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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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TABLE OF CONTENTS

	<u>PAGE</u>
Abstract	1
1. Foreword	2
2. Specifications and Theoretical Foundations for COR 2	4
3. Structure of the Program	6
4. Explanation of the Program	11
4.1 MAIN Program	11
4.2 SUBROUTINE CØCA (JØ, JM, JJA)	17
4.3 FUNCTION CØ(JØ, JM, JJA, FC, FQC)	22
4.4 FUNCTIONS F(X, JØ, JM, JJA) and FT(X)	23
4.5 FUNCTION AC(CL, J)	23
4.6 FUNCTION PRA(JØ, JM, LX, KX, JX, WAA)	23
4.7 FUNCTION RB(UØ, Z)	23
4.8 FUNCTION FQI(JØ, JM, LX, KX, JX, WAA)	23
4.9 FUNCTION FCA (JØ, JM, II, JJA, FCA1, FCAØ)	23
4.10 SUBROUTINE CALI (JØ, JM, JJA, AIT, SWITCH, FQCF, FQCA)	24
4.11 FUNCTION EI(X)	24
4.12 SUBROUTINE AINP (C, IJ, IIMAX, SD)	24
5. Statements of the Program	25
6. Table of Formats for the Data Input Cards	53
7. Outputs	65
8. References	70
APPENDIX 1: NBS Technical Note 521	71
APPENDIX 2: Index of Terms and Symbols	88

	<u>PAGE</u>
APPENDIX 3: Permanent Data File	112

LIST OF FIGURES

Figure No. 1: Structure of COR 2	7
Figure No. 2: Flowsheet of Subroutine CØCA	19

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. Hénoch, 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. Hénoch 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

CORRECTION
FUNCTIONS

PARAMETERS
AND
INTEGRALS

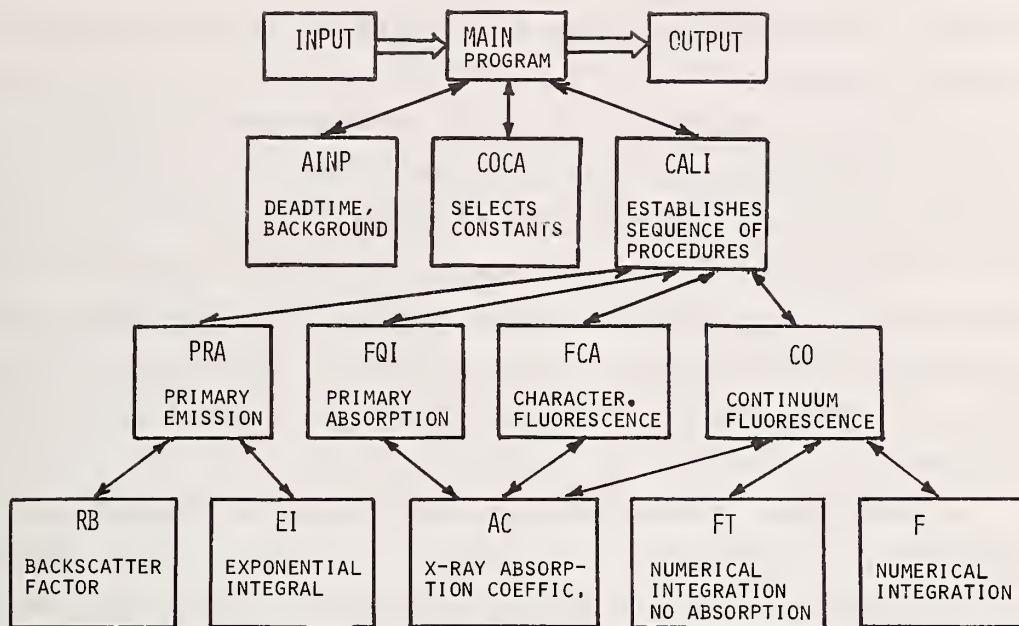


Figure 1. Structure of COR 2.

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:

$$k = \frac{I'_p {}^*f_p {}^* + \Sigma I'_f {}^*f_f {}^* + I'_c {}^*f_c {}^*}{I'_p {}^sf_p {}^s + \Sigma I'_f {}^sf_f {}^s + I'_c {}^sf_c {}^s} \quad (1)$$

in which k is the background- and deadtime-corrected relative x-ray intensity, I' 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, $I'_f f_f$, and

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 Program¹

4.1 MAIN Program

4.1.1 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:

J	atomic number of element
KM(J)	number of x-ray absorption edges
A(J)	atomic weight
FCK12(J)	Coster Kronig coefficients, f12, f23,
FCK23(J)	f13
FCK13(J)	
CI(J)	multiplicative constant for the mass absorption coefficients [4]: C _K if J ≤ 50, C _{KL} if J > 50
ANK(J)	exponent n _K , for the mass absorption coefficients
ANKL(J)	exponent n _{KL} , for the mass absorption coefficients (μ) according to $\mu = C\lambda^n$

loop 350

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

WAV(K,J)	wavelength of absorption jump
R(K,J)	jump ratio
ØME(K,J)	fluorescence yield
LM(K,J)	number of tabulated lines for this level

implied loop

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

CL(L,K,J)	wavelength of line
ZL(L,K,J)	relative intensity of line

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

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 difficulty, 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 concentrations

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:

READ (5,90)

NZ(JJA) its atomic number
C(JJ) its mass fraction

The subprograms CØCA (JJA,JST,JJA) and CALI (JJA,JST,JJA,AIT...) produce the ratio $AIR(JJA) = I_A/I(A)$; 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 (calcu-
late 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:

READ (5,110)

NZ(JJ) atomic number of unanalyzed element
NV(JJ) its valence (empty unless stoichiometry
 is calculated)
CD(1,JJ) its concentration (empty unless
 k-values are calculated)

The decision to calculate k-values from known concentrations is signaled through the input of a "known" concentration value for one element (JJAl) in CD(1,JJ). This tells the program that the C(JJA) values entered for the elements other than JJAl are concentrations rather than k-values, and the k-values of these elements are calculated. But, JJAl 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 JJA1.

The subprogram CØCA (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 CØCA (JØ, JM, JJA)

Arguments:

JØ : 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 N_3 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 λ_q , it can be excited by continuous radiation of a wavelength between the Douane-Hunt limit, λ_0 , and λ_q . 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 λ_0 and λ_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, ω_{eff} .

2) Fluorescence excited by characteristic lines

For each element, except the analyzed element, the characteristic lines at each level are compared with λ_0 ; 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 ω_{eff} of the analyzed element for fluorescence by characteristic lines.

The output of the program consists of: number of sublimits and associated parameters, number of lines which excite fluorescence, and associated parameters; error messages, in case the user has caused the switch NCØ(JJA) to be changed.

4.2.2 Commentary on CØCA (JØ, JM, JJA) (see Figure 2)

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

The switch NCØ(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 λ_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 (λ_0)
KAA	the subscript of the shell emitting the characteristic lines (λ_q)
F ₁₂	the Coster-Kronig coefficients
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)), (λ_0, λ_q) 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.

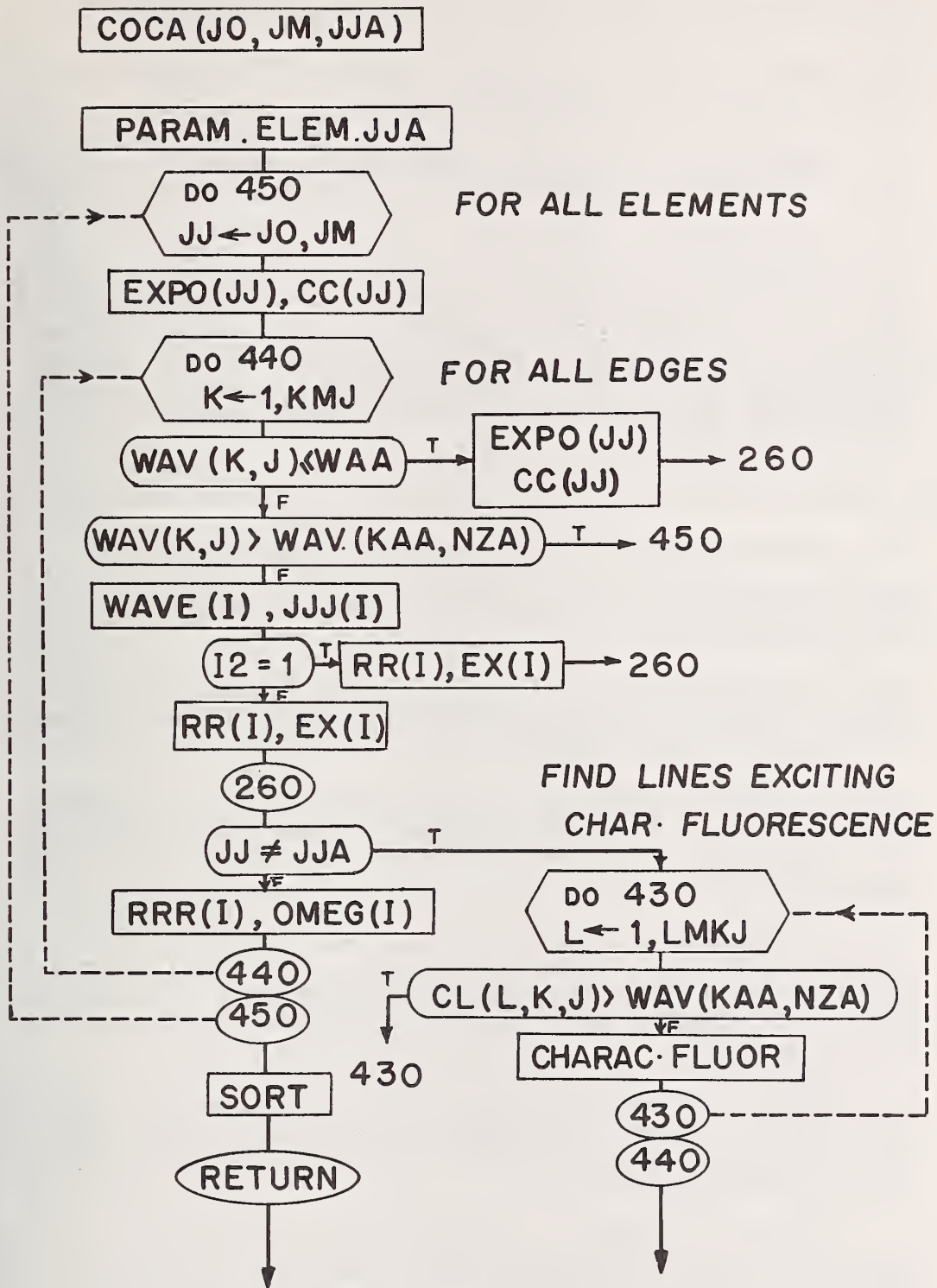


Figure 2. Flowsheet of Subroutine COCA.

Tally I2: 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 (λ_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 $\text{WAV}(K,J) \leq 10^{-6} \text{ \AA}$, 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 λ_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 $NC\emptyset$ (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 $\text{WAA} < \text{WAV}(KMJ) < \text{WAV}(KAA,NZA)$, the tally I2, 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 $\text{WAVE}(I,JJA)$ and $\text{JJJ}(I,JJA)$; 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 K1 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 ω_{eff} . These are stored in RRR(I,JJA) and ØMEG(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 $I \leq IM$, one has assembled the following table:

	number: IM-I3M starting points (continuum fluorescence)	number: I3M line exciting the fluorescence of JJA
WAVE(I,JJA)	X	X
RR(I,JJA)	X	(X)
JJJ(I,JJA)	X	X
RRR(I,JJA)	(X)	0
ØMEG(I,JJA)	(X)	0
EX(I,JJA)	X	(X)
KB(I,JJA)	0	X
LB(I,JJA)	0	X

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 \emptyset MEG(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 $1 \leq I \leq \text{IMA}(\text{JJA})$

EX(I,JJA) (for continuum fluorescence)

RRR(I,JJA)

\emptyset MEG(I,JJA)

WAVE(I,JJA)

JJJ(I,JJA)

RRR(I,JJA) if $\text{IMA}(\text{JJA}) + 1 \leq I \leq \text{MF}(\text{JJA}) + \text{IMA}(\text{JJA}) + 1$

\emptyset MEG(I,JJA) (for characteristic fluorescence)

KB(I,JJA)

LB(I,JJA)

4.3 FUNCTION $C\emptyset(\text{J}\emptyset, \text{JM}, \text{JJA}, \text{FC}, \text{FQC})$

This program calculates the intensity of fluorescence due to the continuum, by means of a numerical integration. $C\emptyset$ is separate from $C\emptyset\text{CA}(\text{J}\emptyset, \text{JM}, \text{JJA})$ because it requires concentrations; therefore it is used in each iteration, while $C\emptyset\text{CA}(\text{J}\emptyset, \text{JM}, \text{JJA})$ is used only once.

4.4 FUNCTIONS F(X,JØ, JM, JJA) and FT(X)

Function F calculates the expression for continuum fluorescence to be numerically integrated in CØ(JØ, JM, JJA).

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 KSTØP 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(JØ, JM, LX, KX, JX, WAA)

Calculates the intensity of primary emission of the line LX, shell KX, of the element of atomic number JX, for a case containing the elements subscripted JØ to JM, where the Duane-Hunt limit associated with the energy of the electrons, λ_0 , is WAA.

4.7 FUNCTION RB(UØ, Z)

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

4.8 FUNCTION FQI(JØ, JM, LX, KX, JX, WAA)

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

4.9 SUBROUTINE FCA (JØ, JM, II, JJA, FCA1, FCAØ)

Calculates the fluorescent intensity FCA1 for a case containing the elements JØ to JM, where the radiation is excited by the line II, and emitted as characteristic radiation of the element JJA.

4.10 SUBROUTINE CALI (JØ, 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 JØ 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

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COR2

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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),COSEC(15),C(15)

DIMENSION KM(100),LM(12,100),EXPO(15,15),CC(15,15),CI(100),ANK(100),ANKL(100),R(12,100)

DIMENSION FCK12(100),FCK23(100),FCK13(100),OME(12,100),IMA(15),WAV1E(120,15),RR(120,15),EX(120,15),MESS(15,15)

DIMENSION KB(120,15),LB(120,15),WA(15),KA(15),JJJ(120,15),RRR(120,115),OMEG(120,15)

DIMENSION FQF(15),FCF(15),FCASF(15),RPF(15),NV(15),AI(15),AKEX(15),CT(15),AIR(15),CD(100,15),SD(100,15),ELNA(100),LI(9,3),CON(15),FQ2C(15),FQCA(15)

COMMON KSTOP,NCO,NIT,MF,A,WAV,CL,ZL,NZ,AK,LA,COSEC,C/B12/KM,LM/B1213/EXPO,CC/B125/CI,ANK,ANKL,R/B126/FCK12,FCK23,FCK13,OME/B1239/IMA,2WAVE,RR,EX,MESS/B1289/KB,LB/B5P/WA,KA,JJJ,RRR,OMEG/BICF/ICOF

COMMON /BINPT/ III,NTAPE/BLT/LOUT,FQF,FCF,FCASF,RPF

DATA (ELNA(KK),KK=3,92)/2HLI,2HBE,1HB,1HC,1HN,1HO,1HF,2HNE,2HNA,2H1MG,2HAL,2HSI,1HP,1HS,2HCL,1HA,1HK,2HCA,2HSC,2HTI,1HV,2HCR,2HMN,2HF2E,2HCO,2HNI,2HCU,2HZN,2HGA,2HGE,2HAS,2HSE,2HBR,2HKR,2HRB,2HSR,1HY,32HZR,2HNB,2HMO,2HTC,2HRU,2HRH,2HPD,2HAG,2HCD,2HIN,2HSN,2HSB,2HTE,14HI,2HXE,2HCS,2HBA,2HLA,2HCE,2HPR,2HND,2HPM,2HSM,2HEU,2HGD,2HTB,2HD5Y,2HHO,2HER,2HTM,2HYB,2HLU,2HHF,2HTA,1HW,2HRE,2HOS,2HIR,2HPT,2HAU,62HHG,2HTL,2HPB,2HBI,2HPO,2HAT,2HRN,2HFR,2HRA,2HAC,2HTH,2HPA,1HU/

DATA LI(1,1)/3HKB1/LI(1,2)/3HKA1/LI(1,3)/3HKA2/LI(2,1)/3HLB3/LI(2,12)/3HLB4/LI(3,1)/3HLG1/LI(3,2)/3HLB1/LI(4,1)/3HLB2/LI(4,2)/3HLA1/L2I(4,3)/3HLA2/LI(9,1)/3HMA1/LI(7,1)/3HMB1/

10 FORMAT (1H ,5X,2HK(,I1,2H)=,F5.4)

20 FORMAT (1H ,19X,A2,I1,A1,I1,5X,F6.4)

30 FORMAT (I3)

40 FORMAT (2I2,F6.3,3F6.4,F6.2,2F4.2)

50 FORMAT (F7.5,2F6.4,I1)

60 FORMAT (2I2,I1,3I2,68X,L1)

70 FORMAT (F7.5,F6.4)

80 FORMAT (I2,10X,F7.3,2I1,F6.4,2I1,F6.4)

90 FORMAT (I2,F5.4)

100 FORMAT (15F5.4)

110 FORMAT (I2,10X,I1,F5.4)

120 FORMAT (/7HELEMENT,I2,4X,9HATOMIC NO,I2,/30X,9HABS COEFF,/30X,5HC(1K)=,F8.2,3X,5HN(K)=,F4.2)

130 FORMAT (18H COMPOUND STANDARD/5H JJA=,I2,4X,4HNZA=,I2/(9X,3HNZ(,I11,2H)=,I2,3X,2HC=,F5.3,3X,3HCC=,F8.2,3X,5HEXPO=,F4.2))

