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Increasing the Efficiency of a Surface Ionization Mass Spectrometer

Thomas Curtis Adams

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This thesis, directed and approved by the candidate's committee, has been accepted by the Graduate Committee of The University of New Mexico in partial fulfillment of the requirements for the degree of

Master of Science in Physics

INCREASING THE EFFICIENCY

Title OF A

SURFACE IONIZATION MASS SPECTROMETER

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1-7-71

Date

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INCREASING THE EFFICIENCY OF A SURFACE IONIZATION MASS SPECTROMETER

BY
THOMAS CURTIS ADAMS
B.S., University of Washington, 1956

THESIS

Submitted in Partial Fulfillment of the
Requirements for the Degree of
Master of Science in Physics
in the Graduate School of
The University of New Mexico
Albuquerque, New Mexico
October, 1970

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ABSTRACT OF THESIS

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An Avco surface ionization mass spectrometer (model 90,000) was installed at the Los Alamos Scientific Laboratory in February, 1968. Since that date this machine has been used as a production instrument for the isotopic analysis of uranium and plutonium samples. During 1969, it was realized that a problem inherent in the ionization mechanism of the instrument was degrading the accuracy of results, and that the number of man-hours expended in reducing data had become excessive. As soon as this situation became apparent, corrective action was initiated to reduce the effect of the ionization problem and to decrease the amount of "people-time" required for data reduction. A relatively sophisticated computer program called "SPECTRE" was written which has improved the accuracy of published results, and which has released two people from the tedious labor of hand data reduction. This paper describes the steps leading to the successful conclusion of this effort, and analyzes the completed computer program in some detail.

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CHAPTER 1

THE INSTRUMENT

The number of types of mass spectrometers in existence is exceedingly large; therefore a rather comprehensive description of the Avco model 90,000 mass spectrometer with which this paper is concerned follows.

The Avco instrument utilizes a single magnetic analyzer to deflect an ion beam through 90 degrees with a 35 centimeter radius.[1] Figure 1 illustrates this ion path, and Figure 2 gives a reasonably good idea of the relative sizes of the ion source, flight tube and beam collector.

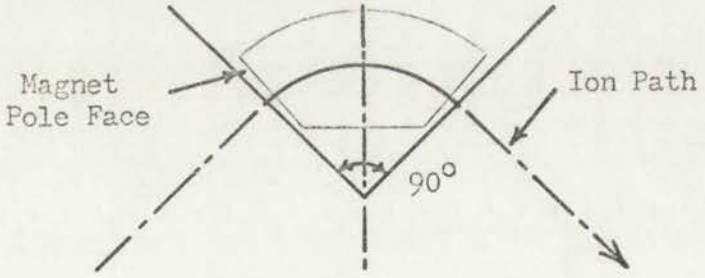

FIGURE 1. Ion optics of the Avco model 90,000 mass spectrometer.

The instrument at the Los Alamos Scientific Laboratory (LASL) is used for isotopic analysis of small quantities of uranium or plutonium. Elemental ions are generated and accelerated through an electrostatic

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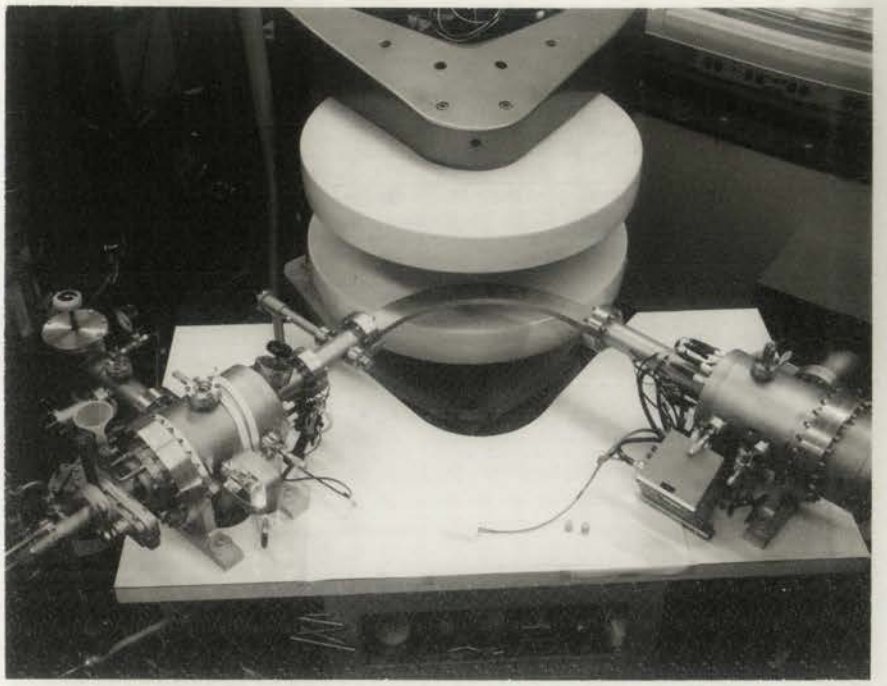
[1] Avco Mass Spectrometers 90,000 Series, Avco Corporation Electronics Division, 2.



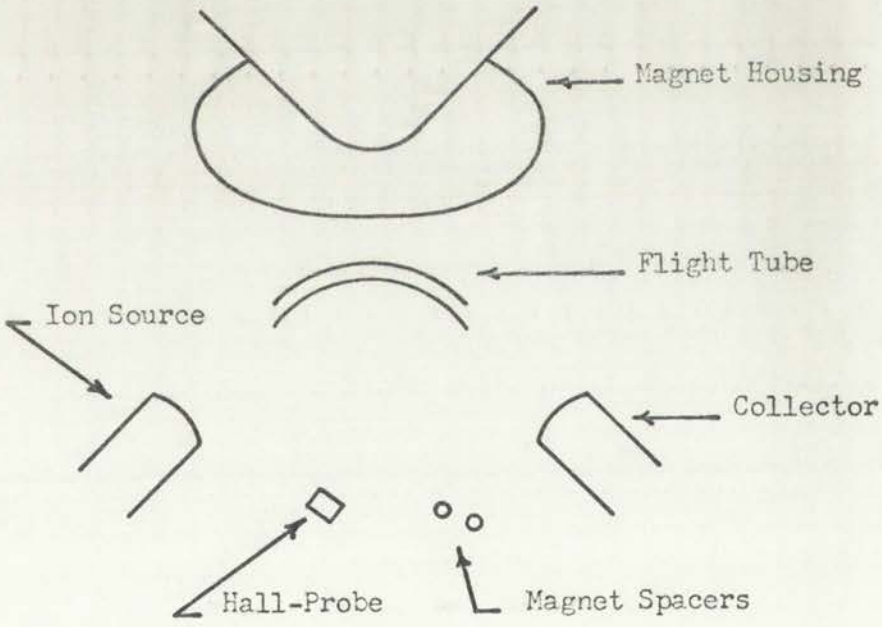


FIGURE 2. A photograph and a diagram of the Avco mass spectrometer located at the Los Alamos Scientific Laboratory (LASL). The magnet housing has been moved back to expose the flight tube. Magnet pole faces are not visible. The magnet spacers are used to keep the pole faces separated by a fixed distance when the magnet is in operation.

thick lensing system to produce a beam which is very nearly parallel. The ion beam is then passed through the magnetic analyzer with magnetic flux density adjusted and source and collector slits set so that only ions of a desired mass number reach the collector. Control during an experimental run is obtained by varying magnetic flux density to select different mass numbers.

As the title of this paper indicates, a surface ionization source is used. A solution of sample material in dilute nitric acid is prepared, and a known amount of this solution is then micropipetted onto two vaporizing filaments and evaporated to dryness. After placing the filaments in position, an electric current is passed through them, heating the sample material and evaporating elemental atoms and ions of this metal (U or Pu). These two side filaments are made of tantalum and serve to produce an atom vapor. A center filament made of rhenium is also used. It is not treated with sample material and serves to ionize a substantial portion of the atoms evaporated from the side filaments. Figure 3 illustrates the physical arrangement of these filaments.

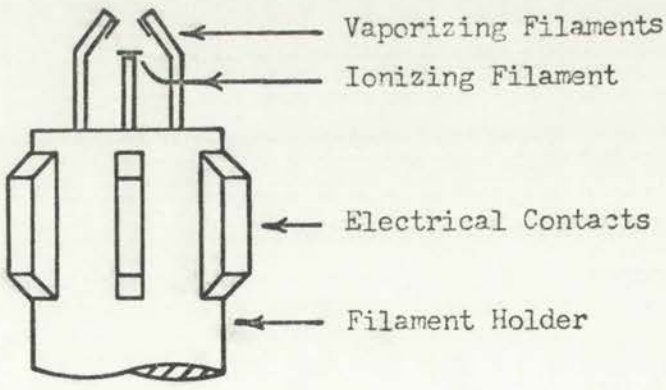


FIGURE 3. LASL filament arrangement.

Surface ionization offers 3 very real advantages over other methods of ion generation (such as electron bombardment):

1. Positive ions are produced with a small energy spread.
2. Sample preparation is relatively simple.
3. Essentially all ions produced are singly charged, which fact allows one to detect ions of a particular mass number rather than ions of a particular charge-to-mass ratio.

This method has the serious disadvantage that ion emission is not constant with time.

As mentioned earlier, an electrostatic lensing system is employed to form a parallel beam of accelerated positive ions. The effective potential through which these ions fall is held constant at a value of 10,000 volts.

The flight tube, a passage through which ions must move to reach the collector, is evacuated to reduce scattering collisions with resident particles. A gas pressure of approximately 5×10^{-8} torr is maintained by pumping during normal operation.

The magnet is water-cooled and is capable of flux densities up to 10,000 gauss. Hall-Probe control permits adjustment to 0.5 gauss over the whole range, and enables any given setting to be relocated within 2 gauss.[2]

At LASL, an 18-stage electrostatically focused electron multiplier is used as a detector (collector).[3] Interstage voltage is held at 110 volts for each stage. A gain of approximately 1.3×10^{5} has been measured,

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[2] Ibid., 2.

[3] As in the literature, the terms "detector" and "collector" are used almost synonymously.

which is sufficient to drive a vibrating reed electrometer. With this set-up, ion beam currents as small as 10^{-16} amperes can theoretically be examined with reasonable accuracy. Isotopic abundance ratios of the order of $10^4/1$ have been regularly measured. It should be noted that a small mass effect has been observed. That is, the average number of secondary electrons produced at the cathode of the electron multiplier varies slightly with the mass of the impinging ion. It has been found adequate to correct for this effect during data reduction.

Now that a general picture of the spectrometer has been established, it is perhaps appropriate to briefly inspect the basic equations involved (Gaussian form). Let the accelerating potential be V, thus allowing a singly charged ion to acquire a kinetic energy eV. This ion will enter the magnetic field with a discrete velocity which is given by

$$eV = \tfrac{1}{2} mv^2 \qquad (1)$$

where m is the mass of the ion, e is the electronic charge, and v is the terminal velocity of the ion after acceleration. The magnetic flux density B is perpendicular to the velocity vector of the ion, therefore the ion under consideration will be deflected into a circular orbit. Balancing forces yields

$$\frac{mv^2}{r} = \frac{e}{c}\left|\vec{v} \times \vec{B}\right| = \frac{evB}{c} \qquad (2)$$

where c is the velocity of light and r is the radius of curvature of the ion path. Eliminating v from equations (1) and (2) yields a general expression relating the magnitude of the magnetic flux density to ion

mass such that only ions of this mass will follow a path which passes through the collector slit:

$$B = \frac{c}{r}\sqrt{\frac{2V}{e}}\quad m^{\frac{1}{2}} \tag{3}$$

Substituting values of r and V for the LASL spectrometer and the accepted values of c and e yields

$$B\ \text{gauss} = \frac{(3 \times 10^{10}\ \frac{\text{cm}}{\text{sec}})}{35\ \text{cm}}\sqrt{\frac{2\,(10^{4}\text{volts})\,(1.66 \times 10^{-24}\ \frac{\text{gm}}{\text{amu}})\,(m\ \text{amu})}{300\ \frac{\text{volts}}{\text{statvolt}}\quad (4.8 \times 10^{-10}\ \text{statcoulomb})}}$$

$$B = 412\ m^{\frac{1}{2}} \tag{4}$$

where the units of m have been changed to atomic mass units. Thus we see that to pass an ion having mass number 235 requires a flux density $B = 412\ \sqrt{235} = 6316$ gauss, and an ion of mass number 234 will reach the collector if the B field is set at $412\ \sqrt{234} = 6302$ gauss. While these figures are not accurate to the number of places given, the difference between them (6316 - 6302 = 14 gauss) is quite representative of the change in flux density required to move from one mass number to an adjacent mass number.

Finite source and collector slit widths mean that ions traveling along paths other than the theoretical line path discussed thus far will also reach the detector. Within reason, this effect is desirable and results in an ion current of detectable magnitude at the collector. In operation the spectrometer is centered on a given mass number by varying magnetic flux density in the vicinity of the magnitude predicted by equation (4) until a maximum output is observed. By sweeping from mass number to mass number it has been well verified that proper velocity ions of adjacent mass number do not reach the collector when the

spectrometer is centered on a particular mass number. The term "proper velocity" is used in the preceding sentence because some ions will suffer energy and direction changing collisions with particles resident in the vacuum system during transit. Some of these will acquire a velocity just right to reach the collector even though they do not have the desired mass number. These unwanted ions are compensated for, to some extent, by ions of desired mass number which fail to reach the collector after experiencing collisions. It is important to keep the vacuum system operating efficiently to reduce collision frequency.

To complete a general understanding of the LASL mass spectrometer it is necessary to discuss the end result or product. With the instrument centered on a particular mass number, the electron multiplier will produce a current proportional to the number of atoms of that mass number present in the sample being analyzed. This current is passed through a resistor to create a d.c. voltage which is fed to a vibrating reed electrometer. The signal is then appropriately scaled and the output of the electrometer is graphically recorded on a moving strip chart. Such a recording is obtained for every mass number for which there are atoms present in the sample. One particular mass number is chosen as a reference, all recorded numbers are converted to a common scale, and atom abundance ratios are calculated by dividing the value associated with each mass number by the value determined for the reference. From this point it is a simple matter to compute the weight percent of the total sample represented by each isotopic species. Results are published (see Table 1) which state the atom ratio and the weight percent of each observed isotope.

