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DESCRIPTION OF A COMPUTER METHOD FOR THE CORRECTION AND PREDICTION OF ELECTRON MICROPROBE DATA

R. H. PACKWOOD

PHYSICAL METALLURGY DIVISION

OCTOBER 1970

Technical Bulletin TB 130

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Information Canada
Ottawa, 1971

Mines Branch Technical Bulletin TB 130

DESCRIPTION OF A COMPUTER METHOD FOR THE CORRECTION AND PREDICTION OF ELECTRON MICROPROBE DATA

by

R. H. Packwood*

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ABSTRACT

A computer method for correcting and predicting electron microprobe data is described. The programme is written in FORTRAN IV language. For convenience the programme is divided into two parts, a correction version and a prediction version, both of which use the same procedures for calculating the effects of absorption (PHILIBERT-DUNCUMB and SHIELDS - HEINRICH), α - and β - line fluorescence (REED), atomic number (DUNCUMB and REED), and bremsstrahlung (SPRINGER). The correction version also includes routines that allow for counter dead-time, background, compound standards, and missing data. The prediction version is employed in general to compute calibration curves for systems under frequent investigation and in particular to calculate the compound standard factors that may be required by the correction version of the programme. Both versions are demonstrated using experimental data and typical analytical situations.

Notes on the practical use of the programmes are appended.

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Direction des mines

Bulletin technique TB 130

DESCRIPTION D'UNE MÉTHODE DE CALCUL SUR ORDINATEUR POUR LA CORRECTION ET LA PRÉDICTION DES DONNÉES D'UNE MICROSONDE ÉLECTRONIQUE

par

R. H. Packwood*

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RÉSUMÉ

L'auteur décrit une méthode de calcul sur ordinateur pour la correction et la prédiction des données d'une microsonde électronique. Le programme est écrit en langage FORTRAN IV. Pour des raisons de commodité, il est divisé en deux parties, la version correction et la version prédiction, les deux utilisant les mêmes procédures pour calculer les effets de l'absorption (PHILIBERT-DUNCUMB et SHIELDS-HEINRICH), de la fluorescence des raies α et β (REED), du numéro atomique (DUNCUMB et REED), et du rayonnement de freinage (SPRINGER). La version correction comprend également les travaux courants qui font entrer en ligne de compte le temps mort des compteurs, le bruit de fond, les composés d'étalonnage et les données manquantes. La version prédiction est employée, d'une manière générale, pour établir les courbes d'étalonnage pour les systèmes qui sont l'objet d'études fréquentes, et, d'une manière plus particulière, pour calculer les facteurs relatifs aux composés d'étalonnage dont on peut avoir besoin pour la version correction du programme. L'auteur donne des exemples pratiques de l'utilisation des deux versions en se servant de données experimentales et de situations d'analyse caractéristiques.

Des notes sur l'utilisation pratique de ces programmes sont jointes au présent bulletin.

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CONTENTS

FIGURE

1. INTRODUCTION

There are currently available a dozen or more computer programmes for correcting electron microprobe data. A review of these by Beaman and Isasi [1] shows that the need for yet another programme would, on the face of things, appear slight. However, when this work commenced (1967), the programmes then in circulation were fewer and, for one reason or another, unsatisfactory. The general intention has been to try to give good flexibility and access by the operator and still keep the amount of key-punching down. In fact, the improvements projected include self-contained absorption coefficients and fluorescence factors, so that only problem identification and specimen and standard data need be "read in" before commencing calculation; this will be at the expense of using larger amounts of memory but, in the light of computer improvements, this is probably not a serious consideration. These programmes are written in FORTRAN IV and are based upon the earlier work of Brown [2] and So and Potts [3]. However, the corrections and changes made have become so extensive that this modified version warrants publication in its own right.

The first is a correction programme that takes raw data and gives values for the "true" concentrations involved, correcting for the effects of absorption, fluorescence, atomic number, bremsstrahlung, dead time background, compound standards, and missing data.

The second is a prediction programme which takes known compositions and predicts probe data. (This is particularly useful in, but not limited to, binary systems.) Also, as weight fractions, the predictions represent the compound standard factors (CSTD) to be used when known compounds are being employed in analyses.

The choice of a separate programme for generating the correction factors for compound standards does not present great difficulty, because most microprobe work tends to be done using a relatively small number of standard compounds and, frequently, at only one or two accelerating potentials. Once calculated, the factors are recorded on the element cards in question and can then be forgotten. As take-off angle, accelerating potential, and compound selection are the personal preference of the individual microprobe operator, no attempt to calculate these compound standard factors has been made.

The particular combination of correction procedures was arrived at by taking into account the general degree of acceptance that the particular procedure had received, the availability of accurate values of physical constants employed in the mathematics, and the over-all ease of use.

The input formats follow closely those actually used in a typical analysis; i.e., numbering for identification, selection of operating conditions, selection of data cards for the elements present, and experimental measurements.

The output formats include all the input information, for purposes of verification in the event of problems arising, together with the corrected data or predicted values.

At the present time no allowance has been made for the various forms of drift, although a beam current record may readily be included on the data input cards, etc. However, the other sources of drift, such as carbon contamination, charging of insulating specimens, electronic changes, etc., would still be present and so militate against a partial compensation scheme.

2. THEORY

When a beam of electrons strikes a target and generates X-rays a series of things happens, both to the escaping X-rays and to the incident electrons. The X-rays recorded in the microprobe detection systems have been subjected to absorption in the target; they are possibly enhanced by fluorescence from the other elements present if their characteristic X-rays generated are of favourable energy, and are affected by any changes in the intensity of the bremsstrahlung. The fraction of the electron beam absorbed by the target and the rate of X-ray production with penetration are also important. The basis for quantitative microprobe analysis is the assumption that the weight fraction of an element present is proportional to the generated X-ray intensity. In order to compute this value from the observed

X-ray intensity, the observed X-ray intensity must be corrected for the above phenomena. The mathematics involved are outlined in the following sections on X-ray absorption, characteristic fluorescence, atomic number effect, and bremsstrahlung fluorescence.

2.1 X-ray Absorption

Philibert [4] proposed the use of an approximate formula, based upon a detailed analysis of the X-ray production process, by incorporating the work of several others, in particular, Castaing [5] and Castaing and Descamps [6, 7]. An alternative derivation has been given by Theisen [8].

In Philibert's correction the fraction of X-rays escaping, $f(\chi)$, is given by:

$$f(\chi) = \frac{1}{\left(1 + \frac{\chi}{\sigma}\right) \cdot \left(1 + \frac{h}{1+h} \cdot \frac{\chi}{\sigma}\right)} ,$$

where $\chi = \frac{\mu}{\rho} \operatorname{cosec} \theta$, $\frac{\mu}{\rho}$ being the X-ray mass absorption coefficient, and θ is the angle of observation, or take-off angle;

σ = a modified Lenard coefficient from Lenard's law; and

h = $1.2\ A/Z^2$, where A and Z are respectively the atomic weight and atomic number of specimens.

For non-elemental specimens the question arises as to how to form $\bar{h}$. Philibert [4] recommends taking a mean based on atomic fractions for $\bar{Z}$. So and Potts [3] use a mean based on weight fractions for A and Z. Theisen [8] uses a mean based on weight fraction and h_i for the various elements:

$$\bar{h} = \sum_i c_i h_i ,$$

c_i being the weight fraction of the ith element. In most circumstances the differences between these values for $\bar{h}$ are small; so, for convenience the So and Potts method will be used here. Versions of the programme with other $\bar{h}$ values can be supplied on request.

In view of the work of Cosslett and Thomas [9], Duncumb and Shields [10] proposed that a different form for σ be used, taking into account that only electrons with energy greater than the critical for X-ray excitation should be considered, and that the range of electrons varied as $V^{-1.5}$; hence:

$$\sigma_{DS} = \frac{2.39 \times 10^5}{V^{1.5} - V_o^{1.5}} ,$$

V being the accelerating potential and V_o the critical excitation potential. The numerical constant was arrived at by fitting the data of Castaing and Descamps and of Green [11]. Heinrich [12] later proposed that sigma be given by:

$$\sigma_H = \frac{4.2 \times 10^5}{V^{1.7} - V_o^{1.7}} .$$

Cards are supplied so that either may be used. The resulting correction factor K is given by:

$$K = \frac{f(\chi)_{sp}}{f(\chi)_{st}} ,$$

with $f(\chi)_{sp}$ and $f(\chi)_{st}$ being the respective functions for specimen and standard.

For the specimen, χ_i becomes

$$\chi_i = \text{cosec}\,\theta_i \cdot \mu_i$$

$$\text{with } \mu_i = \sum_j \left(\frac{\mu}{\rho}\right)_{ij} \cdot C_j$$

With some microprobes, the value for θ_i is a function of the wavelength being examined; consequently θ_i is one of the required input parameters on the Constants card for element i.

2.2 Fluorescence by Characteristic Radiation

For this, the method due to Reed [13] is employed. His treatment is based on Castaing's original work. The changes and simplifications result in a readily usable formula, with γ in the correction factor, $(1-\gamma)$, being given by:

$$\gamma = \sum_j C_j J(A)_{ij} \left(\frac{V/V_{oj} - 1}{V/V_{oi} - 1}\right)^{1.67} \frac{\mu_{ij}}{\mu_j} \left(\frac{\log_e(1+x)}{x} + \frac{\log_e(1+y)}{y}\right)$$

$$\text{where } x = \frac{\mu_i}{\mu_j}\,\text{cosec}\,\theta , \quad y = \frac{\sigma}{\mu_j} ,$$

$$\text{and } J(A)_{ij} = 0.5\, P_{ij} \left(\frac{r_i - 1}{r_i}\right) \omega_j \frac{A_i}{A_j} .$$

P_{ij} is a numerical constant of magnitude dependent upon the radiations involved. A_i is the atomic number of the element i, r_i is the jump ratio for its absorption edge, and w_i is its fluorescence yield. In the light of Reed's comment that the factors in J(A) are none too well known, this programme uses his average values, although the full formula may readily be incorporated if so desired. Also, Reed recommends using Philibert's modified σ; however, using σ_{DS} does not seem to produce any difficulties.

If the fluorescing radiation is a β-line, the J(A) values are set negative for identification by the computer. The J(A) values listed by Reed are for α-line excitation and so need multiplication factors of approximately 0.1 and 0.4 for K_β and L_β lines respectively. These represent average values for the intensity ratio. It may be worth while actually to measure this ratio at the time of the analysis. For convenience the critical excitation potential of the β-line is taken to be 10% greater than that for the α-line.

2.3. Atomic Number Effect

When electrons strike a target there are two ultimate ends in sight: (a) eventual absorption by the target; (b) being backscattered and thus lost so far as X-ray production is concerned. The relative importance of the second process increases with atomic number, hence

an appreciable fraction of the incident beam escapes with significant energy loss to the specimen. Additionally, process (a) varies from element to element in that the stopping power, i.e., rate of energy loss per unit mass thickness, decreases with increasing atomic number. Both the backscatter coefficient R and the stopping coefficient S present difficulties that Duncumb and Reed [14] (DR) solved by empirically fitting the equations to carefully collected data. The results are a matrix of $R_{\alpha\beta}$ values, with α being determined by atomic number and β by $\frac{V}{V_o}$, the overvoltage ratio. The elements of the matrix are stored on pre-punched cards for use in the correction procedure.

For a specimen, $\bar{R}_\beta$ is determined by averaging the weight fractions, i.e.,

$$\bar{R}_\beta = \sum_\alpha R_{\alpha\beta}\, c_\alpha$$

Notice that the $R_{\alpha\beta}$'s are with respect to overvoltage factor β; this is not pointed out in Duncumb and Reed's paper.

The stopping power is given by:

$$S_i = \frac{Z_i}{A_i}\left(\frac{1}{V}\right)\log_e\left(1.166\,\frac{(V+V_o)}{I_i}\right),$$

where I_i is the mean ionization potential. Wilson [15] gives $I = 11.5\ Z$ eV; however, the factor can be used as a disposable constant and this is the DR approach. However, when fitting the data no general allowance was

made for fluorescence by the continuous radiation or bremsstrahlung, and in every case the heavy element was the measured component. A significant biasing of the constants must have been induced. It should be added that this sort of criticism can also be applied to the corrections for absorption and fluorescence by the characteristic radiation. When determining the empirical constants that are involved, the effects of the other possible interactions were, as a rule, minimised but not corrected for properly, either because of the complexity of the calculations required or because of deficiencies in the understanding of the phenomena at that time. As a result, the theoretical treatment of four physical phenomena may have been reduced to three empirical formulae!

The disadvantage of having a table of I_i values is overcome by incorporating the information on the appropriate element cards - see section on Programme Input.

2.4 Bremsstrahlung Fluorescence

With the previous comments in mind, this final correction has been added. The treatment of continuous fluorescence by Henoc [16] and Green [17] has been simplified and improved by Springer [18]. The resultant factor, γ, is composed of the following:

$$\gamma_K = 4.34\times10^{-6} A.\bar{Z}\,\frac{\mu_K^A}{\mu_K}.V_o\left(\frac{r_K-1}{r_K}\right) \quad \text{for K radiation;}$$

$$\gamma_L = 3.13\times10^{-6} A.\bar{Z}\,\frac{\mu_L^A}{\mu_L}.V_o\left(\frac{r_L-1}{r_L}\right) \quad \text{for L radiation,}$$

where μ_K^A refers to the X-ray mass absorption coefficients of component A for the K-edge wavelength, and μ_K the specimen's absorption coefficient for the K-edge wavelength (using the high-energy coefficient); μ_L^A and μ_L are similar constants for the L_{III} edge.