140 FORMAT (11X,4HAIR(,I1,2H)=,F6.4)

150 FORMAT (/12X,3HAI(,I1,2H)=,E10.5)

160 FORMAT (1H0,10H SAMPLE NO,I3,/5X,9HSTANDARDS)

170 FORMAT (/5X,8HPOINT NO,I2)

180 FORMAT (/7X,13HITERATION NO ,I2)


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190  FORMAT (/5H JJA=, I2, 4X, 4HNZA=, I2/(9X, 3HNZ( , I1, 2H)=, I2, 3X, 2HC=, F5.3  A 59
1, 3X, 3HCC=, F8.2, 3X, 5HEXPO=, F4.2)) A 60
200  FORMAT (12X, 3HCT( , I1, 2H)=, F5.3) A 61
210  FORMAT (/10(1X, 3HCT( , I1, 2H)=, F6.4)) A 62
220  FORMAT (1H , 5X, A2, 2X, I2, 3(5X, F6.4)) A 63
230  FORMAT (1H+, 46X, F6.4, 4X, E10.5, 6X, E10.5, 4X, F6.4) A 64
240  FORMAT (1H , 10X, 29HCOMPOUND STANDARD FOR ELEMENT, I2/) A 65
250  FORMAT (1H0, 4X, 7HELEMENT, 4X, 7HAT CONC, 4X, 7HWT CONC, 4X, 7HSTD DEV, 4X  A 66
1, 4HF(X) , 4X, 13HI(P)/(F(X)*C) , 4X, 9HI(C)/I(P) , 4X, 7HF(X) CON, 4X, 10HCHAR  A 67
2 FLUOR, 4X, 7HF(X)CHA) A 68
260  FORMAT (1H0, 24X, 12HITERATION NO, I3) A 69
270  FORMAT (1H+, 46X, F6.4, 4X, E10.5, 6X, E10.5, 4X, F6.4, 4X, E10.5, 5X, F6.4) A 70
280  FORMAT (1H , 10X, A2, A3) A 71
290  FORMAT (80H A 72
1 A 73
) A 74
300  FORMAT (1H1) A 74
310  FORMAT (1H0, 19X, 7HTOTAL =, 2X, F6.4) A 75
320  FORMAT (1H0, 9X, 13HSTOICHIOMETRY//20X, 5HOXIDE, 5X, 5HCONC./) A 76
330  FORMAT (1H0, 4X, 7HELEMENT, 15X, 7HK-VALUE, 14X4HF(X) , 4X, 13HI(P)/(F(X)*  A 77
1C) , 4X, 9HI(C)/I(P) , 4X, 7HF(X) CON, 4X, 10HCHAR FLUOR, 4X, 7HF(X)CHA) A 78
340  FORMAT (1H , 5X, A2, 2X, I2, 16X, F6.4) A 79
CALL DEFTAB A 80
C A 81
C READ DATA INTO THE ELEMENT TABLE A 82
C A 83
READ (5,30) NELM A 84
DO 350 NOE=1, NELM A 85
READ (5,40) J, KM(J) , A(J) , FCK12(J) , FCK23(J) , FCK13(J) , CI(J) , ANK(J) , A 86
INKL(J) A 87
KMJ=KM(J) A 88
DO 350 K=1, KMJ A 89
READ (5,50) WAV(K, J) , R(K, J) , OME(K, J) , LM(K, J) A 90
LMKJ=LM(K, J) A 91
IF (LMKJ.EQ.0) GO TO 350 A 92
READ (5,70) (CL(L, K, J) , ZL(L, K, J) , L=1, LMKJ) A 93
350 CONTINUE A 94
C A 95
C READ IN INITIAL DATA FOR EACH SAMPLE A 96
C A 97
READ (5,30) NECM A 98
DO 1010 NEC=1, NECM A 99
NIT=0 A 100
KSTOP=1 A 101
360 READ (5,60) JJM, JJAM, ND, NPM, LOUT, ICOF, FIRST A 102
NPl=NPM-1 A 103
IF (.NOT.FIRST) GO TO 360 A 104
READ (5,290) A 105
SWITCH=0 A 106
WRITE (6,300) A 107
WRITE (6,290) A 108
WRITE (6,160) NEC A 109
DO 430 JJA=1, JJAM A 110
CON(JJA)=0. A 111
A 112
READ ELEMENT CARDS FOR EACH SAMPLE A 113
A 114
READ (5,80) NZ(JJA) , EO, KA(JJA) , LA(JJA) , COSEC(JJA) , NV(JJA) , NEST, CON  A 115
1(JJA) A 116
NCO(JJA)=1 A 117
WA(JJA)=12.398/EO A 118
C(JJA)=1. A 119

```

C		A 120
C	CALCULATE FLUORESCENCE CONSTANTS FOR PURE ELEMENTS	A 121
C		A 122
	CALL COCA (JJA,JJA,JJA)	A 123
	IF (LOUT.EQ.0) GO TO 370	A 124
	WRITE (6,120) JJA,NZ(JJA),CC(JJA,JJA),EXPO(JJA,JJA)	A 125
370	CONTINUE	A 126
	IF (NCO(JJA).EQ.0) GO TO 1010	A 127
	NZA=NZ(JJA)	A 128
	KAA=KA(JJA)	A 129
	LAA=LA(JJA)	A 130
	IF (NZA.LT.10) LAA=2	A 131
	IF (NZA.LT.40.AND.KAA.EQ.4) LAA=2	A 132
	WRITE (6,280) ELNA(NZA),LI(KAA,LAA)	A 133
C		A 134
C	CALCULATION OF ABSORPTION, ATOMIC NUMBER, AND CONTINUUM	A 135
C	FLUORESCENCE CORRECTIONS FOR THE STANDARDS.	A 136
C	AI = THE TOTAL CORRECTION FACTOR	A 137
C		A 138
	CALL CALI (JJA,JJA,JJA,AIT,SWITCH,FQC,FQCA)	A 139
	IF (KSTOP.EQ.0) GO TO 1010	A 140
	AI(JJA)=AIT	A 141
	AIR(JJA)=1.	A 142
	IF (LOUT.EQ.0) GO TO 380	A 143
	WRITE (6,150) JJA,AI(JJA)	A 144
380	CONTINUE	A 145
	IF (NEST.EQ.0) GO TO 410	A 146
C		A 147
C	READ DATA INPUT FOR COMPOUND STANDARDS AND CALCULATE	A 148
C	FLUORESCENCE CONSTANTS FOR THE COMPOUND STANDARDS.	A 149
C		A 150
	READ (5,100) C(JJA)	A 151
	JST=JJA+NEST	A 152
	JJAS=JJA+1	A 153
	READ (5,90) (NZ(JJ),C(JJ),JJ=JJAS,JST)	A 154
	CALL COCA (JJA,JST,JJA)	A 155
	IF (LOUT.EQ.0) GO TO 390	A 156
	WRITE (6,130) JJA,NZ(JJA),(JJ,NZ(JJ),C(JJ),CC(JJ,JJA),EXPO(JJ,JJA)	A 157
	1,JJ=JJA,JST)	A 158
	GO TO 400	A 159
390	WRITE (6,240) JJA	A 160
400	CONTINUE	A 161
	IF (NCO(JJA).EQ.0) GO TO 1010	A 162
C		A 163
C	CALCULATE CORRECTIONS FOR COMPOUND STANDARDS.	A 164
C	AIR = TOTAL CORRECTION	A 165
C		A 166
	CALL CALI (JJA,JST,JJA,AIT,SWITCH,FQC,FQCA)	A 167
	IF (KSTOP.EQ.0) GO TO 1010	A 168
	AIR(JJA)=AIT/AI(JJA)	A 169
410	IF (LOUT.EQ.0) GO TO 420	A 170
	WRITE (6,140) JJA,AIR(JJA)	A 171
420	CONTINUE	A 172
430	CONTINUE	A 173
C		A 174
C	SORTING ROUTINE FOR ANALYSIS METHOD - NSW DETERMINES METHOD	A 175
C	1 - ALL ELEMENTS ANALYZED	A 176
C	2 - ONE ELEMENT BY STOICHIOMETRY	A 177
C	3 - ONE ELEMENT BY DIFFERENCE	A 178
C	4 - TWO OR MORE ELEMENTS NOT ANALYZED	A 179
C	5 - CALCULATE K-VALUES FROM KNOWN CONCENTRATIONS	A 180

	JJA1=JJAM+1	A 181
	IF (JJM-JJA1) 480,450,440	A 182
	NSW=4	A 183
140	READ (5,110) (NZ(JJ),NV(JJ),CD(1,JJ),JJ=JJA1,JJM)	A 184
150	IF (CD(1,JJA1).GT.1.E-7) GO TO 460	A 185
	IF (NV(JJA1).EQ.0) GO TO 470	A 186
	IF ((JJM-JJA1).NE.0) GO TO 490	A 187
	NSW=2	A 188
	GO TO 490	A 189
160	NSW=5	A 190
	GO TO 490	A 191
170	NSW=3	A 192
	GO TO 490	A 193
180	NSW=1	A 194
190	DO 500 JJA=1,JJAM	A 195
		A 196
		A 197
	CALCULATE FLUORESCENCE CONSTANTS FOR UNKNOWNNS	A 198
		A 199
	CALL COCA (1,JJM,JJA)	A 200
	IF (NCO(JJA).EQ.0) GO TO 1010	A 201
500	CONTINUE	A 202
	SWITCH=1	A 203
	IF (ND.EQ.1) GO TO 530	A 204
		A 205
	READ IN K-VALUES FROM CARDS	A 206
		A 207
	DO 510 NP=1,NPM	A 208
510	READ (5,100) (CD(NP,JJA),JJA=1,JJAM)	A 209
	IF (NSW.NE.5) GO TO 540	A 210
	IF (NPM.EQ.1) GO TO 540	A 211
	DO 520 NP=2,NPM	A 212
520	READ (5,100) (CD(NP,JJ),JJ=JJA1,JJM)	A 213
	GO TO 540	A 214
		A 215
	DATA ARE READ BY THE INPUT SUBROUTINE (AINP)	A 216
		A 217
530	CALL AINP (CD,NPM,JJAM,SD)	A 218
	NP1=NPM-1	A 219
		A 220
	BEGIN CALCULATION OF CONCENTRATIONS FOR EACH UNKNOWN	A 221
		A 222
540	DO 1000 NP=1,NPM	A 223
	NIT=0	A 224
	SC=0.0	A 225
	DO 550 JJA=1,JJAM	A 226
	C(JJA)=CD(NP,JJA)*AIR(JJA)	A 227
	IF (CON(JJA).GT.1.OE-7) C(JJA)=CD(NP,JJA)	A 228
	AKEX(JJA)=C(JJA)	A 229
	SC=SC+C(JJA)	A 230
550	CONTINUE	A 231
	IF (NSW.EQ.5) SC=SC+CD(1,JJA1)	A 232
	GO TO (630,560,580,590,610), NSW	A 233
		A 234
	STOICHIOMETRY CALCULATION	A 235
		A 236
560	C(JJA1)=0.0	A 237
	NZO=NZ(JJA1)	A 238
	DO 570 JJA=1,JJAM	A 239
	NZA=NZ(JJA)	A 240
	CO=C(JJA)/A(NZA)*A(NZO)*NV(JJA)/NV(JJA1)	A 241

	C(JJA1)=C(JJA1)+CO	A 242
570	CONTINUE	A 243
	SC=SC+C(JJA1)	A 244
	GO TO 630	A 245
C		A 246
C	CALCULATE ONE ELEMENT BY DIFFERENCE	A 247
C		A 248
580	C(JJA1)=1.-SC	A 249
	SC=1.	A 250
	GO TO 630	A 251
C		A 252
C	TWO OR MORE ELEMENTS NOT ANALYZED	A 253
C		A 254
590	C(JJM)=0.0	A 255
	NZO=NZ(JJM)	A 256
	NZEX=NZ(JJA1)	A 257
	DO 600 JJA=1, JJAM	A 258
	NZA=NZ(JJA)	A 259
	CO=C(JJA)/A(NZA)*A(NZO)*NV(JJA)/NV(JJM)	A 260
	C(JJM)=C(JJM)+CO	A 261
600	CONTINUE	A 262
	SC=SC+C(JJM)	A 263
	C(JJA1)=(1.-SC)*A(NZEX)*NV(JJM)/(A(NZEX)*NV(JJM)+A(NZO)*NV(JJA1))	A 264
	C(JJM)=C(JJM)+(1.-SC)*A(NZO)*NV(JJA1)/(A(NZEX)*NV(JJM)+A(NZO)*NV(JJA1))	A 265
	SC=1.	A 266
	GO TO 630	A 267
C		A 268
C	CALCULATE K-VALUES FROM KNOWN CONCENTRATIONS	A 269
C		A 270
C		A 271
610	DO 620 JJ=JJA1, JJM	A 272
	C(JJ)=CD(NP, JJ)	A 273
620	CONTINUE	A 274
630	WRITE (6,170) NP	A 275
	DO 640 JJ=1, JJAM	A 276
	WRITE (6,10) JJ, C(JJ)	A 277
640	CONTINUE	A 278
	DO 650 JJ=1, JJM	A 279
	C(JJ)=C(JJ)/SC	A 280
650	CONTINUE	A 281
	NSW2=2	A 282
C		A 283
C	START OF ITERATION LOOP	A 284
C		A 285
660	GO TO (840,670), NSW2	A 286
670	IF (NIT.GT.20) GO TO 840	A 287
	IF (LOUT.EQ.0) GO TO 680	A 288
	WRITE (6,180) NIT	A 289
680	CONTINUE	A 290
	IF (NSW.NE.5) SC=0.0	A 291
	DO 730 JJA=1, JJAM	A 292
	IF (CD(NP, JJA).LT.1.0E-7) GO TO 720	A 293
	IF (LOUT.EQ.0) GO TO 700	A 294
	IF (NIT.EQ.0) GO TO 690	A 295
	GO TO 700	A 296
690	WRITE (6,190) JJA, NZ(JJA), (JJ, NZ(JJ)), C(JJ), CC(JJ, JJA), EXPO(JJ, JJA)	A 297
	1, JJ=1, JJM)	A 298
C		A 299
C	CALCULATE CORRECTIONS FOR UNKNOWNNS	A 300
C		A 301
700	CALL CALI (1, JJM, JJA, AIT, SWITCH, FQC, FQCA)	A 302

	IF (KSTOP.EQ.0) GO TO 1010	A 303
	CT(JJA)=AIT/AI(JJA)	A 304
	IF (CON(JJA).GT.1.OE-7) CT(JJA)=CD(NP,JJA)	A 305
	IF (LOUT.EQ.0) GO TO 710	A 306
710	IF (NIT.EQ.0) WRITE (6,200) JJA,CT(JJA)	A 307
	CONTINUE	A 308
	IF (NSW.EQ.5) GO TO 730	A 309
C		A 310
C	HYPERBOLIC APPROXIMATION FOR CONCENTRATIONS	A 311
C		A 312
	CT(JJA)=AKEX(JJA)*C(JJA)*(1.-CT(JJA))/(AKEX(JJA)*(C(JJA)-CT(JJA))+	A 313
	1CT(JJA)*(1.-C(JJA)))	A 314
	IF (CON(JJA).GT.1.OE-7) CT(JJA)=CD(NP,JJA)	A 315
	SC=SC+CT(JJA)	A 316
	GO TO 730	A 317
720	CT(JJA)=0.	A 318
730	CONTINUE	A 319
	GO TO (790,750,740,770,820), NSW	A 320
740	CT(JJA1)=1.-SC	A 321
	SC=1.	A 322
	GO TO 790	A 323
750	CT(JJA1)=0.0	A 324
	DO 760 JJA=1,JJAM	A 325
	NZA=NZ(JJA)	A 326
	CO=CT(JJA)/A(NZA)*A(NZO)*NV(JJA)/NV(JJA1)	A 327
	CT(JJA1)=CT(JJA1)+CO	A 328
760	CONTINUE	A 329
	SC=SC+CT(JJA1)	A 330
	GO TO 790	A 331
770	CT(JJM)=0.0	A 332
	DO 780 JJA=1,JJAM	A 333
	NZA=NZ(JJA)	A 334
	CO=CT(JJA)/A(NZA)*A(NZO)*NV(JJA)/NV(JJM)	A 335
	CT(JJM)=CT(JJM)+CO	A 336
780	CONTINUE	A 337
	SC=SC+CT(JJM)	A 338
	CT(JJA1)=(1.-SC)*A(NZEX)*NV(JJM)/(A(NZEX)*NV(JJM)+A(NZO)*NV(JJA1))	A 339
	CT(JJM)=CT(JJM)+(1.-SC)*A(NZO)*NV(JJA1)/(A(NZEX)*NV(JJM)+A(NZO)*NV	A 340
	1(JJA1))	A 341
	SC=1.	A 342
790	NSW2=1	A 343
	IF (LOUT.EQ.0) GO TO 800	A 344
	WRITE (6,210) (JJ,CT(JJ),JJ=1,JJM)	A 345
800	CONTINUE	A 346
	DO 810 JJA=1,JJAM	A 347
	CT(JJA)=CT(JJA)/SC	A 348
	IF (CON(JJA).GT.1.OE-7) CT(JJA)=CD(NP,JJA)	A 349
	IF (ABS(CT(JJA)-C(JJA)).GT.1.E-5) NSW2=2	A 350
	C(JJA)=CT(JJA)	A 351
810	CONTINUE	A 352
	C(JJA1)=CT(JJA1)/SC	A 353
	JJA2=JJA1+1	A 354
	C(JJA2)=CT(JJA2)/SC	A 355
	NIT=NIT+1	A 356
C		A 357
C	END OF ITERATION LOOP - IF CONVERGENT , BEGIN WRITING OUTPUT	A 358
C		A 359
	GO TO 660	A 360
820	WRITE (6,330)	A 361
	DO 830 JJA=1,JJAM	A 362
		A 363

C	HYPERBOLIC APPROXIMATION FOR K-VALUES	A 364
C		A 365
	CT(JJA)=1./(1.+(1./AKEX(JJA)-1.)*(1./CT(JJA)-1.)/(1./C(JJA)-1.))	A 366
830	CONTINUE	A 367
	JJMX=JJAM	A 368
	GO TO 890	A 369
840	WRITE (6,250)	A 370
	SACO=0.	A 371
	DO 870 JJ=1,JJM	A 372
	IF (NSW.EQ.5) GO TO 860	A 373
	IF (CON(JJ).GT.1.0E-7) GO TO 860	A 374
	IF (NSW.NE.2) GO TO 850	A 375
	IF (JJ.EQ.JJM) GO TO 860	A 376
850	CT(JJ)=CT(JJ)*SC	A 377
860	CONTINUE	A 378
870	CONTINUE	A 379
	DO 880 JJ=1,JJM	A 380
	NZA=NZ(JJ)	A 381
	SACO=SACO+CT(JJ)/A(NZA)	A 382
880	CONTINUE	A 383
	JJMX=JJM	A 384
890	DO 970 JJ=1,JJMX	A 385
	NZA=NZ(JJ)	A 386
	IF (NSW.EQ.5) GO TO 900	A 387
	SA1=SACO-CT(JJ)/A(NZA)	A 388
	ATCO=CT(JJ)/(CT(JJ)+A(NZA)*SA1)	A 389
	WRITE (6,220) ELNA(NZA),NZA,ATCO,CT(JJ),SD(NP,JJ)	A 390
	GO TO 910	A 391
900	WRITE (6,340) ELNA(NZA),NZA,CT(JJ)	A 392
	CT(JJ)=AKEX(JJ)	A 393
910	IF (JJAM-JJM) 920,930,930	A 394
920	IF (JJ.EQ.JJM) GO TO 940	A 395
930	IF (CT(JJ).GT.1.0E-7) GO TO 950	A 396
940	RPFX=0.	A 397
	FCFX=0.	A 398
	GO TO 970	A 399
950	RPFX=RPF(JJ)/(FQF(JJ)*CT(JJ))	A 400
	FCFX=FCF(JJ)/RPF(JJ)	A 401
	IF (FCASF(JJ).GT.1.0E-12) GO TO 960	A 402
	WRITE (6,230) FQF(JJ),RPFX,FCFX,FQC(JJ)	A 403
	GO TO 970	A 404
960	FCASFX=FCASF(JJ)/RPF(JJ)	A 405
	WRITE (6,270) FQF(JJ),RPFX,FCFX,FQC(JJ),FCASFX,FQCA(JJ)	A 406
970	CONTINUE	A 407
	WRITE (6,310) SC	A 408
	WRITE (6,260) NIT	A 409
	IF (NSW.NE.2) GO TO 1000	A 410
C		A 411
C	WRITE STOICHIOMETRY OUTPUT IF THIS OPTION WAS USED	A 412
C		A 413
	WRITE (6,320)	A 414
	NZA1=NZ(JJM)	A 415
	DO 990 JJ=1,JJAM	A 416
	NZA=NZ(JJ)	A 417
	STOIC=(A(NZA)*NV(JJM)+A(NZA1)*NV(JJ))/(A(NZA)*NV(JJM))*CT(JJ)	A 418
	NY=NV(JJM)	A 419
	NX=NV(JJ)	A 420
	IF (NX.LT.NY) GO TO 980	A 421
	IF (MOD(NX,NY).EQ.1) GO TO 980	A 422
	NX=NX/NY	A 423
	NY=1	A 424

364	380	WRITE (6,20) ELNA(NZA),NY,ELNA(NZA1),NX,STOIC	A	425
365	390	CONTINUE	A	426
366	0000	CONTINUE	A	427
367	010	CONTINUE	A	428
368		STOP	A	429
369		END	A	430-
370		SUBROUTINE COCA (JO,JM,JJA)	B	1
371			B	2
372		DETERMINE ALL THE CONSTANTS NECESSARY FOR A CALCULATION	B	3
373			B	4
374		DIMENSION NCO(15),MF(15),D3(100),WAV(12,100),CL(3,12,100),D4(3,12,	B	5
375		1100),NZ(15),D5(15),N6(15),D7(15),D8(15)	B	6
376		DIMENSION KM(100),LM(12,100),EXPO(15,15),CC(15,15),CI(100),ANK(100	B	7
377		1),ANKL(100),R(12,100)	B	8
378		DIMENSION FCK12(100),FCK23(100),FCK13(100),OME(12,100),IMA(15),WAV	B	9
379		1E(120,15),RR(120,15),EX(120,15),MESS(15,15)	B	10
380		DIMENSION KB(120,15),LB(120,15),WA(15),KA(15),JJJ(120,15),RRR(120,	B	11
381		115),OMEG(120,15)	B	12
382		COMMON N1,NCO,N2,MF,D3,WAV,CL,D4,NZ,D5,N6,D7,D8/B12/KM,LM/B1239/IM	B	13
383		1A,WAVE,RR,EX,MESS/B123/EXPO,CC/B5P/WA,KA,JJJ,RRR,OMEG/B1289/KB,LB/	B	14
384		2B126/FCK12,FCK23,FCK13,OME/B125/CI,ANK,ANKL,R	B	15
385	0	FORMAT (//34H NUMBER OF EDGES GE 12 ARGUMENTS(,I2,1H,,I2,1H,,I2,1	B	16
386		11H) ELEMENT.,I2,16H DISCONTINUITY.,I2)	B	17
387	20	FORMAT (//34H E0 GREATER THAN 30 KV, ARGUMENTS(,I2,1H,,I2,1H,,I2,1	B	18
388		1H))	B	19
389	30	FORMAT (//30H BAD CHOICE FOR E0, ARGUMENTS(,I2,1H,,I2,1H,,I2,1H))	B	20
390	40	FORMAT (3H R(,I2,1H,,I2,28H) MISSING IN DATA,ARGUMENTS(,I2,1H,,I2,	B	21
391		11H,,I2,1H))	B	22
392		NCO(JJA)=1	B	23
393		NSW3=1	B	24
394		I=1	B	25
395		I3=0	B	26
396		NZA=NZ(JJA)	B	27
397		WAA=WA(JJA)	B	28
398		KAA=KA(JJA)	B	29
399		F12=FCK12(NZA)	B	30
400		F23=FCK23(NZA)	B	31
401		F13=FCK13(NZA)	B	32
402		IF (WAA.GT.WAV(KAA,NZA)) WRITE (6,30) JO,JM,JJA	B	33
403		DO 450 JJ=JO,JM	B	34
404		I2=0	B	35
405		MESS(JJ,JJA)=0	B	36
406		J=NZ(JJ)	B	37
407		KMJ=KM(J)	B	38
408		IF (J.GT.50) GO TO 50	B	39
409			B	40
410		INITIALIZATION OF FACTORS FOR THE CALCULATION OF	B	41
411		MASS ABSORPTION COEFFICIENTS.	B	42
412			B	43
413		EXPO(JJ,JJA)=ANK(J)	B	44
414		GO TO 60	B	45
415	50	EXPO(JJ,JJA)=ANKL(J)	B	46
416	50	CC(JJ,JJA)=CI(J)	B	47
417		DO 440 K=1,KMJ	B	48
418		KR1=1+K/2+K/8-(K/3)*(K/5)+((K-8)*(K/8))*2+K/10-(K/11)*2	B	49
419		KR2=1+K/2+K/5-(K/5)*(K/6)+K/9+(K/12)*2	B	50
420		K1=KR1-1-(K/10)*4+(K/12)*3	B	51
421		IF (WAV(K,J).LE.1.E-6) GO TO 440	B	52
422		IF (WAV(K,J).LE.WAA) GO TO 70	B	53
423		IF (WAV(K,J).GT.WAV(KAA,NZA)) GO TO 450	B	54
424		GO TO 140	B	55

70	NNR=R(K,J)	B	56
	IF (KR1.NE.7.AND.NNR.EQ.0) GO TO 560	B	57
	GO TO (80,90,100,110,120,130,570), KR1	B	58
80	IF (J.GT.50) GO TO 440	B	59
	CC(JJ,JJA)=CI(J)/R(K,J)*WAV(K,J)**ANK(J)/WAV(K,J)**ANKL(J)	B	60
	EXPO(JJ,JJA)=ANKL(J)	B	61
	GO TO 440	B	62
90	CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)	B	63
	GO TO 440	B	64
100	CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)*WAV(K,J)**EXPO(JJ,JJA)/WAV(K,J)**2.6	B	65
	EXPO(JJ,JJA)=2.6	B	66
	GO TO 440	B	67
110	CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)	B	68
	MESS(JJ,JJA)=MESS(JJ,JJA)+1	B	69
	GO TO 440	B	70
120	CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)*WAV(K,J)**2.6/WAV(K,J)**2.22	B	71
	EXPO(JJ,JJA)=2.22	B	72
