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ELECTRON MICROPROBE ANALYSIS
PROGRAM FOR BIOLOGICAL SPECIMENS — BIOMAP

Program J201

by

Ben F. Edwards

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ELECTRON MICROPROBE ANALYSIS PROGRAM FOR BIOLOGICAL SPECIMENS — BIOMAP

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ABSTRACT

This program, BIOMAP, is a Univac 1108 compatible program which facilitates the electron probe microanalysis of biological specimens. Input data are x-ray intensity data from biological samples, the x-ray intensity and composition data from a standard sample and the electron probe operating parameters. Output are estimates of the weight percentages of the analyzed elements, the distribution of these estimates for sets of red blood cells and the probabilities for correlation between elemental concentrations. An optional feature statistically estimates the x-ray intensity and residual background of a principal standard relative to a series of standards.

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1. INTRODUCTION

The purpose of this program, BIOMAP, is to facilitate the electron microprobe analysis of biological specimens by computing from microprobe intensity count data and other parameters the quantity of specified chemical elements contained in formed elements of the blood and in micro-thin sections of tissue and gelatin. In addition, BIOMAP estimates background and concentration intensity counts for chemical elements in standards and computes and plots the distributions of elemental concentrations in red blood cell samples.

BIOMAP was developed as part of the Preventative Medicine Division Project 1030, Intracellular Chemical Characterization, which calls for research and development in areas of cellular chemical analysis by micro-X-ray spectrometry and UV microspectrometry. Direction of this effort was provided by Dr. Stephen L. Kimzey, Chief of the Cellular Analytical Section of the Clinical Laboratory, Preventative Medicine Division, NASA-MSC. Electron microprobe data used to test the mathematical model were provided by Mrs. Linda Burns, electron microscopist, The University of Texas Medical School at Galveston. The physical analysis, mathematical modeling, and programming were done by the author.

The atomic constant data and the Fortran-coded algorithm for calculating mass absorption coefficients are from the quantitative electron microprobe analysis program, MAGIC, written by J. W. Colby of Bell Telephone Laboratories, Inc., Allentown, Pennsylvania.

2. PROGRAM DESCRIPTION

2.1 General Description

The central feature of BIOMAP is the computation of absorption factors and the iterative computation of unknown elemental concentrations. Absorption factors quantify the amounts of characteristic X-radiation absorbed by the sample or standard and correctly relate X-ray intensity counts with elemental concentrations in the microprobe equation. Computation of unknown elemental concentrations is accomplished by solving the quantitative equation. This equation is functionally similar to the microprobe equation but involves instead ratios of the intensity counts, absorption factors, and elemental concentrations from unknown and standard samples.

Since a significant degree of variation is characteristic of both input and output data, certain statistical features have also been built into the program. First is a general linear hypothesis subroutine which inputs intensity count and absorption corrected area density data and computes estimates of the residual background and the rate of count increase with area density, along with associated variances. From these estimates and variances an estimate of the most probable intensity count for a given standard and its associated variance can be made. Second, if the unknown sample analyzed is a set of red blood cells (RBC), certain statistical parameters of the sample elemental concentrations are computed and cumulative and frequency functions of these concentrations are plotted.

BIOMAP can be set up to provide the following types of individual or combination analyses:

(1) Analyze microprobe data from a set of standards to statistically estimate the residual background intensity count and the concentration intensity count for the analyzed elements.

(2) Analyze microprobe data from a set of gelatin samples of known or unknown chemical content, obtaining concentration of specified elements.

(3) Analyze microprobe data from a set of red blood cells, obtaining weight percentages and weight percentage distribution plots.

Analyses (2) and (3) depend on input data from a previous type (1) analysis; however, combination analyses of types (1) and (2) and of types (1) and (3) can be made.

The logical sequence of program operations is as follows:

(1) References atomic constant data from block data storage.

(2) Provides by data statement the weight fractions of chemical elements in normal red blood cells and plain gelatin

(3) Reads data cards to input problem information, microprobe parameters, sample and standard data, and program mode

(4) Constructs atomic number arrays for analyzed elements and elements added to standards

(5) Forms symbol, atomic number, and area density arrays for elements in dry gelatin standards

(6) Computes the mass absorption coefficients of the sample and standard elements for the X-ray wavelengths analyzed

(7) Computes partial and total mass absorption coefficients of standard for each analyzed X-ray wavelength

(8) Computes absorption factors for each analyzed X-ray wavelength of standard

(9) Computes area densities of analyzed elements in standard

(10) Computes estimates of statistical parameters for a set of standards and the best linear unbiased estimate of the accumulated count for a specified standard.

For analysis of red blood cells and thin gelatin or tissue samples, the program performs the following operations:

(11) Inputs chemical symbols and intensity counts for analyzed elements in each sample

(12) Forms initial area density arrays for each sample

(13) Computes mass absorption coefficient of sample for lines analyzed

(14) Computes absorption factors for analyzed lines in sample

(15) Computes the absorption correction for each element analyzed

(16) Computes the area density of each analyzed element in the sample

(17) Updates area density and tests against reiteration criterion

(18) Computes the volume density of analyzed elements in gelatin samples

(19) Computes weight fractions of analyzed elements in red blood cell sample set

(20) Computes weight-percentage range, average, variance, and percentage standard deviation over red blood cell set for each analyzed element

(21) Provides cumulative distribution and histogram plots of the weight-percentage distributions.

In operation (1), the atomic constants read from the data tape for each element are the atomic number, the elemental symbol, the critical excitation potentials for the K, L, and M X-ray states, the wavelengths of the $K\alpha$, $L\alpha$, and $M\alpha$ spectral lines, the absorption edge wavelengths, exponents, and empirical constants for mass absorption coefficient equations, and fifth-degree polynomial coefficients for the backscatter factor.

In operation (3), problem information consists of alphanumerics for problem type, problem number, date, submitter's name, and a descriptive title. Microprobe parameters are accelerating potential, beam diameter, beam current, counting time, and counter dead time. Sample information consists of a sample type index, the number of samples to be analyzed, the number of analyzed elements in each sample, and the wet thickness of the samples in microns. Standard information consists of the grams of gelatin per liter used in preparing the standards, the water fraction in the gelatin, the thickness of the wet standard sections, the number of standards input for statistical evaluation, and the symbols of the analyzed elements. If a single standard is used the estimated residual background and intensity count for each standard element is read in with the standard symbols. The program parameters specify whether to print out intermediate results in namelists and the weight options in subroutine GLHFR2. If multiple standards are analyzed to obtain a linear unbiased estimate of the residual background and intensity count for each standard element, the number of elements added to each standard, and their chemical symbol and amounts in grams are read in at the top of the standard analysis loop. Also, at the top of this loop is read the flag for the primary standard and the chemical symbols of the analyzed standard elements and their concentration intensity count. If multiple standards are processed to estimate the primary standard intensity count, microfilm plots are produced of the data points and the fitted line.

2.2 Technical Description

2.2.1 Analysis

In general, X-ray states are excited in microprobe specimens primarily by incident electrons and secondarily by sufficiently energetic X-ray photons resulting from the fluorescent decay of X-ray states. The average number n of specified X-ray states excited in a given atomic species per single-incident electron can be represented as

$$n = n' + n'' \qquad (1)$$

where n' is the average number resulting from primary excitation and n'' is the average number resulting from secondary excitation.

Equation (1) can be expressed in the alternate form

$$n = n'\left(1 + \frac{n''}{n'}\right) = n'f \qquad (2)$$

where $f > 0$ is defined as the fluorescence factor.

The derivation of an expression for n' is of central importance in quantitative microprobe theory and proceeds as follows:

In differential form, the average number of specified X-ray states dn' of energy E_c excited within an electron path length dx is

$$dn' = \delta Q(E(x), E_c)\ dx \qquad (3)$$

where E is the average electron energy over dx; Q is the ionization cross-section of the given atomic X-ray state, a function of E and E_c ; and δ is the number of specified atoms per unit volume of specimen.

In a thick specimen where the energy of the penetrating electron may decay below $3E_c$ while traversing a path length x , Q cannot be considered constant, and

$$n' = \delta \int_0^x Q\ dx = \delta \int_{E_0}^{E} [Q/(dE/dx)]\ dE$$

For a thin low-density specimen, however, one can reasonably assume that entering electrons completely penetrate the target with little loss of energy or scattering. As a consequence, Q is effectively constant and the path length dx can be equated to the sample thickness z. These approximations enable writing Equation (3) as

$$n' = \delta Qz \qquad (4)$$

The average number of states produced in time t by a beam current i_b, considering a fraction of ionizations $(1 - R)$ to be lost as a result of electron backscattering, can be expressed as

$$N' = \phi tR\delta Qz \qquad (5)$$

where ϕ the electron flux equals i_b divided by the electronic charge q_e.

Since the microprobe measures ionizing events caused by X-ray photons resulting from the decay of the excited X-ray states, the microprobe equation relating measured intensity and atomic concentration is

$$I = (\Omega/4\pi)Dwp\phi tafR\delta Qz \qquad (6)$$

These additional factors are defined as follows:

$(\Omega/4\pi)$ is the fraction of the total solid angle intercepted by the X-ray spectrometer, D is the spectrometer-detector efficiency, w is the fluorescence yield of the particular X-ray state, and p is the probability that the photon emitted will be that specified. The factors a and f are the absorption and fluorescence factors respectively and both depend on the chemical and physical configuration of the specimen. The absorption factor a is the probability of a photon not being absorbed as it passes through the sample, and is less than one. The fluorescence factor f accounts for the number of states produced secondarily by X-ray photons with energy greater than E_c, and is greater than one.

A thin standard sample having a known concentration of the specified chemical element would yield a measured intensity

$$I_0 = (\Omega/4\pi) Dwp\phi t a_0 f_0 R_0 z_0 Q \delta_0 \tag{7}$$

By forming the ratios I/I_0 the common factors may be eliminated by division, leaving

$$I_0/I = (a_0/a)(f_0/f)(R_0/R)(z_0/z)\ \delta_0/\delta \tag{8}$$

If the standard is chemically constituted sufficiently similar to the unknown sample, the value of the factors (f_0/f) and (R_0/R), known as the fluorescence and backscatter corrections respectively, become essentially one, leaving

$$I_0/I = (a_0/a)(z_0/z)\ \delta_0/\delta \tag{9}$$

Gelatin-based standards can be chemically constituted similar to a biological specimen but cannot be cut as thin as a red blood cell for instance and, therefore, expressions must be derived for the absorption factor which depends on sample thickness.

An expression for the absorption factor can be simply derived by assuming that X-ray states are produced uniformly over the thickness z, a reasonable assumption since Q is essentially constant for $E \geq 3E_c$. One can start with the differential relation

$$dI = qN \cdot dz \qquad (10)$$

when dI' are the number of photons observed by the detector, N is the number of photons generated per unit path length, and q is the probability of a photon not being absorbed or scattered.

The probability q can be identified from Beer's law

$$i = i_0 e^{-\chi \rho z}$$

as the exponential factor $e^{-\chi \rho z}$ where

$$\chi = \csc \psi \sum w_i \mu_i \qquad (11)$$

and ψ is the angle of emergence of the photons, w_i is the weight fraction of the *ith* element in the sample and μ_i is the mass absorption coefficient of the *ith* element for the specified X-ray photon.

By "integrating over the thickness z the number of photons detected I are

$$I = N \int_0^z e^{-\chi \rho z'} dz' = N(1 - e^{-\chi \rho z})/\chi \rho$$

and the fraction detected (not absorbed) is

$$a = \frac{I}{Nz} = (1 - e^{-\chi\rho z})/\chi\rho z$$

The absorption correction can be expressed as

$$(a_0/a) = \frac{\left(1 - e^{-\chi_0\rho_0 z_0}\right)\chi\rho z}{\left(1 - e^{-\chi\rho z}\right)\chi_0\rho_0 z_0} \tag{12}$$

which, when substituted into the quantitative equation, Equation (9), yields

$$\frac{I_0}{I} = \frac{\left(1 - e^{-\chi_0\rho_0 z_0}\right)\left(\chi\rho z\right)}{\left(1 - e^{-\chi\rho z}\right)\left(\chi_0\rho_0 z_0\right)} \frac{\delta_0 z_0}{\delta z} \tag{13}$$

Since biological specimens are prepared wet and dry under vacuum, it is no longer possible to know the resulting thickness or dry-volume density of a standard element. However, if there is no lateral redistribution of the sample material, the dry area densities $\sigma_0^i = \rho_0^i z_0$ of the standard elements remain invariant and Equation (13) can be written and solved in terms of area densities

$$\sigma^i = \frac{\left(1 - e^{-\chi_0^i\sigma_0}\right)\chi^i\sigma}{\left(1 - e^{-\chi^i\sigma}\right)\chi_0^i\sigma_0} \frac{I^i}{I_0^i} \sigma_0^i \tag{14}$$

Here σ and σ_0 without superscripts represent the total area density of sample and standard respectively, and the superscript i designates quantities specific for the *ith* element.

2.2.2 Method of Solution

If one knows as a zero order approximation the normal average-weight fractions of elements in a biological sample, its total area density, and can analyze simultaneously any elements whose concentrations deviate significantly from normal, then the quantitative microprobe equation used with an iterative computational procedure will provide a higher order estimate of the area densities of the analyzed elements. The iterative procedure is made necessary by the nature of the absorption coefficient which cannot be computed exactly before the solution is obtained. Convergence to solutions lying within the precision of experimental measurement is rapidly achieved, however, by recomputing the absorption factor of the sample subsequent to each iterative area density computation.

A summary of the input data and computational method in mathematical notation is as follows:

I. Computations related to the standard

A. Input data

1. w_i – weight fractions of elements in gelatin ($i = 1, \ldots, L$)

2. h – fraction of water in gelatin

3. g – grams gelatin per liter standard solution

4. t — thickness of wet gelatin slice

5. a_j — gram atoms of standard elements added ($j = 1, \ldots, M$)

6. B_k — accumulated background intensity count for *kth* analyzed element ($k = 1, \ldots, N$)

7. N_k — accumulated intensity count for *kth* analyzed element ($k = 1, \ldots, N$)

8. Atomic constants (J. W. Colby)

B. Computations

1. Compute mass of each element in gelatin.

$$m_i' = w_i(1 - h)g \qquad (i = 1,\ldots,L)$$

2. Compute mass of each added element.

$$m_j'' = a_j A_j \qquad (j = 1,\ldots,M)$$

3. Compute total mass of each element in liter of standard solution.

$$m_i = m_i' + m_i''$$

4. Compute volume density of each element in standard solution.

$$\rho_i = m_i/1000$$

5. Compute area density of each element in dry mounted standard.

$$\sigma_i = \rho_i t$$

6. Compute total area density of dry mounted standard.

$$\sigma = \sum \sigma_i$$

7. Compute weight faction of each element in dry mounted standard.

$$w_i = m_i/\sum m_i = \rho_i/\sum \rho_i = \sigma_i/\sigma$$

8. Compute mass absorption (attenuation) coefficients of *ith* element for Kα line of *kth* element analyzed.

$$\mu_i^k = c(z_i)\lambda_k^{n(z_i)} \quad ; \quad (k = 1, \ldots, N)$$

c and n are constants obtained from J. W. Colby's set of atomic constants.

9. Compute mass absorption coefficient of sample for each element analyzed.

$$\chi^k\sigma = \csc \psi \sum \sigma_i (\mu/\rho_i)^k$$

10. Compute absorption factor of standard for each element analyzed.

$$a_k^o = \left(1 - e^{-\chi^k \sigma}\right) / \chi^k \sigma$$

II. Computation related to the red blood cells

A. Input data

w_i – approximate weight fractions of elements in dry RBCs ($i = 1, \ldots, L$)

$\overline{\sigma}$ – average area density of dry RBC

N_k – accumulated count for k*th* element analyzed, corrected for background ($k = 1, \ldots, N$)

B. Computations

1. Compute approximate average area density of each element in dry red blood cells.

$$\overline{\sigma}_i = w_i \overline{\sigma}$$

2. Compute average mass absorption coefficient of RBC for each element analyzed.

$$\chi^k \overline{\sigma} = \csc \psi \sum \sigma_i (\mu/\rho_i)^k$$

3. Compute average absorption factor of dry red blood cells for k*th* element analyzed.

$$a_k = \left(1 - e^{-\chi^k \overline{\sigma}}\right) / \chi^k \overline{\sigma}$$

4. Compute area density σ_k of kth element analyzed using quantitative equation.

$$\sigma_k = \sigma_k^0 \left(\frac{a_k^0}{a_k}\right)\frac{N_k}{N_k^0}$$

5. Recompute total area density of RBC using new area density values of the N analyzed elements.

$$\bar{\sigma} = \sum_{k=1}^{N}\sigma_k + \sum_{i=1}^{L-N}\sigma_i$$

6. Repeat computations (2) through (5) until the largest σ_k update is less than some arbitrary percent (0.1 percent for example).

7. Compute the final weight fractions of the elements in the RBC.

$$w_i = \frac{\sigma_i}{\bar{\sigma}}$$

3. USAGE

3.1 Input Description

3.1.1 Data and Card Specifications

All integer (I) input is right-justified, alphanumeric (A) input is left-justified, and real number (F) input is unrestricted in its specified fields.

3.1.1.1 Card 1: Title and Run Information
FORMAT(A1,I4,2X,5A3,2X,5A4,2X,6A4)

Code	Type	Columns	Description and Units
IDATE	I	1,10	Date
MISS	I	11,15	Mission identification
MAN	I	16,20	Subject code
JSET	I	21,25	Sample code

3.1.1.2 Card 2: Program Parameters
FORMAT(3I5,F5.0)

Code	Type	Columns	Description and Units
IPRINT	I	1,5	Namelist; write indicator for diagnostic purposes (IPRINT $\leq$ 0 for "no write")
IWT	I	6,10	Weight index for subroutine GLHFR2 [0 – weights are input through calling arguments as 1/(sample variance). 1 – weights are defined as 1. in the subroutine. 2 – weights are calculated in the subroutine as 1/Y(I)].

3.1.1.3 Card 3: Microprobe Parameters
FORMAT(4F10.2)

Code	Type	Columns	Description and Units
AP	F	1,10	Accelerating potential (Kv)
BD	F	11,20	Beam diameter (10^{-4} cm)
CT	F	21,30	Count time (sec)
DT	F	31,40	Dead time (10^{-3} sec)

3.1.1.4 Card 4: Sample Parameters
FORMAT(3I5,F5.0)

Code	Type	Columns	Description and Units
ITYPE	I	1,5	Sample type (1 – RBC, 2-tissue, 3-gelatin standard)
NSAMP	I	6,10	Number of samples
NA	I	11,15	Number elements analyzed
TBIO	F	16,20	Thickness of samples (10^{-4} cm)

3.1.1.5 Card 5: Standard Parameters
FORMAT(3F10.5,I5)

Code	Type	Columns	Description and Units
GEL	F	1,10	Gelatin in liter of standard solution (grams)
H2O	F	11,20	Fraction of water in stock gelatin ($0. \leq H2O \leq 1.$)
TSTD	F	21,30	Thickness of standard section (10^{-4} cm)
NSTD	I	31,35	Number of standard intensity counts

3.1.1.6 Card 6: Single Stand^rd Estimated Data
FORMAT(A2,3X,3F10.0)

Code	Type	Columns	Description and Units
AE(I)	A	1,2	Chemical symbol for I*th* analyzed element (right justified)
BG(I)	F	6,15	Statistically estimated background for I*th* analyzed element
ESC(I)	F	16,25	Statistically estimated intensity count for I*th* analyzed element
SDVESC(I)	F	26,35	Standard deviation of estimated intensity count for I*th* analyzed element.

Note: Program requires one card 6 for each element analyzed. These cards are punched out when program runs statistical analysis of standard data, ITYPE = 0 .

3.1.1.7 Card 7: Standard Chemical Composition
FORMAT(I1,3X,6(A2,1X,F6.1,1X))

Code	Type	Columns	Description and Units
NAD	I	1	Number elements added to standard
ASE(I)	A	5,6	Chemical symbol of added element (right justified)
AMTASE(I)	F	8,13	Amount added element (meq/ℓ)
ASE(n)	A	10n -5, 10n -4	n*th* chemical symbol

Code	Type	Columns	Description and Units
AMTASE(n)	F	10n -2, 10n +3	*nth* amount

Note: Program dimension limitation, n ≤ 6 .

3.1.1.8 Card 8: Standard Intensity Counts
FORMAT(I2,2X,4(A2,1X,F6.0,1X,F6.0,1X))

Code	Type	Columns	Description and Units
IPS	I	1,2	Principal standard indicator (IPS = 1 designates principal standard)
ADSE(1)	A	5,6	Chemical symbol of first analyzed element
SCT(1,ND)		8,13	Intensity count of first analyzed element in ND*th* standard
SCTSD(1,ND)		15,20	Standard deviation of estimated count
ADSE(n)		17n -12, 17n -11	For *nth* element
SCT(n,ND)		17n -9, 17n -8	For *nth* element

Note: Program dimension limitation is n ≤ 10 , *and card space limitation is four elements per card.*

3.1.1.9 Card 9: Biological Elements Analyzed
FORMAT(6(8X,A2))

Code	Type	Columns	Description and Units
ABE(1)	A	9,10	Chemical symbol of first analyzed element
ABE(n)	A	10n - 1, 10n	For *nth* analyzed element

3.1.1.10 Card 10: Sample Intensity Counts
FORMAT(6F10.0)

Code	Type	Columns	Description and Units
CTB(1)	F	1,10	Intensity count of first analyzed element
CTB(n)	F	10n -9, 10n	For *nth* analyzed element

Note: Program dimension limitation is $n \leq 10$, *and card space limitation is* $n \leq 7$ *for cards 9 and 10.*

3.1.2 Tape Specifications

Program tape, NASA-MSC Computation and Analysis Division No. A06690 has one file containing the program with subroutines.

3.2 Program Run Preparation

3.2.1 Deck Setup

3.2.1.1 Punched Program Deck Run

Running the program from a punched program deck requires the following card sequence:

1. NASA-MSC run card (∇ RUN)
2. Message card specifying one tape (∇N MSG 1 TAPE)
3. Microfilm plot control card (∇ PLT)
4. Input tape assign card (∇ ASG A=4483)
5. BIOMAP control card (∇ FOR BIOMAP)
6. BIOMAP program deck
7. GLHFR2 control card (∇ FOR GLHFR2)
8. GLHFR2 subroutine deck
9. IGIVE control card (∇ FOR IGIVE)
10. IGIVE subroutine deck
11. GROP1 control card (∇ FOR GROP1)
12. GROP1 subroutine deck
13. PLOT3 control card (∇ FOR PLOT3)
14. PLOT3 subroutine deck
15. HIS1 control card (∇ FOR HIS1)
16. HIS1 subroutine deck
17. PCORRE control card (∇ FOR PCORRE)
18. PCORRE subroutine deck
19. GAMMA control card (∇ FOR GAMMA)
20. GAMMA subroutine deck
21. FACTOR control card (∇ FOR FACTOR)
22. FACTOR subroutine deck

23. Program execute control card (∇ XQT BIOMAP)

24. Data deck

25. End-of-file control card (∇ EQF)

26. Optional post mortem dump control card (∇E PMD)

3.2.1.2 Tape Run

Running the program from a tape requires the following:

1. NASA-MSC run card (∇ RUN)
2. Message card specifying two tapes (∇N MSG 2 TAPES)
3. Microfilm plot control card (∇ PLT)
4. Input tape assign card (∇ ASG E=$STATP)
5. Program tape assign card (∇ ASG B=   )
6. Complex utility program execute control (∇ XQT CUR) and the four following CUR statements
7. TRW B
8. IN B
9. TRI B
10. TOC
11. Control cards for listing or changing the program or subroutine statements (∇ FOR,* NAME, NAME)
12. Follow with cards described in paragraph 3.2.1.1, sections (23), (24), (25), and (26), as for program deck run.

3.2.2 Special Control Cards

Card 2, the program parameter card, contains (1) IPRINT which must be assigned a nonzero integral value to obtain a namelist printout for diagnostic purposes, and (2) the weighting index IWT to specify the weighting option for subroutine GLHFR2.

3.2.3 Special I/O Devices

None.

3.2.4 Overlay Structure

None.

3.3 Output Description

3.3.1 Printer Output Identification

A run which analyzes a number of standard intensity counts to statistically estimate the intensity count of the primary standard will print out a table giving, for each added element of each standard, the total milli-equivalent amount (residual plus added), the measured intensity count, the area density, the weight percent, the absorption factor; and, for the primary standard, the estimated intensity count with standard deviation, the estimated background count with standard deviation, and the estimated intensity count less the background.

For a run analyzing standard samples relative to a primary sample a table is printed out giving for each analyzed element in each sample the measured intensity count, the absorption factor, the absorption correction, the area density, the weight percent and the calculated concentration of the standard samples.

For a run analyzing a set of red blood cells relative to a primary sample, a table is printed out giving for each analyzed element in each red blood cell the measured intensity count, the area density, and the weight percent; and, for the set, the weight percent range. In addition, a cumulative plot and a histogram of the weight-percent distribution over the set is printed.

3.3.2 Microfilm Output

For each analyzed element in a set of standards a microfilm plot is made which relates the estimated linear relation between the intensity count and the absorption-corrected area density for that element.

3.4 Execution Characteristics

3.4.1 Restrictions

The following analytic restrictions must be observed:

(1) When analyzing a set of standards to estimate a most probable intensity count for the principal standard, assign the integer value of one to the program parameter IWT if the standard data are single-point microprobe intensity counts. If the standard data are average intensity counts over samples taken from each standard and the sample variances, assign the integer value two to IWT.

(2) The number of standard data must be greater than two. If not, the program will stop in the subroutine GLHFR2 after writing a diagnostic message noting this error.

(3) When specific standard or sample data are input (card 10), they are accompanied by the chemical symbol of the corresponding elements (card 9). If these symbols are not found when checked against the array of analyzed element symbols the program stops after writing out a diagnostic statement noting this error.

(4) Principal standard data *must* be last in the sequence of standards.

3.4.2 Running Time/Lines of Output

A multiple-execute analysis of sodium and potassium in sets of 100, 35, 35, and 35 red blood cells ran 1.5 minutes. A combined statistical analysis of five standard averages and sodium and potassium analysis of nine standard samples ran 0.5 minute. Lines of output can be calculated as one line per element analyzed in each standard or red blood cell analyzed. A run performing all analyses of red cell sets outputs cumulative distribution and frequency distribution plots over weight percentage, each of which require three pages per element analyzed.