The term $\frac{r_K-1}{r_K}$ is given by Springer's interpolation formulae,

$$\frac{r_K-1}{r_K} = 0.924 - 1.44\times10^{-3}Z$$

and $$\frac{r_L-1}{r_L} = 0.548 - 2.31\times10^{-3}Z$$

For this calculation only, the programme takes the K-L dividing line to be between Bromine (Br_{35}) and Krypton (Kr_{36}). Therefore, up to and including Bromine, the K-formula is used and, above Bromine, the programme changes to the L-formula.

Because the atomic number and bremsstrahlung effects will occur in the same circumstances, this second correction is available only if the first is also chosen.

3. THE CORRECTION PROGRAMME

The first function performed by the programme is to correct the data for background and dead time. Should these corrections not be needed, the appropriate card fields may be left empty. If compound standards are being employed, the correction factor is applied to the standard reading and then the corrected observed weight fraction or probe ratio is computed. To this ratio (or this times the GUESS factor on the first iteration, as discussed below) is applied the selected set of corrections. The set, which always includes the absorption correction, has, as options, corrections for: (a) fluorescence by the characteristic radiation, (b) atomic number effect, and, if considered appropriate, (c) fluorescence by the continuous radiation or bremsstrahlung.

3.1 The Deadtime and Background Corrections

For high count rates, the X-ray counters are limited by their dead time, τ. The true count rate, N_t, is related to the observed count rate, N_o, by the formula:

$$N_t = N_o / (1 - N_o \cdot \tau)$$

However, if not needed, this routine may be omitted by leaving blank the relevant card fields.

The background corrections for specimen and standard are straightforward subtractions of the recorded off-angle count rates from the appropriate peak readings.

3.2 Determination by Difference

In any specimen, one undetermined element, or group of elements in fixed ratio to one another, may be determined by difference, using only the measurements of the other known elements. The element, or combination of elements, is treated just like those which were measured except that, on the standard card, the intensity is set at 1.0 and the specimen intensity for that element or combination is set at 0.0. It is simple to see how a combination of elements such as $-CO_3$ can be reduced to an effective element by taking the appropriately weighted means of the constants for the two components. At the moment this is still performed manually. Even approximate values for the constants would most probably be sufficient, in view of the fact that the precise values in tabulations are themselves subject to suspicion. It should be noted that in this calculation the totals of the weight fraction are set to be 1.0; should the difference be 0.0 or small, the totals may in fact be greater than 1.0.

3.3 Iteration Procedure

If included in the input, the GUESS factor is employed as a zeroth iteration correction factor, but only then; all subsequent calculations employ the current partly corrected values of the weight fractions.

If the correction factors required by a given problem are known from previous experience, then they should be employed as GUESS factors

to reduce both computation time and the risk of divergence. For a determination by difference calculation, the current difference is employed except when the total of the approximate weight fractions exceeds 1.0; in that instance, the difference is set at 0.0 and the calculation is continued. Using data supplied by Beaman and Isasi [1] for a Co-Cr-Mo alloy, the progress of the iterative procedure is shown in Figure 1. The convergence is oscillatory but well damped. The use of a hyperbolic approximation procedure, after Criss [19], would presumably reduce the oscillations; but these are by no means serious. Iterations are terminated in two ways: (i) when the sum of the magnitudes of the changes in projected weight fractions is less than that required on the precision card, the number taken to reach the required total errors is recorded at the bottom of the corrected results; or (ii) when the maximum number of iterations set by the precision card has been reached, the word LIMIT is printed as a warning. If a difference determination has been made, the position of the element or combination so calculated is noted and the final change in its value is recorded below the iteration record.

3.4 Using Compounds as Standards

When a compound is used as a standard in place of a pure element, the probe ratio, or apparent concentration, is generally too large. If the known composition of the standard is used in the Prediction Programme,

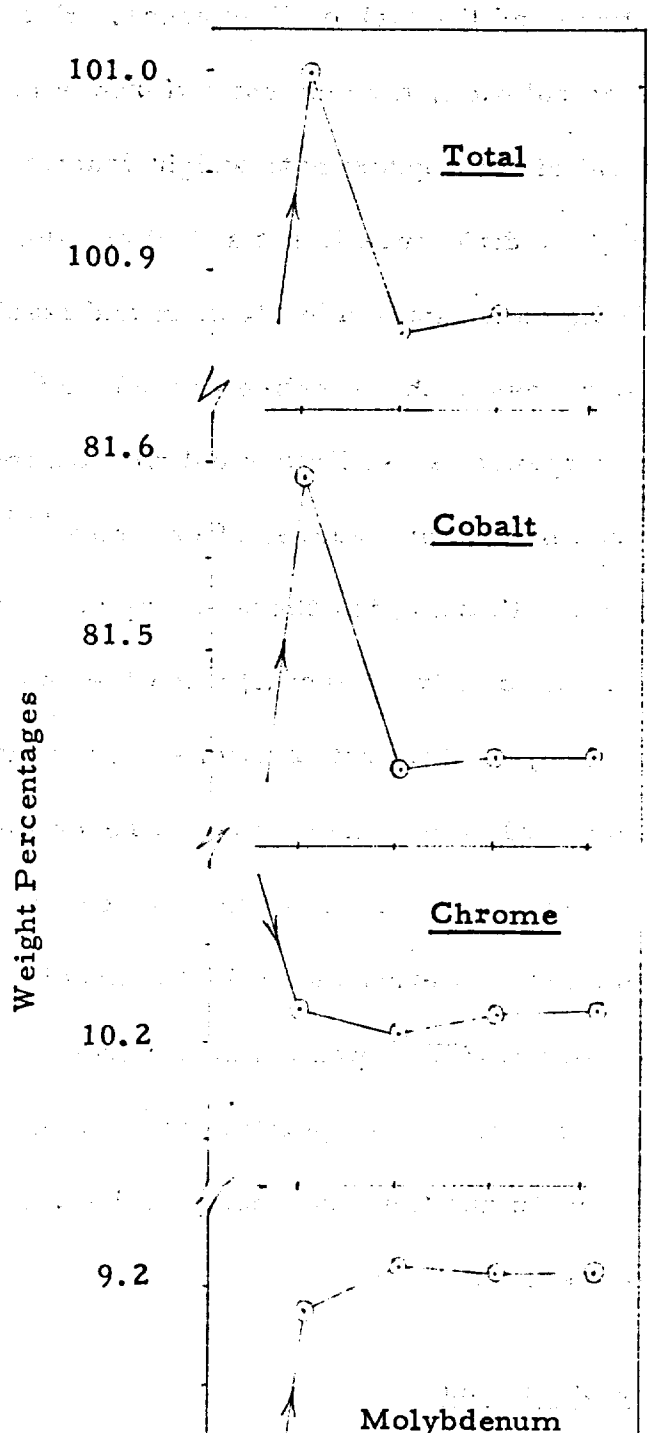

Figure 1. Progressive iterations in the correction of data from a Co-Cr-Mo analysis.

Section 3, the apparent weight fraction of the element in question may be computed and this, together with the observed count rate, enables the count rate to be predicted for the pure element. All that the operator must do, in order to use compound standards for one or more of the elements investigated, is to compute the apparent weight fraction for the operating conditions employed, and punch this on the appropriate element card.

4. THE PREDICTION PROGRAMME

This programme is the converse of the correction programme. All the correction procedures are the same, with the exception of dead time, background, etc., which apply only to real data. Having known values for the weight fractions means that no iterative procedures are needed and, correspondingly, these values can be programmed a good deal faster per output result. The effects of the various degrees of correction are readily seen, for the various possible combinations chosen are all printed out. The simplest application of this programme is predicting calibration curves for binary systems. However, in an investigation of inclusions in steels, a ternary-oxide phase diagram has been constructed, and even higher numbers of elements represent only a keypunch chore. A simple routine for generating calibration tables will be included in later versions of this programme. As mentioned previously, when used with data appropriate to a compound standard this programme gives the CSTD factors

required in the correction programme. Also, the ratios, if predicted to known weight fractions, can be employed as GUESS factors when correcting data from similar specimen material.

5. ACKNOWLEDGEMENTS

The author gratefully acknowledges the assistance of Mrs. V. E. Moore and Mr. K. S. Milliken in this work.

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RHP:(PES)gm

APPENDIX SECTION

COMPLETE PROGRAMME LISTINGS, TOGETHER WITH SAMPLES OF COMPUTER OUTPUT

- - -

NOTE BY AUTHOR:

The arithmetic of the electronic computer is very precise, but this great precision must not be allowed to obscure the fact that the results are no more accurate than the physics upon which the calculations are based. Most probably, an accuracy of $\pm$ 1% of the amount present is all that can be expected at the present.