	MESS(JJ,JJA)=0	B	73
	GO TO 440	B	74
130	CC(JJ,JJA)=CC(JJ,JJA)/R(K,J)	B	75
	GO TO 440	B	76
C		B	77
C	DETERMINE JUMP RATIOS (R) AND EXPONENTS (N) NEEDED BY THE	B	78
C	CONTINUUM FLUORESCENCE CORRECTION	B	79
C		B	80
140	I2=I2+1	B	81
	I=I+1	B	82
	WAVE(I,JJA)=WAV(K,J)	B	83
	JJJ(I,JJA)=JJ	B	84
	RRR(I,JJA)=0.0	B	85
	OMEG(I,JJA)=0.0	B	86
	KB(I,JJA)=0	B	87
	LB(I,JJA)=0	B	88
	IF (I2.EQ.1) GO TO (190,200,210,220,230,240,250,570), KR2	B	89
	GO TO (150,160,170,180,570), K1	B	90
150	RR(I,JJA)=R(K,J)	B	91
	EX(I,JJA)=EX(I-1,JJA)	B	92
	GO TO 260	B	93
160	RR(I,JJA)=R(K,J)*WAV(K,J)**2.6/WAV(K,J)**EX(I-1,JJA)	B	94
	EX(I,JJA)=2.6	B	95
	GO TO 260	B	96
170	RR(I,JJA)=R(K,J)	B	97
	EX(I,JJA)=EX(I-1,JJA)	B	98
	MESS(JJ,JJA)=MESS(JJ,JJA)+1	B	99
	GO TO 260	B	100
180	RR(I,JJA)=R(K,J)*WAV(K,J)**2.22/WAV(K,J)**EX(I-1,JJA)	B	101
	EX(I,JJA)=2.22	B	102
	MESS(JJ,JJA)=0	B	103
	GO TO 260	B	104
190	IF (J.GT.50) GO TO 600	B	105
	RR(I,JJA)=R(K,J)*WAV(K,J)**ANKL(J)/WAV(K,J)**ANK(J)	B	106
	EX(I,JJA)=ANKL(J)	B	107
	GO TO 260	B	108
200	RR(I,JJA)=R(K,J)	B	109
	EX(I,JJA)=EXPO(JJ,JJA)	B	110
	GO TO 260	B	111
210	RR(I,JJA)=R(K,J)*WAV(K,J)**2.6/WAV(K,J)**EXPO(JJ,JJA)	B	112
	EX(I,JJA)=2.6	B	113
	GO TO 260	B	114
220	RR(I,JJA)=R(K,J)	B	115
	EX(I,JJA)=2.6	B	116

	GO TO 260	B 117
230	RR(I,JJA)=R(K,J)	B 118
	EX(I,JJA)=2.6	B 119
	MESS(JJ,JJA)=MESS(JJ,JJA)+1	B 120
	GO TO 260	B 121
240	RR(I,JJA)=R(K,J)*WAV(K,J)**2.22/WAV(K,J)**2.6	B 122
	EX(I,JJA)=2.22	B 123
	MESS(JJ,JJA)=0	B 124
	GO TO 260	B 125
250	RR(I,JJA)=R(K,J)	B 126
	EX(I,JJA)=EXPO(JJ,JJA)	B 127
	GO TO 260	B 128
260	IF (JJ.NE.JJA) GO TO 420	B 129
	KAS=KAA-KAA/6-KAA/7-KAA/9	B 130
	GO TO (270,280,290,300,580,380), KAS	B 131
C		B 132
C	EFFICIENCY RATIOS --	B 133
C	(R-1)/R FOR THE CONTINUUM FLUORESCENCE FOR K-LINES	B 134
C		B 135
270	RRR(1,JJA)=(R(K,J)-1.)/R(K,J)	B 136
	OMEG(1,JJA)=OME(K,J)	B 137
	GO TO 440	B 138
280	KK=K	B 139
	GO TO (310,320,330,340,350,360,370), KK	B 140
290	KK=K+K/2	B 141
	GO TO (310,320,330,340,350,360,370), KK	B 142
300	KK=(K+4)/6*3+K	B 143
	GO TO (310,320,330,340,350,360,370), KK	B 144
310	WRITE (6,30) JO,JM,JJA	B 145
	NSW3=2	B 146
	RKR=1./R(K,J)	B 147
	GO TO 440	B 148
C		B 149
C	(R-1)/R FACTORS FOR THE CONTINUUM FLUORESCENCE CORRECTION FOR	B 150
C	L- AND M-LINES	B 151
C		B 152
C	L1-EDGE	B 153
C		B 154
320	RRR(1,JJA)=(R(K,J)-1.)/R(K,J)	B 155
	OMEG(1,JJA)=OME(K,J)	B 156
	GO TO (440,410), NSW3	B 157
C		B 158
C	L2-EDGE	B 159
C		B 160
330	RRR(1,JJA)=(R(K+1,J)-1.)/R(K,J)/R(K+1,J)	B 161
	OMEG(1,JJA)=OME(K+1,J)*(1.+F12*(R(K,J)-1.)*R(K+1,J)/(R(K+1,J)-1.))	B 162
	GO TO (440,410), NSW3	B 163
340	RRR(I-1,JJA)=(R(K,J)-1.)/R(K,J)	B 164
	OMEG(I-1,JJA)=OME(K,J)	B 165
	GO TO 440	B 166
C		B 167
C	L3-EDGE	B 168
C		B 169
350	RRR(1,JJA)=(R(K+2,J)-1.)/R(K,J)/R(K+1,J)/R(K+2,J)	B 170
	OMEG(1,JJA)=OME(K+2,J)*(1.+F13*(R(K+1,J)*R(K+2,J)*(R(K,J)-1.)/(R(K+2,J)-1.))+F23*(R(K+2,J)*(R(K+1,J)-1.)/(R(K+2,J)-1.))+F12*(R(K+1,J)*R(K+2,J)*(R(K,J)-1.)/(R(K+2,J)-1.)))	B 171
	GO TO (440,410), NSW3	B 172
360	RRR(I-1,JJA)=(R(K+1,J)-1.)/R(K,J)/R(K+1,J)	B 173
	OMEG(I-1,JJA)=OME(K+1,J)*(1.+F23*(R(K,J)-1.)*R(K+1,J)/(R(K+1,J)-1.))	B 174
	1))	B 175
		B 176
		B 177

	GO TO 440	B 178
370	RRR(I-1,JJA)=(R(K,J)-1.)/R(K,J)	B 179
	OMEG(I-1,JJA)=OME(K,J)	B 180
	GO TO 440	B 181
C		B 182
C	M4 - M5 EDGES	B 183
C		B 184
380	IF (K.EQ.1) WRITE (6,30) JO,JM,JJA	B 185
	RRRR=R(KAA,J)-1.	B 186
	DO 390 LLL=K,KAA	B 187
	RRRR=RRRR/R(LLJ,J)	B 188
390	CONTINUE	B 189
	IF (I2.EQ.1) GO TO 400	B 190
	RRR(I-1,JJA)=RRRR	B 191
	OMEG(I-1,JJA)=OMEG(1,JJA)	B 192
	GO TO 440	B 193
400	OMEG(1,JJA)=OME(KAA,J)	B 194
	RRR(1,JJA)=RRRR	B 195
	GO TO 440	B 196
410	RRR(I-1,JJA)=RRR(1,JJA)	B 197
	OMEG(I-1,JJA)=OMEG(1,JJA)	B 198
	RRR(1,JJA)=RRR(1,JJA)*RKR	B 199
	NSW3=1	B 200
	GO TO 440	B 201
420	LMKJ=LM(K,J)	B 202
	IF (LMKJ.EQ.0) GO TO 440	B 203
	DO 430 L=1,LMKJ	B 204
C		B 205
C	TEST FOR ANY CHARACTERISTIC FLUORESCENCE	B 206
C		B 207
C	IF THERE IS A CHARACTERISTIC FLUORESCENCE CORRECTION, THEN	B 208
C	DETERMINE THE (R-1)/R, FLUORESCENT YIELD, LINE NUMBER, EDGE	B 209
C	NUMBER, ELEMENT NUMBER, AND WAVELENGTH FOR THE PARTICULAR	B 210
C	CORRECTION.	B 211
C		B 212
	IF (CL(L,K,J).GT.WAV(KAA,NZA).OR.CL(L,K,J)/WAV(KAA,NZA).LT.0.5) GO	B 213
1	TO 430	B 214
	I=I+1	B 215
	I3=I3+1	B 216
	RRR(I,JJA)=0.0	B 217
	OMEG(I,JJA)=0.0	B 218
	WAVE(I,JJA)=CL(L,K,J)	B 219
	JJJ(I,JJA)=JJ	B 220
	EX(I,JJA)=EX(I-1,JJA)	B 221
	KB(I,JJA)=K	B 222
	LB(I,JJA)=L	B 223
430	CONTINUE	B 224
440	CONTINUE	B 225
450	CONTINUE	B 226
	WAVE(1,JJA)=WAA	B 227
	JJJ(1,JJA)=0	B 228
	RR(1,JJA)=0.	B 229
	EX(1,JJA)=0.	B 230
	LB(1,JJA)=0	B 231
	KB(1,JJA)=0	B 232
	IM=I	B 233
	I3M=I3	B 234
	IM1=IM-1	B 235
	IF (IM1.LT.2) GO TO 550	B 236
	DO 480 I=2,IM1	B 237
	IL=IM-I+1	B 238

	DO 470 II=2, IL	B 239
	IF (WAVE(II, JJA) .GT. WAVE(II+1, JJA)) GO TO 460	B 240
460	GO TO 470	B 241
	T1=WAVE(II, JJA)	B 242
	T2=RR(II, JJA)	B 243
	T3=JJJ(II, JJA)	B 244
	T4=RRR(II, JJA)	B 245
	T5=OMEG(II, JJA)	B 246
	T6=EX(II, JJA)	B 247
	T7=KB(II, JJA)	B 248
	T8=LB(II, JJA)	B 249
	WAVE(II, JJA)=WAVE(II+1, JJA)	B 250
	RR(II, JJA)=RR(II+1, JJA)	B 251
	JJJ(II, JJA)=JJJ(II+1, JJA)	B 252
	RRR(II, JJA)=RRR(II+1, JJA)	B 253
	OMEG(II, JJA)=OMEG(II+1, JJA)	B 254
	EX(II, JJA)=EX(II+1, JJA)	B 255
	KB(II, JJA)=KB(II+1, JJA)	B 256
	LB(II, JJA)=LB(II+1, JJA)	B 257
	WAVE(II+1, JJA)=T1	B 258
	RR(II+1, JJA)=T2	B 259
	JJJ(II+1, JJA)=T3	B 260
	RRR(II+1, JJA)=T4	B 261
	OMEG(II+1, JJA)=T5	B 262
	EX(II+1, JJA)=T6	B 263
	KB(II+1, JJA)=T7	B 264
	LB(II+1, JJA)=T8	B 265
	CONTINUE	B 266
	CONTINUE	B 267
	DO 500 I=2, IM1	B 268
	IF (RRR(I, JJA) .LE. 1.E-7) GO TO 490	B 269
	GO TO 500	B 270
	RRR(I, JJA)=RRR(I-1, JJA)	B 271
	OMEG(I, JJA)=OMEG(I-1, JJA)	B 272
	CONTINUE	B 273
	M4=IM1	B 274
	I=2	B 275
510	IF (LB(I, JJA) .EQ. 0) GO TO 530	B 276
	T1=WAVE(I, JJA)	B 277
	T2=JJJ(I, JJA)	B 278
	T3=KB(I, JJA)	B 279
	T4=LB(I, JJA)	B 280
	T5=RRR(I, JJA)	B 281
	T6=OMEG(I, JJA)	B 282
	DO 520 II=I, M4	B 283
	WAVE(II, JJA)=WAVE(II+1, JJA)	B 284
	RR(II, JJA)=RR(II+1, JJA)	B 285
	JJJ(II, JJA)=JJJ(II+1, JJA)	B 286
	RRR(II, JJA)=RRR(II+1, JJA)	B 287
	OMEG(II, JJA)=OMEG(II+1, JJA)	B 288
	EX(II, JJA)=EX(II+1, JJA)	B 289
	KB(II, JJA)=KB(II+1, JJA)	B 290
	LB(II, JJA)=LB(II+1, JJA)	B 291
520	CONTINUE	B 292
	WAVE(M4+1, JJA)=T1	B 293
	JJJ(M4+1, JJA)=T2	B 294
	KB(M4+1, JJA)=T3	B 295
	LB(M4+1, JJA)=T4	B 296
	RRR(M4+1, JJA)=T5	B 297
	OMEG(M4+1, JJA)=T6	B 298
	M4=M4-1	B 299

	GO TO 540	B 300
530	I=I+1	B 301
540	IF (I.LE.M4) GO TO 510	B 302
550	IMA(JJA)=IM-I3M	B 303
C		B 304
C	SET THE SWITCH FOR THE CHARACTERISTIC FLUORESCENCE CORRECTION	B 305
C		B 306
	MF(JJA)=I3M	B 307
	GO TO 620	B 308
560	WRITE (6,40) K,J,J0,JM,JJA	B 309
	GO TO 610	B 310
570	WRITE (6,10) J0,JM,JJA,J,K	B 311
	GO TO 610	B 312
580	WRITE (6,590)	B 313
590	FORMAT (1H , 'NO PROVISION IS MADE FOR LINES ORIGINATING'/' FRO	B 314
	1M THE M1, M2, OR M3 EDGES.'/)	B 315
	GO TO 560	B 316
600	WRITE (6,20) J0,JM,JJA	B 317
610	NCO(JJA)=0	B 318
	IMA(JJA)=I	B 319
	MF(JJA)=0	B 320
620	RETURN	B 321
	END	B 322
	SUBROUTINE CO (J0,JM,JJA,FC,FQC)	C 1
C		C 2
C	CALCULATION OF CONTINUUM FLUORESCENCE CORRECTION	C 3
C		C 4
	DIMENSION N2(15),N4(15),D5(100),D6(12,100),CL(3,12,100),ZL(3,12,10	C 5
	10),NZ(15),AK(15),LA(15),COSEC(15),C(15)	C 6
	DIMENSION EXPO(15,15),CC(15,15)	C 7
	DIMENSION IMA(15),WAVE(120,15),RR(120,15),EX(120,15),MESS(15,15)	C 8
	DIMENSION WA(15),KA(15),JJJ(120,15),RRR(120,15),OMEG(120,15)	C 9
	DIMENSION EXO(15),CCO(15)	C 10
	COMMON N1,N2,N3,N4,D5,D6,CL,ZL,NZ,AK,LA,COSEC,C/B1239/IMA,WAVE,RR,	C 11
	1EX,MESS/B123/EXPO,CC/B5P/WA,KA,JJJ,RRR,OMEG/B34/EXO,CCO,WAA,ACS	C 12
	IM1=IMA(JJA)-1	C 13
	FCO=0.0	C 14
	FC=0.0	C 15
	NZA=NZ(JJA)	C 16
	KAA=KA(JJA)	C 17
	LAA=LA(JJA)	C 18
	WAA=WAVE(1,JJA)	C 19
	ZMK=0.0	C 20
	ACS=0.0	C 21
	RRRI=RRR(1,JJA)	C 22
	OMEGI=OMEG(1,JJA)	C 23
	DO 10 J=J0,JM	C 24
	EXO(J)=EXPO(J,JJA)	C 25
	CCO(J)=CC(J,JJA)	C 26
	I=NZ(J)	C 27
C		C 28
C	CALCULATE CONSTANTS FOR CONTINUUM FLUORESCENCE	C 29
C		C 30
	ACS=ACS+C(J)*AC(CL(LAA,KAA,NZA),I)*COSEC(JJA)	C 31
	ANZ=NZ(J)	C 32
	AK(J)=3.0E-5	C 33
	ZMK=ZMK+C(J)*ANZ*AK(J)	C 34
10	CONTINUE	C 35
	DO 70 I=1,IM1	C 36
	DO 40 J=J0,JM	C 37
	IF (J.EQ.JJJ(I,JJA)) GO TO 20	C 38

GO TO 40	C	39
20 EXO(J)=EX(I,JJA)	C	40
CCO(J)=CCO(J)/RR(I,JJA)	C	41
IF (J.EQ.JJA) GO TO 30	C	42
GO TO 40	C	43
30 OMEGI=OMEG(I,JJA)	C	44
RRRI=RRR(I,JJA)	C	45
40 CONTINUE	C	46
C	C	47
C SET UP INTERVALS FOR NUMERICAL INTEGRATION	C	48
C	C	49
NIN2=(WAVE(I+1,JJA)-WAVE(I,JJA))/0.02	C	50
NIN=2*NIN2	C	51
H=0.01	C	52
IF (NIN.GE.10) GO TO 50	C	53
H=(WAVE(I+1,JJA)-WAVE(I,JJA))/10.	C	54
NIN=10	C	55
50 ANIN=NIN	C	56
RL=(WAVE(I+1,JJA)-WAVE(I,JJA))-ANIN*H	C	57
BO=WAVE(I,JJA)+RL	C	58
BN=WAVE(I+1,JJA)	C	59
BN1=BN-H	C	60
LKM=NIN-3	C	61
C	C	62
C NUMERICAL INTEGRATION BETWEEN ABSORPTION EDGES	C	63
C TRAPEZOIDAL RULE	C	64
C	C	65
S=0.5*(F(WAVE(I,JJA),JO,JM,JJA)+F(BO,JO,JM,JJA))*RL	C	66
SO=0.5*(FT(WAVE(I,JJA))+FT(BO))*RL	C	67
C	C	68
C SIMPSONS RULE	C	69
C	C	70
S=S+H*(F(BO,JO,JM,JJA)+F(BN,JO,JM,JJA)+4.*F(BN1,JO,JM,JJA))/3.	C	71
SO=SO+H*(FT(BO)+FT(BN)+4.*FT(BN1))/3.	C	72
DO 60 LK=1,LKM,2	C	73
ALK=LK	C	74
BK1=BO+ALK*H	C	75
BK2=BK1+H	C	76
S=S+2.*(2.*F(BK1,JO,JM,JJA)+F(BK2,JO,JM,JJA))*H/3.	C	77
SO=SO+2.*(2.*FT(BK1)+FT(BK2))*H/3.	C	78
60 CONTINUE	C	79
EABI=0.5*ZL(LAA,KAA,NZA)*ZMK*C(JJA)*OMEGI*RRRI	C	80
FI=EABI*S	C	81
FIO=EABI*SO	C	82
C	C	83
C FINAL VALUES OF EMITTED AND GENERATED CONTINUUM FLUORESCENCE	C	84
C	C	85
FC=FC+FI	C	86
FCO=FCO+FIO	C	87
70 CONTINUE	C	88
C	C	89
C F(X) OF THE CONTINUUM	C	90
C	C	91
FQC=FC/FCO	C	92
RETURN	C	93
END	C	94-
FUNCTION F (X,JO,JM,JJA)	D	1
C	D	2
C CALCULATION OF THE INTEGRAL OF THE CONTINUUM CORRECTION FOR	D	3
C THE EMITTED X-RAYS	D	4
C	D	5

	DIMENSION N2(15),N4(15),D5(100),D6(12,100),D7(3,12,100),D8(3,12,10	D	6
	10),N9(15),D10(15),N11(15),D12(15),C(15)	D	7
	DIMENSION EXO(15),CCO(15)	D	8
	COMMON N1,N2,N3,N4,D5,D6,D7,D8,N9,D10,N11,D12,C/B34/EXO,CCO,WAA,AC	D	9
	1S/B410/ACAX,ACX	D	10
	ACAX=CCO(JJA)*X**EXO(JJA)	D	11
	ACX=0.0	D	12
	DO 10 J=J0,JM	D	13
	ACX=ACX+C(J)*CCO(J)*X**EXO(J)	D	14
10	CONTINUE	D	15
	F=ACAX/ACS*(X-WAA)/WAA/X/X*ALOG(1.+ACS/ACX)	D	16
	RETURN	D	17
	END	D	18
	FUNCTION AC (CL,J)	E	1
C		E	2
C	CALCULATION OF THE MASS ABSORPTION COEFFICIENTS	E	3
C		E	4
	DIMENSION N1(15),N3(15),D4(100),WAV(12,100),D5(3,12,100),D6(3,12,1	E	5
	100),N7(15),D8(15),N9(15),D10(15),D11(15)	E	6
	DIMENSION CI(100),ANK(100),ANKL(100),R(12,100)	E	7
	COMMON KSTOP,N1,N2,N3,D4,WAV,D5,D6,N7,D8,N9,D10,D11/B125/CI,ANK,AN	E	8
	1KL,R	E	9
10	FORMAT (//4H MU(,F7.5,1H,,I2,42H) UNKNOWN .MORE THAN 12 EDGES ARE	E	10
	1 CROSSED)	E	11
20	FORMAT (//4H MU(,F7.5,1H,,I2,14H) UNDEFINED,R(,I2,1H,,I2,17H) MISS	E	12
	LING IN DATA)	E	13
	K=1	E	14
C		E	15
C	CONSTANTS FROM OPERATING POTENTIAL TO K-EDGE	E	16
C		E	17
	CC=CI(J)	E	18
	AN=ANK(J)	E	19
	IF (CL.LT.WAV(K,J)) GO TO 100	E	20
C		E	21
C	CONSTANTS FROM K-EDGE TO L1-EDGE FOR ELEMENTS ATOMIC NUMBER 50	E	22
C	AND BELOW	E	23
C		E	24
	IF (J.LE.50) CC=CC/R(K,J)*WAV(K,J)**(ANK(J)-ANKL(J))	E	25
	AN=ANKL(J)	E	26
30	K=K+1	E	27
	IF (WAV(K,J).LE.1.E-7) GO TO 30	E	28
	IF (CL.LT.WAV(K,J)) GO TO 100	E	29
	L=1+K/4-(K/4)*((K-1)/4)+(K/9)*4-(K/10)*2+(K/12)*4	E	30
	NNR=R(K,J)	E	31
	IF (L.NE.3.AND.NNR.EQ.0) GO TO 80	E	32
	GO TO (40,50,60,70), L	E	33
C		E	34
C	ALL CONSTANTS ABOVE L1-EDGE	E	35
C		E	36
40	CC=CC/R(K,J)	E	37
	GO TO 30	E	38
C		E	39
C	ALL CONSTANTS ABOVE L3-EDGE	E	40
C		E	41
50	CC=CC/R(K,J)	E	42
	CC=CC*WAV(K,J)**(ANKL(J)-2.6)	E	43
	AN=2.6	E	44
	GO TO 30	E	45
C		E	46
C	ALL CONSTANTS ABOVE M5-EDGE	E	47
C		E	48

60	CC=CC/R(K,J)	E	49
	CC=CC*WAV(K,J)**(2.6-2.22)	E	50
	AN=2.22	E	51
	GO TO 30	E	52
70	WRITE (6,10) CL,J	E	53
	GO TO 90	E	54
80	WRITE (6,20) CL,J,K,J	E	55
90	AC=1.E-3	E	56
	KSTOP=0	E	57
	RETURN	E	58
100	AC=CC*CL**AN	E	59
	RETURN	E	60
	END	E	61-
	FUNCTION PRA (JO,JM,LX,KX,JX,WAA)	F	1
C		F	2
C	CALCULATION OF PRIMARY INTENSITIES	F	3
C		F	4
	DIMENSION N2(15),N4(15),A(100),WAV(12,100),D5(3,12,100),ZL(3,12,10	F	5
	10),NZ(15),D6(15),N7(15),D8(15),C(15)	F	6
	DIMENSION FCK12(100),FCK23(100),FCK13(100),OME(12,100)	F	7
	COMMON N1,N2,N3,N4,A,WAV,D5,ZL,NZ,D6,N7,D8,C/B126/FCK12,FCK23,FCK1	F	8
	13,OME	F	9
	PRA=0.0	F	10
	UO=WAV(KX,JX)/WAA	F	11
	EM=12.398/WAV(KX,JX)	F	12
	AM=0.0	F	13
	AMLW=0.0	F	14
	DO 10 J=JO,JM	F	15
	I=NZ(J)	F	16
	IF (I.EQ.JX) CX=C(J)	F	17
	RZ=NZ(J)	F	18
	AM=AM+C(J)*RZ/A(I)	F	19
C		F	20
C	CALCULATE MEAN IONIZATION POTENTIAL - J	F	21
C		F	22
	ZJ=9.76*RZ+58.5*(RZ**(-.19))	F	23
	AMLW=AMLW+C(J)*RZ/A(I)*ALOG(1166.*EM/ZJ)	F	24
10	CONTINUE	F	25
C		F	26
C	ALW = LN(V) AW = V ALUOW = LN(UOV) = LN(UO) + LN(V)	F	27
C		F	28
	ALW=AMLW/AM	F	29
	AW=EXP(ALW)	F	30
	ALUOW=ALOG(UO)+ALW	F	31
	T1=(EI(ALUOW)-EI(ALW))*ALW/AW	F	32
C		F	33
C	T2 = THE INTEGRATED VOLTAGE DEPENDENT TERM	F	34
C		F	35
	T2=(UO-1.-T1)*0.76*0.5/AM	F	36
	IF (KX.GT.4) GO TO 90	F	37
	GO TO (20,30,40,60), KX	F	38
C		F	39
C	SELECT THE NUMBER OF ELECTRONS (ZNL) AND THE FLUORESCENT YIELD	F	40
C	(OMED) FOR THE ABSORPTION EDGE PRODUCING THE MEASURED LINE	F	41
C		F	42
C	K-EDGE	F	43
C		F	44
20	ZNL=2.	F	45
	OMED=OME(KX,JX)	F	46
	GO TO 130	F	47
C		F	48

C		L1-EDGE	F	49
C			F	50
30	ZNL=2.		F	51
	OMED=OME(KX,JX)		F	52
	GO TO 130		F	53
C			F	54
C		L2-EDGE	F	55
C			F	56
40	ZNL=2.		F	57
	IF (WAV(KX-1,JX).GT.WAA) GO TO 50		F	58
	OMED=OME(KX,JX)		F	59
	GO TO 130		F	60
50	OMED=OME(KX,JX)*(1.+FCK12(JX))		F	61
	GO TO 130		F	62
C			F	63
C		L3-EDGE	F	64
C			F	65
60	ZNL=4.		F	66
	IF (WAV(KX-2,JX).GT.WAA) GO TO 80		F	67
	IF (WAV(KX-1,JX).GT.WAA) GO TO 70		F	68
	OMED=OME(KX,JX)		F	69
	GO TO 130		F	70
70	OMED=OME(KX,JX)*(1.+0.5*FCK23(JX))		F	71
	GO TO 130		F	72
80	OMED=OME(KX,JX)*(1.+0.5*FCK13(JX)+0.5*FCK23(JX)*(1.+FCK12(JX)))		F	73
	GO TO 130		F	74
C			F	75
C	M-EDGES	NONE OF THE LISTED LINES ARE PRODUCED BY THE M1 AND	F	76
C	M2-EDGES		F	77
C			F	78
90	KXX=1+(KX-4)/3+(KX-4)/5		F	79
	OMED=OME(KX,JX)		F	80
	GO TO (100,110,120), KXX		F	81
C			F	82
C		M3-EDGE	F	83
C			F	84
100	ZNL=2.		F	85
	GO TO 130		F	86
C			F	87
C		M4-EDGE	F	88
C			F	89
110	ZNL=4.		F	90
	GO TO 130		F	91
C			F	92
C		M5-EDGE	F	93
C			F	94
120	ZNL=6.		F	95
130	TO=OMED*ZL(LX,KX,JX)*CX*ZNL/A(JX)		F	96
	PRA=TO*T2		F	97
	RBA=0.0		F	98
	DO 140 J=JO,JM		F	99
	Z=NZ(J)		F	100
	RBA=RBA+RB(UO,Z)*C(J)		F	101
140	CONTINUE		F	102
C			F	103
C	PRA = THE PRIMARY INTENSITY		F	104
C			F	105
	PRA=PRA*RBA		F	106
	RETURN		F	107
	END		F	108-
	FUNCTION RB (UO,Z)		G	1

CALCULATION OF BACKSCATTER -R- FROM DUNCUMBS FIT

