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computer programs EMX and EMX2 for electron microprobe data processing

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COMPUTER PROGRAMS EMX AND EMX2 FOR ELECTRON MICROPROBE DATA PROCESSING

by

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I. INTRODUCTION

Electron probe microanalysis provides a rapid method for the chemical analysis of volumes of the order of $10^{-11}cm^3$ ($10\mu m^3$); however, the process of converting the data, which come from the probe in the form of measured x-ray intensities, into absolute concentrations is long and cumbersome when carried out by conventional methods. Since the task is obviously one for a computer, Fortran-63 programs have been written that not only perform the necessary absorption and fluorescence corrections but also carry out almost the entire data handling operation. With these programs, the amount of data that would come from a normal eight hours of microprobe operation can be processed in a little more than one minute of CDC 3600 computer time, at a fraction of the cost that would be required for an individual to do the work using a desk calculator.

In writing these programs we have tried to satisfy three basic aims: A) versatility, B) use of the most appropriate correction procedures, and C) elimination of all hand calculating and data sorting.

A. Versatility

The programs are suitable for any type of problem from the analysis of a binary alloy to that of a complex mineral system involving as many as twenty elements. They accept any reasonable amount of data in any sequence in which the probe operator wishes to gather them and furnish the results in graphical as well as printed form.

Part of the flexibility of this method comes from the fact that we have written not one but two programs, which may be run together or separately. The first program, EMX, takes raw data from the probe, corrects for deadtime, drift, and background, and calculates the ratio of observed intensities (sample over standard) times the concentration of the element in its standard; the results from EMX are referred to herein as the first approximation.* The output from Program EMX can also be written on magnetic tape or punched on cards for use as input to Program EMX2.

The second program, EMX2, makes corrections for absorption and fluorescence by characteristic radiation. Additional corrections, such as that for atomic number effect, can be added later when a satisfactory correction procedure is determined.

As many as 800 probe data points (each point being made up of from one to 100 separate readings)* may be included in one problem, and any number of problems may be grouped in one computer run. Within each problem, the probe operator may analyze up to nine different elements in the first program. For the second program, output from two or more problems may be grouped together; this allows the analysis of samples containing as many as 20 elements.

Some savings in time and computer costs are made if the two programs are run together, but often this is not desirable. The analyst may wish to look at the first approximations before deciding if the results are worth correcting further. Or he may have analyzed only some of the elements present in the sample and wish to measure or estimate the concentrations of others before correcting for absorption and fluorescence. Another practical advantage of the two-program method is that it effectively increases the storage capacity of the computer and enables one to handle a large amount of data.

Program EMX2 can be modified slightly to run "in reverse." If two cards in the main program are changed**, true concentrations can be entered as input data; the output then shows what the observed intensity ratios will be if the correction procedures used are both valid and complete.

B. Appropriate Correction Procedures

When one is writing a computer program and changing from manual to automatic data processing, it is an opportune time to re-examine all the techniques and formulas used in the correction of microprobe data for quantitative analysis. We would be failing to make use of all the advantages offered by electronic computers if we continued to approach problems from the point of view of a man with a slide rule. Several approximations that were previously tolerated because more rigorous calculations would have been too time consuming are no longer justified.

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*Note that our first approximation is not the "premiere approximation" of Castaing (2) but refers only to the output of the first program (EMX). The first approximation is thus the concentration of the particular element in its standard times the ratio (sample to standard) of observed intensities corrected for deadtime, drift and background but not for absorption or fluorescence.

*For purposes of this discussion, a "reading" is defined as one line of data as it comes from the probe and includes the counting time, sample current, counts on three spectrometers, a six-digit code, and, if desired, an identifying label (NAME). A "data point" is made up of one or more readings of the same sample. All the readings in a data point will be added together to find the average counts per second for that data point. A "data set" includes consecutive probe data points taken without a break. A background or standard peak data point may pertain to all the sample data points within the set, but it will not be used to correct data in another set. Therefore, each data set must contain the necessary standard and background readings.

**Change Statement 11 to `OCON(I) = OCON(I)/(SCF(I)* SCON(I))`. Change fifth statement after Statement 400 to `CON2 = OCON(I)*(FCHI*(1.0 + FL))`. Run with `IMAX = 1`.

Consider, for example, the "simple" formula for fluorescence corrections derived by Wittry (1):

$$I'_f = I_A \left[\frac{U_B \ln U_B - U_B + 1}{U_A \ln U_A - U_A + 1}\right]\left[\frac{X_1{}^B \omega_k{}^B (r_k{}^A - 1) \sin\theta}{2}\right] \left[\frac{X^{-76}(1-C_A)\ln(1+u)}{C_A + (1-C_A)x^3}\right] \qquad (1)$$

This formula was ingeniously arranged to take the form of three separate factors, each dependent upon only one variable. This is a considerable advantage to a person making corrections by hand. A computer cannot readily read values from a graph, but it can evaluate complicated functions extremely quickly. We have worked out a formula for fluorescence corrections which combines Wittry's voltage dependence factor with the formula of Castaing (2), which takes into account the effects of depth of penetration in the sample. Theoretically the combination formula appears more satisfactory than the others, but whether it is a significant improvement remains to be seen.

For the absorption correction the computer program now uses Philibert's (3) formula with Duncumb and Shields' (4) effective sigma, but it is hoped that a correction method based on sounder theoretical considerations can be developed. One of the major advantages of computer handling of microprobe data is that it removes much of the drudgery from the process of accumulating large quantities of analytical data on known samples with a view to evaluating correction methods. The effects of making changes in the correction formulae can readily be seen by simple recycling of the data through the computer. Evaluations of the modified fluorescence correction used in EMX2 and of the absorption correction are being attempted by the analysis of simple known phases, particularly binary alloys. The ability to run the program "in reverse" and generate observed intensities from known compositions proves very valuable in this project.

C. Elimination of Manual Data Processing

Our final aim, which was actually the most difficult to carry out, was to eliminate all hand calculation as well as the need to transfer data to some special form. On the other hand, we did not wish to restrict the probe analyst to following any certain sequence of collecting data. For Program EMX, output from the probe can be on punched paper tape, punched cards, magnetic tape, or typewritten pages which can go directly to the keypunch operator. The data do not need to be rearranged in any way--assuming, of course, that the probe operator did not forget to include the necessary standard and background readings or make some other error. The program user need prepare only one data card for each element analyzed in the problem (the Element Card, see Appendix 2) plus one card giving general information about the entire problem (the Identification Card).

The technique by which this has been accomplished is really the key to the entire EMX program. It consists in the assignment of a six-digit code number to each line-of probe output at the time it comes from the probe. Two digits of the code refer to each of the three spectrometers, one indicating which element of the sample is being analyzed and the other specifying the type of reading--standard peak, sample peak, standard background, sample background, or dead-time data (see Sec. II-A). These code numbers could be written by hand on the data sheet that comes from the probe, but we have actually modified our microprobe by adding a "green box", which is located conveniently for the probe operator and connected to the printout device. By setting the six switches on this box, the operator presets the numbers in the code column before the data is printed or punched.

Because each line of data from the probe is identified by this code number, Program EMX can accept data in any order in which it is run, with no need for it to be arranged into a particular sequence. The operator can take readings on standard peaks first, last, and/or anywhere in the middle of the data. Background data points can appear before and/or after each peak data point, or one background data point (or pair of points) can be subtracted from all peaks for the same element. The user may take one or more readings on each point; in the latter case the computer averages the readings for each data point and computes the standard deviations. It is unnecessary to take the same number of readings on each type of data; one could, for example, take two readings on each sample peak, a large number of readings on the first standard peak (to check probe stability), and some other number of readings on later standard peaks. Data points on samples in any one problem, however, must contain the same number of readings.

Further routine paper work has been eliminated by permanent storage within Program EMX2 of all the various constants necessary for carrying out corrections involving any elements. Of course, this data is not really permanent; it can be changed easily when better values become known. The program does not store all the values of μ/ρ, σ, K-fluorescence yield, critical excitation potential, and absorption jump ratio, but rather the constants necessary for calculating them. Heinrich's (5) method of calculating mass absorption coefficients and absorption jump ratios is used, so his values for absorption edges plus the necessary coefficients and exponents are stored. Also included are the atomic weights and characteristic wavelengths of all the elements (see Sec. III-A).

We chose this method because our computer does not have enough quick access storage space to hold vast numerical tables, and it can re-evaluate functions more economically than it could look up the answers on a tape. For a typical problem involving six elements plus oxygen, the CDC-3600 computer took 10 milliseconds to decide which elements will fluoresce which other elements. Calculation of all the required physical constants, 62 separate variables in all, took 38 milliseconds. This procedure is obviously faster and more economical than looking up numbers in tables and removes the possibility of human error in so doing.

* * *

The remainder of this report is devoted to a detailed description of the two computer programs and how to use them. Neither the history of microprobes nor the theory behind methods of correction for absorption and fluorescence effects will be discussed. For a recent, comprehensive treatment of the latter topic, the reader is referred to Philibert (3). An English translation of this paper is presently being prepared by our group and will be available soon.

Appendix 1 contains Fortran listings of the two programs, and data input specifications are in Appendix 2. Appendix 3 is made up of flow diagrams of most of the routines in the programs for those who wish to understand the logic of the programs and/or modify them.

Programs EMX and EMX2 are written in CDC Fortran-63 and should work in their present form on most CDC 3600 or 1604 computers. After conversion to IBM Fortran they would be suitable for use with other large computers such as IBM 7094.* Such conversion is relatively simple and can be done by any experienced programmer.**

The programs were designed for use with an Applied Research Laboratories electron probe microanalyser. Because the data input routines handle data only in the format in which it comes from our microprobe, further modifications will be required by some users. The graph plotting routines, which were developed by California Computer Products, Inc., for use with their Calcomp 165 incremental plotter, will also have to be replaced with different routines if the program is to be used with another type of equipment. However, the basic method of data processing embodied in programs EMX and EMX2 should be applicable to a wide variety of situations, and it is hoped that they will be useful to most microprobe analysts who wish to use computers for data reduction.

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*Program EMX requires about 23,000 storage locations, of which 11,000 are for the program itself and 12,000 for the data required for 800 data points. Program EMX2 requires 12,650 locations--2,000 for the program, 5,000 for physical constant data, and about 12,000 for data involved in a problem of up to 500 samples with up to 20 elements each. The programs were written without any great effort to save space, and storage requirements could be greatly reduced by modified programming and reduction of the amount of data handled at once. However, modification of the programs for a really small computer would be extremely difficult.

**An IBM Fortran-IV version of these programs is presently being developed by the General Atomic Division of General Dynamics, P.O. Box 608, San Diego. For a listing, contact Tom West.

II. PROGRAM EMX

A. Data Coding and Input

Data from the electron microprobe is read into the computer from either magnetic tape or punched cards. Each card (or tape record) contains one line of output from the probe and consists of 36 digits plus up to eight alphanumeric characters in the format described in Appendix 2. Subroutine EMXINPUT must be modified if data is to be in a different format.

The six-digit KODE* which is part of each line of probe output is the key to this method of handling data in almost any sequence in which they happen to be run. The first, third, and fifth digits of the KODE specify the type of reading on the first, second, and third spectrometers, respectively, as follows:

0 = sample peak
1 = sample background
2 = standard peak
3 = standard background
4 = deadtime data

The second, fourth, and sixth digits are the numbers assigned to the elements being considered in that reading. An element number of zero would indicate that the reading for that spectrometer should be ignored.

A special Break Card, with all zeros in the KODE column, signifies the end of a data set. This card is inserted in the data when there is a time lapse between groups of readings in the same problem. Another special card, with all nines in the KODE column, signifies the end of all data for a problem.

Data can come from the probe directly on punched cards, magnetic tape, punched paper tape, or typewritten data sheets. The best method for any particular laboratory would depend upon the type of operation and what facilities are available. We find that in most cases it is preferable to have punched cards (which are punched from our typewritten data) so that one can easily eliminate faulty data and correct operator errors. For occasional long routine projects, though, we use punched paper tape which is converted directly to magnetic tape.

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*In this discussion, names of variables given in capital letters are the actual names used in the Fortran program.

Figs. 1 and 2 are examples of typewritten data sheets as they come from our microprobe. They illustrate two different types of problems: 1) analysis of six elements of a mineral and 2) analysis for a trace element preceded by a deadtime determination. The comments explain the use of the KODE and possible methods of grouping data.

For oxide and oxyanion systems the amount of oxygen associated with the various elements is calculated by the computer, assuming a known specific stoichiometric relationship and in Program EMX2 these are modified as the element concentrations are modified by the correction procedure. The assignment of oxygen to a particular element is a function of its valence state and this factor (see Appendix 2) is decided by the operator and fed into the program. The program can also handle a second element (for example silicon in silicates) in like manner to oxygen.* In pyroxene analyses, for example, Mg, Fe and Ca can be analysed simultaneously and the corresponding silicon and oxygen contents for each data point can be calculated by the computer. These components which are not experimentally measured, but determined from assumed stoichiometric relationships, are in the following referred to as "stoichiometrically determined components", abbreviated as s.d. components.

B. Data Processing Procedures

Data input is handled by Subroutine EMXINPUT. First a single line of data is read, and the computer uses the KODE to determine the type of data point that the reading is part of. Then any remaining readings in that data point are read. At this stage the computer checks to see that data are grouped according to the specifications on the Identification Card (see Appendix 2) for the problem and that dimension limits are not exceeded. If errors have occurred, the data cannot be processed correctly; so the computer skips over the data for that problem and goes on to the next problem, if any.

If the data point was made up of more than one reading, Subroutine EMXSUM is called to average the readings and compute the standard deviation by two methods: the root mean square (r.m.s.) and the square root of the number of counts ($\sqrt{N}$). If the data point is a standard peak, it is important that the readings do not scatter over too wide a range because a large error in measured intensity of the standard would make all the analyses in the problem worthless. But when automatic data processing is used, the data may go from probe to computer without inspection. Thus the computer checks standard deviations on all standard peaks to see that the r.m.s. value does not exceed the $\sqrt{N}$ value by more than a factor of SLIMIT. The SLIMIT factor is input with the data for each problem, and we suggest a value of 2.0 to 3.0. Setting the limit too low will cause the rejection of some good data, and setting it too high will have the effect of removing this check on data scatter.

For data points other than standard peak, the larger of the standard deviation values calculated is retained, and COUNTS are converted to counts per second. When all data for one problem have been read, control returns to the main program.

The TIME value output of our microprobe is the counting duration of each reading, but for the drift correction one really needs to know the time that has elapsed between the beginning of the data set and each data point. (It must be remembered that the time scale cannot continue over more than one data set because the Break Card between sets may indicate a time lapse of hours.) Therefore each data set is considered to begin at TIME = 0, and the TIME of each data point is changed to the number of seconds elapsed between the beginning of the data set and the median time of that point.

1. Deadtime Correction

The equation used for the deadtime correction is

$$\text{COUNTS} = \frac{\text{OC}}{1.0 - \text{OC}\cdot\text{TAU}}$$

where OC = observed counts and TAU = deadtime in seconds.

A value of TAU may apply only to one of the channels and may vary with time. Thus TAU values are not built into the program but must be read into the computer with data for each problem.

If TAU values are not known, they may be computed from experimental data by Program EMX, either as a separate problem or as part of any other problem. Deadtime data, identified by the numeral "4" in the KODE column, consists of a set of readings on one particular substance over a wide range of sample currents. For each data point, counts per second are divided by sample current, and the resulting values are fit linearly by a least-squares method as a function of sample current, i_s. This is the equivalent of fitting the counts-per-second values with a parabola which goes through the origin, described by the formula $Ai_s + Bi_s^2 = 0$. Then TAU = $-B/A^2$ sec. (Figs. 3 and 4 illustrate output from a deadtime determination).

Since deadtime is a function of photon energy and consequently of the elements analyzed, our first throught in writing Program EMX was to provide a simple means of recalculating TAU at frequent intervals. We soon realized, however, that to obtain a reliable value for TAU one must take many readings at many different sample currents in order to obtain adequate statistics. The current must be measured with an extremely sensitive and properly calibrated meter. Thus we have found that an occasional but thorough determination of deadtime is preferable to frequent quick determinations.

Each Element Card (see Appendix 2) of the input data for Program EMX must contain information about the deadtime correction to be made. TAU, if known, is entered in E format; for example, 2.0E-6 represents a deadtime of 2 x 10^{-6} sec. If deadtime is to be calculated from experimental data, TAU is set equal to zero. Deadtime may be calculated for, say, Element 3 and then this value of TAU used also for Element 5. In this case, TAU for Element 5 would be set equal to 3.0. The computer knows that this is not an actual TAU value, because it expects the actual values to be less than one. A negative value for

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[*] If s.d. components are elements other than oxygen and silicon, subroutine OXYGEN must be modified.

TAU would indicate that no deadtime correction is to be made for that element. (We suggest that a probe analyst who chooses to regard deadtime as negligible is being overly optimistic.) If through some mischance the calculated value of TAU turns out to be negative, no deadtime correction will be made.

2. Drift Correction

Accurate microprobe analyses cannot be expected unless the instrument is operating in a stable manner with a minimum of drift. Program EMX corrects for drift by assuming a linear change with time between successive readings on the same standard. This correction is made with no regard to the amount of drift, and it is left to the discretion of the operator to decide whether the drift rate is low enough to justify correcting and using the data.

Successive data points on a standard were used to monitor drift during probe operation. Between each of these data points for the individual spectrometers,Program EMX corrects the data for the variation in count rate on the standard by assuming drift to be a linear function of time. The elapsed time is measured by the accumulated counting time, and the time between successive readings is assumed to be negligible. If the elapsed time between successive readings is large, a Break Card is inserted into the data at this point. Drift corrections will then be made independently for the data before and after the break. No drift correction is made in the case where the variation between successive data points on the standard is within the deviation found in the successive points. In such a case Program EMX will print out a message indicating that no drift correction has been made.

3. Background

Program EMX incorporates the correction for background by two alternate methods. The method most suitable for the particular problem is selected by the probe operator,and this choice indicated by the appropriate symbol for MBKGD in the lead cards to Program EMX. Background may be measured in a single set of readings for the standard and another set for the sample, and in one scheme (MBKGD = 1) these values are subtracted from each standard and sample reading for the remainder of the problem. Further background data points may be taken at any stage in the probe operation, in which case the new background values are adopted and subtracted from succeeding peak values.

For precise analytical work and particularly for the measurement of minor elements in the range 50 to 10,000 ppm it is necessary to monitor the background more carefully than can be achieved by the above method. In these cases background is measured for each data point on both sample and standard. In the second background method (MBKGD = 0) each peak value must be accompanied by a pair of background data points. The program averages these and subtracts the average value from the peak value. The sequence of background and peak values need not be kept constant (for example, see Fig. 2), but two background values must be associated with each peak value. If one background reading is omitted or an extra value included, the wrong pairs of values will be averaged.

Background values can be measured at the same wavelength as the peak values on a material similar in composition to the sample (or standard) but lacking the element being analyzed. In the absence of such material it is convenient to measure background data points at wavelengths above and below the peak wavelength. In practice, a series of data points are taken over a range of wavelengths in the neighborhood of the peak wavelength. The values of counts versus wavelength are examined to determine the variation in peak and background intensities and to search for any other emission peaks in this range. On the basis of these data, two wavelengths on either side of the peak are chosen ($\lambda + \Delta$, $\lambda - \Delta$) and pairs of background measurements made at these wavelengths. In the EMX program these pairs of data points are averaged to give the background values used.

C. Output

The final printed output from Program EMX consists of a tabulation of the concentrations of elements in each sample or sample point plus a tabulation of the elements measured, combined with appropriate s.d. components,as oxides, for example (see footnote page 4). The element concentrations, of course, are the first approximations; i.e., intensity ratios times the concentration of the element in its standard. Additional printed output includes all input data; input data after readings at each data point were averaged, after deadtime correction, and after correction for drift; and the final measured x-ray intensities in counts per second with statistical errors. Figs. 5-9 are examples of printed output. Some time and paper can be saved by eliminating the intermediate output, but it is often useful to observe the effects of each correction as it is applied.

At the option of the program user, the computer will plot a graph of the concentrations (see Fig. 16). The specific plotting routines used in preparing this plot are usable only with a Calcomp 165 incremental plotter used in conjunction with CDC 3600 and CDC 160-A computers; however, it should be relatively easy for laboratories with other types of computer-plotter facilities to substitute their own plotting routines into the program.

When both programs are run together as a multiple execution job, element concentrations from EMX are written on a scratch tape for input to Program EMX2. If data is to be used for EMX2 input at some other time, it may be recorded on magnetic tape or punched cards.

III. PROGRAM EMX2

A. Basic Correction Procedures

Program EMX2 uses an iterative procedure to calculate composition from the input concentrations, which are first approximations calculated from measured x-ray intensities by Program EMX. The necessary absorption and fluorescence corrections are made on the basis of the original input concentrations and a new composition obtained. This procedure is repeated as many times as specified by the program user or until the percentage change in concentrations from one iteration to the next is less than a specified amount.

The absorption correction used Philibert's (3) formula for $f(\chi)$:

$$f(\chi) = \frac{1+h}{(1+\chi/\sigma)\left[1+h\ (1+\chi/\sigma)\right]} \tag{3}$$

where $h = 1.2\ \bar{A}/\bar{Z}2$, $\bar{A}$ and $\bar{Z}$ being the mean atomic number, $\chi = \mu/_\rho \csc\theta$, $\mu/_\rho$ being the mass absorption coefficient of the target for the measured x-ray line and θ being the take-off angle, and $\sigma = \dfrac{2.39 \times 10^5}{E_o{}^{1.5} - E_c{}^{1.5}}$, the effective σ defined by Duncumb and Shields (4), E_o being applied voltage in kv and Ec the critical excitation potential for the particular element in kv.

The fluorescence correction formula, a combination of those of Castaing (2) and Wittry (1), is as follows (in the case of Element A being fluoresced by Element B):

$$\frac{I_f{}^A}{I^A} = \frac{\omega_k{}^B}{2} \cdot C_B \cdot \left(\frac{r-1}{r}\right)_A \cdot \frac{A}{B} \cdot \frac{\mu_B^A}{\mu_B^{\text{sample}}} \cdot \left[\frac{U_B \ln U_B - U_B + 1}{U_A \ln U_A - U_A + 1}\right] \cdot \left[\frac{\ln(1+u)}{u} + \frac{\ln(1+v)}{v}\right] \tag{4}$$

where I^A is the emergent primary intensity of the characteristic wavelength of element A from direct excitation, I_f^A is the emergent secondary intensity of the same wavelength from fluorescence by element B, W_k^B is the k-fluorescence yield, C_B is the concentration of element B, r is the absorption jump ratio, A and B are the atomic weights of elements A and B, μ_B^A (μ_B^{sample}) mass absorption coefficient of the characteristic radiation of B in A (in the sample), E_c^A and E_c^B are the critical excitation potentials of elements A and B, $U_A = E_o/E_c^A$, $U_B = E_o/E_c^B$, $u = \mu_A^{\text{sample}}/\mu_B^{\text{sample}} \sin\theta = \chi_A/\mu_B^{\text{sample}}$, and $v = \sigma/\mu_B^{\text{sample}}$.

The basic correction formula incorporating absorption and fluorescence corrections is

$$C_A = C_A{}^{(1)}\ \frac{R_S(A)}{R} \tag{5}$$

where $C_A{}^{(1)}$ is the first approximation concentration of element A,

$$C_A{}^{(1)} = \frac{I^A}{I(A)}\ S_A \tag{6}$$

I(A) is the measured intensity of element A in its standard, I^A is the measured intensity of element A in the sample, and S_A is the concentration of the element in its standard. The correction factor R, which depends on the concentrations of all N elements in the sample, is given by

$$R(C_1,\ldots,C_N) = F\ (\chi)\left(1 + \frac{I_f^A}{I^A}\right) \tag{7}$$

The notation $R_S{}^{(A)}$ refers to the correction factor for the standard used for Element A.