- R. H. Packwood

APPENDIX 1 - THE CORRECTION PROGRAMME

```
1*    C     ELECTRON-MICROPROBE DATA CORRECTION - MK 3
2*    C                    R.H.PACKWOOD
3*    C
4*    C       NPROB = PROBLEM NUMBER
5*    C       NCOMP = NUMBER OF COMPONENTS IN THE SPECIMEN
6*    C       PSI = INCIDENT ELECTRON BEAM ANGLE.
7*    C       V = ACCELERATING VOLTAGE
8*    C       ETA = MAXIMUM TOTAL ERROR ON ITERATION
9*    C       ITRN = NUMBER OF ITERATIONS
10*   C       ATNO = ATOMIC NUMBER
11*   C       ATWT = ATOMIC WEIGHT
12*   C       VO = CRITICAL EXCITATION POTENTIAL
13*   C       AVEPOT = MEAN IONISATION POTENTIAL
14*   C       THETA = TAKE OFF ANGLE
15*   C       CSTD = CORRECTION FACTOR FOR COMPOUND STANDARD
16*   C                 ( FROM PROG2 INTENSITY PREDICTION )
17*   C       ABSCO = MASS ABSORPTION COEFFICIENT
18*   C       SIGMA = LENARD COEFFICIENT (DUNCUMB AND SHIELDS)
19*   C       NFLCD = FLUORESCENCE CORRECTION - 0 NO CORRECTION
20*   C                                        - 1 WITH CORRECTION
21*   C       REEDJ = REEDS J(A) FACTOR
22*   C       NBETA = BETA FLUORESCENCE CODE - 0 NONE
23*   C                                      - 1 WITH CORRECTION
24*   C       BABSCO = BETA MASS ABSORPTION COEFFICIENT
25*   C       NATCD = AT.NO. CORRECTION - 0 NONE
26*   C               DUNCUMB + DA-CASA - 1 WITH CORRECTION
27*   C       BSMAT = BACKSCATTER COEF. MATRIX
28*   C       BSCO = BACKSCATTER COEFFICIENT
29*   C       STP = STOPPING COEFFICIENT
30*   C       NBREM = BREMSTRAHLUNG EXCITATION - 0 NONE
31*   C                                        - 1 WITH CORRECTION
32*   C       RKL = IONISATION TERM AND CONSTANT FOR K,L RADN
33*   C       EDGE = MASS ABSORPTION COEFFICIENT AT K,L EDGE
34*   C       NSPEC = NUMBER OF SPECIMENS / OR NUMBER OF TIMES THAT
```

```
C                STANDARDS WILL BE READ
C        NSPOT = NUMBER OF SPOTS PER SET OF STANDARD READINGS
C        STD = STANDARD INTENSITY (CPS)
C        STDBG = STANDARD BACKGROUND (CPS)
C        DT = DEADTIME IN MICROSECONDS
C        SPEC = SPECIMEN INTENSITY (CPS)
C        SPBG = SPECIMEN BACKGROUND (CPS)
C        GUESS = ESTIMATED CORRECTION FACTOR
C
C        INPUT DATA
C
      INTEGER X,Y
      X = 1
      Y = 3
      DIMENSION BSMAT(11,11),ATNO(10),ATWT(10),VO(10),AVEPOT(10),
     1          THETA(10),CSTD(10),ABSCO(10,10),REEDJ(10,10),DT(10),
     2          STD(10),STDBG(10),STINT(10),SPEC(10),SPBG(10),
     3          GUESS(10),SPINT(10),RINT(10),CSC(10),SIGMA(10),
     4          FA100(10),BSCO(10,10),SABSC(10),FA(10),FCT(10),
     5          SBSCO(10),SSTP(10),ATNCT(10),CON1(10),CON2(10),
     6          CON3(10),CON4(10),ERR(10),CONC(10),CON(10),STP(10,10),
     7          EDGE(10,10),SEDGE(10),GA(10),GA100(10),RKL(10),
     8          CON5(10),CON6(10),BABSCO(10,10),BSABSC(10)
      WRITE (Y,201)
  201 FORMAT (1H1,10X,30H ELECTRON-MICROPROBE ANALYSES )
      READ (X,100) ((BSMAT(I,J),J=1,11),I=1,11)
  100 FORMAT (11F6.3)
      READ (X,101) ETA,ITRN
  101 FORMAT (F10.5,I10)
    1 READ (X,102) NPROB,NCOMP,PSI,V,NFLCD,NBETA,NATCD,NBREM
  102 FORMAT (2I5,2F10.3,4I5)
      WRITE (Y,202) NPROB,NCOMP,PSI,V,NFLCD,NBETA,NATCD,NBREM
  202 FORMAT (1H1,17H PROBLEM NUMBER. I6 // 10X,
     1        21H NUMBER OF ELEMENTS = I4 // 10X,
     2        44H INCIDENT ELECTRON BEAM ANGLE W.R.T.NORMAL = F6.2 //,
     3  10X,  24H ELECTRON BEAM VOLTAGE = F6.2 ,4H KV , // 10X,
     4        31H FLUORESCENCE CORRECTION CODE = I3 // 10X,
     5        25H BETA FLUORESCENCE CODE = I3 // 10X,
     6        33H ATOMIC NUMBER CORRECTION CODE = I3 // 10X,
     7        35H BREMSSTRAHLUNG CORRECTION CODE = I3 //)
      READ (X,103) (ATNO(I),ATWT(I),VO(I),AVEPOT(I),
     1                              THETA(I),CSTD(I), I=1,NCOMP)
  103 FORMAT (6F10.4)
      WRITE (Y,203)
  203 FORMAT (1H0,11X,9H AT. NO. ,6X, 9H AT. WT. ,3X,
     1        13H CRITICAL KV ,3X,12H AVE ION KV ,3X,
     2        12H T.O. ANGLE ,4X,17H COMP STD FACTOR // )
      WRITE (Y,204) (ATNO(I),ATWT(I),VO(I),AVEPOT(I),
     1                              THETA(I),CSTD(I),I=1,NCOMP)
  204 FORMAT (6X,6F15.4)
      WRITE (Y,205)
  205 FORMAT (1H0,10X,30H MASS ABSORPTION COEFFICIENTS // )
      DO 2 I = 1,NCOMP
      READ(X,104) (ABSCO(I,J),J=1,NCOMP)
  104 FORMAT (7F10.5)
      WRITE (Y,206) (ABSCO(I,J), J=1,NCOMP )
  206 FORMAT ( 10X,7F15.4 )
    2 CONTINUE
```

```
      IF (NFLCD) 404,404,3
    3 WRITE (Y,207)
  207 FORMAT (1H0,10X,20H NEEDS J(A) FACTORS // )
      DO 4 I = 1,NCOMP
      READ (X,104) (NEEDJ(I,J),J=1,NCOMP)
      WRITE (Y,206) (NEEDJ(I,J),J=1,NCOMP)
    4 CONTINUE
  404 CONTINUE
      IF (NBETA) 303,303,300
  300 WRITE (Y,301)
  301 FORMAT (1H0,10X,30H BETA ABSORPTION COEFFICIENTS //)
      DO 302 I = 1,NCOMP
      READ (X,104)  (BABSCO(I,J),J = 1,NCOMP)
      WRITE (Y,206) (BABSCO(I,J),J = 1,NCOMP)
  302 CONTINUE
  303 CONTINUE
      IF (NGREM) 407,407,405
  405 WRITE (Y,220)
  220 FORMAT (1H0,10X,30H EDGE ABSORPTION COEFFICIENTS //)
      DO 406 I = 1,NCOMP
      READ (X,104) (EDGE(I,J),J = 1,NCOMP)
      WRITE (Y,206) (EDGE(I,J),J = 1,NCOMP)
  406 CONTINUE
  407 CONTINUE
      WRITE (Y,211) NPROB,BETA,ITER
  211 FORMAT (1H0,30X,21H RESULTS FOR PROBLEM I5 //
     1        10X,13H TOTAL ERROR F10.5,5X,
     2        25H MAXIMUM NO. ITERATIONS = I5,// )
C
 1000 READ (X,1001) NSPEC,NSPOT
 1001 FORMAT (2I5)
      DO 219 NS = 1,NSPEC
C
      WRITE (Y,208)
  208 FORMAT (1H1,10X,16H STANDARD (CPS) ,8X,
     1        12H BACKGROUND ,10X, 10H DEADTIME // )
      READ (X,105) (STD(I),STDBG(I),DT(I),I=1,NCOMP)
      WRITE (Y,209) (STD(I),STDBG(I),DT(I),I=1,NCOMP)
  105 FORMAT (3F10.5)
  209 FORMAT (5X,3F20.5)
C
C     DEADTIME-BACKGROUND-COMPOUND STANDARD CORRECTION FACTORS
C
      DO 8 I = 1,NCOMP
      IF (DT(I)) 6,6,5
    5 DT(I) = DT(I) * 0.000001
      STD(I) = STD(I) / (1.0 - STD(I)*DT(I))
      STDBG(I) = STDBG(I) / (1.0 - STDBG(I)*DT(I))
    6 STINT(I) = STD(I) - STDBG(I)
      IF (CSTD(I)) 8,8,7
    7 STINT(I) = STINT(I) / CSTD(I)
    8 CONTINUE
      DO 219 L = 1,NSPOT
      WRITE (Y,210)
  210 FORMAT (1H0,10X,16H SPECIMEN (CPS) ,8X,
     1        12H BACKGROUND ,10X,7H GUESS // )
      READ (X,105) (SPEC(I),SPBG(I),GUESS(I),I=1,NCOMP)
      WRITE (Y,209) (SPEC(I),SPBG(I),GUESS(I),I=1,NCOMP)
```

```
151*          DO 10 I = 1,NCOMP
152*          IF (DT(I)) 9,9,88
153*       88 SPEC(I) = SPEC(I) / (1.0 - SPEC(I)*DT(I))
154*          SPBG(I) = SPBG(I) / (1.0 - SPBG(I)*DT(I))
155*        9 SPINT(I) = SPEC(I) - SPBG(I)
156*       10 CONTINUE
157*     C
158*     C         START CORRECTION PROCEEDURES
159*     C
160*          SRINT = 0.0
161*          DO 11 I = 1,NCOMP
162*          RINT(I) = SPINT(I) / STINT(I)
163*          SRINT = SRINT + RINT(I)
164*       11 CONTINUE
165*          MARK = 0
166*          DO 13 I = 1,NCOMP
167*          IF (RINT(I)) 13,12,13
168*       12 RINT(I) = 1.0 - SRINT
169*          MARK = I
170*       13 CONTINUE
171*     C
172*     C         CALCULATE TERMS FOR STANDARDS
173*     C
174*          IF (L-1) 14,14,17
175*       14 DO 15 I = 1,NCOMP
176*          CSC(I) = COS( PSI/57.2958 )/ SIN( THETA(I)/57.2958 )
177*          CHI = ABSCO(I,1)*CSC(I)
178*          H = 1.2 * ATWT(I) / (ATNO(I)**2)
179*          SIGMA(I) = 239000.0 / (V**1.5 - VO(I)**1.5)
180*          FA100(I) = (1.0 + H)/((1.0 +CHI / SIGMA(I)) *
181*         1                        (1.0 + H*( 1.0 + CHI/SIGMA(I) )))
182*       15 CONTINUE
183*     C
184*     C         Z-1/J MATRIX INTERPOLATION
185*     C
186*          IF (NATCO) 17,17,16
187*       16 DO 117 M = 1,NCOMP
188*          J = IFIX (ATNO(M) / 10.0 ) + 1
189*          DIFFZ = ( ATNO(M)/10.0 ) - AINT ( ATNO(M)/10.0 )
190*          DO 117 N = 1,NCOMP
191*          STP(M,N) = (ATNO(M) / ATWT(M)) *
192*         1                ALOG(0.583 * ((VO(N) + V)/AVEPOT(M)))
193*          K = IFIX ( VO(N) * 10.0 / V ) + 1
194*          DIFFO = ( VO(N) * 10.0 / V ) -
195*         1                AINT ( VO(N) * 10.0 / V )
196*          APROX1 = BSMAT(J,K) - DIFFZ*(BSMAT(J,K) - BSMAT(J+1,K))
197*          APROX2 = BSMAT(J,K+1) - DIFFZ*(BSMAT(J,K+1) - BSMAT(J+1,K+1))
198*          BSCO(M,N) = APROX1 + DIFFO * (APROX2 - APROX1 )
199*      117 CONTINUE
200*       17 CONTINUE
201*          NIT = 0
202*          TRY = 0.0
203*     C
204*     C         KNOWN OR ESTIMATED CORRECTION FACTORS
205*     C
206*          DO 19 I = 1,NCOMP
207*          IF (GUESS(I)) 19,19,18
208*       18 CORC(I) = RINT(I) * GUESS(I)
```

```
209*            GO TO 20
210*         19 CONC(I) = RINT(I)
211*         20 CONTINUE
212*      C
213*      C        ITERATIONS BEGIN HERE
214*      C
215*            IF (ITRN - NIT) 36,36,21
216*         21 NIT = NIT + 1
217*      C
218*      C        ABSORPTION CORRECTION -FA(I)
219*      C             (PHILIBERT-DUNCUMB-SHIELDS)
220*      C
221*      C        ELECTRON MICROPROBE (ED. MCKINLEY) 1964, P284.
222*      C
223*            DO 24 I = 1,NCOMP
224*            SABSC(I) = 0.0
225*            DO 22 J = 1,NCOMP
226*            SABSC(I) = SABSC(I) + CONC(J)*ABSCO(J,I)
227*         22 CONTINUE
228*            SATNO = 0.0
229*            SATWT = 0.0
230*            DO 23 J = 1,NCOMP
231*            SATNO = SATNO + ATNO(J)* CONC(J)
232*            SATWT = SATWT + ATWT(J)* CONC(J)
233*         23 CONTINUE
234*            H = 1.2 * SATWT /(SATNO**2)
235*            SCHI = SABSC(I) * CSC(I)
236*            FA(I) = (1.0 + H) / ((1.0 + SCHI / SIGMA(I)) *
237*           1                    ( 1.0 + H*( 1.0 + SCHI/SIGMA(I))))
238*         24 CONTINUE
239*            IF (NBETA) 82,82,80
240*         80 DO 81 I = 1,NCOMP
241*            BSABSC(I) = 0.0
242*            DO 81 J = 1,NCOMP
243*            BSABSC(I) = BSABSC(I) + CONC(J) * BABSCO(J,I)
244*         81 CONTINUE
245*         82 CONTINUE
246*      C
247*      C        FLUORESCENCE CORRECTION -FCT(I)
248*      C                (REED)
249*      C
250*      C        BRIT.J.APPL.PHYS.,1965,(16) P913.
251*      C
252*            IF (NFLD) 226,226,25
253*         25 DO 26 I = 1,NCOMP
254*            FCT(I) = 0.0
255*            DO 26 J = 1,NCOMP
256*            IF (REEDJ(I,J)) 250,261,261
257*        250 XFCN = (SABSC(I) / BSABSC(J)) * SIN(THETA(I)/57.2958)
258*            YFCN = 239000.0 / ((V**1.5-(VO(J)*1.1)**1.5)*BSABSC(J))
259*            GAMMA = (ALOG(1.0 + XFCN))/XFCN + (ALOG(1.0 + YFCN))/YFCN
260*            FCT(I) = FCT(I) - REEDJ(I,J)*CONC(J)*(BABSCO(I,J)/BSABSC(J))
261*           1          *((V/(VO(J)*1.1)-1.0)**1.67/(V/VO(I)-1.0)**1.67)*GAMMA
262*            GO TO 26
263*        261 CONTINUE
264*            XFCN = ( SABSC(I) / SABSC(J) ) *
265*           1                 SIN(THETA(I)/ 57.2958 )
266*            YFCN = SIGMA(J) / SABSC(J)
```

```
267*          GAMMA = ( ALOG(1.0 + XFCN)) / XFCN
268*         1              + ( ALOG(1.0 + YFCN)) / YFCN
269*          FCT(I) = FCT(I) + REEDJ(I,J)* CONC(J)* ABSCO(I,J)/SABSC(J)*
270*         1       (V/VO(J) - 1.0)**1.67/ (V/VO(I) - 1.0)**1.67 * GAMMA
271*       26 CONTINUE
272*      226 CONTINUE
273*      C
274*      C       ATOMIC NUMBER CORRECTION -ATNCT(I)
275*      C            (DUNCUMB-DA CASA-REED)
276*      C
277*      C       QUANTITATIVE E.P.M.A. (ED. HEINRICH)
278*      C       N.B.S. SPEC. PUBL. 298. 1968, P133.
279*      C
280*          IF (NATCO) 229,229,27
281*       27 DO 28 I = 1,NCOMP
282*          SBSCO(I) = 0.0
283*          SSTP(I) = 0.0
284*          DO 28 J = 1,NCOMP
285*          SBSCO(I) = SBSCO(I) + CONC(J) * BSCO(J,I)
286*          SSTP(I) = SSTP(I) + CONC(J) * STP(J,I)
287*       28 CONTINUE
288*          DO 29 I = 1,NCOMP
289*          ATNCT(I) = (SBSCO(I)*STP(I,I)) / (BSCO(I,I)*SSTP(I))
290*       29 CONTINUE
291*      229 CONTINUE
292*      C
293*      C       BREMSSTRAHLUNG EXCITATION -GA(I)
294*      C            (SPRINGER)
295*      C
296*      C       NEUES JAHRB. MINERAL.,ABHANDL. 1967A,(106) P241.
297*      C
298*          IF(NBREM) 66,66,60
299*       60 DO 64 I = 1,NCOMP
300*          SEDGE(I) = 0.0
301*          IF (ATNO(I)-36.0) 61,62,62
302*       61 RKL(I) = 0.00000434 * (0.924 - 0.00144*ATNO(I))
303*          GO TO 63
304*       62 RKL(I) = 0.00000313 * (0.548 - 0.00231*ATNO(I))
305*       63 CONTINUE
306*          DO 64 J = 1,NCOMP
307*          SEDGE(I) = SEDGE(I)+EDGE(I,J)*CONC(J)
308*       64 CONTINUE
309*          DO 65 I = 1,NCOMP
310*          ALPHA = ABSCO(I,I)*CSC(I) / EDGE(I,I)
311*          GA100(I) = RKL(I)*ATWT(I)*ATNO(I)*VO(I)*
312*         1              (ALOG(1.0 + ALPHA))/ ALPHA
313*          BETA = SABSC(I)*CSC(I)/ SEDGE(I)
314*          GA(I) = RKL(I)*ATWT(I)*SATNO*VO(I)*EDGE(I,I)*
315*         1        (ALOG(1.0 + BETA))/(SEDGE(I)*BETA)
316*       65 CONTINUE
317*       66 CONTINUE
318*      C
319*      C        APPLY CORRECTIONS
320*      C
321*          SUM1 = 0.0
322*          SUM2 = 0.0
323*          SUM3 = 0.0
324*          SUM4 = 0.0
```

```
325*            SUM5 = 0.0
326*            SUM6 = 0.0
327*            DO 34 I = 1,NCOMP
328*            CON2(I) = 0.0
329*            CON3(I) = 0.0
330*            CON4(I) = 0.0
331*            CON5(I) = 0.0
332*            CON6(I) = 0.0
333*            IF (I-MARK) 1301,34,1301
334*       1301 CONTINUE
335*            CON1(I) = RINT(I)* FA100(I) / FA(I)
336*            SUM1 = SUM1 + CON1(I)
337*            RESD1 = 1.0 - SUM1
338*            RESD = RESD1
339*            CON(I) = CON1(I)
340*            IF (NFLCD) 31,31,30
341*         30 CON2(I) = RINT(I)* FA100(I) /
342*           1                  (( 1.0 + FCT(I)) * FA(I))
343*            SUM2 = SUM2 + CON2(I)
344*            RESD2 = 1.0 - SUM2
345*            RESD = RESD2
346*            CON(I) = CON2(I)
347*         31 IF (NATCD) 34,34,32
348*         32 CON3(I) = RINT(I)* FA100(I)/(FA(I)*ATNCT(I))
349*            SUM3 = SUM3 + CON3(I)
350*            RESD3 = 1.0 - SUM3
351*            RESD = RESD3
352*            CON(I) = CON3(I)
353*            IF(NBREM) 71,71,70
354*         70 CON5(I) = RINT(I)*FA100(I)*(1.0 + GA100(I))/
355*           1                (FA(I)*ATNCT(I)*(1.0 + GA(I)))
356*            SUM5 = SUM5 + CON5(I)
357*            RESD5 = 1.0 - SUM5
358*            RESD = RESD5
359*            CON(I) = CON5(I)
360*         71 CONTINUE
361*            IF (NFLCD) 34,34,33
362*         33 CON4(I) = RINT(I)* FA100(I) /
363*           1          ((( 1.0 + FCT(I)) * FA(I) ) * ATNCT(I))
364*            SUM4 = SUM4 + CON4(I)
365*            RESD4 = 1.0 - SUM4
366*            RESD = RESD4
367*            CON(I) = CON4(I)
368*            IF(NBREM) 73,73,72
369*         72 CON6(I) = RINT(I)*FA100(I)*(1.0 + GA100(I))/
370*           1          (FA(I)*ATNCT(I)*(1.0 + FCT(I))*(1.0 + GA(I)))
371*            SUM6 = SUM6 + CON6(I)
372*            RESD6 = 1.0 - SUM6
373*            RESD = RESD6
374*            CON(I) = CON6(I)
375*         73 CONTINUE
376*         34 CONTINUE
377*       C
378*       C       CHECK AGREEMENT
379*       C
380*            TERR = 0.0
381*            DO 42 I = 1,NCOMP
382*            ERR(I) = ABS( CON(I)- CONC(I))
```

```
383*            TERR  = TERR + ERR(I)
384*            IF (I-MARK) 42,421,42
385*        421 TERR = TERR - ERR(MARK)
386*            DELTA = ABS(ERR(MARK) - TRY)
387*            TRY = ERR(MARK)
388*         42 CONTINUE
389*            DO 336 I = 1,NCOMP
390*            CONC(I) = CON(I)
391*        336 CONTINUE
392*      C
393*      C        RESIDUE DETERMINATION
394*      C
395*            IF (MARK) 350,350,35
396*         35 CONTINUE
397*            IF(RESD) 351,352,352
398*        351 RESD = 0.0
399*        352 CONC(MARK) = RESD
400*            ACODE = NFLCD
401*            BCODE = NATCD
402*            CCODE = NBREM
403*            SUM1 = 1.0
404*            SUM2 = 1.0 * ACODE
405*            SUM3 = 1.0 * BCODE
406*            SUM4 = 1.0 * ACODE * BCODE
407*            SUM5 = 1.0 * BCODE * CCODE
408*            SUM6 = 1.0 * ACODE * BCODE * CCODE
409*            CON1(MARK) = RESD1
410*            CON2(MARK) = RESD2 * ACODE
411*            CON3(MARK) = RESD3 * BCODE
412*            CON4(MARK) = RESD4 * ACODE * BCODE
413*            CON5(MARK) = RESD5 * BCODE * CCODE
414*            CON6(MARK) = RESD6 * ACODE * BCODE * CCODE
415*        350 CONTINUE
416*      C
417*            IF (TERR - ETA) 36,36,20
418*      C       OUTPUT CORRECTED DATA
419*      C
420*         36 CONTINUE
421*            WRITE (Y,212) NPROB,NS,L
422*        212 FORMAT (1H0,10X,17H ANALYSIS NUMBER ,2X,I5,1H/,I2,1H/,I2,3X,
423*           1          34H WEIGHT FRACTIONS CORRECTED FOR - // 9X,
424*           2          9H AT. NO. ,3X,10H OBSERVED ,5X,12H ABSORPTION ,
425*           3          3X,12H ABS.FLUORS ,3X,11H ABS.ATNO. ,4X,
426*           4          13H ABS.FL.ATNO ,1X,13H ABS.AT.BREM ,2X,
427*           5          10H ALL FOUR ,2X,9H AT. NO.,/ )
428*            WRITE (Y,213) (ATNO(I),RINT(I),CON1(I),CON2(I),CON3(I),
429*           1                CON4(I),CON5(I),CON6(I),ATNO(I),I=1,NCOMP)
430*        213 FORMAT (1H0,6X,F7.1,3X,7F15.9,F7.1)
431*            WRITE (Y,214) SRINT,SUM1,SUM2,SUM3,SUM4,SUM5,SUM6
432*        214 FORMAT (1H0,6X,8H TOTALS ,7F15.9 // 8X,
433*           1       21H ITERATIONS REQUIRED  )
434*            IF (ITRN-NIT) 215,215,217
435*        215 WRITE (Y,216)
436*        216 FORMAT (1H+,29X,11H **LIMIT** )
437*            GO TO 191
438*        217 WRITE (Y,218) NIT
439*        218 FORMAT (1H+,29X,I6)
440*        191 CONTINUE
```