```

W=1./UO
W2=W**2
W3=W**3
W4=W**4
W5=W**5
Z1=1.0E-02*Z
Z2=1.0E-04*Z**2
Z3=1.0E-06*Z**3
Z4=1.0E-08*Z**4
Z5=1.0E-10*Z**5
R1=-.581+2.162*W-5.137*W2+9.213*W3-8.619*W4+2.962*W5
R2=-1.609-8.298*W+28.791*W2-47.744*W3+46.540*W4-17.676*W5
R3=5.4+19.184*W-75.733*W2+120.05*W3-110.7*W4+41.792*W5
R4=-5.725-21.645*W+88.128*W2-136.06*W3+117.75*W4-42.445*W5
R5=2.095+8.947*W-36.51*W2+55.694*W3-46.079*W4+15.851*W5
RB=1.+R1*Z1+R2*Z2+R3*Z3+R4*Z4+R5*Z5
RETURN
END
FUNCTION FQI (JO,JM,LX,KX,JX,WAA)

```

CALCULATION OF F(X)

```

DIMENSION N2(15),N4(15),A(100),WAV(12,100),CL(3,12,100),D5(3,12,10
10),NZ(15),D6(15),N7(15),COSEC(15),C(15)
COMMON N1,N2,N3,N4,A,WAV,CL,D5,NZ,D6,N7,COSEC,C
H=0.0
ACS=0.0
DO 10 JJ=J0,JM
J=NZ(JJ)
IF (J.EQ.JX) JJA=JJ
RZ=NZ(JJ)

```

CALCULATE THE H OF PHILIBERT AND THE VALUE OF CHI

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H=H+1.2*A(J)*C(JJ)/RZ**2
ACS=ACS+C(JJ)*AC(CL(LX,KX,JX),J)*COSEC(JJA)
CONTINUE

```

CALCULATE SIGMA AND FQI = F(X)

```

SIG=4.5E05/((12.398/WAA)**1.65-(12.398/WAV(KX,JX))**1.65)
FQI=(1.+H)/(1.+ACS/SIG)/(1.+H*(1.+ACS/SIG))
RETURN
END
SUBROUTINE FCA (JO,JM,II,JJA,FCA1,FCA0)

```

CALCULATION OF CHARACTERISTIC FLUORESCENCE CORRECTION

```

DIMENSION N2(15),N3(15),A(100),WAV(12,100),CL(3,12,100),ZL(3,12,10
10),NZ(15),D4(15),LA(15),COSEC(15),C(15),CA(2),CB(2)
DIMENSION KB(120,15),LB(120,15),WA(15),KA(15),JJJ(120,15),RRR(120,
115),OMEG(120,15)
DIMENSION FQF(15),FCF(15),FCASF(15),RPF(15)
COMMON N1,N2,NIT,N3,A,WAV,CL,ZL,NZ,D4,LA,COSEC,C/B5P/WA,KA,JJJ,RRR
1,OMEG/B1289/KB,LB/BLT/LOUT,FQF,FCF,FCASF,RPF
FORMAT (/13X,5HWAVE=,F7.5,4X,5HACBA=,F6.1,4X,4HACA=,F6.1,4X,4HACB=
1,F6.1/(30X,4HCAI=,E10.5,14X,4HCBI=,E10.5))
NZA=NZ(JJA)

```

G 2
G 3
G 4
G 5
G 6
G 7
G 8
G 9
G 10
G 11
G 12
G 13
G 14
G 15
G 16
G 17
G 18
G 19
G 20
G 21
G 22-
H 1
H 2
H 3
H 4
H 5
H 6
H 7
H 8
H 9
H 10
H 11
H 12
H 13
H 14
H 15
H 16
H 17
H 18
H 19
H 20
H 21
H 22
H 23
H 24
H 25
H 26-
I 1
I 2
I 3
I 4
I 5
I 6
I 7
I 8
I 9
I 10
I 11
I 12
I 13
I 14