3.4.3 Accuracy/Validity

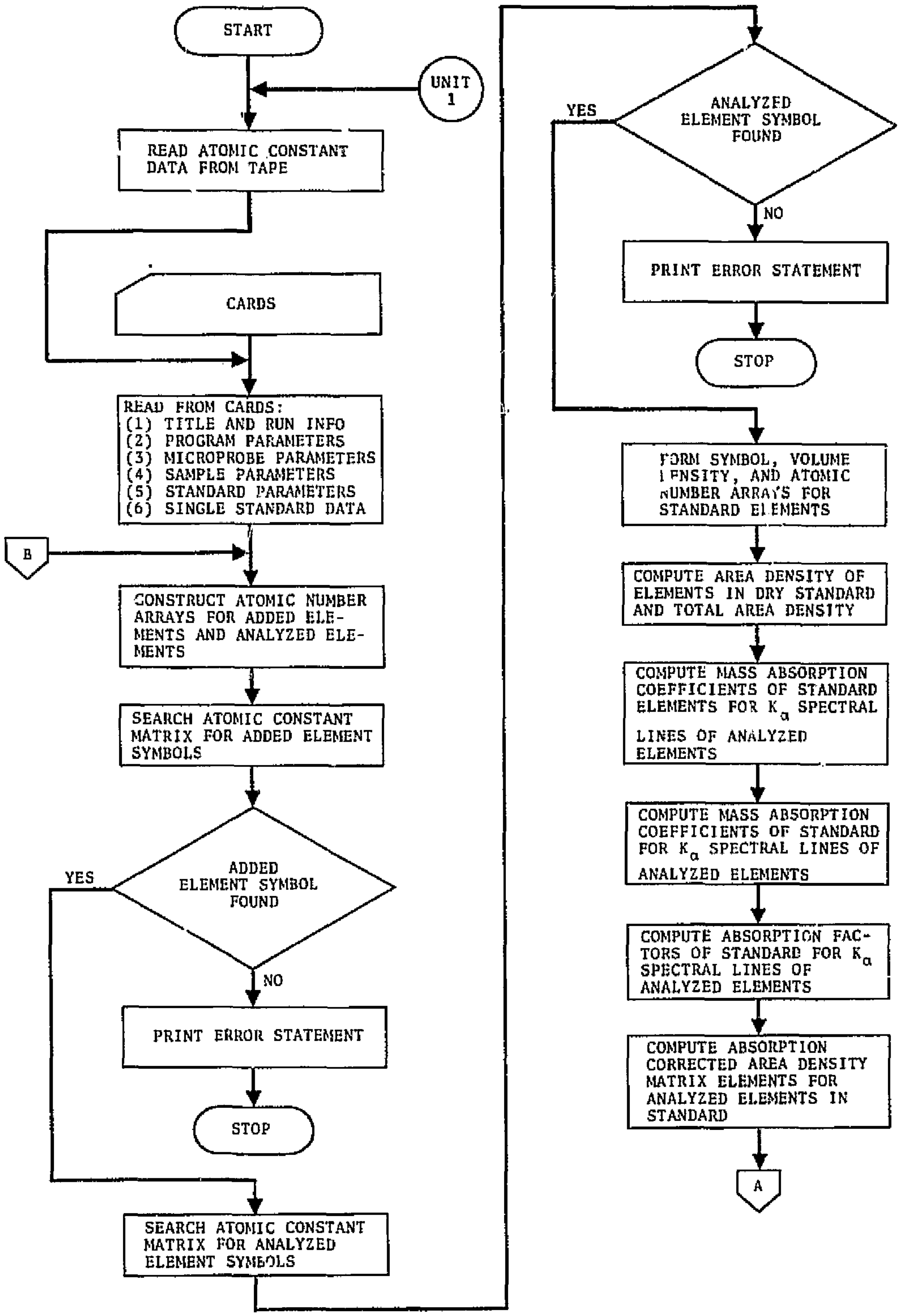
Arithmatic operations are single-precision, which is quite adequate for the four significant figure iterative criterion of the area density computation. This computational precision is an order of magnitude better than the precision of experimental measurement.

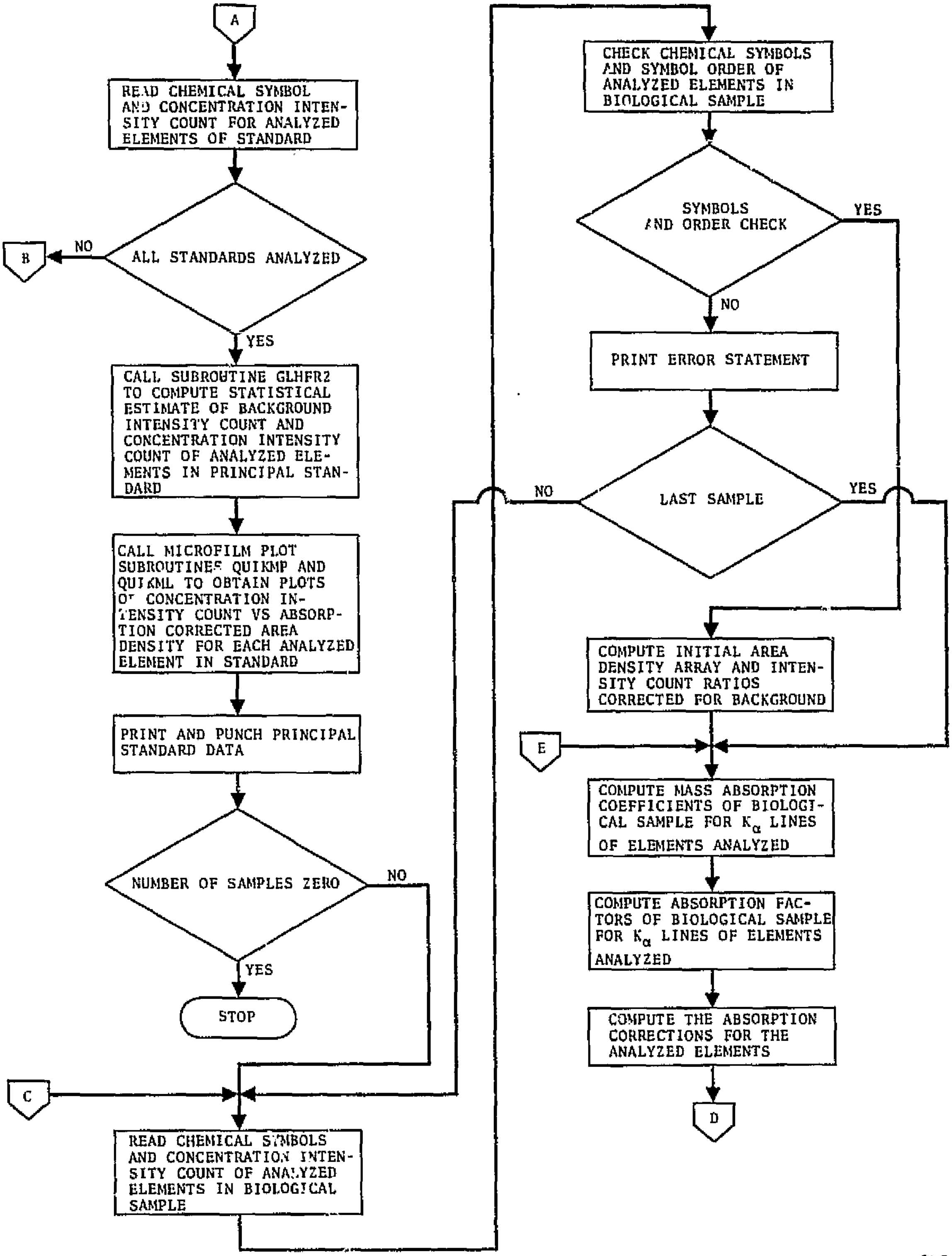
4. REFERENCE INFORMATION

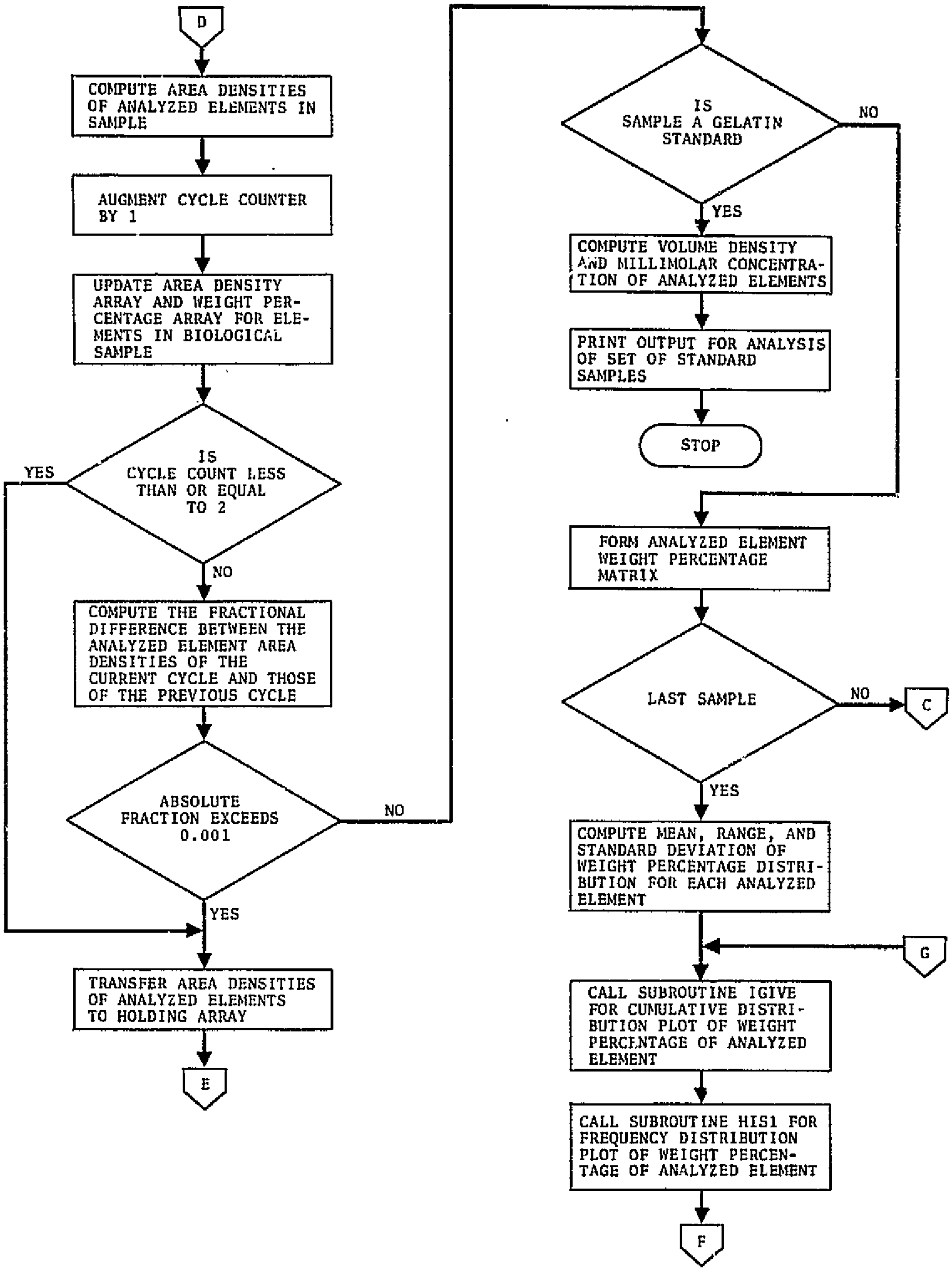
4.1 Detailed Flow Chart of BIOMAP

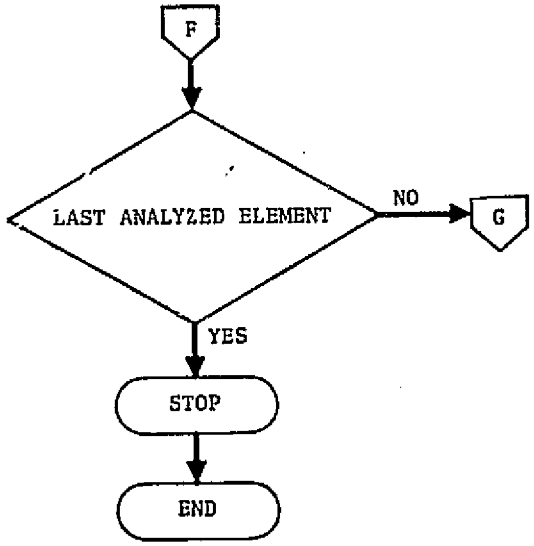
The detailed flow chart of BIOMAP is shown on the following pages.

DETAILED FLOW CHART OF BIOMAP




A
READ CHEMICAL SYMBOL AND CONCENTRATION INTENSITY COUNT FOR ANALYZED ELEMENTS OF STANDARD
ALL STANDARDS ANALYZED
NO
B
YES
CALL SUBROUTINE GLHFR2 TO COMPUTE STATISTICAL ESTIMATE OF BACKGROUND INTENSITY COUNT AND CONCENTRATION INTENSITY COUNT OF ANALYZED ELEMENTS IN PRINCIPAL STANDARD
CALL MICROFILM PLOT SUBROUTINES QUIKMP AND QUIKML TO OBTAIN PLOTS OF CONCENTRATION INTENSITY COUNT VS ABSORPTION CORRECTED AREA DENSITY FOR EACH ANALYZED ELEMENT IN STANDARD
PRINT AND PUNCH PRINCIPAL STANDARD DATA
NUMBER OF SAMPLES ZERO
NO
YES
STOP
C
READ CHEMICAL SYMBOLS AND CONCENTRATION INTENSITY COUNT OF ANALYZED ELEMENTS IN BIOLOGICAL SAMPLE
CHECK CHEMICAL SYMBOLS AND SYMBOL ORDER OF ANALYZED ELEMENTS IN BIOLOGICAL SAMPLE
SYMBOLS AND ORDER CHECK
YES
NO
PRINT ERROR STATEMENT
LAST SAMPLE
NO
YES
COMPUTE INITIAL AREA DENSITY ARRAY AND INTENSITY COUNT RATIOS CORRECTED FOR BACKGROUND
E
COMPUTE MASS ABSORPTION COEFFICIENTS OF BIOLOGICAL SAMPLE FOR K_α LINES OF ELEMENTS ANALYZED
COMPUTE ABSORPTION FACTORS OF BIOLOGICAL SAMPLE FOR K_α LINES OF ELEMENTS ANALYZED
COMPUTE THE ABSORPTION CORRECTIONS FOR THE ANALYZED ELEMENTS
D


D
COMPUTE AREA DENSITIES OF ANALYZED ELEMENTS IN SAMPLE
AUGMENT CYCLE COUNTER BY 1
UPDATE AREA DENSITY ARRAY AND WEIGHT PERCENTAGE ARRAY FOR ELEMENTS IN BIOLOGICAL SAMPLE
IS CYCLE COUNT LESS THAN OR EQUAL TO 2
YES
NO
COMPUTE THE FRACTIONAL DIFFERENCE BETWEEN THE ANALYZED ELEMENT AREA DENSITIES OF THE CURRENT CYCLE AND THOSE OF THE PREVIOUS CYCLE
ABSOLUTE FRACTION EXCEEDS 0.001
NO
YES
TRANSFER AREA DENSITIES OF ANALYZED ELEMENTS TO HOLDING ARRAY
E
IS SAMPLE A GELATIN STANDARD
NO
YES
COMPUTE VOLUME DENSITY AND MILLIMOLAR CONCENTRATION OF ANALYZED ELEMENTS
PRINT OUTPUT FOR ANALYSIS OF SET OF STANDARD SAMPLES
STOP
FORM ANALYZED ELEMENT WEIGHT PERCENTAGE MATRIX
LAST SAMPLE
NO
C
YES
COMPUTE MEAN, RANGE, AND STANDARD DEVIATION OF WEIGHT PERCENTAGE DISTRIBUTION FOR EACH ANALYZED ELEMENT
G
CALL SUBROUTINE IGIVE FOR CUMULATIVE DISTRIBUTION PLOT OF WEIGHT PERCENTAGE OF ANALYZED ELEMENT
CALL SUBROUTINE HIS1 FOR FREQUENCY DISTRIBUTION PLOT OF WEIGHT PERCENTAGE OF ANALYZED ELEMENT
F


F
LAST ANALYZED ELEMENT
NO
G
YES
STOP
END

4.2 Symbol Definitions

Math	Code	Type	Description
$x^n\sigma$	ABC(n)	F	Mass absorption coefficient of biological sample for n*th* analyzed element.
$(a_0/a)_n$	ABCO(n)	F	Absorption correction for n*th* analyzed element.
	ABCS(n)	F	Mass absorption coefficient of standard for n*th* analyzed element.
	ABE(n)	I	Chemical symbol of n*th* analyzed element in biological sample.
μ_m^n	AC(n,m)	F	Mass absorption coefficient of m*th* element for Kα line of n*th* analyzed element.
σ	ADB	F	Area density of biological sample.
σ_n	ADNB(m)	F	Area density of m*th* element in biological sample.
σ_m^0	ADNS(m)	F	Area density of m*th* element in standard.
σ^0	ADS	F	Area density of standard.
	ADSE(n)	I	Chemical symbol of n*th* analyzed element in standard.
	AE(n)	I	Chemical symbol of n*th* analyzed element in single standard.

Math	Code	Type	Description
a_n	AFB(n)	F	Absorption factor of biological sample for *nth* analyzed element.
a_n^0	AFS(n)	F	Absorption factor of standard for *nth* analyzed element.
	AMTASE(ℓ)	F	Amount in millimoles per liter of *ℓth* element added to standard.
w_m^0	AMTGEL(m)	F	Approximate weight percentage of *mth* element in dry gelatin. Literal list in data statement.
w_{nc}	AMTRBD(m)	F	Approximate weight fraction of *mth* element in normal dry red blood cell. Literal list in data statement.
E_0	AP	F	Kinetic energy of focused electrons given in Kev. Also electron gun accelerating potential. Not used in calculation.
	ARATIO	F	Ratio of effective area of excitation on the standard to that of the biological sample. Assigned a value of 1.0 for this version of BIOMAP.

Math	Code	Type	Description
	ASE(ℓ)	I	Chemical symbol of *ℓth* element added to standard.
	BD	F	Beam diameter (10^{-4} cm).
	BG(n)	F	Background intensity count for n*th* analyzed element in standard. *Note: Concentration intensity count for biological samples are assumed to be background corrected.*
	BIOEL(m)	I	Chemical symbol of m*th* element in normal biological cells. Literal list in data statement.
z_m	BIOZ(m)	I	Atomic number of m*th* element in normal biological cells. Literal list in data statement.
	COEF(k)	F	k*th* component of coefficient array for given analyzed element returned to BIOMAP from GLHFR2. COEF(1) is the estimated background intensity count (intercept) and COEF(2) is the estimated rate of concentration intensity count increase with absorption corrected area density (slope).

Math	Code	Type	Description
C	CON	F	Empirical constant C used in computing mass absorption coefficient ($re^{\kappa} = C\lambda_{\kappa}^{n}$). Obtained from atomic constants.
	CONC(n)	F	Concentration of *nth* analyzed element in gelatin sample (millimoles/liter).
I/I_0	CR(n)	F	Concentration intensity count ratio for *nth* analyzed element (sample count/standard count).
$\csc\psi$	CSCTH	F	Cosecant of 52.5 degrees the angle of X-ray emergence. Fixed parameter set equal to 1.2605.
	CT	F	Counting time for sample and standard (seconds).
I_n	CTB(n)	F	Concentration intensity count of *nth* analyzed element in biological sample.
	DATE	A	Date of computer run request.
	DEL(n)	F	Fractional difference between area densities of *nth* analyzed element as computed in two adjacent iterative cycles.
ρ_ℓ	PENAD(ℓ)	F	Volume density of *ℓth* element added to standard ($grams/cm^3$).
ρ_m	DENS(m)	F	Volume density of *mth* element in gelatin ($grams/cm^3$).

Math	Code	Type	Description
	DRYGEL	F	Concentration of anhydrous gelatin in standard base (grams/cm^3).
	DT	F	Counter dead time (10^{-6} seconds). Not used in computation.
λ	EDGE	F	Absorption edge wavelengths λ used in computation of mass absorption coefficients ($\mu^{\kappa} = C\lambda_{\kappa}^{\eta}$). Obtained from atomic constants.
	ESC(n)	F	Statistically estimated concentration intensity count for *nth* analyzed element of single standard.
η	EX	F	Exponent η of absorption wavelength λ used in computation of mass absorption coefficients ($\mu^{\kappa} = C\lambda_{\kappa}^{\eta}$). Obtained from atomic constants.
	F	F	An array of weight percentage frequencies falling in each interval or group. Returned from statistical subroutines IGIVE and HIS1.
	GEL	F	Concentration of stock gelatin in gelatin standard (grams/liter).
	HZO	F	Fraction of water in stock gelatin.

Math	Code	Type	Description
	ICOUNT	I	Iterative cycle counter for sample element area density computation.
	ICS	I	Array of chemical symbols for the chemical elements.
	INDX	I	Holder for sample number of principal standard. Always last standard in sequence.
	IPS	I	Flag identifying principal standard. Always last standard in sequence.
	ITITX ITITY	I and I	Data statement arrays containing abscissa and ordinate titles for microfilm plot of concentration intensity count vs absorption corrected area density.
	ITIT1 ITIT2	I and I	Data statements containing histogram of print plot headings.
	ITYPE	I	Type designator for sample to be analyzed (RBC-1, TISSUE-2, GELATIN-3).
	MDIM	I	Dimension of concentration intensity count and absorption corrected area density array input to subroutine GLHFR2.
	NA	I	Number elements analyzed.
	NAD	I	Number elements added to standard.

Math	Code	Type	Description
	NAME	A	Name of run requester.
	NBE	I	Number of biological elements.
	NG	I	Number of weight percentage groups. Fixed in program.
	NPROB	I	Problem number in title and run information (Card 1).
	NSAMP	I	Number of biological samples to be analyzed.
	NSE	I	Number of elements in standard.
	NSTD	I	Number sets of standard concentration intensity count data used in statistical estimates.
	NZ	I	Atomic number symbol used in computation of mass absorption coefficient.
	NZA(ℓ)	I	Atomic number of *ℓth* chemical element added to standard.
	NZAE(n)	I	Atomic number of n*th* analyzed element in standard.
	NZSE(m)	I	Atomic number of m*th* chemical element in standard.
	P(i,j)	F	j*th* atomic constant of i*th* atomic number chemical element (i = 1,100 and j = 1,36).
	PABC	F	Partial absorption coefficient of standard or sample.

Math	Code	Type	Description
	POE	F	Power of e (base of natural log); used in computing absorption factors.
	Q R	F and F	Arrays containing coordinates of endpoints of microfilm plotted line fitted to concentration intensity count vs absorption corrected area density data.
	RHOB2(n)	F	Computed volume density of n*th* analyzed element in gelatin sample.
	SCT(n)	F	Concentration intensity count of n*th* analyzed element in standard.
	SDEV	F	Standard deviation of RBC population distribution.
	SDVERR(n)	F	Estimated standard deviation of error in intensity count measurements for n*th* analyzed element.
	SDVESC(n)	F	Standard deviation of error in estimated concentration intensity count for n*th* analyzed element.
	SE	A	Chemical symbol array for elements in gelatin.
	SIGB1(n) SIGB2(n)	F and F	Area density of n*th* analyzed element in sample as computed

Math	Code	Type	Description
			in current and previous iterative cycles, respectively.
σ_n^0	SIGS(n)	F	Area density of *nth* analyzed element in standard.
	STEP	F	Width of weight percentage groups in cumulative and frequency distribution plots.
	SUM1 SUM2	F and F	Cumulative sums used in computing RBC distribution statistics.
	SX(i,j)	F	Absorption corrected area density of j*th* element in i*th* standard.
	TAG	A	Problem type identification.
	TBIO	F	Thickness of biological sample (10^{-4} cm).
	TITLE	A	Descriptive title of run.
	TSTD	F	Thickness of gelatin standard (10^{-4} cm).
	VAR	F	Variance of weight percentage distribution of analyzed element in RBC sample.
	VARCOV(i,j)	F	ij element of covariance matrix returned from GLHFR2.
	VARERR	F	Estimated measurement error variance returned from GLHFR2.
λ_K	WAVE	F	Wavelength of $K\alpha$ X-ray photon emitted by analyzed element.

Math	Code	Type	Description
w_m	WFBE(m)	F	Weight fraction of *mth* element in biological sample.
	WM	F	Array of statistical weights used in GLHFR2.
	WTPMX(i,s)	F	Weight percentage of *jth* analyzed element in *ith* RBC.
	X(i)	F	Weight percentage of specified element in *ith* RBC.
	XBAR	F	Mean weight percentage of specified element in RBC set.
	XL,XR	F	Left and right marginal values of absorption corrected area density in microfilm plot.
	XM	F	Array of absorption corrected area densities.
	XMAX XMIN	F	Maximum and minimum weight percentage of specified analyzed element in RBC sample.
	XMX	F	Maximum absorption corrected area density of specified analyzed element in set of standards.
	YB,YT	F	Top and bottom marginal values of intensity count for microfilm plot.
	YM	F	Array of intensity counts for specified analyzed element over set of standards.
	YMX	F	Maximum intensity count of specified analyzed element in set of standards.

4.3 Subprogram Documentation

4.3.1 STAT-CAT Statistical Subroutine

Documentation of the following subroutines can be found in the NASA-MSC Computation and Analysis Division Statistical Catalogue: IGIVE, GROT1, TLOT3, HIS1.

4.3.2 Subroutine GLHFR2

Documentation follows.

SUBROUTINE GLHFR2

IDENTIFICATION

Name/Title	—	GLHFR2 (General Linear Hypothesis Statistical Model of Full Rank Two)
Author/Date	—	B. F. Edwards, March 1971
Documented by/Date	—	B. F. Edwards, March 1971
Organization/Installation	—	LEC/NASA-MSC
Machine Identification	—	UNIVAC 1108
Source Language	—	FORTRAN V

PURPOSE

The purpose of this subroutine is to compute best linear unbiased estimates (BLUE) of parameters associated with a linear statistical model of full rank two. This model has the form $y = X\beta + e$ where Y is a random n-vector of weighted observations (measurements), X is an nx2-matrix of weighted known fixed independent quantities (experimental parameters), β is a 2-vector of unknown coefficients (intercept and slope), and e is an unknown random n-vector of measurement errors which satisfies either Case (1): e is distributed $N(0,\sigma^2 I)$, with σ^2 unknown, or Case (2): e is a random vector such that $E(e) = 0$ and $cov(e) = E(ee') = \sigma^2 I$, with σ^2 unknown.

USAGE

- Calling Sequence

CALL GLHFR2(N,X,Y,W,M,EB,EVAR,VAREB)

Math	Code	Type	Description
n	N	I	Number of observations.
$\{x_i\}$	X	F	n-array of known experimental constants.
$\{y_i\}$	Y	F	n-array of observations.
$\{w_i\}$	W	F	n-array of weighting coefficients.
	M	I	Calling program dimension of the X, Y, and W arrays.
$\hat{\beta}$	EB	F	2-array of linear coefficient estimate.
$\hat{\sigma}^2$	EVAR	F	Estimate of equivalent homegeneous error variance.
$cov(\hat{\beta})$	VAREB	F	4-array of variance-covariance matrix elements for cov $\hat{\beta}$ in the order: 11, 12, 21, 22.

- Data In/Out

Data is input or output through argument lists and the printed namelist HATS which contains N and EVAR and the elements of EB and VAREB.

- Error Messages

An error message is printed out and the program stops if N is not greater than 2.