TABLE 1. Result of a Typical Analysis

Mass Number	Atom Ratio	Weight Percent
234	0.0116 ± 0.0004	1.08 ± 0.04
235 (reference)	1.00000 ± 0.00000	93.3 ± 0.2
236	0.00219 ± 0.00008	0.206 ± 0.007
238	0.057 ± 0.002	5.4 ± 0.2

CHAPTER 2

THE PROBLEM

As mentioned in Chapter 1, the only serious disadvantage inherent in the surface ionization method of ion generation is that ion emission is not constant with time. Total beam current falls off as time passes because of sample depletion. Irregular long term fluctuations (longer than 10 seconds) are often observed, and are attributed to complex heat transfer characteristics at the side filaments. A moment's reflection yields the inescapable conclusion that, if total beam current is not constant, then a measurement taken at some particular time is proportional to the atom abundance of the isotope in question only with respect to total beam current at that time. The ratio of such a measurement to another measurement made for the reference isotope at another time when beam current was different certainly does not give the atom abundance ratio of these two species!

One way to eliminate the problem of changing beam current is to build a dual collector. By measuring the ion currents contributed by two different isotopes simultaneously, it becomes a trivial job to calculate the relative abundance ratio. This method has drawbacks. An additional set of detecting, amplifying, and recording equipment is required. Calibration of the relative gain of each of the two channels can be troublesome. Physically mounting a second collector on an already established instrument requires careful planning and time.

At LASL neither time nor funding was available to install a dual collector, and an alternate solution was initially adopted. A large number of reference isotope measurements were made during each analysis. It then became possible to infer from the strip chart, which showed the reference measurements in their proper time relationship, what the reference isotope measurement would have been at any time (see Figure 4). With this information it was possible to divide any measurement by the value for the reference isotope obtained from the strip chart for the same time, and to obtain a fairly accurate value for the isotopic ratio associated with that measurement. By repeating the measurement of each isotope several times (6 to 8) large errors were averaged out and meaningful answers obtained.

It was only after this system had been in use for about 6 months and a sufficient number of standards[1] had been run that it became clear that the accuracy of results was not adequate. The girl reducing the strip chart information simply was not able to draw in the complete reference isotope curve with sufficient accuracy. Also, a background measurement taken immediately before and after each isotopic measurement had to be averaged and graphically subtracted from the isotopic measurement. None of the background correction techniques attempted proved to be completely satisfactory.

A second and equally serious problem occurred in connection with data handling. The Avco mass spectrometer at LASL is a production instrument used to analyze approximately 800 samples a year. During most of 1969 one person was involved half-time in reading strip charts. During

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[1]Standards are isotopic samples of accurately known composition, usually supplied by the National Bureau of Standards (NBS).

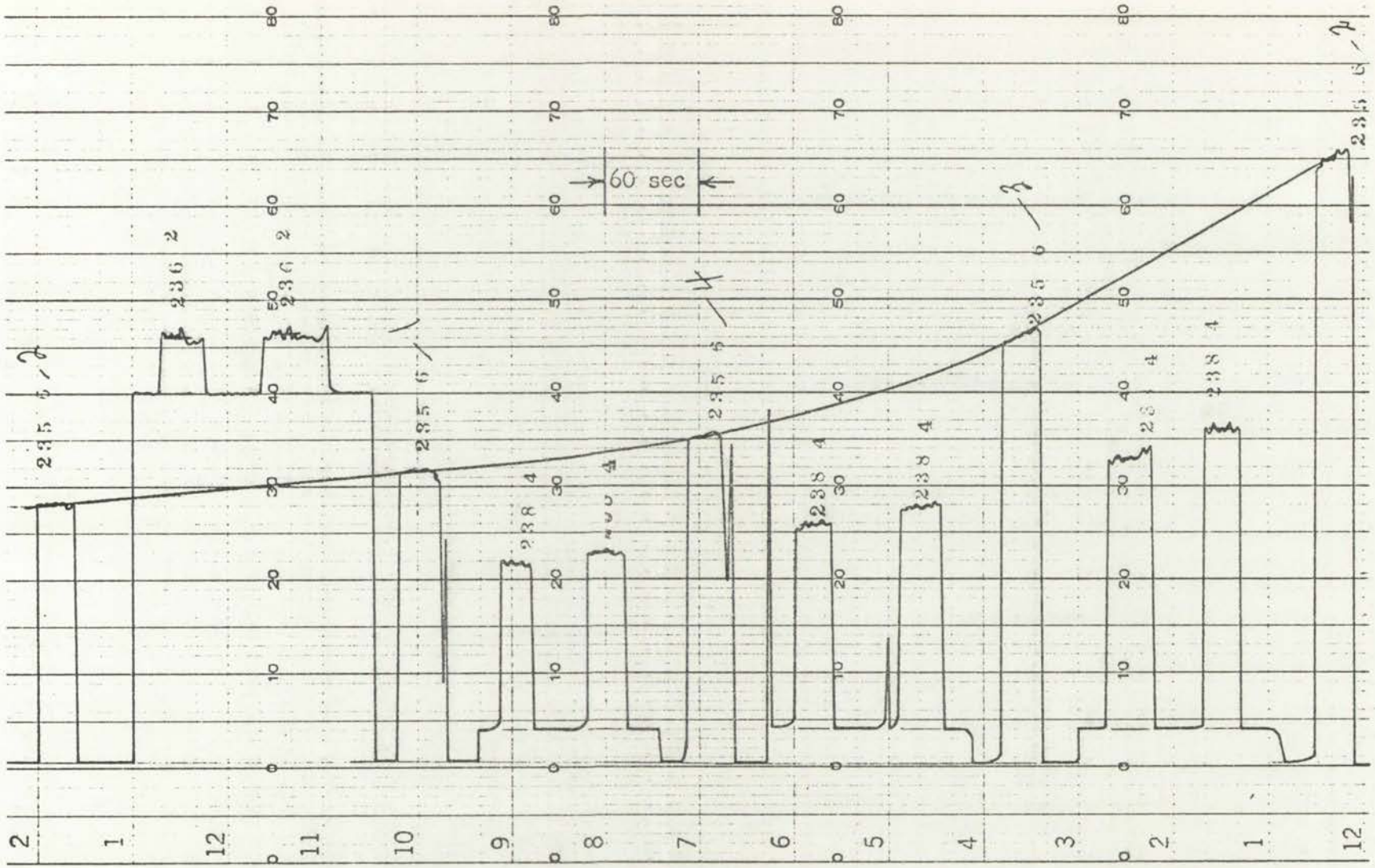

FIGURE 4. A portion of a strip chart. This particular chart was obtained at the same time as the data used in producing the material for Appendices E and F. A description of the sample material used may be found in Appendix F. Peak height is plotted in the vertical direction and time is measured from right to left (the result of chart drive direction). Five reference peaks (mass number 235) and 8 isotope peaks (6 for 238, 2 for 236) are illustrated. The number following each mass number (e.g., 238 4) is a scale factor.

a single analysis many measurements of each mass number present were taken to eliminate bad measurements and to obtain sufficient information for error statistics; and the reading of the resultant strip charts was a time consuming job. Another person was employed full time in performing calculations and determining statistical uncertainty. A secretary devoted a significant portion of her time to typing the correspondence necessary to disseminate results. The number of man-hours expended in checking numbers and proofreading correspondence was appreciable.

An instrument producing information required by other organizations to successfully accomplish their assigned tasks cannot be allowed to shut down. To solve a severe manpower problem while at the same time improving the accuracy of published results, all without spending any money, is not an easy proposition.

A major step forward occurred when a counter with paper tape digital output which had been originally purchased for use with the Avco spectrometer was rediscovered.[2] This subsystem had been in use when the Avco was first employed, but was universally disliked and distrusted by the spectrometer operators. The counter did nothing more than total the number of pulses of the output signal from a voltage-to-frequency converter driven by the vibrating reed electrometer for some set period, usually 10 seconds. The operator had to manually adjust the scale factor dial, set a mass number indicator, position a switch to a special setting if the mass number being measured was to be the reference mass number, and push a button to print this information on tape. Then

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[2]This digital system had been used under a previous supervisory administration. The reasons stated for its lack of success and subsequent fall from favor have been obtained from the operators themselves and from results published during the period of use.

the operator successively adjusted the magnetic field to record the first background, the mass number center measurement and the second background.[3] Measurement times were automatically recorded.

The operator had to complete this procedure for each measurement of each mass number, while at the same time annotating the moving strip chart. Time between successive measurements averaged between 40 and 80 seconds.

When the digital output system was first used, occasional operator errors in positioning the many adjustable indicators destroyed both results and operator confidence. A straight line approximation was used to obtain reference isotope values corresponding to the times of measurement of other mass number isotopes. Results were poor, and the project was abandoned in favor of a return to the strip chart method.

Nevertheless, the rediscovery of this equipment was of the greatest importance. The obvious way to solve the existent manpower problem was to have the large computers at the LASL Central Computer Facility do all the calculational work, and computers require digital data. It remained necessary to figure out a procedure to make the operator's job tenable, and a method whereby the computer would produce more accurate results.

---

[3] One background would be taken at a mass number setting slightly less than that for the isotope being examined and the other at a setting somewhat higher than the setting for this isotope.

CHAPTER 3

EARLY ATTEMPTS AT A SOLUTION

The first step in solving the problems associated with the Avco mass spectrometer was to place the paper tape digital output system back into business. To make the operators' lives less hectic, several unnecessary manual operations were eliminated (e.g., positioning a switch to indicate if the mass number being measured corresponded to the reference isotope), and the remaining operations were ordered and simplified. An excellent least-squares curve fitting routine[1] was located, and program SPECTRE was conceived.

Before the first line of SPECTRE was written it was necessary to define in general terms the architecture the finished program was to possess. The basic idea was to let the computer do the same job the strip chart analyst had been doing graphically (hopefully the computer would perform with greater accuracy). That is, the computer would examine the set of measurements belonging to the reference isotope and the times at which each measurement was taken, and would then use the already

---

[1]This least-squares routine was written on October 15, 1959, by R.H. Moore and R.K. Ziegler of the Los Alamos Scientific Laboratory. It was initially distributed as LASL Report Serial LA-2367 with the title, "The Solution of the General Least-Squares Problem with Special Reference to High-Speed Computers." The original routine has been modified many times by many people, and acquired the name "PACKAGE" at some stage of its evolution. For this application it was extensively modified and greatly reduced in length, thereby receiving the name "PARCEL."

extant least-squares subroutine to fit a curve to these experimental points. The program would also examine the background readings and correct all isotope measurements accordingly. It was decided to break SPECTRE down into a relatively short parent program and several subroutines so as to make debugging and future change as simple as possible. The modular flowchart contained in Appendix C, section I, is essentially a block diagram of program SPECTRE as it was initially conceived, with the exception of subroutine MEMO which was a later addition. At this point it would be wise for the reader to look at Appendix C.

That portion of program SPECTRE which caused the greatest concern early in this project was the least-squares curve fitting subroutine, called "PARCEL" (see footnote, page 14). A mathematical function of the form

$$YT = f(P(1), P(2), P(3), P(4), Z) \qquad (5)$$

has to be supplied to subroutine PARCEL, where YT is reference value, the P(i) are constant parameters to be determined and Z is time.[2] PARCEL then returns the values of the P(i) which yield the best fit. Once in possession of these parameters it is possible to use Equation (5) to calculate a reference value (also called a "reference peak height") for any desired time. Isotope abundance ratios can then be calculated by dividing each isotope measurement (often referred to as an "isotope peak height") by the reference peak height obtained for the same time. The problem arises when one attempts to pick a function.

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[2] From this point on upper case letters are used for all variable names and symbols, even though occasionally contrary to standard practice, in order to remain in close accordance with the program listings which are restricted to upper case lettering (Appendices C through F).

Three sets of actual data were selected where measurements associated with the reference mass number (235) varied with time in the wildest manner ever observed. It was felt that if a function YT could be found such that a good curve fit would result for each of these three experimental runs, then that function would work for any experimental run. Numerous polynomial and exponential functions were tried. The P(i) were allowed to become exponents as well as coefficients in many of the functions attempted. Some of the failures were spectacular (see Figure 5). For the most part, however, the fitted curves followed the experimental points fairly well. Fairly well was not good enough.

A brief digression is again in order. By this time everything possible was being done with the aid of the computer, including the print-out of all trial curves. A typewriter plotting routine was located

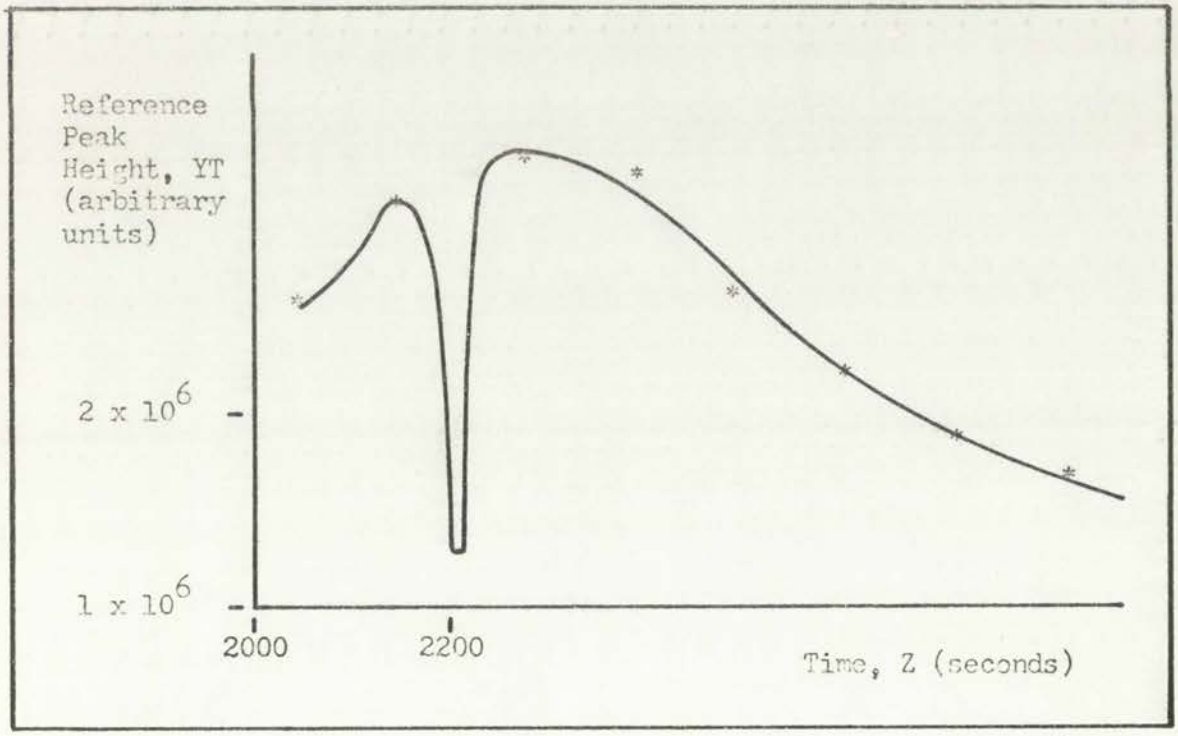

FIGURE 5. An unsuccessful reference curve fit.

and highly modified to plot both experimental points and the fitted curve.[3] This code, called subroutine "Graphic", enabled trial curves to be seen and trial functions to be evaluated quickly without hand plotting (see Appendix F, pages 130, 132, and 134). Such typewriter plots are actually produced by high speed printer equipment attached to the computer and are available much more quickly than plots made on conventional x-y plotters or photographic plotting devices.