	KAA=KA(JJA)	I 15
	LAA=LA(JJA)	I 16
	JJB=JJJ(II,JJA)	I 17
	NZB=NZ(JJB)	I 18
	KBB=KB(II,JJA)	I 19
	LBB=LB(II,JJA)	I 20
C		I 21
C	ABSORPTION COEFFICIENT OF EXCITING RADIATION (B) IN THE	I 22
C	EXCITED ELEMENT (A)	I 23
C		I 24
	ACBA=AC(CL(LBB,KBB,NZB),NZA)	I 25
	H=0.0	I 26
	ACA=0.0	I 27
	ACB=0.0	I 28
	DO 20 I=JO, JM	I 29
	J=NZ(I)	I 30
	RJ=J	I 31
C		I 32
C	ABSORPTION COEFFICIENT OF RADIATION A IN THE SAMPLE X COSEC	I 33
C	THETA	I 34
C		I 35
	ACA=ACA+AC(CL(LAA,KAA,NZA),J)*COSEC(JJA)*C(I)	I 36
C		I 37
C	ABSORPTION COEFFICIENT OF RADIATION B IN THE SAMPLE	I 38
C		I 39
	ACB=ACB+AC(CL(LBB,KBB,NZB),J)*C(I)	I 40
	H=H+1.2*A(J)*C(I)/RJ**2	I 41
20	CONTINUE	I 42
	SIG=4.5E05/((12.398/WA(JJA))**1.65-(12.398/WAV(KBB,NZB))**1.65)	I 43
	FQIB=(1.+H)/(1.+ACA/SIG)/(1.+H*(1.+ACA/SIG))	I 44
	CA(1)=(1.+H)*SIG	I 45
	CA(2)=-CA(1)	I 46
	CB(1)=SIG	I 47
	CB(2)=SIG*(1.+1./H)	I 48
C		I 49
C	CALCULATE CONSTANTS IN EQUATION AND THE PRIMARY INTENSITY	I 50
C		I 51
	FCAL=OMEG(II,JJA)*RRR(II,JJA)*ZL(LAA,KAA,NZA)*ACBA*C(JJA)*0.5*PRA(I 52
	1JO, JM, LBB, KBB, NZB, WA(JJA))	I 53
	FCAO=FCAL/ACB	I 54
C		I 55
C	S1 AND S0 ARE THE INTEGRATIONS OF THE EMITTED AND GENERATED	I 56
C	FACTORS RESPECTIVELY IN THE CRISS EQUATION	I 57
C		I 58
	S2=FQIB*ALOG(1.+ACA/ACB)/ACA	I 59
	IF (LOUT.EQ.0) GO TO 30	I 60
	IF (NIT.EQ.0) WRITE (6,10) CL(LBB,KBB,NZB),ACBA,ACA,ACB,CA(1),CB(1	I 61
	1),CA(2),CB(2)	I 62
30	CONTINUE	I 63
	S1=0	I 64
	S0=0	I 65
	DO 40 I=1,2	I 66
	S1=S1+CA(I)/(CB(I)+ACA)*ALOG(1.+CB(I)/ACB)/CB(I)	I 67
	S0=S0+CA(I)/CB(I)*ALOG(1.+CB(I)/ACB)/CB(I)*ACB	I 68
40	CONTINUE	I 69
C		I 70
C	FCAL IS THE CHARACTERISTIC FLUORESCENCE FACTOR EMITTED	I 71
C		I 72
	FCAL=FCAL*(S1+S2)	I 73
	FCAO=FCAO*(S0+FQIB)	I 74
	RETURN	I 75

	END	I	76-
	SUBROUTINE CALI (JO, JM, JJA, AIT, SWITCH, FQCF, FQCA)	J	1
C		J	2
C	DETERMINE SUBROUTINES TO BE CALLED TO CALCULATE THE TOTAL	J	3
C	EMITTED RADIATION FOR EITHER STANDARDS OR SAMPLES	J	4
C		J	5
	INTEGER SWITCH	J	6
	DIMENSION N2(15), MF(15), D3(100), D4(12,100), D5(3,12,100), D6(3,12,10	J	7
10	10), NZ(15), D7(15), LA(15), D8(15), C(15), FQCF(15), FQCA(15)	J	8
	DIMENSION KB(120,15), LB(120,15), WA(15), KA(15), JJJ(120,15), RRR(120,	J	9
	115), OMEG(120,15)	J	10
	DIMENSION IMA(15), WAVE(120,15), RR(120,15), EX(120,15), MESS(15,15)	J	11
	DIMENSION FQF(15), FCF(15), FCASF(15), RPF(15)	J	12
	COMMON N1, N2, NIT, MF, D3, D4, D5, D6, NZ, D7, LA, D8, C/B1239/IMA, WAVE, RR, EX	J	13
	1, MESS/B5P/WA, KA, JJJ, RRR, OMEG/B1289/KB, LB/BLT/LOUT, FQF, FCF, FCASF, RP	J	14
	2F	J	15
	COMMON /BICF/ ICOF	J	16
10	FORMAT (6X, 2HI=, I2, 3X, 5HWAVE=, F7.5, 3X, 3HRR=, F5.3, 3X, 4HJJJ=, I2, 3X, 4	J	17
	1HRRR=, F5.3, 3X, 5HOMEG=, F5.3, 3X, 3HEX=, F5.3, 3X, 3HLB=, I1, 3X, 3HKB=, I1)	J	18
20	FORMAT (/5H JJA=, I1, 8X, 3HRP=, E10.5, 3X, 3HFQ=, F6.4, 3X, 3HFC=, E10.5, 3X	J	19
	1, 4HFQC=, F6.4/)	J	20
30	FORMAT (71X, 5HFCA1=, E10.5, 2X, 6HFQCA1=, F6.4)	J	21
40	FORMAT (//6X, 5HMESS(, I2, 1H, , I2, 2H)=, I2, 67H .M4 EDGE IS CROSSED, ABS	J	22
	1ORPTION COEFFICIENTS MAY NOT BE MEANINGFUL)	J	23
50	FORMAT (1H+, 19X, 5HAT NO, I3, 4X, 5HF(X)=, F6.4, 4X, 14HI(P)/(F(X)*C)=, E1	J	24
	10.5, 4X, 10HI(C)/I(P)=, E10.5, 4X, 10HF(X), CONT=, F6.4)	J	25
	IMAM=IMA(JJA)+MF(JJA)	J	26
	IF (LOUT.EQ.0) GO TO 60	J	27
	IF (NIT.EQ.0) WRITE (6,10) (I, WAVE(I, JJA), RR(I, JJA), JJJ(I, JJA), RRR	J	28
	1(I, JJA), OMEG(I, JJA), EX(I, JJA), LB(I, JJA), KB(I, JJA), I=1, IMAM)	J	29
	GO TO 60	J	30
60	CONTINUE	J	31
	DO 70 JJ=JO, JM	J	32
	IF (MESS(JJ, JJA).EQ.0) GO TO 70	J	33
	WRITE (6,40) JJ, JJA, MESS(JJ, JJA)	J	34
70	CONTINUE	J	35
	IF (ICOF.EQ.1) GO TO 80	J	36
C		J	37
C	FC = EMITTED RADIATION DUE TO FLUORESCENCE BY THE CONTINUUM	J	38
C		J	39
	CALL CO (JO, JM, JJA, FC, FQC)	J	40
	GO TO 90	J	41
80	FC=0.	J	42
	FQC=0.	J	43
90	RPO=PRA(JO, JM, LA(JJA), KA(JJA), NZ(JJA), WA(JJA))	J	44
	FQ=FQI(JO, JM, LA(JJA), KA(JJA), NZ(JJA), WA(JJA))	J	45
C		J	46
C	RP = THE EMITTED PRIMARY INTENSITY	J	47
C		J	48
	RP=RPO*FQ	J	49
	FCAS=0.0	J	50
	FCASO=0.0	J	51
	IF (LOUT.EQ.0) GO TO 100	J	52
	WRITE (6,20) JJA, RP, FQ, FC, FQC	J	53
100	CONTINUE	J	54
	FCFX=FC/RP	J	55
C		J	56
C	RPFX = THE NORMALIZED GENERATED PRIMARY INTENSITY	J	57
C		J	58
	RPFX=RP/(FQ*C(JJA))	J	59
C		J	60

C	WRITE DATA FOR STANDARDS	J	61
C		J	62
	IF (SWITCH.EQ.0) WRITE (6,50) NZ(JJA),FQ,RPFX,FCFX,FQC	J	63
	FQCF(JJA)=FQC	J	64
	FQF(JJA)=FQ	J	65
	FCF(JJA)=FC	J	66
	RPF(JJA)=RP	J	67
	IF (MF(JJA).EQ.0) GO TO 130	J	68
C		J	69
C	CHARACTERISTIC FLUORESCENCE CORRECTION - THE VALUE OF MF IS SET	J	70
C	IN SUBROUTINE COCA	J	71
C		J	72
	IO=IMA(JJA)+1	J	73
	DO 120 I=IO,IMAM	J	74
	CALL FCA (JO, JM, I, JJA, FCA1, FCA0)	J	75
	IF (FCA0.LT.1.0E-12) GO TO 110	J	76
	FQCA1=FCA1/FCA0	J	77
	IF (LOUT.EQ.0) GO TO 110	J	78
	WRITE (6,30) FCA1,FQCA1	J	79
110	CONTINUE	J	80
C		J	81
C	FCAS = TOTAL EMITTED RADIATION DUE TO CHARACTERISTIC	J	82
C	FLUORESCENCE	J	83
C		J	84
	FCAS=FCAS+FCA1	J	85
	FCAS0=FCAS0+FCA0	J	86
120	CONTINUE	J	87
	IF (FCAS0.LT.1.0E-12) GO TO 130	J	88
	FQCA(JJA)=FCAS/FCAS0	J	89
C		J	90
C	AIT = TOTAL EMITTED RADIATION	J	91
C		J	92
130	AIT=RP+FC+FCAS	J	93
	FCASF(JJA)=FCAS	J	94
	RETURN	J	95
	END	J	96-
	FUNCTION EI (X)	K	1
C		K	2
C	EXPONENTIAL INTEGRAL	K	3
C		K	4
	EI=ALOG(X)+X	K	5
	TN=X	K	6
	N=1	K	7
10	AN=N	K	8
	IF (AN.GT.2.*X.AND.TN.LT.1.E-06) GO TO 20	K	9
	TN=TN*X*AN/(AN+1.)**2	K	10
	EI=EI+TN	K	11
	N=N+1	K	12
	GO TO 10	K	13
20	RETURN	K	14
	END	K	15-
	FUNCTION FT (X)	L	1
C		L	2
C	CALCULATION OF THE INTEGRAL OF THE CONTINUUM FLUORESCENCE	L	3
C	CORRECTION FOR GENERATED X-RAYS	L	4
C		L	5
	DIMENSION D1(15),D2(15)	L	6
	COMMON /B34/ D1,D2,WAA,DACS/B410/ACAX,ACX	L	7
	FT=ACAX/ACX*(X-WAA)/WAA/X/X	L	8
	RETURN	L	9
	END	L	10-

	SUBROUTINE AINP (C,IJ,IIMAX,SD)	M	1
	DOUBLE PRECISION SUM,SSUM,SUMS,FSD	M	2
	DIMENSION NUMBER(1000),NTABL(100,8),MCO(8),NCODE(100,7),T(100),ICO	M	3
	1N(7,2),NSTD(12,2,7,2),SNSTD(7,2),CSTD(7,2),SPH(5,7),SPHC(5,7),PHC(M	4
	2100,7),C(100,6),PEAK(7),KK(5),TIM(5),SD(100,7),SUM(6,7),SSUM(6,7),	M	5
	3SUMS(6,7),FSD(6,7)	M	6
	COMMON /BINPT/ III,NTAPE	M	7
10	FORMAT (4I2,I5,I2)	M	8
20	FORMAT (10I8)	M	9
30	FORMAT (1H0,8HELEMENT ,I1,34H - STANDARD DEVIATION OF PEAK FOR ,I2	M	10
	1,11H POINTS IS ,F6.4)	M	11
40	FORMAT (1H0,8HELEMENT ,I1,40H - STANDARD DEVIATION OF BACKGROUND F	M	12
	10R ,I2,11H POINTS IS ,F6.4)	M	13
	III=510	M	14
	NIND=0	M	15
C		M	16
C	READ DATA FROM MAG TAPE AND SET UP TABLE	M	17
C		M	18
	READ (5,10) NC,NM,NTC,NAV,ND,NTRA	M	19
	NC1=NC-1	M	20
	NS=6	M	21
	M=NC*ND	M	22
	IF (NTC.EQ.1) GO TO 60	M	23
	INDEX=0	M	24
	CALL PTLOAD (NUMBER,M,NS,NC)	M	25
	DO 50 NROW=1,ND	M	26
	DO 50 NCOL=1,NC	M	27
	INDEX=INDEX+1	M	28
	NTABL(NROW,NCOL)=NUMBER(INDEX)	M	29
50	CONTINUE	M	30
	GO TO 80	M	31
C		M	32
C	READ DATA FROM CARDS AND SET UP TABLE	M	33
C		M	34
60	DO 70 NROW=1,ND	M	35
	READ (5,20) (NTABL(NROW,NCOL),NCOL=1,NC)	M	36
70	CONTINUE	M	37
80	CONTINUE	M	38
C		M	39
C	SEPARATE MANUAL DATA ENTRY INTO 6 VARIABLES	M	40
C		M	41
	DO 110 NROW=1,ND	M	42
	MCO(1)=NTABL(NROW,NM)	M	43
	DO 100 I=1,6	M	44
	IK=6-I	M	45
	IF (MCO(I).EQ.0) GO TO 90	M	46
	ITEN=10**IK	M	47
	IF (MCO(I).LT.ITEN) GO TO 90	M	48
	NCODE(NROW,I)=MCO(I)/ITEN	M	49
	IF (IK.EQ.0) GO TO 100	M	50
	MCO(I+1)=MCO(I)-NCODE(NROW,I)*ITEN	M	51
	GO TO 100	M	52
90	NCODE(NROW,I)=0	M	53
	MCO(I+1)=MCO(I)	M	54
100	CONTINUE	M	55
110	CONTINUE	M	56
C		M	57
C	SET UP TABLES OF STANDARDS AND BACKGROUNDS FOR ALL ELEMENTS	M	58
C		M	59
	DO 130 I=1,NC1	M	60
	DO 120 J=1,2	M	61

	SUM(I,J)=0	M	62
	SSUM(I,J)=0	M	63
	ICON(I,J)=0	M	64
	SNSTD(I,J)=0	M	65
120	CONTINUE	M	66
130	CONTINUE	M	67
	DO 160 NROW=1,ND	M	68
	DO 150 I=1,NC1	M	69
	PHC(NROW,I)=0	M	70
	IF (NCODE(NROW,I).EQ.0) GO TO 150	M	71
	T(NROW)=1000	M	72
	IF (NCODE(NROW,I).NE.6) GO TO 140	M	73
	ICON(I,1)=ICON(I,1)+1	M	74
	IIC=ICON(I,1)	M	75
	NSTD(IIC,1,I,1)=NROW	M	76
	NSTD(IIC,2,I,1)=NTABL(NROW,I)	M	77
	GO TO 150	M	78
140	CONTINUE	M	79
	IF (NCODE(NROW,I).NE.7) GO TO 150	M	80
	ICON(I,2)=ICON(I,2)+1	M	81
	IIC=ICON(I,2)	M	82
	NSTD(IIC,1,I,2)=NROW	M	83
	NSTD(IIC,2,I,2)=NTABL(NROW,I)	M	84
150	CONTINUE	M	85
160	CONTINUE	M	86
C		M	87
C	AVERAGE STANDARDS AND BACKGROUNDS AND CORRECT FOR DEAD TIME	M	88
C		M	89
	DO 200 I=1,NC1	M	90
	DO 190 J=1,2	M	91
	IF (ICON(I,J).EQ.0) GO TO 190	M	92
	IC=ICON(I,J)	M	93
	DO 170 IIC=1,IC	M	94
	NR=NSTD(IIC,1,I,J)	M	95
	SNSTD(I,J)=SNSTD(I,J)+NSTD(IIC,2,I,J)/(ICON(I,J)*T(NR))	M	96
	SUM(I,J)=SUM(I,J)+NSTD(IIC,2,I,J)	M	97
	SSUM(I,J)=SSUM(I,J)+NSTD(IIC,2,I,J)**2	M	98
	CSTD(I,J)=DEADT(SNSTD(I,J),I,NIND)	M	99
	IF (NTRA.EQ.1) GO TO 170	M	100
	CSTD(I,J)=CSTD(I,J)*T(NR)	M	101
170	CONTINUE	M	102
	SUMS(I,J)=SUM(I,J)**2/ICON(I,J)	M	103
	ASUM=SUM(I,J)/ICON(I,J)	M	104
	STSD=DSQRT((SSUM(I,J)-SUMS(I,J))/(ICON(I,J)-1))/ASUM	M	105
	SSTSD=SNGL(STSD)	M	106
	IF (J.EQ.2) GO TO 180	M	107
	WRITE (6,30) I,ICON(I,J),SSTSD	M	108
	GO TO 190	M	109
180	WRITE (6,40) I,ICON(I,J),SSTSD	M	110
190	CONTINUE	M	111
200	CONTINUE	M	112
	IF (NAV.EQ.1) GO TO 260	M	113
C		M	114
C	AVERAGE DATA ON INDIVIDUAL PHASES AND CORRECT FOR DEAD TIME	M	115
C		M	116
	DO 250 I=1,NC1	M	117
	DO 210 J=1,5	M	118
	KK(J)=0	M	119
	SUM(J,I)=0	M	120
	SSUM(J,I)=0	M	121
	TIM(J)=0	M	122

	SPH(J,I)=0	M 123
210	CONTINUE	M 124
	DO 220 NROW=1,ND	M 125
	IF (NCODE(NROW,I).EQ.0.OR.NCODE(NROW,I).GE.6) GO TO 220	M 126
	J=NCODE(NROW,I)	M 127
	KK(J)=KK(J)+1	M 128
	SPH(J,I)=SPH(J,I)+NTABL(NROW,I)/T(NROW)	M 129
	TIM(J)=TIM(J)+T(NROW)	M 130
	SUM(J,I)=SUM(J,I)+NTABL(NROW,I)	M 131
	SSUM(J,I)=SSUM(J,I)+NTABL(NROW,I)**2	M 132
220	CONTINUE	M 133
	DO 240 J=1,5	M 134
	SPHC(J,I)=DEADT(SPH(J,I)/KK(J),I,NIND)	M 135
	IF (NTRA.EQ.1) GO TO 230	M 136
	SPHC(J,I)=SPHC(J,I)*TIM(J)/KK(J)	M 137
230	CONTINUE	M 138
	SUMS(J,I)=SUM(J,I)**2/KK(J)	M 139
	ASUM=SUM(J,I)/KK(J)	M 140
	FSD(J,I)=DSQRT((SSUM(J,I)-SUMS(J,I))/(KK(J)-1))/ASUM	M 141
240	CONTINUE	M 142
250	CONTINUE	M 143
	GO TO 290	M 144
C		M 145
C	CORRECT FOR DEAD TIME ON INDIVIDUAL DETERMINATIONS	M 146
C		M 147
260	DO 280 NROW=1,ND	M 148
	DO 270 I=1,NC1	M 149
	IF (NCODE(NROW,I).EQ.0.OR.NCODE(NROW,I).GE.6) GO TO 270	M 150
	PHC(NROW,I)=DEADT(NTABL(NROW,I)/T(NROW),I,NIND)	M 151
	IF (NTRA.EQ.1) GO TO 270	M 152
	PHC(NROW,I)=PHC(NROW,I)*T(NROW)	M 153
270	CONTINUE	M 154
280	CONTINUE	M 155
290	CONTINUE	M 156
C		M 157
C	PEAK MINUS BACKGROUND ON STANDARDS	M 158
C		M 159
	DO 300 I=1,NC1	M 160
	IF (ICON(I,1).EQ.0) GO TO 300	M 161
	PEAK(I)=CSTD(I,1)-CSTD(I,2)	M 162
300	CONTINUE	M 163
	IF (NAV.EQ.1) GO TO 340	M 164
C		M 165
C	DETERMINE K-VALUES ON AVERAGED PHASES	M 166
C		M 167
	IJ=0	M 168
	DO 330 J=1,5	M 169
	II=0	M 170
	DO 320 I=1,NC1	M 171
	IF (SPHC(J,I)) 320,320,310	M 172
310	II=II+1	M 173
	IF (II.EQ.1) IJ=IJ+1	M 174
	C(IJ,II)=(SPHC(J,I)-CSTD(I,2))/PEAK(I)	M 175
	SD(IJ,II)=SNGL(FSD(J,I))	M 176
	IIMAX=II	M 177
320	CONTINUE	M 178
330	CONTINUE	M 179
	RETURN	M 180
C		M 181
C	DETERMINE K-VALUES ON INDIVIDUAL POINTS	M 182
C		M 183