- Storage

  Code: 252 octal

  Data: 143 octal (M = 25)

METHOD

If a quantity to be measured (μ) is known to depend linearly on a quantity (x) over a given range (x', x''), the functional relationship between μ and x is given by

$$\mu = a + bx \quad ; \quad (x' \leq x \leq x'') \tag{1}$$

where a and b are constant parameters. If a pair of points (x_1, μ_1) and (x_2, μ_2) are known which satisfy the relation (1), then a and b can be computed.

If, however, for fixed x, say x_i, one successively attempts to measure $\mu(x_i)$ but obtains fluctuating values y_{ij} where the subscript j denotes the *jth* measurement at x_i, then y_{ij} can be equated to the true value $\mu(x_i)$ plus an error e_{ij},

$$y_{ij} = \mu(x_i) + e_{ij}$$

or

$$y_{ij} = a + bx_i + e_{ij} \tag{2}$$

Solving Equation (2) for the error term yields

$$e_{ij} = y_{ij} - a - bx_i \tag{3}$$

If (A), the e_{ij} are normally distributed with mean 0 and variance σ_i^2, that is $e_{ij} \sim N(0,\sigma_i^2)$, or (B), the expectation of e_{ij} is 0 and the expectation of $(e_{ij})^2$ is σ_i^2; and, furthermore, for either (A) or (B) the σ_i^2 are equal for every i, then point and interval estimates of the parameters a and b and $\mu(x)$ can be made provided that the total number of measurement is greater than two and $i > 1$.

If the σ_i^2 are not equal, e_{ij} in Equation (3) may be transformed to $e_{ij}^* \sim N(0,1)$ so that all σ_i^2 are equal to unity. This transformation consists of multiplying (3) by $1/\sigma_i$ to obtain

$$e_{ij}^* = y_{ij}/\sigma_i - (a + bx_i)/\sigma_i$$

In general the σ_i are not known and estimates of σ_i, s_i must be obtained from independent measurements or as functions of y_i

$$e_{ij}^* = y_{ij}/s_i - (a + bx_i)/s_i \tag{4}$$

with e_{ij}^* distributed with variance σ^{*2} only approximately equal to one.

The n measurements (4) can be combined into the matrix equation

$$e = Y - X\beta \tag{5}$$

where e and Y are n-vectors;

X is a nx2-matrix with row elements $(\sqrt{w_i}\ , \ x_i\sqrt{w_i})$ where w_i , the weighting factor, is $1/s_i^2$; and β is the 2-vector of parameters a and b . Estimates of a and b can be obtained from estimators derived, in case (A) by the maximum-likelyhood method or, in case (B), by the least-squares method. In the least-squares method

$$\sum_1^n e_K^{*2} = e'e = (Y - X\beta)'(Y - X\beta) \tag{6}$$

Differentiating with respect to β and setting to zero yields

$$\partial(e'e)/\partial\beta = 2X'Y - 2X'X\beta = 0$$

and the unbiased estimate of β , $\hat{\beta}$ is the matrix solution

$$\hat{\beta} = (X'X)^{-1}X'Y \tag{7}$$

An estimate of σ^{*2} , the expectation of (e_{ij}^{*2}) following from (6), is $\sigma^{*2} = (Y - X_\beta)'(Y - X\beta)/n$. Slight modification produces an unbiased estimate:

$$\sigma^{*2} = (Y - X\hat{\beta})'(Y - X\hat{\beta})/(n - 2)$$

or

$$(Y'Y - \hat{\beta}'X'Y)/(n - 2) \tag{8}$$

Expansion of (7) yields:

$$a = \hat{\beta}_1 = \left(\sum w_i y_i \sum w_i x_i^2 - \sum w_i x_i \sum w_i x_i y_i\right) \Big/ D$$

$$b = \hat{\beta}_2 = \left(\sum w_i \sum w_i x_i y_i - \sum w_i x_i \sum w_i y_i\right) \Big/ D$$

with

$$D = \sum w_i \sum w_i x_i^2 - \left(\sum w_i x_i\right)^2 \tag{9}$$

Expansion of (8) yields:

$$\hat{\sigma}^{*2} = \left(\sum w_i y_i^2 - a\sum w_i y_i - b\sum w_i x_i y_i\right) \tag{10}$$

The variance-covariance matrix of $\hat{\beta}$ is given by

$$\text{cov}(\hat{\beta}) = (X'X)^{-1}\sigma^{*2} \cong (X'X)^{-1}\hat{\sigma}^{*2}$$

and yields

$$\hat{\sigma}_a^2 = \hat{\sigma}^{*2} \sum w_i x_i^2 / D$$

$$\hat{\sigma}_{ab}^2 = \hat{\sigma}_{ba}^2 = -\hat{\sigma}^{*2} \sum w_i x_i / D$$

$$\hat{\sigma}_b^2 = \hat{\sigma}^{*2} \sum w_i / D \tag{11}$$

In this subroutine the n-arrays of measurements Y , known fixed constants X , and precalculated weighting coefficients W are input through the calling arguments and the estimates in equations (9), (10), and (11) are calculated and output, also through the calling arguments.

- Symbol Definition

Math	Code	Type	Definition
D^{-1}	DETINV	F	Reciprocal of the determinant $D = \|X'X\| = \|S\|$.
$(X'X)^{-1}$	SINV11, SINV12, SINV22	F	The 11, 12, and 22 elements of the $(X'X)^{-1}$ or S^{-1} matrix.
w_i	WW	F	Working symbol for the weighting coefficient w_i .
x_i	XX	F	Working symbol for the fixed parameter x_i .
y_i	YY	F	Working symbol for the measurement y_i .
$w_i x_i$	WX	F	Product symbol.
$w_i x_i^2$	WXX	F	Product symbol.
$w_i x_i y_i$	WXY	F	Product symbol.
$w_i y_i$	WY	F	Product symbol.
$w_i y_i^2$	WYY	F	Product symbol.
$\sum w_i$	SUMW	F	Sum of the w_i .
$\sum w_i x_i$	SUMWX	F	Sum of the products $w_i x_i$.
$\sum w_i x_i^2$	SUMWXX	F	Sum of the products $w_i x_i^2$.
$\sum w_i x_i y_i$	SUMWXY	F	Sum of the products of $w_i x_i y_i$.

Math	Code	Type	Definition
$\sum w_i y_i^2$	SUMWYY	F	Sum of the products $w_i y_i^2$.
$\sum w_i^2$	SUMWW	F	Sum of the products w_i^2.
X'Y	XTY1, XTY2	F	Components of the vector (X'Y).

- References

F. A. Graybill, *An Introduction to Linear Statistical Models*, Vol. 1, McGraw-Hill Book Company, Inc., New York (1961), Chapter 6.

C. A. Bennett and N. L. Franklin, *Statistical Analyses in Chemistry and the Chemical Industry*, John Wiley and Sons, New York (1954), Section 6.27.

RESTRICTIONS

- Analytic

The number of observations (measurements) must be greater than two.

- Hardware

None.

- Operational

None.

ACCURACY

The subprogram uses single-precision accuracy. There is no loss of significance in the output.

VALIDATION PLAN

Mathematical equations were checked out by showing, when the weighting coefficients were equal to unity, that they reduced to the least-squares line-fitting formula. Operational checks were made by showing that the straight line estimates correctly fit the data sets.

CODING INFORMATION

- Special Program Constants

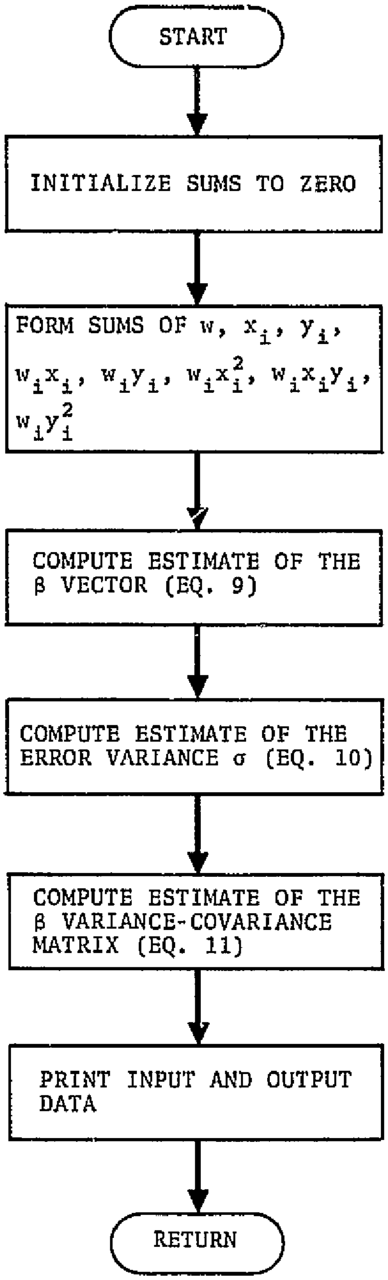
  None.

- Timing

  The subroutine has not been timed.

DETAILED FLOW CHART

- See the following page.


START
INITIALIZE SUMS TO ZERO
FORM SUMS OF w, x_i, y_i, $w_i x_i$, $w_i y_i$, $w_i x_i^2$, $w_i x_i y_i$, $w_i y_i^2$
COMPUTE ESTIMATE OF THE β VECTOR (EQ. 9)
COMPUTE ESTIMATE OF THE ERROR VARIANCE σ (EQ. 10)
COMPUTE ESTIMATE OF THE β VARIANCE-COVARIANCE MATRIX (EQ. 11)
PRINT INPUT AND OUTPUT DATA
RETURN

SOURCE LISTING

See the following pages.

```
* FOR,* GLHFR2,GLHFR2                                                    19 NOV 71                  10:21:11.187
UNIVAC 1108 FORTRAN V LEVEL 2206 0024A    -(EXEC8 LEVEL E1201000 9A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:11

     SUBROUTINE GLHFR2     ENTRY POINT 000241

     STORAGE USED: CODE(1) 000305; DATA(0) 000150; BLANK COMMON(2) 000000

     EXTERNAL REFERENCES (BLOCK, NAME)

      0003    NWDU$
      0004    NI02$
      0005    NWNL$
      0006    NSTOP$
      0007    NERR3$

     STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

      0000    000065 1F        0001    000050 10L       0001    000035 117G      0001    000205 12L       0001    000045 127G
      0001    000214 13L       0001    000065 144G      0000    000105 2F        0000    000074 3F        0001    000042 8L
      0000 R  000017 DETINV    0000    000033 HATS      0000 I  000000 I         0000    000121 INJP$     0000 R  000020 SINV11
      0000 R  000021 SINV12    0000 R  000022 SINV22    0000 R  000001 SUMW      0000 R  000002 SUMWX     0000 R  000004 SUMWXX
      0000 R  000005 SUMWXY    0000 R  000003 SUMWY     0000 R  000006 SUMWYY    0000 R  000011 WW        0000 R  000012 WX
      0000 R  000014 WXX       0000 R  000015 WXY       0000 R  000013 WY        0000 R  000016 WYY       0000 R  000023 XTY1
      0000 R  000024 XTY2      0000 R  000007 XX        0000 R  000010 YY
```



```
00101            SUBROUTINE GLHFR2(N,X,Y,W,M,IW,EB,EVAR,VAREB)
00101      C * N        = NUMBER OF OBSERVATIONS
00101      C * X        = ARRAY OF KNOWN INDEPENDENT VARIABLE VALUES
00101      C * Y        = ARRAY OF OBSERVED DEPENDENT VARIABLE VALUES
00101      C * W        = ARRAY OF WEIGHT VALUES
00101      C * M        = DIMENSION OF INPUT ARRAYS: X,Y,W.
00101      C * EB       = ESTIMATES OF LINEAR COEFFICIENTS
00101      C * EVAR     = ESTIMATE OF ERROR VARIANCE
00101      C * VAREB    = ELEMENTS OF VARIANCE MATRIX FOR ESTIMATED LIN. COEFFICIENTS
00101      C
00101      C     IW = 0  WEIGHTS ARE INPUT THROUGH CALLING ARGUMENTS (1/SAMPLE VAR)
00101      C     IW = 1  WEIGHTS ARE DEFINED AS 1. IN GLHFR2
00101      C     IW = 2  WEIGHTS ARE CALCULATED IN GLHFR2 AS 1./Y(I) (1/POISSON VAR)
00101      C
00103            DIMENSION X(M),Y(M),W(M),EB(2),VAREB(2,2)
00104            NAMELIST/HATS/N,EB(1),EB(2),EVAR,VAREB(1,1),VAREB(1,2),VAREB(2,1),
00104           1                VAREB(2,2)
00105            WRITE(6,1)
00107          1 FORMAT(1H0,///,10X,'SUBROUTINE GLHFR2',///)
00110            IF(N.LE.2) GO TO 12
00112            IF(IW.EQ.1) GO TO 8
00114            IF(IW.LT.1) GO TO 10
00116            DO 7 I = 1,N
00121            W(I) = 1./Y(I)
00122          7 CONTINUE
```

```
00124           GO TO 10
00125         8 CONTINUE
00126           DO 9 I = 1,N
00131           W(I) = 1.
00132         9 CONTINUE
00134        10 CONTINUE
00135           SUMW    = 0.
00136           SUMWX   = 0.
00137           SUMWY   = 0.
00140           SUMWXX  = 0.
00141           SUMWXY  = 0.
00142           SUMWYY  = 0.
00142     C * FORM SUMS
00143           DO 11 I = 1,N
00146           XX = X(I)
00147           YY = Y(I)
00150           WW = W(I)
00151           WX = WW * XX
00152           WY = WW * YY
00153           WXX = WX * XX
00154           WXY = WX * YY
00155           WYY = WY * YY
00156           SUMW = SUMW + WW
00157           SUMWX = SUMWX + WX
00160           SUMWY = SUMWY + WY
00161           SUMWXX = SUMWXX + WXX
00162           SUMWXY = SUMWXY + WXY
00163           SUMWYY = SUMWYY + WYY
00164        11 CONTINUE
00164     C * FORM S-INVERSE MATRIX (S = X'X) AND X'Y VECTOR
00166           DETINV = 1./(SUMW*SUMWXX - SUMWX*SUMWX)
00167           SINV11 = SUMWXX * DETINV
00170           SINV12 = -SUMWX * DETINV
00171           SINV22 = SUMW * DETINV
00172           XTY1 = SUMWY
00173           XTY2 = SUMWXY
00173     C * COMPUTE BETA VECTOR, ERROR VARIANCE, AND VARIANCE-COVARIANCE MATRIX
00173     C     FOR BETA VECTOR
00174           EB(1) = SINV11*XTY1 + SINV12*XTY2
00175           EB(2) = SINV12*XTY1 + SINV22*XTY2
00176           EVAR = (SUMWYY - (EB(1)*XTY1 + EB(2)*XTY2))/FLOAT(N - 2)
00177           VAREB(1,1) = EVAR * SINV11
00200           VAREB(1,2) = EVAR * SINV12
00201           VAREB(2,1) = VAREB(1,2)
00202           VAREB(2,2) = EVAR * SINV22
00202     C * PRINT INPUT AND OUTPUT DATA
00203           WRITE(6,HATS)
00206           GO TO 13
00207        12 CONTINUE
00210           WRITE(6,3)
00212         3 FORMAT(1H1,///,10X,'ERROR - N MUST BE GREATER THAN 2')
00213           STOP
00214        13 CONTINUE
00215           WRITE(6,2)
00217         2 FORMAT(1H0,//,10X,'RETURN TO CALLING ROUTINE',/////)
00220           RETURN
00221           END
```

1/71

END OF COMPILATION: NO DIAGNOSTICS.

```
GLHFR2         SYMBOLIC       19 NOV 71  10:20:33  0  01641245  14  82  (DELETED)
GLHFR2  CODE   RELOCATABLE    19 NOV 71  10:20:33  1  01644251  18   1  (DELETED)
                                                   0  01643441  14  28
```

GLHFR2-14
4-30

4.4 Program Listings

The program listings are shown on the following pages.

@FOR,* BIOMAP,BIOMAP 19 NOV 71 10:20:51. 61

UNIVAC 1108 FORTRAN V LEVEL 2206 0024A -(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:20:51

MAIN PROGRAM

STORAGE USED: CODE(1) 002710; DATA(0) 015041; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 P 00702G

EXTERNAL REFERENCES (BLOCK, NAME)

0004 GLMFR2
0005 QUIKMP
0006 QUIKML
0007 HIST
0010 IGIVE
0011 CORAN
0012 PCORRE
0013 NRDU$
0014 NI01$
0015 NI02$
0016 NWDU$
0017 EXP
0020 NWNL$
0021 NEXP6$
0022 SQRT
0023 NWDC$
0024 NSTOP$

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	014145 101F	0000	014157 102F	0001	001522 1027G	0000	014401 103F	0000	014176 104F
0001	001537 1041G	0001	001630 1075G	0001	000527 11L	0001	001636 1103G	0001	001171 111L
0001	001657 1117G	0001	000566 112L	0001	001666 1123G	0001	001034 113L	0001	001702 1136G
0001	001711 1145G	0001	001726 1157G	0001	001573 116L	0001	001737 1165G	0001	001762 1177G
0001	000514 12L	0001	001765 1203G	0001	002003 1213G	0001	002034 1225G	0001	002037 1230G
0001	002072 1246G	0001	002105 1256G	0001	002114 1264G	0001	002140 1275G	0001	000563 13L
0001	002152 1307G	0001	0[illegible]170 1320G	0001	002176 1326G	0001	002250 1356G	0001	002266 1371G
0001	000550 14L	0001	00[illegible]24 1415G	0001	000010 142G	0001	002355 1430G	0001	002377 1445G
0001	002407 1455G	0001	0024[illegible] [illegible]470G	0001	002547 1514G	0001	002550 1517G	0001	002615 1535G
0001	000026 154G	0001	002633 1541G	0000	014052 2F	0000	014055 202F	0000	014046 203F
0000	014040 204F	0000	014066 205F	0000	014103 206F	0000	014032 207F	0000	014020 208F
0000	014025 210F	0000	014214 211F	0000	014231 212F	0000	014241 213F	0000	014313 215F
0000	014330 216F	0000	014417 221F	0000	014427 222F	0000	014445 223F	0000	014517 224F
0000	014661 225F	0000	014673 226F	0000	014726 227F	0001	000660 23L	0000	014534 231F
0000	014606 232F	0000	014616 233F	0000	014113 241F	0001	000654 25L	0001	000162 253G
0001	000177 265G	0000	014377 3F	0000	014075 305F	0001	000245 311L	0001	000306 312L
0001	000466 32L	0001	000470 321L	0001	000345 322G	0001	000364 327G	0001	000400 340G
0001	000315 35L	0001	000422 353G	0001	000441 365G	0001	000451 375G	0001	002662 38L
0001	002664 39L	0000	014036 4F	0001	000501 415G	0001	000504 420G	0001	000762 44L
0001	000535 442G	0001	000540 445G	0001	001022 45L	0001	000777 47L	0001	000573 470G
0001	001003 48L	0001	001010 49L	0000	014062 5F	0001	001013 50L	0001	000607 501G

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0001   000624 5I1G     0001   000632 514G     0001   000672 5366     0001   000703 5456     0001   000714 5556
0001   000733 562G     0001   000743 5666     0001   001120 57L      0000   014415 5BF      0000   014045 6F
0001   001652 61L      0001   001047 626G     0001   001052 632G     0001   001720 64L      0001   001070 642G
0001   001721 65L      0001   001106 651G     0001   001111 654G     0001   001130 667G     0001   001756 67L
0000   014030 7F       0001   001747 70L      0001   001150 703G     0001   001214 721G     0001   001235 724G
0001   002136 73L      0001   001300 737G     0001   001361 767G     0001   002046 77L      0000   014015 8F
0001   002144 81L      0001   002164 86L      0001   002313 98L      0001   002227 99L      0001   002704 999L
0000 R 011363 ABC      0000 R 011407 ABCO     0000 R 011255 ABCS     0000 I 000064 ABE      0000 R 010663 AC
0000 R 013527 ADB      0000 R 011203 ADNB     0000 R 011551 ADNS     0000 R 013531 ADS      0000 I 000032 AE
0000 R 011375 AFB      0000 R 011301 AFS      0000 R 011503 AMTASE   0000 R 011457 AMTGEL   0000 R 011471 AMYRBC
0000 R 000110 ANIO     0000 I 000076 ANSE     0000 R 013547 AP       0000 R 013530 ARATIO   0000 I 000024 ASE
0000 R 013550 BD       0000   013734 BDATA    0000 R 011313 BG       0000 I 000000 BIOEL    0000 I 000012 BIOZ
0000 R 013461 CC       0000 R 010621 COEF     0000 R 013576 CON      0000 R 011537 CONC     0000 R 013501 CP
0000 R 011351 CR       0000 R 013541 CSCTH    0000 R 013551 CT       0000 R 011325 CTB      0000 R 013441 CV
0000 R 013524 C1       0000 R 013525 C12      0000 R 013526 C2       0000 R 011433 DEL      0000 R 011517 DENAD
0000 R 011143 DENS     0000   013622 DIST     0000 R 013566 DRYGEL   0000 R 013552 DT       0000 R 013575 EDGE
0000 R 011337 ESC      0000 R 007130 ESCMX    0000 R 013577 EX       0000 R 012524 F        0000 R 013557 GEL
0000   013702 GLMID    0000 R 013560 H20      0000 I 013523 I        0000 I 013533 ICOUNT   0003 I 000144 ICS
0000 I 013521 IDATE    0000 I 013602 INDX     0000 I 013545 IPRINT   0000 I 013564 IPS      0000 I 010633 ITITX
0000 I 010647 ITITY    0000 I 013553 ITYPE    0000 I 013546 INT      0000 I 013565 J        0000 I 013621 JA
0000 I 013544 JSET     0000 I 013570 K        0000 I 013574 M        0000 I 013543 MAN      0000 I 013603 MDIM
0000 I 013542 MISS     0000 I 013567 N        0000 I 013555 NA       0000 I 013563 NAD      0000 I 013614 NBE
0000 I 013562 ND       0000 I 013617 NG       0000 I 013613 NS       0000 I 013554 NSAMP    0000 I 013571 NSE
0000 I 013532 NSTD     0000 I 013573 NZ       0000 I 011511 NZA      0000 I 011243 NZAE     0000 I 011123 NZSE
0003 R 000000 P        0000 R 013600 PABG     0000 R 013620 PCOR     0012 R 000000 PCORRE   0000 R 013601 POE
0000 R 010631 Q        0000 R 010627 R        0000 R 011421 RHOB2    0000 R 010114 SCT      0000 R 011615 SCTSD
0000   013645 SDATA    0000 R 013540 SDEV     0000 R 011603 SDVERR   0000 R 011571 SDVESC   0000 I 000044 SE
0000 R 011445 SIGB1    0000 R 011525 SIGB2    0000 R 011267 SIGS     0000   013774 STAT     0000 R 013615 SUM1
0000 R 013616 SUM2     0000 R 007522 SX       0000 R 013556 TBIO     0000 R 012575 TITLE1   0000 R 013561 TSTD
0000 R 013537 VAR      0000 R 010623 VARCOV   0000 R 013604 VARERR   0000 R 013572 WAVE     0000 R 011223 WFBE
0000 R 010570 WM       0000 R 011163 WPSE     0000 R 012207 X        0000 R 013536 XBAR     0000 R 013607 XL
0000 R 010506 XM       0000 R 013535 XMAX     0000 R 013534 XMIN     0000 R 013605 XMX      0000 R 013610 XR
0000 R 012611 Y        0000 R 013435 YAVG     0000 R 013611 YB       0000 R 010537 YM       0000 R 013606 YMX
0000 R 013612 YT
```

```
00100     C * INITIALIZE AND INPUT BASIC PARAMETERS
00101           INTEGER BIOEL,BIOZ,ASE,AE,SE,ABE,ANSE
00103           DIMENSION ANIO(6,6,100),ESCMX(10,25)
00104           DIMENSION SX(10,25),SCT(10,25),XM(25),YM(25),WM(25),ANSE(10),
00104          1        COEF(2),VARCOV(2,2),R(2),Q(2),ITITX(12),ITITY(12)
00105           COMMON/P/P
00106           DIMENSION P(100,36),AC(10,16),SE(16),NZSE(16),DENS(16),WPSE(16),
00106          1 ADNB(16),WFBE(16),AE(10),NZAE(10),ABCS(10),SIGS(10),AFS(10),
00106          2 ABE(10),BG(10),CTB(10),ESC(10),CR(10),ABC(10),AFB(10),ABCO(10),
00106          3 RHOB2(10),DEL(10),SIGB1(10),BIOEL(10),BIOZ(10),AMTGEL(10),
00106          4 AMYRBC(10),ASE(6),AMTASE(6),NZA(6),DENAD(6),SIGB2(10),CONC(10),
00106          5 ADNS(16),SDVESC(10),SDVERR(10),SCTSD(10,25)
00107           DIMENSION X(205),F(41),TITLE1(12)
00110           DIMENSION Y(101,4),YAVG(4),CV(4,4),CC(4,4),CP(4,4)
00111           DIMENSION ICS(100)
00112           DIMENSION IDATE(2)
00113           EQUIVALENCE (P(1,2),ICS(1))
00114           DATA BIOEL /' H',' C',' N',' O','NA',' P',' S','CL',' K','FE'/
00116           DATA BIOZ /1,6,7,8,11,15,16,17,19,26/
00120           DATA AMTGEL/07.29,42.72,15.03,34.74,00.00,00.00,00.22,00.00,00.00,
```