Meanwhile, the thought had occurred that if the reference isotope curve were fitted in smaller segments the fit should be better. Some segmented fitting was already being done. Occasionally during a run the beam current would fall to an unacceptably low level and the operator would increase the current through the two evaporative filaments to raise ion beam intensity. When this event occurred all measurements following the increase in filament temperature (FILTEMP) had to be considered separately when obtaining individual measurement ratios. A new program section was written which assigned synthetic FILTEMPs to each measurement so that the reference peak height curve would be fitted in sections of four to eight reference measurements each. The function (a modified Gaussian) which had been giving the best results to date was inserted and the refurbished source deck submitted to the computer. The results were very discouraging.

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[3]This routine, by reputation, was plagiarized from a graduate student at Princeton who in turn had plagiarized it from some other source. Not knowing where credit belongs, the current version here at LASL is called "GRAPHIC" and is used without reference to antecedents or credit.

CHAPTER 4

SUCCESS AND THE LETTER

After considerable soul-searching, it was concluded that perhaps a polynomial might be more efficient at handling the shorter segments, many of which did not resemble any portion of a Gaussian curve. Almost immediately a number of functions were found which gave excellent results. Several weeks were required to arrive at a choice, and as arbitrary as the selected polynomial may appear, it gave the best overall fit for all data selections tested:

$$YT = P(1)Z^{-3/2} + P(2)Z^{-1/2} + P(3)Z^{1/2} + P(4)Z^{3/2} \qquad (6)$$

Typical values for the P(i),i=1,4, may be found in Appendix F, pages 129, 131, and 133.

At this stage the "Weight Percent" column shown in Table 1 was not regularly included in the published report of a completed sample analysis. A survey of users revealed that several were performing the conversion from atom ratio to weight percent by hand, as they required this information on a routine basis.

During the survey just mentioned the group secretaries were asked to comment on procedural changes that might make their job easier or which might result in less delay in mailing the results. None of the relatively large number of suggestions received was of real value, but the volume caused one to ponder the possibility of having the computer write the

entire report.

As a result of this survey, subroutine MEMO was written and added to program SPECTRE. The coding necessary to have the computer calculate weight percent as well as atom ratio for each mass number examined was straightforward. Programing to have the computer write the letter report took considerably more effort. In having the computer draft a letter, it was necessary to program a good many logical decisions so that the computer could pick and choose the proper items to be included in any particular report. The distribution, for instance, varies widely depending on sample type. It was also necessary to ensure that the report was compositionally correct and consistantly in a format acceptable to the clerical staff, group and division leaders, and to the users (no easy task). A copy of the computer report as programed in subroutine MEMO and as presently used appears in Figure 6.

When this report is returned from the computer, it is only necessary for the Supervisor of the Mass Spectrometer Section (Dr. R.M. Tisinger) to indicate his approval by initialing the signature block. The secretary on duty will then add a group symbol, Xerox an appropriate number of copies, and send the report on its way.

Today such letter reports are being published at the rate of approximately 800 per year. If one counts the 6 copies of each report (average) sent to different users as separate reports, then it is fair to say that program SPECTRE produces almost 5000 highly accurate mass spectrometer analysis reports each year and requires essentially no hand labor once the spectrometer run has been completed.

LOS ALAMOS SCIENTIFIC LABORATORY
UNIVERSITY OF CALIFORNIA
LOS ALAMOS, NEW MEXICO 87544

OFFICE MEMORANDUM

TO : DISTRIBUTION DATE: 4 SEP 70

FROM : R. M. TISINGER

SUBJECT: MASS SPECTROMETER ANALYSIS (SPECIAL)
(SAMPLE SERIAL NUMBER)
(NBS-930)

SYMBOL :

AN ANALYSIS OF THE SAMPLE DESCRIBED ABOVE WAS COMPLETED ON 31 AUG 70. THIS ANALYSIS WAS PERFORMED USING THE AVCO MASS SPECTROMETER. RESULTS ARE TABULATED BELOW WITH UNCERTAINTY EXPRESSED AT THE NINETY-FIVE PERCENT CONFIDENCE LEVEL. ATOM RATIO IS THE NUMERICAL RATIO OF THE NUMBER OF ATOMS OF SPECIFIED MASS NUMBER TO THE NUMBER OF ATOMS OF MASS NUMBER 235.

MASS NUMBER	ATOM RATIO	WEIGHT PERCENT
234	.01165 +- .00039	1.0822 +- .0361
235	1.00000 +- 0.00000	93.2936 +- .1672
236	.00219 +- .00008	.2055 +- .0073
238	.05735 +- .00186	5.4187 +- .1757

R. M. TISINGER
GROUP W-7

DISTRIBUTION:

W- 7 W. H. CHAMBERS
W- 7 R. M. TISINGER

FIGURE 6. The computer produced letter report of program SPECTRE. This particular example of the SPECTRE report was produced along with the material contained in Appendices E and F. A description of the sample material used may be found in Appendix F, pages 124 and 139.

CHAPTER 5

PROGRAM SPECTRE

The background for this program has been covered in preceding chapters. Program variables, flowcharts, a program listing, and an example of standard output are contained in appendices. Several important aspects of this program, however, remain to be discussed.

Program SPECTRE was not coded in the American Standards Association (ASA) FORTRAN IV programing language. It was coded in a version of FORTRAN IV espoused by the Control Data Corporation (CDC). While these two languages are essentially similar, several very important differences exist: ASA FORTRAN IV may be used on almost any computer. CDC FORTRAN IV is usable only on those few machines especially programed to accept this language. The CDC version permits 7-character variable and routine names. The ASA version allows a maximum of 6 characters in such names. Buffer handling statements are not the same. The methods of writing and operating with logical arithmetic statements are quite different. Other differences exist.

This discrepancy is not fatal. If one were to attempt to compile a SPECTRE source deck on a machine other than the CDC-6600 or CDC-7600 machines at LASL, strange things would occur. Most other machines will truncate all names to 6 characters. All other machines will print diagnostic remarks to be identified with program statements which are not understood. A good program analyst could then correct the imperfect

statements and rename the variables and routines having names requiring changes. The corrected source program should then compile properly and the new user would have a viable program similar to SPECTRE.

The author learned his programing from scratch, and now knows enough to do future coding with ASA standard programing languages exclusively.

Two different criteria have been used for the identification of anomalous measurements. Chauvenet's Criterion was initially applied, and was felt to have resulted in the elimination of good data.[1] Grubbs' table for a 10% 2-sided significance level has been used for the past several months, and has proven eminently satisfactory.[2] When using a 10% 2-sided significance table, the desired result is that there will be only a 10% probability of erroneously rejecting a good observation from either the high or the low measurement side. It should be pointed out that both of these criteria are based on an assumed normal (Gaussian) population or distribution. It has been recognized that mass spectrometer measurements are not normally distributed, but it is felt that the actual distribution is sufficiently close to normal so that it is reasonable to apply such criteria.

Computer time is expensive. The computer run made to obtain the material for Appendices E and F required exactly 8.8 seconds of central processer time. If program SPECTRE were run 800 times each year with similar data, less than 2 hours of computer time would be used annually. SPECTRE is economical.

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[1] Yardley Beers, Introduction to the Theory of Error, 23-24.

[2] Frank E. Grubbs, "Procedures for Detecting Outlying Observations in Samples," 2-5.

Initially it was decided that a basic 3% error plus a calculated statistical uncertainty (expressed at the 95% confidence level) would be shown for each isotope atom ratio listed on the published report. It was hoped that as experience was gained the magnitude and nature of non-statistical errors inherent in the procedure and material system would become apparent, and could perhaps be eliminated. It was intended that, when the magnitude of the actual irreducible nonstatistical error became known, the 3% arbitrarily assigned error should be accordingly reduced. While it was realized that assigning too large an uncertainty could be as bad as assigning too little, in this instance it was most important to the users that the accuracy of results be evaluated pessimistically. The numbers appearing in Figures 6 and 16 include the aforementioned arbitrary 3% error.

Recent checks against NBS standards have indicated that the non-statistical error is now less than 1% (compare the numbers stated for weight percent on page 138 with those given on page 139). The maximum uncertainty considered acceptable for Avco mass spectrometer results is 1%. SPECTRE is now producing consistantly accurate and timely results.

CHAPTER 6

CONCLUSIONS

I shall use the first person throughout this chapter, as the opinions expressed are entirely my own.

There was a time when the mass spectrometer was almost exclusively a tool of the chemist. That time has passed. At Los Alamos, the Supervisor of the Mass Spectrometry Section, Dr. R.M. Tisinger, is a physicist, as is his principal assistant. The other national laboratories with which I am familiar have physicists, as well as scientists from other disciplines, attached to their mass spectrometer organizations. Today, the mass spectrometer must be considered, among many other things, as a research instrument for the physicist.

A report recently published by the National Academy of Sciences contains the following note:

> Experience at Brookhaven and Berkeley has shown that a programmer [sic] can produce between 10 and 20 debugged and documented lines of program per day, depending on such factors as experience, when he is working on reasonably straight forward programming. When working on a complicated monitor system he would be considerably less productive.[1]

A quick count of the number of lines in program SPECTRE, skipping comment statements and ignoring subroutines PARCEL and GRAPHIC which were not wholly written for use with SPECTRE, yields the figure 380. Assuming the

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[1] On-Line Data-Acquisition Systems in Nuclear Physics, 1969, National Academy of Sciences, 15.

statement quoted on the previous page is accurate, then an experienced programer working at his maximum rate would have taken 19 full working days to write SPECTRE. I knew absolutely nothing about computers or programing when I started this project. It took me longer than 19 days. By the time modifications necessary to make PARCEL and GRAPHIC function with SPECTRE were completed and the entire program was put on-line as a tested and proven piece of production software, I should estimate the time expenditure as close to 6 man-months and the work involved as more than would have been required for 15 hours of course-work (exclusive of the time spent producing this report).

Six months of effort must be balanced against what was accomplished. The staff-member who was engaged full-time reducing data has now been assigned to another task which cannot be done by a machine. The girl who was working half-time reading strip charts was caught in the recent personnel reduction at LASL and was discharged. The secretaries who used to type 800 reports each year have expressed their appreciation on several occasions. The users have commented in writing that report accuracy is noticeably higher, that they are receiving results promptly for the first time, and that the weight percent column in the letter report has saved considerable "busy-work" on their part. I have become somewhat proficient in programing and in using a computer for data handling and analysis. I have also learned a great deal about mass spectrometers and their employment. It is perhaps also fair to say that I have gained some knowledge of technical report writing. I am more than satisfied.

SPECTRE is not the end. Improvement must continue. While program SPECTRE has placed the LASL Avco mass spectrometer on a par with the best of the dual collector machines, this instrument should be able to handle

a larger number of samples daily, and accuracy could be further improved. The next step will most probably be to change from magnetic field to electric field control. That is, instead of varying the magnetic flux density to determine which mass number reaches the collector, the ion accelerating electric field will be adjusted to accomplish the same result. The advantage in making this switch is that the change from one mass number to another can be made much more quickly without having to fight the tremendous inductance of the magnet coils. As soon as funding is available it is planned to interface the spectrometer to a small local computer. Rapid mass number selection under computer direction and control should greatly increase accuracy and sample through-put, and will have the additional advantage of allowing some degree of on-line data reduction.

I have enjoyed this project in all of its facets without reservation, and I look forward to the next.

APPENDIX A

FLOWCHART SYMBOLS

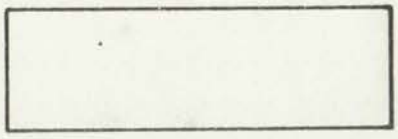
A flowchart is a diagram that shows the operations performed in an information processing system (usually a computer), and the sequence in which these operations are performed. Appendix C contains a modular flowchart for program SPECTRE, which stresses the logic flow of the program and its principal subroutines. Appendix D contains a detailed flowchart for program SPECTRE, which illustrates every step performed throughout the entire program.

It has long been recognized that uniformity in the meaning and use of symbols would enhance understanding and utility of the flowchart. To this end, the International Organization for Standardization (ISO) published a document entitled, Recommendation on Flowchart Symbols for Information Processing. The United States of America Standards Institute (USASI) has also promulgated a recommended set of flowchart symbols. Large companies in the business, such as IBM and CDC, have distributed manuals with their versions and their recommended extensions. All of these suggested groupings of flowcharting symbols are similar, but none are identical.