340	IJ=0	M 184
	DO 370 NROW=1,ND	M 185
	II=0	M 186
	DO 360 I=1,NC1	M 187
	IF (PHC(NROW,I)) 360,360,350	M 188
350	II=II+1	M 189
	IF (II.EQ.1) IJ=IJ+1	M 190
	C(IJ,II)=(PHC(NROW,I)-CSTD(I,2))/PEAK(I)	M 191
	SD(IJ,II)=1./SQRT(NTABL(NROW,I))	M 192
	IIMAX=II	M 193
360	CONTINUE	M 194
370	CONTINUE	M 195
	RETURN	M 196
	END	M 197-
	FUNCTION DEADT (COUNT,IND,NIND)	N 1
C		N 2
C	CORRECTION OF RAW INTENSITIES FOR DEAD TIME	N 3
C	THIS MAY BE EXPANDED TO INCLUDE MORE THAN THE TWO DETECTORS	N 4
C	USED HERE	N 5
C		N 6
C		N 7
	IF (NIND.EQ.0) GO TO 10	N 8
	IF (IND.GT.NIND) GO TO 20	N 9
C		N 10
C	DEAD TIME OF FIRST DETECTOR	N 11
C		N 12
10	DEADT=COUNT/(1-COUNT*3.2E-6)	N 13
	NIND=IND	N 14
	GO TO 30	N 15
C		N 16
C	DEAD TIME OF SECOND DETECTOR	N 17
C		N 18
20	DEADT=COUNT/(1-COUNT*2.8E-6)	N 19
30	CONTINUE	N 20
	RETURN	N 21
	END	N 22-
	SUBROUTINE PTLOAD (NUMBER,M,NS,NC)	O 1
C		O 2
C	READ DATA FROM MAGNETIC TAPE - USE ONLY ON UNIVAC 1108 FORTRAN5	O 3
C		O 4
	COMMON /BINPT/ III,NTAPE	O 5
	DIMENSION NUMBER(M),NEOF(1)/056/,ICLK(2)/040,015/,IOCT(10)/060,061	O 6
	1,062,063,064,065,066,067,070,071/	O 7
	DIMENSION FMT(2)	O 8
	DATA (FMT(I),I=1,2)/('1H , ','9I10) '/	O 9
10	FORMAT (1H1)	O 10
20	FORMAT (1H0)	O 11
30	FORMAT (1H0,20X,'DIRECT LISTING OF DATA INPUT VIA PTLOAD')	O 12
	IF (NC.GT.5) GO TO 40	O 13
	FLD(0,6,FMT(2))=FLD(6*NC,6,'012345')	O 14
	GO TO 50	O 15
40	FLD(0,6,FMT(2))=FLD(6*(NC-6),6,'678900')	O 16
50	CONTINUE	O 17
	DO 60 I=1,M	O 18
60	NUMBER(I)=0	O 19
	NTAPE=7	O 20
	WRITE (6,10)	O 21
	DO 130 I=1,M	O 22
70	ICOUNT=1	O 23
	DO 120 J=1,NS	O 24
	NCHK=0	O 25

80	CALL CHAR (N)	0	26
	IF (N.EQ.NEOF(1)) GO TO 140	0	27
	IF (.NOT.(N.EQ.ICHK(1).OR.N.EQ.ICHK(2))) GO TO 90	0	28
	IF (ICOUNT.EQ.1) GO TO 80	0	29
	IF (ICOUNT.EQ.2) GO TO 70	0	30
	NUMBER(I)=0	0	31
	GO TO 130	0	32
90	DO 100 K=1,11	0	33
	IF (K.EQ.11) NCHK=NCHK+1	0	34
	IF (NCHK.EQ.5000) GO TO 160	0	35
	IF (K.EQ.11) GO TO 80	0	36
	IF (N.EQ.IOCT(K)) GO TO 110	0	37
100	CONTINUE	0	38
110	NUMBER(I)=NUMBER(I)*10+IABS(K-1)	0	39
	ICOUNT=ICOUNT+1	0	40
120	CONTINUE	0	41
130	CONTINUE	0	42
	WRITE (6,30)	0	43
	WRITE (6,20)	0	44
140	WRITE (6,FMT) (NUMBER(I),I=1,M)	0	45
	GO TO 170	0	46
150	FORMAT (1H , 'INPUT ERROR TERMINATION')	0	47
160	WRITE (6,150)	0	48
	STOP	0	49
170	RETURN	0	50
C		0	51
C		0	52
	SUBROUTINE CHAR (N)	0	53
	COMMON /BINPT/ III,NTAPE	0	54
	DIMENSION INCOME(510),INPUT(170)	0	55
	IF (III.NE.510) GO TO 200	0	56
	CALL NTRAN (NTAPE,2,170,INPUT,L)	0	57
180	IF (L+1) ,180	0	58
	IF (L) 210	0	59
	I=1	0	60
	DO 190 J=1,510,3	0	61
	INCOME(J)=(AND(FLD(6,6,INPUT(I)),7)*16)+(AND(FLD(0,6,INPUT(I)),15)	0	62
	1)	0	63
	INCOME(J+1)=(AND(FLD(18,6,INPUT(I)),7)*16)+(AND(FLD(12,6,INPUT(I))	0	64
	1,15))	0	65
	INCOME(J+2)=(AND(FLD(30,6,INPUT(I)),7)*16)+(AND(FLD(24,6,INPUT(I))	0	66
	1,15))	0	67
190	I=I+1	0	68
	III=0	0	69
200	III=III+1	0	70
	N=INCOME(III)	0	71
	RETURN	0	72
210	N=-1	0	73
	RETURN	0	74
	END	0	75-
	SUBROUTINE DEFTAB	P	1
10	FORMAT (1H1,9X, 'DEFINITIONS OF HEADINGS USED IN OUTPUT'///)	P	2
20	FORMAT (1H ,4X, 'F(X)',16X, 'ABSORPTION CORRECTION FACTORS FOR EITHE	P	3
	1R STANDARDS OR SAMPLES.')	P	4
30	FORMAT (1H ,4X, 'I(P)/(F(X)*C)',7X, 'PRIMARY X-RAY GENERATION FROM E	P	5
	1LITHER STANDARD OR SAMPLE IN PHOTONS PER ELECTRON.')	P	6
40	FORMAT (1H ,4X, 'I(C)/I(P)',11X, 'RATIO OF EMITTED X-RAYS EXCITED BY	P	7
	1 THE CONTINUUM TO THE EMITTED PRIMARY X-RAYS.')	P	8
50	FORMAT (1H ,4X, 'F(X),CONT',11X, 'ABSORPTION CORRECTION FACTOR FOR T	P	9
	1HE CONTINUUM IN THE STANDARD.')	P	10
60	FORMAT (1H ,4X, 'F(X)CON',13X, 'SAME AS F(X),CONT BUT FOR THE SAMPLE	P	11

	1.')	P	12
70	FORMAT (1H ,4X,'CHAR FLUOR',10X,'CHARACTERISTIC FLUORESCENCE CORRECTION FACTOR.')	P	13
		P	14
80	FORMAT (1H ,4X,'F(X)CHA',13X,'ABSORPTION CORRECTION FACTOR FOR THE 1 CHARACTERISTIC FLUORESCENCE CORRECTION.')	P	15
		P	16
90	FORMAT (1H 4X,'AT CONC',13X,'ATOM FRACTION.'/5X,'WT CONC',13X,'MASS FRACTION.')	P	17
		P	18
100	FORMAT (1H ,4X,'STD DEV',13X,'STANDARD DEVIATION OF THE DATA - NOT 1 USED WHEN INPUT IS INTENSITY RATIOS.')	P	19
		P	20
110	FORMAT (1H ,4X,'K(1)...K(N)',9X,'INTENSITY RATIOS.')	P	21
120	FORMAT (1H ,4X,'TOTAL',15X,'TOTAL OF MASS FRACTIONS OBTAINED.')	P	22
130	FORMAT (1H ,4X,'ITERATION NO',8X,'THE NUMBER OF ITERATIONS REQUIRE 1D FOR CONVERGENCE.')	P	23
		P	24
140	FORMAT (1H0,9X,'WHEN THE STOICHIOMETRY OPTION IS USED.'/9X,'A TABLE OF THE FORMULAS OF THE POSTULATED'/9X,'COMPOUNDS, AND THEIR MASS FRACTIONS AS'/9X,'FOUND IN THE ANALYSIS IS PRINTED OUT.'//////////3)	P	25
		P	26
		P	27
	WRITE (6,10)	P	28
	WRITE (6,20)	P	29
	WRITE (6,30)	P	30
	WRITE (6,40)	P	31
	WRITE (6,50)	P	32
	WRITE (6,60)	P	33
	WRITE (6,70)	P	34
	WRITE (6,80)	P	35
	WRITE (6,90)	P	36
	WRITE (6,100)	P	37
	WRITE (6,110)	P	38
	WRITE (6,120)	P	39
	WRITE (6,130)	P	40
	WRITE (6,140)	P	41
	RETURN	P	42
	END	P	43
		P	44

6. Table of Formats for the Data Input Cards

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

* - Right justified in field

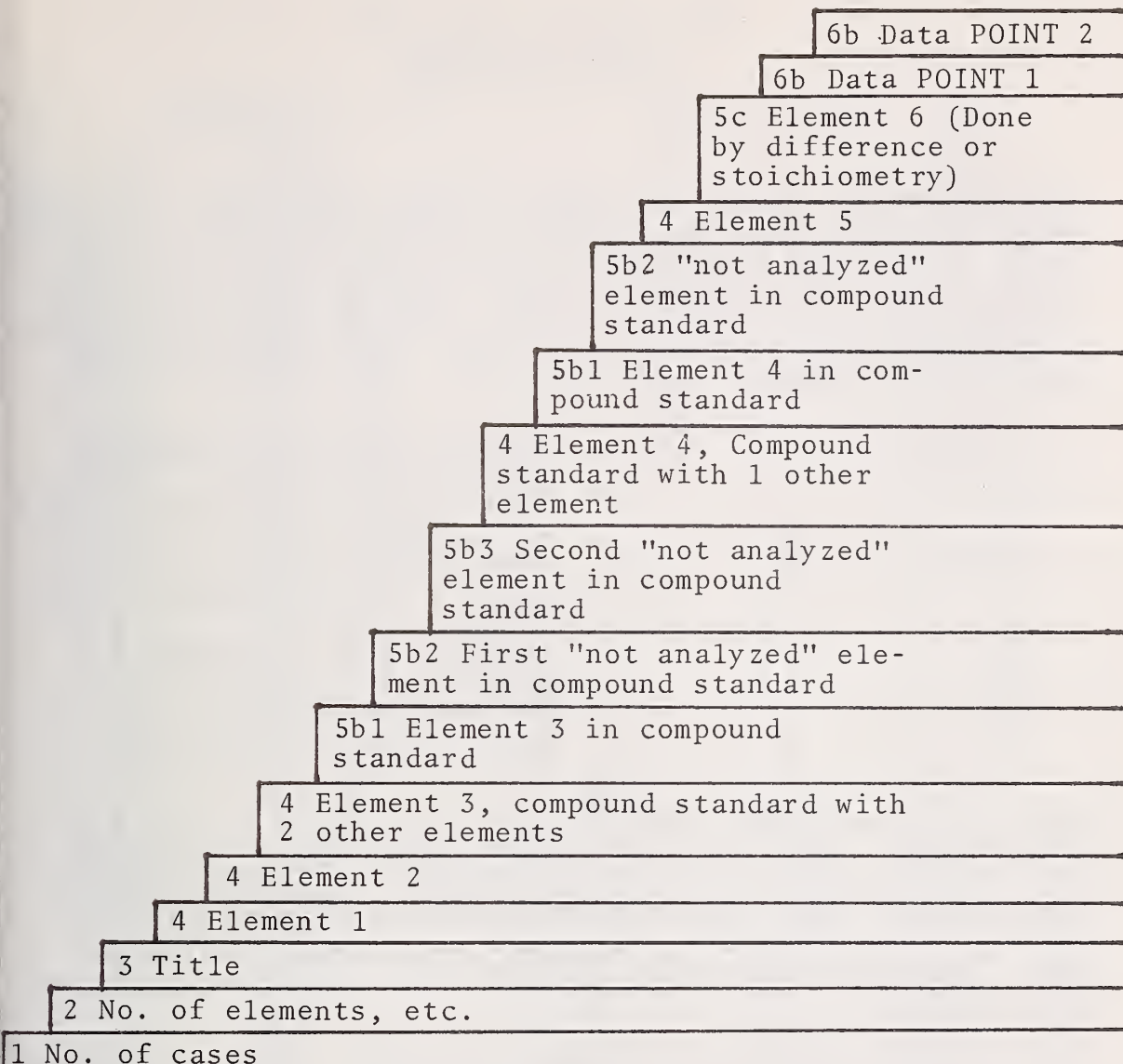
<u>Card no.</u>	<u>When used</u>	<u>Cols.</u>	<u>Format</u>	<u>Description</u>
				If K-edge: 1 - $K_{\beta_{1,3}}$ 2 - K_{α_1}
				If L_{III} -edge: 1 - L_{β_2} 2 - L_{α_1}
				etc.
		22-27	(F6.4)	Cosecant of the x-ray emergence angle.
		28	(I1)	Valence of element if one element is calculated by stoichiometry.
		29	(I1)	If a compound standard was used, enter the number of additional elements in the standard.
		30-35	(F6.4)	Any number greater than 0 will fix the concentration of this element at whatever value is entered on cards 6a.
5a(1)	Element was from a compound standard		(F5.4)	If present, must follow card 4. Weight fraction of analyzed element in compound standard.

<u>Card no.</u>	<u>When used</u>	<u>Cols.</u>	<u>Format</u>	<u>Description</u>
5a(2)	Element was from a compound standard	1-2*	(I2)	If present, must follow card 5a(1). Atomic number of the other element in compound standard.
		3-7	(F5.4)	Weight fraction of this element in compound standard. If more than one other element is present, this card is repeated for each.
5b	Element not analyzed	1-2*	(I2)	Atomic number of element.
		13	(I1)	Valence if calculation by stoichiometry.
		14-18	(F5.4)	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.
6a	Input is either k-values or weight fractions	Fields of 5 (15F5.4)		The k-values or weight fractions for each element (element 1 is first, etc.) measured are on one card for each point.
6b(1)	Input is raw data through subroutine AINP	1-2*	(I2)	Total number of 6-digit numbers read per data point. (Max. of 6 plus code)

<u>Card no.</u>	<u>When used</u>	<u>Cols.</u>	<u>Format</u>	<u>Description</u>
		3-4*	(I2)	Position of manual data entry for coding the line. (Must be in the last position.)
		5-6*	(I2)	Blank - read data from magnetic tape via PTLOAD (or tape reading routine supplied by user). 1 - read data from cards.
		7-8*	(I2)	Blank - average data on each phase for each element. 1 - do each point individually.
		9-13*	(I2)	Total number of lines of input including all samples and standards
		14-15*	(I2)	Blank - calculate k-values from total counts. 1 - calculate k-values from counts/sec.

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*	(10I8)	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.

Options for Data Code
for Raw Data
(Subroutine AINP)

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:

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

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.

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.

DEFINITIONS OF HEADINGS USED IN OUTPUT

F(X)	ABSORPTION CORRECTION FACTORS FOR EITHER STANDARDS OR SAMPLES.
I(P)/(F(X)*C)	PRIMARY X-RAY GENERATION FROM EITHER STANDARD OR SAMPLE IN PHOTONS PER ELECTRON.
I(C)/I(P)	RATIO OF EMITTED X-RAYS EXCITED BY THE CONTINUUM TO THE EMITTED PRIMARY X-RAYS.
F(X),CONT	ABSORPTION CORRECTION FACTOR FOR THE CONTINUUM IN THE STANDARD.
F(X)CON	SAME AS F(X),CONT BUT FOR THE SAMPLE.
CHAR FLUOR	CHARACTERISTIC FLUORESCENCE CORRECTION FACTOR.
F(X)CHA	ABSORPTION CORRECTION FACTOR FOR THE CHARACTERISTIC FLUORESCENCE CORRECTION.
AT CONC	ATOM FRACTION.
WT CONC	MASS FRACTION.
STD DEV	STANDARD DEVIATION OF THE DATA - NOT USED WHEN INPUT IS INTENSITY RATIOS.
K(1)...K(N)	INTENSITY RATIOS.
TOTAL	TOTAL OF MASS FRACTIONS OBTAINED.
ITERATION NO	THE NUMBER OF ITERATIONS REQUIRED FOR CONVERGENCE.

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
STANDARDS

CUKA1 AT NO 29 F(X)= .9836 I(P)/(F(X)*C)= .11546-02 I(C)/I(P)= .39533-01 F(X)CONTE= .9069
 AULA1 AT NO 79 F(X)= .9710 I(P)/(F(X)*C)= .31759-03 I(C)/I(P)= .65730-01 F(X)CONTE= .6783

POINT NO 1
K(1)=.8401
K(2)=.1570

ELEMENT	AT CONC	WT CONC	STD DEV	F(X)	I(P)/(F(X)*C)	I(C)/I(P)	F(X)CON	CHAR FLUOR	F(X)CHA
CU 29	.9259	.8062	.0000	.9746	.11850-02	.49077-01	.7493	.10A20-01	.8115
AU 79	.0741	.2001	.0000	.9488	.25009-03	.42123-01	.4725		

TOTAL = 1.0063

ITERATION NO 3

POINT NO 2
K(1)=.6622
K(2)=.3323

ELEMENT	AT CONC	WT CONC	STD DEV	F(X)	I(P)/(F(X)*C)	I(C)/I(P)	F(X)CON	CHAR FLUOR	F(X)CHA
CU 29	.8244	.6971	.0000	.9659	.12280-02	.56082-01	.6963		
AU 79	.1756	.4009	.0000	.9543	.26957-03	.49526-01	.5246		

TOTAL = 1.0080

ITERATION NO 3

POINT NO 3
K(1)=.4634
K(2)=.5286

ELEMENT	AT CONC	WT CONC	STD DEV	F(X)	I(P)/(F(X)*C)	I(C)/I(P)	F(X)CON	CHAR FLUOR	F(X)CHA
CU 29	.6753	.4036	.0000	.9574	.12832-02	.63753-01	.6426		
AU 79	.3247	.6016	.0000	.9599	.28311-03	.55954-01	.5758		

TOTAL = 1.0052

ITERATION NO 3

POINT NO 4
K(1)=.2462
K(2)=.7525

ELEMENT	AT CONC	WT CONC	STD DEV	F(X)	I(P)/(F(X)*C)	I(C)/I(P)	F(X)CON	CHAR FLUOR	F(X)CHA
CU 29	.4386	.2027	.0000	.9493	.13419-02	.71093-01	.5866		
AU 79	.5614	.8041	.0000	.9655	.29762-03	.61349-01	.6266		

TOTAL = 1.0068

ITERATION NO 3

SPRINGWATER OLIVINE 20KV

SAMPLE NO 2
STANDARDS

COMPOUND	AT NO 12	F(X)E	STN DEV	F(X),CONTE	I(C)/I(P)E	F(X)CON	F(X)CHA
VCKA1	AT NO 12	F(X)E .8213	.0000	.89406-03		.5574	
STANDARD FOR ELEMENT 1							
S1K11	AT NO 12	F(X)E .6156	.0000	.97003-03		.3775	
S1K11	AT NO 14	F(X)E .8717	.0000	.17074-02		.5044	
STANDARD FOR ELEMENT 2							
FEK11	AT NO 14	F(X)E .7578	.0000	.18184-02		.4051	
FEK11	AT NO 26	F(X)E .9756	.0000	.24877-01		.7754	

POINT NO 1
K(1)E .1512
K(2)E .1164
K(3)E .1200

ELEMENT	AT CONC	WT CONC	STN DEV	F(X)	I(P)/(F(X)*C)	I(C)/I(P)	F(X)CON	CHAR FLUOR	F(X)CHA
MO 12	.2356	.2615	.0000	.4770	.00817-02	.13000-02	.3729	.36622-02	.5481
SI 14	.1411	.1810	.0000	.5657	.61591-02	.20591-02	.3149		
FE 26	.0527	.1343	.0000	.9775	.17490-02	.42195-01	.5302		
O 8	.5706	.4168	.0000						

TOTAL E .9935

ITERATION NO 5

STOICHIOMETRY

8. References

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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* ;

$$n_A = N_{Av} \cdot \rho \cdot \frac{C_A}{A} \int_{E_0}^0 \frac{Q}{-dE/dx} dE \quad (1)$$

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]:

$$Q = b \cdot \pi e^4 \cdot z_l \cdot \frac{\ln U}{U} \cdot E^{-2} \quad (2)$$

$$S = -\frac{1}{\rho} \cdot \frac{dE}{dx} = 2\pi e^4 \cdot N_{Av} \cdot \frac{Z}{A} \cdot \frac{1}{E} \ln \left(\frac{\alpha E}{J} \right) \quad (3)$$

The values of some parameters of these equations are, however, poorly known. Héroc 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 α 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:

$$J = 9.76 Z + 58.5 Z^{-0.19} \quad (4)$$

* A list of symbols used is appended.