```
00120              1                00,00/
00122              DATA AMTRBC/.0721,.5368,.1671,.2006,.0012,.0030,.0038,.0048,.0114,
00122             1             .0031/
00124              DATA TITLE1/'CONCENTRATION FREQUENCY DISTRIBUTION',6*' '/
00126              DATA (ITITX(I),I=1,12)/72H ABSORPTION-FACTOR * AREA-DENSITY (10**-
00126             16)                        /
00130              DATA (ITITY(I),I=1,12)/72H ACCUMULATED COUNT (10**3)
00130             1                          /
00132              NAMELIST/DIST/C1,C12,C2,ADB,AMATIO
00133              NAMELIST/SDATA/DENAD,DENS,ADNS,ADS,SIGS,AC,ABCS,AFS,WPSE
00134              NAMELIST/GLMIO/NSTD,XM,YM,WM,BG,ESC,SDVESC,SDVERR
00135              NAMELIST/BDATA/ABC,AFB,ABCO,CR,SIGS,SIGB2,ADNB,ADB,WFBE,ICOUNT
00136              NAMELIST/STAT/XMIN,XMAX,XBAR,VAR,SDEV
00137              CSCTH = 1.2605
00137        C
00137        C * LIST OF OPTIONS
00137        C    IPRINT = 0  NO NAMELIST PRINTOUT (TYPICAL)
00137        C    IPRINT = 1  PRINT NAMELISTS CONTAINING INTERMEDIATE CALCULATIONS
00137        C    IWT = 0  WEIGHTS ARE INPUT THROUGH CALLING ARGUMENTS (1/SAMPLE VAR)
00137        C    IWT = 1  WEIGHTS ARE DEFINED AS 1. IN GLMFR2
00137        C    IWT = 2  WEIGHTS ARE CALCULATED IN GLMFR2 AS 1./Y(I) (1/POISSON VAR)
00137        C    ITYPE = 0  ONLY STATISTICAL ANALYSIS OF STANDARD DATA PERFORMED
00137        C    ITYPE = 1  SAMPLES ARE RED BLOOD CELLS
00137        C    ITYPE = 2  SAMPLES ARE BIOLOGICAL TISSUE SECTIONS
00137        C    ITYPE = 3  SAMPLES ARE GELATIN SECTIONS
00137        C
00137        C * INPUT PROBLEM INFORMATION
00140              READ(5,8) IDATE,MISS,MAN,JSET
00151            8 FORMAT(2A5,I5,A5,A5)
00152              WRITE(6,208) IDATE,MISS,MAN,JSET
00163          208 FORMAT (' CARD 1 ',2A5,I5,A5,A5)
00163        C
00163        C * INPUT PROGRAM PARAMETERS
00164              READ(5,4) IPRINT,IWT
00170              WRITE(6,210) IPRINT,IWT
00174          210 FORMAT(' CARD 2 ',3I5)
00174        C
00174        C * INPUT MICROPROBE PARAMETERS
00175              READ(5,7) AP,BD,CT,DT
00203            7 FORMAT (4F10.2)
00204              WRITE(6,207) AP,BD,CT,DT
00212          207 FORMAT(' CARD 3 ',4F10.2)
00212        C
00212        C * INPUT SAMPLE INFORMATION
00213              READ(5,4) ITYPE,NSAMP,NA,TBIO
00221            4 FORMAT(3I5,F5.0)
00222              WRITE(6,204) ITYPE,NSAMP,NA,TBIO
00230          204 FORMAT(' CARD 4 ',3I5,F5.0)
00231              TBIO = TBIO*1.0E-04
00231        C
00231        C * INPUT STANDARD DATA
00232              READ(5,6) GEL,H2O,TSTD,NSTD
00240            6 FORMAT(3F10.5,I5)
00241              WRITE(6,203) GEL,H2O,TSTD,NSTD
00247          203 FORMAT(' CARD 5 ',3F10.5,I5)
00250              TSTD = TSTD*1.0E-04
00261              READ(5,2) (AE(I),BG(I),ESC(I),SDVESC(I),I=1,NA)
00262            2 FORMAT(A2,3X,3F10.0)
```

```
00263             WRITE(6,202) (AE(I),BG(I),ESC(I),SDVESC(I),I=1,NA)
00274         202 FORMAT(' CARD 6 ',A2,3X,3F10.0)
00274       C
00274       C * COMPUTE RBC AREA DENSITY AND CURRENT INTERCEPT RATIO
00275             IF(ITYPE.NE.1) GO TO 35
00277 *DIAGNOSTIC*  THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
00277             IF(BD.EQ.0.)GO TO 311
00301             CI = 1. - EXP(-0.5/0.75**2)
00302             CI2 = 1. - EXP(-4.5/0.75**2)
00303             C2 = CI2 - CI
00304             ADB = 32.*(.01728*CI + .48272*C2/8.)*.0001/CI2/3.14159
00305             GO TO 312
00306         311 CONTINUE
00307             CI = 1. - EXP(-4.5/((.5*BD)**2))
00310             CI2 = 1. - EXP(-0.5*(3.75**2)/((.5*BD)**2))
00311             C2 = CI2 - CI
00312             ADB = 32.*(0.5*CI/9. + 0.5*C2/(3.75**2 - 9.))*0.0001/CI2/3.14159
00313         312 CONTINUE
00314             ARATIO = 1.0/CI2
00315             WRITE(6,DIST)
00320          35 CONTINUE
00320       C
00320       C
00320       C * THIS LOOP FORMS ATOMIC NUMBER AND SYMBOL ARRAYS, AND COMPUTES AREA
00320       C   DENSITY AND ABSORPTION COEFFICIENTS FOR EACH ANALYZED ELEMENT IN
00320       C   EACH STANDARD
00320       C
00321             DO 111 ND = 1,NSTD
00324             READ(5,5) NAD,(ASE(I),AMTASE(I),I = 1,NAD)
00334           5 FORMAT(I1,3X,6(A2,1X,F6.0,1X))
00335             WRITE(6,205) NAD,(ASE(I),AMTASE(I),I=1,NAD)
00345         205 FORMAT(' CARD 7 ',I1,3X,6(A2,1X,F6.0,1X))
00346             IF(NSTD.EQ.1) GO TO 321
00350             READ(5,305) IPS,(ANSE(I),SCT(I,ND),SCTSD(I,ND),I=1,NA)
00361         305 FORMAT(I2,2X,4(A2,1X,F6.0,1X,F6.0,1X))
00362             WRITE(6,206) IPS,(ANSE(I),SCT(I,ND),SCTSD(I,ND),I=1,NA)
00373         206 FORMAT(' CARD 8 ',I2,2X,4(A2,1X,F6.0,1X,F6.0,1X))
00374             DO 32 I = 1,NA
00377             IF(ANSE(I).EQ.AE(I)) GO TO 32
00401             WRITE(6,241) ND,NSTD
00405         241 FORMAT(1H0,5X,'ANALYZED ELEMENT CHECK ARRAYS ANSE(I) AND AE(I), I
00405            1 = 1,NA, ARE NOT IDENTICAL.',/,5X,'CHECK CARDS 7 AND 8 FOR STANDAR
00405            2DS',I3,' THROUGH',I3)
00406             GO TO 999
00407          32 CONTINUE
00411         321 CONTINUE
00411       C
00411       C * CONSTRUCT ATOMIC NUMBER ARRAYS NZA(I) AND NZAE(I) FOR ADDED ELEMENTS
00411       C   AND ANALYZED ELEMENTS
00412             IF(ND.NE.1) GO TO 112
00414             DO 11 I = 1,NAD
00417             DO 12 J = 1,100
00422             IF(ICS(J).NE.ASE(I)) GO TO 12
00424             NZA(I) = J
00425             GO TO 11
00426          12 CONTINUE
00430             IF(NZA(I).NE. 0) GO TO 11
00432             WRITE(6,101) I
```

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```
00435      101 FORMAT(1H0,10X,'ADDED ELEMENT SYMBOL',13,1X,'WAS NOT FOUND')
00436          GO TO 999
00437       11 CONTINUE
00441          DO 13 I = 1,NA
00444          DO 14 J =1,100
00447          IF(ICS(J).NE.AE(I)) GO TO 14
00451          NZAE(I) = J
00452          GO TO 13
00453       14 CONTINUE
00455          IF(NZAE(I).NE.0) GO TO 13
00457          WRITE(6,102) I
00462      102 FORMAT(1H0,10X,'ANALYZED ELEMENT SYMBOL',13,1X,'WAS NOT FOUND')
00463          GO TO 999
00464       13 CONTINUE
00464    C
00464    C * FORM SYMBOL, DENSITY AND ATOMIC NUMBER ARRAYS FOR STANDARD ELEMENTS
00466      112 CONTINUE
00467          DO 21 I = 1,10
00472          DRYGEL = GEL*(1.0 - H2O)*1.0E-03
00473          SE(I) = BIOEL(I)
00474          NZSE(I) = BIOZ(I)
00475          DENS(I) = DRYGEL*AMTGEL(I)*1.0E-02
00476       21 CONTINUE
00500          DO 22 I = 1,NAD
00503          N = NZA(I)
00504          DENAD(I) = AMTASE(I)*P(N,1)*1.0E-06
00505       22 CONTINUE
00507          K = 10
00510          DO 23 I = 1,NAD
00513          DO 24 J = 1,K
00516          IF(ASE(I).EQ.SE(J)) GO TO 25
00520       24 CONTINUE
00522          K = K+1
00523          NZSE(K) = NZA(I)
00524          SE(K) = ASE(I)
00525          DENS(K) = DENAD(I)
00526          GO TO 23
00527       25 CONTINUE
00530          DENS(J) = DENS(J) + DENAD(I)
00531       23 CONTINUE
00531    C
00531    C * CALCULATE AREA DENSITY OF DRY STANDARD
00533          NSE = K
00534          ADS = 0.
00535          DO 51 I = 1,NSE
00540          ADNS(I) = DENS(I)*TSTD
00541          ADS = ADS + ADNS(I)
00542       51 CONTINUE
00544          DO 52 I = 1,NSE
00547          WPSE(I) = 100.*ADNS(I)/ADS
00550       52 CONTINUE
00552          IF(ND.NE.1) GO TO 113
00552    C
00552    C * COMPUTE ELEMENTAL MASS ABSORPTION COEFFICIENTS FOR ANALYZED LINES
00554          DO 41 I = 1,NA
00557          N = NZAE(I)
00560          WAVE = P(N,6)
00561          DO 41 J = 1,NSE
```

```
00564            NZ = NZSE(J)
00565            DO 43 M = 9,17
00570            EDGE = P(NZ,M)
00571            IF(WAVE.LT.EDGE) GO TO 44
00573         43 CONTINUE
00575            CON = P(NZ,30)
00576            EX = 2.22
00577            GO TO 45
00600         44 CON = P(NZ,M+12)
00601            IF(M-10)46,47,48
00604         46 EX = P(NZ,19)
00605            GO TO 45
00606         47 EX = P(NZ,20)
00607            GO TO 45
00610         48 IF(M-13)47,49,50
00613         49 EX = 2.60
00614            GO TO 45
00615         50 IF(M.LT.17) GO TO 49
00617            EX = 2.33
00620         45 AC(I,J) = CON*WAVE**EX
00621         41 CONTINUE
00621      C
00621      C * COMPUTE MASS ABSORPTION COEFFICIENT OF STANDARD FOR ANALYZED LINES
00624        113 CONTINUE
00625            DO 53 I = 1,NA
00630            ABCS(I) = 0.
00631            DO 53 J = 1,NSE
00634            PABC = AC(I,J)*ADNS(J)
00635            ABCS(I) = ABCS(I) + PABC
00636         53 CONTINUE
00636      C
00636      C * COMPUTE ABSORPTION FACTORS FOR ANALYZED LINES IN STANDARD
00641            DO 54 I = 1,NA
00644            POE = ABCS(I)*CSCTH
00645            AFS(I) = (1. - EXP(-POE))/POE
00646         54 CONTINUE
00646      C
00646      C * COMPUTE AREA DENSITIES FOR ANALYZED ELEMENTS IN STANDARD
00650            DO 55 I = 1,NA
00653            DO 56 J = 1,NSE
00656            IF(NZAE(I).EQ.NZSE(J)) GO TO 57
00660         56 CONTINUE
00662         57 CONTINUE
00663            SIGS(I) = ADNS(J)
00664         55 CONTINUE
00666            DO 114 I = 1,NA
00671            SX(I,ND) = AFS(I) * SIGS(I)
00672        114 CONTINUE
00674            IF(IPRINT.NE.0) WRITE(6,SDATA)
00700            IF(NSTD.EQ.1) GO TO 116
00700      C * LOAD ANALYSIS INPUT-OUTPUT MATRIX
00702            DO 31 I = 1,NA
00705            AMIO(I,1,ND) = AMTASE(I)
00706            AMIO(I,2,ND) = 100.*SIGS(I)/ADS
00707            AMIO(I,3,ND) = SIGS(I)
00710            AMIO(I,4,ND) = AFS(I)
00711         31 CONTINUE
00713            IF(IPS.NE.1) GO TO 111
```

```
00715          INDX = ND
00716      111 CONTINUE
00716    C
00716    C * COMPUTE ESTIMATES OF STATISTICAL PARAMETERS FOR SET OF STANDARDS
00716    C   AND COMPUTE MOST PROBABLE COUNT FOR THE PRINCIPAL STANDARD
00720          DO 115 I = 1,NA
00723          DO 117 ND = 1,NSTD
00726          XM(ND) = SX(I,ND)
00727          YM(ND) = SCT(I,ND)
00730          IF(IWT.EQ.0) WM(I) = 1.0/SCTSD(I,ND)**2
00732      117 CONTINUE
00734          MDIM = 25
00735          CALL GLHPR2(NSTD,XM,YM,WM,MDIM,IWT,COEF,VARERR,VARCOV)
00736          DO 34 ND=1,NSTD
00741          ESCMX(I,ND) = COEF(1) + COEF(2) SX(I,ND)
00742          ANIO(1,5,ND) = SCT(I,ND)
00743          ANIO(1,6,ND) = ESCMX(I,ND)
00744       34 CONTINUE
00746          BG(I) = COEF(1)
00747          ESC(I)= COEF(1) + COEF(2)*SX(I,INDX)
00750          SDVESC(I) = SQRT(ABS(VARCOV(1,1) + VARCOV(2,2)*SX(I,INDX)**2))
00751          SDVERR(I) = SQRT(ABS(VARERR))
00752          IF(IPRINT.NE.0) WRITE(6,GLHIO)
00756          PUNCH 2,(AE(I),BG(I),ESC(I),SDVESC(I))
00756    C
00756    C * MICROFILM STANDARD COUNT VS. ABSORPTION-FACTOR * AREA-DENSITY
00764          XMX = 0.
00765          YMX = 0.
00766          DO 118 J = 1,NSTD
00771          XM(J) = XM(J)*1.0E+06
00772          YM(J) = YM(J)*1.0E-03
00773          IF(XM(J).GT.XMX) XMX = XM(J)
00775          IF(YM(J).GT.YMX) YMX = YM(J)
00777      118 CONTINUE
01001          XL = 0.
01002          XR = XMX
01003          YB = 0.
01004          IF(COEF(1).LT.0.) YB = COEF(1)*1.0E-03
01006          YT = YMX
01007          Q(1) = 0.
01010          Q(2) = XMX
01011          R(1) = COEF(1)*1.0E-03
01012          R(2) = R(1) + COEF(2)*1.0E-09*XMX
01013          CALL QUIKMP(-1,XL,XR,YB,YT,1H*,ITITX,ITITY,NSTD,XM,YM)
01014          CALL QUIKML(0,XL,XR,YB,YT,1H ,ITITX,ITITY,-2,Q,R)
01015          WRITE(17,104) NZA(I)
01020      104 FORMAT(1H+,38X,'ACCUMULATED-COUNT VS CORRECTED AREA-DENSITY FOR EL
01020         1EMENT WITH Z = ',I2)
01021      115 CONTINUE
01023          WRITE(6,211)
01025      211 FORMAT(1H1,' STATISTICAL ANALYSIS OF MICROPROBE DATA FROM A SET OF
01025         1 STANDARDS')
01026          DO 89 I=1,NSTD
01031          WRITE(6,212) AE(I)
01034      212 FORMAT(1H0,//,1X,A2,' IS THE ELEMENT ANALYZED')
01035          WRITE(6,213)
01037      213 FORMAT(1H0,'  NUMBER ',6X,'CONCENTRATION',2X,'  WEIGHT  ',5X,
01037         1 '  AREA  ',8X,'ABSORPTION',5X,'MEASURED',7X,'ESTIMATED',/,1X,
```

```
01037          2 ' STANDARD',6X,'  IN MEQ/L  ',2X,'PERCENTAGE',5X,'DENSITY',8X,
01037          3 '  FACTOR  ',5X,' COUNT  ',7X,'  COUNT  ')
01040            DO 94 ND = 1,NSTD
01043            WRITE(6,215) ND,ANID(I,1,ND),ANID(I,2,ND),ANID(I,3,ND),
01043          1 ANID(I,4,ND),ANID(I,5,ND),ANID(I,6,ND)
01054      215 FORMAT(1H0,3X,I3,9X,3X,F5.1,7X,1X,E8.3,6X,2X,E8.3,5X,3X,F6.5,6X,
01054          1 2X,F6.0,7X,2X,F6.0)
01055       94 CONTINUE
01057            WRITE(6,216) BG(I),CT,SDVESC(I),NSTD
01065      216 FORMAT(1H0,1X,F6.0,' IS THE ESTIMATED RESIDUAL BACKGROUND FOR A ',
01065          1 F4.0,' SECOND COUNT TIME.',//,1X,F6.0,' IS THE ESTIMATED ERROR ST
01065          2ANDARD DEVIATION FOR INTENSITY COUNT ON',/,8X,'THE PRINCIPAL STAND
01065          3ARD (STANDARD NUMBER ',I3,')')
01066       89 CONTINUE
01070      116 CONTINUE
01071            IF(NSAMP.EQ.0) GO TO 999
01071    C
01071    C
01071    C * PERFORM ANALYSIS OF ONE SAMPLE EACH TIME THROUGH LOOP
01071    C
01071    C
01071    C * CHECK SYMBOLS AND SYMBOL ORDER OF COUNT DATA
01073            READ(5,3) (ABE(I),I=1,NA)
01101        3 FORMAT (6(8X,A2))
01102            DO 61 I = 1,NA
01105            IF(AE(I).EQ.ABE(I)) GO TO 61
01107            WRITE(6,103) NA
01112      103 FORMAT (1H0,10X,'CHEMICAL SYMBOL OR SYMBOL ORDER IS IN ERROR FOR N
01112          *A = ',I2)
01113            GO TO 999
01114       61 CONTINUE
01116            DO 99 NS = 1,NSAMP
01121            READ(5,58) (CTB(I),I=1,NA)
01127       58 FORMAT (6F10.0)
01127    C
01127    C * FORM INITIAL DENSITY ARRAY FOR BIOLOGICAL ELEMENTS,
01127    C   CORRECT COUNTS FOR BACKGROUND AND FORM COUNT RATIOS
01130            NBE = NSE
01131            IF(ITYPE - 2)63,64,65
01134       63 CONTINUE
01135            DO 66 I = 1,10
01140            WFBE(I) = AMTRBC(I)
01141            ADNB(I) = WFBE(I)*ADB
01142       66 CONTINUE
01144            DO 69 I = 1,NA
01147            CR(I) = CTB(I)/(ESC(I) - BG(I))
01150       69 CONTINUE
01152            GO TO 67
01152    C
01152    C * SPACE LEFT HERE FOR COMPUTING TISSUE DENSITY ARRAY
01153       64 CONTINUE
01154            GO TO 67
01154    C
01155       65 CONTINUE
01156            DO 62 I = 1,NA
01161            CR(I) = (CTB(I)-BG(I))/(ESC(I)-BG(I))
01162       62 CONTINUE
01162    C
```

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01164          DO 68 I = 1,NBE
01167          ADNB(I) = ADNS(I)*TBIO/TSTD
01170       68 CONTINUE
01172          ADB = ADS*TBIO/TSTD
01173       67 CONTINUE
01173    C
01173    C * COMPUTE MASS ABSORPTION COEFF. OF BIO. SAMPLE FOR LINES ANALYZED
01174          ICOUNT = 0
01175       70 CONTINUE
01176          DO 71 I = 1,NA
01201          ABC(I) = 0.
01202          DO 71 J = 1,NBE
01205          PABC = AC(I,J)*ADNB(J)
01206          ABC(I) = ABC(I) + PABC
01207       71 CONTINUE
01207    C
01207    C * COMPUTE ABSORPTION FACTORS FOR ANALYZED LINES IN BIOLOGICAL SAMPLE
01212          DO 72 I = 1,NA
01215          POE = ABC(I)*CSCTH
01216          AFB(I) = (1. - EXP(-POE))/POE
01216    C
01216    C * COMPUTE THE ABSORPTION CORRECTION ARRAY FOR THE ANALYZED ELEMENTS
01217          ABCO(I) = AFS(I)/AFB(I)
01217    C
01217    C * COMPUTE AREA DENSITY ARRAY OF ANALYZED ELEMENTS IN BIOLOGICAL SAMPLE
01220          SIGB2(I) = SIGS(I)*CR(I)*ARATIO*ABCO(I)
01221       72 CONTINUE
01223          ICOUNT = ICOUNT + 1
01223    C
01223    C * UPDATE AREA DENSITY AND WEIGHT FRACTION ARRAYS OF BIOLOGICAL SAMPLE
01224          DO 75 I = 1,NA
01227          DO 76 J = 1,NBE
01232          IF(NZAE(I).EQ.NZSE(J)) GO TO 77
01234       76 CONTINUE
01236       77 CONTINUE
01237          ADNB(J) = SIGB2(I)
01240       75 CONTINUE
01242          IF(ITYPE.EQ.3) ADNB(8)=(ADNB(5)/22.997+ADNB(9)/39.100)*35.457
01244          ADB = 0.
01245          DO 78 I = 1,NBE
01250          ADB = ADB + ADNB(I)
01251       78 CONTINUE
01251    C
01251    C * TEST FOR REITERATION CRITERION
01253          IF(ICOUNT.LE.2) GO TO 73
01255          DO 74 I = 1,NA
01260          DEL(I) = (SIGB2(I)-SIGB1(I))/SIGB2(I)
01261       74 CONTINUE
01263          DO 33 I = 1,NA
01266          IF(ABS(DEL(I)).GT.0.001.AND.ICOUNT.LT.10) GO TO 73
01270       33 CONTINUE
01272          GO TO 81
01273       73 CONTINUE
01274          DO 80 I = 1,NA
01277          SIGB1(I) = SIGB2(I)
01300       80 CONTINUE
01302          GO TO 70
01303       81 CONTINUE
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01304          IF(ITYPE.NE.3) GO TO 86
01306          DO 82 I = 1,NA
01311          N = NZA(I)
01311     C
01311     C * COMPUTE THE VOLUME DENSITY OF ANALYZED ELEMENTS IN GELATIN SAMPLES
01312          RHOB2(I) = SIGB2(I)/TBIO
01313          CONC(I) = RHOB2(I)*1.0E+06/P(N,I)
01314       82 CONTINUE
01316       86 CONTINUE
01316     C
01316     C * FORM WEIGHT PERCENT MATRIX ATPMA(NSAMP,NA)
01317          DO 79 I = 1,NBE
01322          AFBE(I) = ADNBE(I)/ADB
01323       79 CONTINUE
01323     C * LOAD ANALYSIS INPUT-OUTPUT MATRIX
01325          DO 88 I = 1,NA
01330          ANIO(I,1,NS) = CTB(I)
01331          ANIO(I,2,NS) = AFB(I)
01332          ANIO(I,3,NS) = ABCO(I)
01333          ANIO(I,4,NS) = SIGB2(I)
01334          ANIO(I,5,NS) = 100.*SIGB2(I)/ADB
01335          ANIO(I,6,NS) = CONC(I)
01336       88 CONTINUE
01340          IF(NS.GT.2) GO TO 99
01342          IF(IPRINT.NE.0) WRITE(6,BDATA)
01346       99 CONTINUE
01350          IF(ITYPE.EQ.1) GO TO 98
01352          WRITE(6,221)
01354      221 FORMAT(1H1,' ANALYSIS OF GELATIN-BASE SAMPLES')
01355          DO 87 I = 1,NA
01360          WRITE(6,222) ABE(I),BG(I)
01364      222 FORMAT(1H0,//,30X,A2,' IS THE ELEMENT ANALYZED',
01364         1 /,30X,I5,' IS THE BACKGROUND COUNT')
01365          WRITE(6,223)
01367      223 FORMAT(1H0,' SAMPLE',8X,'INTENSITY',6X,'ABSORPTION',5X,'ABSORPTION
01367         1',8X,' AREA  ',5X,'  WEIGHT  ',5X,'CONCENTRATION',/,1X,' NUMBER',
01367         2 8X,'  COUNT ',7X,'  FACTOR  ',5X,'CORRECTION',8X,'DENSITY',5X,
01367         3 'PERCENTAGE',5X,'  IN MEQ/L   ')
01370          DO 87 NS = 1,NSAMP
01373          WRITE(6,224) NS,ANIO(I,1,NS),ANIO(I,2,NS),ANIO(I,3,NS),
01373         1 ANIO(I,4,NS),ANIO(I,5,NS),ANIO(I,6,NS)
01404      224 FORMAT(1H ,1X,2X,I3,10X,1X,F6.0,8X,2X,F6.5,7X,2X,F6.5,7X,E10.5,5X,
01404         1 2X,F4.2,9X,F5.1)
01405       87 CONTINUE
01410          GO TO 999
01411       98 CONTINUE
01412          WRITE(6,231)
01414          DO 90 K = 1,NA
01417      231 FORMAT(1H1,16(/),45X,'QUANTITATIVE ANALYSIS OF RBG SET',5(/),40X,'
01417         1.  INPUT-OUTPUT TABLE',3(/),40X,'2.  CONCENTRATION FREQUENCY DIST
01417         *RIBUTION',3(/),40X,'3.  CONCENTRATION CUMULATIVE DISTRIBUTION',3(/
01417         *),40X,'4.  CONCENTRATION CORRELATION ANALYSIS')
01420          WRITE(6,232) ABE(K)
01423      232 FORMAT(1H1,///,30X,A2,' IS THE ELEMENT ANALYZED')
01424          WRITE(6,233)
01426      233 FORMAT(1H0,' SAMPLE',8X,'INTENSITY',6X,'ABSORPTION',5X,'ABSORPTION
01426         1',8X,' AREA  ',5X,'  WEIGHT  ',5X,/,1X,' NUMBER',
01426         2 8X,'  COUNT ',7X,'  FACTOR  ',5X,'CORRECTION',8X,'DENSITY',5X,
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01426            3 *PERCENTAGE*)
01427            DO 97 NS = 1,NSAMP
01432            WRITE(6,224) NS,ANIO(K,1,NS),ANIO(K,2,NS),ANIO(K,3,NS),ANIO(K,4,NS
01432           *),ANIO(K,5,NS)
01442         97 CONTINUE
01442      C
01442      C * COMPUTE STATISTICAL PARAMETERS AND PRINT CUMULATIVE DISTRIBUTION AND
01442      C   HISTOGRAM OF SAMPLE SET DISTRIBUTION
01444            DO 91 J = 1,NSAMP
01447            X(J) = ANIO(K,5,J)
01450         91 CONTINUE
01452            XMAX = X(1)
01453            XMIN = X(1)
01454            DO 92 I = 2,NSAMP
01457            IF(X(I).GT.XMAX) XMAX = X(I)
01461            IF(X(I).LT.XMIN) XMIN = X(I)
01463         92 CONTINUE
01465            SUM1 = 0.
01466            SUM2 = 0.
01467            DO 93 I = 1,NSAMP
01472            SUM1 = SUM1 + X(I)
01473            SUM2 = SUM2 + X(I)*X(I)
01474         93 CONTINUE
01476            XBAR = SUM1/NSAMP
01477            VAR = (SUM2 - NSAMP*XBAR*XBAR)/(NSAMP-1)
01500            SDEV = SQRT(VAR)
01501            NG = NSAMP/5
01502            CALL HIST(X,NSAMP,NG,XMIN,XMAX,F,0,TITLE1)
01503            CALL IGIVE(X,NSAMP,NG,XMIN,XMAX,F,1,0)
01504            WRITE(6,STAT)
01507         90 CONTINUE
01511            IF(NA.EQ.1)GO TO 999
01511      C
01511      C * PERFORM CORRELATION ANALYSIS BETWEEN ANALYZED CHEMICAL ELEMENTS
01511      C
01513            DO 36 I = 1,NA
01516            DO 36 K = 1,NSAMP
01521            Y(K,I) = ANIO(I,5,K)
01522         36 CONTINUE
01525            CALL CORAN(Y,NSAMP,NA,0,0,YAVG,CV,PCOR,101,4)
01526            WRITE(6,225)
01530        225 FORMAT(1H1,///,30X,'CONCENTRATION CORRELATION ANALYSIS',///)
01531            WRITE(6,226)
01533        226 FORMAT(1H0,10X,'CHEMICAL',10X,' VARIANCE ',10X,'CORRELATION',10X,
01533           1 'CORRELATION',/,11X,'ELEMENTS',10X,'COVARIANCE',10X,'COEFFICIENT'
01533           2 ,10X,'PROBABILITY')
01534            DO 37 I = 1,NA
01537            JA = 1
01540            DO 37 J = JA,NA
01543            CC(I,J) = CV(I,J)/SQRT(CV(I,I)*CV(J,J))
01544            IF(I.EQ.J) GO TO 38
01546            CP(I,J) = 1.0 - PCORRE(CC(I,J),NSAMP)
01547            GO TO 39
01550         38 CONTINUE
01551            CP(I,J) = 1.0
01552         39 CONTINUE
01553            WRITE(6,227) ABE(I),ABE(J),CV(I,J),CC(I,J),CP(I,J)
01562        227 FORMAT(1H0,10X,A2,' - ',A2,F19.4,2F21.4)
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01563   542*       37 CONTINUE
01566   543*      999 STOP
01567   544*          END