In Program EMX2 Eq.5 is solved for the concentrations C_J by the Gauss-Seidel iteration method, which has produced rapid convergence for all cases encountered so far. The second-approximation concentrations $C_J{}^{(2)}$ are calculated as follows: The concentration $C_1{}^{(2)}$ of element 1 is calculated using a correction factor R evaluated with the first-approximation concentrations $C_J{}^{(1)}$. The concentration $C_2{}^{(2)}$ of element 2 is then calculated using a correction factor R evaluated with first-approximation concentrations for elements 2 through N, but with the second-approximation value for C_1. The procedure continues in this manner, with R always using the best available (i.e. the most recently calculated) values for the C's. For the second approximation this procedure is expressed by the formula

(8)

This method would be prohibitively time consuming for hand calculation, but is natural for computer calculation.

B. Physical Constants

Data necessary for the calculation of the various constants pertaining to absorption and fluorescence corrections involving almost any elements are stored by Subroutine CONSTANT. Below are listed the data, sources of data, and methods of calculating the required constants:

1. SINTHETA. Sine of the takeoff angle, which with our microprobe is 52.5°.

2. Atomic weights (A). From reports prior to 1960 of the Commission of Atomic Weights, International Union of Pure and Applied Chemistry.

3. Characteristic wavelengths (LAMBDA). For each element we have included only one characteristic wavelength, the one which we customarily use for analyzing the particular element. For elements with atomic numbers 5-35, LAMBDA is the weighted Kα wavelength ($K\alpha_1$ given twice the weight of $K\alpha_2$); for atomic numbers 36-82, $L\alpha_1$; and for atomic numbers 83 to 90-92, Mβ. Wavelength data are from Bearden (7).

4. Mass absorption coefficients (MU) are calculated by Heinrich's (5) method: $MU = C\lambda^n$ where λ is the wavelength of the radiation being observed and the coefficients (C) and exponents (EXP) are those determined by Heinrich. Values for absorption edges (EDGE) are also from Heinrich's tables (5). It should be noted that the data are not complete for all elements. As of now, Program EMX2 cannot be used for the analysis of extremely light elements (atomic numbers less than 12). Values for C and EXP are also unavailable for the regions between the M_4 and M_5 absorption edges and beyond the N_1 edge. The computer will calculate mass absorption coefficients as if the absorption curves for these regions were merely continuations of those for the M_3 to M_4 and M_5 to N_1 regions. This is a very rough approximation and will introduce greater than usual errors when analyses involve elements such that the characteristic wavelength of one falls within the unknown absorption region of the other.

5. Absorption jump ratios (R) used in the fluorescence corrections are calculated from Heinrich's data (5) by the formula $R = (C_k/C_{kl}) \lambda_k^{(n_k - n_{kl})}$, where C and n refer to the absorption curve of the element fluoresced and λ_k = the characteristic wavelength of the fluorescing element. The absorption jump ratio is commonly calculated at the absorption edge, but this unnecessary approximation is not made by Program EMX2 (see Compton and Allison(8), p. 542, or Philibert (3), p. 55).

6. K-fluorescence yields (OMEGA) are calculated from the formula

$$\left(\frac{W_k}{1 - W_k}\right) 1/4 = A + BZ + CZ^3 \qquad (9)$$

using the coefficients of Hagedoorn and Wapstra(9), $A = -0.064$, $B = 0.034$, $C = -1.03 \times 10^{-6}$. Because acceptable values of the L-fluorescence yields and ratios of K to L intensities are not easily evaluated at the present time (Philibert(3))*, only K-K fluorescence is considered. Corrections for K-L, L-K, and L-L fluorescence can be added to the program if reliable data become available.

C. Input

Except for the few introductory data cards (see below and Appendix 2), the input to Program EMX2 consists of the punched card or magnetic tape output from Program EMX. If no more than nine elements are involved in each problem, there will be one card (or tape record) for each sample or point on the sample, and Program EMX2 can be run with Program EMX as a multiple-execution job. For samples involving 10 to 18 different elements, however, the data must be run through the first program as two separate problems, one including nine elements and the other including the remainder. The punched card output must then be put together so that the two cards for each sample are together in the data deck for EMX2.

Sometimes samples contain elements such as carbon that cannot be analyzed directly by many microprobe facilities. Concentrations of such elements must be considered in the total composition, however, if absorption and fluorescence corrections are to be made. The probe operator can estimate the concentrations of elements which were not or could not be analyzed and add them to the data cards for EMX2 after the concentrations of the other elements, setting NFIX on the Identification Card (see Appendix 2) equal to the number of such elements. Concentrations of these fixed elements will be used in calculating average atomic number, etc., but will not themselves be corrected.

For a particular element i the correction factor R(i) combines the absorption and fluorescence corrections for the standard (see section IIIA). The value of R(i) depends on the composition of the standard and the operating voltage. To solve Equation 5, Program EMX2 will calculate R^i for the unknown, but the values of R(i), the correction factors (SCF) for the elements in their standards, must be read into the program on the Element Cards (Appendix 2). Thus before any analyses of actual samples are corrected, the necessary correction factors must be calculated. This is done by considering the standard as a separate problem, with an Element Card for each element of the standard on which SCF is set equal to zero. The operating voltage (EO) for this problem is set equal to that actually used in the analyses. The computer will calculate each SCF value and punch new Element Cards containing all the necessary information including the SCF. These cards may be saved for use as Element Cards in any problem in which the same standard and EO were used. The most efficient procedure is to build up a file of Element Cards for all the standards commonly used (pure element standards as well as mineral or alloy standards) with correction factors evaluated for all EO which are likely to be used.

D. Computer Method

After the preliminary calculations of the physical constants (listed under Sec. IIIB, above) by Subroutine SETUP, the computer looks at the first SCF (see Sec. IIIC) to see if the correction factors for the standard are known. If they are not (i.e., if SCF = 0), the problem is assumed to be one of determining the correction factors for a particular standard. In this case the program calculates the SCF, punches new element cards, and proceeds to the next problem. If the SCF do not equal zero, the computer proceeds to the sample data and reads in the first approximation concentrations (OCON(J), J = 1 to NEL, where NEL = number of elements analyzed) for one sample or point on the sample. Subroutine OXYGEN is called to calculate the concentrations of oxygen (OCON(NELP1)) and silicon (OCON(NEPL2)) (if O or SI factors present) as a function of the concentrations of the other elements. Concentrations of all elements and their total are printed, and the computer then proceeds to the corrections themselves.

The first step is the storage of all OCON in CON and the multiplication of each OCON by its SCF. Now OCON is not the first approximation but a product of the first approximation and the R correction factor for the standard according to Equation

---

*There is some difference of opinion about this; see Reed (10).

5. This product will remain constant throughout the iterations.

FCHI, the absorption correction factor, is calculated in Function ABSORB.

Function FLUOR(NN) calculates the fluorescence correction term, which may include the fluorescence effects of from zero to four other elements. Subroutine SETUP has previously determined which elements fluoresce each of the elements analyzed in the problem. For simplicity, the former may include only the four elements nearest in atomic number whose $K\alpha$ lines are less than the K absorption edge of the element in question. Thus, for example, in determining which elements might fluoresce Fe ($Z = 26$), the program looks only for elements in the problem with atomic numbers in the range 28-31. Although fluorescence by elements with higher atomic numbers or by the $K\beta$ line of Co ($Z = 27$) might be significant, these are not taken into consideration.

In the Fortran notation of the computer program, the function calculated by Function FLUOR(NN) is

$$\mathrm{FLUOR} = \sum_{j=1}^{\mathrm{NF(NN)}} \mathrm{CON}_{L} \cdot \mathrm{U}_{\mathrm{NN},J} \cdot \frac{\mathrm{ULC + V}}{\mathrm{FMUBAR}}$$

where L is index of fluorescing element, NN is index of element fluoresced, NF is number of elements fluorescing NN, FMUBAR is mass absorption coefficient of alloy for wavelength of element L, MUBAR is mass absorption coefficient of alloy for wavelength of element NN,

$$\mathrm{ULC} = \frac{\ln\ (1\ +\ \mathrm{MUBAR/(FMUBAR \cdot SINTHETA)}}{\mathrm{MUBAR/(FMUBAR \cdot SINTHETA)}}$$

$$\mathrm{V} = \frac{\ln\ (1 + \mathrm{SIGMA/FMUBAR})}{\mathrm{SIGMA/FMUBAR}}$$

and U is the U from Subroutine SETUP, a variable which contains all the parameters of the fluorescence correction equation except those that depend on the concentrations of elements. Note: U here is <u>not</u> just E0/EC.

A new approximation (CON2) is then calculated according to Eqn. 8, which in Fortran notation is written as CON2 = OCON(I)/(FCHI*(1.0 + FL)). DELCON, the change in the concentration of Element 1 that resulted from this formula, is calculated; concentrations of s.d. components (if any) are modified, and the value of CON2 replaces CON(I). Then the procedure is repeated for all the other elements. Note that the estimated composition, from which FCHI and FL are calculated, changes with the correction of each element; the same estimated composition does not carry through an entire iteration. The results of each correction are printed out (see Fig. 13), and the total of concentrations is printed after each iteration.

The limits of the iteration have been read into the computer from the Problem Card, with IMIN and IMAX specifying the minimum and maximum number of iterations to be performed. Within these limits, the correction procedure will be iterated until DELCON for any element present in amounts greater than one percent does not change by more than DMIN from one iteration to the next.

No method for calculating estimated errors in the final results is included in the program.

E. OUTPUT

Final output for Program EMX2 is in the same format as that from Program EMX, including the optional graph. (If more than ten elements are included in the problem, there will be two graphs because too many lines on one plot would be undecipherable.)

Concentrations in weight percent shown for each element and the total for all the elements analyzed are those calculated by the correction procedures described above. They are not normalized to sum to 100 percent. The information that the total corrected concentrations for a particular problem vary quite markedly from 100 percent can give a useful indication of how well the microprobe was working, how carefully the analyses were performed, or perhaps how the computer correction method needs to be revised. We do not believe that this valuable information should be lost.

Printed output from EMX2 begins with the input data from the Identification and Element Cards as well as all the mass absorption coefficients, wavelengths, etc., determined by Subroutine SETUP. Next comes one printed page for each sample or point on the sample showing the first approximations (those read in), and the concentrations, $f(\chi)$, and fluorescence correction values calculated in each iteration, plus the change in the concentration of each element from one iteration to the next. Figs. 11 to 16 are examples of printed output from Program EMX2.

ACKNOWLEDGMENTS

The development of these computer programs can be directly attributed to the innate laziness of the microprobe operators at the La Jolla Microprobe Laboratory. We thank Drs. W. R. Frazer and G. Arrhenius for many helpful and stimulating discussions and the staff of the UCSD Computer Center for their invaluable assistance. The programs were developed under the sponsorship in equal parts of the National Aeronautics and Space Administration (grantnumber NsG-317-63) and the United States Air Force Office of Scientific Research (contract AFOSR-631-64). The generous support of these agencies is gratefully acknowledged.

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002000	000377	028955	047217	022521	212223	Marj.	Standard for Elements 1, 2 and 3 on spectrometers 1, 2 and 3, respectively. NAME indicates that the mineral standard used was Marjalahti. Identifying names are optional; this column could have been left blank.
002000	000377	028880	047936	022628	212223	↓	
002000	000378	028897	047741	022623	212223		
002000	000378	029020	046930	022373	212223		
002000	000377	029544	047491	022558	212223		
002000	000377	029735	047164	022712	212223		
002000	000377	029771	047482	022530	212223		
002000	000377	000586	000287	000503	313233		Background readings for standard, above and below peak.
000200	000377	000489	000221	000427	313233		
002000	000377	000717	000249	000089	111213		Sample background readings.
002000	000377	000868	000327	000081	111213		
002000	000377	034633	038649	000116	010203	1	Sample readings on all three spectrometers.
002000	000377	036125	041653	000138	010203	2	
002000	000377	038196	042098	000141	010203	3A	
002000	000377	036543	039488	000147	010203	3B	
002000	000377	046622	040533	000110	010203	3C	
002000	000377	028242	046361	022460	212223	marj.	Standard readings repeated. Computer will interpolate between this and previous group of standard readings to correct for drift.
002000	000377	038824	046663	022570	212223	↓	
002000	000377	028525	046817	022492	212223		
					000000		"BREAK" Card: indicates end of a data set.
002000	000377	000164	070293	019544	202526	andesine	Standard peak for elements 5 and 6 on spectrometers 2 and 3, respectively. Zero in the second column of the KODE indicates that reading on spectrometer 1 is to be ignored.
002000	000377	000154	070625	019317	202526	↓	
002000	000377	000161	069911	019636	202526		
002000	000300	201090	002560	000164	240000	Mn100	Standard for Element 4 on spectrometer 1; other spectrometers ignored.
002000	000300	201295	002524	000162	240000	↓	
002000	000300	200767	002709	000142	240000		
002000	000300	202077	002612	000181	240000		
002000	000300	202517	002538	000171	240000		
002000	000350	000493	000149	000187	141516		First sample background reading. Will be averaged with the one that comes after the sample readings. Note that pairs of background readings need not appear consecutively.
002000	000350	045393	013670	012138	040506	1	
002000	000350	043481	012899	012285	040506	2	
002000	000350	044873	012964	012301	040506	3A	
002000	000350	042892	013854	012355	040506	3B	
002000	000350	037200	018717	012266	040506	3C	
002000	000350	000508	001631	000279	141516		
002000	000300	001529	002530	000137	340000		
002000	000300	001717	002619	000146	340000		
002000	000300	200927	002689	000120	240000	Mn100	
002000	000300	200519	000298	000161	240000	↓	
002000	000377	000263	069380	019736	003536	andesine	
002000	000377	000234	069246	019154	003536	↓	
					999999		Card signalling the end of the data for this problem.

Figure 1. Data sheet as it comes from the microprobe illustrating the use of the six-digit code. The columns, from left to right, are counting time in hundredths of a second, sample current in μa x 10^{-4}, counts on spectrometers 1, 2 and 3, the six-digit code (KODE), and, if desired, a name for identification (NAME). In this problem NS = 1, so each reading on the sample is a separate data point. MBKGD = 1 so background data points do not accompany each individual peak data point.

```
000100    000800    003837    000000    000000    410000
001000    000780    003712    000000    000000    410000
001000    000760    003654    000000    000000    410000
```

Deadtime data on Spectrometer 1. Printout columns for spectrometers 2 and 3 were not used, so turned off. NDT = 1, so each reading is one data point. Of course many more dead time data points would be taken.

```
000000    000013    000476    000000    000000    000000
```

"BREAK" Card. Numbers which happened to get printed in cols. 2 and 3 will be ignored.

```
002000    000000    000374    000000    000000    310000
002000    000000    000384    000000    000000    310000
002000    000000    120118    000000    000000    210000
002000    000000    119402    000000    000000    210000
002000    000000    120751    000000    000000    210000
002000    000000    121284    000000    000000    210000
002000    000000    000391    000000    000000    310000
002000    000000    000397    000000    000000    310000
```

Standard peak and background readings. For this problem NS was set equal to 2, so standard background, sample background, and sample peak data points will be taken in pairs which will be averaged. Note that readings in this problem were taken over different time intervals.

```
010000    000000    000699    000000    000000    110000
010000    000000    000690    000000    000000    110000
010000    000000    000568    000000    000000    110000
010000    000000    000551    000000    000000    110000
010000    000000    000695    000000    000000    010000
010000    000000    000688    000000    000000    010000
```

First sample. MBKGD equals 0, so a pair of background data points will be taken with each sample.

```
010000    000000    000669    000000    000000    010000
010000    000000    000669    000000    000000    010000
010000    000000    000696    000000    000000    110000
010000    000000    000700    000000    000000    110000
010000    000000    000591    000000    000000    110000
010000    000000    000585    000000    000000    110000
```

Second sample. Note that background points were taken before the first sample but after this sample. Computer will keep track of which background goes with which sample.

```
002000    000000    117977    000000    000000    210000
002000    000000    118404    000000    000000    210000
002000    000000    117931    000000    000000    210000
002000    000000    118216    000000    000000    210000

010000    000000    000692    000000    000000    110000
010000    000000    000681    000000    000000    110000
010000    000000    000708    000000    000000    010000
010000    000000    000721    000000    000000    010000
010000    000000    000501    000000    000000    110000
010000    000000    000519    000000    000000    110000
```

A standard peak data point taken again to check for drift. Because MBKGD equals 0 but no background readings were taken for this standard peak, this data point will not be corrected for background. But that doesn't matter because this point is used only for the drift correction.

```
000000    000000    000000    000000    000000    999999
```

Figure 2. Data as it comes from the microprobe illustrating the use of the six-digit code. First three readings are part of a data set used to measure deadtime. The remaining readings refer to a problem in which NS = 2 so that each standard background, sample peak and sample background data point comprises two readings which will be averaged. MBKGD = 0, so each peak data point is accompanied by a pair of background data points.

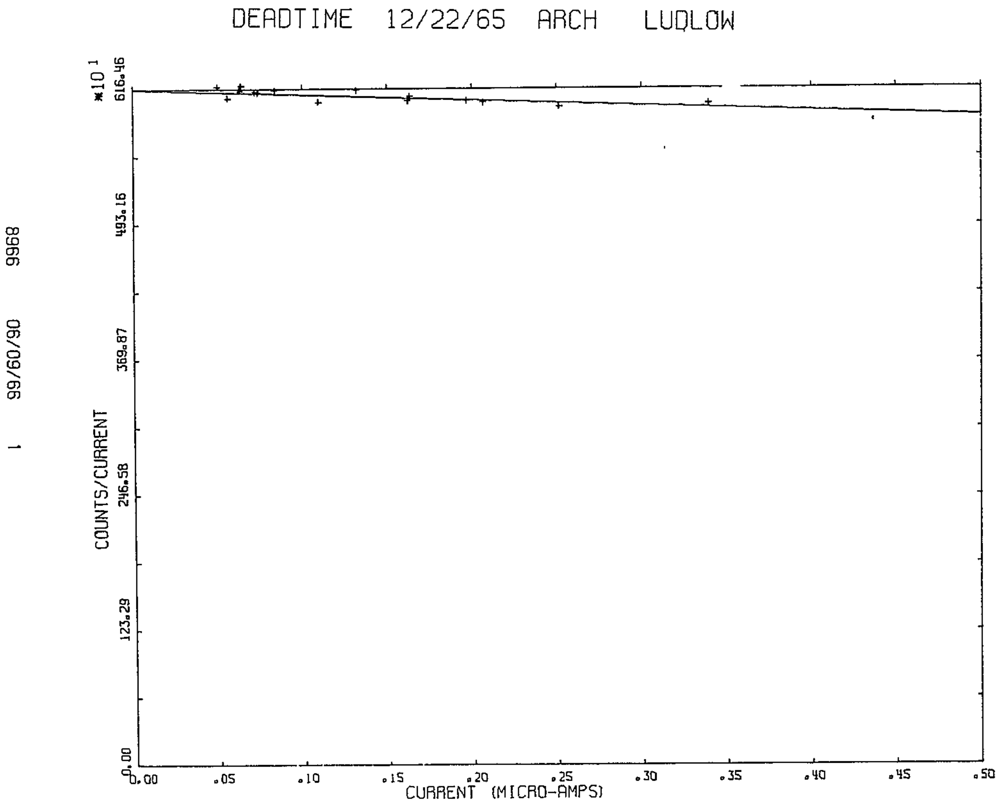

Figure 3. Sample of the type of plot drawn by the computer for deadtime data points. Counting rate divided by sample current is plotted against sample current. If there were no deadtime the points would plot on a horizontal straight line. The slope of the line (least squares fit to the plotted points) is a measure of the deadtime. The equation of the line is used to derive the constants for the parabola approximated in a plot of counting rate versus sample current, and hence to estimate the deadtime (Section IIB).

```
COEFFICIENTS OF Y=B1+B2*X+ETC AND ERRORS

B( 1)=  5.7233994E 02 ERRB= 2.517E 00 B( 2)= -1.5635789E 00 ERRB= 1.211E 00 B(

SIGMA =   1.3125602E 00

COEFFICIENTS OF Y=T1*P1+T2*P2+ETC AND ERRORS

T( 1)=  5.6942390E 02 ERRT= 1.110E 00 T( 2)= -1.5635789E 00 ERRT= 1.211E 00 T(

   I          X(I)             F(I)             Y(I)             DELY(I)            W(I)

   1    4.9885000E-01    5.7572417E 02    5.7155995E 02    -4.1642160E 00    3.4658959E-02
   2    5.6215000E-01    5.6755314E 02    5.7146098E 02     3.9078309E 00    3.9619197E-02
   3    6.4215000E-01    5.7899245E 02    5.7133589E 02    -7.6565585E 00    4.4363273E-02
   4    7.3995000E-01    5.7368741E 02    5.7118297E 02    -2.5044406E 00    5.1592556E-02
   5    6.3105000E-01    5.7745028E 02    5.7135324E 02    -6.0970368E 00    4.3712854E-02
   6    7.2105000E-01    5.6632688E 02    5.7121252E 02     4.8856380E 00    5.0227084E-02
   7    8.3880000E-01    5.7319981E 02    5.7102841E 02    -2.1713983E 00    5.8534562E-02
   8    1.0954500E 00    5.7223059E 02    5.7062712E 02    -1.6034717E 00    5.1148626E-02
   9    1.3187500E 00    5.6693839E 02    5.7027797E 02     3.3395826E 00    9.3043620E-02
  10    1.6354000E 00    5.7161856E 02    5.6978286E 02    -1.8357003E 00    1.1443995E-01
  11    2.0698000E 00    5.7289352E 02    5.6910365E 02    -3.7898709E 00    1.4451551E-01
  12    1.6243000E 00    5.6769070E 02    5.6980022E 02     2.1095222E 00    1.1444965E-01
  13    1.9687000E 00    5.6100472E 02    5.6926172E 02     8.2569992E 00    1.4036958E-01
  14    2.5175500E 00    5.6699966E 02    5.6840355E 02     1.4038905E 00    1.7760504E-01
  15    3.3996500E 00    5.6917624E 02    5.6702432E 02    -2.1519188E 00    2.3891721E-01


FOR ELEMENT 12 ON SPECTROMETER 3, TAU =  4.77E-06 SECONDS
```

Figure 4. Output of deadtime calculation from Program EMX.

```
PROBLEM NO.    18      SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966

NO. OF ELEMENTS = 5
 0 DEADTIME READINGS PER SET
 2 SAMPLE READINGS PER SET
BACKGROUND READING METHOD = 1
SIGMA FOR STANDARD PEAK MAY NOT EXCEED  3,0 * SQRTF(N)


        ATOMIC   PER CENT W          TAJ     OXYGEN   SILICON
ELEMENT NUMBER  OF STANDARD                  FACTOR    FACTOR

   1      25      34.970000   1,60E-05    .29110        -0      MNO
   2      20       6.980000   2,00E-06    .39220        -0      CAO
   3      13      14.700000   2,00E-06    .88960        -0      AL2O3
   4      26       8.700000   1,60E-05    .28650        -0      FEO
   5      14      18.800000   2,00E-06   1,13900        -0      SIO2
```

Figure 5. Output from Program EMX. First output page showing problem description.

```
PROBLEM NO.     18      SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966

                                 INPUT DATA
             NAME       TIME   CURRENT      SPEC 1       SPEC 2       SPEC 3     KODE

   1                  20.00          0      82609        27242           53   210000
   1                  20.00          0      83333        27554           59   210000
   1                  20.00          0      81919        27580           54   210000
   1                  20.00          0      82353        27778           62   210000
   1                  20.00          0      82898        27674           67   210000
   2                  20.00          0        295        60848        18813   202223
   2                  20.00          0        280        60669        18580   202223
   2                  20.00          0        287        60744        18685   202223
   2                  20.00          0        313        60603        18996   202223
   2                  20.00          0        287        59902        18594   202223
   3                  20.00          0      45685        11379        11872   010203
   3                  20.00          0      45679        11379        11649   010203
   4                  20.00          0      45231        11307        11789   010203
   4                  20.00          0      45221        11314        11820   010203
   5                  20.00          0      44891        10515        11886   010203
   5                  20.00          0      45595        10525        11974   010203
   6                  20.00          0      44192        12028        11876   010203
   6                  20.00          0      44215        12215        11977   010203
   7                  20.00          0      45040        12840        11905   010203
   7                  20.00          0      45022        12616        11756   010203
   8                  20.00          0      39273        14946        11825   010203
   8                  20.00          0      38805        15069        11828   010203
   9                  20.00          0      44900        12495        11831   010203
   9                  20.00          0      44371        12478        11799   010203
  10                  20.00          0      46359        11800        12004   010203
  10                  20.00          0      45724        11691        11951   010203
  11                  20.00          0      45120        12941        11895   010203
  11                  20.00          0      45004        12911        11780   010203
  12                  20.00          0   ---52604        10574        11695   010203
  12                  20.00          0      52448        10457        11767   010203
  13                  20.00          0        270        61696        18608   202223
  13                  20.00          0        302        60964        18678   202223
  14                  20.00          0      81351        27847           76   212020
  14                  20.00          0      80984        27808           51   212020
  15                  20.00          0      45272        11313        11930   010203
  15                  20.00          0      45801        11459        11604   010203
  16                  20.00          0      54102        10271        11781   010203
  16                  20.00          0      54381        10070        11926   010203
  17                  20.00          0      52073        10510        11930   010203
  17                  20.00          0      51502        10468        11615   010203
  18                  20.00          0      52731        10313        11464   010203
  18                  20.00          0      52212        10341        11826   010203
  19                  20.00          0      52819         8888        11689   010203
  19                  20.00          0      53108         9048        11855   010203
  20                  20.00          0      52501        10685        11628   010203
```