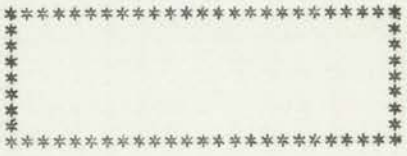
An effort has been made to use only those symbols common to all of the major recommended groupings. The flowchart contained in Appendix D was computer produced directly from a complete SPECTRE source program by a

TABLE 2. Flowchart Symbols Used in Appendices C and D

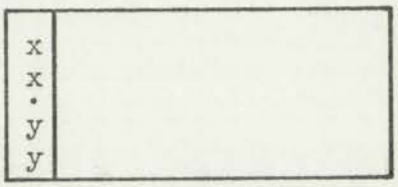
1. Process



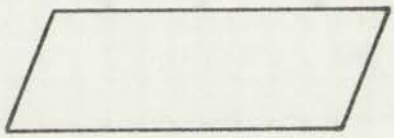
2. Comment/Annotation
(non-standard)



3. Predefined Process/Subroutine



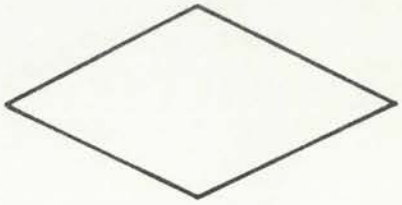
4. Input/Output



5. Connector/Transfer

6. Exit

7. Decision



standard flowcharting code called "AUTOFLOW."[1] It was impractical to remove one non-standard symbol from this flowchart; therefore, the comment/annotation symbol has been plainly marked "non-standard" in Table 2 and has been used in the flowcharts appearing in both Appendix C and Appendix D.

An illustrated listing of symbols to be used, such as appears in Figure 2, is really not sufficient for complete understanding of the use of these symbols. The remaining paragraphs of this Appendix will be employed to explain in detail the specific varities of symbol usage.

Each flowchart symbol, except for certain unconditional transfers, has a symbol number which is printed above and to the right of the symbol. Within each flowchart page (in Appendix D each flowchart page takes up two physical pages), the symbols are numbered consecutively starting with 1. A symbol may also have a FORTRAN statement number associated with it. If so, the number is printed above and to the left of the symbol.

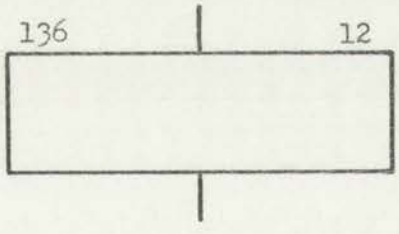


FIGURE 7. Symbol number 12. This symbol is associated with FORTRAN statement number 136.

If a symbol initiates a new path of flow, meaning that control does not pass down from the previous symbol, then the FORTRAN statement number associated with the symbol initiating the new path is printed in a small

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[1]AUTOFLOW was produced by Applied Data Research, Inc., of Princeton, New Jersey, for use at Goddard Space Center, Greenbelt, Maryland.

box above the symbol.

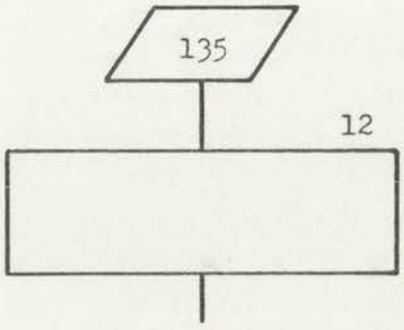

FIGURE 8. A symbol which begins a new path of flow. Symbol number 12 corresponds to FORTRAN statement number 135 in the source program.

Many references to symbols are shown in the form xx.yy where xx is the flowchart page number[2] on which the symbol appears and yy is the number of the referenced symbol. If the symbol is on the current page, the xx is omitted and only the symbol number is printed.

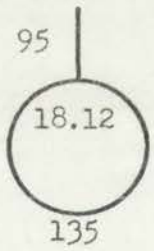

FIGURE 9. A connector or transfer. This transfer has been generated by FORTRAN statement number 95. Control is being transferred to symbol number 12 on flowchart page 18, which corresponds to FORTRAN statement number 135 in the source program.

When a call is made to a subroutine, the flowchart page and symbol number at which the subroutine flowchart begins are included within the

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[2]In Appendix D the flowchart page number is assigned by the computer and is different from the usual physical page number.

predefined process/subroutine symbol generated by the call statement. If the word NONE appears instead, then a flowchart of the subroutine being called does not exist at the flowchart level under consideration.

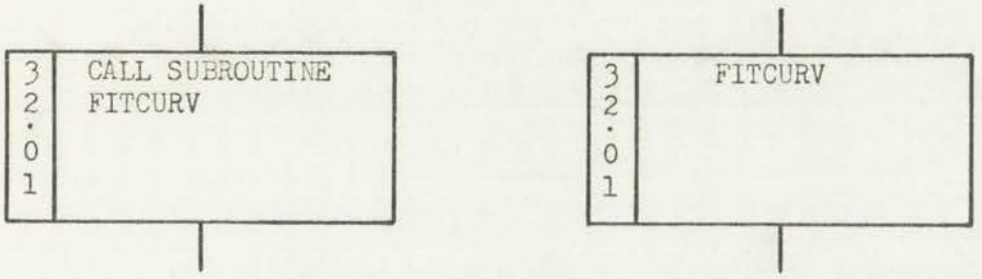

FIGURE 10. Symbols used to call a subroutine. A flowchart for subroutine FITCURV may be found starting with symbol number 1 on flowchart page 32.

An example of the decision symbol is shown in Figure 11. Each possible path leading from the decision is labeled according to the condition it represents (HIGH, LOW, EQUAL, YES, NO, etc.). If possible, a line is drawn to show the path to the specified destination. If a line cannot be drawn, then a connector/transfer symbol is used.

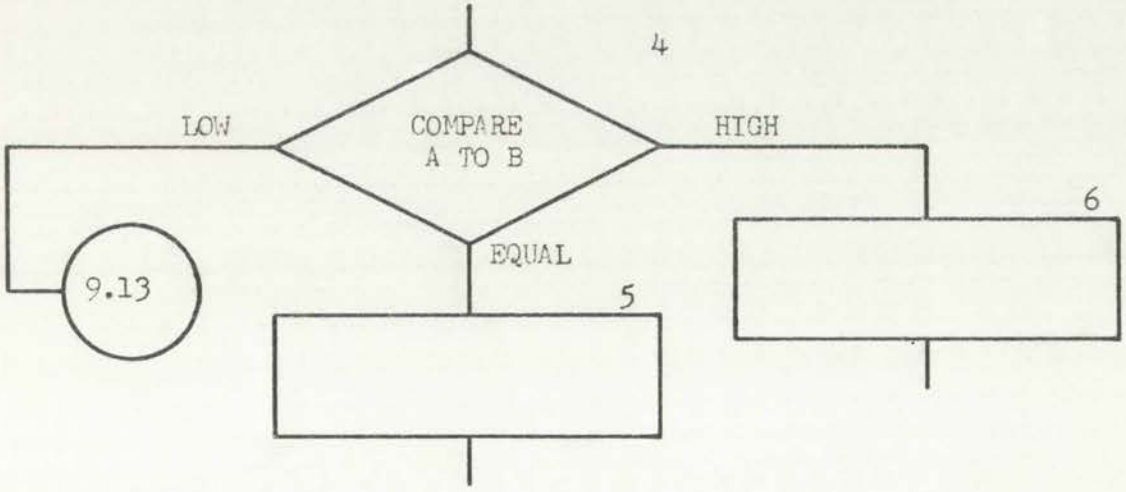

FIGURE 11. A decision wherein A is being compared to B. Note that, if A is low, then the path followed goes to the 13th symbol on flowchart page 9.

Additional information is provided through the use of in-connectors. An in-connector indicates that there is a transfer of control to that symbol from the symbol specified by the in-connector.

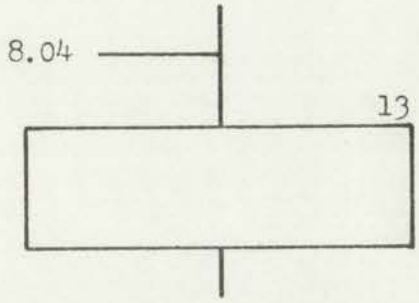

FIGURE 12. An in-connector. The in-connector illustrated indicates that control is transferred to this point from the fourth symbol on flowchart page 8.

The detailed flowchart contained in Appendix D uses asterisks to convey information. If there is more than one transfer to a given point, the in-connector at that point will contain an asterisk following information describing the first transfer. An asterisk found imbedded in a connecting line means that there are additional transfers to the terminal point of the connecting line besides that shown by the line itself. In both of these instances information describing the other transfers may be found in the cross reference listing immediately preceding the flowchart in Appendix D (a further discussion of this cross reference listing may be found on page 51, paragraph 1).

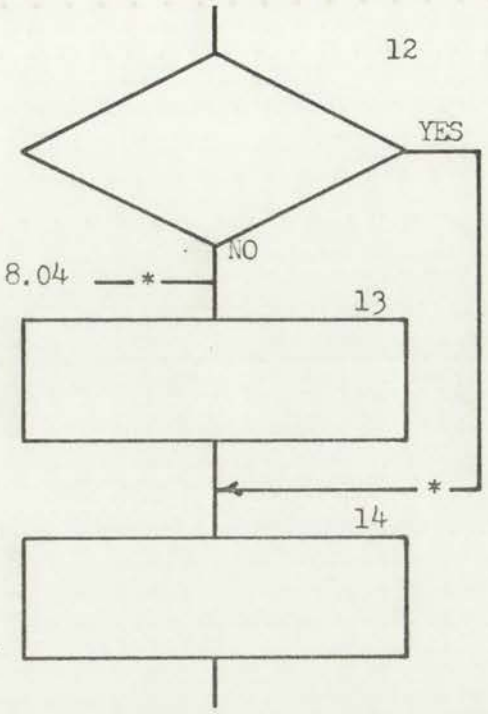

FIGURE 13. An example of the asterisk convention. The in-connector indicates that control is transferred to symbol 13 from symbol 4 on page 8. The right most connecting line indicates that for the YES condition control is transferred from decision symbol 12 to symbol 14. The asterisks found in each of these lines mean that there are transfers to symbols 13 and 14 other than those shown.

Column break indicators are used to show that the flow has been broken because the bottom of a column has been reached. In all such cases the flow is continued at the top of the next column.

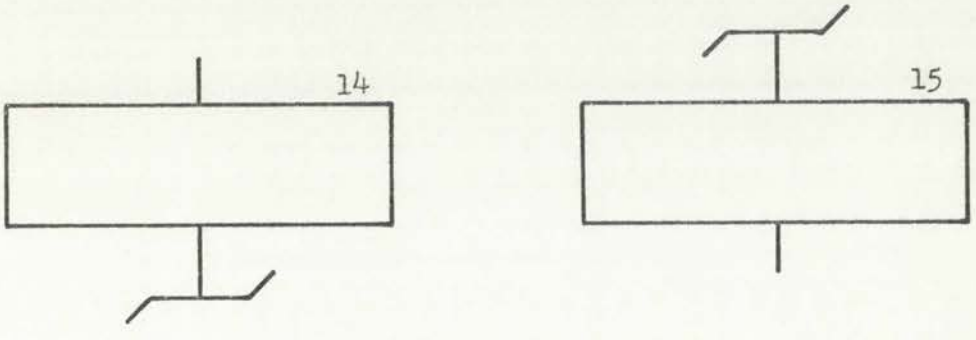

FIGURE 14. Column break indicators. These indicators show that control passes from the left to the right column.

APPENDIX B

VARIABLE MEANINGS

Meanings for all of the variables used in program SPECTRE are given in the following list. This list is divided into four sections: one section for the parent program and a section for each of the subroutines FITCURV, ANALYZE and MEMO. In those cases where a particular variable is used in more than one routine, it is defined only in the section pertaining to the routine of first use. Several variables change meaning during the course of the program's logic flow. Such variables are redefined at the point in the list where the change takes place. Within a section, variables are defined in strict order of appearance in the detailed flowchart contained in Appendix D.

It should be noted that seven-character variable names are occasionally used, in direct conflict with the American Standards Association (ASA) standard for the FORTRAN IV computer language which specifies a maximum of six characters (see page 21, paragraph 2).

I. Parent Program Variables

	Name	Meaning
1.	TITLE (1)	is the date of the mass spectrometer run.
2.	TITLE (2), (3), (4)	is the assigned serial number of the sample being analyzed.
3.	TITLE (5)	is sample type (PRESHOT, POSTSHOT and SPECIAL are the only types permitted).
4.	TITLE (6)	is shot name when a specific test shot is involved (e.g., TRINITY).
5.	TITLE (7)	is the spectrometer used in the analysis (e.g., AVCO).
6.	TITLE (8)	is the name of a person to be added to the distribution list (at present only ANDERSON or JAYNES are allowed).
7.	FILTEMP (I)	is the sequence number of the filament temperature at which the Ith measurement was taken. That is, if the thirteenth measurement were made with the filament temperature adjusted to its second value, then FILTEMP (13) = 2.
8.	SCALE (I)	is an integer which indicates the scale of the Ith measurement ($1 \leq$ SCALE (I) ≤ 10).
9.	MASS (I)	is the mass number associated with the Ith measurement.

10.	HOUR (I,J) MINUTE (I,J) SECOND (I,J) *	are the constituents of the time of the I,Jth measurement.
11.	SUMTIME (I,J)*	is the duration in seconds (integration time) of the counting period of the I,Jth measurement.
12.	PEAK (I,J)*	is the value of the I,Jth measurement (total pulse count or counts per second).
13.	N	is the total number of peak height measurements.
14.	K, KA, KB, and KC	are convenient indices used in connection with a data printout.
15.	BACKGND (I)	is a calculated background value for the time of the Ith peak height measurement.
16.	PEAK (I)	is the value of the Ith peak height. This value has been corrected for background and has been adjusted to a common scale.
17.	TIME (I)	is the time of the Ith peak height measurement normalized such that TIME (1) = 2000 seconds.
18.	J	is changed at this point to the sequence number (index I) of the first measurement belonging to the FILTEMP segment under consideration (see variable 24 on the following page).
19.	L	is the sequence number of the FILTEMP under consideration.
20.	M	is the sequence number of the synthetic FILTEMP segment under consideration.

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*J = 1 refers to the preceding background measurement.
J = 2 refers to the peak height measurement.
J = 3 refers to the following background measurement.

The term "measurement" has been used somewhat ambiguously to refer in some instances to a group of two backgrounds plus a peak height (index I), and in other cases to refer to just one of these three (index I,J). This ambiguity soon disappears, as peak height is corrected for background immediately after data printout, and the term "measurement" refers to a unique peak height (index I) from that point on.

21.	NREF	is a counter used to count the number of reference measurements processed at various program stages.[1]
22.	K	is the sequence number (index I) of the last measurement belonging to the FILTEMP or FILTEMP segment under consideration.
23.	KEEP	is the total number of measurements taken at the FILTEMP under consideration.
24.	KOUNT	is the number of segments into which a group of measurements taken at the FILTEMP under consideration is to be divided. This division is programmed so that the reference peak height curve will be fitted in sections containing between 4 and 8 reference measurements each. When KOUNT equals 0 or 1 then the group of measurements is to be left undivided.
25.	JUMP	is an indicator which is set to value 5 whenever the next segment is to contain 5 reference measurements.
26.	INVERT	is a counter which counts from N down to J and is used only as an index for other variables.