      END OF COMPILATION:          1 DIAGNOSTICS.
    BIOMAP           SYMBOLIC                                     19 NOV 71  10:20:22   0  01550342   14   599  (DELETED)
    BIOMAP  CODE     RELOCATABLE                                  19 NOV 71  10:20:22   1  01575466   31     1  (DELETED)
                                                                                        0  01567242   14   230
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UNIVAC 1108 FORTRAN V LEVEL 2206 0024A   *(EXEC8 LEVEL E1201000 9A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:03

    BLOCK DATA

    STORAGE USED: CODE(1) 000000; DATA(0) 000001; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   P      007020

    STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000 I 000000 J        0003 R 000000 P


00101          BLOCK DATA
00102          COMMON/P/P(100,36)
00103          DATA(P(  1,J),J=1,36)/  1.008,2H H,  .014,  .000,  .000,
00103         *   .000,   .000,   .000,999.000,999.000,999.000,
00103         *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00103         * .00, .00,   .000,   .00,
00103         *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00103         *   .10040331E01,  -.51088296E-2,   .11210435E-2,
00103         *  -.11886645E-3,   .58783235E-5,  -.10814580E-6/
00105          DATA(P(  2,J),J=1,36)/  4.003,2HHE,  .025,  .000,  .000,
00105         *   .000,   .000,   .000,999.000,999.000,999.000,
00105         *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00105         * .00, .00,   .000,   .00,
00105         *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00105         *   .10059710E01,  -.72186701E-2,   .14225233E-2,
00105         *  -.14111192E-3,   .66914290E-5,  -.11980717E-6/
00107          DATA(P(  3,J),J=1,36)/  6.939,2HLI,  .055,  .000,  .000,
00107         *228.000,   .000,   .000,226.500,999.000,999.000,
00107         *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00107         *2.89,2.73,   .135,   .00,
00107         *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00107         *   .10085917E01,  -.10267098E-1,   .19859984E-2,
00107         *  -.19498321E-3,   .91950060E-5,  -.16415851E-6/
00111          DATA(P(  4,J),J=1,36)/  9.012,2HBE,  .11 ,  .000,  .000,
00111         *114.000,   .000,   .000,111.000,999.000,999.000,
00111         *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00111         *2.86,2.73,   .350,   .03,
00111         *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00111         *   .10118990E01,  -.14245909E-1,   .28139926E-2,
00111         *  -.28115022E-3,   .13437611E-4,  -.24230872E-6/
00113          DATA(P(  5,J),J=1,36)/ 10.811,2H B,  .188,  .000,  .000,
00113         * 67.600,   .000,   .000, 65.000,999.000,999.000,
00113         *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00113         *2.85,2.73,   .740,   .05,
00113         *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00113         *   .10153513E01,  -.18509068E-1,   .36845955E-2,
00113         *  -.36908500E-3,   .17648432E-4,  -.31814955E-6/
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00115        DATA(P(  6,J),J=1,36)/ 12.011,2H C,  .284,  .000,  .000,
00115       * 44.700,   .000,   .000, 43.680,646.000,837.000,
00115       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00115       *2.84,2.73,  1.350,   .07,
00115       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00115       *    .10194912E01,  -.23691256E-1,   .48299246E-2,
00115       *  -.49167499E-3,   .23763496E-4,  -.43147054E-6/
00117        DATA(P(  7,J),J=1,36)/ 14.007,2H N,  .402,  .000,  .000,
00117       * 31.600,   .000,   .000, 30.970,435.000,556.000,
00117       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00117       *2.83,2.73,  2.210,   .11,
00117       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00117       *    .10240059E01,  -.29437535E-1,   .61336705E-2,
00117       *  -.63335989E-3,   .30898140E-4,  -.56450887E-6/
00121        DATA(P(  8,J),J=1,36)/ 15.999,2H O,  .532,  .000,  .000,
00121       * 23.620,   .000,   .000, 23.320,309.000,390.000,
00121       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00121       *2.82,2.73,  3.800,   .17,
00121       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00121       *    .10284491E01,  -.35199635E-1,   .74029714E-2,
00121       *  -.76721469E-3,   .37474747E-4,  -.68485588E-6/
00123        DATA(P(  9,J),J=1,36)/ 18.998,2H F,  .685,  .000,  .000,
00123       * 18.320,   .000,   .000, 17.800,228.000,285.000,
00123       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00123       *2.81,2.73,  4.980,   .23,
00123       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00123       *    .10335608E01,  -.41864660E-1,   .89623295E-2,
00123       *  -.93928911E-3,   .46210902E-4,  -.84851553E-6/
00125        DATA(P( 10,J),J=1,36)/ 20.183,2HNE,  .867,  .000,  .000,
00125       * 14.610,   .000,   .000, 14.302,174.000,216.000,
00125       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00125       *2.80,2.73,  6.770,   .43,
00125       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00125       *    .10390854E01,  -.49116664E-1,   .10703538E-1,
00125       *  -.11347223E-2,   .56245408E-4,  -.10379363E-5/
00127        DATA(P( 11,J),J=1,36)/ 22.990,2HNA, 1.072,  .000,  .000,
00127       * 11.910,   .000,   .000, 11.480,136.000,168.000,
00127       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00127       *2.79,2.73,  9.050,   .55,
00127       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00127       *    .10442524E01,  -.56049932E-1,   .12310874E-1,
00127       *  -.13096987E-2,   .65021843E-4,  -.12007768E-5/
00131        DATA(P( 12,J),J=1,36)/ 24.312,2HMG, 1.305,  .000,  .000,
00131       *  9.890,   .000,   .000,  9.512,109.000,133.000,
00131       *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00131       *2.79,2.73, 11.750,   .89,
00131       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00131       *    .10499678E01,  -.63725293E-1,   .14165778E-1,
00131       *  -.15179592E-2,   .75701770E-4,  -.14020889E-5/
00133        DATA(P( 13,J),J=1,36)/ 26.982,2HAL, 1.560,  .000,  .000,
00133       *  8.339,   .000,   .000,  7.951, 89.000,108.000,
00133       * 94.000,   .000,   .000,   .000,   .000,   .000,   .000,
00133       *2.78,2.73, 14.870,  1.18,
00133       *   .00,   .00,   .00,   .00,   .00,   .00,   .00,   .00,
00133       *    .10555687E01,  -.71366787E-1,   .15998293E-1,
00133       *  -.17221065E-2,   .86106462E-4,  -.15973201E-5/
00135        DATA(P( 14,J),J=1,36)/ 28.086,2HSI, 1.839,  .000,  .000,
00135       *  7.125,   .000,   .000,  6.795, 73.000, 88.000,
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00135    * 78.100,    .000,    .000,    .000,    .000,    .000,    .000,
00135    *2.77,2.73, 18.500,  1.54,
00135    *  1.92,  1.40,   .00,    .00,    .00,    .00,    .00,    .00,
00135    *    .10614996E+1,  -.79481125E-1,    .17990243E-1,
00135    *  -.19476968E-2,    .97735756E-4,  -.18172641E-5/
00137     DATA(P( 15,J),J=1,36)/ 30.974,2H P, 2.146,  .000,   .000,
00137    *  6.157,   .000,    .000,  5.787, 61.000, 74.000,
00137    * 65.700,448.000,    .000,    .000,    .000,    .000,    .000,
00137    *2.77,2.73, 22.500,  1.96,
00137    *  2.32,  1.70,   .00,    .00,    .00,    .00,    .00,    .00,
00137    *   .10669823E01,  -.87160349E-1,    .19826554E-1,
00137    *  -.21511782E-2,    .10805634E-3,  -.20101752E-5/
00141     DATA(P( 16,J),J=1,36)/ 32.064,2H S, 2.472,  .000,   .000,
00141    *  5.372,    .000,    .000,  5.018, 52.000, 62.000,
00141    * 55.900,371.000,    .000,    .000,    .000,    .000,    .000,
00141    *2.76,2.73, 27.000,  2.43,
00141    *  2.78,  2.03,   .00,    .00,    .00,    .00,    .00,    .00,
00141    *    .10730906E+1,  -.95653415E-1,    .21945883E-1,
00141    *  -.23934257E-2,    .12061383E-3,  -.22485010E-5/
00143     DATA(P( 17,J),J=1,36)/ 35.453,2HCL, 2.822,  .200,   .000,
00143    *  4.728,    .000,    .000,  4.379, 44.400, 53.000,
00143    * 48.100,311.000,    .000,    .000,    .000,    .000,    .000,
00143    *2.76,2.73, 21.700,  2.98,
00143    *  3.29,  2.40,   .00,    .00,    .00,    .00,    .00,    .00,
00143    *    .10785866E+1,  -.10350823E-0,    .23847383E-1,
00143    *  -.26056655E-2,    .13142932E-3,  -.24513120E-5/
00145     DATA(P( 18,J),J=1,36)/ 39.948,2HAR, 3.203,  .245,   .000,
00145    *  4.192,    .000,    .000,  3.871, 38.400, 45.400,
00145    * 41.700,263.000,    .000,    .000,    .000,    .000,    .000,
00145    *2.75,2.73, 36.900,  3.62,
00145    *  3.86,  2.81,  1.02,    .00,    .00,    .00,    .00,    .00,
00145    *    .10843163E+1,  -.11171609E-0,    .25877882E-1,
00145    *  -.28357953E-2,    .14327976E-3,  -.26751186E-5/
0014      DATA(P( 19,J),J=1,36)/ 39.102,2H K, 3.607,  .294,   .000,
00147    *  3.741,    .000,    .000,  3.437, 33.400, 39.300,
00147    * 36.400,225.000,    .000,    .000,    .000,    .000,    .000,
00147    *2.75,2.73, 42.500,  4.31,
00147    *  4.49,  3.27,  1.04,    .00,    .00,    .00,    .00,    .00,
00147    *    .10905924E+1,  -.12063515E-0,    .28167494E-1,
00147    *  -.31023589E-2,    .15726734E-3,  -.29428020E-5/
00151     DATA(P( 20,J),J=1,36)/ 40.080,2HCA, 4.038,  .346,   .000,
00151    *  3.358, 36.330,    .000,  3.070, 29.300, 34.300,
00151    * 32.000,194.000,    .000,    .000,    .000,    .000,    .000,
00151    *2.74,2.73, 48.400,  5.10,
00151    *  5.18,  3.77,  1.09,    .00,    .00,    .00,    .00,    .00,
00151    *    .10957041E+1,  -.12824494E-0,    .30009781E-1,
00151    *  -.33062601E-2,    .16760103E-3,  -.31357004E-5/
00153     DATA(P( 21,J),J=1,36)/ 44.956,2HSC, 4.493,  .402,   .000,
00153    *  3.031,  3.350,    .000,  2.757, 25.800, 30.100,
00153    * 28.300,168.000,    .000,    .000,    .000,    .000,    .000,
00153    *2.74,2.73, 55.100,  5.99,
00153    *  5.93,  4.31,  1.16,    .00,    .00,    .00,    .00,    .00,
00153    *    .11017056E+1,  -.13696826E-0,    .32247540E-1,
00153    *  -.35671997E-2,    .16128079E-3,  -.33972774E-5/
00155     DATA(P( 22,J),J=1,36)/ 47.900,2HTI, 4.966,  .456,   .000,
00155    *  2.749, 27.420,    .000,  2.497, 22.900, 26.600,
00155    * 25.200,147.000,    .000,    .000,    .000,    .000,    .000,
00155    *2.73,2.73, 62.100,  7.00,
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00155      *  6.75,  4.90,  1.27,   .00,   .00,   .00,   .00,   .00,
00155      *    .11071053E+1,  -.14503819E-0,   .34272999E-1,
00155      *  -.37984818E-2,   .19324299E-3,  -.36238298E-5/
00157       DATA(P( 23,J),J=1,36)/ 50.942,2H V, 5.465,  .513,  .000,
00157      *  2.504, 24.250,   .000,  2.269, 20.400, 23.700,
00157      * 22.600,129.000,   .000,   .000,   .000,   .000,   .000,
00157      *2.73,2.73, 69.800,  8.02,
00157      *  7.64,  5.55,  1.40,   .00,   .00,   .00,   .00,   .00,
00157      *    .11122885E+1,  -.15291673E-0,   .36249910E-1,
00157      *  -.40240437E-2,   .20490146E-3,  -.38444978E-5/
00161       DATA(P( 24,J),J=1,36)/ 51.996,2HCR, 5.989,  .575,  .000,
00161      *  2.290, 21.640,   .000,  2.070, 18.300, 21.200,
00161      * 20.300,114.000,   .000,   .000,   .000,   .000,   .000,
00161      *2.73,2.73, 78.000,  9.18,
00161      *  8.60,  6.24,  1.55,   .00,   .00,   .00,   .00,   .00,
00161      *    .11173811E+1,  -.16072637E-0,   .38216673E-1,
00161      *  -.42488985E-2,   .21653707E-3,  -.40649120E-5/
00163       DATA(P( 25,J),J=1,36)/ 54.938,2HMN, 6.539,  .640,  .000,
00163      *  2.102, 19.450,   .000,  1.896, 16.500, 19.000,
00163      * 18.300,101.000,   .000,   .000,   .000,   .000,   .000,
00163      *2.72,2.73, 86.700, 10.45,
00163      *  9.64,  6.99,  1.74,   .00,   .00,   .00,   .00,   .00,
00163      *    .11228161E+1,  -.16898721E-0,   .40360369E-1,
00163      *  -.44993125E-2,   .22969024E-3,  -.43166765E-5/
00165       DATA(P( 26,J),J=1,36)/ 55.847,2HFE, 7.112,  .708,  .000,
00165      *  1.936, 17.590,   .000,  1.743, 14.900, 17.100,
00165      * 16.600, 90.400,   .000,   .000,   .000,   .000,   .000,
00165      *2.72,2.73, 95.800, 11.75,
00165      * 10.75,  7.79,  1.95,   .00,   .00,   .00,   .00,   .00,
00165      *    .11276951E+1,  -.17663497E-0,   .42308399E-1,
00165      *  -.47236532E-2,   .24135446E-3,  -.45383431E-5/
00167       DATA(P( 27,J),J=1,36)/ 58.933,2HCO, 7.709,  .779,  .000,
00167      *  1.789, 15.972,   .000,  1.608, 13.500, 15.300,
00167      * 15.100, 81.000,   .000,   .000,   .000,   .000,   .000,
00167      *2.71,2.73,105.500, 13.25,
00167      * 11.94,  8.65,  2.17,  1.62,  1.33,  1.13,  1.21,   .00,
00167      *    .11322651E+1,  -.18395174E-0,   .44157222E-1,
00167      *  -.49350709E-2,   .25228900E-3,  -.47453614E-5/
00171       DATA(P( 28,J),J=1,36)/ 58.710,2HNI, 8.333,  .855,  .000,
00171      *  1.658, 14.561,   .000,  1.488, 12.300, 14.100,
00171      * 13.800, 72.800, 89.800,   .000,   .000,   .000,   .000,
00171      *2.71,2.73,115.900, 14.80,
00171      * 13.22,  9.57,  2.44,  1.83,  1.51,  1.27,  1.35,   .00,
00171      *    .11371069E+1,  -.19162685E-0,   .46154723E-1,
00171      *  -.51685125E-2,   .26459800E-3,  -.49799246E-5/
00173       DATA(P( 29,J),J=1,36)/ 63.540,2HCU, 8.979,  .931,  .000,
00173      *  1.541, 13.336,   .000,  1.380, 11.270, 12.800,
00173      * 12.600, 65.800, 80.700,   .000,   .000,   .000,   .000,
00173      *2.71,2.73,126.800, 16.45,
00173      * 14.06, 10.54,  2.73,  2.06,  1.70,  1.44,  1.50,   .00,
00173      *    .11413851E+1,  -.19865793E-0,   .47943894E-1,
00173      *  -.53739138E-2,   .27519651E-3,  -.51818297E-5/
00175       DATA(P( 30,J),J=1,36)/ 65.370,2HZN, 9.659, 1.020,  .000,
00175      *  1.435, 12.254,   .000,  1.283, 10.330, 11.870,
00175      * 11.600, 59.600, 72.800,   .000,   .000,   .000,   .000,
00175      *2.70,2.73,138.000, 18.25,
00175      * 15.60, 11.20,  3.05,  2.31,  1.90,  1.61,  1.67,   .00,
00175      *    .11459284E+1,  -.20602679E-0,   .49873140E-1,
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00175     *    -.56008203E-2,   .28708880E-3,  -.54095790E-5/
00177      DATA(P( 31,J),J=1,36)/ 69.720,2HGA,10.367, 1.115,  .000,
00177     *  1.340, 11.292,   .000,  1.196,  9.540, 10.930,
00177     * 11.100, 54.200, 65.900,   .000,   .000,   .000,   .000,
00177     *2.70,2.73,149.800, 20.20,
00177     * 17.25, 12.40,  3.39,  2.58,  2.12,  1.80,  1.84,   .00,
00177     *     .11478795E+1,  -.21274740E-0,   .51595230E-1,
00177     *    -.57985485E-2,   .29740762E-3,  -.56055460E-5/
00201      DATA(P( 32,J),J=1,36)/ 72.590,2HGE,11.103, 1.217,  .000,
00201     *  1.254, 10.436,   .000,  1.117,  8.730,  9.940,
00201     * 10.190, 49.400, 59.900, 59.900, 87.200, 87.500,   .000,
00201     *2.70,2.73,162.200, 22.15,
00201     * 16.95, 13.60,  3.76,  2.87,  2.36,  2.01,  2.03,   .00,
00201     *     .11536303E+1,  -.21919364E-0,   .53240959E-1,
00201     *    -.59875809E-2,   .30720397E-3,  -.57911966E-5/
00203      DATA(P( 33,J),J=1,36)/ 74.922,2HAS,11.867, 1.323,  .000,
00203     *  1.176,  9.671,   .000,  1.045,  8.107,  9.124,
00203     *  9.390, 45.100, 54.500, 54.500, 79.300, 79.600,   .000,
00203     *2.67,2.73,175.400, 24.25,
00203     * 20.75, 14.90,  4.28,  3.18,  2.62,  2.23,  2.23,   .00,
00203     *     .11573725E+1,  -.22566962E-0,   .54918893E-1,
00203     *    -.61823614E-2,   .31737448E-3,  -.59849408E-5/
00205      DATA(P( 34,J),J=1,36)/ 78.960,2HSE,12.658, 1.436,  .000,
00205     *  1.105,  8.990,   .000,   .980,  7.506,  8.416,
00205     *  8.670, 41.400, 49.800, 49.800, 72.400, 72.700,   .000,
00205     *2.69,2.73,189.400, 26.40,
00205     * 22.55, 16.20,  4.69,  3.52,  2.90,  2.46,  2.45,   .00,
00205     *     .11614338E+1,  -.23259068E-0,   .56772836E-1,
00205     *    -.64026937E-2,   .32906607E-3,  -.62101708E-5/
00207      DATA(P( 35,J),J=1,36)/ 79.909,2HBR,13.474, 1.550,  .000,
00207     *  1.040,  8.375,   .000,   .920,  6.970,  7.800,
00207     *  8.000, 38.000, 45.600, 45.600, 66.200, 66.500,435.000,
00207     *2.69,2.73,205.000, 28.80,
00207     * 24.60, 17.70,  5.13,  3.88,  3.20,  2.72,  2.67,   .00,
00207     *     .11647587E+1,  -.23852879E-0,   .58300775E-1,
00207     *    -.65788478E-2,   .33821259E-3,  -.63836742E-5/
00211      DATA(P( 36,J),J=1,36)/ 83.800,2HKR,14.326, 1.675,  .000,
00211     *   .980,  7.817,   .000,   .866,  6.460,  7.210,
00211     *  7.430, 35.000, 41.900, 41.900, 60.700, 61.000,388.000,
00211     *2.68,2.73,219.300, 31.25,
00211     * 26.90, 19.15,  5.60,  4.26,  3.52,  2.99,  2.91,   .00,
00211     *     .11691128E+1,  -.24456573E-0,   .59884880E-1,
00211     *    -.67641065E-2,   .34793024E-3,  -.65693448E-5/
00213      DATA(P( 37,J),J=1,36)/ 85.470,2HRB,15.200, 1.804,  .110,
00213     *   .926,  7.318,   .000,   .816,  5.998,  6.643,
00213     *  6.890, 32.400, 38.600, 38.600, 55.700, 56.000,347.000,
00213     *2.68,2.73,235.500, 33.90,
00213     * 28.80, 20.80,  6.10,  4.68,  3.86,  3.28,  3.17,   .00,
00213     *     .11709729E+1,  -.25004494E-0,   .61292183E-1,
00213     *    -.69259219E-2,   .35631424E-3,  -.67281444E-5/
00215      DATA(P( 38,J),J=1,36)/ 87.620,2HSR,16.105, 1.940,  .133,
00215     *   .875,  6.863,   .000,   .770,  5.583,  6.172,
00215     *  6.387, 29.900, 35.600, 35.600, 51.300, 51.600,312.000,
00215     *2.68,2.73,251.300, 36.50,
00215     * 31.20, 22.40,  6.62,  5.12,  4.22,  3.59,  3.44,   .00,
00215     *     .11741581E+1,  -.25585365E-0,   .62832654E-1,
00215     *    -.71071908E-2,   .36585727E-3,  -.69109110E-5/
00217      DATA(P( 39,J),J=1,36)/ 88.905,2H Y,17.038, 2.080,  .157,
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00217     *   .829,  6.449,   .000,   .728,  5.232,  6.755,
00217     *  5.961, 27.800, 32.900, 32.900, 47.400, 47.700,280.000,
00217     *2.67,2.73,268.100, 39.30,
00217     * 33.50, 24.10,  7.18,  5.58,  4.61,  3.72,  3.73,   .00,
00217     *    .11770344E+1,  -.26131707E-0,   .64271033E-1,
00217     *   -.72754659E-2,   .37467899E-3,  -.70793358E-5/
00221      DATA(P( 40,J),J=1,36)/ 91.220,2HZR,17.998, 2.222,  .180,
00221     *   .786,  6.071,   .000,   .000,  4.867,  5.378,
00221     *  5.538, 25.800, 30.400, 30.400, 43.800, 44.100,253.000,
00221     * .00,2.73,   .000, 42.30,
00221     * 36.15, 25.95,  7.78,  6.08,  5.02,  4.28,  4.03,  4.71,
00221     *    .11796608E+1,  -.26647782E-0,   .65619469E-1,
00221     *   -.74320920E-2,   .38284436E-3,  -.72346211E-5/
00223      DATA(P( 41,J),J=1,36)/ 92.906,2HNB,18.986, 2.371,  .205,
00223     *   .746,  5.724,   .000,   .000,  4.581,  5.026,
00223     *  5.223, 24.000, 28.200, 28.200, 40.600, 40.900,229.000,
00223     * .00,2.73,   .000, 45.50,
00223     * 38.90, 27.90,  8.39,  6.61,  5.46,  4.65,  4.34,  4.99,
00223     *    .11822348E+1,  -.27157331E-0,   .66965759E-1,
00223     *   -.75897910E-2,   .39181497E-3,  -.73925412E-5/
00225      DATA(P( 42,J),J=1,36)/ 95.940,2HMO,20.000, 2.520,  .227,
00225     *   .709,  5.407,   .000,   .000,  4.278,  4.718,
00225     *  4.913, 22.400, 26.300, 26.300, 37.700, 38.000,208.000,
00225     * .00,2.72,   .000, 48.80,
00225     * 41.45, 29.75,  9.05,  7.17,  5.42,  5.05,  4.68,  5.28,
00225     *    .11842622E+1,  -.27629940E-0,   .68213642E-1,
00225     *   -.77345334E-2,   .39865100E-3,  -.75356802E-5/
00227      DATA(P( 43,J),J=1,36)/ 99.000,2HTC,21.044, 2.677,  .253,
00227     *   .675,  5.115,   .030,   .000,  4.000,  4.436,
00227     *  4.632, 20.900, 24.400, 24.900, 35.000, 35.300,189.000,
00227     * .00,2.72,   .000, 52.10,
00227     * 44.50, 31.95,  9.74,  7.75,  6.41,  5.47,  5.03,  5.58,
00227     *    .11865511E+1,  -.28073108E-0,   .69337845E-1,
00227     *   -.78629479E-2,   .40525687E-3,  -.76600245E-5/
00231      DATA(P( 44,J),J=1,36)/101.070,2HRU,22.117, 2.838,  .279,
00231     *   .643,  4.896,   .000,   .000,  3.830,  4.180,
00231     *  4.369, 19.500, 22.800, 22.800, 32.600, 32.900,172.000,
00231     * .00,2.72,   .000, 55.60,
00231     * 47.50, 34.10, 10.47,  8.39,  6.93,  5.91,  5.39,  5.88,
00231     *    .11891661E+1,  -.28582484E-0,   .70728004E-1,
00231     *   -.80272821E-2,   .41410560E-3,  -.78306457E-5/
00233      DATA(P( 45,J),J=1,36)/102.905,2HRH,23.220, 3.004,  .307,
00233     *   .613,  4.597,   .000,   .000,  3.626,  3.942,
00233     *  4.130, 18.300, 21.300, 21.400, 30.500, 30.800,157.000,
00233     * .00,2.72,   .000, 59.30,
00233     * 50.70, 36.40, 11.24,  9.05,  7.47,  6.38,  5.78,  6.20,
00233     *    .11910248E+1,  -.29001153E-0,   .71813822E-1,
00233     *   -.81541762E-2,   .42055990E-3,  -.79525062E-5/
00235      DATA(P( 46,J),J=1,36)/106.400,2HPD,24.350, 3.173,  .335,
00235     *   .585,  4.368,   .000,   .000,  3.428,  3.724,
00235     *  3.908, 17.200, 19.900, 20.200, 28.500, 28.800,144.000,
00235     * .00,2.72,   .000, 63.10,
00235     * 53.95, 38.70, 12.03,  9.74,  8.05,  6.87,  6.18,  6.52,
00235     *    .11927643E+1,  -.29403836E-0,   .72858036E-1,
00235     *   -.82741678E-2,   .42675529E-3,  -.80694272E-5/
00237      DATA(P( 47,J),J=1,36)/107.870,2HAG,25.514, 3.351,  .367,
00237     *   .559,  4.154,   .000,   .000,  3.254,  3.514,
00237     *  3.698, 16.100, 18.700, 19.000, 26.600, 26.900,132.000,
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00237   * .00,2.71,   .000, 67.30,
00237   * 57.50, 41.30, 12.87, 10.47,  8.65,  7.39,  6.60,  6.86,
00237   *   .11947527E+1,  -.2983381 2E-0,   .74010313E-1,
00237   *  -.84098317E-2,   .43388270E-3,  -.82056113E-5/
00241    DATA(P( 48,J),J=1,36)/112.400,2HCD,26.711, 3.538,  .404,
00241   *    .535,  3.956,   .000,   .000,  3.085,  3.326,
00241   *  3.504, 15.200, 17.500, 17.900, 25.080, 25.300,121.000,
00241   * .00,2.71,   .000, 71.00,
00241   * 60.70, 43.60, 13.76, 11.24,  9.29,  7.94,  7.04,  7.20,
00241   *   .11963425E+1,  -.30214036E-0,   .74997902E-1,
00241   *  -.85231364E-2,   .43972116E-3,  -.83155519E-5/
00243    DATA(P( 49,J),J=1,36)/114.820,2HIN,27.940, 3.730,  .443,
00243   *    .512,  3.772,   .000,   .000,  2.926,  3.147,
00243   *  3.324, 14.300, 16.500, 16.900, 23.400, 23.700,111.000,
00243   * .00,2.71,   .000, 75.50,
00243   * 64.50, 46.30, 14.68, 12.05,  9.96,  8.51,  7.50,  7.55,
00243   *   .11979666E+1,  -.30597371E-0,   .76011181E-1,
00243   *  -.86410679E-2,   .44586184E-3,  -.84321082E-5/
00245    DATA(P( 50,J),J=1,36)/118.690,2HSN,29.200, 3.929,  .485,