Figure 6. Output from Program EMX. Second output page showing raw probe data and code identification of data points.

```
PROBLEM NO.     18      SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966                        PAGE  3
                         AVERAGED DATA

                REL.                 SPECTROMETER 1              SPECTROMETER 2              SPECTROMETER 3
                TIME   CURRENT   CTS/SEC      SIGMA          CTS/SEC      SIGMA          CTS/SEC      SIGMA

   1              50         0    4131.1       10.7  2 1          0           0  0 0          0           0  0 0
   2             150         0         0          0  2 0     3027.7         7.5  2 2      936.7         3.5  2 3
   3             220         0    2284.1        7.6  0 1      569.0         3.8  0 2      588.0         3.9  0 3
   4             260         0    2261.3        7.5  0 1      565.5         3.8  0 2      590.2         3.8  0 3
   5             300         0    2262.2       12.4  0 1      526.0         3.6  0 2      596.5         3.9  0 3
   6             340         0    2210.2        7.4  0 1      606.1         3.9  0 2      596.3         3.9  0 3
   7             380         0    2251.6        7.5  0 1      636.4         4.0  0 2      591.5         3.8  0 3
   8             420         0    1951.9        8.3  0 1      750.4         4.3  0 2      591.3         3.8  0 3
   9             460         0    2231.8        9.4  0 1      624.3         4.0  0 2      590.8         3.8  0 3
  10             500         0    2327.1        7.6  0 1      587.3         3.8  0 2      598.9         3.9  0 3
  11             540         0    2253.1        7.5  0 1      646.3         4.0  0 2      591.9         3.8  0 3
  12             580         0    2626.3        8.1  0 1      525.8         3.6  0 2      586.5         3.8  0 3
  13             620         0         0          0  2 0     3066.5        12.9  2 2      932.2         4.8  2 3
  14             660         0    4058.4       10.1  2 1          0           0  2 0          0           0  2 0
  15             700         0    2276.8        9.4  0 1      569.3         3.8  0 2      588.4         5.8  0 3
  16             740         0    2712.1        8.2  0 1      508.5         3.6  0 2      592.7         3.8  0 3
  17             780         0    2589.4       10.1  0 1      524.5         3.6  0 2      588.6         5.6  0 3
  18             820         0    2623.6        9.2  0 1      516.4         3.6  0 2      582.3         6.4  0 3
  19             860         0    2648.2        8.1  0 1      448.4         3.3  0 2      588.6         3.8  0 3
  20             900         0    2622.5        8.1  0 1      532.3         3.6  0 2      578.9         3.8  0 3
  21             940         0    2735.7        8.3  0 1      516.7         3.6  0 2      581.3         3.8  0 3
  22             980         0    2670.5        8.2  0 1      510.4         5.4  0 2      581.0         3.8  0 3
  23            1020         0    2650.7       10.0  0 1      472.5         3.4  0 2      574.1         3.8  0 3
  24            1060         0    2995.2       14.6  0 1      417.4         3.5  0 2      581.7         3.8  0 3
  25            1100         0         0          0  2 0     2958.7         8.6  2 2      899.6         4.7  2 3
  26            1140         0    3939.9       10.4  2 1          0           0  2 0          0           0  2 0
  27            1180         0      37.8        1.0  3 1          0           0  0 0          0           0  0 0
  28            1220         0      32.5         .9  3 1          0           0  0 0          0           0  0 0
  29            1260         0         0          0  3 0       68.7         1.3  3 2       12.1          .5  3 3
  30            1300         0         0          0  3 0       64.5         1.3  3 2       18.3          .7  3 3
  31            1340         0      25.0         .8  1 1       73.6         1.4  1 2       11.8          .5  1 3
  32            1380         0      25.9        1.3  1 1       66.7         1.3  1 2        9.3          .5  1 3

  33              20         0    4156.3       10.2  2 1          0           0  2 0          0           0  2 0
  34              60         0         0          0  2 0     3101.6         8.8  2 2      945.2         5.0  2 3
  35             100         0    3066.5        8.8  0 1      447.4         5.9  0 2      608.9         3.9  0 3
  36             140         0    3212.4       10.8  0 1      418.1         3.2  0 2      598.5         3.9  0 3
  37             180         0    3021.5        8.7  0 1      467.3         4.8  0 2      606.5         3.9  0 3
  38             220         0    3139.2        8.9  0 1      422.7         3.3  0 2      599.9         3.9  0 3
  39             260         0    2972.9        8.6  0 1      464.5         3.4  0 2      599.9         3.9  0 3
  40             300         0    3306.5       21.8  0 1      374.0         3.1  0 2      605.7         3.9  0 3
  41             340         0    3342.1        9.1  0 1      384.4         3.1  0 2      603.0         3.9  0 3
  42             380         0    3207.2        9.0  0 1      394.6         3.1  0 2      596.2         3.9  0 3
  43             420         0    3215.5        9.0  0 1      383.1         3.1  0 2      594.9         3.9  0 3
  44             460         0    3249.6        9.0  0 1      349.1         3.0  0 2      583.9         3.8  0 3
  45             500         0         0          0  2 0     3033.1         8.7  2 2      936.1         4.8  2 3
  46             540         0    4134.7       10.2  2 1          0           0  2 0          0           0  2 0
  47             580         0    3220.5       19.4  0 1      348.3         3.0  0 2      591.9         3.8  0 3
```

Figure 7. Output from Program EMX. Averaged data. Columns from left to right are data point number, relative time (for drift correction), sample current (not measured in this problem), averaged count rate in counts per second for each data point on spectrometer 1, error, code number showing type of reading, element number, averaged count rate on spectrometer 2, etc.

```
PROBLEM NO.    18      SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966
                              CONCENTRATIONS CORRECTED FOR DEADTIME, DRIFT, AND BACK
                        SAMPLE CORRECTED   CONCEN-  RELATIVE              GROUND
    E      SAMPLE     CURRENT   CTS/SEC    TRATION    ERROR

  1  1   STD              0     4388.3    .34970       ,002
  3  1                    0     2357.8    .18789       ,004
  4  1                    0     2336.1    .18616       ,004
  5  1                    0     2339.9    .18647       ,006
  6  1                    0     2286.5    .18221       ,004
  7  1                    0     2334.3    .18602       ,004
  8  1                    0     2012.7    .16039       ,005
  9  1                    0     2318.7    .18477       ,005
 10  1                    0     2425.7    .19330       ,004
 11  1                    0     2347.8    .18710       ,004
 12  1                    0     2761.7    .22007       ,004
 15  1                    0     2343.6    .18676       ,005
 16  1                    0     2824.5    .22508       ,004
 17  1                    0     2697.1    .21493       ,004
 18  1                    0     2741.8    .21849       .004
 19  1                    0     2776.3    .22124       ,004
 20  1                    0     2755.2    .21936       ,004
 21  1                    0     2888.5    .23018       ,004
 22  1                    0     2823.5    .22500       ,004
 23  1                    0     2808.9    .22384       ,004
 24  1                    0     3204.4    .25535       ,005

  2  2   STD              0     2979.5    .06980       ,003
  3  2                    0      498.3    .01167       ,008
  4  2                    0      494.3    .01158       ,008
  5  2                    0      454.2    .01064       ,009
  6  2                    0      533.5    .01250       ,008
  7  2                    0      563.1    .01319       ,008
  8  2                    0      675.8    .01583       ,007
  9  2                    0      549.7    .01288       ,008
 10  2                    0      512.2    .01200       ,008
 11  2                    0      570.1    .01336       ,008
 12  2                    0      450.0    .01054       ,009
 15  2                    0      499.8    .01171       ,008
 16  2                    0      438.9    .01028       ,009
 17  2                    0      454.8    .01066       ,009
 18  2                    0      446.7    .01047       ,009
 19  2                    0      378.6    .00887       ,010
 20  2                    0      462.7    .01084       ,009
 21  2                    0      447.1    .01047       ,009
 22  2                    0      440.8    .01033       ,013
 23  2                    0      402.7    .00943       ,009
 24  2                    0      347.5    .00814       ,011
```

Figure 8. Output from Program EMX. First approximation. Columns from left to right are data point number, element number, sample current, count rate in counts per second corrected for deadtime, drift and background, corresponding composition (first approximation) and statistical error.

```
PROBLEM NO.    18      SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966

                       CONCENTRATIONS CORRECTED FOR DEADTIME, DRIFT, AND BACK
                                                                      GROUND
           TOTAL        25         20         13         26         14
          55.1833    18.7891     1.1674     9.2061     8.8023    17.2184
          56.5262    18.6158     1.1580     9.2412    10.1431    17.3682
          56.6706    18.6466     1.0641     9.3413    10.3872    17.2315
          57.3713    18.2205     1.2498     9.3385    11.2715    17.2909
          57.0652    18.6017     1.3190     9.2619    10.6624    17.2201

          58.3307    16.0391     1.5832     9.2587    14.0259    17.4238
          57.8720    18.4771     1.2877     9.2495    11.4579    17.3998
          58.2862    19.3300     1.1999     9.3792    11.1632    17.2139
          58.2711    18.7095     1.3356     9.2675    11.5483    17.4102
          57.0318    22.0074     1.0543     9.1825     7.4855    17.3021

          57.2659    18.6760     1.1708     9.2112    10.6452    17.5625
          58.0152    22.5078     1.0281     9.2803     7.6470    17.5519
          57.6675    21.4926     1.0655     9.2156     8.3213    17.5724
          57.3793    21.8494     1.0465     9.1139     7.7834    17.5860
          57.0401    22.1240      .8870     9.2152     7.3558    17.4581

          57.9029    21.9561     1.0840     9.0600     8.2380    17.5648
          58.2234    23.0179     1.0474     9.0991     7.4067    17.6523
          57.4976    22.4998     1.0326     9.0947     7.4176    17.4529
          57.2470    22.3840      .9435     8.9834     7.3607    17.5754
          57.8181    25.5354      .8142     9.1043     4.6985    17.6657

          58.4975    25.3499      .8650     9.4608     5.1888    17.6330
          59.0397    26.6425      .7999     9.3045     4.5568    17.7360
          59.0839    24.9774      .9150     9.4385     6.0359    17.7171
          58.7357    26.0216      .8144     9.3422     5.0292    17.5282
          58.7214    24.5735      .9129     9.3518     6.2747    17.6085

          59.0574    27.5203      .7055     9.4517     3.6528    17.7271
          59.0784    27.8477      .7315     9.4180     3.4825    17.5988
          58.1192    26.6558      .7570     9.3182     3.9613    17.4169
          57.7727    26.7513      .7319     9.3055     3.7337    17.2503
          56.9297    27.0646      .6544     9.1388     2.8657    17.2062

          57.0592    26.7837      .6362     9.1823     3.0256    17.4313
          56.8160    27.8768      .5787     9.0779     2.0738    17.2087
          56.4300    26.0319      .6555     9.2305     3.1105    17.4015
          56.2167    27.3320      .5705     9.0234     2.0134    17.2773
          56.2717    26.7507      .5634     8.8692     2.8402    17.2483

          56.4949    27.5216      .4786     9.0119     1.9081    17.5747
          56.2432    28.7223      .4996     8.9815      .8430    17.1969
          57.1427    27.2230      .6346     9.0060     2.7017    17.5774
          57.0323    26.8648      .6313     8.9811     3.2180    17.3371
          56.9173    28.5053      .4643     9.0080     1.2703    17.6694
```

Figure 9. Output from Program EMX. First approximation. Concentrations in weight percent, elements identified by atomic number.

```
PROBLEM NO.    18      SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966

                 CONCENTRATIONS CORRECTED FOR DEADTIME, DRIFT, AND BACK
                                                                   GROUN
         TOTAL       MNO        CAO        AL203       FEO        SIO2
       91.4341    24.2586     1.6253     17.3958     11.3241    36.8302
       93.3087    24.0348     1.6121     17.4621     13.0490    37.1505
       93.4286    24.0746     1.4815     17.6513     13.3631    36.8581
       94.3966    23.5245     1.7400     17.6461     14.5008    36.9853
       93.9054    24.0167     1.8364     17.5013     13.7171    36.8339

       95.7213    20.7081     2.2041     17.4953     18.0443    37.2695
       95.0851    23.8557     1.7927     17.4779     14.7406    37.2182
       95.5324    24.9570     1.6705     17.7230     14.3614    36.8205
       95.6244    24.1559     1.8594     17.5119     14.8568    37.2404
       93.8720    28.4137     1.4677     17.3513      9.6301    37.0092

       94.4096    24.1126     1.6300     17.4056     13.6951    37.5663
       95.4088    29.0599     1.4314     17.5360      9.8379    37.5436
       94.9392    27.7491     1.4834     17.4139     10.7053    37.5875
       94.5182    28.2098     1.4570     17.2216     10.0134    37.6164
       94.0183    28.5643     1.2349     17.4131      9.4632    37.3428

       95.1457    28.3475     1.5092     17.1198     10.5981    37.5710
       95.6573    29.7184     1.4582     17.1937      9.5288    37.7582
       94.5470    29.0495     1.4376     17.1854      9.5427    37.3317
       94.2519    28.8999     1.3135     16.9751      9.4695    37.5938
       95.1373    32.9688     1.1335     17.2035      6.0446    37.7869

       96.2030    32.7292     1.2042     17.8771      6.6754    37.7170
       96.8932    34.3981     1.1136     17.5818      5.8623    37.9374
       97.0193    32.2484     1.2738     17.8350      7.7651    37.8970
       96.3463    33.5965     1.1338     17.6531      6.4701    37.4929
       96.4060    31.7268     1.2709     17.6712      8.0724    37.6646

       96.9912    35.5314      .9822     17.8599      4.6993    37.9184
       96.8927    35.9541     1.0183     17.7963      4.4802    37.6438
       95.4407    34.4282     1.0539     17.6077      5.0962    37.2547
       94.8430    34.5386     1.0190     17.5836      4.8033    36.8984
       93.6136    34.9430      .9111     17.2687      3.6868    36.8041

       93.9952    34.5805      .8858     17.3509      3.8925    37.2856
       93.4285    35.9918      .8057     17.1537      2.6679    36.8094
       93.1880    33.6098      .9126     17.4420      4.0017    37.2219
       92.6797    35.2884      .7943     17.0506      2.5903    36.9562
       92.6294    34.5378      .7843     16.7592      3.6539    36.8942

       93.2753    35.5331      .6664     17.0289      2.4548    37.5922
       92.6188    37.0833      .6955     16.9714      1.0845    36.7841
       94.1226    35.1476      .8835     17.0177      3.4758    37.5981
       93.7587    34.6851      .8789     16.9706      4.1400    37.0840
       93.9003    36.8032      .6465     17.0214      1.6342    37.7949

       94.6211    34.2531      .9794     17.7184      4.6581    37.0121
       94.7495    37.0218      .7655     17.6435      1.4096    37.9090
       95.6673    38.5120      .6120     17.8083       .9866    37.7484
       94.8211    37.6485      .7903     17.8053      1.2288    37.3481
       95.7229    37.9347      .7728     17.9946      1.2009    37.8199
```

Figure 10. Output from Program EMX. First approximation. Concentrations in weight percent, expressed as oxides.

```
PROBLEM NO.    18    SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966      20 K

                ------STANDARD FOR ELEMENT Z------    OXYGEN    SILICON
 NL     Z     CONCENTRATION      F(CHI)*(1+FLUOR)    FACTOR     FACTOR

  1    25        .349690               .964476       .291100         -0      MNO
  2    20        .069800               .874575       .399200         -0      CAO
  3    13        .147000               .599711       .889600         -0      AL203
  4    26        .087000               .974452       .286500         -0      FEO
  5    14        .188000               .528008      1.139000         -0      SIO2


              MASS ABSORPTION COEFFICIENTS---MU/RHO

EMITTER= 25     20     13     26     14
ABSORBER
 25       79    286   3419     64   2225
 20      371    139   1669    296   1086
 13      117    432    386     93   3493
 26       89    321   3844     71   2502
 14      145    531    504    115    328
  8       31    116   1505     25    966
```

Figure 11. Output from Program EMX2. First output page showing for each element an identifying number, atomic number, concentration of the element in its standard, the correction factor (R) for the 20 kv operating voltage (see Section IIIA), oxygen factor, silicon factor, and formula of the oxide. Calculated mass absorption coefficients are shown in the lower table.

```
PROBLEM NO.    18    SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966      20 KV



             NUMBER OF
           FLUORESCING
NL     Z      ELEMENTS    ELEMENT NUMBER AND ABSORPTION JUMP RATIO OF FLUORESCING
                                                                          ELEMENTS
 1    25          0
 2    20          0
 3    13          1      5  13.902
 4    26          0
 5    14          0
 6     8         -0



 Z    LAMBDA      EC     SIGMA    OMEGA        U

25    2.1020   6.539    3286.5    .2600    3.059
20    3.3590   4.038    2938.7    .1201    4.953
13    8.3400   1.559    2731.6    .0195   12.827
26    1.9370   7.113    3391.4    .2925    2.812
14    7.1260   1.838    2748.7    .0273   10.881
 8        -0    .827    2694.7    .0018   24.198



LAMBDA = WAVELENGTH OF EMISSION LINE
Z = ATOMIC NUMBER
R = ABSORPTION JUMP RATIO
EC = CRITICAL EXCITATION VOLTAGE (KV)
OMEGA = K FLUORESCENCE YIELD
U = EO/EC
```

Figure 12. Output from Program EMX2. Table showing what elements will fluoresce what other elements and the calculated values of the parameters required for the corrections.

```
PROBLEM NO.    18    SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966      20 K


 NIT     Z        CON      DELCON      F(CHI)    I/I(FL)

   0    25    ,278500
   0    20    ,007315
   0    13    ,094180
   0    26    ,034820
   0    14    ,176000
   0     8    ,378214
   0   TOT    ,969029

   1    25    ,277636   -,000864    ,967478          0
   1    20    ,007258   -,000057    ,881503          0
   1    13    ,115107    ,020927    ,488548    ,004368
   1    26    ,034843    ,000023    ,973821          0
   1    14    ,175498   -,000502    ,529520          0
   1     8    ,395990
   1   TOT   1,006330

   2    25    ,277947    .000311    ,966396          0
   2    20    ,007290    ,000032    ,877580          0
   2    13    ,116129    ,001023    ,484339    ,004176
   2    26    ,034844    ,000001    ,973792          0
   2    14    ,175743    ,000245    ,528780          0
   2     8    ,397283
   2   TOT   1,009235

   3    25    ,277972    ,000025    ,966309          0
   3    20    ,007292    ,000002    ,877322          0
   3    13    ,116197    ,000067    ,484059    ,004172
   3    26    ,034844    ,000001    ,973775          0
   3    14    ,175776    ,000033    ,528680          0
   3     8    ,397389
   3   TOT   1,009470
```

Figure 13. Output from Program EMX2. Correction of a single data point. Columns from left to right are the number of iterations, atomic number, concentration, the change in concentration from the previous estimate, the absorption correction factor and the fluorescence correction factor. Output from EMX gives the first estimate, and three successive iterations are shown.

```
PROBLEM NO,    18    SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966       20 KV

                    CONCENTRATIONS CORRECTED FOR ABSORPTION AND FLUORESCENCE

       TOTAL      25          20          13          26          14          8
     93,3768    18,7288     1,1547     10,9273      8,7990     16.6490     37.1180
     96,1455    18,5739     1,1493     11,1592     10,1428     17,0273     38,0929
     96.5022    18,6034     1,0564     11,3131     10,3927     16.9508     38.1858
     97.8950    18.1859     1.2428     11,4043     11,2786     17.1186     38.6648
     97.1211    18.5622     1.3101     11,2639     10,6667     16,9777     38.3404

     99.8837    16.0280     1.5777     11,4635     14,0524     17,4111     39.3509
     98.8205    18.4510     1.2818     11.3624     11,4714     17.2868     38.9671
     99,6544    19,3027     1.1954     11.5879     11,1720     17.1999     39.1963
     99.6049    18,6856     1.3306     11.4349     11,5640     17,3604     39.2295
     96,8116    21.9537     1.0463     11.1276      7,4876     16.9910     38.2055

     97,6590    18,6423     1.1641     11,2189     10,6568     17,3221     38.6548
     98,9539    22,4654     1,0229     11,3598      7,6522     17,3949     39.0588
     98.2569    21,4451     1,0600     11,2451      8,3259     17.3567     38.8241
     97.5696    21.7993     1,0403     11,0804      7,7861     17.3046     38.5588
     96,9564    22.0603      .8808     11.1623      7,3568     17,1506     38.3456

     98,4979    21,9154     1,0781     11,0927      8,2432     17,3580     38.8105
     99.1520    22,9757     1,0419     11,1640      7,4123     17.4843     39.0738
     97,6577    22,4470     1.0264     11,0772      7,4208     17.1865     38.4998
     97.1199    22.3219      .9370     10.9100      7,3624     17.2519     38.3367
     98,2413    25.4750      .8093     11,0863      4,6991     17.4026     38.7691

     99.9853    25,2997      .8614     11.6012      5,1925     17.5380     39.4925
    100.8515    26.5903      .7972     11,4786      4,5605     17.6944     39.7305
    101.2307    24,9433      .9127     11,6692      6,0422     17.7306     39.9326
    100.2286    25,9674      .8111     11.5013      5,0323     17.4663     39.4503
    100.3386    24.5256      .9095     11.5202      6,2801     17.5563     39.5468

    101.0406    27,4685      ,7035     11.6526      3,6556     17.7046     39.8559
    100,9470    27.7972      ,7292     11.6197      3,4844     17.5776     39.7389
     98.9010    26,6034      .7529     11,3837      3,9621     17.2473     38,9516
     98.1012    26.6759      .7272     11.3295      3,7342     17.0314     38.6030
     96,2212    26,9678      ,6489     11,0179      2,8647     16.8257     37.8961

     96,6407    26.6923      ,6313     11,0732      3,0250     17.0544     38.1645
     95.8910    27.7789      ,5736     10.9251      2,0727     16.7894     37.7513
     95,4990    25,9379      .6497     11,0479      3,1093     16.9357     37.8186
     94,7149    27,2225      ,5648     10,7778      2,0112     16.7482     37.3903
     94,6782    26.6446      .5578     10,6243      2,8375     16.7231     37.2908

     95.3665    27,4145      .4743     10,7855      1,9065     17,0524     37.7333
     94,5974    28,6018      ,4945     10,7242       ,8421     16.6573     37.2775
     96,6447    27,1306      ,6296     10,8672      2,7010     17,1696     38,1466
     96.3126    26,7688      ,6261     10,8474      3,2166     16.9424     37.9112
     96.1899    28,4059      ,4605     10,8219      1,2692     17,1991     38.0333

     97,7583    26,4536      .6988     11,3771      3,6209     17.0500     38.5580
     97.4588    28,5788      .5460     11,2490      1,0957     17,3591     38.6303
     98.9293    29,7418      .4372     11,4558       ,7668     17.4308     39.0969
     97.7847    29,0691      .5638     11,3884       ,9550     17,1653     38.6431
     98.9956    29,2985      ,5521     11,5592       ,9335     17,4626     39.1896
```