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[1] From this point on a distinction is made between the terms "reference measurement" (or peak height) and "isotope measurement" (or peak height). "Isotope" is to be understood to apply to all mass numbers except the reference mass number. "Reference" is to be used only in connection with the reference mass number.

II. Subroutine FITCURV Variables

	Name	Meaning
1.	START	is the sequence number of the first measurement belonging to the FILTEMP under consideration.
2.	FILNUM	is the sequence number of the FILTEMP under consideration.
3.	K	is now the mass number index. The mass number associated with any value of K is K + 230 (i.e. K = 1 corresponds to mass number 231). K is restricted to integral values from K = 1 to K = 15.
4.	TOTAL (K)	is a counter used to count the number of measurements of the Kth isotope processed through completion of the FILTEMP under consideration.
5.	COUNT (K)	is a counter used to count the number of measurements of the Kth isotope processed through completion of the FILTEMP previous to the FILTEMP currently under consideration.
6.	REFPEAK (I)	is the value of the Ith reference peak height belonging to the FILTEMP under consideration.
7.	REFTIME (I)	is the time of the Ith reference measurement belonging to the FILTEMP under consideration.
8.	M	is the value of TOTAL (K) and is used only as a do loop index.
9.	ISOPEAK (K,M)	is the value of the Mth peak height for the Kth isotope.
10.	ISOTIME (K,M)	is the time of the Mth measurement of the Kth isotope.
11.	J	is the value of COUNT (K) + 1 and is used as a test element and as a do loop index.
12.	REFVALU	is the calculated value of reference peak height based on the fitted reference curve at a time corresponding to one of the isotope measurements.
13.	RATIO (K,I)	is the isotopic ratio of the Ith measurement of the Kth isotope belonging to the FILTEMP under consideration.

14.	XPLOT (I)	is a time in seconds. The current FILTEMP curve is divided into 99 equal increments for smooth plotting. XPLOT (1), XPLOT (2), ..., XPLOT (100) are the boundary times of these increments.
15.	YPLOT (I)	is the calculated value of reference peak height based on the fitted reference curve at time XPLOT (I).
16.	REFPLOT (I)	is the calculated value of reference peak height based on the fitted reference curve at time REFTIME (I).
17.	DIFFER (I)	is the percentage difference between REFPEAK (I) and REFPLOT (I) (A measure of the quality of reference curve fit).

III. Subroutine ANALYZE Variables

	Name	Meaning
1.	FUDGE	is a constant determined experimentally which is used in correcting for the mass effect (see page 4, paragraph 5).
2.	ISOMASS	is the mass number of the isotope under consideration.
3.	FACTOR	is a multiplicative correction applicable to the isotope under consideration.
4.	BINGO	is an indicator which is set to value 99.0 whenever an isotopic ratio is statistically found to be an "outlier."
5.	SUM	is the sum of the isotopic ratios for all measurements made of the isotope under consideration.
6.	AVE	is the average isotopic ratio of the isotope under consideration.
7.	SUMSQ	is the sum of squares of the statistical deviation in the isotopic ratios for all measurements made of the isotope under consideration.
8.	DEV (K,I)	is the statistical deviation of the Ith isotopic ratio of the Kth isotope.
9.	PERDEV (K,I)	is the percentage deviation in the Ith isotopic ratio of the Kth isotope.
10.	SIGMA (K)	is the standard deviation (root mean square deviation) of the individual isotopic ratios calculated for the Kth isotope.
11.	SIGBAR (K)	is the standard deviation of the average isotopic ratio of the Kth isotope (standard deviation of the sampling distribution).

12.	UNRATIO*	is an uncorrected isotopic ratio.
13.	DSIGMA	is the deviation of an isotopic ratio expressed in units of standard deviations. This quantity is immediately printed for record purposes.
14.	RATIO (K)	is a variable in common with the parent program and all other subroutines. It is therefore used briefly to pass the value of AVE on to subroutine MEMO.
15.	RATIO (K,2)	is used in the same manner as RATIO (K). It passes the value of SIGBAR (K) on to subroutine MEMO.
16.	UNAVE*	is an uncorrected average isotopic ratio.
17.	UNSIGMA*	is an uncorrected standard deviation of individual isotopic ratios for a particular mass number.
18.	UNSIGBR*	is an uncorrected standard deviation of an average isotopic ratio for a particular mass number.
19.	REJECT (M)	is the maximum number of standard deviations by which a given isotopic ratio may differ from the average isotopic ratio without being considered an "outlier" in a sample consisting of M ratios.[1]
20.	TEST	is the value of REJECT (M) and is used as a test element.

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*Variables marked with an asterisk are purposely returned to the uncorrected state with respect to the mass effect, and are immediately printed for record purposes.

[1]Grubbs, "Procedures for Detecting Outlying Observations in Samples," 2-5.

IV. Subroutine MEMO Variables

	Name	Meaning
1.	ATOMRAT (K)	is the average isotopic ratio of the Kth isotope.
2.	ATOMERR (K)	is the uncertainty (expressed at the 95% confidence level) in ATOMRAT (K).
3.	TFACTOR (M)	is the percentile value for Student's t (0.95) distribution with (M-1) degrees of freedom.
4.	RATIO (K)	is changed in meaning early in this subroutine. The third statement following program statement number 30 is "RATIO(K)=ATOMRAT(K)*FLOAT(K+230)/ MASS." From this statement on, RATIO (K) is the most probable mass ratio of the Kth isotope. "Mass ratio" is intended to mean the ratio of the mass of atoms of the Kth isotope to the mass of atoms of the reference isotope in any amount of sample material.
5.	RATIO (K,2)	is changed in meaning at the same point as RATIO (K). From this point on RATIO (K,2) is the uncertainty (expressed at the 95% confidence level) in RATIO (K).
6.	SUM	is used in subroutine MEMO as the sum of the mass ratios for all isotopes.
7.	SUMSQ	is used in subroutine MEMO as the sum of squares of the uncertainties in the mass ratios for all isotopes.
8.	ERROR1	is the root mean square uncertainty formed by taking the square root of SUMSQ.
9.	ERROR (K)	is the uncertainty (expressed at the 95% confidence level) in PERCENT (K) (see immediately below).
10.	PERCENT (K)	is the weight percent of the sample material contributed by the Kth isotope.
11.	NUMBER	is the number of copies of the final written letter report which the computer is to prepare.

12.	NDAY	is used initially to contain a 6 digit date (i.e., 072470 corresponding to July 24, 1970). This variable is quickly emptied of all but the 2 day digits (i.e., 24). The exact date is supplied by the computer and corresponds to the day of processing.
13.	NMONTH	is a 2 digit month (i.e., 07).
14.	NYEAR	is a 2 digit year (i.e., 70).
15.	MONTH (I)	is the 3 letter month corresponding to NMONTH (i.e., JUL corresponds to NMONTH = 07).
16.	MASSNUM	is the mass number corresponding to a given value of K (i.e., 235 corresponds to K = 5).

APPENDIX C

MODULAR FLOWCHART FOR PROGRAM SPECTRE

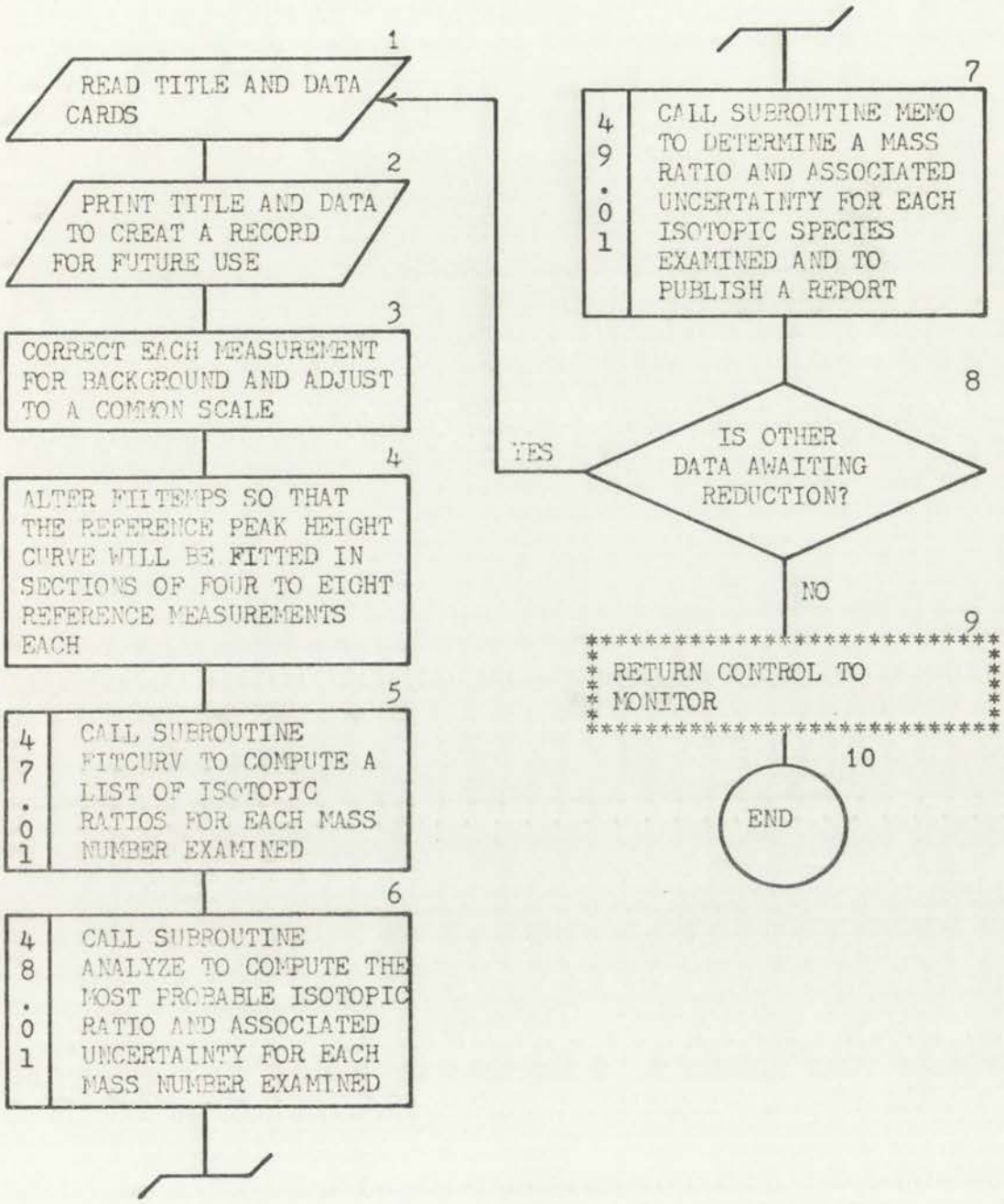
The following modular flowchart is perhaps the most important item appearing in this report. A detailed flowchart, such as that given in Appendix D, is excellent for correcting program "bugs" and evaluating the effect of individual statements, but is so complex as to be of questionable value to one not already familiar with the particulars of the program being considered. A modular program, on the other hand, stresses the logic flow of a program and allows one to quickly grasp the series of intended operations and desired results.

This flowchart has been broken into four self-sufficient parts. The flowchart for the parent program completely describes SPECTRE in modular terms. The flowcharts for subroutines FITCURV, ANALYZE and MEMO go one step further in detailing the methods used to perform those functions called for in the parent program flowchart. Subroutine FITCURV uses two other subroutines called PARCEL and GRAPHIC. Modular flowcharts for PARCEL and GRAPHIC are not included as these subroutines are adaptations of routines already in existance (see footnotes on pages 14 and 17), and the explanations of each appearing in the FITCURV flowchart are quite adequate to establish logic flow.

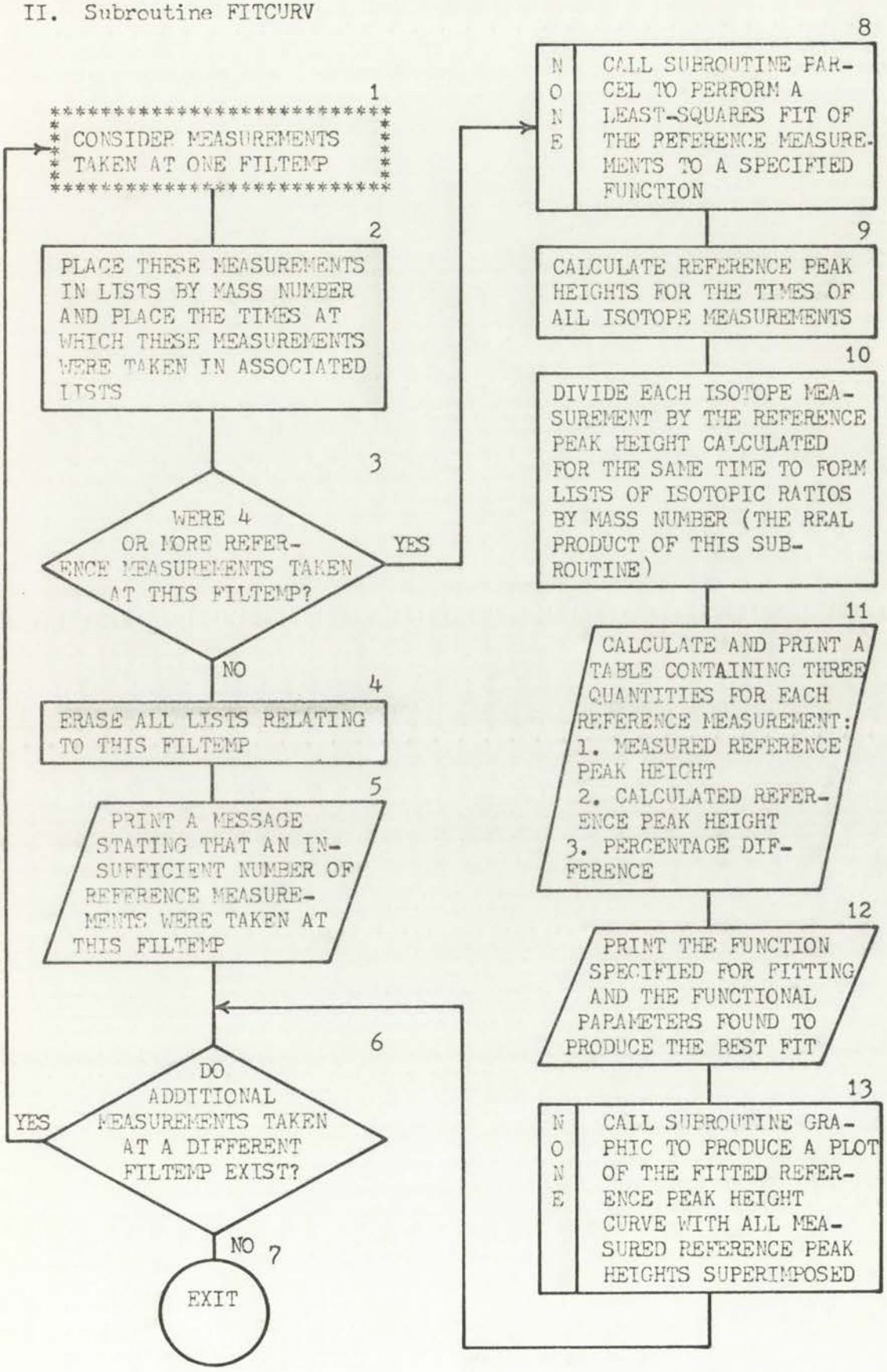
The symbols and the numbering convention employed are the same as those used with the detailed flowchart of Appendix D (see Appendix A for symbol descriptions). Page references are to be applied to the usual

physical page numbers appearing at the bottom of each page (special computer assigned flowchart page numbers are used for reference purposes in Appendix D). The variable FILTEMP has been used by name throughtout the flowchart. All measurements taken at the original filament temperature are assigned a FILTEMP code of 1; all measurements taken after the spectrometer operator changes the filament current to obtain a different filament temperature are assigned a code of 2. If the operator should change the filament temperature again, then measurements at that temperature would be coded with a FILTEMP of 3, etc.