Another expression for J has been proposed by Duncumb *et al.* [12]:

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

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:

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

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

$$n_A = \frac{1}{2} \frac{C_A}{A} z_{\ell} b \frac{1}{M} \left\{ U_0 - 1 - \frac{\ell_n V}{V} [EI(\ell_n(U_0 V)) - EI(\ell_n V)] \right\} \quad (7)$$

in which EI is the exponential integral:

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

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]:

$$\begin{aligned}
 R = & 1.0000 + \\
 & + (-.581 + 2.162W - 5.137W^2 + 9.213W^3 - 8.619W^4 + 2.962W^5) \times 10^{-2}Z + \\
 & + (-1.609 - 8.298W + 28.791W^2 - 47.744W^3 + 46.540W^4 - 17.676W^5) \times 10^{-4}Z^2 + \\
 & + (5.400 + 19.184W - 75.733W^2 + 120.050W^3 - 110.700W^4 + 41.792W^5) \times 10^{-6}Z^3 + \\
 & + (-5.725 - 21.645W + 88.128W^2 - 136.060W^3 + 117.750W^4 - 42.445W^5) \times 10^{-8}Z^4 + \\
 & + (2.095 + 8.947W - 36.510W^2 + 55.694W^3 - 46.079W^4 + 15.851W^5) \times 10^{-10}Z^5
 \end{aligned} \tag{9}$$

where $W = 1/U_O = E_O/E_k$. 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, ω_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}):

$$I'_{Ap} = n_A \cdot R \cdot \omega_m \cdot p_{mn} \tag{10}$$

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]

$$1/f(\chi) = (1 + \frac{\chi}{\sigma}) (1 + \frac{h}{1+h} \cdot \frac{\chi}{\sigma}); \quad h = 1.2 \frac{A}{Z^2} \tag{11}$$

The factor $f(\chi)$ is the ratio between attenuated and unattenuated primary radiation: $F(\chi) = I_p/I'_p$. Expressions for the coefficient σ , which depends on the electron energy, were pro-

posed by Duncumb and Shields [18] and by Heinrich [19]. We presently use the following equation:

$$\sigma = \frac{4.5 \times 10^5}{E_o^{1.65} - E_k^{1.65}} \quad (12)$$

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]:

$$r_f \equiv \frac{I_{fA}}{I_{pA}} = C_B \cdot \frac{I'_{pA}}{I'_{pA}} \cdot \frac{r_A - 1}{r_A} \cdot \frac{\omega_B}{2} \cdot \frac{\mu(A, BK\alpha)}{\mu(AB, BK\alpha)} \cdot \frac{A}{B} \left[\frac{\ell_n(1+u)}{u} + \frac{\ell_n(1+v)}{v} \right] \quad (13)$$

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'_{pB}/I'_{pA} 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 $K\alpha$ lines by $K\beta$ 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 $f(\chi)$ [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

Hénoch 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 Hénoch'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:

$$C^* = k \cdot k_Z^* \cdot k_A^* \cdot k_F^* \quad (14)$$

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 Héroc 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

$$K = \frac{I^*}{I} = \frac{I_p^* + I_c^* + \Sigma I_f^*}{I_p + I_c + \Sigma I_f} \quad (15)$$

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:

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

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

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

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 oxydic systems is presently in progress.

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List of Symbols

A, B	atomic weights of elements A, B
C	mass fraction ("concentration")
E	kinetic energy of the electron
E_0	initial kinetic energy of the electron, operating voltage
E_k	excitation potential of line k
I	attenuated (emergent) intensity of radiation
I'	intensity of generated radiation, before attenuation
J	mean ionization potential
M	variable used for stopping power calculation (eq. 6-7)
N_{Av}	Avogadro's number
Q	ionization cross-section
R	correction factor for electron backscattering
S	stopping power
U	$= E/E_k$
U_0	$= E_0/E_k$
V	variable used for stopping power calculation (eq. 6-7)
W	$= 1/U_0$
Z	atomic number
a	constant in the hyperbolic approximation
b	constant in the calculation of the ionization cross-section
c	constant in the calculation of σ
e	charge of electron

$f(\chi)$	correction factor for absorption of primary radiation
h	$= 1.2(A/Z^2)$ in Philibert's equation. For multi-element targets, $h = \sum_i C_i A_i / Z_i^2$
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
α	constant in Bethe's equation for energy loss of electrons
θ	emergence angle of measured x-rays
μ	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
ρ	density of specimen
σ	coefficient for electron energy effect in Philibert's equation
χ	$= \mu \operatorname{cosec} \theta$
ω	$=$ fluorescence yield

Subscripts and superscripts:

A,B elements A, B
i tally in integration
l electron shell l
* 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 1. 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

<u>Program Variable Name</u>	<u>Common Symbols</u>	<u>Remarks</u>
A(J)	A, B, etc.	Atomic weight of element, the atomic number of which is J
AI(JJA)	I(A)	Total emerging x-ray intensity from pure element A (See definition for JJA)
AIR(JJA)	$I_A^S/I(A)$	Ratio of emerging x-ray intensities from a compound standard, s, and from pure A
AIT	I_A^x	Total emerging x-ray intensity from the specimen for element A
AK(JJA)	K_A	Continuum efficiency constant (Kramer's constant)
AKEX(JJA)	$k_A = I_A^*/I(A)$	Ratio of experimental x-ray intensities emerging from specimen and pure A
ANK(J)	n_K	Exponent for calculating absorption coefficients for element J; in the equation: $\mu(J, \lambda) = C\lambda^n$ for $\lambda < \lambda_K$ edge
ANKL(J)	n_{KL}	same, for $\lambda_K < \lambda < \lambda_{L_I}$
ATCO		Atomic fraction of each analyzed element
C(JJA),	$k_A, k_B \dots$	1. At start of the first iteration, and in the calculation of k-values: x-ray intensity ratio for each element.
	$C_A, C_B \dots$	2. In all other instances: successive estimates of weight fraction of each element.

CC(JJ,JJA)	C_i	Absorption coefficient constant in $\mu(JJ,\lambda_{JJA})$ (definitions for JJ and JJA below).
CD(NP,JJA)	k_j	1. Experimental x-ray intensity ratio for point NP, and line of JJA.
	C_j	2. (In the calculation of k-values) given concentration of element JJ.
CI(J)	C_j (from $\mu=C_j\lambda^n$)	Absorption coefficient constant for element of atomic number J
CL(L,K,J)	λ	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)	$\text{csc } \psi$	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_o	Operating potential, in kV

EX(II,JJA)	n_i	Value of exponent for the absorption coefficient in $\mu=C\lambda^n$, selected and stored by CØCA. II = subinterval number, JJA = element label
EXPO(JJ,JJA)	n_i	Value of the exponent for the absorption coefficient at the wavelength λ_0 , corresponding to E_0 [kV]: $(\lambda_0 = \frac{12.398}{E_0})$
FCASF(JJ)	ΣI_f	Sum of emitted fluorescence intensities excited by characteristic lines, for element JJ
FCASFX	$\Sigma I_f/I_p$	Sum of emitted characteristic fluorescence intensities, divided by the emitted primary intensity.
FCF(JJ)	I_c	Emitted fluorescence intensity excited by the continuum, for element JJ
FCFX	I_c/I_p	Emitted continuum-fluorescence intensity divided by the emitted primary intensity
FCK12(J) FCK13(J) FCK23(J)	f_{12} f_{13} f_{23}	Coster-Kronig coefficients stored in the permanent data file for each element
FIRST		Logical variable used to label the first input card of a sample
FQC(JJ)	$f_c, f_c(\chi)$	Absorption factor, $f(\chi)$, for fluorescence excited by the continuum
FQCA(JJ)	$f_f, f_f(\chi)$	Absorption factor, $f(\chi)$, for the fluorescence x-ray intensity excited by characteristic lines

FQF(JJ)	$f_p, f_p(\lambda), f(\lambda)$	Absorption factor for primary radiation, element JJ
ICOF		Switch to eliminate correction for continuum fluorescence
III		Constant needed for reading magnetic tape input via PTLOAD (not operative unless PTLOAD is used)
IMA(JJA)		Number of sublimits need in the calculation of fluorescence excited by the continuum
J	Z	Subscript for atomic number
JJ		Subscript for order in which the element appears in the input data (arbitrary) \equiv "element label"
JJA		Label JJ of the element being measured
JJA1, JJA2		Element labels of unanalyzed elements
JJAM		Number of analyzed elements
JJAS		$JJA + \underline{1}$
JJJ(I, JJA)		Label of the element which emits the line of wavelength WAVE(I, JJA)
JJM		Number of elements in a case
JJMX		Either JJAM or JJM, depending on the variant of the program
JST		Number of elements contained in a compound standard
K		Subscript: level number (edge)

KA(JJA) KAA	K, L _I , L _{II} , ... K, L _I , L _{II} , ...	Number of the level of the analyzed element which emits the measured line
KB(I, JJA)	K, L _I , L _{II} , ...	Number of the level emitting the line WAVE(I, JJA)
KK		Diverse switches
KM(J) KMJ		Number of absorption edges listed in the permanent data file, for element J
KSTOP		Switch for termination of program
L		Subscript for CL(L, K, J). Position in the sequence in which the lines are filed in the permanent data file. This sequence restarts after each edge.
LA(JJA)		Subscript: Position of measured line in permanent data file.
LB(I, JJA)		Subscript: Position of exciting line in permanent data file.
LI(KAA, LAA)	alphabetic	Name of analyzed line (KA ₁ , MB ₁ , ..., etc.)
LM(K, J) LMKJ		Number of lines listed in the series K, of the element of atomic number J (K=level number of the edge).
LOUT		Switch for output 2.
MESS(JJ, JJA)		Switch for writing error message
MF(JJA)		Number of characteristic lines which excite fluorescent emission
NCO(JJA)		Switch for error termination due to insufficient data

ND		Switch for input method
NEC		Case number
NECM		Number of cases in a run
NELM		Number of elements listed in table
NEST	= $\text{JST} - \underline{1}$	Number of additional elements in a compound standard (not including the analyzed element)
NIT		Number of iteration
NOE		Running number of element for reading permanent data file.
NP		Index: data point number in any case
$\text{NP}\underline{1} \equiv \text{NPM} - \underline{1}$		Total number of data points minus <u>1</u>
NPM		Total number of data points
NSW		Switch determining the variant of the program to be used
NSW2		Switch set for terminating iterations
NTAPE		Magnetic tape assignment (for PTLOAD only)
$\text{NV}(\text{JJ})$		Valence of element number JJ
NX NY		Subscripts for stoichiometry printout
$\text{NZ}(\text{JJ})$	Z_A, Z_B, \dots	Atomic number of element JJ

NZA		Atomic number for a particular element
NZA1		
NZEX		
NZO		
OME(K,J)	$\omega_q(J)$	Fluorescence yield for level number K of element of atomic number J
OMEG(I,JJA)	ω_{eff}	Effective yield for ionization produced by photons (corrected for Coster-Kronig effects)
R(K,J)	r_q	Jump ratio at edge number K of element of atomic number J
RPF(JJ)	I_p	Emitted primary intensity of element number JJ
RPFX	I'_p	Generated primary intensity of an element
RR(I,JJA)	r_i	Absorption jump ratio associated with line of wavelength WAVE(I,JJA)
RRR(I,JJA)	$(r_{i-1})/r_j$	Jump-efficiency ratio for element JJA
SA <u>1</u>		Auxiliary variable in calculation of atomic concentration
SACO	$\Sigma(C_i/A_i)$	Sum of the weight fractions divided by their respective atomic weights
SC	ΣC_i	Summation of the weight fractions
SD(NP,JJ)	$\frac{\sigma_k}{k}$	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)	λ_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_{qm}	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, \dots or N_1, N_2, \dots are dummy variables used only to keep variables in COMMON in order.

Additional Variables in AINP

ASUM		Average value of a set of peak- or background-intensity measurements
C(IJ,II)	k_j	$C(IJ,II) = CD(NP,JJA)$
COUNT		Count-rate, in cts/sec, for dead-time correction
CSTD(I,J)		Intensity of standard, corrected for dead-time
DEADT(---)		Function used to make dead-time correction
FSD(J,I)		Double-precision standard relative deviation of counts collected for each element in each point
I		Index
IC		$IC = ICON(I,J)$
ICON(I,J)		Number of times standards or backgrounds are read
II,IIC	Index	
IIMAX		$IIMAX = JJAM$ (number of elements analyzed)
IJ		$IJ = NPM$ (total number of data points)
IK		$IK = 6 - I$ (tally for separating of codes for scalers)
IND		Variable for dead-time determination
INDEX		An index for setting up a table of all the input data
ITEN		$ITEN = 10^{IK}$ auxiliary variable for scaler code separation

KK(J)	Counter for number of determinations in each point
M	$M + NC * ND$
MCO(I)	Variable used in separating data code
NAV	Output code: if 0, print: average of measurement for each point if <u>1</u> ,: handle all data individually as separate points
NC	Number of scalers used in a measurement
NC <u>1</u>	$NC\underline{1} = NC - \underline{1}$
NCODE(NROW, I)	$NCODE(NROW, I) = MCO(I) / ITEN$
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	$NR = NSTD(IIC, \underline{1}, I, J)$
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

NTC	If NTC=0, data are on magnetic tape If NTC= <u>1</u> , data are on cards
NTRA	If NTRA=0, calculate using total counts If NTRA= <u>1</u> , calculate using counts/sec
NUMBER(INDEX)	List of numbers returned by magnetic-tape reading subroutine PTLOAD
PEAK(I)	Peak minus background for standards
PHC(NROW,I)	Peak intensity of specimen
SNSTD(I,J)	Sum of the standard intensities (peak or background)
SPH(J,I)	Sum of peak intensities on each point of the specimen
SPHC(J,I)	Average peak intensity on each point of the specimen
SSTSD	Conversion of STSD from double precision to single
SSUM(I,J)	Sum of the squares of all peak and background measurements for each standard (double precision)
STSD	Relative double precision standard deviation for signals from each standard and background
SUM(I,J)	Sum of all peak and background measurements for each standard (double precision)
SUMS(I,J)	$SUMS(I,J) = [SUM(I,J)]^2 / ICON(I,J)$ (double precision)
T(NR)	Time in seconds
TIM(J)	Summation of times in each point

Additional Variables in COCA

F $\overline{12}$ F $\overline{13}$ F $\overline{23}$	f $\overline{12}$ f $\overline{13}$ f $\overline{23}$	Coster-Kronig coefficients
I		Subscript: index of sub- limits of the wavelength ranges
I2		Number of absorption edges of one element between λ_o and λ_m
I3		Number of the exciting line (char. fluor.)
I3M		Total number of exciting lines (char. fluor.)
II		Subscript: index of sub- limits
IL		IM-I+ <u>1</u>
IM		Variable value for I in loop
IM <u>1</u>		IM <u>1</u> = IM- <u>1</u>
JM		For pure element standard: JM = JJA For compound standard: JM = JST For specimen: JM = JJM
JO		For all standards: JO = JJA For all specimens: JO = <u>1</u>

K1
KR1
KR2

Auxiliary variables related
to shells and subshells:

<u>K</u>	<u>KR1</u>	<u>KR2</u>	<u>K1</u>
1	1	1	0
2	2	2	1
3	2	2	1
4	3	3	2
5	2	4	1
6	2	4	1
7	2	4	1
8	4	5	3
9	5	6	4
10	6	7	1
11	6	7	1
12	7	8	5

M4

Variable M4 = IM1

NNR

r_1

Jump ratio: NNR = R(K,J)

T1 to T8

Temporary storage

WAA

λ_0

λ_0 wavelength: WAA = WA(JJA)

Additional Variables in CALI

FCAS	ΣI_f^*	Total fluorescence intensity excited by characteristic lines (emitted)
FCASO	$\Sigma I'_f^*$	Total fluorescence intensity excited by characteristic lines (generated)
FQ	$f_p, f(\chi)$	Absorption factor for primary emission
FQCA <u>1</u>	$f_f, f(\chi)_{char}$	FQCA <u>1</u> = FQCA(JJ)
FQCF(JJA)	$f_c f(\chi)_c$	FQCF(JJA) \equiv FQC(JJ)
IMAM		IMAM = IMA(JJA)
IO		IO = IMA(JJA) + <u>1</u>
RP	I_p	Emerging primary intensity = RPF(JJ)
RPO	I'_p	Generated primary intensity

Additional Variables for FCA

ACA	χ_A^*	$\chi_A^* = A \sum_{B \dots} C_B \mu(B, A \text{ qm}) X$ $X \operatorname{cosec} \psi$
ACB	χ_B^*	$\chi_B^* = A \sum_{B \dots} C_A \mu(A, B \text{ qm}) X$ $X \operatorname{cosec} \psi$
ACBA	μ_B^A	$\mu_B^A = C_i^A (\lambda_B)^{n_i^A}$
CA(I), CB(I)	a_i, b_i	Coefficients of expansion of the depth-distribution function $\phi(\rho z)$ (according to Criss [5]): $\phi(\rho z) = \sum_i a_i \exp [-b_i \rho z]$
FCA $\underline{1}$	I_f	Fluorescence intensity excited by a characteristic line (emitted)
FCAO	I_f'	Fluorescence intensity excited by a characteristic line (generated)
FQIB	f_f	Absorption factor in fluorescence intensity excited by a characteristic line
H	h	h from Philibert's absorption correction equation
JJB		Number of the exciting element
KBB		$KBB = KB(I, JJA)$
LBB		$LBB = LB(I, JJA)$
NZB		Atomic number of exciting element
RJ		Conversion of J from integer to real mode