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441*            IF (MARK) 219,219,192
442*        192 WRITE (Y,193) MARK,DELTA
443*        193 FORMAT (1H0,6X,29H CHANGE IN REMAINDER ELEMENT ,I2,3H = ,F10.9
444*        219 CONTINUE
445*      C
446*      C       SPACE SETS OF ANALYSES WITH BLANK CARDS AND THE
447*      C       NEW INSPEC-INSPOT INSTRUCTIONS.
448*      C
449*      C       START A NEW PROBLEM, IE. DIFFERENT ELEMENTS, KV,
450*      C       OR WAVELENGTH, ETC., WITH A 1 IN COLUMNS 1-5
451*      C
452*      C       END CALCULATIONS WITH A -1 IN COLUMNS 1-5
453*      C
454*            READ (X,107) NLSET
455*        107 FORMAT (I5)
456*            IF (NLSET) 56,1000,1
457*         56 STOP
458*            END

END OF UNIVAC 1108 FORTRAN V COMPILATION.      0 *DIAGNOSTIC* MESSAGE(S)
```

PROBLEM NUMBER. 100

MANGANESE-IRON-SULPHIDES

NUMBER OF ELEMENTS = 3

INCIDENT ELECTRON BEAM ANGLE W.R.T.NORMAL = .00

ELECTRON BEAM VOLTAGE = 25.00 KV

FLUORESCENCE CORRECTION CODE = 1

BETA FLUORESCENCE CODE = 0

ATOMIC NUMBER CORRECTION CODE = 1

BREMSSTRAHLUNG CORRECTION CODE = 0

AT. NO.	AT. WT.	CRITICAL KV	AVE ION KV	T.O. ANGLE	COMP STD FACTOR
16.0000	32.0700	2.4700	.1800	20.0000	.3664
25.0000	54.9400	6.5370	.3160	20.0000	.0000
26.0000	55.8500	7.1110	.3320	20.0000	.0000

MASS ABSORPTION COEFFICIENTS

239.4000	210.1000	167.4000
1029.5000	79.5000	63.5000
1157.5000	89.4000	71.4000

REEDS J(A) FACTORS

.0000	.0320	.0320
.0000	.0000	.0145
.0000	.0000	.0000

RESULTS FOR PROBLEM 100

TOTAL ERROR .00050 MAXIMUM NO. ITERATIONS = 20

STANDARD (CPS)	BACKGROUND	DEADTIME
3639.50000	.00000	.00000
11680.90002	.00000	.00000
11739.90002	.00000	.00000

SPECIMEN (CPS)	BACKGROUND	GUESS
1201.20000	.00000	.00000
3384.50000	.00000	.00000
452.60000	35.20000	.00000

ANALYSIS NUMBER 100/ 1/ 1 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO.,
16.0	.120926611	.148046399	.147545485	.133244868	.132794036	.000000000	.000000000	16.0
25.0	.289746508	.282333989	.282174710	.297511574	.297343731	.000000000	.000000000	25.0
26.0	.035553965	.034479603	.034479603	.035724853	.035724853	.000000000	.000000000	26.0
TOTALS	.446229078	.464859989	.464199796	.466481294	.465862617	.000000000	.000000000	

ITERATIONS REQUIRED 4

STANDARD (CPS)	BACKGROUND	DEADTIME
3463.50000	.00000	.00000
10210.50000	.00000	.00000
9811.50000	.00000	.00000

SPECIMEN (CPS)	BACKGROUND	GUESS
1936.70000	.00000	.00000
5036.00000	.00000	.00000
685.30000	35.20000	.00000

ANALYSIS NUMBER 100/ 1/ 1 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO.'
16.0	.204681443	.334113564	.332963798	.302823626	.301781535	.000000000	.000000000	16.0
25.0	.493217763	.516655646	.516359083	.548407882	.548093095	.000000000	.000000000	25.0
26.0	.066258982	.068074607	.068074607	.071051271	.071051271	.000000000	.000000000	26.0
TOTALS	.764358165	.918843813	.917397484	.922282778	.920925900	.000000000	.000000000	

ITERATIONS REQUIRED 6

SPECIMEN (CPS)	BACKGROUND	GUESS
1985.39999	.00000	.00000
5313.50000	.00000	.00000
511.40000	35.20000	.00000

ANALYSIS NUMBER 100/ 1/ 2 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO.'
16.0	.209821737	.349332027	.348117020	.316596803	.315497641	.000000000	.000000000	16.0
25.0	.520395566	.548216179	.547946393	.581882171	.581595831	.000000000	.000000000	25.0
26.0	.058727004	.060611192	.060611192	.063258795	.063258795	.000000000	.000000000	26.0
TOTALS	.788944453	.958159395	.956674598	.961739764	.960352257	.000000000	.000000000	

ITERATIONS REQUIRED 6

CHROMIUM-COBALT-MOLYBDENUM WITH DIFFERENCE DETERMINATION

PROBLEM NUMBER, 101

NUMBER OF ELEMENTS = 3

INCIDENT ELECTRON BEAM ANGLE W.R.T.NORMAL = .00

ELECTRON BEAM VOLTAGE = 20.00 KV

FLUORESCENCE CORRECTION CODE = 1

BETA FLUORESCENCE CODE = 0

ATOMIC NUMBER CORRECTION CODE = 0

BREMSSTRAHLUNG CORRECTION CODE = 0

AT. NO.	AT. WT.	CRITICAL KV	AVE ION KV	T.O. ANGLE	COMP STD FACTOR
24.0000	52.0100	5.9880	.3010	52.5000	.0000
27.0000	58.9400	7.7090	.3470	52.5000	.0000
42.0000	95.9500	2.5250	.5670	52.5000	.0000

MASS ABSORPTION COEFFICIENTS

68.2000	382.0000	919.6000
127.4000	64.9000	1327.3000
462.4000	236.3000	728.0000

REEDS J(A) FACTORS

.9000	.1320	.0000
.8000	.0000	.0000
.0140	.0180	.0000

RESULTS FOR PROBLEM 101

TOTAL ERROR .00050 MAXIMUM NO. ITERATIONS = 20

STANDARD (CPS)	BACKGROUND	DEADTIME
1.00000	.00000	.00000
23127.00000	127.00000	.00000
12066.00000	60.00000	.00000

SPECIMEN (CPS)	BACKGROUND	GUESS
.00000	.00000	.00000
18517.00000	138.00000	.00000
986.00000	62.00000	.00000

ANALYSIS NUMBER 101/ 1/ 1 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO.
24.0	.123913950	.094333112	.094460547	.000000000	.000000000	.000000000	.000000000	24.0
27.0	.799086951	.813033223	.813033223	.000000000	.000000000	.000000000	.000000000	27.0
42.0	.077000000	.092633670	.092506231	.000000000	.000000000	.000000000	.000000000	42.0
TOTALS	.876086950	1.000000000	1.000000000	.000000000	.000000000	.000000000	.000000000	

ITERATIONS REQUIRED 3

CHANGE IN REMAINDER ELEMENT 1 = .002190113

PROBLEM NUMBER = 102

COPPER-ZINC
WITH BETA FLUORESCENCE

NUMBER OF ELEMENTS = 2

INCIDENT ELECTRON BEAM ANGLE W.R.T.NORMAL = .00

ELECTRON BEAM VOLTAGE = 25.00 KV

FLUORESCENCE CORRECTION CODE = 1

BETA FLUORESCENCE CODE = 1

ATOMIC NUMBER CORRECTION CODE = 1

BREMSSTRAHLUNG CORRECTION CODE = 0

AT. NO.	AT. WT.	CRITICAL KV	AVE ION KV	T.O. ANGLE	COMP STD FACTOR
29.0000	63.5400	8.9800	.3770	20.0000	.0000
30.0000	65.3800	9.6600	.3920	20.0000	.0000

MASS ABSORPTION COEFFICIENTS

53.7000	44.2000
59.5000	49.0000

REEDS J(A) FACTORS

.0000	-.0200
.0000	.0000

BETA ABSORPTION COEFFICIENTS

.0000	255.5000
.0000	37.0000

RESULTS FOR PROBLEM 102

TOTAL ERROR .00050 MAXIMUM NO. ITERATIONS = 20

STANDARD (CPS)	BACKGROUND	DEADTIME
6426.93002	.00000	.00000
7207.50000	.00000	.00000

SPECIMEN (CPS)	BACKGROUND	GUESS
5756.00040	.00000	.00000
667.00000	.00000	.00000

ANALYSIS NUMBER 102/ 1/ 1 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO.
29.0	.895921819	.895708278	.894369520	.895835705	.894496746	.000000000	.000000000	29.0
30.0	.091778466	.091249961	.091249961	.091136577	.091136577	.000000000	.000000000	30.0
TOTALS	.987700284	.986958236	.985619478	.986972280	.985633321	.000000000	.000000000	

ITERATIONS REQUIRED 2

STANDARD (CPS)	BACKGROUND	DEADTIME
6482.40002	.00000	.00000
6944.70011	.00000	.00000

SPECIMEN (CPS)	BACKGROUND	GUESS
4271.00000	.00000	.00000
2383.00000	.00000	.00000

ANALYSIS NUMBER 102/ 2/ 1 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO.
29.0	.656860907	.660333112	.655780815	.660681419	.656126723	.000000000	.000000000	29.0
30.0	.343139369	.341846611	.341846611	.341538336	.341538336	.000000000	.000000000	30.0
TOTALS	1.002000272	1.002179712	.997627422	1.002219751	.997665055	.000000000	.000000000	

ITERATIONS REQUIRED 2

STANDARD (CPS)	BACKGROUND	DEADTIME
6462.40002	.00000	.00000
6944.70031	.00000	.00000

SPECIMEN (CPS)	BACKGROUND	GUESS
5227.00000	.00000	.00000
12062.00000	.00000	.00000

ANALYSIS NUMBER 102/ 3/ 1 WEIGHT FRACTIONS CORRECTED FOR -

AT. NO.	OBSERVED	ABSORPTION	ABS.FLUORS	ABS.ATNO.	ABS.FL.ATNO	ABS.AT.BREM	ALL FOUR	AT. NO..
29.0	.806337155	.806607127	.804035701	.806834772	.804262623	.000000000	.000000000	29.0
30.0	.181721311	.180758699	.180758899	.180556674	.180556674	.000000000	.000000000	30.0
TOTALS	.988058463	.987366021	.984794594	.987391442	.984819293	.000000000	.000000000	

ITERATIONS REQUIRED 2

APPENDIX 2 - THE PREDICTION PROGRAMME