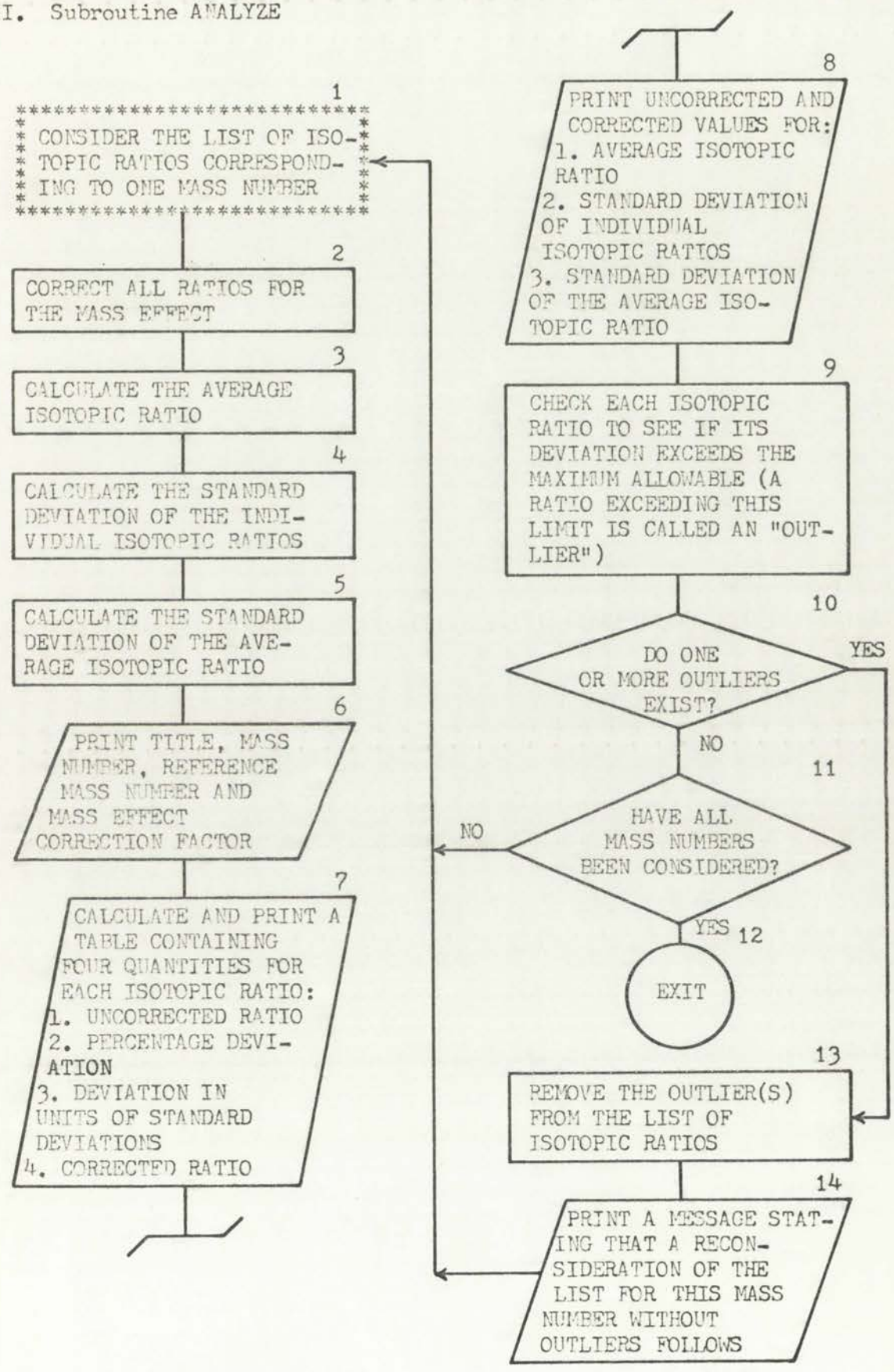
I. The Parent Program:



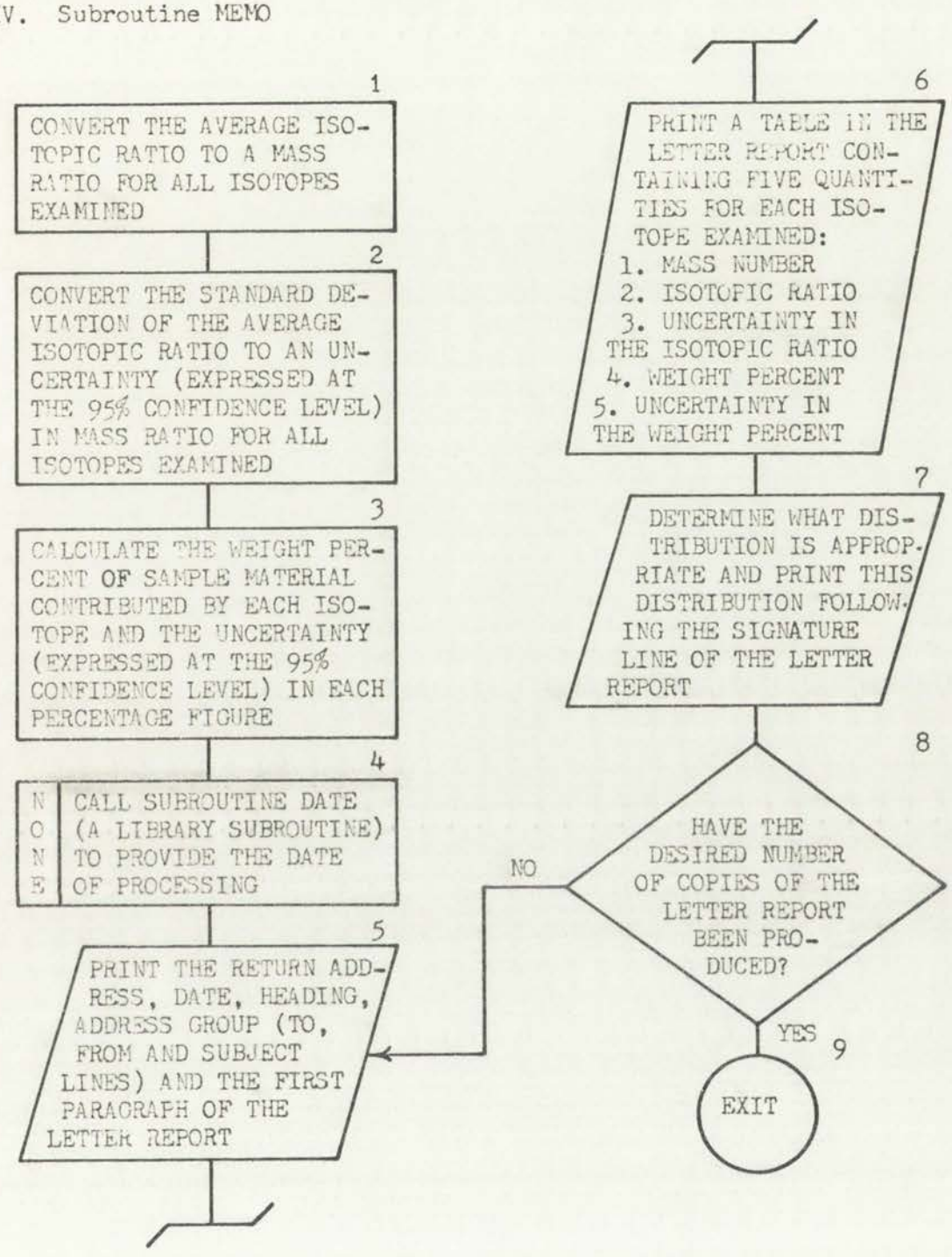
II. Subroutine FITCURV



III. Subroutine ANALYZE



IV. Subroutine MEMO



APPENDIX D

DETAILED FLOWCHART FOR PROGRAM SPECTRE

This flowchart was produced directly from a complete SPECTRE source program by a standard flowcharting code called "AUTOFLOW" (see footnote page 29). Sections are included for subroutines PARCEL and GRAPHIC because they actually form an integral part of program SPECTRE, even though they were not wholly written for this application (PARCEL and GRAPHIC are also included in the complete listing appearing in Appendix E). With exception of subroutines PARCEL and GRAPHIC, every step and symbol of the entire flowchart has been checked for accuracy and proper usage. The flowchart is without a flaw!

Flowcharting is normally accomplished before a program is written as an aid for the coder. Many times, however, flowcharting is performed "after-the-fact" so as to allow a user to understand a program more thoroughly or to enable a program analyst to explain a program to others more efficiently. AUTOFLOW is so good that no-one familiar with its capability would consider flowcharting an already extant program by hand.

It is important to note that a flowchart page number is assigned by the computer and is placed in the upper right-hand corner of each flowchart page. Two physical pages are required to form one flowchart page. The computer assigned numbers are important in that all sequencing and referencing within the flowchart itself is keyed to these numbers. A normal page number appears at the bottom of each physical page.

Confusion should not result as the physical page numbers in this Appendix are all larger than the largest of the flowchart page numbers.

Before the flowchart begins, a section called "Cross-Reference Listing" has been included. This listing gives the flowchart page and symbol or "box" number of all symbols corresponding to statements in the source program having a FORTRAN statement number (label). It also lists, in a column headed "References", all other symbols which transfer to each listed symbol. An example of such a listing is shown in Figure 15 below:

CROSS-REFERENCE LISTING

PAGE BOX	LABEL	REFERENCES		
DECK PARCEL				
SUBROUTINE PARCEL				
7.01	PARCEL	4.25*		
7.14	1			
7.16		7.18		
7.24	2	7.21	9.25	9.27

FIGURE 15. A sample cross-reference listing. This listing describes subroutine PARCEL. Symbol 7.01 is the starting symbol of PARCEL and it is referenced by a call statement in symbol 4.25. The asterisk next to this reference indicates a subroutine call. Statement number 1 has been assigned page-and-symbol number 7.14 and there are no transfers to this symbol. Symbol 7.16 has no statement number, but is referenced by symbol 7.18 (a normal occurance in do loops and logical IF statements). Statement number 2 has been assigned symbol 7.24 and is referenced by symbols 7.21, 9.25 and 9.27.

The parent program and subroutines are each preceded by a table of contents, which lists all FORTRAN statement numbers appearing in the source program in numerical order. The page and box number of the symbol corresponding to each statement number are also listed.