S1

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

AC(CL,J)	μ_λ	Mass absorption coefficient of element J, for the wavelength: $\lambda = CL$ (function)
ACS	χ_A^*	$\chi_A^* = A_{A,B...} C_B \mu(B,A \text{ qm}) X$ $X \text{ cosec } \psi$
ALK		Conversion of LK from integer to real mode
ANIN		Conversion of NIN from integer to real mode
ANZ	Z_A	Conversion of NZ from integer to real mode
BK1 BK2 BN BN1 BO		Sublimits used in the computation of the definite integral over wavelength
CCO(J)	C_i	Value of C_i (constant for calculation of μ) for element J, as a function of wavelength
EABI		Auxiliary variable in the calculation of fluorescence excited by the continuum
EXO(J)	n_i	Value of exponent n_i for element J
F(X,JO,JM,JJA)		Auxiliary function for numerical integration (emitted)
FC	I_f	Fluorescence intensity excited by the continuum (emitted)
FCO	I'_f	Fluorescence intensity excited by the continuum (generated)
FI		Step in calculation of FC

FIO		Step in calculation of FCO
FT(X,JO,JM,JJA)		Auxiliary function for numerical integration, case without absorption
H	$\Delta\lambda$	Wavelength increment for integration
IM <u>1</u>		IM <u>1</u> = IMA(JJA)
LK		Index
LKM		Limit of LK
NIN		Number of intervals used in the integration
NIN2		NIN = 2*NIN2
OMEGI	ω_{eff}	Effective yield in a given interval of wavelength
RL		Remainder after wavelength interval is divided
RRRI	$(r_{i-1})/r_j$	RRRI = RRR(I,JJA)
S		Step in calculation of fluorescence excited by the continuum (emitted)
SO		Step in calculation of fluorescence excited by the continuum (generated)
ZMK	K_A, \bar{K}	Efficiency constant for continuum production

Additional Variables in RB

R <u>1</u> to R5		Auxiliary variables in calculation of backscatter
W	$\frac{1}{U_0}$	Reciprocal of overvoltage
W2 to W5	$(\frac{1}{U_0})^2$ to $(\frac{1}{U_0})^5$	Powers of W
Z <u>1</u> to Z5		$Z_1 = \frac{1}{10} Z$; ... $Z_5 = \frac{1}{10} Z^5$

Additional Variables in FQI

H	h	h from Philibert's equation
SIG	σ	$\sigma = 4.5 \times 10^5 / (E_0^{1.65} - E_q^{1.65})$

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 $\ln(U_o V)$ $\ln(U_o V) = \ln(U_o) + \ln(V)$

ALW $\ln(V)$ $\ln(V) = \sum_{A,B,\dots} C_i \frac{Z_i}{A_i} \ln X$
 $\times \left(\frac{1 \cdot 166 E}{J_i} \right) / \sum_{A,B,\dots} C_i \frac{Z_i}{A_i}$

AM M $M = \sum_{A,B,\dots} C_i \frac{Z_i}{A_i}$

AMLW $M \ln(V)$ $M \ln(V) = \sum_{A,B,\dots} C_i \frac{Z_i}{A_i} \ln X$
 $\times \left(\frac{1 \cdot 166 E}{J_i} \right)$

AW V $V = \exp [ALW]$

CX C_A Concentration of analyzed
element

EI $ei(x)$ Function: $ei(x) = \int_{-\infty}^x \frac{e^{-V}}{V} dV$

EM	E_1	1 energy level
JX	Z_A	Atomic number
KX		Subscript: level number (edge) = K
KXX		KX must be greater than 4:
	$\frac{KX}{5}$	$\frac{KXX}{1}$
	6	1
	7	2
	8	2
	9	3
LX		Subscript: line number = L
OMED	ω_{eff}	Effective fluorescence yield for ionization produced by electrons
RB	R	Backscatter factor
RBA		$RBA = \sum_{A,B} C_A \cdot R_A$
RZ	Z_A	Conversion of NZ from integer to real
UO	$\frac{E_o}{E_1} = U_o$	Overvoltage
Z	Z_A	Atomic number
ZJ	J_A	Mean excitation potential
ZNL	Z_{n1}	Number of electrons in a shell

Additional Variables in F

ACAX	μ_A^A	Mass absorption coefficient, pure element: $\mu(A, A_{qm}) = C_i (\lambda_Z)^{n_i}$
ACX	μ_λ^*	Mass absorption coefficient, specimen $\mu(*, A_\lambda) = \sum_{A, B, \dots} C_A [C_i^A (\lambda)^{n_i^A}]$
X		Whichever sublimit is used in the calling routine (BK <u>1</u> , BK2, BN, BN <u>1</u> , or BO)

APPENDIX 3
Permanent Data File

Permanent Data File

Types of cards for data input to the permanent data table

<u>Card No.</u>	<u>When Used</u>	<u>Cols.</u>	<u>Format</u>	<u>Description</u>
1	once at beginning of table	1-3*	(I3)	Number of elements in permanent data table
2	first card for each element	1-2*	(I2)	atomic number
		3-4*	(I2)	number of absorption edges listed in table
		5-10	(F6.3)	atomic weight
		3 fields of 6	(3F6.4)	Coster-Kronig coefficients f_{12}, f_{23}, f_{13}
		(11-28)		
29-34		(F6.2)	absorption constant C_i	
		2 fields of 4 (35-42)	(2F4.2)	absorption exponents n_K, n_{KL}
3	card for each edge	1-7	(F7.5)	wavelength at absorption edge
		8-13	(F6.4)	jump for the edge
		14-19	(F6.5)	fluorescent yield ω
		20	(I1)	number of lines listed for the edge
4	card for each line	1-7	(F7.5)	wavelength of line
		8-13	(F6.4)	weight of the line with respect to the sum of line intensities in its series

*Number must be right justified in the field.

67			
1 1 1007			1 290
200.			
3 1 6939			14 288
120.			
4 1 9012			35 286
111.			
5 1 1081			74 285
676			
6 2 12011			135 284 273
4368 2622	00091		
447 1			
99			
7 2 14007			221 283 273
3099 2576	00151		
316 1			
99			
8 2 16			38 282 273
2332 24	00221		
2362 1			
99			
9 2 19			49 281 273
17913 1933	1		
1832 1			
99			
11 2 2299			905 279 273
11569 184	025 2		
11575 12			
119101 88			
99			
12 2 2431			1175 279 273
95122 15	028 2		
95207 12			
989 88			
99			
13 2 2698			1487 278 273
79481 14	038 2		
79605 12			
83393 88			
99			
14 2 2809			185 277 273
6738 1296	038 2		
67530 12			
712542 88			
99			
15 3 30974			225 277 273
5784 1232	08 2		

5796	12		
61568	88		
00			
94			
16 2 32064			27 276 273
5019 1167	083 2		
50316 12			
53722 88			
757			
17 2 35453			317 276 273
43971 1112	1 2		
44034 12			
47278 88			
609			
19 3 39102			425 275 273
34365 101	155 2		
34539 12			
37414 88			
00			
421			
20 3 4008			484 274 273
30703 96	165 2		
30897 12			
33584 88			
00			
3513			
21 3 4496			551 274 273
2762 929	17 2		
27796 12			
30309 88			
00			
3014			
22 3 479			621 273 273
24973 887	213 2		
25139 12			
27485 88			
00			
2729			
23 3 5094			698 273 273
22694 8703	242 2		
22844 12			
250356 88			
00			
238882			
24 2 52			78 273 273
20702 8497	272 2		
208487 12			
22897 88			
167			
25 2 5494			867 272 273
18964 824	291 2		

19102	126		
21018	874		
1624			
26 3 5585			9580 272 273
174346	8108	32	2
175661	102		
193604	895		
00			
17202			1
1726	857		
27 3 5894			1055 271 273
160815	7962	35	2
162079	10		
178897	88		
00			
15618			
28 3 5869			11590 271 273
148807	7769	38	2
150014	107		
165791	893		
00			
14242			1
14271	857		
29 5 6354			12680 271 273
138059	7659	415	2
139222	12		
154056	88		
112709	117		
13014	139		
13288	573	00561	
13336	1		
110.6			
30 4 6538			138 270 273
12834	7505	45	2
129525	12		
143516	88		
1106	117		
11862	139		
12131			
31 5 6972			1498 270 273
11958	7376	469	2
120789	12		
134008	88		
9517	117		1
10365	1		
10828	139		1
11023	1		
111	4246	006	1
11292	1		
99			
32 5 7259			1622 270 273
111658	7299	51	2
112894	12		

125405	88		
8773	117		2
9581	59		
9640	41		
9924	139		1
10175	1		
10187	4605	006	1
104361	1		
99			

33 5 7492			1754	269	273
1045	722	548	2		
10573	12				
117588	88				
8107	117		1		
8929	1				
9125	139		1		
94141	1				
9367	4661	006	1		
96709	1				
99					

34 5 7896			1894	269	273
97974	718	585	2		
99218	12				
110477	88				
7503	117		1		
8321	1				
8407	139		1		
87358	1				
8646	4583	006	1		
899					
99					

35 5 79909			205	269	273
9204	7142	628	2		
93279	12				
103974	88				
6959	117		1		
7767	1				
7753	139		1		
81251	1				
7984	4524	006	1		
83746	1				
99					

37 5 8547			2355	268	273
8157	7018	68	2		
82868	12				
92555	88				
5998	117	008	2		
67876	59				
68207	41				
6644	139	024	1		
70759	1				
6865	439	024	1		
73183	1				
38265					

38 5 8762			2513	268	273
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76973	6976	7	2
78292	16		
87526	84		
5592	117	008	2
63672	59		
64026	41		
6173	139	024	1
66239	1		
6387	4314	024	1
68628	1		

345

39 5 8891				57	2681	267	273
72766	695	719	2				
74072	16						
82884	84						
5217	117	008	2				
59832	59						
60186	41						
5756	139	024	1				
6212	1						
5962	424	024	1				
64488	1						

3147

40 5 9122				57	2851	267	273
68883	696	737	2				
70173	16						
78593	84						
4879	117	008	2				
5633	59						
56681	41						
5378	139	024	2				
53843	10						
5836	90						
5579	4166	024	2				
55863	7						
60705	93						

288

41 5 9291				56	3039	267	273
65298	7035	754	2				
66576	16						
7462	84						
4575	117	008	2				
53102	59						
53455	41						
5031	139	024	2				
50361	10						
54923	90						
523	4123	024	2				
52379	7						
57243	93						

2627

42 5 9595				55	3241	266	272
61978	694	77	2				
63229	16						
7093	84						
4304	117	001	2				

50133 59
 50488 41
 4719 139 003 2
 47258 10
 517708 90
 4913 3979 03 2
 49232 7
 540655 93
 245

44 51011 23 15 54 3671 266 272
 56051 6049 799 2
 57248 15
 64308 85
 3835 117 01 2
 44866 58
 4523 36
 418 139 03 2
 41822 16
 462058 83
 4369 3897 03 2
 43718 16
 484575 84
 211932

45 5102905 23 15 54 3902 266 272
 53395 658 812 2
 54561 15
 61328 85
 3629 117 01 2
 42522 58
 42888 36
 39425 139 03 2
 39437 16
 437414 83
 41299 3839 03 2
 4131 16
 459743 84
 198368

46 51064 3 17 5 4142 265 272
 5092 695 822 2
 52052 15
 58545 85
 34369 117 01 2
 40346 58
 40711 36
 37228 139 03 2
 37246 16
 414622 83
 39074 380 03 2
 390887 16
 436767 84
 18532

47 510788 314 20 457 439 265 271
 48589 673 833 2
 49707 15
 55941 85
 3254 117 00352

383313	58						
387023	36						
3514	139	025	2				
35226	16						
393473	83						
3698	371	021	2				
370335	16						
415443	84						
1724							
48 511240	42	25		36	4648	265	271
46407 6855		819					
30489	117	05	2				
364495	58						
3682	36						
33257	139	06	2				
333564	16						
373823	83						
35047	372	02	2				
351408	16						
395635	84						
1608							
49 511482	46	30		25	4914	264	271
44371 689		845					
29260	117	05	2				
346984	58						
350697	36						
31473	139	06	2				
316213	16						
355531	83						
33237	361	02	2				
333838	16						
377192	84						
1505							
50 511869	5	26		26	5188	264	271
4246	592	84					
27769	117	03	2				
33058	58						
33433	36						
29831	139	06	2				
30012	16						
33849	83						
31557	3539	05	2				
31751	16						
35999	84						
14028							
51 512176	586	12			842		270
40668	58	862					
26388	117		2				
315258	58						
319014	36						
28294	139	069	2				
285159	16						
322567	83						
30003	346	049	2				
302335	16						
343941	84						

1313

52	51276	31	13	885	27
	3897	58	87		
	25101	117	04	2	
	30089	58			
	30466	36			
	26882	139	07	2	
	27124	16			
	30768	83			
	28558	3403	06	2	
	28822	16			
	32892	84			

1234

53	51269	63	23	94	270
	37381	57	895		
	2388	117	05	2	
	291207	58			
	287429	36			
	25542	139	09	2	
	258244	16			
	293744	83			
	27196	339	07	2	
	375053	16			
	31486	84			

11544

55	5132905	628	175	1034	269
	34451	55	89		
	21673	117	2		
	26285	58			
	26666	36			
	23139	139	2		
	2348	16			
	26837	83			
	2474	3251	05	2	
	25118	16			
	28924	84			

101957

56	513734	66	26	109	269
	33104	55	87		
	20678	117	2		
	25164	58			
	25553	36			
	22048	139	2		
	22415	16			
	256821	83			
	23629	323	05	2	
	240435	16			
	277595	84			

155

57	913891	66	26	1144	268
	31844	55	9		
	1978	117	2		
	24105	59			
	24493	39			
	21053	139	2		

21418	16		
24589	84		
2261	3168	05	2
2303	16		
26657	84		
90629	116		
10272	1207		
110106	1158		
14535	1895		
14795	1895		
60 914424	62		132 267
28453	53		
1739	117	2	
21268	59		
21669	39		
1844	139	2	
18779	16		
21669	84		
19967	3044	07	2
2036	16		
23704	84		
78668	116		
88242	1207		
9559	1158		
123856	1895		
126769	1895		
701017304	518		199 263
20224	475	94	
11818	117	2	
145233	61		
149138	39		
12428	139	34	2
126769	15		
147565	85		
13862	2691	20	2
14155	16		
167189	84		
51701	116		
57029	1207		
63547	1158		
78668	1895		
81086	1895		
254579			
72101785	55		214 262
18982	47		
10997	117	28	2
13530	61		
13920	39		
11548	139	25	2
11790	15		
13741	85		
12972	264	25	2
13264	16		
15696	84		
4774	116	005	
5249	1207	0084	
58926	1158	00451	

6768	1				
72376	1892	017	1		
7601	1				
74777	1892	019	1		
7840	1				
2317					
731018095	55	2	19	222	262
18394	47	946			
10613	117	28	2		
130678	61				
134581	39				
11137	139	25	2		
113794	15				
132698	85				
12553	2615	25	2		
128454	16				
152197	84				
4585	116	005			
502	1207	0084			
565	1158	00451			
6312	1				
687	1892	017	1		
7023	1				
7128	1892	019	1		
7252	1				
2105					
741018392	0386		258	231	261
17837	47	0945			
102467	117	0305	2		
126269	61				
130162	39				
10745	139	0311	2		
109855	15				
128181	85				
12155	260	22	2		
124460	1593				
147639	8407				
4407	116	005			
4815	1207	0084			
5435	1158	00451			
6092	1				
659	1895	017	1		
6757	1				
683	1895	019	1		
6983	1				
2105					
75101862	325		458	239	261
17302	47	951			
9894	117	11	2		
122031	61				
125917	39				
10371	139	33	2		
106099	15				
123858	85				
11773	2574	20	2		
12066	16				
14329	84				

4236	116	005			
462	1207	0084			
5234	1158	00451			
5885	1				
633	1895	017	1		
6504	1				
656	1895	019	1		
6729	1				
199					
76101902	3		46	247	260
16787	46				
9558	117	1	2		
117955	61				
121844	39				
10014	139	35	2		
102503	15				
119727	85				
11408	2544	21	2		
116979	16				
13912	84				
4071	116	005			
4433	1207	0084			
5043	1158	00451			
5682	1				
6073	1904	017	1		
6267	1				
630	1904	019	1		
6490	1				
1890					
77101922	19		46	256	26
16292	46				
9236	117	10	2		
114085	61				
117958	39				
9671	139	37	2		
99085	18				
115781	82				
11058	252	23	2		
113532	17				
135128	82				
3915	116	005			
4260	1207	0084			
4861	1158	00451			
55	1				
583	1895	017	1		
6038	1				
605	1895	019	1		
6262	1				
179					
781019523	17		50	263	259
15818	46				
8931	117	35	2		
110394	61				
114223	39				
93414	140	31	2		
95797	18				
111990	82				

10723	248		275	2		
110200	17					
131304	82					
3774	116		005			
4414	1207		0084			
471	1158		00451			
5319	1					
5665	1895		017	1		
5828	1					
581	1895		019	1		
6047	1					
172						
791019697	25	22	51	272		259
015359	46					
086376	117	08	2			
106785	61					
110651	39					
090259	139	343	2			
92650	18					
108353	82					
10400	247	31	2			
107022	18					
127640	82					
3616	116		005			
3936	1207		0084			
4518	1158		00451			
5145	1					
5374	1895		017	1		
5624	1					
5584	1895		019	1		
584	1					
1627						
801020059	158	08	647	281		258
14918	46	96				
8353	117		2			
103358	61					
107222	39					
8722	139	39	2			
89646	18					
104868	82					
10091	2438	40	2			
103975	18					
12412	82					
3478	116		005			
3783	1207		0084			
4355	1158		00451			
4978	1					
5157	1895		017	1		
5431	1					
536	1895		019	1		
5645	1					
154012						
811020437	17	25	56	289		258
14495	45					
80786	117	09	2			
100062	61					
103918	39					

8435	139	43	2
86752	18		
101513	82		
9795	2404	27	2
101031	18		
120739	82		
33471	116	005	
36297	1207	0084	
41933	1158	00451	
4823	1		
49889	1888	017	1
5249	1		
5189	1888	019	1
546	1		
14664			

821020719	16	6	298	257
14088	56			
78168	117	37	2	
96911	61			
10075	39			
81566	139	24	2	
83973	18			
98291	82			
95112	2394	35	2	
98221	18			
117501	82			
321967	116	005		
348827	1207	0084		
404318	1158	00451		
4674	1			
479502	1895	017	1	
5076	1			
499114	1895	019	1	
5286	1			
13874				

8310209	19	59	307	256
13694	45	963		
7571	117	12	2	
93855	61			
97690	39			
7887	139	32	2	
81311	18			
95198	82			
9234	236	35	2	
95518	183			
114386	817			
3094	116	005		
3359	1207	0084		
3904	1158	00451		
4532	1			
4572	1895	017	1	
4909	1			
4764	1895	019	1	
5118	1			
132				

901223204	21	458	377	253
11037	42	963		

6059	117		2		
75479	61				
79257	39				
6299	139	56	2		
65313	21				
76521	79				
7607	194	39	2		
79354	19				
956	81				
2393	116	005			
2572	1207	0084			
3068	1158	00451			
3679	1				
3557	1895	017	1		
3941	1				
3729	1895	019	1		
41381	1				
9371					
10688					
12928					
921223803	1			55	397
10723	42	963			253
5695	117	25	2		
71029	61				
74799	39				
5919	139	59	2		
61477	21				
71998	79				
7223	2069	44	2		
75468	19				
91064	81				
2235	116	005			
2394	1207	0084			
2884	1158	00451			
3479	1				
3333	1888	017	1		
3716	1				
3497	1888	019	1		
391	1				
8614					
9747					
11898					

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