```
1*      C
2*      C     ELECTRON-MICROPROBE DATA PREDICTION - MK 4
3*      C                    AND
4*      C          COMPOUND STANDARD FACTOR (CSTD)
5*      C                  BY R.H.PACKWOOD.  AFTER  S.S.SO.
6*      C
7*      C          BSMAT = BACKSCATTER COEF. MATRIX
8*      C          LAMDT = ALPHA FACTOR - 0 NONE
9*      C                  LACHANCE          1 WITH
10*     C                    + TRAILL       -1 ONLY
11*     C          IPROB = PROBLEM NUMBER
12*     C          ICOMP = NUMBER OF COMPONENTS IN THE SPECIMEN
13*     C          NSPOT = NUMBER OF SPOTS
14*     C          PSI = INCIDENT ELECTRON BEAM ANGLE
15*     C          V = ACCELERATING VOLTAGE
16*     C          ATNO = ATOMIC NUMBER
17*     C          ATWT = ATOMIC WEIGHT
18*     C          VO = CRITICAL EXCITATION POTENTIAL
19*     C          AVEPOT = MEAN IONISATION POTENTIAL
20*     C          THETA = TAKE OFF ANGLE
21*     C          ABSCO = MASS ABSORPTION COEFFICIENT
22*     C          SIGMA = LENARD COEFFICIENT (DUNCUMB AND SHIELDS)
23*     C          WTFT = WEIGHT FRACTION OF EACH COMPONENT
24*     C          NFLCD = FLUORESCENCE CORRECTION - 0 NO CORRECTION
25*     C                                          - 1 WITH CORRECTION
26*     C          REEDJ = REEDS J(A) FACTOR
27*     C          NBETA = BETA FLUORESCENCE CODE - 0 NONE
28*     C                                         - 1 WITH CORRECTION
29*     C          BABSCO = BETA MASS ABSORPTION COEFFICIENT
30*     C          NATCD = AT.NO. CORRECTION - 0 NONE
31*     C                  DUNCUMB + DA-CASA - 1 WITH CORRECTION
32*     C          BSCO = BACKSCATTER COEFFICIENT
33*     C          STP = STOPPING COEFFICIENT
34*     C          NBREM = BREMSTRAHLUNG EXCITATION - 0 NONE
35*     C                                           - 1 WITH CORRECTION
36*     C          RKL = IONISATION TERM AND CONSTANT FOR K,L RADN
37*     C          EDGE = MASS ABSORPTION COEFFICIENT AT K,L EDGE
38*     C          G1,2,3,4 = ALPHA FACTORS AS PER CORRECTION
```

```
39*    C                              SCHEDULE
40*    C
41*          INTEGER X,Y
42*          X = 1
43*          Y = 3
44*          DIMENSION ATNO(10),ATWT(10),VO(10),ABSCO(10,10),CSC(10),
45*         1          WTFTN(100,10),F100A(10),SABSC(10),FA(10),FCT(10),
46*         2          RINT1(10),RINT2(10),REEDJ(10,10),SIGMA(10),
47*         3          RINT3(10),RINT4(10),ATNCT(10),BSMAT(11,11),STP(10,10),
48*         4          BSCO(10,10),SBSCO(10),SSTP(10),AVEPOT(10),THETA(10),
49*         5          EDGE(10,10),SEDGE(10),GA(10),GA100(10),
50*         6          RKL(10),RINT5(10),RINT6(10),BABSCO(10,10),BSABSC(10)
51*          DIMENSION G1(15,2),G2(15,2),G3(15,2),G4(15,2)
52*    C
53*    C        INPUT DATA
54*    C
55*     5     READ (X,100) (( BSMAT(I,J),J=1,11 ), I=1,11 )
56*     100   FORMAT (11F6.3 )
57*         1 READ(X,2) LAMDT,NPROB,NCOMP,NSPOT,PSI,V,NFLCD,NBETA,NATCD,NBREM
58*         2 FORMAT (4I5,2F10.3,4I5)
59*           READ (X,3) (ATNO(I),ATWT(I),VO(I),AVEPOT(I),THETA(I),I=1,NCOMP)
60*     3     FORMAT (5F10.4)
61*           DO 5 I = 1,NCOMP
62*           READ (X,4) (ABSCO(I,J),J=1,NCOMP)
63*     4     FORMAT (7F10.3)
64*     5     CONTINUE
65*           DO 6 I = 1,NSPOT
66*           READ (X,4) (WTFTN(I,J),J=1,NCOMP)
67*     6     CONTINUE
68*           IF (NFLCD) 90,90,7
69*     7     DO 9 I = 1,NCOMP
70*           READ (X,4) (REEDJ(I,J),J=1,NCOMP)
71*     9     CONTINUE
72*           IF (NBETA) 82,82,80
73*        80 DO 81 I = 1,NCOMP
74*           READ (X,4) (BABSCO(I,J),J = 1,NCOMP)
75*        81 CONTINUE
76*        82 CONTINUE
77*        90 IF (NBREM) 93,93,91
78*        91 DO 92 I = 1,NCOMP
79*           READ (X,4) (EDGE(I,J),J = 1,NCOMP)
80*        92 CONTINUE
81*        93 CONTINUE
82*    C
83*    C        CALCULATE ABSORPTION CORRECTION TERMS
84*    C
85*    C
86*    C        CALCULATE F100A(CHI) OF EACH ELEMENT IN THE STANDARD
87*    C
88*     10    DO 11 I = 1,NCOMP
89*           CSC(I) = COS(PSI/57.2958)/SIN(THETA(I)/57.2958)
90*           CHI = ABSCO(I,I) * CSC(I)
91*           H = 1.2 * ATWT(I) / (ATNO(I)**2)
92*           SIGMA(I) = 239000.0 / (V**1.5 - VO(I)**1.5 )
93*           F100A(I) = (1.0 + H)/((1.0 +CHI / SIGMA(I)) *
94*          1                      (1.0 + H*( 1.0 + CHI/SIGMA(I) )))
95*     11    CONTINUE
96*    C
```

```
      C       ITERATION FOR EACH SPOT
      C
            DO 525 L = 1,NSPOT
      C
      C       CALCULATE FA(CHI) OF EACH ELEMENT IN THE SPECIMEN
      C
      C       ELECTRON MICROPROBE (ED. MCKINLEY) 1964, P284.
      C
            DO 14 I = 1,NCOMP
            SABSC(I) = 0.0
            DO 12 J = 1,NCOMP
            SABSC(I) = SABSC(I) + WTFTN(L,J)*ABSCO(J,I)
         12 CONTINUE
            SATNO = 0.0
            SATWT = 0.0
            DO 13 J = 1,NCOMP
            SATNO = SATNO + ATNO(J) * WTFTN(L,J)
            SATWT = SATWT + ATWT(J) * WTFTN(L,J)
         13 CONTINUE
            H = 1.2 * SATWT/ (SATNO**2)
            SCHI = SABSC(I) * CSC(I)
            FA(I) = (1.0 + H) / ((1.0 + SCHI / SIGMA(I)) *
           1                     ( 1.0 + H*( 1.0 + SCHI/SIGMA(I))))
         14 CONTINUE
            IF (NBETA) 151,151,15
         15 DO 150 I = 1,NCOMP
            BSABSC(I) = 0.0
            DO 150 J = 1,NCOMP
            BSABSC(I) = BSABSC(I) + WTFTN(L,J) * BABSCO(J,I)
        150 CONTINUE
        151 CONTINUE
      C
      C       CALCULATE REEDS FLUORESCENCE CORRECTION TERM - FCT(I)
      C
      C       BRIT. J. APPL. PHYS., 1965,(16) P913.
      C
            IF (NFLCO) 19,19,16
         16 DO 18 I = 1,NCOMP
            FCT(I) = 0.0
            DO 18 J = 1,NCOMP
            IF (REEDJ(I,J)) 17,170,170
         17 XFCN = (SABSC(I) / BSABSC(J)) * SIN(THETA(I)/57.2958)
            YFCN = 239000.0 / ((V**1.5-(VO(J)*1.1)**1.5)*BSABSC(J))
            GAMMA = (ALOG(1.0 + XFCN))/XFCN + (ALOG(1.0 + YFCN))/YFCN
            FCT(I) = FCT(I) - REEDJ(I,J)*WTFTN(L,J)*(BABSCO(I,J)/BSABSC(J))
           1         *((V/(VO(J)*1.1)-1.0)**1.67/(V/VO(I)-1.0)**1.67)*GAMMA
            GO TO 18
        170 CONTINUE
            XFCN = (SABSC(I) / SABSC(J)) * SIN(THETA(I)/57.2958)
            YFCN = SIGMA(J) / SABSC(J)
            GAMMA = (ALOG(1.0 + XFCN)) / XFCN + (ALOG(1.0 + YFCN)) / YFCN
            FCT(I) = FCT(I) + REEDJ(I,J)*WTFTN(L,J)*ABSCO(I,J)/SABSC(J)*
           1         (V/VO(J) - 1.0)**1.67 / (V/VO(I) - 1.0)**1.67 * GAMMA
         18 CONTINUE
      C
      C       CALCULATE DUNCUMBS ATOMIC NO. CORRECTION TERMS
      C
      C       QUANTITATIVE E.P.M.A. (ED. HEINRICH)
```