CROSS-REFERENCE LISTING

PAGE BOX	LABEL	REFERENCES	
1.03	5	3.15	
1.06	10		
1.11		1.18	
1.14	80	1.05	
1.16	40		
1.20	50	1.13	
1.22		1.25	
1.23	52		
1.30	55	1.32	
1.34	58	1.28	
1.35		2.05	
1.36		1.38	
1.37	60		
2.04	70		
2.08	200		
2.09	210	3.10	
2.11		2.14	
2.14	220	2.12	
2.17	230	2.11	
2.18	240	2.16	
2.21	250	2.19	3.21
2.24		3.01	
3.01	260	2.24	
3.03	270	2.26	2.27
3.04	300	2.21	
3.05	310	3.06	
3.13	75	3.08	
3.16		3.18	
3.17	320		
3.21	330		

```
     DECK FITCURV
     SUBRCUTINE FITCURV
4.01          FITCURV       3.13*
4.04                        4.06
4.05          10
4.08          20            6.14
4.10                        4.17
4.12          40            4.10
4.13          50
4.14          60            4.12
4.17          80            4.13
4.19          100           4.11
4.22          105           4.23
4.25          120           4.19
4.26          200
4.27          205           4.30      5.09
5.03          220           4.28
5.04                        5.07
5.06          230
5.12          235           4.29
5.13                        5.15
5.14          240
5.19                        5.21
5.20          250
5.23          260           5.02
5.25          300
6.01          306           5.25
6.02          310           6.04
6.07          324
6.08          325           6.10
6.13          328           5.26
6.15          340           6.13


     DECK PARCEL
     SUBRCUTINE PARCEL
7.01          PARCEL        4.25*
```

CROSS-REFERENCE LISTING

PAGE BOX	LABEL	REFERENCES			
7.05	2000	7.06			
7.10	2010	7.11			
7.14	1				
7.16		7.18			
7.17	10				
7.24	2	7.21	9.25	9.27	
7.26		7.33			
7.27		7.29			
7.28	20				
7.32	30				
7.35	3				
7.38		8.17			
8.05	4	8.06			
8.06	60				
8.10		8.15			
8.11	70	8.12			
8.14	80				
8.17	90				
8.20	7				
8.22	11				
8.24	12	9.02			
8.25	13	8.31			
8.28	14				
8.29	15	8.27			
9.01	16				
9.02	140	8.26	8.27	8.28	8.29
9.06	17				
9.08		9.11			
9.10	18	9.08			
9.11	160	9.09			
9.16	19	9.04	9.09	9.13	
9.17	170	9.18			
9.24	21	9.20			
9.27	22	9.24			

```
      DECK GRAPHIC
      SUBRCUTINE GRAPHIC
10.01         GRAPHIC      6.12*
10.04         73
10.05                      10.07
10.06         75
10.10                      10.12
10.11         76
10.17         1            10.26
10.19         2
10.20         3            10.18
10.21         4
10.22         5            10.20
10.23         6
10.24         7            10.22
10.25         8
10.26         9            10.24
10.27         10
10.30                      10.28
10.33                      10.31
10.34         90
10.35         12
10.36         14           10.35
10.37         15           10.34     11.01
10.40         17
10.41         18           10.36     10.39     11.01
10.42         19
10.43         20
11.01         13
11.02         21           10.42
11.03         22           10.41     10.43
11.06         24
11.07         25           10.43     11.02     11.05
11.09                      11.11
```

CROSS-REFERENCE LISTING

PAGE BOX	LABEL	REFERENCES		
11.10	600			
11.14		11.19		
11.15		11.17		
11.16	26			
11.22	30			
11.24		12.17		
12.02	31			
12.03	32			
12.04	33	12.01		
12.05	34			
12.06	35	12.04		
12.08	36			
12.09	37	12.07		
12.10	38	12.03	12.05	12.08
12.11		12.14		
12.13	39			
12.14	40	12.12		
12.17	41	12.02		
13.02		13.05		
13.04	610			
13.05	620	13.03		
13.08	42			
13.09	43	16.28		
13.11		14.21		
13.12	44			
13.14		13.17		
13.17	45			
14.01	47	13.11		
14.03		14.06		
14.06	48			
14.11		14.09		
14.14		14.11		
14.17		14.14		
14.21	50	13.21	14.18	
15.01	51	16.28		
15.04		15.01		

```
15.05          53          13.08     14.23
15.07          54
15.08          55          15.06
15.10          56
15.11          57          15.09
15.13          58
16.01          59          15.12
16.02          60          15.13
16.04          61          16.05
16.09          62
16.10          63          16.08
16.12                      16.26
16.14          65          16.13
16.15          66          16.29
16.16          67          16.18
16.18          68
16.19          69          16.17
16.21                      16.23
16.22          70
16.25          71
16.28          72          16.17
16.29          64
```

```
      DECK ANALYZE
      SUBRCUTINE ANALYZE
17.01          ANALYZE      3.14*
17.04          20          17.07     18.15
17.05          30
17.08          40          17.05
17.09          45          17.10
17.12          50          18.34
17.14          60          17.15
17.19                      17.21
```

CROSS-REFERENCE LISTING

PAGE BOX	LABEL	REFERENCES	
17.20	70		
17.24	72		
18.01	74	17.23	
18.02	80	17.24	
18.07		18.10	
18.08	110		
18.13	220	18.12	18.33
18.15	230	17.06	
18.22	140		
18.23	145	18.30	18.31
18.24	150		
18.26		18.28	
18.27	160		
18.31	170	18.23	
18.34	180		

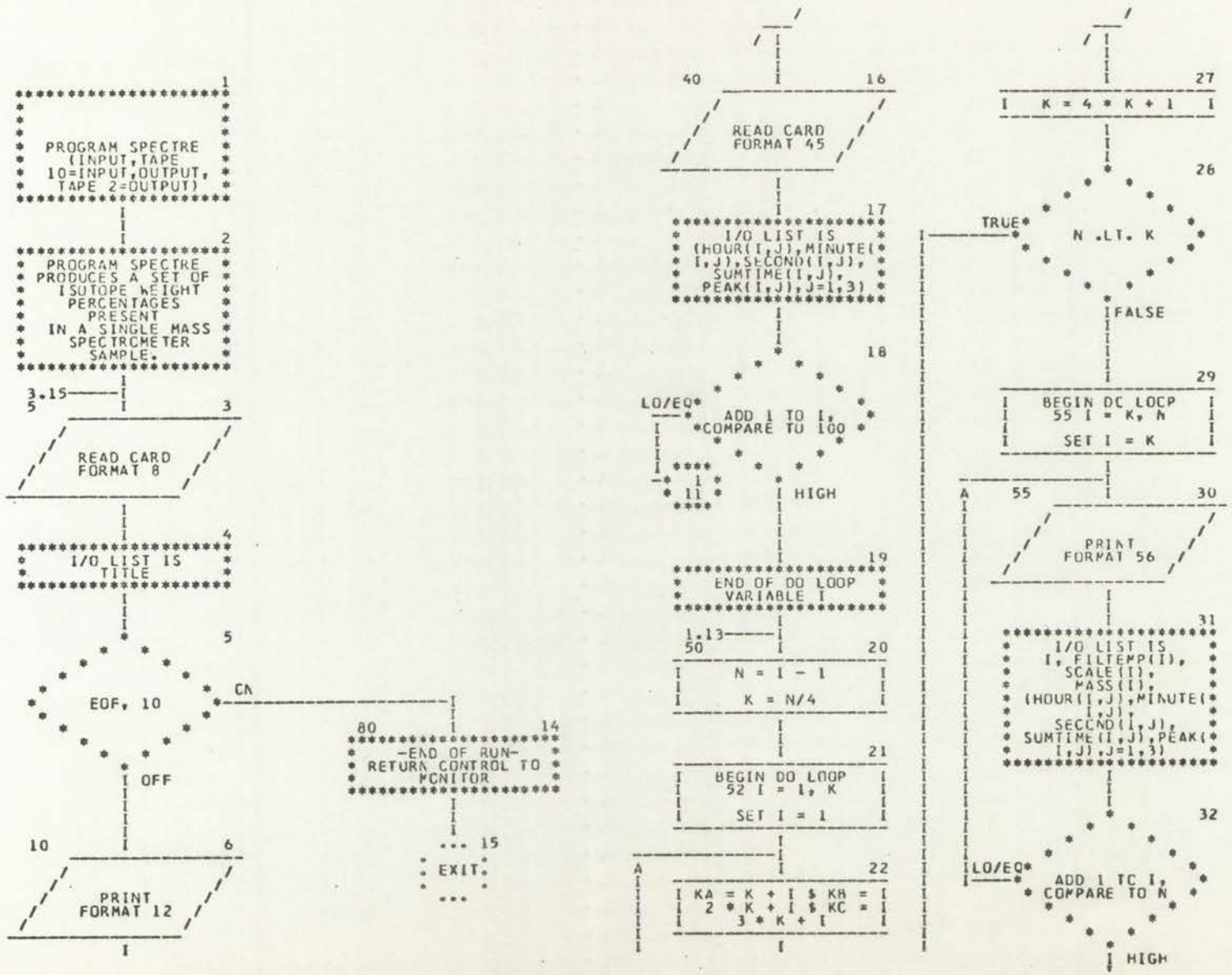
DECK MEMC

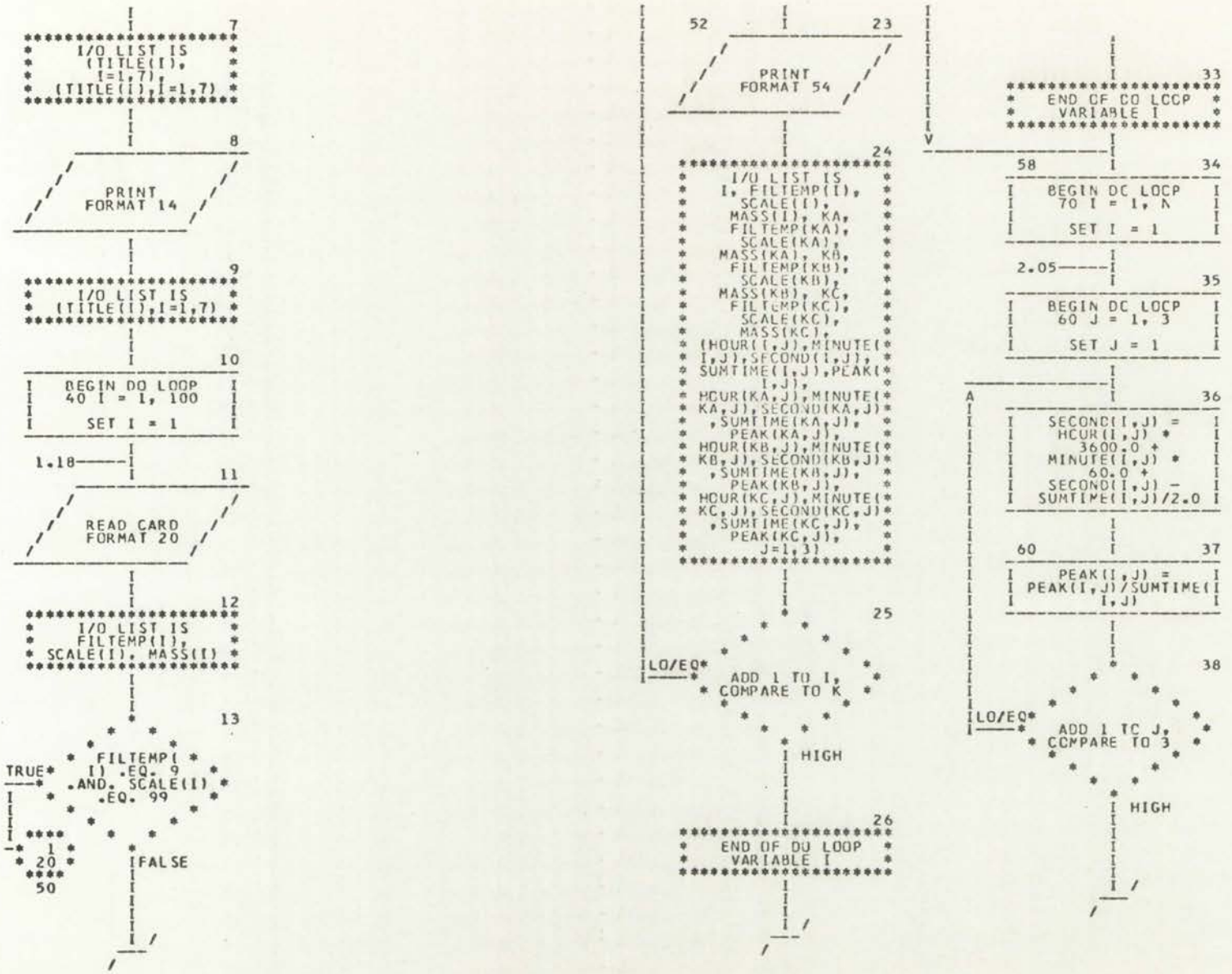
SUBROUTINE MEMO

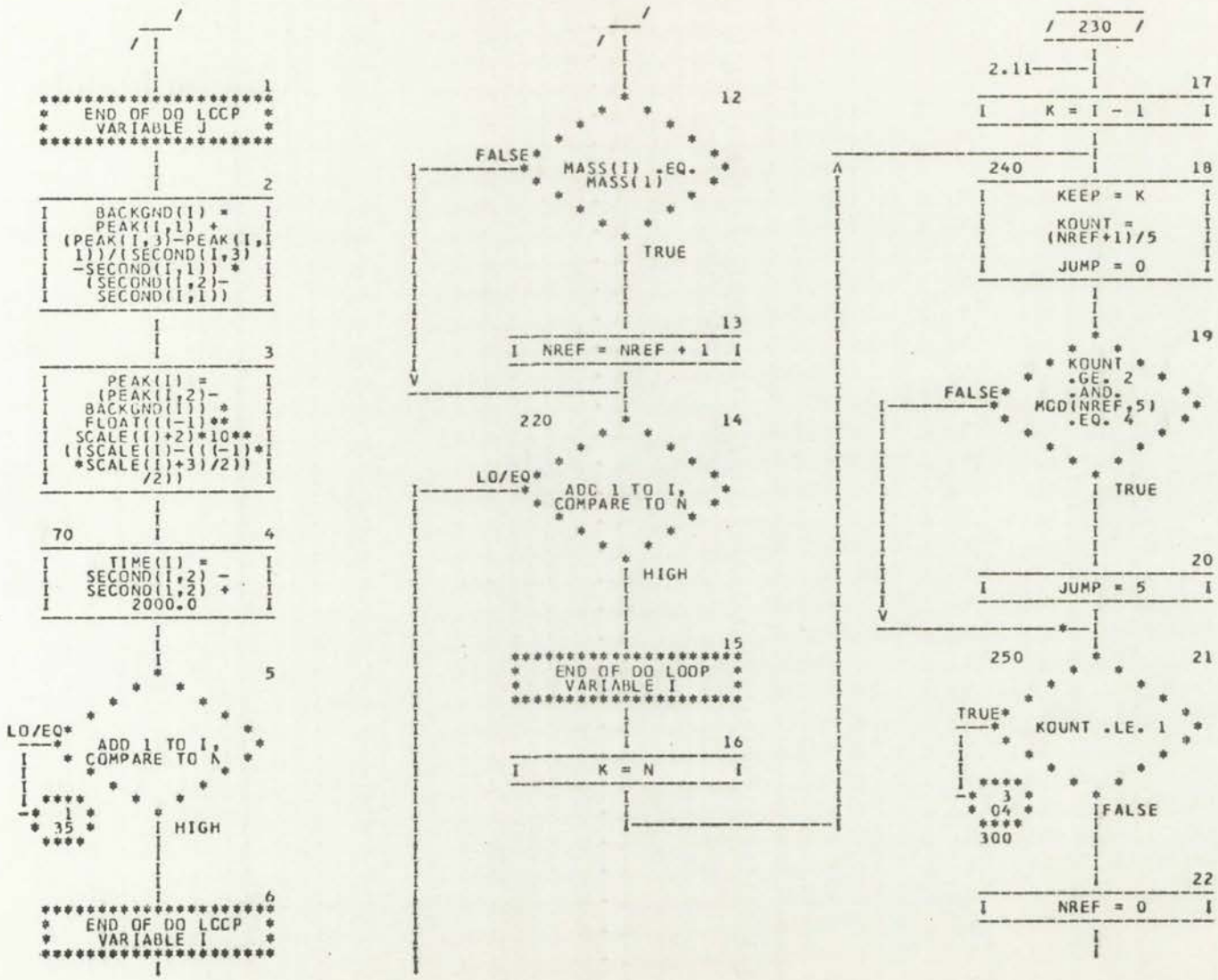
19.01	MEMO	3.15*	
19.04	10	19.06	19.11
19.07	30	19.04	
19.10	40		
19.13	42	19.05	
19.15	45	19.17	20.03
20.01	60	19.15	
20.02	70		
20.05	72	19.16	
20.09	75	20.33	
20.13	160	20.15	20.19
20.16	180	20.13	
20.19	200		
20.21	210	20.14	
20.25	230	20.22	
20.26	250	20.23	