00245   *    .491,  3.600,   .000,   .000,  2.777,  2.982,
00245   *  3.156, 13.500, 15.500, 16.000, 22.000, 22.300,102.000,
00245   * .00,2.71,   .000, 79.60,
00245   * 68.00, 48.80, 15.65, 12.90, 10.66,  9.12,  7.98,  7.92,
00245   *   .11993437E+1,  -.30948490E-0,   .76919675E-1,
00245   *  -.87447912E-2,   .45118225E-3,  -.85319507E-5/
00247    DATA(P( 51,J),J=1,36)/121.750,2HSB,30.491, 4.132,  .528,
00247   *    .470,  3.439,   .000,   .000,  2.639,  2.830,
00247   *  3.000, 12.700, 14.600, 15.100, 20.700, 21.000, 94.500,
00247   * .00,2.70,   .000, 84.20,
00247   * 71.95, 51.70, 16.66, 13.79, 11.40,  9.75,  8.48,  8.29,
00247   *   .12009430E+1,  -.31323344E-0,   .77921033E-1,
00247   *  -.88619739E-2,   .45730267E-3,  -.86483224E-5/
00251    DATA(P( 52,J),J=1,36)/127.600,2HTE,31.814, 4.341,  .572,
00251   *    .000,  3.289,   .000,   .000,  2.511,  2.687,
00251   *  2.855, 12.000, 13.700, 14.300, 19.500, 19.800, 87.400,
00251   * .00,2.70,   .000, 88.50,
00251   * 75.65, 54.30, 17.72, 14.73, 12.17, 10.42,  9.00,  8.67,
00251   *   .12018719E+1,  -.31616079E-0,   .78646660E-1,
00251   *  -.89414455E-2,   .46124193E-3,  -.87202734E-5/
00253    DATA(P( 53,J),J=1,36)/126.904,2H I,33.169, 4.557,  .619,
00253   *    .000,  3.149,   .000,   .000,  2.389,  2.553,
00253   *  2.719, 11.400, 13.000, 13.600, 18.400, 18.600, 80.900,
00253   * .00,2.70,   .000, 94.00,
00253   * 80.35, 57.70, 18.82, 15.70, 12.98, 11.11,  9.54,  9.07,
00253   *   .12033234E+1,  -.31969351E-0,   .79586506E-1,
00253   *  -.90510771E-2,   .46695024E-3,  -.88285360E-5/
00255    DATA(P( 54,J),J=1,36)/131.300,2HXE,34.561, 4.782,  .672,
00255   *    .000,  3.017,   .000,   .000,  2.279,  2.429,
00255   *  2.592, 10.800, 12.300, 12.900, 17.300, 17.600, 75.800,
00255   * .00,2.69,   .000, 98.30,
00255   * 84.00, 60.30, 19.97, 16.72, 13.82, 11.84, 10.11,  9.47,
00255   *   .12043486E+1,  -.32269275E-0,   .80351472E-1,
00255   *  -.91369972E-2,   .47129416E-3,  -.89091136E-5/
00257    DATA(P( 55,J),J=1,36)/132.905,2HCS,35.985, 5.012,  .726,
00257   *    .000,  2.893,   .000,   .000,  2.167,  2.314,
00257   *  2.474, 10.202, 11.600, 12.300, 16.400, 16.700, 69.600,
00257   * .00,2.69,   .000,103.40,
00257   * 88.40, 63.40, 21.16, 18.20, 14.70, 12.60, 10.69,  9.88,
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00257      *     .12050686E+1,  -.32530850E-0,   .80986977E-1,
00257      *  -.92051588E-2,    .47460641E-3,  -.89685973E-5/
00261       DATA(P( 56,J),J=1,36)/137.340,2HBA,37.441, 5.247,  .781,
00261      *     .000,  2.776,   .000,    .000,  2.068,  2.204,
00261      *  2.363,  9.557, 10.845, 11.700, 15.500, 15.800, 64.700,
00261      * .00,2.69,    .000,109.00,
00261      * 93.15, 68.90, 22.41, 19.30, 16.00, 13.40, 11.30, 10.33,
00261      *     .12067242E+1,  -.32900286E-0,    .82008362E-1,
00261      *  -.93273968E-2,    .48108562E-3,  -.90930444E-5/
00263       DATA(P( 57,J),J=1,36)/138.910,2HLA,38.925, 5.483,  .832,
00263      *     .000,  2.646, 14.880,    .000,  1.973,  2.103,
00263      *  2.258,  9.092, 10.321, 11.100, 14.700, 15.300, 60.200,
00263      * .00,2.68,    .000,114.40,
00263      * 97.80, 70.20, 23.70, 20.40, 16.90, 14.23, 11.93, 10.77,
00263      *     .12073441E+1,  -.33145458E-0,    .82601011E-1,
00263      *  -.93905069E-2,    .48413151E-3,  -.91473894E-5/
00265       DATA(P( 58,J),J=1,36)/140.120,2HCE,40.443, 5.723,  .883,
00265      *     .000,  2.562, 14.040,    .000,  1.889,  2.011,
00265      *  2.164,  8.614,  9.692, 10.488, 13.900, 14.200, 56.100,
00265      * .00,2.68,    .000,120.00,
00265      *102.50, 73.60, 25.05, 21.60, 17.90, 15.50, 12.58, 11.21,
00265      *     .12081738E+1,  -.33412713E-0,    .83274484E-1,
00265      *  -.94649978E-2,    .48784260E-3,  -.92153705E-5/
00267       DATA(P( 59,J),J=1,36)/140.907,2HPR,41.991, 5.964,  .931,
00267      *     .000,  2.463, 13.343,    .000,  1.811,  1.924,
00267      *  2.077,  8.188,  9.258,  9.957, 13.200, 13.500, 52.400,
00267      * .00,2.68,    .000,125.50,
00267      *107.30, 77.00, 26.47, 22.80, 18.90, 16.30, 13.26, 11.66,
00267      *     .12092009E+1,  -.33701009E-0,    .84027708E-1,
00267      *  -.95508844E-2,    .49222610E-3,  -.92971968E-5/
00271       DATA(P( 60,J),J=1,36)/144.240,2HND,43.569, 6.207,  .978,
00271      *     .000,  2.370, 12.680,    .000,  1.735,  1.843,
00271      *  1.995,  7.841,  8.773,  9.499, 12.500, 12.800, 48.900,
00271      * .00,2.67,    .000,132.00,
00271      *112.80, 81.00, 27.93, 24.10, 20.00, 17.20, 13.96, 12.13,
00271      *     .12099524E+1,  -.33954793E-0,    .84664822E-1,
00271      *  -.96289422E-2,    .49569714E-3,  -.93604813E-5/
00273       DATA(P( 61,J),J=1,36)/147.000,2HPM,45.184, 6.459, 1.027,
00273      *     .000,  2.282, 12.000,    .000,  1.665,  1.767,
00273      *  1.918,  7.513,  8.376,  9.115, 11.900, 12.200, 45.800,
00273      * .00,2.67,    .000,138.50,
00273      *118.50, 85.00, 29.44, 25.40, 21.00, 18.20, 14.69, 12.60,
00273      *     .12105265E+1,  -.34185231E-0,    .85223556E-1,
00273      *  -.96803457E-2,    .49855048E-3,  -.94111665E-5/
00275       DATA(P( 62,J),J=1,36)/150.350,2HSM,46.834, 4.716, 1.080,
00275      *     .000,  2.200, 11.470,    .000,  1.599,  1.703,
00275      *  1.845,  7.178,  8.023,  8.705, 11.300, 11.600, 42.800,
00275      * .00,2.67,    .000,143.50,
00275      *122.50, 88.00, 31.01, 26.70, 22.20, 19.10, 15.44, 13.09,
00275      *     .12112732E+1,  -.34432930E-0,    .85842550E-1,
00275      *  -.97478089E-2,    .50187181E-3,  -.94713023E-5/
00277       DATA(P( 63,J),J=1,36)/151.960,2HEU,48.519, 6.977, 1.131,
00277      *     .000,  2.121, 10.960,    .000,  1.536,  1.626,
00277      *  1.775,  6.856,  7.642,  8.331, 10.604, 10.893, 40.100,
00277      * .00,2.66,    .000,150.00,
00277      *128.00, 92.00, 32.63, 28.10, 23.30, 20.10, 16.22, 13.85,
00277      *     .12120667E+1,  -.34684891E-0,    .86483300E-1,
00277      *  -.98189600E-2,    .50541107E-3,  -.95360529E-5/
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00301    DATA(P( 64,J),J=1,36)/157.250,2HGD,50.239, 7.243, 1.185,
00301    *   .000,  2.047, 10.460,   .000,  1.477,  1.561,
00301    *  1.710,  6.566,  7.322,  7.997, 10.111, 10.408, 37.700,
00301    * .00,2.66,   .000,157.00,
00301    *134.00, 96.30, 34.31, 29.60, 24.50, 21.20, 17.02, 14.30,
00301    *    .12127247E+1,  -.34919322E-0,   .87066293E-1,
00301    *  -.98822415E-2,   .50850492E-3,  -.95918031E-5/
00303    DATA(P( 65,J),J=1,36)/158.924,2HYB,51.996, 7.514, 1.241,
00303    *   .000,  1.977, 10.000,   .000,  1.421,  1.501,
00303    *  1.649,  6.292,  7.011,  7.685,  9.692,  9.957, 35.400,
00303    * .00,2.65,   .000,163.50,
00303    *140.00,100.30, 36.06, 31.10, 25.80, 22.30, 17.85, 14.80,
00303    *    .12127314E+1,  -.35074627E-0,   .87372184E-1,
00303    *  -.99069886E-2,   .50934800E-3,  -.96014292E-5/
00305    DATA(P( 66,J),J=1,36)/162.500,2HDY,53.789, 7.790, 1.295,
00305    *   .000,  1.909,  9.590,   .000,  1.365,  1.438,
00305    *  1.579,  6.088,  6.715,  7.383,  9.258,  9.528, 33.200,
00305    * .00,2.65,   .000,170.50,
00305    *146.00,104.50, 37.86, 32.60, 27.00, 23.40, 18.70, 15.30,
00305    *    .12133589E+1,  -.35301358E-0,   .87932110E-1,
00305    *  -.99672405E-2,   .51226374E-3,  -.96535232E-5/
00307    DATA(P( 67,J),J=1,36)/164.930,2HHO,55.618, 8.071, 1.351,
00307    *   .000,  1.845,  9.200,   .000,  1.317,  1.390,
00307    *  1.535,  5.820,  6.453,  7.128,  8.899,  9.155, 31.300,
00307    * .00,2.65,   .000,176.50,
00307    *151.00,108.50, 39.76, 34.30, 28.50, 24.50, 19.59, 15.85,
00307    *    .12139149E+1,  -.35518014E-0,   88459015E-1,
00307    *  -.10022942E-1,   .51492197E-3,  -.97003804E-5/
00311    DATA(P( 68,J),J=1,36)/167.260,2HER,57.486, 8.358, 1.409,
00311    *   .000,  1.784,  8.820,   .000,  1.268,  1.338,
00311    *  1.482,  5.581,  6.175,  6.834,  8.509,  8.773, 29.500,
00311    * .00,2.64,   .000,184.00,
00311    *157.00,113.00, 41.69, 35.90, 29.80, 25.70, 20.50, 16.30,
00311    *    .12146044E+1,  -.35747802E-0,   .89032710E-1,
00311    *  -.10085203E-1,   .51795901E-3,  -.97549555E-5/
00313    DATA(P( 69,J),J=1,36)/168.934,2HTM,59.390, 8.648, 1.468,
00313    *   .000,  1.727,  8.480,   .000,  1.222,  1.288,
00313    *  1.433,  5.366,  5.931,  6.559,  8.155,  8.433, 27.800,
00313    * .00,2.64,   .000,192.50,
00313    *165.00,118.00, 43.69, 37.70, 31.20, 27.00, 21.44, 16.85,
00313    *    .12148819E+1,  -.35927922E-0,   .89432538E-1,
00313    *  -.10123145E-1,   .51957020E-3,  -.97802340E-5/
00315    DATA(P( 70,J),J=1,36)/173.040,2HYB,61.332, 8.944, 1.528,
00315    *   .000,  1.672,  8.149,   .000,  1.182,  1.243,
00315    *  1.386,  5.161,  5.686,  6.331,  7.836,  8.086, 26.200,
00315    * .00,2.63,   .000,199.00,
00315    *170.00,122.00, 45.79, 39.60, 32.70, 28.30, 22.40, 17.45,
00315    *    .12153540E+1,  -.36129034E-0,   .89909077E-1,
00315    *  -.10172036E-1,   .52182912E-3,  -.98188948E-5/
00317    DATA(P( 71,J),J=1,36)/174.970,2HLU,63.314, 9.244, 1.589,
00317    *   .000,  1.620,  7.840,   .000,  1.140,  1.199,
00317    *  1.341,  4.972,  5.475,  6.112,  7.545,  7.777, 24.700,
00317    * .00,2.63,   .000,206.00,
00317    *176.00,126.00, 47.92, 41.30, 34.20, 29.60, 23.40, 18.00,
00317    *    .12156477E+1,  -.36307693E-0,   .90307117E-1,
00317    *  -..0209896E-1,   .52343868E-3,  -.98441733E-5/
00321    DATA(P( 72,J),J=1,36)/178.?90,2HHF,65.351, 9.561, 1.662,
00321    *   .000,  1.570,  7.539,   .000,  1.100,  1.155,
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00321     * 1.273, 4.753, 5.211, 5.861, 7.190, 7.427, 23.400,
00321     * .00,2.62,   .000,214.00,
00321     *183.00,131.00, 50.13, 43.20, 35.80, 30.90, 24.43, 18.55,
00321     *   .12154608E+1,  -.36428607E-0,   .90505064E-1,
00321     *  -.10220122E-1,   .52344101E-3,  -.98366072E-5/
00323      DATA(P( 73,J),J=1,36)/180.948,2HTA,67.416, 9.881, 1.735,
00323     *   .000,  1.523,  7.252,   .000,  1.061,  1.114,
00323     * 1.255,  4.569,  5.015,  5.637,  6.898,  7.128, 22.100,
00323     * .00,2.62,   .000,222.00,
00323     *190.00,136.00, 52.44, 45.20, 37.50, 32.40, 25.48, 19.05.
00323     *   .12159710E+1,  -.36629272E-0,   .90982914E-1,
00323     *  -.10269132E-1,   .52569993E-3,  -.98751425E-5/
00325      DATA(P( 74,J),J=1,36)/183.850,2H W,69.525,10.207, 1.809,
00325     *   .000,  1.476,  6.983,   .000,  1.025,  1.075,
00325     * 1.216,  4.405,  4.823,  5.351,  6.640,  6.871, 20.900,
00325     * .00,2.61,   .000,231.00,
00325     *197.00,142.00, 54.79, 47.20, 39.10, 33.80, 26.57, 19.60,
00325     *   .12160664E+1,  -.36780047E-0,   .91288388E-1,
00325     *  -.10274373E-1,   .52658096E-3,  -.98855744E-5/
00327      DATA(P( 75,J),J=1,36)/186.200,2HRE,71.676,10.535, 1.883,
00327     *   .000,  1.433,  6.729,   .000,   .990,  1.037,
00327     * 1.177,  4.231,  4.625,  5.253,  6.357,  6.594, 19.800,
00327     * .00,2.61,   .000,239.00,
00327     *204.00,147.00, 57.21, 49.30, 40.90, 35.30, 27.68, 20.10,
00327     *   .12162924E+1,  -.36944044E-0,   .91638446E-1,
00327     *  -.10325525E-1,   .52778749E-3,  -.99024310E-5/
00331      DATA(P( 76,J),J=1,36)/190.200,2HOS,73.870,10.871, 1.960,
00331     *   .000,  1.391,  6.490,   .000,   .956,  1.001,
00331     * 1.140,  4.064,  4.443,  5.060,  6.106,  6.357, 18.800,
00331     * .00,2.60,   .000,247.00,
00331     *211.00,152.00, 59.70, 51.50, 42.60, 36.90, 28.83, 20.45,
00331     *   .12164927E+1,  -.37103456E-0,   .91975689E-1,
00331     *  -.10355104E-1,   .52891276E-3,  -.99177405E-5/
00333      DATA(P( 77,J),J=1,36)/192.200,2HIR,76.111,11.215, 2.040,
00333     *   .000,  1.351,  6.262,   .000,   .923,   .967,
00333     * 1.106,  3.915,  4.273,  4.873,  5.880,  6.094, 17.800,
00333     * .00,2.60,   .000,256.00,
00333     *219.00,157.00, 62.27, 53.70, 44.50, 38.40, 30.01, 21.35,
00333     *   .1216448 E 1,  -.37232566E-0,   .92206717E-1,
00333     *  -.10369834E-1,   .52916608E-3,  -.99150839E-5/
00335      DATA(P( 78,J),J=1,36)/195.090,2HPT,78.395,11.564, 2.122,
00335     *   .000,  1.313,  6.097,   .000,   .893,   .934,
00335     * 1.072,  3.774,  4.114,  4.710,  5.665,  5.880, 16.900,
00335     * .00,2.59,   .000,263.00,
00335     *225.00,161.00, 64.92, 56.00, 46.40, 40.10, 31.22, 21.95,
00335     *   .12166262E+1,  -.37385374E-0,   .92521310E-1,
00335     *  -.10396112E-1,   .53008972E-3,  -.99261415E-5/
00337      DATA(P( 79,J),J=1,36)/196.967,2HAU,80.725,11.919, 2.206,
00337     *   .000,  1.276,  5.840,   .000,   .863,   .903,
00337     * 1.040,  3.620,  3.939,  4.522,  5.415,  5.629, 16.000,
00337     * .00,2.59,   .000,272.00,
00337     *232.00,167.00, 67.64, 58.30, 48.30, 41.80, 32.47, 22.50,
00337     *   .12165537E+1,  -.37506962E-0,   .92727244E-1,
00337     *  -.10407273E-1,   .53013023E-3,  -.99190720E-5/
00341      DATA(P( 80,J),J=1,36)/200.590,2HHG,83.102,12.284, 2.295,
00341     *   .000,  1.241,  5.648,   .000,   .835,   .872,
00341     * 1.008,  3.482,  3.779,  4.349,  5.280,  5.413, 15.200,
00341     * .00,2.58,   .000,281.00,
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00341     *240.00,172.00, 70.55, 60.80, 50.40, 43.60, 33.74, 23.10,
00341     *     .12168427E+1,  -.37668729E-0,   .93074918E-1,
00341     *  -.10438059E-1,    .53130952E-3,  -.99352219E-5/
00343      DATA(P( 81,J),J=1,36)/204.370,2HTL,85.530,12.658, 2.389,
00343     *  .000,  1.207,  5.460,   .000,   .808,   .843,
00343     *   .979,  3.349,  3.632,  4.201,  4.998,  5.200, 14.500,
00343     * .00,2.58,   .000,289.00,
00343     *247.00,177.00, 73.60, 63.50, 52.60, 45.40, 35.05, 23.80,
00343     *     .12163706E+1,  -.37730162E-0,   .93097985E-1,
00343     *  -.10423575E-1,    .52983896E-3,  -.98970304E-5/
00345      DATA(P( 82,J),J=1,36)/207.190,2HPB,88.004,13.035, 2.484,
00345     *   .000,  1.175,  5.286,   .000,   .782,   .815,
00345     *   .950,  3.218,  3.484,  4.042,  4.797,  4.994, 13.800,
00345     * .00,2.57,   .000,298.00,
00345     *255.00,183.00, 76.64, 66.10, 54.70, 47.30, 36.40, 24.40,
00345     *     .12165289E+1,  -.37879550E-0,   .93375385E-1,
00345     *  -.10444440E-1,    .53043012E-3,  -.99009676E-5/
00347      DATA(P( 83,J),J=1,36)/208.980,2HBI,90.526,13.419, 2.580,
00347     *   .000,  1.144,  5.118,   .000,   .757,   .789,
00347     *   .923,  3.099,  3.355,  3.902,  4.612,  4.808, 13.100,
00347     * .00,2.56,   .000,307.00,
00347     *262.00,188.00, 79.94, 68.90, 57.10, 49.30, 37.78, 25.10,
00347     *     .12163048E+1,  -.37972516E-0,   .93481243E-1,
00347     *  -.10441240E-1,    .52960776E-3,  -.98758701E-5/
00351      DATA(P( 84,J),J=1,36)/210.000,2HPO,93.105,13.814, 2.683,
00351     *   .000,  1.114,   .000,   .000,   .732,   .763,
00351     *   .897,  2.987,  3.228,  3.768,  4.443,  4.625, 12.500,
00351     * .00,2.56,   .000,316.00,
00351     *270.00,194.00, 83.51, 72.00, 59.70, 51.60, 39.19, 25.80,
00351     *     .12162142E+1,  -.38078475E-0,   .9363544 E-1,
00351     *  -.10444839E-1,    .52918168E-3,  -.98580644E-5/
00353      DATA(P( 85,J),J=1,36)/210.000,2HAT,95.730,14.214, 2.787,
00353     *   .000,  1.085,   .000,   .000    .709,   .739,
00353     *   .872,  2.876,  3.099,  3.635,  4.274,  4.459, 11.900,
00353     * .00,2.55,   .000,325.00,
00353     *278.00,199.00, 87.27, 75.20, 62.30, 53.90, 40.64, 26.60,
00353     *     .12159491E+1,  -.38159627E-0,   .93700707E-1,
00353     *  -.10435835E-1,    .52801124E-3,  -.98265155E-5/
00355      DATA(P( 86,J),J=1,36)/222.000,2HRN,98.404,14.619, 2.892,
00355     *   .000,  1.057,   .000,   .000,   .000,   .715,
00355     *   .848,  2.767,  2.987,  3.512,  4.118,  4.304, 11.400,
00355     * .00, .00,   .000,   .00,
00355     *286.00,205.00, 91.21, 78.50, 65.20, 56.30, 42.12, 27.40,
00355     *     .12157631E+1,  -.38245738E-0,   .93781710E-1,
00355     *  -.10428660E-1,    .52693137E-3,  -.97957573E-5/
00357      DATA(P( 87,J),J=1,36)/223.000,2HFR,99.999,15.031, 3.000,
00357     *   .000,  1.030,   .000,   .000,   .000,   .000,
00357     *   .825,  2.672,  2.876,  3.387,  3.960,  4.146, 10.900,
00357     * .00, .00,   .000,   .00,
00357     *  .00,210.00, 95.35, 82.20, 68.10, 58.90, 43.64, 28.30,
00357     *     .12154980E+1,  -.38317627E-0,   .93812287E-1,
00357     *  -.10914340E-1,    .52542775E-3,  -.97562306E-5/
00361      DATA(P( 88,J),J=1,36)/226.000,2HRA,99.999,15.444, 3.105,
00361     *   .000,  1.005,   .000,   .000,   .000,   .000,
00361     *   .803,  2.577,  2.773,  3.279,  3.826,  4.012, 10.330,
00361     * .00, .00,   .000,   .00,
00361     *   .00,   .00, 99.70, 86.00, 71.20, 61.50, 45.20, 29.60,
00361     *     .12152710E+1,  -.38389122E-0,   .93841732E-1,
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00361        *  -.10399707E-1,   .52389489E-3,  -.97160320E-5/
00363         DATA(P( 89,J),J=1,36)/227.000,2HAC,99.999,15.871, 3.219,
00363        *   .000,   .980,   .000,   .000,   .000,   .000,
00363        *   .782,  2.484,  2.672,  3.170,  3.689,  3.874,  9.917,
00363        * .00, .00,   .000,   .00,
00363        *   .00,   .00,104.30, 89.90, 74.50, 64.40, 46.80, 30.80,
00363        *   .12147446E+1,  -.38422579E-0,   .93736649E-1,
00363        *  -.10366131E-1,   .52125077E-3,  -.96528447E-5/
00365         DATA(P( 90,J),J=1,36)/232.038,2HTH,99.999,16.300, 3.332,
00365        *   .000,   .956,  4.138,   .000,   .000,   .000,
00365        *   .761,  2.401,  2.577,  3.080,  3.573,  3.745,  9.492,
00365        * .00, .00,   .000,   .00,
00365        *   .00,   .00,109.40, 94.30, 78.10, 67.50, 48.43, 31.30,
00365        *   .12144461E+1,  -.38470334E-0,   .93676150E-1,
00365        *  -.10338165E-1,   .51890803E-3,  -.95955593E-5/
00367         DATA(P( 91,J),J=1,36)/231.000,2HPA,99.999,16.733, 3.442,
00367        *   .000,   .933,  4.022,   .000,   .000,   .000,
00367        *   .741,  2.313,  2.479,  2.980,  3.443,  3.614,  9.048,
00367        * .00, .00,   .000,   .00,
00367        *   .00,   .00,114.50, 98.70, 81.80, 70.70, 50.10, 32.40,
00367        *   .12141867E+1,  -.38518625E-0,   .93618155E-1,
00367        *  -.10310382E-1,   .51656738E-3,  -.95381638E-5/
00371         DATA(P( 92,J),J=1,36)/238.030,2H U,99.999,17.166, 3.552,
00371        *   .000,   .911,  3.910,   .000,   .000,   .000,
00371        *   .722,  2.235,  2.394,  2.882,  3.300,  3.496,  8.614,
00371        * .00, .00,   .000,   .00,
00371        *   .00,   .00,120.70,104.00, 86.20, 74.50, 51.80, 33.60,
00371        *   .12136379E+1,  -.38523477E-0,   .93400300E-1,
00371        *  -.10259636E-1,   .51284025E-3,  -.94524676E-5/
00373         DATA(P( 93,J),J=1,36)/237.000,2HNP,99.999,17.610, 3.666,
00373        *   .000,   .889,   .000,   .000,   .000,   .000,
00373        *   .704,  2.160,  2.313,  2.798,  3.220,  3.387,  8.264,
00373        * .00, .00,   .000,   .00,
00373        *   .00,   .00,127.10,109.50, 90.80, 78.50, 53.55, 34.90,
00373        *   .12132721E+1,  -.38541490E-0,   .93224943E-1,
00373        *  -.10214318E-1,   .50944719E-3,  -.93724557E-5/
00375         DATA(P( 94,J),J=1,36)/244.000,2HPU,99.999,18.057, 3.778,
00375        *   .000,   .868,   .000,   .000,   .000,   .000,
00375        *   .000,  2.090,  2.229,  2.718,  3.114,  3.279,  7.946,
00375        * .00, .00,   .000,   .00,
00375        *   .00,   .00,135.40,116.50, 96.70, 83.60, 55.34, 36.40,
00375        *   .12129555E+1,  -.38554609E-0,   .93025923E-1,
00375        *  -.10165025E-1,   .50577731E-3,  -.92868595E-5/
00377         DATA(P( 95,J),J=1,36)/243.000,2HAM,99.999,18.504, 3.887,
00377        *   .000,   .848,   .000,   .000,   .000,   .000,
00377        *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00377        * .00, .00,   .000,   .00,
00377        *   .00,   .00,   .00,   .00,   .00,   .00, 57.16,   .00,
00377        *   .12121478E+1,  -.38503844E-0,   .92595935E-1,
00377        *  -.10082912E-1,   .50016353E-3,  -.91610882E-5/
00401         DATA(P( 96,J),J=1,36)/247.000,2HCM,99.999,18.930, 3.971,
00401        *   .000,   .000,   .000,   .000,   .000,   .000,
00401        *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00401        * .00, .00,   .000,   .00,
00401        *   .00,   .00,   .00,   .00,   .00,   .00, 59.02,   .00,
00401        *   .12120562E+1,  -.38515389E-0,   .92377782E-1,
00401        *  -.10029525E-1,   .49619796E-3,  -.90686890E-5/
00403         DATA(P( 97,J),J=1,36)/247.000,2HBK,99.999,19.452, 4.132,
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00403   676*        *   .000,   .000,   .000,   .000,   .000,   .000,
00403   677*        *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00403   678*        * .00, .00,   .000,   .00,
00403   679*        *   .00,   .00,   .00,   .00,   .00,   .00, 60.93,   .00,
00403   680*        *   .12111570E+1,  -.38516915E-0,   .92113495E-1,
00403   681*        *  -.99686496E-2,   .49175555E-3,  -.89659807E-5/
00405   682*        DATA(P( 98,J),J=1,36)/251.000,2HCF,99.999,19.930, 4.253,
00405   683*        *   .000,   .000,   .000,   .000,   .000,   .000,
00405   684*        *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00405   685*        * .00, .00,   .000,   .00,
00405   686*        *   .00,   .00,   .00,   .00,   .00,   .00, 62.88,   .00,
00405   687*        *   .12116747E+1,  -.38481987E-0,   .91711283E-1,
00405   688*        *  -.98877028E-2,   .48610964E-3,  -.08382285E-5/
00407   689*        DATA(P( 99,J),J=1,36)/254.000,2HES,99.999,20.410, 4.374,
00407   690*        *   .000,   .000,   .000,   .000,   .000,   .000,
00407   691*        *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00407   692*        * .00, .00,   .000,   .00,
00407   693*        *   .00,   .00,   .00,   .00,   .00,   .00, 64.87,   .00,
00407   694*        *   .12112694E+1,  -.38416493E-0,   .91188729E-1,
00407   695*        *  -.97887777E-2,   .47936640E-3,  -.86873597E-5/
00411   696*        DATA(P(100,J),J=1,36)/253.000,2HFM,99.999,20.900, 4.498,
00411   697*        *   .000,   .000,   .000,   .000,   .000,   .000,
00411   698*        *   .000,   .000,   .000,   .000,   .000,   .000,   .000,
00411   699*        * .00, .00,   .000,   .00,
00411   700*        *   .00,   .00,   .00,   .00,   .00,   .00, 66.70,   .00,
00411   701*        *   .12111340E+1,  -.38363683E-0,   .90693365E-1,
00411   702*        *  -.96920170E-2,   .47269068E-3,  -.85370948E-5/
00413   703*        END