```
C       N.B.S. SPEC. PUBL. 298. 1968, P133.
C
 19   IF (NATCD) 119,119,102
102   DO 111 N = 1,NCOMP
      J = IFIX (ATNO(M) / 10.0 ) + 1
      DIFFZ = ( ATNO(M)/10.0 ) - AINT ( ATNO(M)/10.0 )
      DO 111 N = 1,NCOMP
      K = IFIX ( VO(N) * 10.0 / V ) + 1
      DIFFU = ( VO(N) * 10.0 / V ) -
     1                    AINT ( VO(N) * 10.0 / V )
      APROX1 = BSMAT(J,K) - DIFFZ*( BSMAT(J,K)
     1                              -BSMAT(J+1,K))
      APROX2 = BSMAT(J,K+1) - DIFFZ*( BSMAT(J,K+1)
     1                              -BSMAT(J+1,K+1))
      BSCO(M,N) = APROX1 + DIFFU * (APROX2 - APROX1 )
      STP(M,N) = (ATNO(M) / ATWT(M)) *
     1                    ALOG(0.583 * ((VO(N) + V)/AVEPOT(M)))
111   CONTINUE
C
C       CALCULATE ATOMIC NO. TERMS FOR SPECIMENS - ATNCT(I)
C
      DO 115 I = 1,NCOMP
      SBSCO(I) = 0.0
      SSTP(I) = 0.0
      DO 115 J = 1,NCOMP
      SBSCO(I) = SBSCO(I) + WTFTN(L,J) * BSCO(J,I)
      SSTP(I) = SSTP(I) + WTFTN(L,J)*STP(J,I)
115   CONTINUE
      DO 116 I = 1,NCOMP
      ATNCT(I) = (SBSCO(I)*STP(I,I)) / (BSCO(I,I)*SSTP(I))
116   CONTINUE
C
C       CALCULATE SPRINGERS BREMSSTRAHLUNG CORRECTION - GA(I)
C
C       NEUES JAHRB. MINERAL.,ABHANDL. 1967A,(106) P241
C
      IF(NBREM) 66,66,60
60    DO 64 I = 1,NCOMP
      SEDGE(I) = 0.0
      IF (ATNO(I)-36.0) 61,62,62
61    RKL(I) = 0.00000434 * (0.924 - 0.00144*ATNO(I))
      GO TO 63
62    RKL(I) = 0.00000313 * (0.548 - 0.00231*ATNO(I))
63    CONTINUE
      DO 64 J = 1,NCOMP
      SEDGE(I) = SEDGE(I)+EDGE(I,J)*WTFTN(L,J)
64    CONTINUE
      DO 65 I = 1,NCOMP
      ALPHA = ABSCO(I,I)*CSC(I) / EDGE(I,I)
      GA100(I) = RKL(I)*ATWT(I)*ATNO(I)*VO(I)*
     1            (ALOG(1.0 + ALPHA))/ ALPHA
      BETA = SABSC(I)*CSC(I)/ SEDGE(I)
      GA(I) = RKL(I)*ATWT(I)*SATNO*VO(I)*EDGE(I,I)*
     1          (ALOG(1.0 + BETA))/(SEDGE(I)*BETA)
65    CONTINUE
66    CONTINUE
C
C       CALCULATE MEASURED RELATIVE INTENSITIES
```

```
      C
  119 SRIN1 = 0.0
      SRIN2 = 0.0
      SRIN3 = 0.0
      SRIN4 = 0.0
      SRIN5 = 0.0
      SRIN6 = 0.0
      SWTFT = 0.0
      DO 20 I = 1,NCOMP
      RINT1(I) = WTFTN(L,I) * FA(I) * 100.0 / F100A(I)
      RINT2(I) = WTFTN(L,I) * (1.0+FCT(I)) * FA(I) * 100.0 / F100A(I)
      RINT3(I) = WTFTN(L,I)*FA(I)*ATNCT(I)*100.0/F100A(I)
      RINT4(I) = WTFTN(L,I)*(1.0+FCT(I))*FA(I)*ATNCT(I)
     1                *100.0 / F100A(I)
      RINT5(I) = RINT3(I)*(1.0+GA(I))/(1.0+GA100(I))
      RINT6(I) = RINT4(I)*(1.0+GA(I))/(1.0+GA100(I))
      SRIN1 = SRIN1 + RINT1(I)
      SRIN2 = SRIN2 + RINT2(I)
      SRIN3 = SRIN3 + RINT3(I)
      SRIN4 = SRIN4 + RINT4(I)
      SRIN5 = SRIN5 + RINT5(I)
      SRIN6 = SRIN6 + RINT6(I)
      SWTFT = SWTFT + WTFTN(L,I)
   20 CONTINUE
      C
      C        TRAILL-LACHANCE ALPHA FACTORS
      C
      IF ( LANOT ) 21,95,21
   21 DO 22 I=1,NCOMP
      G2(L,I) = 0.0
      G3(L,I) = 0.0
      G4(L,I) = 0.0
      G1(L,I)=(WTFTN(L,I)-RINT1(I)/100.0)/((RINT1(I)/100.0)
     1        *(1.0-WTFTN(L,I)))
      IF (NFLCD) 212,212,211
  211 CONTINUE
      G2(L,I)=(WTFTN(L,I)-RINT2(I)/100.0)/((RINT2(I)/100.0)
     1        *(1.0-WTFTN(L,I)))
  212 CONTINUE
      IF (NATCD) 215,215,213
  213 CONTINUE
      G3(L,I)=(WTFTN(L,I)-RINT3(I)/100.0)/((RINT3(I)/100.0)
     1        *(1.0-WTFTN(L,I)))
      IF (NFLCD) 215,215,214
  214 CONTINUE
      G4(L,I)=(WTFTN(L,I)-RINT4(I)/100.0)/((RINT4(I)/100.0)
     1        *(1.0-WTFTN(L,I)))
  215 CONTINUE
   22 CONTINUE
   95 CONTINUE
      C
      C        OUTPUT
      C
      IF (L-1) 25,25,380
   25 WRITE (Y,26) NPROB,NCOMP,NSPOT,PSI,V,NFLCD,NBETA,NATCD,NBREM
   26 FORMAT (1H1,16H PROBLEM NUMBER I6 // 5X,12H INPUT DATA // 10X,
     1        23H NUMBER OF COMPONENTS = I4 // 10X,18H NUMBER OF SPOTS =
     2        I4 // 10X,42H LENARD COEFFICIENT (DUNCUMB AND SHIELDS) //
```

```
271*          3       10X,31H INCIDENT ELECTRON BEAM ANGLE = F6.2 //
272*          4       10X,24H ELECTRON BEAM VOLTAGE = F6.2  // 10X,
273*          5       31H FLUORESCENCE CORRECTION CODE = I3 // 10X,
274*          6        25H BETA FLUORESCENCE CODE = I3 // 10X,
275*          7       30H ATOMIC NO. CORRECTION CODE = I3 // 10X,
276*          8       33H BREMSSTRAHLUNG CORRECTION CODE = I3 // )
277*           WRITE (Y,27)
278*     27    FORMAT (1H0,10X,9H AT. NO. ,11X,9H  AT. WT. ,10X,
279*          1       13H CRITICAL KV. ,6X,13H AVE.EXC.KV. ,8X,
280*          2       12H T.O. ANGLE. // )
281*           WRITE (Y,28) (ATNO(I),ATWT(I),VO(I),AVEPOT(I),THETA(I),I=1,NCOMP
282*     28    FORMAT (5F20.4)
283*           WRITE (Y,29)
284*     29    FORMAT (1H0,10X,30H MASS ABSORPTION COEFFICIENTS  //)
285*           DO 31 I = 1,NCOMP
286*           WRITE (Y,30) (ABSCO(I,J),J=1,NCOMP)
287*     30    FORMAT (5F20.5)
288*     31    CONTINUE
289*           WRITE (Y,32)
290*     32    FORMAT (1H0,10X,34H WEIGHT FRACTION OF EACH COMPONENT  //)
291*           DO 33 I = 1,NSPOT
292*           WRITE (Y,30) (WTFTN(I,J),J=1,NCOMP)
293*     33    CONTINUE
294*           IF(NFLCO) 351,351,343
295*     343   WRITE (Y,344)
296*     344   FORMAT (1H0,10X,19H REEDS J(A) FACTOR  //)
297*           DO 35 I = 1,NCOMP
298*           WRITE (Y,30) (REEDJ(I,J),J=1,NCOMP)
299*     35    CONTINUE
300*     351   CONTINUE
301*           IF (NBETA) 332,332,330
302*      330  WRITE (Y,333)
303*      333  FORMAT (1H0,10X,30H BETA ABSORPTION COEFFICIENTS // )
304*           DO 331 I = 1,NCOMP
305*           WRITE (Y,30) (BABSCO(I,J), J = 1,NCOMP)
306*      331  CONTINUE
307*      332  CONTINUE
308*           IF (NATCO) 355,355,345
309*      345  WRITE (Y,346)
310*      346  FORMAT (1H0,10X,35H ELEMENTS BACKSCATTER COEFFICIENTS //)
311*           DO 347 I = 1,NCOMP
312*           WRITE (Y,30) ( BSCO(I,J),J = 1,NCOMP )
313*      347  CONTINUE
314*           WRITE (Y,348)
315*     348   FORMAT(1H0,10X,32H ELEMENTS STOPPING COEFFICIENTS  //)
316*           DO 349 I = 1,NCOMP
317*           WRITE (Y,30) ( STP(I,J),J = 1,NCOMP )
318*      349  CONTINUE
319*           IF (NBREM) 403,403,400
320*      400  WRITE (Y,401)
321*      401  FORMAT (1H0,10X,30H EDGE ABSORPTION COEFFICIENTS //)
322*           DO 402 I = 1,NCOMP
323*           WRITE (Y,30) (EDGE(I,J), J = 1,NCOMP)
324*      402  CONTINUE
325*      403  CONTINUE
326*     355   WRITE (Y,36)
327*     36    FORMAT (1H1,12H OUTPUT DATA  //)
328*     360   CONTINUE
```

```
      IF (LANDT) 525,38,38
   38 CONTINUE
      WRITE (Y,39) L
   39 FORMAT (1H0,5X,12H SPOT NUMBER I3)
   40 WRITE (Y,41) (ATNO(I),I=1,NCOMP)
   41 FORMAT (1H0,   15H ATOMIC NUMBERS,34X,4F20.1 //
     1        51X,4F20.5 // 51X,2F20.5  //)
      WRITE (Y,46) SWTFT,(WTFTN(L,I),I=1,NCOMP)
   46 FORMAT (1H0,16H WEIGHT FRACTION,14X,   5F20.5 // 51X,4F20.5 //
     1       51X,2F20.5  //)
      WRITE (Y,47) SRIN1,(RINT1(I),I=1,NCOMP)
   47 FORMAT (1H0,21H REL. INT., ABS. COR.,9X,5F20.3 // 51X, 4F20.3 //
     1        51X,2F20.3  //)
      IF (NFLCD) 50,50,48
   48 WRITE (Y,49) SRIN2,(RINT2(I),I=1,NCOMP)
   49 FORMAT (1H0,30H REL. INT., ABS. AND FL. CORS.,5F20.3 // 51X,4F20.3
     1       //51X,2F20.3 //)
   50 CONTINUE
      IF (NATCD) 510,510,501
  501 WRITE (Y,502) SRIN3,(RINT3(I),I=1,NCOMP)
  502 FORMAT(1H0, 30H REL.INT., ABS + AT.NO. CORS. ,
     1       5F20.3 // 51X, 4F20.3 // 51X, 2F20.3//)
      IF(NFLCD) 510,510,503
  503 WRITE (Y,504) SRIN4,( RINT4(I),I=1,NCOMP)
  504 FORMAT(1H0, 30H REL.INT., ABS.FL.+AT.NO CORS. ,
     1       5F20.3 // 51X, 4F20.3 // 51X, 2F20.3 ////)
  510 CONTINUE
      IF (NBREM) 524,524,520
  520 WRITE (Y,521) SRIN5,(RINT5(I),I = 1,NCOMP)
  521 FORMAT (1H0,29H REL.INT.,ABS.+AT.NO.+BREMS. , 1X,
     1       5F20.3 // 51X,4F20.3 // 51X,2F20.3 ////)
      IF (NFLCD) 524,524,522
  522 WRITE (Y,523) SRIN6,(RINT6(I),I = 1,NCOMP)
  523 FORMAT (1H0,22H ALL FOUR CORRECTIONS ,8X,
     1       5F20.3 // 51X,4F20.3 // 51X,2F20.3 ////)
  524 CONTINUE
  525 CONTINUE
      IF (LANDT) 37,373,37
   37 CONTINUE
      WRITE (Y,370) (ATNO(I),I=1,NCOMP)
  370 FORMAT (1H1,20X,5H ATNO,F6.1,40X,5H ATNO,F6.1/)
      WRITE (Y,371)
  371 FORMAT (1H0,15H GERRYS ALPHAS //,1X,8H WT FTN ,
     1       5X,4H G1 ,6X,4H G2 ,6X,4H G3 ,6X,4H G4 ,5X,
     2       8H WT FTN ,5X,4H G1 ,6X,4H G2 ,6X,4H G3 ,6X,
     3       4H G4 ,/)
  372 CONTINUE
      WRITE (Y,375) (((WTFTN(L,I),G1(L,I),G2(L,I),G3(L,I),G4(L,I),
     1       I=1,NCOMP),L=1,NSPOT))
  375 FORMAT (10F10.5)
  373 CONTINUE
C
C        SPACE DATA SETS WITH BLANK CARDS,
C                END WITH 1 IN COLS 1-5.
C
      READ (X,52) NLSET
   52 FORMAT (I5)
      IF (NLSET) 54,1,54
```