Figure 14. Output from Program EMX2. Concentrations in weight percent identified by atomic number after correction for absorption and fluorescence.

```
PROBLEM NO.    18    SPESSARTINE RUTHERFORD PEGMATITE ARCH MAR 1966      20 KV

                         CONCENTRATIONS CORRECTED FOR ABSORPTION AND FLUORESCENCE

          TOTAL  MNO          CAO          AL203       FEO          SI02
         93.3768    24,1808      1.6157     20,6482     11,3199     35.6122
         96.1455    23,9808      1.6081     21,0864     13,0488     36.4214
         96,5022    24,0189      1.4781     21,3772     13,3703     36,2577
         97,8950    23.4798      1,7390     21,5496     14,5099     36.6167
         97.1211    23.9657      1,8331     21,2843     13,7228     36.3152

         99.8837    20.6938      2.2076     21,6615     18,0784     37.2424
         98.8205    23.8220      1.7935     21,4704     14,7580     36.9766
         99.6544    24,9218      1.6727     21,8966     14,3728     36,7906
         99.6049    24.1249      1,8617     21,6073     14,8770     37.1338
         96.8116    28,3444      1.4640     21.0267      9,6328     36.3437

         97.6590    24,0690      1.6288     21.1992     13,7100     37.0520
         98,9539    29.0051      1.4312     21,4654      9,8445     37,2076
         98.2569    27.6878      1.4832     21.2487     10,7112     37.1261
         97.5696    28.1451      1.4556     20.9375     10,0169     37.0145
         96.9564    28.4821      1.2325     21.0922      9,4645     36,6851

         98.4979    28,2950      1.5084     20.9608     10,6049     37,1288
         99.1520    29.6640      1.4578     21.0954      9,5360     37.3988
         97.6577    28.9813      1.4361     20,9314      9,5469     36,7620
         97.1199    28,8198      1.3111     20,6156      9,4717     36.9017
         98.2413    32,8907      1,1324     20,9486      6,0453     37.2242

         99.9853    32,6645      1.2053     21,9216      6,6802     37,5138
        100.8515    34.3307      1.1155     21.6899      5,8671     37,8483
        101.2307    32.2043      1.2771     22,0502      7,7733     37,9258
        100.2286    33.5265      1.1350     21,7328      6,4740     37.3603
        100.3386    31,6650      1.2726     21,7686      8,0794     37.5530

        101.0406    35,4646       .9843     22.0187      4,7029     37,8702
        100.9470    35,8889      1.0203     21,9565      4,4827     37,5986
         98,9010    34,3477      1,0534     21,5107      5,0972     36,8920
         98.1012    34,4412      1,0175     21,4083      4,8041     36,4301
         96.2212    34,8181       .9080     20.8195      3,6854     35,9902

         96,6407    34,4625       .8833     20,9239      3,8916     36,4794
         95,8910    35.8654       .8026     20,6441      2.6665     35.9124
         95.4990    33.4884       ,9090     20,8761      4,0001     36.2254
         94.7149    35,1470       .7903     20,3657      2,5875     35.8244
         94.6782    34.4009       .7805     20,0757      3,6505     35,7707

         95,3665    35,3949       .6636     20.3802      2,4527     36.4751
         94.5974    36,9277       .6919     20,2644      1,0834     35,6299
         96.6447    35.0284       .8810     20,5347      3,4749     36.7258
         96.3126    34,5512       .8761     20.4973      4,1381     36.2399
         96.1899    36,6749       ,6443     20.4490      1,6328     36,7889

         97,7583    34.1542       .9778     21.4982      4,6583     36.4699
         97.4588    36,8981       ,7639     21,2561      1,4096     37.1311
         98,9293    38,3997       .6117     21,6470       ,9865     37,2844
         97,7847    37,5311       .7889     21,5196      1,2286     36,7165
         98,9956    37,8273       .7725     21,8423      1,2010     37.3525
```

Figure 15. Output from Program EMX2. Concentrations expressed as oxides.

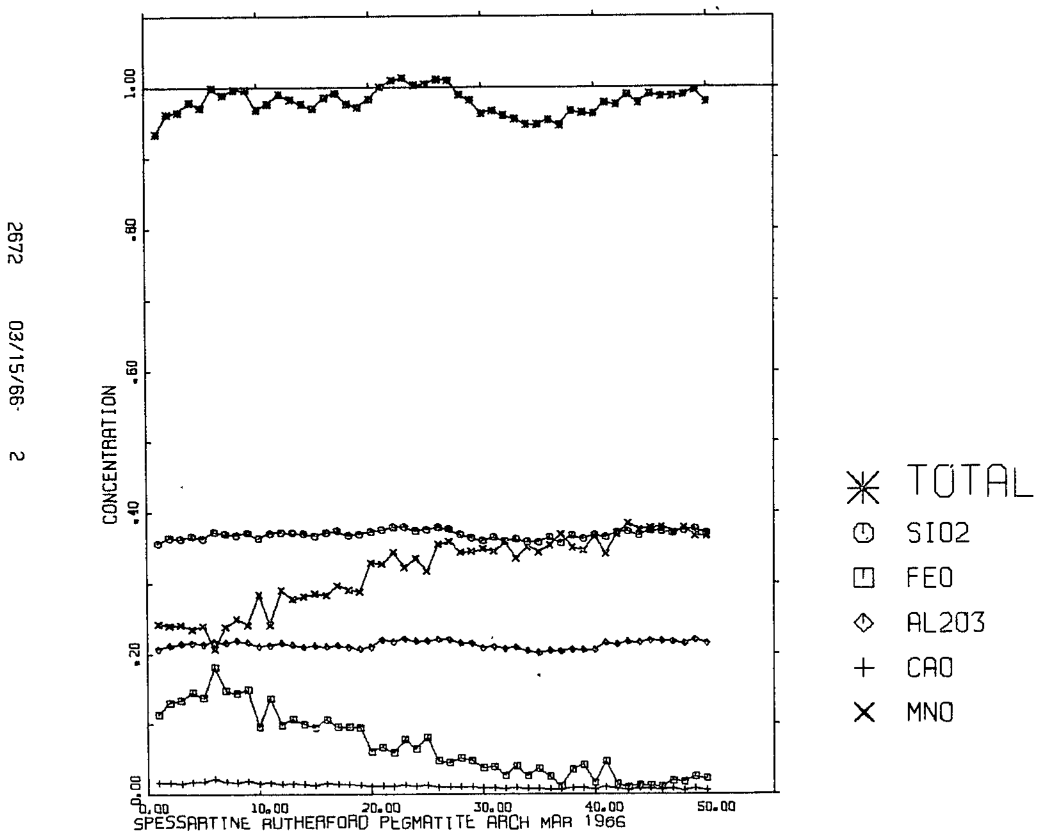

Figure 16. Output from Program EMX2. Plot of concentrations of oxides after correction. Similar plots can be obtained as the output of Program EMX. The analytical data in this problem are from Sinkankas and Reid (6).

```
      PROGRAM EMX
      COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),TAU(9),
     1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
     2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
     3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
     4   YMAX, O(9), SI(9)
      COMMON/1775/CON(500,9),DINFO(200,7),NLD(200,3)                      4500
      EQUIVALENCE(TIME,XINFO), (CON,DINFO),(CON(1401),NLD),(NAME2,TIME),
     1   (TOTAL,CURRENT)
      DEAD(T,OC) = OC/(1.0 - OC*T)
      NPAGE = 0
      JB = 2223642020202020B
C
C READ AND AVERAGE DATA FOR ONE PROBLEM
C
    1 CALL EMXINPUT (XMAX)
      IF(ISTOP) 95,2
    2 IF(.NOT.NS)55,3
    3 CALL EMXHEAD
      PRINT 200
  200 FORMAT(25X,13HAVERAGED DATA/)
      PRINT 201
  201 FORMAT(15X,6H  REL.,16X,14HSPECTROMETER 1,
     1  11X,14HSPECTROMETER 2,11X,14HSPECTROMETER 3/15X,16H  TIME    CURR
     2ENT,3X,3(17HCTS/SEC      SIGMA,8X)/)
C
C FIND RELATIVE TIME, PRINT AVERAGED DATA AND STANDARD DEVIATIONS.
C
      DO 5 M = 2,MNUM
      M1 = NUM(M-1)
      M2 = NUM(M) - 1
      T = 0.0
      DO 4 I = M1,M2
      T = T + TIME(I)
      TIME(I) = T - .5*TIME(I)
      PRINT 205, I, NAME(I), TIME(I), CURRENT(I), (COUNTS(I,J), ERR(I,J
     1   ), KD(I,J), NL(I,J),J=1,3)
  205 FORMAT(I5,2X,A8,F6.0,F10.4,3(F10.1,F10.1,I3,I2))
      IF(XMODF(I,50))4,21
   21 CALL EMXHEAD
      PRINT 200
      PRINT 201
    4 CONTINUE
    5 PRINT 310
  310 FORMAT ()
      IF(.NOT.NR)56,53
   53 IA= 0
   55 CALL EMXHEAD
      IFIRST = IA+ 1
      PRINT 203
      PRINT 201
  203 FORMAT(14H0DEADTIME DATA)
      DO 54 IA= IFIRST,NR
      PRINT 204, DINFO(IA),DINFO(IA,2),DINFO(IA,5),NLD(IA),DINFO(IA,3),
     1   DINFO(IA,6),NLD(IA,2),DINFO(IA,4),DINFO(IA,7),NLD(IA,3)
  204 FORMAT(21X,F10.4,3(2F10.1,I5))
      IF(.NOT.XMODF(IA,50))55,54
   54 CONTINUE
C
C COMPUTE DEADTIME CORRECTION COEFFICIENTS WHERE NECESSARY AND CORRECT FOR
```

```
C DEADTIME
C
   56 LAST = NUM(MNUM) - 1
      DO 7 L = 1,NEL
      ENCODE (5,320,NP(L))NO(L)
  320 FORMAT(2X,I3)
      KEY(L) = 0
      IF(TAU(L))7,6
    6 CALL DEADTIME(L, XMAX)
    7 CONTINUE
      IF(.NOT.NS)1,17
   17 DO 13 NN = 1,NEL
      JLAST = 3
      MM = NN
      IF(TAU(NN).LT.0.0)13,8
    8 IF(TAU(NN).LT.1.0)10,9
    9 MM = TAU(NN)
   10 TT = TAU(MM)
      DO 15 JX= 1,JLAST
      DO 15 IX= 1,LAST
      IF(NL(IX,JX).NE.NN)15,11
   11 JLAST = JX
      COUNTS(IX,JX) = DEAD(TT,COUNTS(IX,JX))
   15 CONTINUE
   13 CONTINUE
      CALL EMXHEAD
      PRINT 275
  275 FORMAT(25X,34HDATA AFTER CORRECTION FOR DEADTIME/)
      PRINT 201
      PRINT 276, (I3, (COUNTS(I3,J3),ERR(I3,J3),J3=1,3),I3=1,LAST)
  276 FORMAT (I5,26X,3(2F10.1,5X))
C
C FIND TWO SUCCESSIVE STANDARDS AND INTERPOLATE BETWEEN TO CORRECT FOR DRIFT
C
      DO 35 MX= 2,MNUM
      M1X= NUM(MX-1)
      M2X = NUM(MX) - 1
      DO 35 JJ= 1,3
      DO 16 I1 = M1X,M2X
      IF(KD(I1,JJ).EQ.2.AND.NL(I1,JJ))18,16
   16 CONTINUE
      GO TO 35
   18 I2 = I1 + 1
      NL1 = NL(I1,JJ)
   20 DO 22 I4= I2,M2X
      IF(KD(I4,JJ).EQ.2.AND.NL(I4,JJ).EQ.NL1)24,22
   22 CONTINUE
      GO TO 35
   24 I2 = I4
      CALL DRIFT (I1,I2,JJ,IFLAG)
      K1 = I2 + 1
      IF(KD(K1,JJ).NE.2)28,27
   27 I1 = K1
      GO TO 18
   28 IF(IFLAG)30,32
   30 I2 = K1 + 1
      GO TO 20
   32 I1 = I2
      GO TO 18
   35 CONTINUE
```

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```
      CALL EMXHEAD
      PRINT 277
  277 FORMAT(25X,31HDATA AFTER CORRECTION FOR DRIFT/)
      PRINT 201
      PRINT 276, (I5,(COUNTS(I5,J5),ERR(I5,J5),J5=1,3),I5=1,LAST)
C
C SUBTRACT BACKGROUND FROM SAMPLES AND STANDARDS
C
      CALL RKGD(1)
      CALL BKGD(3)
   37 CALL FMXHEAD
      PRINT 210
  210 FORMAT(25X,60HCONCENTRATIONS CORRECTED FOR DEADTIME, DRIFT, AND BA
     1CKGROUND//                                21X,36HSAMPLE CORRECTED   CONC
     1EN-  RELATIVE/6X,51HE     SAMPLE   CURRENT   CTS/SEC   TRATION
     2ERROR/)
      DO 39 JP= 1,3
      DO 38 IP= 1,LAST
   38 ERR(IP,JP) = ERR(IP,JP)/COUNTS(IP,JP)
      DO 39 IQ = 1,500
   39 CON(IQ,JP) = 0.0
      DO 50 MY= 2,MNUM
      M1Y= NUM(MY-1)
      M2Y = NUM(MY) - 1
      DO 50 JY= 1,3
      DO 40 NNN= 1,NEL
      DO 400IY= M1Y,M2Y
      IF(KD(IY,JY).EQ.2.AND.NL(IY,JY).EQ.NNN)42,400
  400 CONTINUE
   40 CONTINUE
      GO TO 50
   42 STD = 1.0/COUNTS(IY,JY)
      SE = ERR(IY,JY)**2
      PRINT 310
      PRINT 213, IY,NNN,JB,CURRENT(IY),COUNTS(IY,JY),WTPC(NNN),FRR(IY,JY)
     1    )
  213 FORMAT (I5,I2,2X,A8,F10.4,F10.1,F10.5,F10.3)
      DO 45 IZ = M1Y,M2Y
      IF(KD(IZ,JY).OR.NL(IZ,JY).NE.NNN)45,43
   43 KN = KEY(NNN) = KEY(NNN) + 1
      IF(KN.LE.500)44,430
  430 PRINT 240,NNN
  240 FORMAT(//55H DIMENSION EXCEEDED----FURTHER DATA OMITTED FOR ELEMEN
     1T,I3//)
      GO TO 40
   44 CON(KN,NNN) = COUNTS(IZ,JY)*STD*WTPC(NNN)
      NAME2(KN) = NAME(IZ)
      E = SQRTF(ERR(IZ,JY)**2 + SE)
      PRINT 213, IZ,NNN,NAME(IZ),CURRENT(IZ),COUNTS(IZ,JY),CON(KN,NNN),E
   45 CONTINUE
      GO TO 40
   50 PRINT 310
      KEY1 = KEY2 = KEY(1)
      DO 58 JZ= 2,NEL
      IF(KEY(JZ).EQ.KEY2)58,57
   57 PRINT 250, JZ
  250 FORMAT(////77H NUMBER OF SAMPLE DATA POINTS OF ELEMENT 1 DOES NOT
     1EQUAL NUMBER FOR ELEMENT ,I1)
      KEY2 = XMAX0F(KEY2,KEY(JZ))
   58 CONTINUE
```

```
      DO 62 I = 1,KEY2
      TOTAL(I) = 0.0
      DO 60 J = 1,NEL
   60 TOTAL(I) = TOTAL(I) + CON(I,J)
   62 CONTINUE
      CALL PPLOT (NP)
      DO 72 I = 1,KEY2
      DO 71 J = 1,NEL
      IF(CON(I,J).LT.0.0)69,71
   69 CON(I,J) = 0.0
   71 CONTINUE
   72 WRITE (3,214) NAME2(I),(CON(I,J),J=1,NEL)
  214 FORMAT(A8,9(3PE8.0))
      END FILE 3
      IF(IOX)91,1
   91 DO 92 IC= 1,KEY2
      TOTAL(IC)= 0.0
      DO 92 JC= 1,NEL
      CON(IC,JC) = CON(IC,JC)*(1.0 + O(JC) + SI(JC))
   92 TOTAL(IC) = TOTAL(IC) + CON(IC,JC)
      CALL PPLOT (NOM)
      GO TO 1
   95 END FILE 3
      END
      SUBROUTINE EMXINPUT (XMAX)
      COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),TAU(9).
     1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
     2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
     3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
     4   YMAX, O(9), SI(9)
      COMMON/1775/DINFO(200,7),NLD(200,3),DUMMY(1995),X(101,5)          4500
      EQUIVALENCE (TIME,XINFO), (NAME2,TIME),(TOTAL,CURRENT)
C
C THIS SUBROUTINE READS DATA FOR ONE PROBLEM AND CALLS S.R. EMXSUM TO AVERAGE
C
      ICHECK = 1111111111112020B
    1 READ 100, NPROB, ID, NEL, NDT, NS, MBKGD, SLIMIT, IG, XMAX,YMAX
  100 FORMAT (I6,6A8,4I2,F3.0,I2,2F3.0)
      IF(NPROB)5,3
    3 ISTOP = 1
      RETURN
    5 CALL EMXHEAD
      ISTOP = IOX = 0
      PRINT 200, NEL, NDT, NS, MBKGD, SLIMIT
  200 FORMAT (18H NO. OF ELEMENTS =,I2/I3,26H DEADTIME READINGS PER SET/
     1   I3,24H SAMPLE READINGS PER SET/28H BACKGROUND READING METHOD =,
     2I2/39H SIGMA FOR STANDARD PEAK MAY NOT EXCEED, F5.1,11H * SQRTF(N)
     3   ///10X,50HATOMIC   PER CENT W          TAU    OXYGEN   SILICON/
     4   60H ELEMENT  NUMBER  OF STANDARD                  FACTOR    FACTOR
     5   /)
      READ  102,(NO(I),WTPC(I),TAU(I),O(I),SI(I),NOM(I),I=1,NEL)
  102 FORMAT(1X,I3,F6.0, E15.5,2F10.0,5X,A5)
      PRINT 202, (I,NO(I),WTPC(I),TAU(I),O(I),SI(I),NOM(I),I=1,NEL)
  202 FORMAT (I5,I9,5X,2PF10.6,0PE11.2,2F10.5,5X,A5)
      DO 907 I = 1,NEL
      IF(O(I))908,907
  907 CONTINUE
      GO TO 1111
  908 IOX = 1
      DO 909 I = 1,NEL
```

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```
     IF(SI(I))1000,909
 909 CONTINUE
     GO TO 1111
1000 IOX = -IOX
1111 CONTINUE
     CALL EMXHEAD
     PRINT 204
 204 FORMAT(25X,11H INPUT DATA/5X,68H       NAME       TIME    CURRENT
    1SPEC 1     SPEC 2     SPEC 3     KODE/)
     N = NR = 0
     IB = 1212121212122020B
     M = NUM(1) = 1
   7 N = N + 1
     IF(N.GT.800)90,8
   8 READ (2,104) (X(1 ,J),J=1,5),KODE,NAME(N)
 104 FORMAT (F6.2,F6.3,3F6.0,A6,A8)
   9 IF(KODE.EQ.ICHECK)96,10
  10 IF(KODE.NE.IB)12,11
  11 M = M + 1
     PRINT 310
 310 FORMAT()
     NUM(M) = N
     IF(M.EQ.25)96,8
  12 PRINT 206, N, NAME(N), (X(1,J),J=1,5), KODE
 206 FORMAT (I5,2X,A8,F10.2,F10.3,3F10.0,2X,A6)
     DECODE (8,300,KODE) (KD(N,J), NL(N,J),J=1,3)
 300 FORMAT (6I1, 2X)
     IF(KD(N).GE.2)25,13
  13 IF(NS.NE.1)17,14
  14 XINFO(N) = X
     X = 1.0/X
     DO 15 J = 1,3
     K = J + 2
  15 ERR(N,J) =   SQRTF(X(1,K))*X
     DO 16 J = 2,5
  16 XINFO(N,J) = X(1,J)*X
     GO TO 7
  17 DO 20 I = 2,NS
     READ (2,104) (X(I,J),J=1,5),JKODE,JUNK
     PRINT 206, N, JUNK, (X(I,J),J=1,5),JKODE
     IF(JKODE.EQ.KODE)20,19
  19 PRINT 208
 208 FORMAT(//51H ERROR IN GROUPING DATA--FURTHER PROCESSING DELETED)
  65 IF(JKODE.EQ.ICHECK)1,95
  20 CONTINUE
     CALL EMXSUM (N, NS)
     GO TO 7
  25 IF(KD(N).NE.4)28,26
  26 NR = NR + 1
     IF(NR.GT.200)90,27
  27 DO 50 I = 2,NDT
     READ (2,104) (X(I,J),J=1,5),JKODE,JUNK
     PRINT 206, NR,JUNK, (X(I,J),J=1,5),JKODE
     IF(JKODE.NE.KODE)19,50
  50 CONTINUE
     CALL EMXSUM (N,NDT)
     DO 55 J = 1,7
     K = J + 1
  55 DINFO(NR,J) = XINFO(N,K)
     DO 60 J = 1,3
```

```
   60 NLD(NR,J) = NL(N,J)
      GO TO 8
   28 DO 61 J = 1,3
      IF(KD(N,J).EQ.2)62,61
   61 CONTINUE
      GO TO 13
   62 I = 1
   29 I = I + 1
      IF(I.GT.101)90,30
   30 READ (2,104) (X(I,J),J=1,5),JKODE,JUNK
      IF(JKODE.NE.KODE)31,75
   75 PRINT 206, N, JUNK, (X(I,J),J=1,5),JKODE
      GO TO 29
   31 NX = I - 1
      CALL EMXSUM (N, NX)
      IF(.NOT.ISTOP)32,64
   64 ISTOP =0
      GO TO 65
   32 KODE = JKODE
      N = N + 1
      IF(N.GT.800)90,42
   42 NAME(N) = JUNK
      DO 43 J = 1,5
   43 X(1,J) = X(I,J)
      GO TO 9
   90 PRINT 250
  250 FORMAT (///52H ERROR--DIMENSION EXCEEDED--DATA CANNOT BE PROCESSED
     1/)
   95 READ 150, JKODE
  150 FORMAT(30X,A6)
      IF(JKODE.EQ.ICHECK)1,95
   96 MNUM = M + 1
      NUM(MNUM) = N
      END
      SUBROUTINE EMXHEAD
      COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),DCA(9),
     1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
     2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26);MNUM,NAME(800),
     3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
     4   YMAX, O(9), SI(9)
      EQUIVALENCE (TIME,XINFO), (NAME2,TIME),(TOTAL,CURRENT)
C
C PAGE HEADING ROUTINE
C
      NPAGE = NPAGE + 1
      PRINT 200, NPROB, ID, NPAGE
  200 FORMAT(12H1PROBLEM NO. I6,5X,6A8,30X,4HPAGE I3/)
      END
      SUBROUTINE EMXSUM (NY,NX)
      COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),DCA(9),
     1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
     2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
     3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
     4   YMAX, O(9), SI(9)
      COMMON/1775/DUMMY(3990),SUM(5),X(101,5)                                4500
      EQUIVALENCE (TIME,XINFO), (NAME2,TIME),(TOTAL,CURRENT)
C
C THIS SUBROUTINE AVERAGES DATA SETS, COMPUTES STANDARD DEVIATIONS,
C AND CONVERTS TO COUNTS PER SECOND.
C
```

```
      N = NY
      XN = FLOATF(NX)
      DO 5 JJ= 1,5
      SUM(JJ)= 0.0
      DO 5 I = 1,NX
    5 SUM(JJ) = SUM(JJ) + X(I,JJ)
      TIME(N) = SUM
      X = 1.0/SUM
      CURRENT(N) = SUM(2)*X
      DO 20 J = 1,3
      K = J + 2
      IF(NL(N,J))9,7
    7 COUNTS(N,J) = ERR(N,J) = 0.0
      GO TO 20
    9 TEST = SQRTF(SUM(K))*X
      S = SUM(K)/XN
      DEV = 0.0
      DO 10 I = 1,NX
   10 DEV = DEV + (X(I,K) - S)**2
      DEV = SQRTF(DEV)*X
      IF(KD(N,J).NE.2)15,11
   11 IF(DEV.LE.SLIMIT*TEST)15,12
   12 DEV = DEV/TEST
      PRINT 200,DEV
  200 FORMAT(////32H SCATTER IN STANDARD READING IS ,F4.1,33H * SQRTF(N)
     1--FURTHER DATA OMITTED////)
      ISTOP = 1
      RETURN
   15 ERR(N,J) = MAX1F(DEV,TEST)
      XINFO(N,K) = SUM(K)*X
   20 CONTINUE
      END
      SUBROUTINE DEADTIME(N, XMAX)
      COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),TAU(9),
     1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
     2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
     3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
     4   YMAX, O(9), SI(9)
      COMMON/1775/DINFO(200,7),NLD(200,3),DELY(200),Y(200),B(2),SB(2),
     1   DUMMY(2096)                                                    4500
      EQUIVALENCE (DCTS,DINFO(201)),  (DE,DINFO(801))
      EQUIVALENCE (TIME,XINFO), (NAME2,TIME),(TOTAL,CURRENT)
      DIMENSION DCTS(200,3),DE(200,3)
      DO 5 J = 1,3
      DO 5 I1 = 1,NR
      IF(NLD(I1,J).EQ.N)6,5
    5 CONTINUE
      PRINT 250, N
  250 FORMAT(///29H NO DEADTIME DATA FOR ELEMENT,I2,38H---NO DEADTIME CO
     1RRECTION WILL BE MADE)
      TAU(N) = -1.0
      RETURN
    6 I2 = I1 + 1
        DO 8 I = I2,NR
      IF(NLD(I,J).EQ.N)8,10
    8 CONTINUE
      I2 = NR
      ND = NR - I1 + 1
      GO TO 11
   10 I2 = I - 1
```

```
      ND = I - I1
   11 DO 15 I = I1,I2
      DCTS(I,J) = DCTS(I,J)/DINFO(I)
   15 DE(I,J) = (DINFO(I)/DE(I,J))**2
      CALL EMXHEAD
      CALL LSQ (ND,1,SIG,DINFO(I1),DCTS(I1,J),DE(I1,J),Y(I1). DELY,B,SB)
      TAU(N) = -B(2)/B**2
      PRINT 200, NO(N), J, TAU(N)
  200 FORMAT(////13H FOR ELEMENT ,I2,16H ON SPECTROMETER,I2,
     1    8H, TAU = ,E9.2,8H SECONDS)
      DX = XMAX*.10
      DY = .125*B
      DIV = 100. * XMAX
      CALL CCAXIS (0.,0.,14HCOUNTS/CURRENT,14,8.,90.,0.,DY,12.5)
      CALL CCAXIS(0.,8.,20HCURRENT (MICRO-AMPS),-20,10.,0.,0.,DX,-DIV)
      CALL CCAXIS (10.,0.,14 ,-1,8.,90.,0.,DY,-12.5)
      CALL CCAXIS (0.,0.,20HCURRENT (MICRO-AMPS),-20,10.,0.,0.,DX,DIV)
      CALL CCSYMBOL (1.,10.,.21,ID,0.,48)
      CALL P2LINE (DINFO(I1),DCTS(I1,J),ND,1,-1,3,.07,0.0,DX,0.0,DY)
      YNEW = (B + XMAX*B(2))/DY
      CALL CCPLOT (10.,YNEW,3)
      CALL CCPLOT (0.,8.,2)
      CALL CCPLOT (0,0,-3)
      END
      SUBROUTINE LSQ (M,IW,SIGMA,X,F2,W,Y,DELY,B,SB)
C
C    SHORT VERSION OF E2 UCSD LSQPOL--FOR FITTING WITH STRAIGHT LINE ONLY.
C    FTN 63
C    JANUARY. 1966
C
      DIMENSION S(2), X(200), F2(200), ST(2), SB(2), F(200), PM(200),
     1    P(200), B(2), DELY(200), W(200), A(2,2), T(2), Y(200)
      LL = 0
      A = A(2,2) = 1.0
      FBAR = XBAR = FM = 0.0
      DO 10 I = 1,M
      IF(IW)1009,1010
 1010 W2 = W(I) = 1.0
      GO TO 1011
 1009 W2 = SQRTF(W(I))
 1011 FM = FM + W(I)
      F(I) = W2*F2(I)
      PM(I) = W2
      FBAR = FBAR + F(I)*PM(I)
   10 XBAR = XBAR + X(I)*PM(I)**2
      XBAR = XBAR/FM
      T(1) = FBAR/FM
      A(2,1) = -XBAR
      PXF = PXP = 0.0
      DO 20 I = 1,M
      P(I) = (X(I) - XBAR)*PM(I)
      PXF = PXF + P(I)*F(I)
   20 PXP = PXP + P(I)**2
      T(2) = PXF/PXP
      S(1) = PMXPM = FM
      B(1) = T(1) *A(1,1) + T(2)*A(2,1)
      B(2) = T(2)*A(2,2)
  165 SIG2 = 0.0
      DO 180 I = 1,M
      Y(I) = B(1) + B(2)*X(I)
```