        END OF COMPILATION:          NO  DIAGNOSTICS.
      DBLOCK              SYMBOLIC                19 NOV 71  10:20:30   0  01575525   14   703  (DELETED)
      DBLOCK  CODE        RELOCATABLE             19 NOV 71  10:20:30   1  01641227   14     1  (DELETED)
                                                                        0  01620707   14   600
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UNIVAC 1108 FORTRAN V LEVEL 2206 0024A   -(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:19

   SUBROUTINE HIS1        ENTRY POINT 000271

   STORAGE USED: CODE(1) 000342; DATA(0) 000460; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   GROP1
    0004   PLOT3
    0005   DMPBUF
    0006   NWDUS
    0007   NI01S
    0010   NI02S
    0011   NERR3S

   STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000021 121G      0001   000054 133G      0001   000132 154G      0001   000150 165G      0001   000161 172G
    0000   000337 20F       0001   000207 200G      0000   000375 21F       0001   000235 211G      0000   000410 23F
    0000   000333 30F       0001   000064 4L        0001   000101 5L        0000 R 000000 B         0000 R 000145 FF
    0000 R 000316 FMT       0000 I 000322 I         0000 I 000332 IND       0000   000430 INJP$     0000 I 000312 IR
    0000 I 000331 IS        0000 I 000321 J         0000 I 000327 NN        0000 I 000323 NT        0000 R 000326 R
    0000 R 000324 STEP      0000 R 000325 VK        0000 R 000330 XX


00101          SUBROUTINE  HIS1(X,N,NG,XMIN,XMAX,F,INX,TITLE)
00101     C----------------------------------------------------------------------
00101     C  CALCULATES AND PLOTS ON THE PRINTER A HISTOGRAM FROM A SET
00101     C    OF DATA POINTS FROM GROUPED OR UNGROUPED DATA POINTS.
00101     C----------------------------------------------------------------------
00103          DIMENSION X(N),F(NG ),B(101),FF(101),IR(3),FMT(4)
00103         1  , TITLE(12)
00104          DATA FMT(1)/6H(13X,1/,FMT(2)/6HPE8.3,/,FMT(3)/6H2X     /,FMT(4)/6H
00104         1      /,(B(J),J=1,101)/101*1HI/
00112          DATA(IR(I),I=1,3)/0,1,1/
00112     C----------------------------------------------------------------------
00112     C  TESTS WHETHER THE DATA POINTS ARE GROUPED OR UNGROUPED, IF THE LATTER,
00112     C    CALLS GROUP SUBROUTINE TO GROUP THE DATA POINTS.
00112     C----------------------------------------------------------------------
00114          NT = 17
00115          IF(INX.EQ.0) NT = 6
00117          WRITE(NT,30) TITLE
00125       30 FORMAT(1H1,///,50X,12A6,///)
00126          CALL GROP1(X,N,NG,XMIN,XMAX,F)
00127          STEP = (XMAX - XMIN)/NG
00127     C----------------------------------------------------------------------
00127     C  FINDS MAXIMUM FREQUENCY AND COMPUTES THE K FACTOR FOR EXPANDING OF PLOT.
00127     C----------------------------------------------------------------------
00130          VK=1.
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00131         R = F(1)
00132         DO 3 I=2,NG
00135       3 R=AMAX1(R,F(I))
00137       4 IF((R/N*VK).GT.1.)  GO TO 5
00141         VK=VK+1.
00142         GO TO 4
00143       5 VK=VK-1.
00143   C-----------------------------------------------------------------------
00143   C  WRI  .  OUT ARGUEMENTS AND HEADING FOR PLOT.
00143   C-----------------------------------------------------------------------
00144      20 FORMAT(20X,5HSTEP=F15.8/20X,29HCENTERPOINT OF INITIAL GROUP=F15.8,
00144        110X,20HNO. OF OBSERVATIONS=I5    /20X,27HCENTERPOINT OF FINAL GROUP
00144        2=F15.8,10X,14HNO. OF GROUPS=I5/20X,9HK FACTOR=F6.0//)
00145         WRITE(NT,20)STEP,XMIN,N,XMAX,NG,VK
00155         DO 1 I=1,101
00160       1 FF(I)=I-1
00162      21 FORMAT(8X,10HPERCENTAGE,5X,1H0,10(7X,I3)/23X,10(1H+,9H*********),1
00162        1H+)
00163         WRITE(NT,21) (I,I=10,100,10)
00163   C-----------------------------------------------------------------------
00163   C  COMPUTES VALUE FOR EACH GROUP AND PLOTS THREE LINES FOR EACH GROUP WITH
00163   C    THE VALUE PRINTED OUT ON THE SECOND LINE.
00163   C-----------------------------------------------------------------------
00171         DO 2 I=1,NG
00174         NN=100*VK*(F(I)/N)
00175         XX=XMIN+(I-1)*STEP
00176         IS=0
00177         DO 2 J=1,3
00202         IND=IR(J)
00203       2 CALL PLOT3(IND,IS,XX,B,FF,NN,FMT,INX)
00203   C-----------------------------------------------------------------------
00203   C  WRITES OUT TRAILER INFORMATION ON GRAPH.
00203   C-----------------------------------------------------------------------
00206      23 FORMAT(23X,10(1H+,9H*********),1H+/8X,10HPERCENTAGE,5X,1H0,10(7X,I
00206        13))
00207         WRITE(NT,23) (I,I=10,100,10)
00215         IF(NT.EQ. 17) CALL DMPBUF
00217         RETURN
00220         END

      END OF COMPILATION:        NO  DIAGNOSTICS.
    HIS1           SYMBOLIC                        19 NOV 71  10:20:36   0  01644273    14     63  (DELETED)
    HIS1    CODE   RELOCATABLE                     19 NOV 71  10:20:36   1  01647117    20      1  (DELETED)
                                                                         0  01646055    14     39
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UNIVAC 1108 FORTRAN V LEVEL 2206 0024A   *(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:16

   SUBROUTINE IGIVE      ENTRY POINT 000353

   STORAGE USED: CODE(1) 000426; DATA(0) 000165; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   GROP1
    0004   PLOT3
    0005   DMPBUF
    0006   NWDU$
    0007   N102$
    0010   N101$
    0011   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

   0000   000034 10F     0000   000033 101F    0001   000036 126G    0001   000076 146G    0001   000105 152G
   0001   000164 167G    0000   000046 20F     0001   000212 201G    0000   000100 21F     0001   000243 212G
   0001   000313 225G    0000   000114 23F     0001   000320 231G    0001   000124 5L      0001   000131 6L
   0000 R 000000 B       0000 R 000001 FF      0000 R 000014 FMT     0000 I 000022 I      0000 I 000002 IF
   0000 I 000030 IND     0000   000136 INJP$   0000 I 000130 IR      0000 I 000026 IS     0000 I 000024 I1
   0000 I 000025 I2      0000 I 000032 J       0000 I 000027 NG1     0000 I 000023 NN     0000 I 000020 NT
   0000   000130 R       0000 R 000021 STEP    0000 R 000031 XX


 00101      1*          SUBROUTINE IGIVE(X,N,NG,XMIN,XMAX,F,ICUM,INX)
 00101      2*    C---------------------------------------------------------------------
 00101      3*    C  CALCULATES AND PLOTS ON THE PRINTER A CUMULATIVE FREQUENCY POLYGON
 00101      4*    C    FROM A SET OF DATA POINTS.
 00101      5*    C---------------------------------------------------------------------
 00103      6*          DIMENSION X(1),F(1),B(1),FF(1),IF(10),FMT(4)
 00104      7*          EQUIVALENCE (R,IR)
 00104      8*    C---------------------------------------------------------------------
 00104      9*    C  FILLS THE B ARRAY WITH 'X' TO BE PRINTED FOR THE PLOT.
 00104     10*    C---------------------------------------------------------------------
 00105     11*          DATA FMT(1)/6H(13X,1/,FMT(2)/6HPE8.3,/,FMT(3)/6H2X     /,FMT(4)/6H
 00105     12*         1     /,B(1)/1HX/
 00113     13*          NT=17
 00114     14*          IF(INX.EQ.0) NT=6
 00116     15*          WRITE (NT,101)
 00120     16*      101 FORMAT(1H1)
 00121     17*          WRITE(6,10)
 00123     18*       10 FORMAT (///,50X,'CONCENTRATION CUMULATIVE DISTRIBUTION',///)
 00123     19*    C---------------------------------------------------------------------
 00123     20*    C  COMPUTE FREQUENCY VALUES AT EACH PERCENTILE FOR PRINTOUT AT TOP
 00123     21*    C    OF PLOT
 00123     22*    C---------------------------------------------------------------------
 00124     23*          STEP=(XMAX-XMIN)/NG
```

```
00125            DO 3 I=1,10
00130          3 IF(I)=I*N/10
00130     C-----------------------------------------------------------------------
00130     C  TESTS WHETHER DATA POINTS ARE GROUPED OR UNGROUPED,IF THE LATTER,
00130     C    CALLS GROUP SUBROUTINE TO GROUP THE DATA POINTS.
00130     C-----------------------------------------------------------------------
00132            CALL GROP1(X,N,NG,XMIN,XMAX,F)
00132     C-----------------------------------------------------------------------
00132     C  WRITES OUT ARGUMENTS AND HEADING FOR THE PLOT.
00132     C-----------------------------------------------------------------------
00133         20 FORMAT(20X,5HSTEP=F15.8/20X,29HCENTERPOINT OF INITIAL GROUP=F15.8,
00133           110X,20HNO. OF OBSERVATIONS=I5   /20X,27HCENTERPOINT OF FINAL GROUP
00133           2=F15.8,10X,14HNO. OF GROUPS=I5//)
00134            WRITE (NT,20) STEP,XMIN,N,XMAX,NG
00143         21 FORMAT(8X,10HPERCENTAGE,5X,1H0,10(7X,I3)//8X,9HFREQUENCY,6X,1H0,10
00143           1(7X,I3))
00143     C-----------------------------------------------------------------------
00143     C  COMPUTES ACCUMULATED FREQUENCIES BOTTOM UP, OR TOP DOWN
00143     C-----------------------------------------------------------------------
00144            WRITE (NT,21) (I, I=10,100,10), (IF(I), I=1,10)
00156            NN=1
00157            IF(ICUM.EQ.-1) GO TO 5
00161            I1=2
00162            I2=NG
00163            GO TO 6
00164          5 I1=NG-1
00165            I2=1
00166          6 DO 1 I=I1,I2,ICUM
00171          1 F(I)=F(I)+F(I-ICUM)
00171     C-----------------------------------------------------------------------
00171     C  COMPUTES VALUE FOR EACH GROUP AND PLOTS EACH FREQUENCY WITH FIVE
00171     C    CONNECTING POINTS.
00171     C-----------------------------------------------------------------------
00173            IR=4
00174            IS=1
00175            NG1=NG+1
00176            IF(ICUM.EQ.1) NG1=NG
00200            DO 2 I=1,NG1
00203            IND=0
00204            XX = XMIN + I*STEP
00205            IF(ICUM.EQ.-1) XX = XMIN + (I-1)*STEP
00207            IF(I.EQ.NG1) IR=0
00211            DO 2 J=0,IR
90214            FF(I)=((5.0-J)*F(I)+J*F(I+1))/5.0
00215            FF(I)=FF(I)/N*100.
00216            CALL PLOT3(IND,IS,XX,B,FF,NN,FMT,INX)
00217          2 IND=1
00217     C-----------------------------------------------------------------------
00217     C  WRITES OUT FREQUENCY AND PERCENTAGE AT BOTTOM OF GRAPH
00217     C-----------------------------------------------------------------------
00222         23 FORMAT(8X,9HFREQUENCY,6X,1H0,10(7X,I3)//8X,10HPERCENTAGE,5X,1H0,10
00222           1(7X,I3))
00223            WRITE (NT,23) (IF(I),I=1,10), (I, I=10,100,10)
00235            IF(NT.EQ.17) CALL DMPBUF
00237            RETURN
00240            END

      END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
IGIVE            SYMBOLIC                19 NOV 71  10:20:39  0  01647143  14  79  (DELETED)
IGIVE   CODE     RELOCATABLE             19 NOV 71  10:20:39  1  01652255  20   1  (DELETED)
                                                              0  01651265  14  36
```

```
@FOR,* GROP1,GROP1                                                                    19 NOV 71        10:21:19.606
UNIVAC 1108 FORTRAN V LEVEL 22U6 0024A    =(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:19

    SUBROUTINE GROP1      ENTRY POINT 000114

    STORAGE USED: CODE(1) 000131; DATA(0) 000027; BLANK COMMON(2) 000000

    EXTERNAL REFERENCES (BLOCK, NAME)

     0003    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000022 104G        0001   000026 113G       0001   000100 9L        0000 I 000001 I          0000   000010 INJP$
     0000 I 000003 K           0000 R 000000 STEP     0000 R 000002 Z          0000 R 000004 ZK


 00101       1*            SUBROUTINE  GROP1(X,N,NG,XMIN,XMAX,F)
 00103       2*            DIMENSION X(1),F(1)                                     GROUP
 00104       3*            STEP=(XMAX-XMIN)/NG
 00105       4*            DO 6 I=1,NG
 00110       5*          6 F(I)=0.0                                                GROUP
 00112       6*            DO 9 I=1,N                                              GROUP
 00112       7*      C-------------------------------------------------------------
 00112       8*      C     IN WHICH GROUP DOES THE POINT FALL                      GROUP
 00112       9*      C-------------------------------------------------------------
 00115      10*            Z=(X(I)-XMIN)/STEP
 00116      11*            K=Z
 00117   *DIAGNOSTIC*  THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
 00117      12*            IF(X(I).EQ.XMIN) K=1
 00121      13*            ZK=K
 00122      14*            IF(ZK.LT.Z) K=K+1
 00124      15*            IF(K.LE.0) GO TO 9
 00126      16*            IF(K.GT.NG) GO TO 9
 00126      17*      C-------------------------------------------------------------
 00126      18*      C     CALCULATION OF FREQUENCIES FOR EACH POINT FOR EACH GROUP   GROUP
 00126      19*      C-------------------------------------------------------------
 00130      20*            F(K)=F(K)+1.0
 00131      21*          9 CONTINUE
 00133      22*            RETURN                                                  GROUP
 00134      23*            END                                                     GROUP

      END OF COMPILATION:          1 DIAGNOSTICS.
    GROP1          SYMBOLIC                        19 NOV 71  10:20:41  -0  01652301    14    23  (DELETED)
    GROP1    CODE  RELOCATABLE                     19 NOV 71  10:20:41   1  01653217    14     1  (DELETED)
                                                                        -0  01653003    14    10
```

```
UNIVAC 1108 FORTRAN V LEVEL 2206 0024A    -(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:21

     SUBROUTINE PLOT3      ENTRY POINT 000240

     STORAGE USED: CODE(1) 000263; DATA(0) 000213; BLANK COMMON(2) 000000

     EXTERNAL REFERENCES (BLOCK, NAME)

      0003    NWDU$
      0004    NIO1$
      0005    NIO2$
      0006    NERR3$

     STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

      0001     000211 10L        0000     000163 101F        0001     000015 122G       0001     000036 134G       0001     000061 147G
      0001     000064 153G       0001     000076 162G        0001     000101 166G       0001     000112 174G       0001     000052 2L
      0001     000202 214G       0001     000220 224G        0001     000073 4L         0001     000107 6L         0001     000165 7L
      0001     000142 9L         0000 R 000000 A             0000 R 000154 AXIS        0000 R 000153 BLANK       0000 R 000145 FMT
      0000 I 000161 I            0000     000172 INJP$       0000 I 000162 J           0000 I 000160 NT          0000 R 000155 PLUS
      0000 R 000156 STAR         0000 R 000157 ZERO


 00101              SUBROUTINE PLOT3(IND,IS,X,B,F,N,FRM,INX)
 00103              DIMENSION A(101),B(1),F(1),FRM(4),FMT(6)
 00104              DATA FMT(5) /6H,101A1/,FMT(6) /1H)/
 00107          101 FORMAT(23X,101A1)                                              PLOT1
 00110              DATA BLANK/1H /,AXIS/1HI/,PLUS/1H+/,STAR/1H*/,ZERO/1H0/         PLOT1
 00116              NT = 17
 00117              IF(INX.EQ.0) NT = 6
 00121              DO 11 I=1,4
 00124           11 FMT(I)=FRM(I)
 00126              A(101)=AXIS                                                    PLOT1
 00127              IF(IND.EQ.1)A(101)=PLUS                                        PLOT1
 00131              IF(IS.EQ.1) GO TO 2                                            PLOT1
 00133              DO 1 I=2,100                                                   PLOT1
 00134            1 A(I)=BLANK                                                     PLOT1
 00140              A(1) =AXIS                                                     PLOT1
 00141              IF(IND.EQ.1) A(1)=PLUS                                         PLOT1
 00143              GO TO 6                                                        PLOT1
 00144            2 IF (IND.EQ.1) GO TO 4                                          PLOT1
 00146              DO 3 I=1,91,10                                                 PLOT1
 00151              A(I)=AXIS                                                      PLOT1
 00152              DO 3 J=1,9                                                     PLOT1
 00155            3 A(I+J)=STAR                                                    PLOT1
 00160              GO TO 6                                                        PLOT1
 00161            4 DO 5 I=1,91,10                                                 PLOT1
 00164              A(I)=PLUS                                                      PLOT1
 00165              DO 5 J=1,9                                                     PLOT1
 00170            5 A(I+J)=BLANK                                                   PLOT1
```

```
00173    28*       6 DO 7 I=1,N                                          PLOT1
00174    29*         J=F(I)+1.5                                          PLOT1
00177    30*         IF((J.LT.1).OR.(J.GT.101)) GO TO 7                  PLOT1
00201    31*         IF(A(J).LT.BLANK.OR.A(J).GT.BLANK)  GOTO9           PLOT1
00203    32*         A(J)=B(I)                                           PLOT1
00204    33*         GO TO 7                                             PLOT1
00205    34*       9 A(J)=ZERO                                           PLOT1
00206    35*       7 CONTINUE                                            PLOT1
00210    36*         IF(IND.NE.1) GO TO 10                               PLOT1
00212    37*         WRITE(NT,101) (A(I),I=1,101)
00220    38*         RETURN                                              PLOT1
00221    39*      10 WRITE(NT,FMT) X,(A(I),I=1,101)
00230    40*         RETURN                                              PLOT1
00231    41*         END                                                 PLOT1

      END OF COMPILATION:        NO  DIAGNOSTICS.
    PLOT3           SYMBOLIC              19 NOV 71  10:20:43  0  01653235  14   41  (DELETED)
    PLOT3   CODE    RELOCATABLE           19 NOV 71  10:20:43  1  01654763  17    1  (DELETED)
                                                               0  01654333  14   20
```

```
@ FOR,* PCORRE,PCORRE                                                              19 NOV 71          10:21:24.111
UNIVAC 1108 FORTRAN V LEVEL 2206 0024A    -(EXEC8 LEVEL E1201000*A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:24

     FUNCTION PCORRE      ENTRY POINT 000267

     STORAGE USED: CODE(1) 000276; DATA(0) 000052; BLANK COMMON(2) 000000

     EXTERNAL REFERENCES (BLOCK, NAME)

       0003   GAMMA
       0004   DSQRT
       0005   DATAN
       0006   NERR3$

     STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

       0001   000025 13L       0001   000052 134G      0001   000007 15L      0001   000214 161G      0001   000046 31L
       0001   000146 41L       0001   000202 51L       0001   000247 57L      0001   000254 60L      0000 D 000013 DENOM
       0000 D 000007 FI        0000 D 000011 FNUM      0000 R 000020 FREE      0003 R 000000 GAMMA     0000 I 000021 I
       0000 I 000017 IMAX      0000   000033 INJP$     0000 I 000016 NEVEN     0000 I 000015 NFREE     0000 R 000000 PCORRE
       0000 D 000001 R2        0000 D 000005 SUM       0000 D 000003 TERM