```
387*          54 STOP
388*             END

END OF UNIVAC 1108 FORTRAN V COMPILATION.     0 *DIAGNOSTIC* MESSAGE(S)
```

PROBLEM NUMBER 103

IRON-SULPHUR BINARY
WITH THE LACHANCE ALPHA FACTORS

INPUT DATA

NUMBER OF COMPONENTS = 2

NUMBER OF SPOTS = 12

LENARD COEFFICIENT (DUNCUMB AND SHIELDS)

INCIDENT ELECTRON BEAM ANGLE = .00

ELECTRON BEAM VOLTAGE = 20.00

FLUORESCENCE CORRECTION CODE = 1

BETA FLUORESCENCE CODE = 0

ATOMIC NO. CORRECTION CODE = 1

BREMSSTRAHLUNG CORRECTION CODE = 0

AT. NO. K	AT. WT.	CRITICAL KV.	AVE.EXC.KV.	T.O. ANGLE.
16.0000	32.0700	2.4700	.1800	38.5000
26.0000	55.8500	7.1110	.3320	38.5000

MASS ABSORPTION COEFFICIENTS

239.40000	167.40000
1157.50000	71.40000

WEIGHT FRACTION OF EACH COMPONENT

.05000	.95000
.10000	.90000
.20000	.80000
.30000	.70000
.40000	.60000
.50000	.50000
.53000	.47000
.60000	.40000
.70000	.30000
.80000	.20000
.90000	.10000
.95000	.05000

REED'S J(A) FACTOR

.00000	.03200
.01000	.00000

ELEMENTS BACKSCATTER COEFFICIENTS

.90436	.93242
.85823	.87918

ELEMENTS STOPPING COEFFICIENTS

2.13903	2.23270
1.71094	1.79635

OUTPUT DATA

SPOT NUMBER 1			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.05000	.95000
REL. INT., ABS. COR.	98.104	3.337	94.767
REL. INT., ABS. AND FL. CORS.	98.112	3.345	94.767
REL.INT., ABS + AT.NO. CORS.	97.754	3.834	93.920
REL.INT., ABS.FL.+AT.NO CORS.	97.763	3.843	93.920
SPOT NUMBER 2			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.10000	.90000
REL. INT., ABS. COR.	96.352	6.793	89.559
REL. INT., ABS. AND FL. CORS.	96.367	6.808	89.559
REL.INT., ABS + AT.NO. CORS.	95.717	7.740	87.977
REL.INT., ABS.FL.+AT.NO CORS.	95.734	7.757	87.977
SPOT NUMBER 3			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.20000	.80000
REL. INT., ABS. COR.	93.306	14.088	79.217
REL. INT., ABS. AND FL. CORS.	93.333	14.116	79.217
REL.INT., ABS + AT.NO. CORS.	92.275	15.793	76.482
REL.INT., ABS.FL.+AT.NO CORS.	92.306	15.823	76.482
SPOT NUMBER 4			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.30000	.70000
REL. INT., ABS. COR.	90.917	21.944	68.973
REL. INT., ABS. AND FL. CORS.	90.954	21.981	68.973
REL.INT., ABS + AT.NO. CORS.	89.694	24.212	65.482

REL.INT., ABS.FL.+AT.NO CORS.	89.735	24.254	65.482
SPOT NUMBER 5			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.40000	.60000
REL. INT., ABS. COR.	89.253	30.425	58.827
REL. INT., ABS. AND FL. CORS.	89.298	30.471	58.827
REL.INT., ABS + AT.NO. CORS.	88.005	33.061	54.944
REL.INT., ABS.FL.+AT.NO CORS.	88.053	33.110	54.944
SPOT NUMBER 6			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.50000	.50000
REL. INT., ABS. COR.	88.392	39.613	48.778
REL. INT., ABS. AND FL. CORS.	88.441	39.662	48.778
REL.INT., ABS + AT.NO. CORS.	87.249	42.408	44.840
REL.INT., ABS.FL.+AT.NO CORS.	87.301	42.461	44.840
SPOT NUMBER 7			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.53000	.47000
REL. INT., ABS. COR.	88.305	42.520	45.783
REL. INT., ABS. AND FL. CORS.	88.353	42.570	45.783
REL.INT., ABS + AT.NO. CORS.	87.212	45.322	41.890
REL.INT., ABS.FL.+AT.NO CORS.	87.265	45.375	41.890
SPOT NUMBER 8			
ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.60000	.40000
REL. INT., ABS. COR.	88.424	49.597	38.827
REL. INT., ABS. AND FL. CORS.	88.474	49.647	38.827
REL.INT., ABS + AT.NO. CORS.	87.481	52.336	35.145
REL.INT., ABS.FL.+AT.NO CORS.	87.534	52.389	35.145

SPOT NUMBER 9

ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.70000	.30000
REL. INT., ABS. COR.	89.459	60.486	28.973
REL. INT., ABS. AND FL. CORS.	89.506	60.533	28.973
REL.INT., ABS + AT.NO. CORS.	88.772	62.938	25.834
REL.INT., ABS.FL.+AT.NO CORS.	88.820	62.986	25.834

SPOT NUMBER 10

ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.80000	.20000
REL. INT., ABS. COR.	91.625	72.408	19.217
REL. INT., ABS. AND FL. CORS.	91.664	72.446	19.217
REL.INT., ABS + AT.NO. CORS.	91.210	74.324	16.886
REL.INT., ABS.FL.+AT.NO CORS.	91.249	74.363	16.886

SPOT NUMBER 11

ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.90000	.10000
REL. INT., ABS. COR.	95.077	85.518	9.559
REL. INT., ABS. AND FL. CORS.	95.100	85.541	9.559
REL.INT., ABS + AT.NO. CORS.	94.906	86.626	8.280
REL.INT., ABS.FL.+AT.NO CORS.	94.930	86.649	8.280

SPOT NUMBER 12

ATOMIC NUMBERS		16.0	26.0
WEIGHT FRACTION	1.00000	.95000	.05000
REL. INT., ABS. COR.	97.341	92.574	4.767
REL. INT., ABS. AND FL. CORS.	97.354	92.587	4.767
REL.INT., ABS + AT.NO. CORS.	97.268	93.168	4.101
REL.INT., ABS.FL.+AT.NO CORS.	97.281	93.181	4.101

ATNO 16.0

GERRYS ALPHAS

WT FTN	G1	G2	G3	G4
.05000	.52455	.52089	.32005	.31687
.10000	.52454	.52096	.32441	.32126
.20000	.52452	.52107	.33301	.32994
.30000	.52449	.52116	.34148	.33847
.40000	.52445	.52123	.34982	.34685
.50000	.52441	.52126	.35802	.35510
.55000	.52440	.52130	.36645	.35754
.60000	.52436	.52132	.36609	.36320
.70000	.52431	.52133	.37403	.37117
.80000	.52424	.52132	.38183	.37899
.90000	.52415	.52129	.38951	.38668
.95000	.52411	.52126	.39329	.39046

ATNO 26.0

WT FTN	G1	G2	G3	G4
.95000	.04912	.04912	.22998	.22998
.90000	.04921	.04921	.22998	.22998
.80000	.04941	.04941	.22998	.22998
.70000	.04962	.04962	.23000	.23000
.60000	.04985	.04985	.23005	.23005
.50000	.05009	.05009	.23013	.23013
.47000	.05016	.05016	.23016	.23016
.40000	.05035	.05035	.23024	.23024
.30000	.05062	.05062	.23038	.23038
.20000	.05092	.05092	.23056	.23056
.10000	.05125	.05125	.23078	.23078
.05000	.05142	.05142	.23090	.23090

PROBLEM NUMBER 104

COMPOUND STANDARD CALCULATION FOR CALCIUM CARBONATE

INPUT DATA

NUMBER OF COMPONENTS = 3

NUMBER OF SPOTS = 1

LENARD COEFFICIENT (DUNCUMB AND SHIELDS)

INCIDENT ELECTRON BEAM ANGLE = .00

ELECTRON BEAM VOLTAGE = 20.00

FLUORESCENCE CORRECTION CODE = 0

BETA FLUORESCENCE CODE = 0

ATOMIC NO. CORRECTION CODE = 1

BREMSSTRAHLUNG CORRECTION CODE = 0

AT. NO.	AT. WT.	CRITICAL KV.	AVE.EXC.KV.	T.O. ANGLE.
6.0000	12.0100	.2830	.2460	20.0000
8.0000	16.0000	.5310	.1270	20.0000
20.0000	40.0800	4.0380	.2390	20.0000

MASS ABSORPTION COEFFICIENTS

2270.00000	13500.00000	42.10000
5300.00000	1250.00000	115.10000
45000.00000	16000.00000	139.40000

WEIGHT FRACTION OF EACH COMPONENT

.12000	.48000	.40000

ELEMENTS BACKSCATTER COEFFICIENTS

.96073	.96155	.97189
.94765	.94874	.96252
.85069	.85904	.88628

ELEMENTS STOPPING COEFFICIENTS

1.93471	1.94078	2.01956
2.26639	2.27297	2.35182
1.94636	1.95292	2.03162

OUTPUT DATA

SPOT NUMBER 1

ATOMIC NUMBERS		6.0	8.0	20.0
WEIGHT FRACTION	1.00000	.12000	.48000	.40000
REL. INT., ABS. COR.	47.036	.633	5.717	40.686
REL.INT., ABS + AT.NO. CORS.	46.299	.555	5.949	39.795

PROBLEM NUMBER 105

INPUT DATA

MAGNESIUM-ZINC BINARY CALIBRATION CALCULATION

NUMBER OF COMPONENTS = 2

NUMBER OF SPOTS = 26

LENARD COEFFICIENT (DUCUMB AND SHIELDS)

INCIDENT ELECTRON BEAM ANGLE = .00

ELECTRON BEAM VOLTAGE = 15.00

FLUORESCENCE CORRECTION CODE = 0

BETA FLUORESCENCE CODE = 0

ATOMIC NO. CORRECTION CODE = 1

BREMSSTRAHLUNG CORRECTION CODE = 0

AT. NO.	AT. WT.	CRITICAL KV.	AVE.EXC.KV.	T.O. ANGLE.
12.0000	24.3200	1.3030	.1330	20.0000
30.0000	65.3800	9.6600	.3920	20.0000

MASS ABSORPTION COEFFICIENTS

465.60000	32.40000
9507.00000	49.00000

WEIGHT FRACTION OF EACH COMPONENT

.99500	.00500
.99000	.01000
.98000	.02000
.97000	.03000
.95000	.05000
.90000	.10000
.85000	.15000
.80000	.20000
.75000	.25000
.70000	.30000
.65000	.35000
.60000	.40000
.55000	.45000
.50000	.50000
.45000	.55000
.40000	.60000
.30000	.70000
.25000	.75000
.20000	.80000

.15000	.85000
.10000	.90000
.05000	.95000
.03000	.97000
.02000	.98000
.01000	.99000
.00500	.99500

ELEMENTS BACKSCATTER COEFFICIENTS

.92815	.97818
.80485	.92156

ELEMENTS STOPPING COEFFICIENTS

2.10651	2.31070
1.46296	1.65285

OUTPUT DATA

SPOT NUMBER 1			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.99500	.00500
REL. INT., ABS. COR.	97.244	96.741	.503
REL.INT., ABS + AT.NO. CORS.	97.207	96.825	.382
SPOT NUMBER 2			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.99000	.01000
REL. INT., ABS. COR.	94.649	93.644	1.005
REL.INT., ABS + AT.NO. CORS.	94.571	93.806	.765
SPOT NUMBER 3			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.98000	.02000
REL. INT., ABS. COR.	89.897	87.887	2.010
REL.INT., ABS + AT.NO. CORS.	89.726	88.192	1.533
SPOT NUMBER 4			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.97000	.03000
REL. INT., ABS. COR.	85.668	82.653	3.015
REL.INT., ABS + AT.NO. CORS.	85.390	83.085	2.305
SPOT NUMBER 5			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.95000	.05000
REL. INT., ABS. COR.	78.527	73.503	5.024
REL.INT., ABS + AT.NO. CORS.	78.006	74.147	3.859
SPOT NUMBER 6			
ATOMIC NUMBERS		12.0	30.0

WEIGHT FRACTION	1.00000	.90000	.10000
REL. INT., ABS. COR.	66.309	56.262	10.046
REL.INT., ABS + AT.NO. CORS.	65.070	57.265	7.806
SPOT NUMBER 7			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.85000	.15000
REL. INT., ABS. COR.	59.349	44.283	15.066
REL.INT., ABS + AT.NO. CORS.	57.331	45.485	11.845
SPOT NUMBER 8			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.80000	.20000
REL. INT., ABS. COR.	55.636	35.553	20.083
REL.INT., ABS + AT.NO. CORS.	52.842	36.861	15.982
SPOT NUMBER 9			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.75000	.25000
REL. INT., ABS. COR.	54.051	28.953	25.098
REL.INT., ABS + AT.NO. CORS.	50.525	30.307	20.219
SPOT NUMBER 10			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.70000	.30000
REL. INT., ABS. COR.	53.929	23.819	30.110
REL.INT., ABS + AT.NO. CORS.	49.739	25.177	24.562
SPOT NUMBER 11			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.65000	.35000
REL. INT., ABS. COR.	54.643	19.729	35.119
REL.INT., ABS + AT.NO. CORS.	50.079	21.064	29.015
SPOT NUMBER 12			

ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.60000	.40000
REL. INT., ABS. COR.	56.534	16.407	40.126
REL.INT., ABS + AT.NO. CORS.	51.283	17.698	33.585
SPOT NUMBER 13			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.55000	.45000
REL. INT., ABS. COR.	58.795	13.665	45.130
REL.INT., ABS + AT.NO. CORS.	53.173	14.896	38.277
SPOT NUMBER 14			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.50000	.50000
REL. INT., ABS. COR.	61.501	11.369	50.132
REL.INT., ABS + AT.NO. CORS.	55.623	12.527	43.096
SPOT NUMBER 15			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.45000	.55000
REL. INT., ABS. COR.	64.554	9.423	55.131
REL.INT., ABS + AT.NO. CORS.	58.548	10.498	48.049
SPOT NUMBER 16			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.40000	.60000
REL. INT., ABS. COR.	67.883	7.756	60.127
REL.INT., ABS + AT.NO. CORS.	61.884	8.740	53.144
SPOT NUMBER 17			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.30000	.70000
REL. INT., ABS. COR.	75.169	5.057	70.112
REL.INT., ABS + AT.NO. CORS.	69.625	5.835	63.788

SPOT NUMBER 18			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.25000	.75000
REL. INT., ABS. COR.	79.053	3.953	75.100
REL.INT., ABS + AT.NO. CORS.	73.970	4.617	69.353
SPOT NUMBER 19			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.20000	.80000
REL. INT., ABS. COR.	83.062	2.977	80.085
REL.INT., ABS + AT.NO. CORS.	78.613	3.521	75.092
SPOT NUMBER 20			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.15000	.85000
REL. INT., ABS. COR.	87.176	2.108	85.068
REL.INT., ABS + AT.NO. CORS.	83.541	2.526	81.015
SPOT NUMBER 21			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.10000	.90000
REL. INT., ABS. COR.	91.379	1.331	90.048
REL.INT., ABS + AT.NO. CORS.	88.749	1.616	87.133
SPOT NUMBER 22			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.05000	.95000
REL. INT., ABS. COR.	95.657	.632	95.025
REL.INT., ABS + AT.NO. CORS.	94.235	.777	93.457
SPOT NUMBER 23			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.03000	.97000
REL. INT., ABS. COR.	97.387	.371	97.016