2243

```
 175 DELY(I) = Y(I) - F2(I)
 180 SIG2 = SIG2 + (DELY(I)**2)*W(I)
     SIG2 = SIG2/(M - 2)
     SIGMA = SQRTF(SIG2)
     S(2) = PXP
     DO 499 I = 1,2
 499 ST(I) = SIGMA/SQRTF(S(I))
     DO 501 I = 1,2
     SB(I) = 0.0
     DO 500 J = 1,2
 500 SB(I) = SB(I) + (A(J,I)*ST(J))**2
 501 SB(I) = SQRTF(SB(I))
 192 PRINT 1,(I,B(I),SB(I),I=1,2)
   1 FORMAT (36H0COEFFICIENTS OF Y=B1+B2X AND ERRORS//    2(3H B(I2,
    1    2H)=E15.7,6H ERRB=E10.3))
 185 PRINT 186, SIGMA
 186 FORMAT (8H0SIGMA =E16.7)
 670 PRINT 2, (I,X(I),F2(I),Y(I),DELY(I),W(I),I=1,M)
   2 FORMAT(47H0  I              X(I)              F(I)
    137HY(I)              DELY(I)           W(I)//(I6,5E16.7))
 190 CONTINUE
     END
     SUBROUTINE DRIFT (I1,I2,J,IFLAG)
     COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),DCA(9),
    1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
    2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
    3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
    4   YMAX, O(9), SI(9)
     EQUIVALENCE (TIME,XINFO), (NAME2,TIME),(TOTAL,CURRENT)
     IF(ABSF(COUNTS(I1,J) - COUNTS(I2,J)).LE.MAX1F(ERR(I1,J),ERR(I2,J)
    1  ))90,2
   2 T = TIME(I1)
     CF = (COUNTS(I2,J)/COUNTS(I1,J) - 1.0)/(TIME(I2) - T)
   5 K1 = I1 + 1
     K2 = I2 - 1
     IFLAG = 0
     DO 10 I = K1,K2
  10 COUNTS(I,J) = COUNTS(I,J)/(1.0 + CF*(TIME(I)-T))
     RETURN
  90 PRINT 200, I1,I2,J
 200 FORMAT(//31H DRIFT BETWEEN STANDARDS LINES ,I3,5H AND ,I3,
    1   14H, SPECTROMETER,I2,
    1   51H IS WITHIN COUNTING ERROR--NO DRIFT CORRECTION MADE)
     IFLAG = 1
     END
     SUBROUTINE BKGD (KKD)
     COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),DCA(9),
    1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
    2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
    3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
    4   YMAX, O(9), SI(9)
     EQUIVALENCE (TIME,XINFO), (NAME2,TIME),(TOTAL,CURRENT)
C
C THIS SUBROUTINE LOCATES BACKGROUND READINGS AND SUBTRACTS THEM FROM
C THE APPROPRIATE PEAK.
C
     KODE = KKD
     MODE = KODE - 1
     DO 50 J = 1,3
     DO  50 M = 2,MNUM
```

```
      M1 = NUM(M-1)
      M2 = NUM(M) - 1
      J1 = M1
    3 DO 5 I1 = M1,M2
      IF(KD(I1,J).EQ.KODE.AND.NL(I1,J))8,5
    5 CONTINUE
      GO TO 50
    8 I2 = I1 + 1
      J2 = M2
      NL1 = NL(I1,J)
      DO 10 I = I2,M2
      IF(KD(I,J).EQ.KODE.AND.NL(I,J).EQ.NL1)12,10
   10 CONTINUE
      B = COUNTS(I1,J)
      EBSQ = ERR(I1,J)**2
      GO TO 17
   12 I2 = I
      J2 = I2 + 1
      DO 13 I = J2,M2
      IF(KD(I,J).EQ.KODE.AND.NL(I,J).EQ.NL1)15,13
   13 CONTINUE
      J2 = M2
      GO TO 22
   15 J2 = I - 1
   22 B =  (COUNTS(I1,J) + COUNTS(I2,J))* .5
      EBSQ = (ERR(I1,J)**2 + ERR(I2,J)**2)*.25
   17 IF(.NOT.MBKGD)30,23
   23 DO 25 I = J1,J2
      IF(KD(I,J).NE.MODE.OR.NL(I,J).NE.NL1)25,24
   24 COUNTS(I,J) = COUNTS(I,J) - B
      ERR(I,J) = SQRTF(ERR(I,J)**2 + EBSQ)
   25 CONTINUE
      J1 = J2 + 2
      GO TO 41
   30 DO 35 I = J1,J2
      IF(KD(I,J).EQ.MODE.AND.NL(I,J).EQ.NL1)40,35
   35 CONTINUE
      PRINT 205, I1, I2
  205 FORMAT(//38H NO SAMPLE DATA FOR BACKGROUND, LINES ,I3,I6)
      GO TO 41
   40 COUNTS(I,J) = COUNTS(I,J) - B
      ERR(I,J) = SQRTF(ERR(I,J)**2 + EBSQ)
      J1 = I + 1
   41 IF(J2.GE.M2)50,42
   42 I1 = J2 + 1
      GO TO 8
   50 CONTINUE
      END
      SUBROUTINE PPLOT (N)
      COMMON SLIMIT,NPROB,ID(6),NEL,MBKGD,NR,NO(10),WTPC(10),TAU(9),
     1   NOM(9),TIME(800),CURRENT(800),COUNTS(800,3),ERR(800,3),
     2   XINFO(800,8),KD(800,3),NL(800,3),ISTOP,NUM(26),MNUM,NAME(800),
     3   NAME2(500), KEY(9), NP(9), KEY2, IOX, NS, IG, TOTAL(500),
     4   YMAX, O(9), SI(9)
      COMMON/1775/CON(500,9),DINFO(200,7),NLD(200,3)
      DIMENSION IPREF(9), X(500), N(20)
      EQUIVALENCE(TIME,XINFO), (CON,DINFO),(CON(1401),NLD),(NAME2,TIME),
     1   (TOTAL,CURRENT), (X,ERROR)
      DATA (IPREF = 4,3,5,0,1,2,6,7,9)
      CALL EMXHEAD
```

```
      PRINT 220, (N(L),L=1,NEL)
  220 FORMAT(25X,60HCONCENTRATIONS CORRECTED FOR DEADTIME, DRIFT, AND BA
     1CKGROUND//15X,5HTOTAL,10(5X,A5))
      DO 10 I = 1,KEY2
      PRINT 256, NAME2(I), TOTAL(I),(CON(I,JJ), JJ = 1,NEL)
  256 FORMAT(2X,A8,11(2PF10.4))
      IF(XMODF(I.5))10,5
    5 IF(XMODF(I,45))8,7
    7 CALL EMXHEAD
      PRINT 220, (N(K),K=1,NEL)
      GO TO 10
    8 PRINT 400
  400 FORMAT ()
   10 CONTINUE
   14 IF(IG)15,90
   90 RETURN
   15 IF(N.NE.NP)30,16
   16 IF(IOX)90,30
   30 YLEN = 8.6614
      YYMAX = YMAX*1.1
      XLEN = FLOATF((KEY2+7)/8)
      PX1 = XLEN + 1.0
      PX2 = XLEN + 1.5
      CALL CCPLOT(XLEN+3.0,0,0)
   33 DO 35 IA= 1,KEY2
   35 X(IA) = IA
      PY1 = .8924
      PY2 = .7874
      DX = 8.0
      DY = YYMAX/YLEN
      DO 40 J = 1,NEL
      CALL P2LINE (X, CON(1,J), KEY(J), 1,1,IPREF(J),.07,0.0,DX.0.0.DY)
      CALL CCSYMBOL (PX1,PY1,.21,IPREF(J),0.0,-1)
      CALL CCSYMBOL (PX2,PY2,.21,N(J),0.0,5)
      PY1 = PY1 + .5
      PY2 = PY2 + .5
   40 CONTINUE
      CALL P2LINF (X, TOTAL, KEY2, 1,1,11,.07,0.0,DX,0.0,DY)
      CALL CCSYMBOL (PX1,PY1  ,.35,11,0.0,-1)
      CALL CCSYMBOL (PX2,PY2,  .35,5HTOTAL,0.0,5)
      CALL CCAXIS (0.,0.,60HCONCENTRATIONS CORRECTED FOR DEADTIME, DRIFT
     1, AND BACKGROUND,60,YLEN,90.0,0.0,DY,12.7)
      CALL CCAXIS (XLEN,0.,ID,8,YLEN,90.,0.,DY,-12.7)
      CALL CCAXIS (0.,7,874,ID,-48,XLEN,0.0,0.0,8.0 ,-8.0)
      CALL CCAXIS (0.,0.,ID,-48,XLEN,0.0,0.0,8.0 ,8.0)
      CALL CCAXIS (0.,YLEN ,ID,-48,XLEN,0.0,0.0,8.0 ,-8.0)
      DO 50 IC= 1,KEY2
      IF(NAME2(IC).EQ.1H )50,45
   45 PX = X(IC)*,125
      CALL CCSYMBOL (PX,YLEN,.14,NAME2(IC),45.,8)
   50 CONTINUE
      CALL CCPLOT(0,0,-3)
      END
      SUBROUTINE P2LINE(X,Y,N,K,J,L,H,XMIN,DX,YMIN,DY)
CLINE   VERSION 5 COPYRIGHT 1964 CALIFORNIA COMPUTER PRODUCTS           LINE0010
      DIMENSION X(1), Y(1)
C                                                                       LINE0030
C             X  IS THE NAME OF THE ARRAY OF ORDINATE VALUES.(SEE NOTE) LINE0040
C             Y  IS THE NAME OF THE ARRAY OF ABSCISSA VALUES.(SEE NOTE) LINE0050
C             N  IS THE NUMBER OF POINTS IN THE ARRAY                   LINE0060
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C             K   IS THE REPEAT CYCLE OF A MIXED ARRAY (NORMALLY = 1).    LINE0070
C             J   IS THE ALTERNATE NUMBER OF DATA POINT TO PLOT A SYMBOL.LINE0080
C                  J WILL = 0 FOR LINE PLOT,NEGATIVE FOR POINT PLOT,      LINE0090
C                  J = 1 FOR POINT FOR EVERY DATA POINT,2 FOR EVERY OTHERLINE0100
C             L   IS AN INTEGER DESCRIBING SYMBOL TO BE USED, SEE SYMBOL LINE0110
C                  ROUTINE FOR LIST                                       LINE0120
C                                                                         LINE0160
      NP = N * K + 1                                                      LINE0170
      NQ = NP + K                                                         LINE0180
      NO = NP - K                                                         LINE0190
      I3 = 3                                                              LINE0240
      CALL CCWHERE(XN,YN)                                                 LINE0250
      I2 = -1                                                             LINE0260
      XN = XN * DX + XMIN                                                 LINE0270
      YN = YN * DY + YMIN                                                 LINE0280
      DX1 = ABSF(X(1)-XN)                                                 LINE0290
      DY1 = ABSF(Y(1)-YN)                                                 LINE0300
      DX2 = ABSF(X(NO)-XN)                                                LINE0310
      DY2 = ABSF(Y(NO)-YN)                                                LINE0320
      DX1 = MAX1F(DX1,DY1)                                                LINE0330
      DX2 = MAX1F(DX2,DY2)                                                LINE0340
      KK = K                                                              LINE0350
       NA=NT=J $ IF(NT) 100,101,102
  100 NT=-NT
  102 NA = (N-1)/NT                                                       LINE0370
  101 NA = NA * NT + NT +1 - N                                            LINE0380
      IF (DX1-DX2) 10,10,20                                               LINE0390
   10 NO = 1                                                              LINE0400
      KK = -KK                                                            LINE0410
      NA = NT                                                             LINE0420
   20 NV = 2                                                              LINE0430
      NW = -2                                                             LINE0440
      KL = 2                                                              LINE0450
      IF (J) 30,40,50                                                     LINE0460
   30 NV = 3                                                              LINE0470
      NW = -1                                                             LINE0480
      KL = 1                                                              LINE0490
      GO TO 50                                                            LINE0500
   40 NA = NP                                                             LINE0510
   50 DO 90 I = 1,N                                                       LINE0520
          IF (NA-NT) 65,60,70                                             LINE0530
   60 CALL CCSYMBOL((X(NO)-XMIN)/DX,(Y(NO)-YMIN)/DY,H,L,0.0,I2)           LINE0540
          NA = 1                                                          LINE0550
          GO TO 80                                                        LINE0560
   65     GO TO (75,70),KL                                                LINE0570
   70 CALL CCPLOT((X(NO)-XMIN)/DX,(Y(NO)-YMIN)/DY,I3)                     LINE0580
   75     NA = NA + 1                                                     LINE0590
   80     I3 = NV                                                         LINE0600
          I2 = NW                                                         LINE0610
   90     NO = NO + KK                                                    LINE0620
      RETURN                                                              LINE0630
      END                                                                 LINE0640
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```
      PROGRAM EMX2
      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCF(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      COMMON/PP/NAME2(500), Y(500,20), TOT(500)
      NTOTAL = 5H  TOT
      CALL CONSTANT
    1 NPAGE = IOX = 0
      CALL SETUP
      IF(SCF)9,4
    4 DO 5 I = 1,NEL
    5 CON(I) = SCON(I)
      CALL OXYGEN
      PRINT 200
  200 FORMAT(11X,53H------STANDARD FOR ELEMENT Z------   OXYGEN   SILICO
     1N/94H NL    Z   CONCENTRATION     F(CHI)*(1+FLUOR)   FACTOR    FAC
     2TOR               F(CHI)    I(FL)/I/)
      DO 6 I = 1,NEL
      FCHI = ABSORR(I)
      FL = FLUOR(I)
      SCF(I) = FCHI*(1.0+FL)
      PUNCH 302,  I, NZ(I), SCON(I), SCF(I), O(I), SI(I),NOM(I)
  302 FORMAT(2I5,4F10.6,5X,A5)
    6 PRINT 202,  I, NZ(I), SCON(I), SCF(I), O(I), SI(I), FCHI, FL
  202 FORMAT(I3,I5,F13.6,F20.6,F13.6,F10.6, 10X, 2F10.6)
      GO TO 1
    9 NS = 0
    8 READ (3,100) NAME,(OCON(I), I = 1,NEL)
  100 FORMAT (A8,9E8.0/8X,9E8.0)
      IF(EOF,3)75,7
    7 DO 11 I = 1,NVAR
      CON(I) = OCON(I)
   11 OCON(I) = OCON(I)*SCF(I)
      CALL OXYGEN
      NIT = 0
      CALL PAGE
      PRINT 204, NAME
  204 FORMAT(10X, A8//50H  NIT    Z        CON     DELCON    F(CHI)    I/I(
     1FL)/)
      DO 12 I = 1,NEL
   12 PRINT 206, NIT, NZ(I), CON(I)
  206 FORMAT(2I5,4F10.6)
   16 TOTAL = 0.0
      DO 17 I = 1,NELP2
   17 TOTAL = TOTAL + CON(I)
      IF(IOX)18,20
   18 PRINT 206, NIT, NZ(NELP1), CON(NELP1)
      IF(IOX.GT.0)20,19
   19 PRINT 206, NIT, NZ(NELP2), CON(NELP2)
   20 PRINT 208, NIT,NTOTAL, TOTAL
  208 FORMAT (I5,A5,F10.6)
      IF(NIT.LT.IMIN)26,27
   27 IF(NIT.EQ.IMAX)85,29
   29 DO 31 I = 1,NVAR
      IF(CON(I).GT..01.AND.DELCON(I).GT.DMIN)26,31
   31 CONTINUE
      GO TO 85
   26 PRINT 400
  400 FORMAT()
      NIT = NIT + 1
```

```
      DO 25 I = 1,NVAR
      FCHI = ABSORB(I)
      FL = FLUOR(I)
      CON2 = OCON(I)/(FCHI*(1.0 + FL))
      DELCON(I) = CON2 - CON(I)
      IF (O(I))21,24
   21 CON(NELP1) = CON(NELP1) + DELCON(I)*O(I)
      IF(SI(I))22,24
   22 CON(NELP2) = CON(NELP2) + DELCON(I)*SI(I)
   24 CON(I) = CON2
   25 PRINT 206, NIT, NZ(I), CON2, DELCON(I), FCHI, FL
      GO TO 16
   85 NS = NS + 1
      IF(NS.LE.500)86,60
   60 PRINT 260
  260 FORMAT(///57H DIMENSION EXCEEDED--REMAINING POINTS CANNOT BE CORRE
     1CTED)
   62 READ (3,110)NAME
   10 FORMAT(A8)
      IF(EOF,3)75,62
   86 NAME2(NS) = NAME
      TOT(NS) = TOTAL
      DO 40 J = 1,NELP2
   40 Y(NS,J) = CON(J)
      GO TO 8
   75 CALL PRNTPLOT (NP, NELP2)
      IF(IOX)50,1
   50 DO 76 J = 1,NEL
      XX = 1.0 + O(J) + SI(J)
      DO 76 I = 1,NS
   76 Y(I,J) = Y(I,J)*XX
      CALL PRNTPLOT (NOM,NEL)
      GO TO 1
      END


      SUBROUTINE CONSTANT
      TYPE REAL LAMBDA, MU
      COMMON/DATA/A(92), LAMBDA(92), EDGE(92,7), C(92,8), EXP(92), WAVL,
     1   SINTHETA,  AWK, BWK, CWK, CSIG, XSIG                            DATA
      DATA (A = 1.008,4.003,6.939,9.012,10.810,12.011,14.007,15.999,      A
     1   19.000,20.183,22.990,24.310,26.980,28.090,30.974,32.064,35.453, A
     2   39.948,39.102,40.080,44.960,47.900,50.940,52.,54.94,55.85,58.93 A
     3   ,58.71,63.54,65.37,69.72,72.59,74.92,78.96,79.909,83.8,85.47,    A
     4  87.62,88.905,91.22,92.91,95.94,98.,101.1,102.905,106.4,107.87,    A
     5   112.4,114.82,118.69,121.75,127.6,126.9,131.3,132.905,137.34,     A
     6   138.91,140.12,140.91,144.24,147.,150.35,152.,157.25,158.92,      A
     7   162.5,164.93,167.26,168.93,173.04,174.97,178.49,180.95,183.85,   A
     8   186.2,190.2,192.2,195.09,196.97,200.59,204.37,207.19,208.98)     A
      DATA (A(84) = 210.,210.,222.,223.,226.,227.,232.04,231.,238.03)     A84
      DATA(LAMBDA(5) = 67.6,44.7,31.6,23.62,18.32,14.61,11.91,9.89,8.34, LAMBDA
     1   7.126,6.157,5.373,4.728,4.192,3.742,3.359,3.031,2.749,2.504,     LAMBDA
     2   2.29,2.102,1.937,1.79,1.658,1.541,1.436,1.341,1.255,1.176,1.105 LAMBDA
     3   ,1.04,7.817)                                                    LAMBDA
      DATA (LAMBDA(37)= 7.318,6.863,6.449,6.07,5.724,5.407,5.115,4.846,  LMDA37
     1   4.597,4.368,4.154,3.956,3.772,3.6,3.439,3.289,3.149,3.017,2.892 LMDA37
     2   ,2.776,2.666,2.561,2.463,2.37,2.282,2.2,2.121,2.047,1.977,1.909 LMDA37
     3   ,1.845,1.784,1.727,1.672,1.62,1.57,1.522,1.476,1.433,1.391,     LMDA37
     4   1.351,1.313,1.276,1.313,1.207,1.175,4.909,6(0.),3.941,3.827,   LMDA37
     5   3.716)                                                          LMDA37
      DATA (EXP(3) = 2.88,2.86,2.85,2.84,2.83,2.82,2.81,2.80,2.79,2.79,   EXP
```

```
 1    2.78,2.77,2.77,2.76,2.76,2.75,2.75,2.74,2.74,3(2.73),2(2.72),   EXP
 2    3(2.71),3(2.7),3(2.69),6(2.73),5(2.72),4(2.71),3(2.7),3(2.69),  EXP
 3    3(2.68),3(2.67),2(2.66),3(2.65),2(2.64),2(2.63),2(2.62),2(2.61) EXP
 4    ,2.6,2.6,2.59,2.59,2.58,2.58,2.57,10(2.6))                      EXP
  DATA (EDGE = 9(15.), 14.3,11.569,9.512,7.951,6.745,5.787,5.018,    EDGE
 1    4.379,3.871,3.437,3.07,2.757,2.497,2.269,2.07,1.896,1.743,      EDGE
 2    1.608,1.488,1.38,1.283,1.196,1.117,1.045,.98,.92,6.46,5.998,    EDGE
 3    5.583,5.232,4.867,4.581,4.298,4.06,3.83,3.626,3.428,3.254,3.085EDGE
 4    ,2.926,2.777,2.639,2.511,2.389,2.274,2.167,2.068,1.973,1.889,   EDGE
 5    1.811,1.735,1.665,1.599,1.536,1.477,1.421,1.365,1.317,1.268,    EDGE
 6    1.222,1.182,1.14,1.1,1.061,1.025,.99,.956,.923,.893,.863,.835,  EDGE
 7    .808,.782,3.099,6(0.),2.401,2.313,2.235)                        EDGE
  DATA (EDGE(104) = 16(15.), 14.24, 11.27, 10.3,                      EDGE104
 1                            9.54,8.73,8.107,7.506,6.97,7.21,6.643,   EDG5104
 1    6.172,5.755,5.378,5.026,4.718,4.436,4.18,3.942,3.724,3.514,3.32  EDGE104
 2 6,3.147,2.982,2.83,2.687,2.553,2.429,2.314,2.204,2.103,2.011,       EDGE104
 3    1.924,1.843,1.767,1.703,1.626,1.561,1.501,1.438,1.39,1.338,       EDGE104
 4    1.288,1.243,1.199,1.155,1.114,1.075,1.037,1.001,.967,.934,.903,   EDGE104
 5    .872,.843,.815,3.355,6(0.),2.577,2.479,2.394)                     EDGE104
  DATA (EDGE(214) = 11.87)
  DATA (EDGE(215) = 10.9,9.94,9.124,8.416,7.8,7.43,6.89,6.387,5.961,  EDGE215
 1    5.538,5.223,4.913,4.632,4.369,4.13,3.908,3.698,3.504,3.324,       EDGE215
 2    3.156,3.,2.855,2.719,2.592,2.474,2.363,2.258,2.164,2.077,1.995,   EDGE215
 3    1.918,1.845,1.775,1.71,1.649,1.579,1.535,1.482,1.433,1.386,       EDCE215
 4    1.341,1.297,1.255,1.216,1.177,1.14,1.106,1.072,1.04,1.008,.979,   EDGE215
 5    .95,3.902,6(0.),3.08,2.98,2.882)                                  EDGE215
  DATA (EDGE(308) = 10.2,9.39,8.67,8.,20(10.),9.557,9.042,8.614,      EDGE308
 1    8.188,7.831,7.513,7.178,6.856,6.566,6.292, 6.088,5.82,5.581,      EDGE308
 2    5.366,5.161,4.972,4.753,4.569,4.405,4.231,4.064,3.915,3.774,      EDGE308
 3    3.62,3.482,3.349,3.218,4.808,6(0.),3.745,3.614,3.496)             EDGE308
  DATA (EDGE(401) = 3(10.)), (EDGE(424) = 10.8,10.3,9.642,9.258,      EDGE401
 1    8.773,8.376,8.023,7.642,7.322,7.011,6.715,6.453,6.179,5.931,      EDGE401
 2    5.686,5.475,5.211,5.015,4.823,4.625,4.443,4.273,4.114,3.939,      EDGE401
 3    3.779,3.632,3.484,10.,6(0.),3(10.))                               EDGE401
  DATA (EDGE(611) = 6(10.),9.957,9.528,9.115,8.773,8.433,8.086,7.777 EDGE611
 1    ,7.427,7.128,6.871,6.594,6.357,6.094,5.88,5.629,5.413,5.2,        EDGE611
 2    4.994), (EDGE(518) = 10.4,9.957,9.499,9.115,8.705,8.331,7.997,    EDGE611
 3    7.685,7.383,7.128,6.834,6.559,6.331,6.112,5.861,5.637,5.451,      EDGE611
 4    5.253,5.06,4.873,4.71,4.522,4.349,4.201,4.042)                    EDGE611
  DATA (C(3) = .135,.35,.74,1.35,2.21,3.8,4.9,6.77,9.05,11.75,14.87, C3
 1    18.5,22.5,27.,31.7,36.9,42.5,48.4,55.1,62.1,69.8,78.,86.7,        C3
 2    95.8,105.5,115.9,126.8,138.,149.8,162.2,175.4,189.4,205.,31.25,   C3
 3    33.9,36.5,39.3,42.3,45.5,48.5,52.1,55.6,59.3,63.1,67.3,71.,75.5   C3
 4    ,79.6,84.2,88.5,94.,98.3,103.4,109.,114.4,120.,125.5,132.,        C3
 5    138.5,143.5,150.,157.,163.5,170.5,176.5,184.,192.5,199.,206.,     C3
 6    214.,222.,231.,239.,247.,256.,263.,272.,281.,289.,298.,79.94,     C3
 7     6(0.),109.4,114.5,120.7)                                         C3
  DATA (C(104) = .89,1.18,1.54,1.96,2.43,2.98,3.62,4.31,5.1,5.99,     C104
 1    7.,8.02,9.18,10.45,11.75,13.25,14.8,16.45,18.25,20.2,22.15,       C104
 2    24.25,26.4,28.8,26.7,28.8,31.2,33.5,36.15,38.9,41.45,44.5,47.5,   C104
 3    50.7,53.95,57.5,60.7,64.5,68.,71.95,75.65,80.35,84.,88.4,93.15,   C104
 4    97.8,102.5,107.3,112.8,118.5,122.5,128.,134.,140.,146.,151.,157   C104
 5 .,165.,170.,176.,183.,190.,197.,204.,211.,219.,225.,232.,240.,       C104
 6    247.,255.,68.9,6(0.),94.3,98.7,104.),(C(214)=15,6)                C104
  DATA (C(215) = 17.25,18.95,20.75,22.55,24.6,19.15,20.8,22.4,24.1,   C215
 1    25.95,27.9,29.75,31.95,34.1,36.4,38.7,41.3,43.6,46.3,48.8,51.7,   C215
 2    54.3,57.7,60.3,63.4,66.9,70.2,73.6,77.,81.,85.,88.,92.,96.3,      C215
 3    100.3,104.5,108.5,113.,118.,122.,126.,131.,136.,142.,147.,152.,   C215
 4    157.,161.,167.,172.,177.,183.,57.1,6(0.),78.1,81.8,86.2)          C215
  DATA (C(308)=13.6,14.9,16.2,17.7,5.6,6.1,6.62,7.18,7.78,8.39,9.05,  C308
 1    9.74,10.47,11.24,12.03,12.87,13.76,14.68,15.65,16.66,17.72,       C308
 2    18.82,19.97,21.16,22.41,23.7,25.05,26.47,27.93,29.44,31.01,       C308
```

```
     3   32.63,34.31,36.06,37.86,39.76,41.69,43.69,45.79,47.92,50.13,      C308
     4 52.44,54.79,57.21,59.7,62.27,64.92,67.64,70.55,73.6,76.64.49.3.      C308
     5   6(0.),67.5,70.7,74.5)                                              C308
      DATA (C(401) = 4.28,4.69,5.13), (C(424) = 19.3,20.4,21.6,22.8,        C401
     1   24.1,25.4,26.7,28.1,29.6,31.1,32.6,34.3,35.9,37.7.39.6,41.3,       C401
     2   43.2,45.2,47.2,49.3,51.5,53.7,56.,58.3,60.8,63.5,66.1.25.1,        C401
     3   6(0.),31.3,32.4,33.6), (C(518) = 17.9,18.9,20.,21.,22.2,23.3,      C401
     4   24.5,25.8,27.,28.5,29.8,31.2,32.7,34.2,35.8,37.5,39.1,40.9,        C401
     5   42.6,44.5,46.4,48.3,50.4,52.6,54.7)                                C401
      DATA ( C(611) = 16.3,17.2,18.2,19.1,20.1,21.2,22.3,23.4,24.5,         C611
     1   25.7,27.,28.3,29.6,30.9,32.4,33.8,35.3,36.9,38.4,40.1,41.8,        C611
     2   43.6,45.4,47.3), (C(709)= 14.8,15.3,15.85,16.3,16.85,17.45,        C611
     3   18.,18.55,19.05,19.6,20.1,20.45,21.35,21.95,22.5,23.1,23.8,        C611
     4   24.4)                                                              C611
      SINTHETA = .79335
      AWK = -.064
      BWK = .034
      CWK = -1.03E-6
      WAVL = 12397.7
      CSIG = 2.39E+5
      XSIG = 1.5
      END


      SUBROUTINE SETUP
      TYPE REAL LAMBDA, MU
      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCF(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      COMMON/DATA/A(92), LAMBDA(92), EDGE(92,7), C(92,8), EXP(92), WAVL,
     1   SINTHETA, AWK, BWK, CWK, CSIG, XSIG                              DATA
      DIMENSION X(20),Y(20), CR(20), XR(20)
      READ 100, NPROB, ID, NEL, EO, NFIX, IMIN, IMAX, IG, YMAX, DMIN
      IF(EOF,50)3,5
    3 STOP
    5 CALL PAGE
      PRINT 200
      READ 102, (NZ(I), SCON(I), SCF(I), O(I), SI(I),NOM(I),I=1,NEL)
      PRINT 202, (I,NZ(I),SCON(I),SCF(I),O(I),SI(I),NOM(I),I=1,NEL)
      LF = 1
      NVAR = NEL - NFIX
      DO 7 I = 1,NEL
      IF(O(I))8,7
    7 CONTINUE
      NELP1 = NELP2 = NEL
       GO TO 11
    8 IOX = 1
      NELP1 = NEL + 1
      NZ(NELP1) = 8
      DO 9 I = 1,NEL
      IF(SI(I))10,9
    9 CONTINUE
      NELP2 = NELP1
      GO TO 11
   10 NELP2 = NELP1 + 1
      NZ(NELP2) = 14
      IOX = -IOX
   11 DO 20 I = 1,NVAR
      N = 0
```

```
      IF(NZ(I).GE.36)20,12
   12 IF(NZ(I).GT.21)15,13
   13 N1 = NZ(I) + 1
      GO TO 16
   15 N1 = NZ(I) + 2
   16 N2 = N1 + 3
      DO 18 J = 1,NELP2
      IF(NZ(J).LT.N1.OR.NZ(J).GT.N2)18,17
   17 N = N + 1
      LF = 0
      NZF(I,N) = J
   18 CONTINUE
   20 NF(I) = N
      DO 40 I = 1,NELP2
      N1 = NZ(I)
      Z(I) = FLOATF(N1)
      ENCODE (6,320,NP(I))N1
      X = EXP(N1)
      IF(N1.GT.35)23,21
   21 X(2) = X(3) = X(4) = 2.73
      X(5) = 2.60
      GO TO 27
   23 X(3) = X(2) = X
      IF(N1.GT.82)25,24
   24 X(4) = X(5) = 2.60
      GO TO 27
   25 X(5) = 2.22
      X(4) = 2.60
   27 X(6) = X(7) = 2.60
      X(8) = 2.22
      EC(I) = WAVL/EDGE(N1) * .001
      SIGMA(I) = CSIG/(EO**XSIG - EC(I)**XSIG)
      DO 35 J = 1,NELP2
      N2 = NZ(J)
      Y(J) = LAMBDA(N2)
      DO 30 K = 1,7
      IF(Y(J).LE.EDGE(N1,K))35,30
   30 CONTINUE
      K = 8
   35 MU(J,I) = C(N1,K)*Y(J)**X(K)
      IF(LF)40,38
   38 CR(I) = C(N1)/C(N1,2)
      XR(I) = X - X(2)
      YY= (AWK + BWK*Z(I) + CWK*Z(I)**3)**4
      WK(I) = YY/(1.0 + YY)
   40 U(I) = EO/EC(I)
      PRINT 500
      PRINT 208, (NZ(I),I=1,NVAR)
      PRINT 209
      DO 42 I = 1,NELP2
   42 PRINT 210, NZ(I), (MU(J,I),J=1,NVAR)
      CALL PAGE
      IF(LF)65,45
   45 PRINT 204
      DO 47 I = 1,NELP2
      N1 = NF(I)
      DO 46 J = 1,N1
      N2 = NZF(I,J)
   46 R(I,J) = CR(I)*Y(N2)**XR(I)
   47 PRINT 206, I, NZ(I), N1, (NZF(I,J),R(I,J),J=1,N1)
      PRINT 212
      PRINT 214, (NZ(I),Y(I),EC(I),SIGMA(I),WK(I),U(I),I=1,NELP2)
```

```
      GO TO 67
   65 PRINT 213
      PRINT 216, (NZ(I),Y(I),EC(I),SIGMA(I),I=1,NELP2)
   67 CONTINUE
      PRINT 218
      IF(LF)72,69
   69 DO 70 I = 1,NELP2
      X(I) = U(I)*LOGE(U(I)) - U(I) + 1.0
      WK(I) = WK(I)*.5
   70 EC(I) = POWRF(EC(I),0.3)
      DO 71 I = 1,NELP2
      N = NZ(I)
      M = NF(I)
      DO 71 J = 1,M
      L = NZF(I,J)
      K = NZ(L)
   71 U(I,J) = (X(L)*(R(I,J)-1.0)*WK(L)*EC(I)*A(N)*MU(L,I))/(X(I)*R(I,J)
     1    *EC(L)*A(K))
   72 CONTINUE
      PRINT 500
  100 FORMAT (I6,6A8,I3,F3.0,4I2,2F5.0)
  102 FORMAT(5X,I5,4F10.6,5X,A5)
  200 FORMAT(11X,53H------STANDARD FOR ELEMENT Z------   OXYGEN   SILICO
     1N/64H NL     Z   CONCENTRATION      E(CHI)*(1+FLUOR)  FACTOR    FAC
     2TOR/)
  202 FORMAT(I3,I5,F13.6,F20.6,E13.6,F10.6,5X,A5)
  204 FORMAT(////13X,9HNUMBER OF/11X,11HFLUORESCING/ 89H NL    Z      EL
     1EMENTS   ELEMENT NUMBER AND ABSORPTION JUMP RATIO OF FLUORESCING E
     2LEMENTS/)
  206 FORMAT(I3,I5,I10,4(I7,F8.3))
  208 FORMAT(10X,37HMASS ABSORPTION COEFFICIENTS---MU/RHO//9H EMITTER=,
     1    I3,18I6)
  209 FORMAT (9H ABSORBER)
  210 FORMAT (I4,F8.0,18F6.0)
  213 FORMAT (///28H  Z   LAMBDA      EC    SIGMA/)
  212 FORMAT (///44H  Z   LAMBDA      EC    SIGMA   OMEGA      U/)
  214 FORMAT  (I3,F9.4,F7.3,F9.1,      F8.4,F8.3)
  216 FORMAT  (I3,F9.4,F7.3,F9.1)
  218 FORMAT (///37H LAMBDA = WAVELENGTH OF EMISSION LINE/
     1        18H Z = ATOMIC NUMBER/26H R = ABSORPTION JUMP RATIO/
     2   38H EC = CRITICAL EXCITATION VOLTAGE (KV)/29H OMEGA = K FLUORES
     3CENCE YIELD/10H U = EO/EC)
  320 FORMAT(2X,I3)
  500 FORMAT(///)
      END
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```
      SUBROUTINE PAGE
      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCE(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      NPAGE = NPAGE + 1
      PRINT 200, NPROB, ID, EO, NPAGE
  200 FORMAT(12H1PROBLEM NO.,I6,3X,6A8,5X,F2.0,3H KV, 10X,4HPAGE,I3/)
      END
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      SUBROUTINE OXYGEN
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      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCF(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      IF(IOX)5,2,10
   10 CON(NELP1) = 0.0
      DO 12I = 1,NEL
   12 CON(NELP1) = CON(NELP1) + CON(I)*O(I)
      GO TO 2
    5 CON(NELP1) = CON(NELP2) = 0.0
      DO 7 I = 1,NEL
      CON(NELP1) = CON(NELP1) + CON(I)*O(I)
    7 CON(NELP2) = CON(NELP2) + CON(I)*SI(I)
    2 RETURN
      END



      FUNCTION ABSORB (N)
      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCF(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      COMMON/DATA/A(92), LAMBDA(92), EDGE(92,7), C(92,8), EXP(92), WAVL,
     1   SINTHETA,  AWK, BWK, CWK, CSIG, XSIG
      TYPE REAL MUBAR,MU
      ABAR = ZBAR = MUBAR = 0.0
      DO 10 I = 1,NELP2
      N1 = NZ(I)
      MUBAR = MUBAR + MU(N,I)*CON(I)
      ABAR = ABAR + A(N1)*CON(I)
   10 ZBAR = ZBAR + Z(I)*CON(I)
      H = 1.2 * ABAR/ZBAR**2
      CHI = MUBAR/(SINTHETA*SIGMA(N)) + 1.0
      ABSORB=(1.0 + H)/(CHI*(1.0 + H*CHI))
      END



      FUNCTION FLUOR(NN)
      TYPE REAL MU, MUBAR
      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCF(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      COMMON/DATA/A(92), LAMBDA(92), EDGE(92,7), C(92,8), EXP(92), WAVL,
     1   SINTHETA,  AWK, BWK, CWK, CSIG, XSIG                           DATA
      N = NN
      FLUOR = 0.0
      IF(NF(N))3,2
    2 RETURN
    3 M = NF(N)
      DO 25 J = 1,M
      L = NZF(N,J)
      IF(NZ(L).GT.35)5,7
    5 PRINT 200, NZ(L)
  200 FORMAT(//58H FLUORESCENCE CORRECTION CANNOT BE CALCULATED FOR ELEM
     1ENT ,I2//)
      GO TO 25
```

```
    7 FMUBAR = 0.0
      DO 10 I = 1,NELP2
   10 FMUBAR = FMUBAR + CON(I)*MU(L,I)
      V = SIGMA(L)/FMUBAR
      V = LOGF(1.0 + V)/V
      ULC = MUBAR/(FMUBAR*SINTHETA)
      ULC = LOGF(1.0 + ULC)/ULC
      FLUOR = FLUOR + CON(L)*U(N,J)*(ULC + V)/FMUBAR
   25 CONTINUE
      END


      SUBROUTINE PRNTPLOT (N,NO)
      COMMON NPROB, ID(6), NEL, EO, NZ(20), SCON(20), SCF(20), MUBAR,
     1   O(20), IOX, NELP1, NF(20), NZF(20,4), Z(20), R(20,4), EC(20),
     2   SIGMA(20), WK(20), MU(20,20), U(20,4), SI(20), NVAR, NELP2,
     3   OCON(20), CON(20), DELCON(20), NOM(20),  NS, NP(20), IMIN,
     4   IMAX, IG, YMAX, DMIN
      COMMON/PP/NAME2(500), Y(500,20), TOT(500)
      DIMENSION IPREF(9), X(500), N(20)
      DATA (IPREF = 4,3,5,0,1,2,6,7,9)
      IF(NO.LE.10)3,1
    1 N1 = N3 = 1
      N2 = 10
      GO TO 4
    3 N1 = 1
      N3 = 0
      N2 = NO
    4 CALL PAGE
      PRINT 220, (N(I),I=N1,N2)
  220 FORMAT(25X,56HCONCENTRATIONS CORRECTED FOR ABSORPTION AND FLUORESC
     1ENCE//15X,5HTOTAL,10(5X,A5))
      DO 10 I = 1,NS
      PRINT 256,NAME2(I), TOT(I), (Y(I,J),J=N1,N2)
  256 FORMAT(2X,A8,11(2PF10.4))
      IF(XMODF(I,5))10,5
    5 IF(XMODF(I,45))8,7
    7 CALL PAGE
      PRINT 220, (N(K),K=N1,N2)
      GO TO 10
    8 PRINT 400
  400 FORMAT ()
   10 CONTINUE
      IF(N3)11,14
   11 N1 = 11
      N2 = NO
      N3 = 0
      GO TO 4
   14 IF(IG)15,90
   90 RETURN
   15 IF(N.NE.NP)30,16
   16 IF(IOX)90,30
   30 YLEN = 8.6614
      YYMAX = YMAX*1.1
      XLEN = FLOATF((NS+7)/8)
      PX1 = XLEN + 1.0
      PX2 = XLEN + 1.5
      CALL CCPLOT(XLEN+3.0,0,0)
      DY = YYMAX/YLEN
   33 DO 35 I = 1,NS
   35 X(I) = I
```

```
      NX = XMINOF(NO,9)
      PY1 = .8924
      PY2 = .7874
      DO 40 J = 1,NX
      CALL P2LINE (X,Y(1,J),NS,1,1,IPREF(J),.07,0.0,8.0,0.0,DY)
      CALL CCSYMBOL (PX1,PY1,.21,IPREF(J),0.0,-1)
      CALL CCSYMBOL (PX2,PY2,.21,N(J),0.0,5)
      PY1 = PY1 + .5
      PY2 = PY2 + .5
   40 CONTINUE
      CALL P2LINE (X,TOT,NS,1,1,11,.07,0.0,8.0,0.0,DY)
      CALL CCSYMBOL (PX1,PY1  ,.35,11,0.0,-1)
      CALL CCSYMBOL (PX2,PY2,  .35,5HTOTAL,0.0,5)
      CALL CCAXIS (0.,0.,ID,-48,XLEN,0.0,0.0,8.0 ,8.0)
      CALL CCAXIS (XLEN,0.,14H CONCENTRATION,14,YLEN ,90.,0.0,DY,-12.7)
      CALL CCAXIS (0.,YLEN ,ID,-48,XLEN,0.0,0.0,8.0 ,-8.0)
      CALL CCAXIS (0.,7.874,ID,-48,XLEN,0.0,0.0,8.0 ,-8.0)
      CALL CCAXIS (0.,0.,14H CONCENTRATION,14,YLEN ,90.,0.0,DY,12.7)
      DO 50 I = 1,NS
      IF(NAME2(I).EQ.1H )50,45
   45 PX = X(I)*.125
      CALL CCSYMBOL (PX,YLEN,.14,NAME2(I),45.0,8)
   50 CONTINUE
      CALL CCPLOT (0,0,-3)
      END
```