   00101      1*           FUNCTION PCORRE (R,NPTS)
   00103      2*           DOUBLE PRECISION R2, TERM, SUM, FI, FNUM, DENOM
   00103      3*     C
   00103      4*     C     PURPOSE
   00103      5*     C       EVALUATE PROBABILITY FOR NO CORRELATION BETWEEN TWO VARIABLES
   00103      6*     C
   00103      7*     C     USAGE
   00103      8*     C       RESULT = PCORRE (R, NPTS)
   00103      9*     C
   00103     10*     C     DESCRIPTION OF PARAMETERS
   00103     11*     C       R    - LINEAR CORRELATION COEFFICIENT
   00103     12*     C       NPTS - NUMBER OF DATA POINTS
   00103     13*     C
   00103     14*     C
   00103     15*     C         EVALUATE NUMBER OF DEGREES OF FREEDOM
   00103     16*     C
   00104     17*           NFREE = NPTS - 2
   00105     18*           IF (NFREE) 13,13,15
   00110     19*        13 PCORRE = 0.
   00111     20*           GO TO 60
   00112     21*        15 R2 = R**2
   00113     22*           IF (1.-R2) 13,13,17
   00114     23*        17 NEVEN = 2*(NFREE/2)
   00117     24*           IF (NFREE - NEVEN) 21,21,41
   00117     25*     C
   00117     26*     C         NUMBER OF DEGREES OF FREEDOM IS EVEN
   00117     27*     C
   00122     28*        21 IMAX = (NFREE-2)/2
```

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```
00123          FREE = NFREE
00124          TERM = ABS (R)
00125          SUM = TERM
00126          IF (IMAX) 60,26,31
00131       26 PCORRE = 1. - TERM
00132          GO TO 60
00133       31 DO 36 I=1,IMAX
00134          FI = I
00137          FNUM = IMAX - I + 1
00140          DENOM = 2*I + 1
00141          TERM = -TERM * R2 * FNUM/FI
00142       36 SUM = SUM + TERM/DENOM
00144          PCORRE = 1.12837917 * (GAMMA((FREE+1.)/2.)/GAMMA(FREE/2.))
00145          PCORRE = 1. - PCORRE*SUM
00146          GO TO 60
00146    C
00146    C        NUMBER OF DEGREES OF FREEDOM IS ODD
00146    C
00147       41 IMAX = (NFREE-3)/2
00150          TERM = ABS(R) * DSQRT(1.-R2)
00151          SUM = DATAN(R2/TERM)
00152          IF (IMAX) 57,45,51
00155       45 SUM = SUM + TERM
00156          GO TO 57
00157       51 SUM = SUM + TERM
00160          DO 56 I=1,IMAX
00163          FNUM = 2*I
00164          DENOM = 2*I + 1
00165          TERM = TERM * (1.-R2) * FNUM/DENOM
00166       56 SUM = SUM + TERM
00170       57 PCORRE = 1. - 0.63661977724*SUM
00171       60 RETURN
00172          END

     END OF COMPILATION:        NO  DIAGNOSTICS.
    PCORRE          SYMBOLIC                        19 NOV 71  10:20:46   0  01655004   14    61  (DELETED)
    PCORRE   CODE   RELOCATABLE                     19 NOV 71  10:20:46   1  01657200   17     1  (DELETED)
                                                                          0  01656532   14    21
```

```
@FOR,* GAMMA,GAMMA                                                          19 NOV 71          10:21:26.858
UNIVAC 1108 FORTRAN V LEVEL 2206 0024A    -(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:27

   FUNCTION GAMMA        ENTRY POINT 000131

   STORAGE USED: CODE(1) 000135; DATA(0) 000041; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   FACTOR
    0004   DLOG
    0005   DEXP
    0006   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000042 123G      0001    000067 134G      0001    000026 31L      0001    000056 44L      0001    000061 51L
    0001   000117 60L       0003 R  000000 FACTOR    0000 D  000005 FI       0000 R  000000 GAMMA    0000 I  000011 I
    0000   000027 INJP$     0000 I  000007 N         0000 D  000001 PROD     0000 D  000003 SUM      0000 R  000010 XN

 00101          FUNCTION GAMMA (X)
 00103          DOUBLE PRECISION PROD,SUM,FI
 00103       C
 00103       C  PURPOSE
 00103       C    CALCULATE THE GAMMA FUNCTION FOR INTEGERS AND HALF-INTEGERS
 00103       C
 00103       C  USAGE
 00103       C    RESULT = GAMMA (X)
 00103       C
 00103       C  DESCRIPTION OF PARAMETERS
 00103       C    X - INTEGER OR HALF-INTEGER
 00103       C
 00103       C      INTEGERIZE ARGUMENT
 00103       C
 00104          N = X - .25
 00105          XN = N
 00106          IF (X-XN-.75) 31,31,21
 00106       C
 00106       C      ARGUMENT IS INTEGER
 00106       C
 00111       21 GAMMA = FACTOR(N)
 00112          GO TO 60
 00112       C
 00112       C      ARGUMENT IS HALF-INTEGER
 00112       C
 00113       31 PROD = 1.77245385
 00114          IF (N) 44,44,33
 00117       33 IF (N-10) 41,41,51
 00122       41 DO 43 I=1,N
 00125          FI = I
```

```
00126        43 PROD = PROD * (FI-.5)
00130        49 GAMMA = PROD
00131           GO TO 60
00132        51 SUM = 0.
00133           DO 54 I=II,N
00136           FI = I
00137        54 SUM = SUM + DLOG(FI-.5)
00141           GAMMA = PROD * 639383.8623 * DEXP(SUM)
00142        60 RETURN
00143           END

    END OF COMPILATION:         NO  DIAGNOSTICS.
    GAMMA           SYMBOLIC                                  19 NOV 71  10:20:48   0  01657221    14    40  (DELETED)
    GAMMA   CODE    RELOCATABLE                               19 NOV 71  10:20:48   1  01660551    17     1  (DELETED)
                                                                                    0  01660301    14    12
```

```
@ FOR,* FACTOR,FACTOR                                                     19 NOV 71          10:21:28.892
UNIVAC 1108 FORTRAN V LEVEL 2206 0024A    -(EXEC8 LEVEL E12010009A)
THIS COMPILATION WAS DONE ON 19 NOV 71 AT 10:21:29

   FUNCTION FACTOR        ENTRY POINT 000102

   STORAGE USED: CODE(1) 000104; DATA(0) 000027; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003    DLOG
    0004    DEXP
    0005    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000022 114G      0001    000044 124G      0001    000040 31L      0001    000070 40L      0000 R 000000 FACTOR
    0000 D  000001 FI        0000 I  000005 I         0000    000015 INJP$    0000 D  000003 SUM


 00101          FUNCTION FACTOR (N)
 00103          DOUBLE PRECISION FI,SUM
 00103     C
 00103     C    PURPOSE
 00103     C       CALCULATES FACTORIAL FUNCTION FOR INTEGERS
 00103     C
 00103     C    USAGE
 00103     C       RESULT = FACTOR (N)
 00103     C
 00103     C    DESCRIPTION OF PARAMETERS
 00103     C       N - INTEGER ARGUMENT
 00103     C
 00104          FACTOR = 1.
 00105          IF (N-1) 40,40,13
 00110       13 IF (N-10) 21,21,31
 00110     C
 00110     C          N LESS THAN 11
 00110     C
 00113       21 DO 23 I=2,N
 00116          FI = I
 00117       23 FACTOR = FACTOR * FI
 00121          GO TO 40
 00121     C
 00121     C          N GREATER THAN 10
 00121     C
 00122       31 SUM = 0.
 00123          DO 34 I=11,N
 00126          FI = I
 00127       34 SUM = SUM + DLOG(FI)
 00131          FACTOR = 3628800. * DEXP(SUM)
 00132       40 RETURN
 00133          END
```

```
     END OF COMPILATION:        NO  DIAGNOSTICS.
  FACTOR          SYMBOLIC                                    19 NOV 71  10:20:50  0  01660572    14    32  (DELETED)
  FACTOR  CODE    RELOCATABLE                                 19 NOV 71  10:20:50  1  01661670    16     1  (DELETED)
                                                                                   0  01661472    14     9
```

19 NOV 71 10:2,:30 IDENT H3 ACCOUNT L04878 CARDS IN 40 CARDS OUT 0 PAGES 92 ELAPSED TIME 0 1 37

UNIVAC-1106-PROCESSOR-1-EXEC-II-LEVEL-6.5-MSC117A-NASA-SPECIAL

-UNIVAC-1106-PROCESSOR-I-EXEC-II-LEVEL-6.5-MSC117A-NASA-SPECIAL--*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*

4.5 Sample Input/Output

Sample input and output are shown on the following pages.

```
CARD 1    10-13-71    15    A   R+00
CARD 2      0     0
CARD 3       10.00         1.50      50.00        1.00
CARD 4      1    35     2    0.
CARD 5   112.00000      .14000  16.00000      1
CARD 6   K              0.       2366.          94.
CARD 6   5              0.        947.          50.
$DIST
C1        =      .99964455E+00,
C12       =      .99999627E+00,
C2        =      .33172946E-03,
ADB       =      .56603072E-04,
ARATIO    =      .1000002[illegible]01,
$END
CARD 7 4    NA      5.   S      0.   K     10. CL     15.
```

QUANTITATIVE ANALYSIS OF RBC SET

1. INPUT-OUTPUT TABLE

2. CONCENTRATION FREQUENCY DISTRIBUTION

3. CONCENTRATION CUMULATIVE DISTRIBUTION

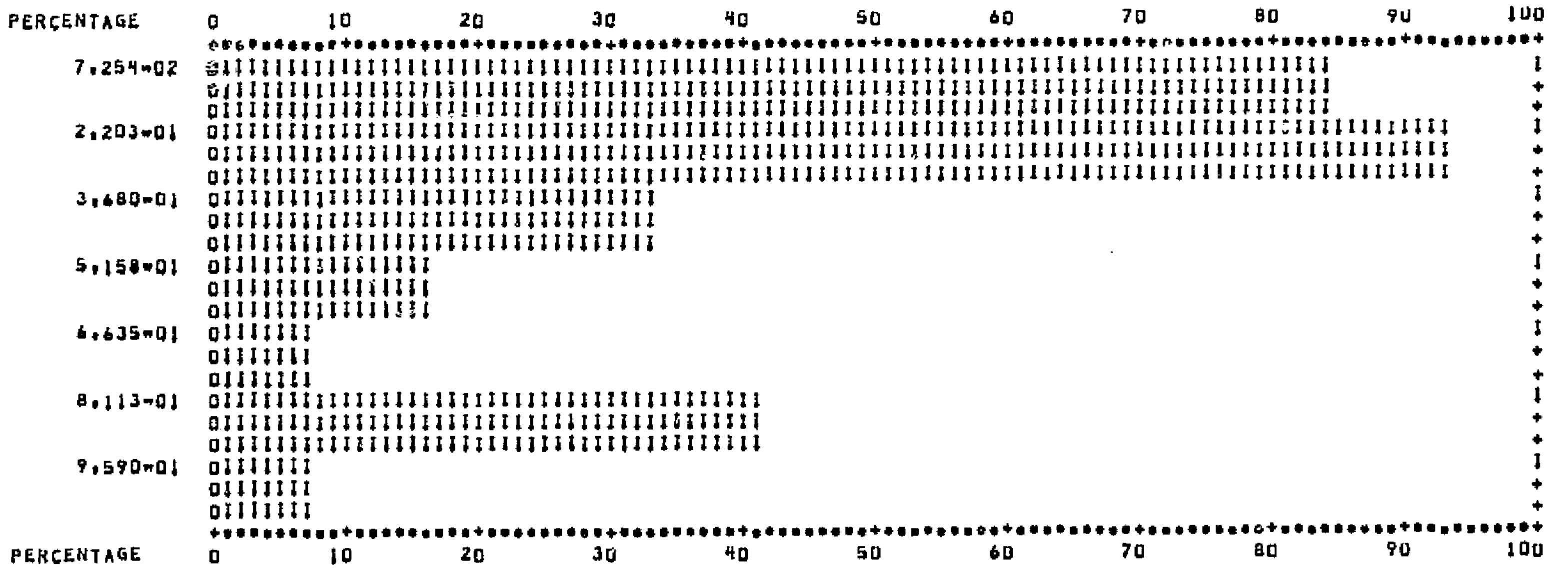
4. CONCENTRATION CORRELATION ANALYSIS

K IS THE ELEMENT ANALYZED

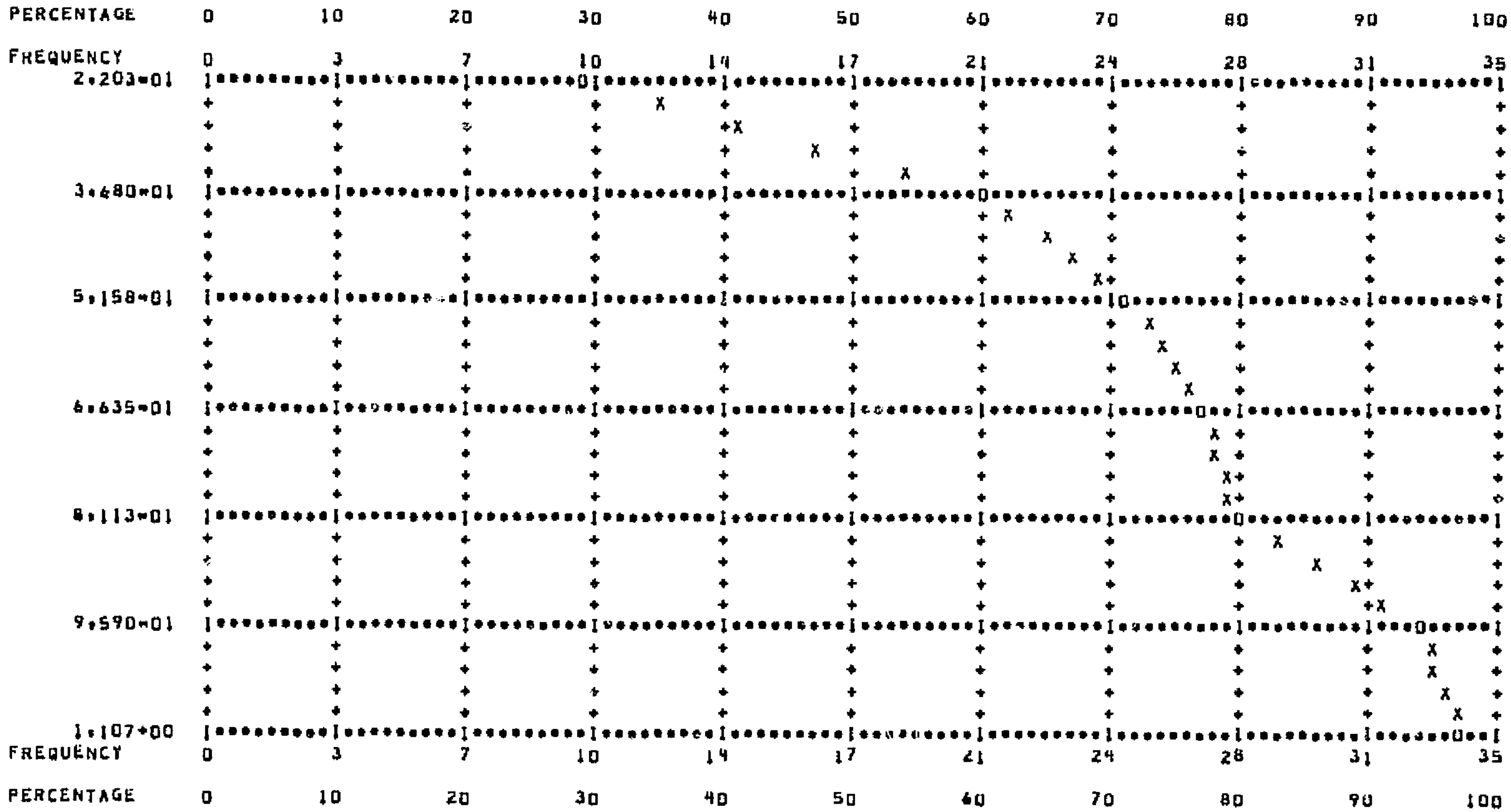
SAMPLE NUMBER	INTENSITY COUNT	ABSORPTION FACTOR	ABSORPTION CORRECTION	AREA DENSITY	WEIGHT PERCENTAGE
1	648.	.99669	.99336	.17021-06	.30
2	179.	.99682	.99323	.47012-07	.08
3	181.	.99668	.99338	.47544-07	.09
4	563.	.99670	.99335	.14788-06	.27
5	383.	.99670	.99335	.10060-06	.18
6	762.	.99668	.99338	.20016-06	.36
7	354.	.99667	.99339	.92988-07	.17
8	244.	.99672	.99333	.64090-07	.12
9	811.	.99674	.99331	.21302-06	.39
10	683.	.99683	.99322	.17938-06	.33
11	980.	.99674	.99332	.25741-06	.47
12	2317.	.99666	.99339	.60863-06	1.11
13	1663.	.99672	.99333	.48934-06	.89
14	1840.	.99669	.99336	.48332-06	.87
15	1924.	.99670	.99335	.50538-06	.91
16	269.	.99679	.99327	.70652-07	.13
17	243.	.99680	.99326	.63822-07	.12
18	245.	.99692	.99313	.64340-07	.12
19	1758.	.99673	.99332	.46176-06	.85
20	1815.	.99671	.99334	.47674-06	.87
21	2143.	.99676	.99330	.56287-06	1.02
22	1647.	.99672	.99333	.43261-06	.79
23	1381.	.99677	.99328	.36272-06	.66
24	1126.	.99664	.99342	.29578-06	.54
25	486.	.99680	.99325	.12764-06	.23
26	461.	.99675	.99331	.12109-06	.22
27	873.	.99675	.99330	.22930-06	.42
28	600.	.99678	.99328	.15759-06	.29
29	984.	.99672	.99333	.25846-06	.47
30	150.	.99673	.99332	.39399-07	.07
31	693.	.99694	.99311	.18199-06	.34
32	590.	.99679	.99327	.15496-06	.29
33	272.	.99680	.99326	.71439-07	.13
34	543.	.99685	.99321	.14261-06	.2[illegible]
35	699.	.99687	.99319	.18358-06	.34

CONCERN FREQUENCY DISTRIBUTION

STEP= .14774365
CENTERPOINT OF INITIAL GROUP= .07254016 NO. OF OBSERVATIONS= 35
CENTERPOINT OF FINAL GROUP= 1.10674572 NO. OF GROUPS= 7
K FACTOR= 3.



```
STEP=        .14774365
CENTERPOINT OF INITIAL GROUP=        .07254016          NO. OF OBSERVATIONS=   35
CENTERPOINT OF FINAL GROUP=      1.10674572          NO. OF GROUPS=    7
```

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XMIN   =     .72540159E-01,
XMAX   =     .11067457E+01,
XBAR   =     .41988858E+00,
VAR    =     .94091450E-01,
SDEV   =     .30674330E+00,
$END
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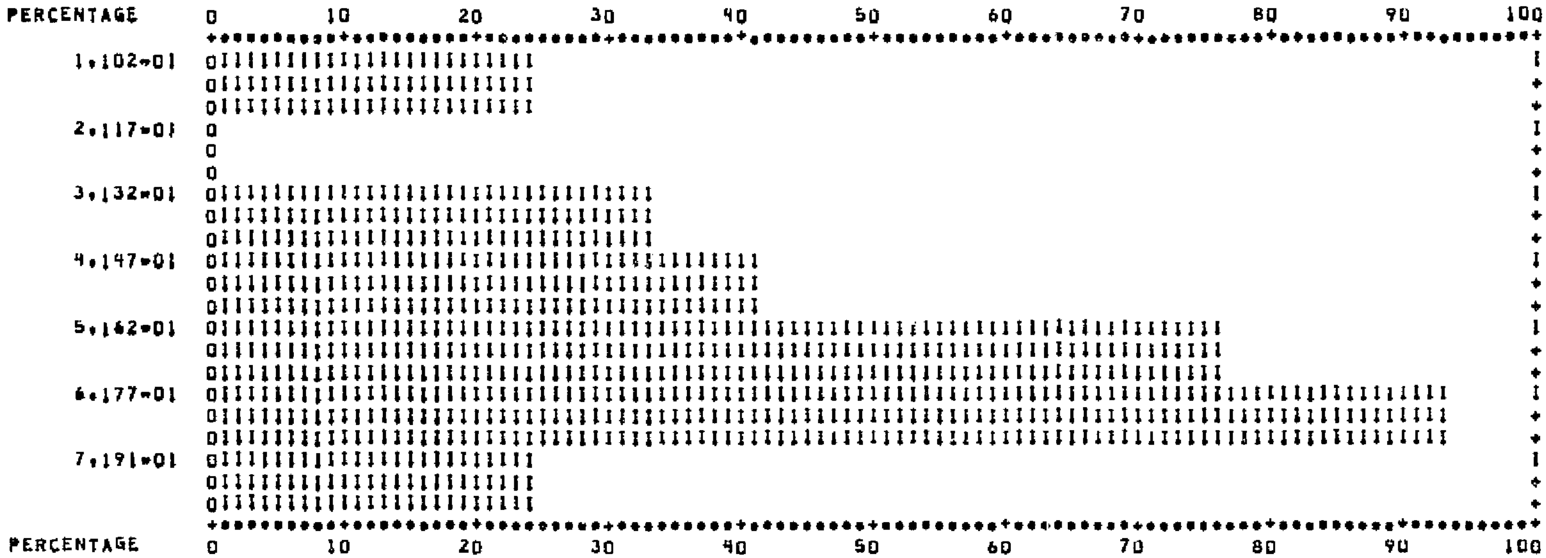
S IS THE ELEMENT ANALYZED

SAMPLE NUMBER	INTENSITY COUNT	ABSORPTION FACTOR	ABSORPTION CORRECTION	AREA DENSITY	WEIGHT PERCENTAGE
1	715.	.99178	.98294	.25162-06	.45
2	268.	.99186	.98286	.94305-07	.17
3	1019.	.99189	.98283	.35856-06	.64
4	915.	.99191	.98281	.32196-06	.58
5	989.	.99194	.98278	.34799-06	.63
6	1094.	.99193	.98279	.38494-06	.70
7	1194.	.99196	.98276	.42011-06	.76
8	995.	.99199	.98273	.35008-06	.64
9	887.	.99199	.98273	.31208-06	.57
10	522.	.99203	.98269	.18365-06	.34
11	980.	.99202	.98270	.34479-06	.63
12	1147.	.99192	.98280	.40359-06	.73
13	836.	.99192	.98280	.29416-06	.53
14	935.	.99189	.98283	.32900-06	.59
15	845.	.99186	.98286	.29734-06	.54
16	621.	.99196	.98276	.21850-06	.40
17	644.	.99201	.98271	.22658-06	.41
18	181.	.99208	.98264	.63677-07	.12
19	967.	.99201	.98271	.34022-06	.62
20	1006.	.99197	.98275	.35396-06	.65
21	712.	.99194	.98278	.25052-06	.46
22	890.	.99193	.98279	.31316-06	.57
23	673.	.99194	.98278	.23680-06	.43
24	1287.	.99193	.98279	.45284-06	.82
25	614.	.99200	.98272	.21603-06	.39
26	925.	.99202	.98270	.32544-06	.59
27	883.	.99202	.98270	.31067-06	.57
28	832.	.99205	.98267	.29271-06	.54
29	1068.	.99204	.98268	.37575-06	.69
30	1103.	.99209	.98263	.38804-06	.71
31	169.	.99213	.98259	.59453-07	.11
32	964.	.99215	.98257	.33912-06	.63
33	986.	.99219	.98254	.34685-06	.65
34	768.	.99220	.98252	.27015-06	.51
35	726.	.99222	.98250	.25538-06	.48

CONCENN FREQUENCY DISTRIBUTION

STEP= .10148651
CENTERPOINT OF INITIAL GROUP= .11021756 NO. OF OBSERVATIONS= 35
CENTERPOINT OF FINAL GROUP= .82062310 NO. OF GROUPS= 7
K FACTOR= 3.



STEP= .10148651
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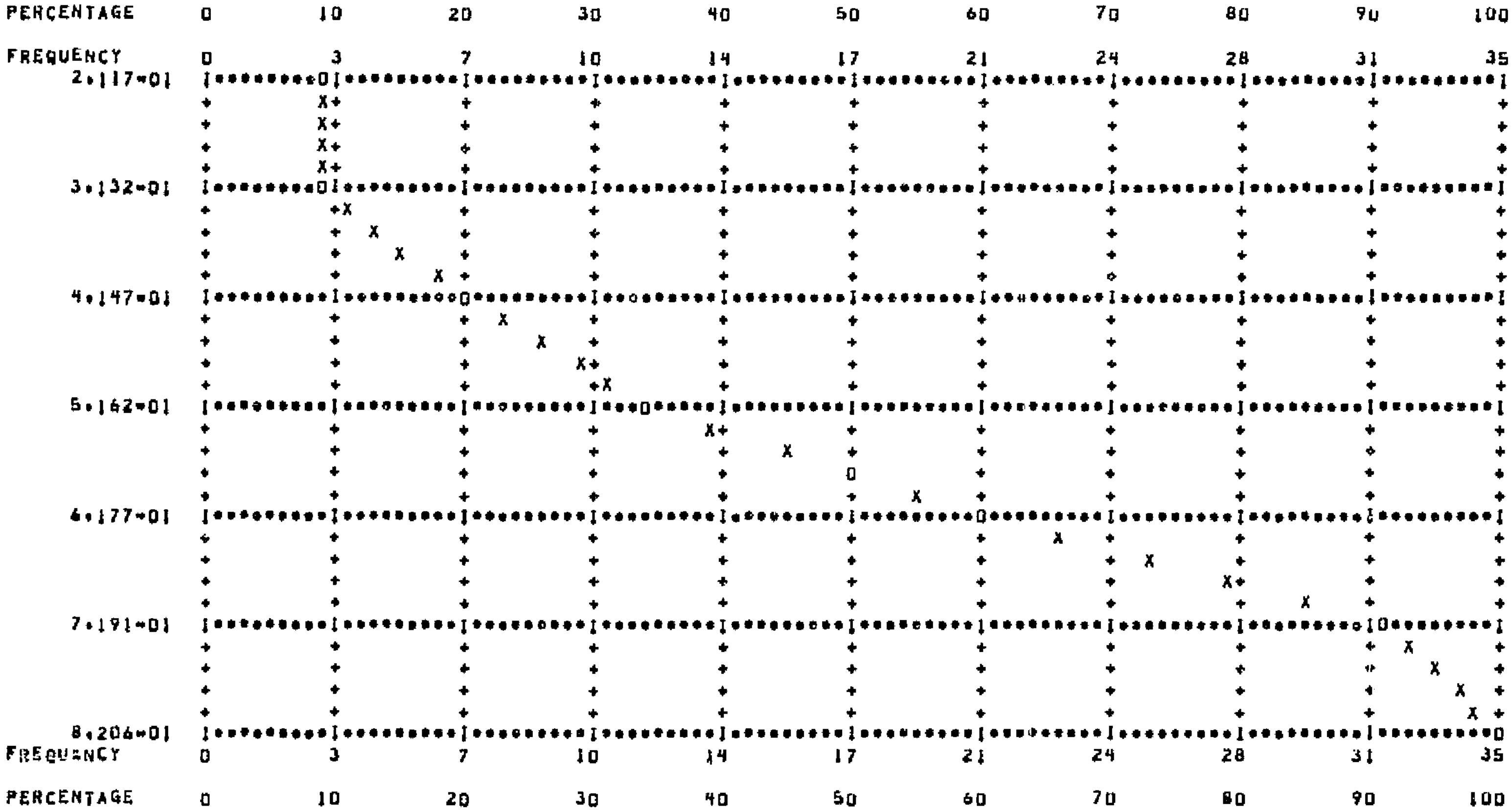
CENTERPOINT OF FINAL GROUP= .82062310 NO. OF GROUPS= 7

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XMAX  =  .82062310E+00,
XBAR  =  .53821459E+00,
VAR   =  .28260567E-01,
SDEV  =  .16810880E+00,
$END
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CONCENTRATION CORRELATION ANALYSIS

CHEMICAL ELEMENTS	VARIANCE COVARIANCE	CORRELATION COEFFICIENT	CORRELATION PROBABILITY
K - K	.0941	1.0000	1.0000
K - S	.0112	.2164	.7883
S - S	.0283	1.0000	1.0000

4.6 References

1. Andersen, C. A., "An Introduction to the Electron Probe Microanalyzer and its Applications to Biochemistry," Methods of Biochemical Analysis, Vol. XV, Interscience Publ. (1967), p. 147.

2. Colby, J. W., Advances in X Ray Analysis, 11, 287 (1968).

3. Earle, K. M. and Tousimis, A. J., "X-Ray and Electron Probe Analysis in Biomedical Research," Prog. in Anal. Chem., Vol. 3, Plenum Press, N. Y. (1969).

4. Heinrich, K.F.J., Ed., "Quantitative Electron Probe Microanalysis," NBS Spec. Publ. 298, 1968.