REL.INT., ABS + AT.NO. CORS.	96.507	.460	96.048
SPOT NUMBER 24			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.02000	.98000
REL. INT., ABS. COR.	98.256	.245	98.010
REL.INT., ABS + AT.NO. CORS.	97.660	.304	97.356
SPOT NUMBER 25			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.01000	.99000
REL. INT., ABS. COR.	99.127	.121	99.005
REL.INT., ABS + AT.NO. CORS.	98.824	.151	98.673
SPOT NUMBER 26			
ATOMIC NUMBERS		12.0	30.0
WEIGHT FRACTION	1.00000	.00500	.99500
REL. INT., ABS. COR.	99.563	.060	99.503
REL.INT., ABS + AT.NO. CORS.	99.411	.075	99.336

EOF

APPENDIX 3 - INPUT REQUIREMENTS

3.1 INPUT LIST FOR CORRECTION PROGRAMME (With Notes on the Selection of Parameters):

(a) Machine control cards for the Univac 1108 terminal at the Department of Energy, Mines and Resources.

(b) Comment cards (C in first column) identifying the various names employed in the programme and the correction mode numbers.

(c) Programme reader and printer identification numbers. These must be punched by the user and inserted in the programme deck. As supplied, the reader is identified with x = 1 and the printer by y = 3. These are directly after the card Integer X, Y at the beginning of the programme.

(d) Programme deck.

(e) Univac 1108 data input card.

(f) Eleven backscatter matrix cards (blue).

(g) Total error and maximum number of iteration card - supplied as 0.0005, 20.

(h) Problem card with:

(i) problem number
(ii) number of elements
(iii) angle of incidence of the electron beam, with respect to the normal, to the specimen surface, in degrees.
(iv) accelerating voltage, in kilovolts
* (v) α-line characteristic fluorescence correction code
* (vi) β-line characteristic fluorescence correction code
* (vii) atomic number correction code
* (viii) bremsstrahlung fluorescence correction code (only in combination with (vii)

* These corrections are chosen by placing a 1 in the relevant field or omitted by placing a 0.

(i) Element cards with:

(i) atomic number
(ii) atomic weight
(iii) critical excitation potential of the line used for analysis, in kilovolts

(iv) average ionization potential in kilovolts - taken from the Duncumb and Reed tabulation. (N.B: The latter is in electron volts.)
(v) take-off angle - in degrees.
(vi) compound standard factor, i.e., the corrected weight fraction from the prediction programme
(vii) element symbol - not read into computer

(j) α-line absorption coefficient array

A series of cards, one or two per element for each element in the problem. The order of the cards and of the coefficients on each card must be the same as the order chosen for inserting the element cards. If Heinrich's tables are to be employed, there is great convenience in taking the natural order of increasing atomic number. The absorption coefficients in Heinrich's tables are then in the same array on the page as is required on the series of input cards; i.e., reading left to right along the respective element's row in the table gives each card's coefficients. Proceeding down the page gives the corresponding rows for the other elements.

(k) Fluorescence coefficient array

These are found from Reed's table, keeping the same order as for the absorption array, i.e., radiation fluorescing or being absorbed down each column per absorber across the rows. The leading diagonal of the array will contain only zeros, i.e., no self-fluorescence is possible.

β-line coefficients should be denoted by a minus sign so that the computer will recognize it as such.

The recorded J(A) factors are for α-lines and must be multiplied by the relative intensity ratios for β-lines. These are approximately 0.1 and 0.4 for K and L radiations respectively.

(l) β-line absorption coefficient array

If β-line fluorescence is to be computed, then for each β-line the appropriate absorption coefficients are inserted in the column of the exciter line. Other spaces in the array can be set equal to zero or merely left blank.

(m) K- or L-edge absorption coefficients

These are read from Springer's table. Care must be taken to ensure that the appropriate value is used for lines adjacent to the

low-energy side of the edge; it may prove better to use the higher energy coefficient.

(n) Number of analyses cards

(i) number of specimens - or number of times that standards are recorded
(ii) number of spots per set of standard readings

(o) Standard cards - one per element in the order of the element cards

(i) standard intensity - counts per second
(ii) background - counts per second
(iii) dead time - microseconds. May be omitted if not needed.

(p) Specimen cards - one per element in order of the element cards

(i) intensity of element from specimen - in counts per second
(ii) background intensity from specimen - in counts per second
(iii) guess factor - this is for cases of severe corrections which may cause excessive or divergent iterations or where previous experience, e.g., the prediction programme, has shown that such and such a factor is approximately correct, and so save computer time on slower machines.

(q) Whatnext card - this has a blank, a 1 or a -1 in the first five columns and is used to route the calculations so that the ratio of standard to specimen readings can be varied and so that the elements involved can be altered.

3.2 INPUT LIST FOR PREDICTION PROGRAMME

For simplicity, only the changes will be noted.

(g) Delete - not required for this programme

(h) Problem card with:

(i) problem number
(ii) number of elements or components
(iii) number of analyses
(iv) angle of incident electron beam, with respect to the normal, from the specimen surface - in degrees

(v) accelerating voltage - in kilovolts
(vi) α-line characteristic fluorescence correction code
(vii) β-line characteristic fluorescence correction code
(viii) atomic number correction code
(ix) bremsstrahlung fluorescence correction code (only if (viii) is also chosen)

(j,k) Weight fraction cards. (Insert between (j) and (k).)

A series of cards, one or two per analytical point, recording the required weight fractions. The order of the weight fractions must be the same as that of the element cards.

(n), (o), (p) Delete - not required for this programme.

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APPENDIX 4 - CARD FORMATS AND DEFINITIONS OF SYMBOLS

(The number of cards is noted in parentheses beside the card title.)

(11) Duncumb and Read Back-Scatter Matrix Cards (11 F6.3)

(Blue cards, already punched. If shuffled, replace in order of decreasing magnitude of contents.)

(1) Precision Card (F10.3, I10)

ETA		ITRN	
1	10	11	20
0.0005			20

ETA = maximum sum of moduli of errors on iteration as a weight fraction.

ITRN = maximum number of iterations.

(2) Correction Problem Card (2I5, 2F10.3, 4I5)

NPROB		NCOMP		PSI		V		NFLCD		NBETA		NATCD		NBREM	
1	5	6	10	11	20	21	30	31	35	36	40	41	45	46	50
	100		3		0.0		25.0		1		0		1		0

NPROB = problem number
NCOMP = number of elements
PSI = incident electron beam angle with respect to the normal to the specimen, in degrees
V = accelerating potential, in kilovolts
* NFLCD = fluorescence code
* NBETA = β-line fluorescence code
* NATCD = atomic number correction code
* NBREM = bremsstrahlung fluorescence code

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* 1 for correction, 0 for omit.

For the Prediction programme the Precision Card is omitted and the Problem Card becomes:

(1) Prediction Problem Card (5X, 3I5, 2F10.3, 4I5)

	NPROB	NCOMP	NSPOT	PSI	V	NFLCD	NBETA	NATCD	NBREM
1 5	6 10	11 15	16 20	21 30	31 40	41 45	46 50	51 55	56 60
	104	3	1	0.0	20.0	0	0	1	0

NSPOT = number of sets of predicted data.

(NCOMP) Element Cards (6F10.4) (5F10.4 for Prediction Prog.)

ATNO	ATWT	VO	AVEPOT	THETA	(CSTD)		
1 10	11 20	21 30	31 40	41 50	51 60		76 80
12.0	24.32	1.303	0.133	20.0			Mg

ATNO = atomic number
ATWT = atomic weight
VO = X-ray line critical excitation potential, in kilovolts
AVEPOT = mean ionization potential in kilovolts, after Duncumb and Reed
THETA = take-off angle, in degrees
CSTD = compound standard factor from Prediction programme

End of card shows element symbol in non-read field.

(NCOMP) α-Mass Absorption Cards (7F10.3)

	E_1	E_2	
	1 10	11 20	21
A_1	463.6	32.4	
A_2	9507.0	49.0	

E_1, E_2, etc; = EMITTER 1,2
A_1, A_2, etc; = ABSORBER 1,2

The prediction programme has the following cards for weight fractions:

(NSPOT) Weight Fraction Cards (7F10.3)

W_1 1 10	W_2 11 20	W_3 21 30	
0.995	0.005		
0.99	0.01		

W_1, 2, etc; = weight fraction of element 1, 2

(NCOMP) Reed J (A) Factor Cards (7F10.3)

	λ_1 1 10	λ_2 11 20	λ_3 21 30	
F_1	0.0	0.132	0.0	
F_2	0.0	0.0	0.0	
F_3	0.018	0.018	0.0	

λ_1, λ_2, etc; = fluorescing wavelength 1, 2
F_1, F_2, etc; = element fluoresced 1, 2

(NCOMP) β-Mass Absorption Cards (7F10.3)

	B_1 1 10	B_2 11 20	21
A_1	0.0	255.5	
A_2	0.0	37.0	

A_1, A_2, etc. = β-absorber 1, 2
B_1, B_2, etc. = β-emitter 1, 2

(Zn Kβ in Cu and Zn used as illustration.)

(NCOMP) K- or L-Edge Mass Absorption Cards (7F10.3)

	KL_1 1 10	KL_2 11 20	21
A_1			
A_2			

KL_1, KL_2 = critical excitation wavelength 1, 2
A_1, A_2 = absorber 1, 2

(i) Number of Analyses Card (2I5)

NSPEC 1 5	NSPOT 6 10	
1	1	

NSPEC = number of specimens or times that standards are recorded.
NSPOT = number of analyses per set of standard readings.

(NSPEC) Standard Cards (3F10.3)

	STD 1 10	STDBG 11 20	DT 21 30	
*	1.0	0.0	0.0	
	23127.0	127.0	0.0	
	12060.0	60.0	0.0	

STD = standard intensity in cps.
STBDG = standard background in cps.
DT = deadtime in microseconds; may be omitted if desired.

(* Difference determination)

(NSPOT) Specimen Cards (3F10.3)

	SPEC 1 10	SPBG 11 20	GUESS 21 30	
*	0.0	0.0	0.0	
	18517.0	138.0		
	98.6	62.0		

SPEC = specimen intensity cps.
SPBG = specimen background cps.
GUESS = estimated correction factor for faster computation - may be omitted if desired.

(* Difference determination)

(1) Whatnext Card (I5)

NLSET 1 5	
-1	

For Correction Programme:

NLSET = 0 (blank), start new Number of Analyses Card
= 1, start new Problem Card
= -1, end calculations

For Prediction Programme:

NLSET = 0 (blank), start new Problem Card
= 1, end calculations

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ADDENDUM TO THE PREDICTION PROGRAMME

A routine for calculating theoretical values of Lachance's α-factors [1] from the predicted intensities has been incorporated into the Prediction programme.

In the α-factor method the weight fraction C_A, of component A, is related to the relative intensity R_A by

$$C_A = R_A (1 + C_B \alpha_{AB})$$

for the binary A-B, and by

$$C_A = R_A (1 + C_B \alpha_{AB} + C_C \alpha_{AC})$$

for the ternary A-B-C etc.

In ternary and higher systems the α-factors may be derived from the appropriate binary systems; therefore only the latter systems need be computed.

The routine is obtained when either a +1 or a -1 is inserted in columns 1-5 of the Problem Card.

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(1) G. R. Lachance, Geol. Surv. Canada, Paper No. 64-50 (1964).

These values of the LANDT code give respectively the α-factors in addition to, or instead of, the predicted intensity data. Leaving the LANDT code blank causes the α-factors to be omitted. Up to 15 compositions may be computed at any one time.

The changes in the α's with varying degrees of correction can readily be seen in columns G1-G4. These are equivalent to the correction combinations chosen, although for the time being the effects of bremsstrahlung have been neglected.

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RHP:(PES) gm