APPENDIX 2: INPUT SPECIFICATIONS

A. Data Cards for Program EMX

Columns	Description
IDENTIFICATION CARD:	One at the beginning of each problem.
1-6	NPROB (problem number). Up to six digits (all numerals), right justified*, no decimal point.
8-54	ID - alphanumeric information (letters, numbers, symbols) for problem identification.

NOTE: NPROB and ID will appear as a heading on each page of output and on any graphs associated with this problem. If NPROB = 0, the program will terminate.

Columns	Description
56	NEL (total number of elements analyzed in this problem). NEL $\leq$ 9.
57-58	NDT (number of readings in each deadtime data point). NDT $\leq$ 99. Right justified, no decimal point. If no deadtime data, NDT = 0.
59-60	NS (number of readings in each sample peak, sample background or standard background data point). NS $\leq$ 99. Right justified, no decimal point. If the problem involves only the calculation of deadtime, NS = 0.

NOTE: If readings are not grouped according to NS and NDT specifications, program will print an error message and move on the next problem, if any, without making any calculations; or, if the total number of consecutive equivalent readings happens to be evenly divisible by NS (or NDT for deadtime readings), it will group data incorrectly. Standard peak data points may be made up of a variable, unspecified number of readings $\leq$ 100. If one data point includes both standard peak and standard background data, it will be handled as "standard peak".

Columns	Description
62	MBKGD (method of taking background readings). If MBKGD = 0, the program expects to find a pair of background data points for each sample or standard peak data point. If MBKGD = 1, one pair of background data points is averaged and the result subtracted from all of the appropriate peaks until the time when another pair appears or until the end of the data set. If no background points are given, no background will be subtracted from the points in that data set. There will be no indication of this in the final output.

CAUTION: Background data points are assumed to occur in pairs (not necessarily adjacent), which are averaged to find true background. Reading down each spectrometer column, the first two background points (wherever they may be) are assumed to make up the first pair, and so on. If there is an odd number of background points, the last one will be used alone as a true background. This means that if one member of the first pair is omitted, all further points will be grouped incorrectly.

In BKGD Method 0, the omission of a background or peak data point will cause all succeeding background points to be subtracted from the wrong peaks.

Columns	Description
62-65	SLIMIT (limit of scatter allowed within a standard peak data point). Either right-justified integer or the decimal point must be included. If in any standard peak data point $\sigma > \text{SLIMIT}\cdot\sqrt{N}$ (where σ = root mean square, N = number of counts) the computer will print an error message and move on to data for the next problem, if any. It is suggested that SLIMIT = 2 to 3.
67	IG. If IG = 1, computer will make a plot of the concentration of each element or oxide and total concentration of all elements analyzed at each point on the sample. If IG = 0 or blank, no plot will be made.
68-70	XMAX--(the value of the current at the right-hand edge of the deadtime curve plot). Whenever deadtime is calculated, a plot is made of counts/current as a function of current, and a value must be given for XMAX. For ease in reading values from the plot, XMAX should be a number with only one significant figure. Decimal point required. If no deadtime data, may be left blank.
71-73	YMAX (maximum y-value on concentration plot, which will be increased by 10 percent by the program). Decimal point required. If IG = 0, may be left blank. Example: if elements analyzed are expected to total 100%, set YMAX = 1.0. Plot will show concentrations up to 110%.

ELEMENT CARD: One "element card" is needed for each element analyzed in the problem. Cards must be arranged so that NL's (see below) are consecutive integers from 1 to NEL. If elements analyzed are not numbered this way in probe output, NEL must be changed and dummy cards must be made for the missing elements. For example, if only three elements are being analyzed but these are numbered 2,

---

*"Right-justified" means that the rightmost digit of a number is in the farthest right column allowed for the number; any blank columns are on the left of the number.

3, and 6 in the probe data, NEL must be set equal to 6 and there must be an element card (with NL in column 1) for Elements 1, 4 and 5 as well as for the elements analyzed. (This will take more computer time than if the elements analyzed had been numbered 1, 2 and 3 in the first place.)

Columns	Description
1	NL (the element code number assigned to this element at the time probe data was taken). Elements may be numbered in any order, without regard to atomic number, order in which analyzed, etc.
2-4	NO(NL) (atomic number of the element). Right-justified, no decimal point.
5-10	WTPC(NL) (concentration of element in its standard). NOTE: If, for example, standard contains 25 percent Fe, WTPC = .25. Decimal point required; may appear anywhere within the field.
11-25	TAU(NL) (deadtime in <u>seconds</u>). E-format; exponent of 10 must be in Col. 25; decimal point required. If TAU is to be computed by the program, put a zero somewhere within Cols. 11-22. If deadtime correction is to be omitted, put any negative number (with decimal point) somewhere within Cols. 11-22. If the TAU from some other element is to be used for this element, set TAU = NL of the element from which the TAU is to be used.
26-35	O(NL) (Oxygen factor). The oxide concentrations will be calculated as CON(NL)*(1 + O(NL)). Decimal point required; may be left blank if no oxygen. Example: to convert silicon concentration into concentration of SIO_2, O = 1.139.
36-45	SI(NL) (silicon factor). If silicon is not analyzed for, silicon concentrations can be calculated in same manner as oxygen concentrations. Decimal point required, or may be left blank.
51-55	NOM(NL) (name of oxide or other element combination to be used in headings on printout and plots. Example: Al_2O_3.)

PROBE DATA RECORDS: One card or magnetic tape record for each reading from probe. If records are on magnetic tape, they must be written in BCD.

Columns	Description	
PROBE DATA RECORDS (Continued)		
1-6	Time (in hundredths of sec.)	No decimal points. If a column is left out in the output from probe, it must contain zeros or blank spaces.
7-12	Current	
13-18	Scanner 1 counts	
19-24	Scanner 2 counts	
25-30	Scanner 3 counts	
31-36	KODE (a set of six code digits to identify the element and type of reading. NL = identifying number of the element being analyzed for, and may be any arbitrary number from 1 to 9. If NL = 0, that reading for that scanner will be disregarded. KD = type of reading. If KD = 0, sample peak 1, sample background 2, standard peak 3, standard background 4, deadtime reading Col. 31 KD, 32 NL for Scanner 1 33 KD, 34 NL for Scanner 2 35 KD, 36 NL for Scanner 3	
37-44	NAME (alphanumeric information for identification of a data point) May be left blank.	

BREAK CARD: Data sets must be separated by a "break" card, which contains zeros in Columns 31-36. Any data in other columns will be ignored.

After the last data card for each problem, there must be a card with 999999 in columns 31-36.

After the 999999 card of the last problem for the computer run, there must be one blank card. (Or if data records are on tape, blank card must be after last ELEMENT CARD of last problem.)

B. <u>Data Cards for Program EMX2</u>

Columns	Description
IDENTIFICATION CARD: One at the beginning of each problem.	
1-6	NPROB (problem number). Up to six digits (all numerals), right justified, no decimal point.
7-54	ID - alphanumeric information (letters, numbers, symbols) for problem identification.

NOTE: NPROB and ID will appear as a heading on each page of output and on any graphs associated with this problem. If DATA RECORDS (see below) are on punched cards, only one problem may be run at one time. If DATA RECORDS are on magnetic tape, any number of problems may be run at once, as long as DATA RECORDS are all on one tape. In this case, data cards should be followed by one blank card.

Columns	Description
55-57	NEL - number of elements for each sample to be read from DATA RECORDS. NEL $\leq$ 20.
58-60	EO - operating voltage in KV. Right justified, no decimal point.
61-62	NFIX - number of fixed elements. Concentrations for these elements will be read from data records and used in corrections but will not themselves be corrected. All "fixed elements" must appear after the other elements on ELEMENT CARDS and DATA RECORDS. Right justified, no decimal.
63-64	IMIN - minimum number of iterations. Right justified, no decimal.
65-66	IMAX - maximum number of iterations. Right justified, no decimal.
68	IG. IG = 1 if a graph is to be plotted, IG = 0 if no graph desired.
69-73	Maximum Y-value on graph (which will be increased by 10 percent by the program). If IG = 0, may be left blank. Decimal point required.
74-78	DMIN. The calculation will be iterated at least IMIN and no more than IMAX times. Between these limits, iteration will stop when concentrations of no elements present in amounts greater than one percent change more than DMIN from one iteration to the next.

ELEMENT CARD: One needed for each element in the problem. Cards must be arranged in same order as element concentrations appear on DATA RECORDS. No element card is needed for oxygen, the concentration of which will be calculated on the basis of the other element concentrations. (Silicon can be calculated in the same manner; then no element card or probe data would appear for silicon.)

Columns	Description
6-10	NZ(I) - atomic number of element i. Right justified, no decimal.
11-20	SCON(I) - concentration of element i in its standard. Decimal point required.
21-30	SCF(I) - correction factor for the standard of the ith element: f(chi) $\cdot$ $(1 + I_{f}i/I_{i})$. If SCF = 0, all SCF for this problem must = 0. In this case correction factors are calculated for the standard, and new ELEMENT CARDS are punched for later use (see Sec. IIIC). Decimal point required.
31-40	O(I) - oxygen factor: the oxygen concentration in the sample will be calculated as $\Sigma CON_{i}O_{i}; i = 1, NEL$. Oxide concentrations will be calculated as $CON_{i}(1 + O_{i})$. Decimal point required, or may be left blank if no oxygen.
41-50	SI(I) - silicon factor. If silicon is not analyzed for, silicon concentrations can be calculated in same manner as oxygen concentrations. Decimal point required, or may be left blank.
56-60	NOM(I) - name of oxide or other element combination to be used in headings on printout and plots. Example: Al_2O_3

PROBE DATA RECORDS: any number up to 500. May be on punched cards or on magnetic tape on Logical Unit 3.

1-8	NAME - alphanumeric information to identify the sample or sample point. May be left blank.
9-16 17-24 25-32 33-40 41-48 49-56 57-64 65-72 73-80	Observed concentrations $(I_A/I(A))$ of elements in sample. Must appear in same order as element cards, with fixed elements last. E8.0 format - for example, 33.3 percent would appear as 3330E-04. 5 ppm would appear as 0005E-06.

If the problem includes more than 9 elements, two records (cards) may be included for each sample or sample point. The concentration of the 10th element would appear in columns 9-16 of the second card; the 11th, in columns 17-24 etc.

C. Special Tapes

To make EMX and EMX2 as flexible as possible in input and output operations, the use of several special tapes is built into the programs. These tapes must be provided, bypassed, or equivalenced to some standard I/O unit; they cannot be ignored.

Data from the microprobe is read into Program EMX from Tape 2. If probe data is actually to be on punched cards, Tape 2 must be equivalenced on the appropriate control card to the standard input unit.

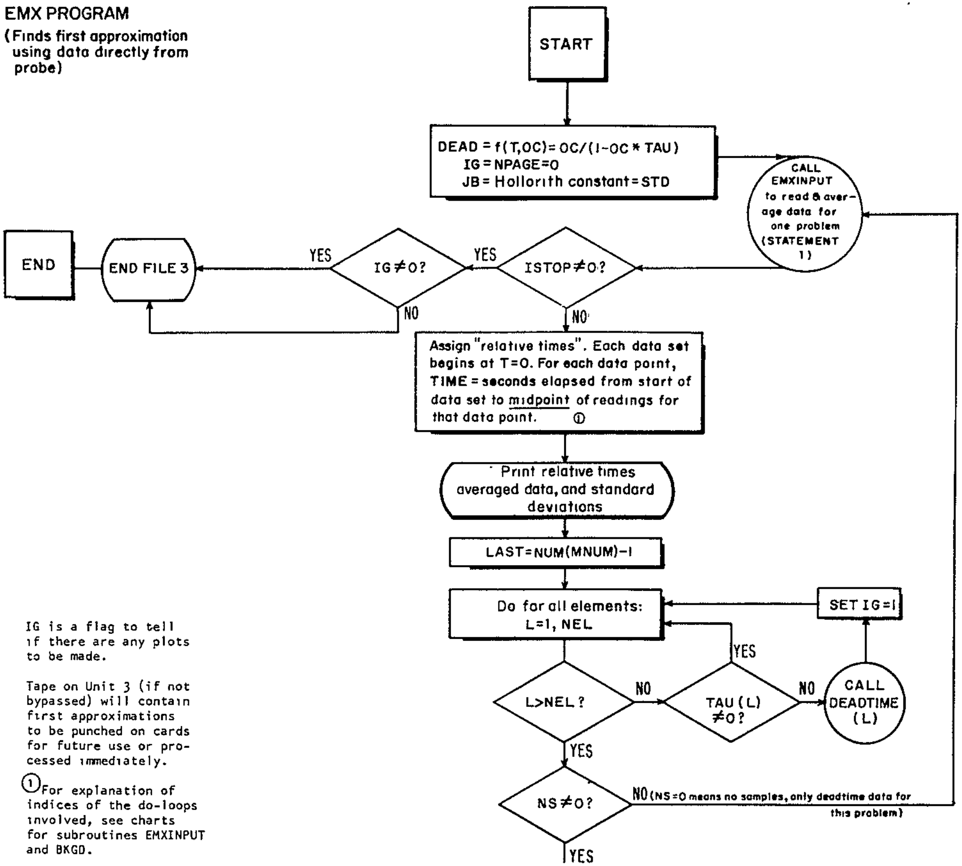
Results from Program EMX that are to be used as input for Program EMX2 will be written on Tape 3. If the user prefers to receive this output in the form of punched cards, Tape 3 may be equivalenced to the standard punch unit or cards may be punched later from the tape. If both programs are being run together as a multiple-execution job, this intermediate output could most economically be on a standard scratch tape; then Tape 3 would be equivalenced to the standard scratch tape. This tape must be rewound between the execution of EMX and EMX2. If EMX is being run alone and no such output is desired because no further corrections are to be made to the data, the program user must specify that Tape 3 be bypassed.

If input to Program EMX2 is to be entirely from punched cards, Tape 3 must be equivalenced to the standard input unit.

A special tape must be provided for plotting information when plots are desired.

EMX PROGRAM

(Finds first approximation using data directly from probe)



IG is a flag to tell if there are any plots to be made.

Tape on Unit 3 (if not bypassed) will contain first approximations to be punched on cards for future use or processed immediately.

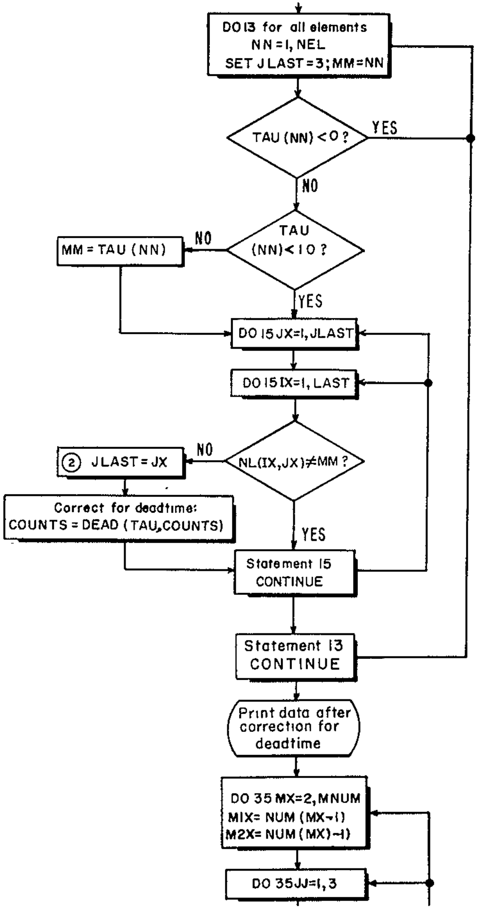
① For explanation of indices of the do-loops involved, see charts for subroutines EMXINPUT and BKGD.

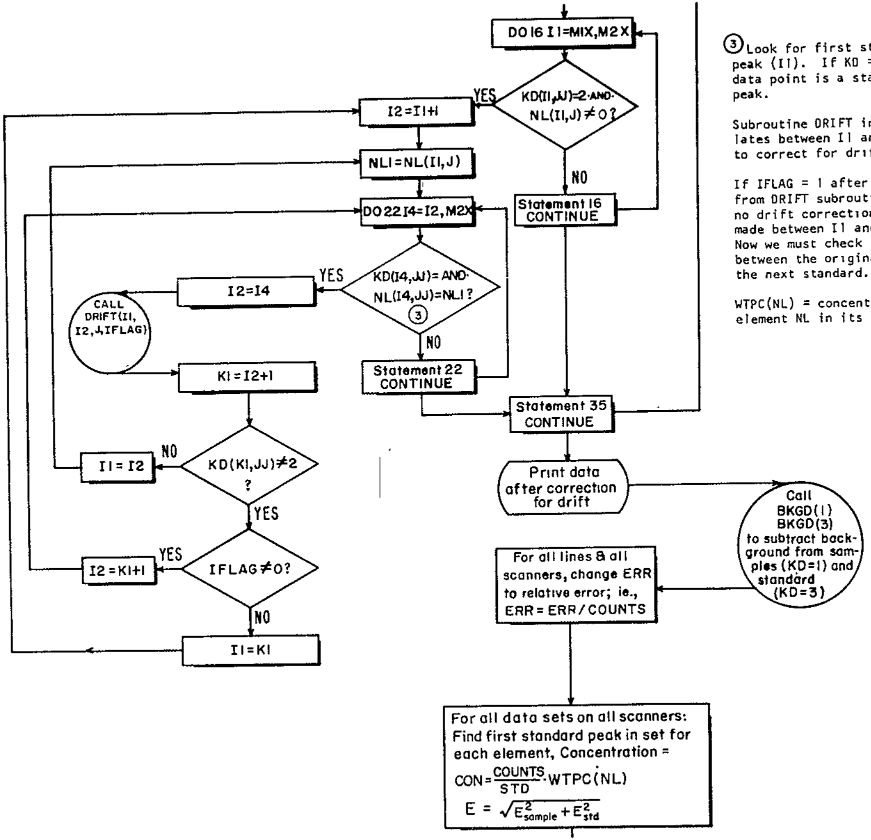
LAST = index of last line of data for this problem.

NN = element number

Note: if TAU<0, it means don't correct for deadtime. If TAU = 0, find correct TAU using data. If TAU>1, use TAU from element tau.

② Once a sample no. NN is found, it is assumed that all of that element will be on the same scanner.



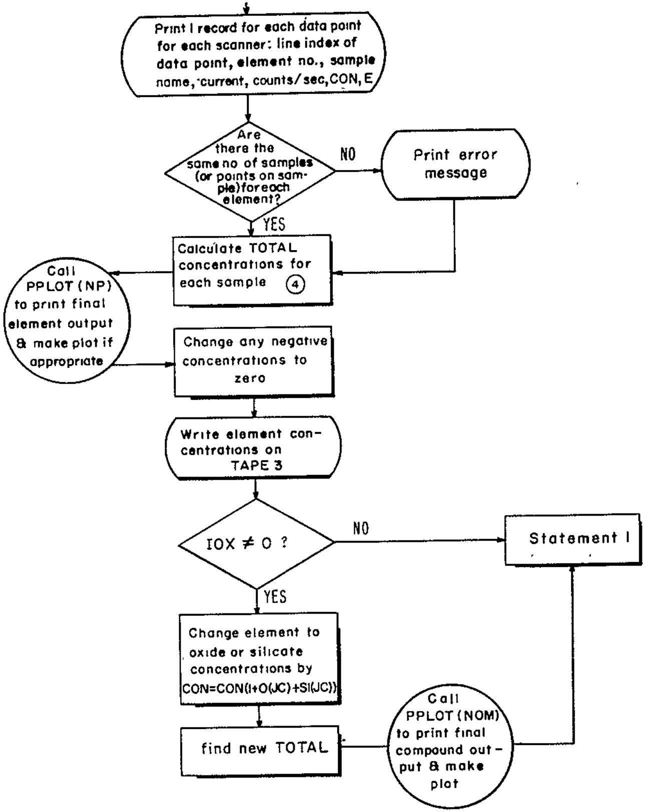


③ Look for first standard peak (I1). If KD = 2, data point is a standard peak.

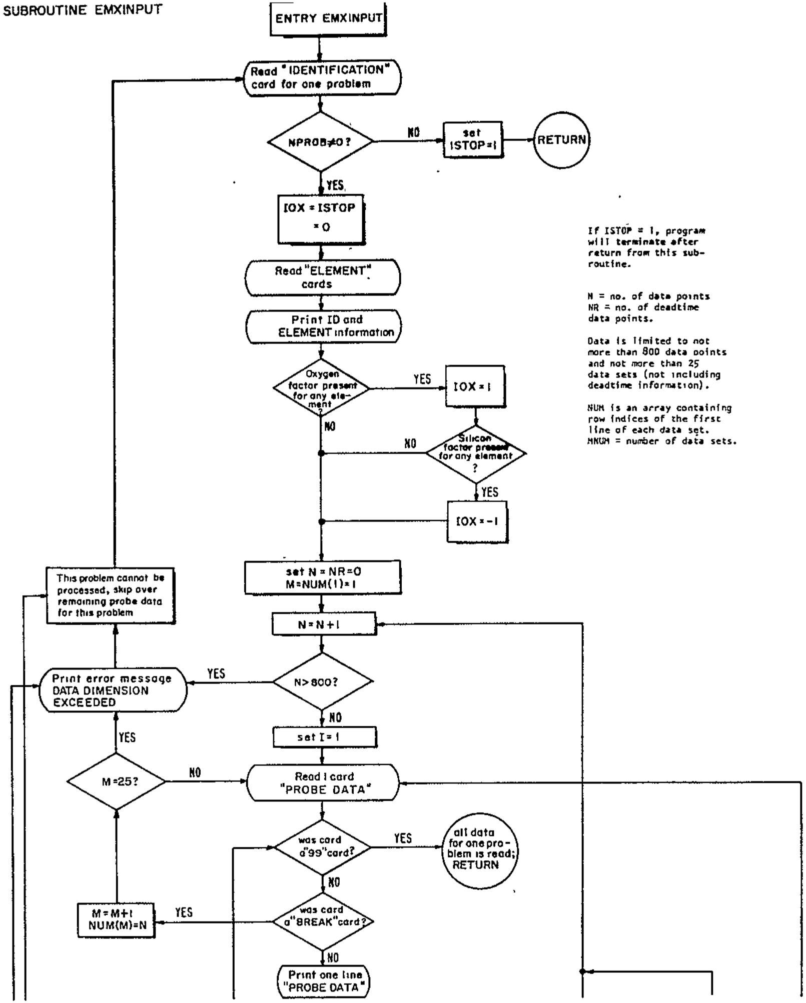
Subroutine DRIFT interpolates between I1 and I2 to correct for drift.

If IFLAG = 1 after return from DRIFT subroutine, no drift correction was made between I1 and I2. Now we must check for drift between the original I1 and the next standard.

WTPC(NL) = concentration of element NL in its standard.


Print I record for each data point for each scanner: line index of data point, element no., sample name, current, counts/sec, CON, E
Are there the same no of samples (or points on sample) for each element?
NO
Print error message
YES
Calculate TOTAL concentrations for each sample ④
Call PPLOT (NP) to print final element output & make plot if appropriate
Change any negative concentrations to zero
Write element concentrations on TAPE 3
IOX ≠ 0 ?
NO
Statement I
YES
Change element to oxide or silicate concentrations by CON=CON(I+O(JC)+SI(JC))
find new TOTAL
Call PPLOT (NOM) to print final compound output & make plot

SUBROUTINE EMXINPUT

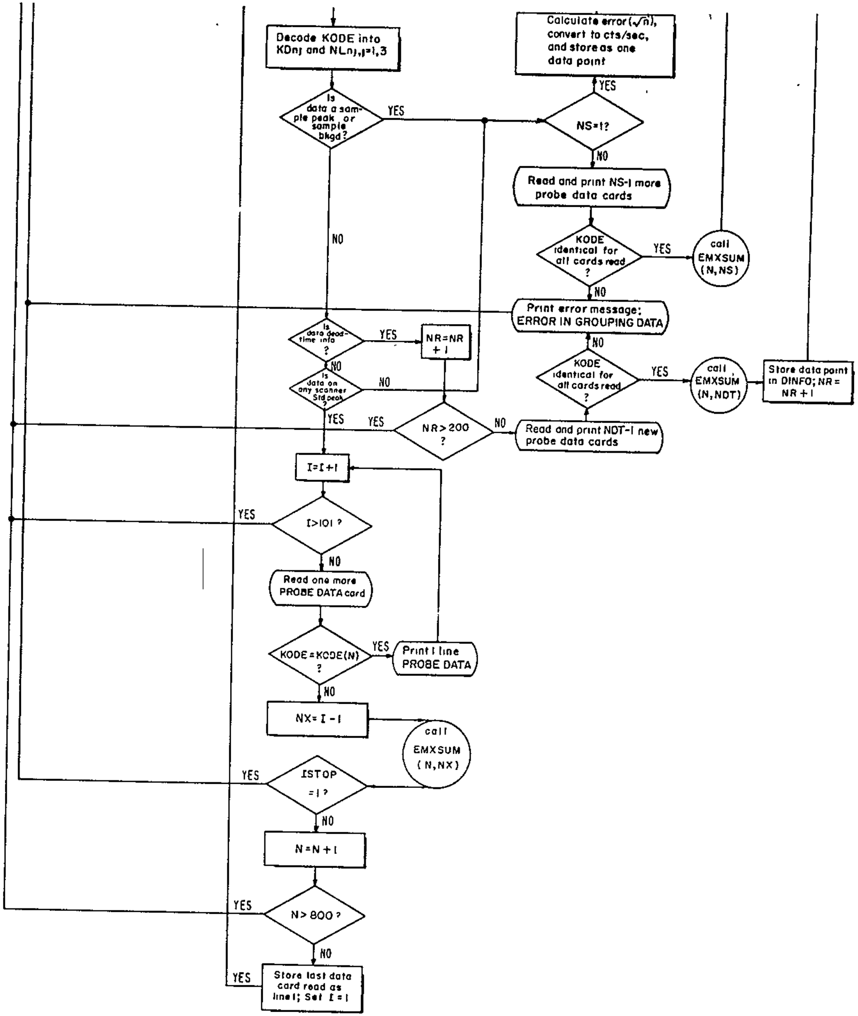


If ISTOP = 1, program will terminate after return from this subroutine.

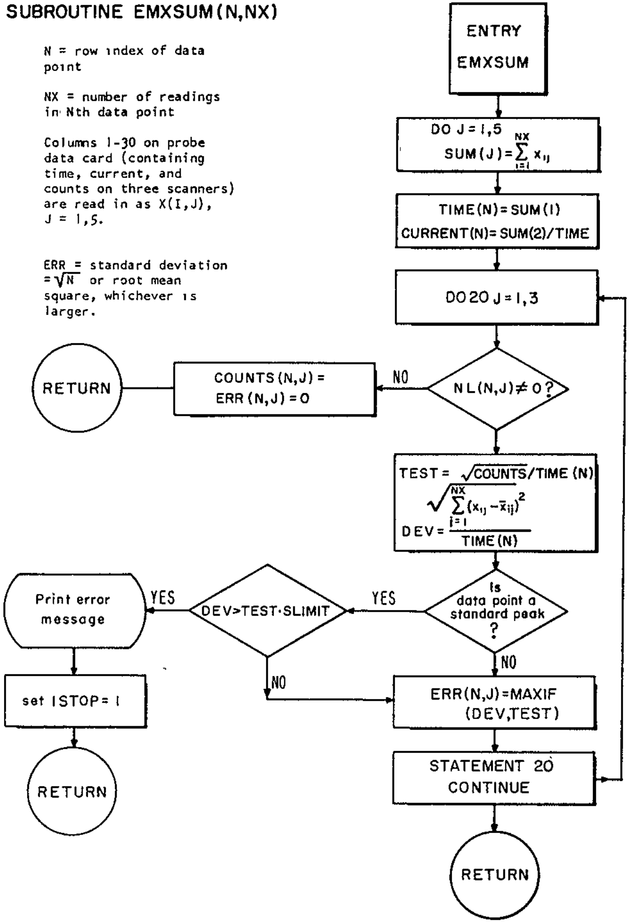
N = no. of data points
NR = no. of deadtime data points.

Data is limited to not more than 800 data points and not more than 25 data sets (not including deadtime information).

NUM is an array containing row indices of the first line of each data set.
MNUM = number of data sets.


Decode KODE into KDnj and NLnj, j=1,3
Is data a sample peak or sample bkgd?
YES
NO
NS=1?
YES
Calculate error (√n), convert to cts/sec, and store as one data point
NO
Read and print NS-1 more probe data cards
KODE identical for all cards read ?
YES
call EMXSUM (N,NS)
NO
Print error message; ERROR IN GROUPING DATA
NO
KODE identical for all cards read ?
YES
call EMXSUM (N,NDT)
Store data point in DINFO; NR = NR + 1
Is data dead-time info ?
YES
NR=NR + 1
NO
Is data on any scanner Std peak ?
NO
YES
YES
NR > 200 ?
NO
Read and print NDT-1 new probe data cards
I=I+1
YES
I>101 ?
NO
Read one more PROBE DATA card
KODE = KODE(N) ?
YES
Print 1 line PROBE DATA
NO
NX= I - 1
call EMXSUM (N,NX)
YES
ISTOP =1 ?
NO
N=N+1
YES
N> 800 ?
NO
YES
Store last data card read as line 1; Set I = 1

SUBROUTINE EMXSUM(N,NX)



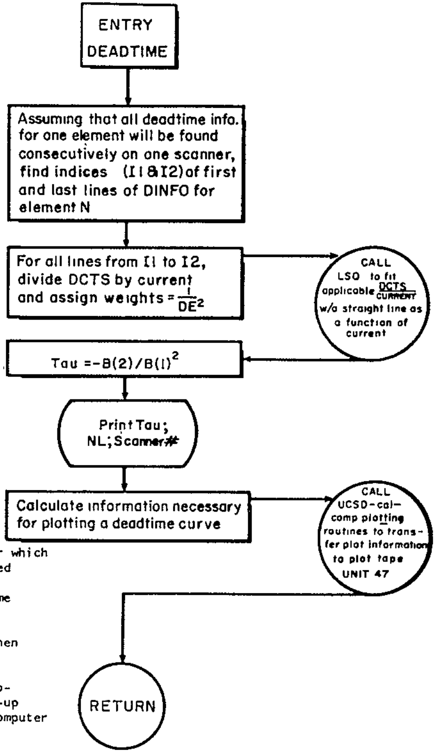
N = row index of data point

NX = number of readings in Nth data point

Columns 1-30 on probe data card (containing time, current, and counts on three scanners) are read in as X(I,J), J = 1,5.

ERR = standard deviation = $\sqrt{N}$ or root mean square, whichever is larger.

SUBROUTINE DEADTIME(N)



N = no. of element for which TAU is to be calculated

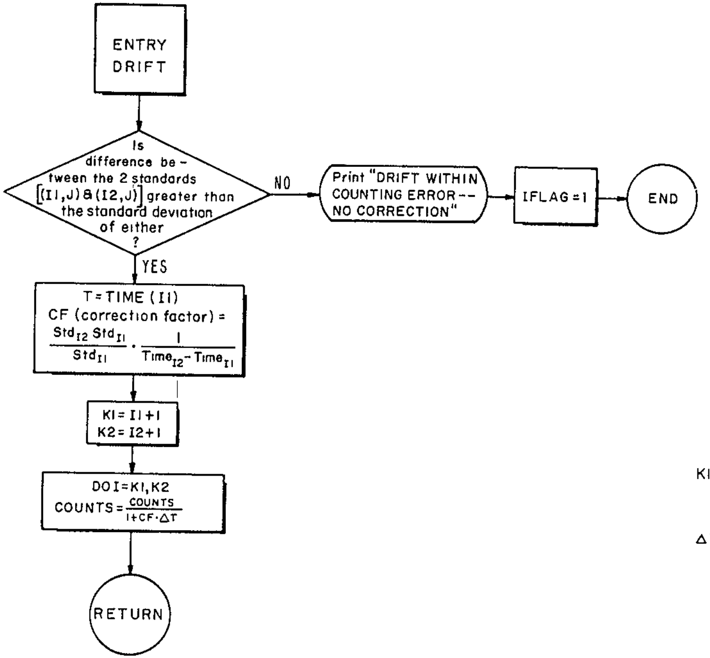
DCTS = counts (deadtime information)

DE = error in DCTS, then weight.

LSQ adapted from a subroutine LSQPOL (write-up available from UCSD Computer Center).

B(1) and B(2) are coefficients of x where f(x) = B(1) + B(2)X. Calculated by LSQ subroutine.

Subroutine DRIFT (I1,I2,J,IFLAG)



K1-K2 are limits within which to correct for drift

ΔT = TIME(I) - T

SUBROUTINE BKGD(KODE)

J = no. of scanner

Subroutine is done twice, once for KODE=3 (standard bkgd) and once for KODE=1 (sample bkgd).

M1 and M2 are indices of first and last lines of a data set

J1 is first line to look on for a sample from which to subtract B.

① Look for an appropriate background reading.

I1 = line of first of a background pair.

NL1 = element to which I1 applies.

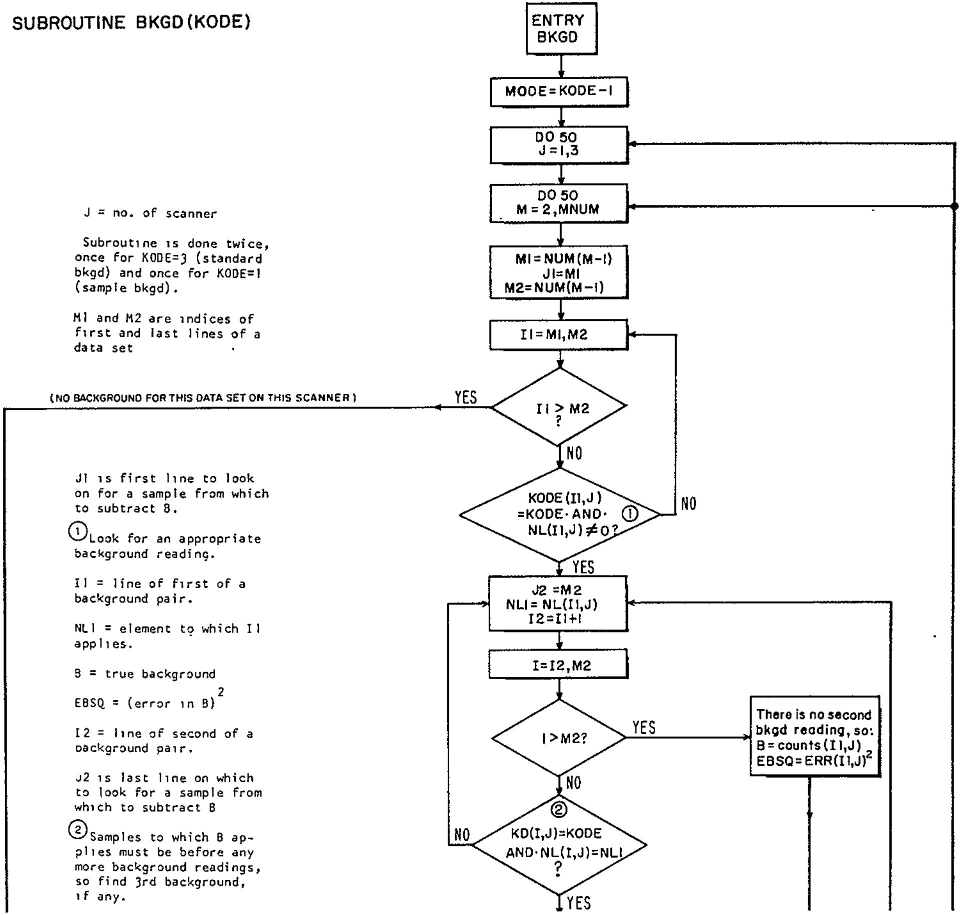
B = true background

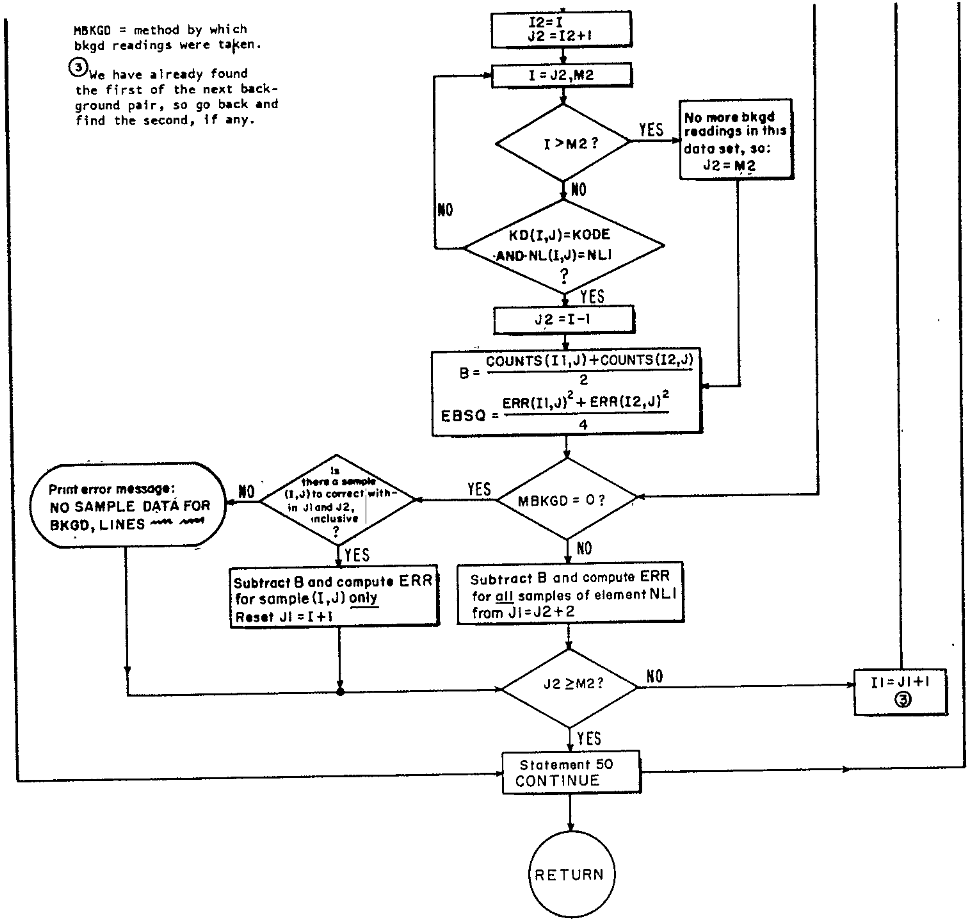
EBSQ = $(\text{error in } B)^2$

I2 = line of second of a background pair.

J2 is last line on which to look for a sample from which to subtract B

② Samples to which B applies must be before any more background readings, so find 3rd background, if any.

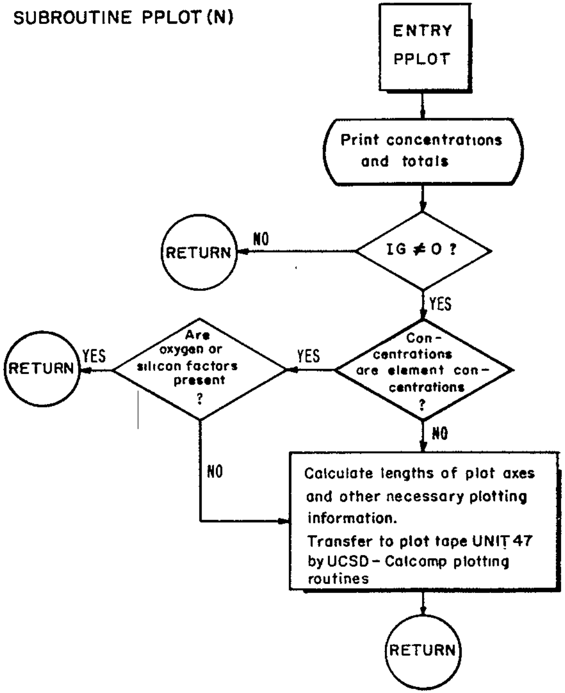




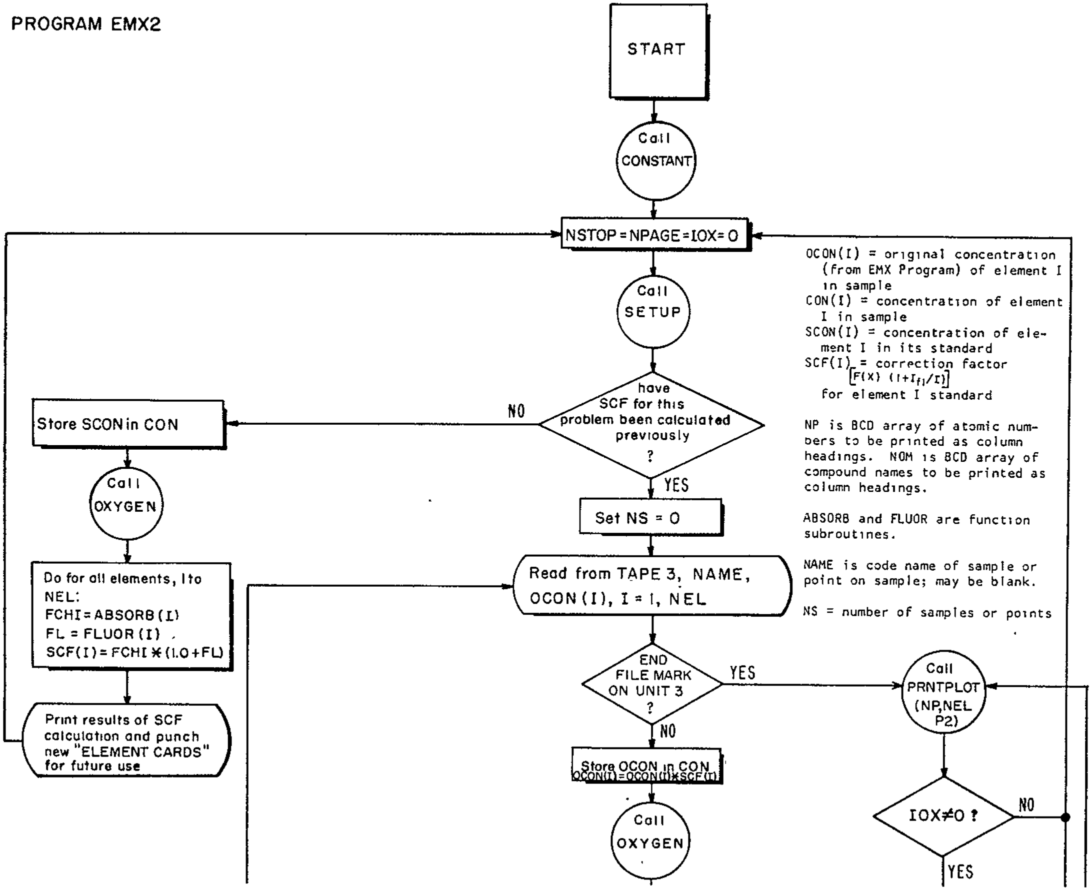
MBKGD = method by which bkgd readings were taken.

③We have already found the first of the next background pair, so go back and find the second, if any.

SUBROUTINE PPLOT (N)



PROGRAM EMX2



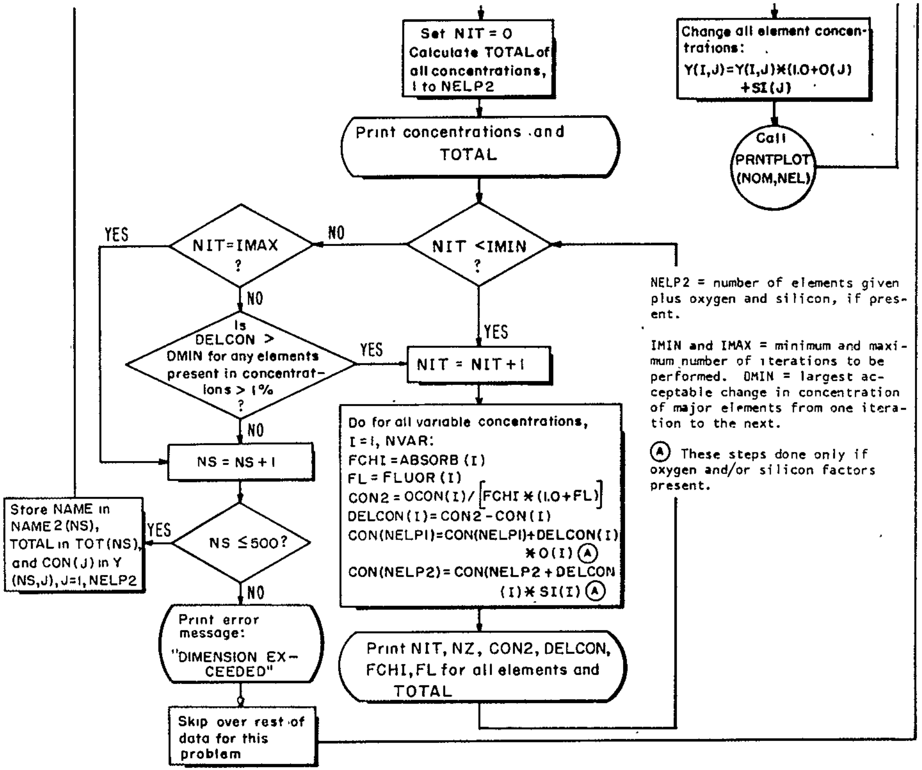
OCON(I) = original concentration (from EMX Program) of element I in sample
CON(I) = concentration of element I in sample
SCON(I) = concentration of element I in its standard
SCF(I) = correction factor $[F(X)\ (1+I_{fl}/I)]$ for element I standard

NP is BCD array of atomic numbers to be printed as column headings. NOM is BCD array of compound names to be printed as column headings.

ABSORB and FLUOR are function subroutines.

NAME is code name of sample or point on sample; may be blank.

NS = number of samples or points

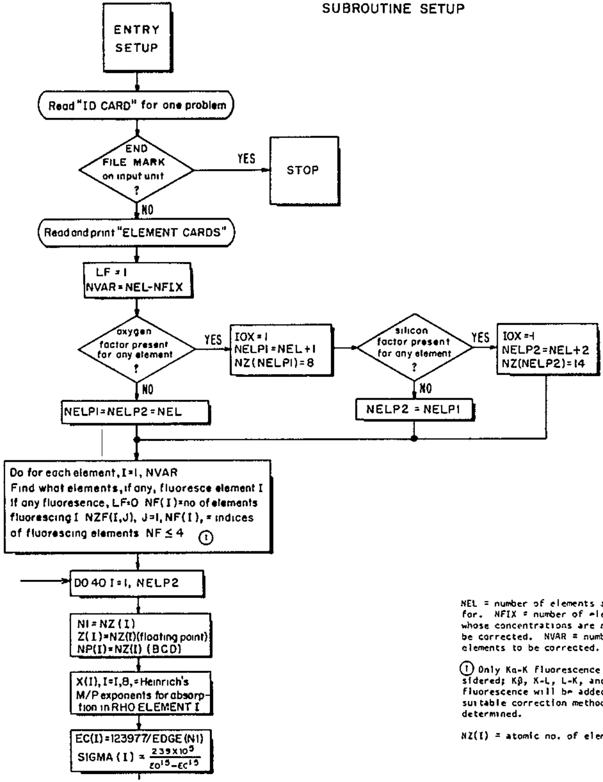


NELP2 = number of elements given plus oxygen and silicon, if present.

IMIN and IMAX = minimum and maximum number of iterations to be performed. DMIN = largest acceptable change in concentration of major elements from one iteration to the next.

Ⓐ These steps done only if oxygen and/or silicon factors present.

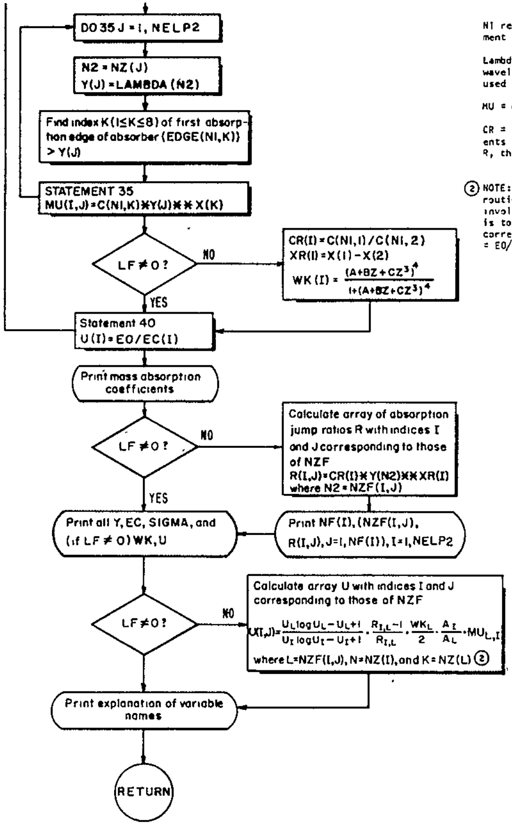
SUBROUTINE SETUP



NEL = number of elements analyzed for. NFIX = number of elements whose concentrations are not to be corrected. NVAR = number of elements to be corrected.

① Only Kα-K fluorescence is considered; Kβ, K-L, L-K, and L-L fluorescence will be added as suitable correction methods are determined.

NZ(I) = atomic no. of element I



N1 refers to atomic no. of element as absorber, N2, as emitter.

Lambda array contains the one wavelength (either k, L, or M) used for each element.

MU = mass absorption coefficient.

CR = ratio of Heinrich coefficients to be used in calculating R, the absorption jump ratio.

② NOTE: after exit from this subroutine, U is an expression involving many variables which is to be used in fluorescence corrections. IT IS NO LONGER = E0/EC.