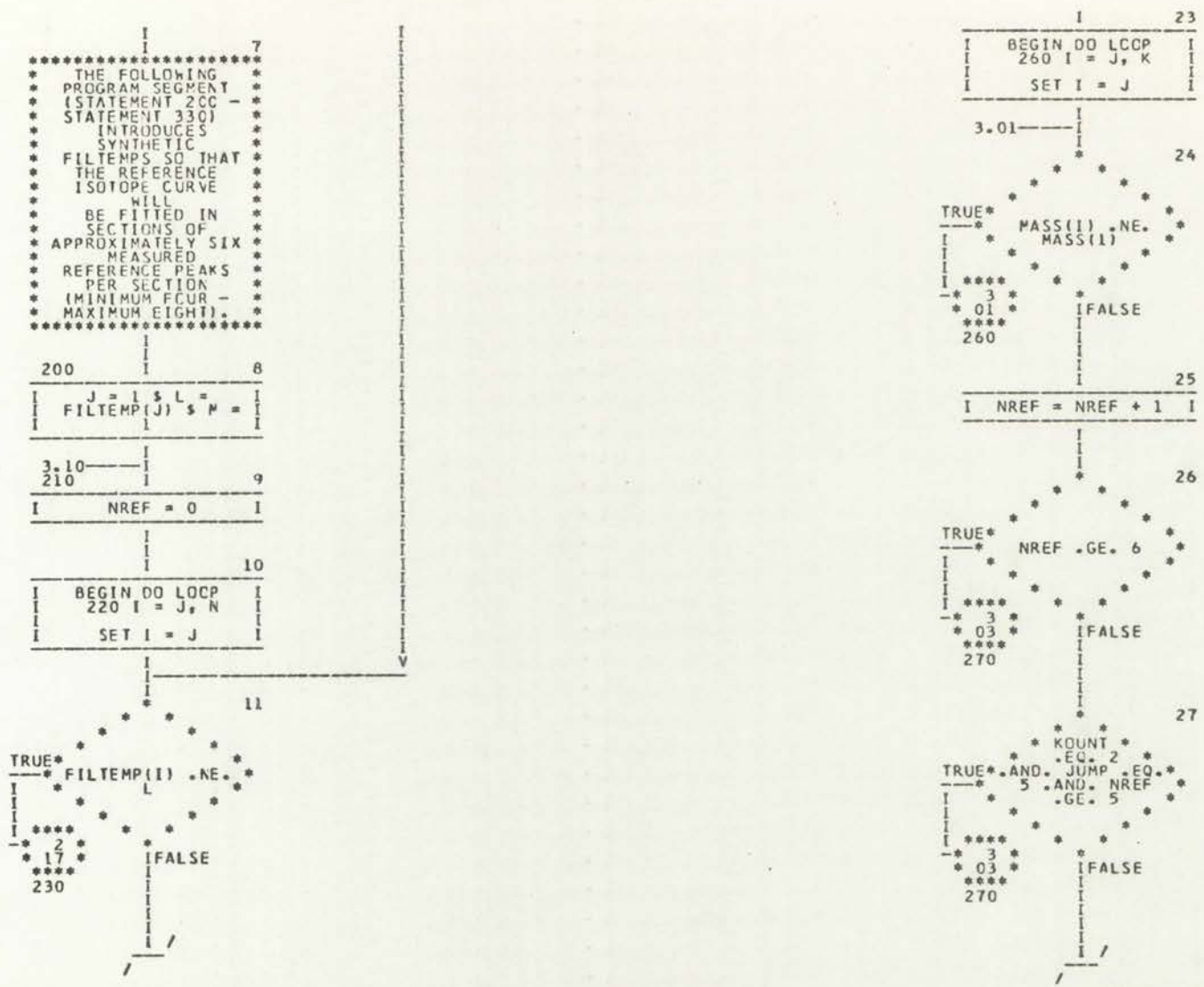
20.29		20.27	
20.31	270	20.24	20.29
20.34	300	20.24	

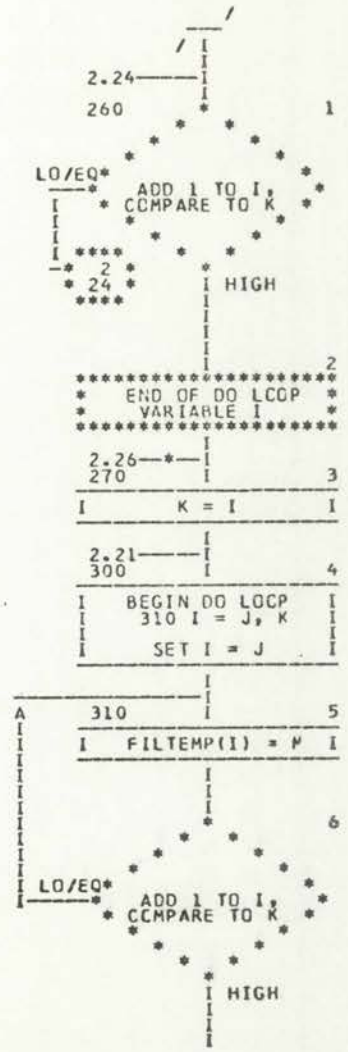
TABLE OF CONTENTS

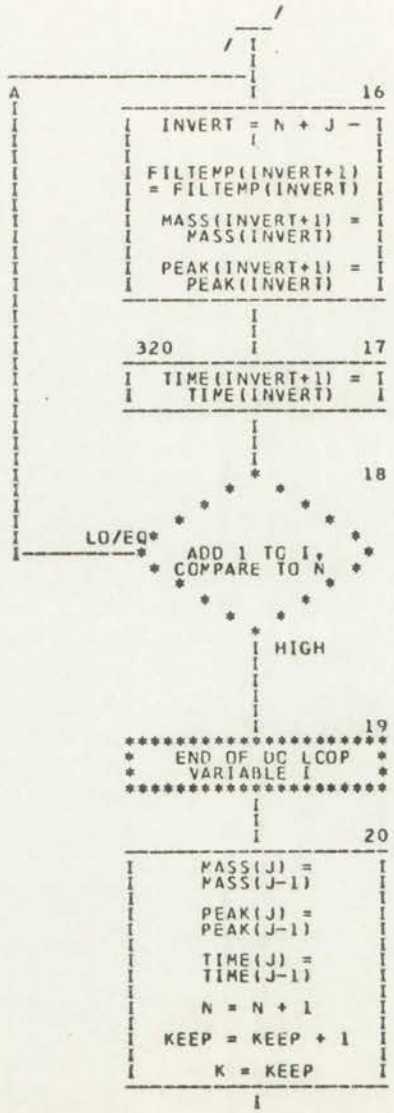

1
PROGRAM SPECTRE (INPUT,TAPE 10=INPUT,OUTPUT, TAPE 2=OUTPUT)
2
PROGRAM SPECTRE PRODUCES A SET OF ISOTOPE WEIGHT PERCENTAGES PRESENT IN A SINGLE MASS SPECTROMETER SAMPLE.
3.15
5
3
READ CARD FORMAT 8
4
I/O LIST IS TITLE
5
EOF, 10
CR
OFF
80
14
-END OF RUN- RETURN CONTROL TO MONITOR
... 15
EXIT.
10
6
PRINT FORMAT 12
40
16
READ CARD FORMAT 45
17
I/O LIST IS (HOUR(I,J),MINUTE(I,J),SECOND(I,J), SUMTIME(I,J), PEAK(I,J),J=1,3)
18
LO/EQ
ADD 1 TO I, COMPARE TO 100
11
HIGH
19
END OF DO LOOP VARIABLE I
1.13
50
20
N = I - 1
K = N/4
21
BEGIN DO LOOP 52 I = 1, K
SET I = 1
A
22
KA = K + I $ KB = 2 * K + I $ KC = 3 * K + I
27
K = 4 * K + 1
26
TRUE
N .LT. K
FALSE
29
BEGIN DO LOOP 55 I = K, N
SET I = K
A
55
30
PRINT FORMAT 56
31
I/O LIST IS I, FILTEMP(I), SCALE(I), MASS(I), (HOUR(I,J),MINUTE(I,J), SECOND(I,J), SUMTIME(I,J),PEAK(I,J),J=1,3)
32
LO/EQ
ADD 1 TO I, COMPARE TO N
HIGH

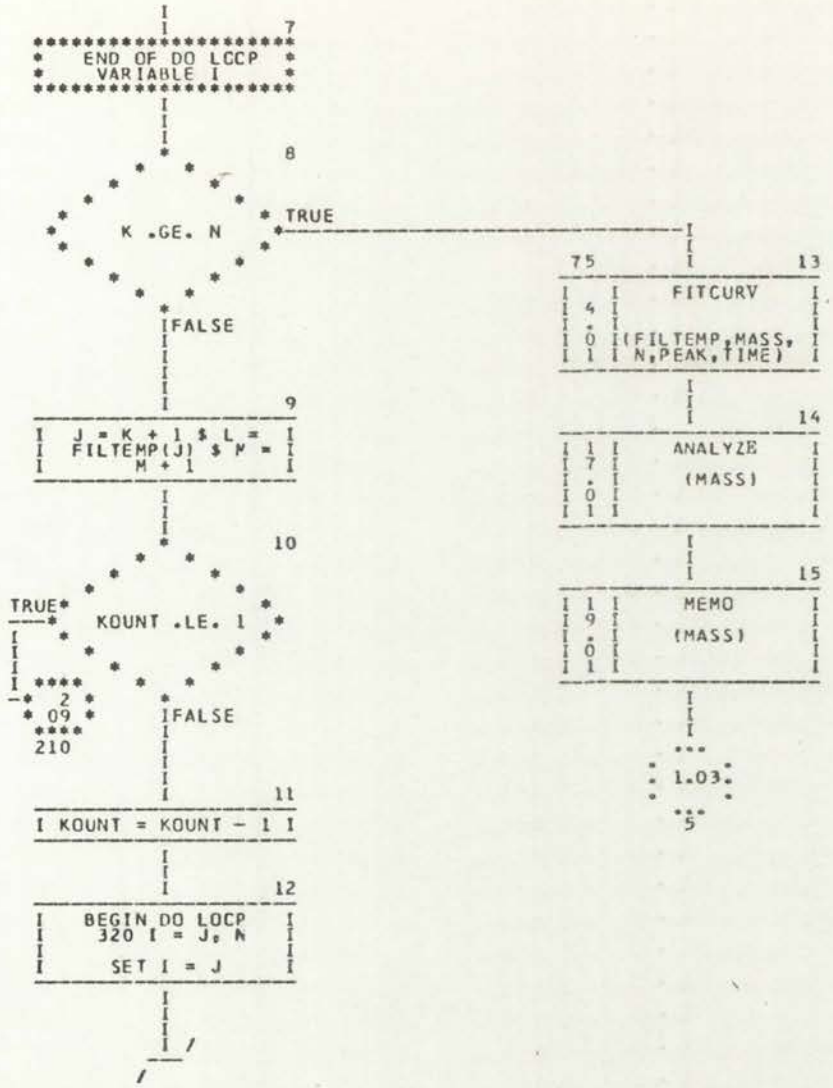

7
I/O LIST IS
(TITLE(I),
I=1,7),
(TITLE(I),I=1,7)
8
PRINT
FORMAT 14
9
I/O LIST IS
(TITLE(I),I=1,7)
10
BEGIN DO LOOP
40 I = 1, 100
SET I = 1
1.18
11
READ CARD
FORMAT 20
12
I/O LIST IS
FILTEMP(I),
SCALE(I), MASS(I)
13
FILTEMP(
I) .EQ. 9
.AND. SCALE(I)
.EQ. 99
TRUE
FALSE
1
20
50
52
23
PRINT
FORMAT 54
24
I/O LIST IS
I, FILTEMP(I),
SCALE(I),
MASS(I), KA,
FILTEMP(KA),
SCALE(KA),
MASS(KA), KB,
FILTEMP(KB),
SCALE(KB),
MASS(KB), KC,
FILTEMP(KC),
SCALE(KC),
MASS(KC),
(HOUR(I,J),MINUTE(
I,J),SECOND(I,J),
SUMTIME(I,J),PEAK(
I,J),
HOUR(KA,J),MINUTE(
KA,J),SECOND(KA,J)
,SUMTIME(KA,J),
PEAK(KA,J),
HOUR(KB,J),MINUTE(
KB,J),SECOND(KB,J)
,SUMTIME(KB,J),
PEAK(KB,J),
HOUR(KC,J),MINUTE(
KC,J),SECOND(KC,J)
,SUMTIME(KC,J),
PEAK(KC,J),
J=1,3)
25
LO/EQ
ADD 1 TO I,
COMPARE TO K
HIGH
26
END OF DO LOOP
VARIABLE I
33
END OF DO LOOP
VARIABLE I
58
34
BEGIN DO LOOP
70 I = 1, N
SET I = 1
2.05
35
BEGIN DO LOOP
60 J = 1, 3
SET J = 1
A
36
SECOND(I,J) =
HOUR(I,J) *
3600.0 +
MINUTE(I,J) *
60.0 +
SECOND(I,J) -
SUMTIME(I,J)/2.0
60
37
PEAK(I,J) =
PEAK(I,J)/SUMTIME(I
I,J)
38
LO/EQ
ADD 1 TO J,
COMPARE TO 3
HIGH


END OF DO LOOP VARIABLE J
BACKGND(I) = PEAK(I,1) + (PEAK(I,3)-PEAK(I,1))/(SECOND(I,3)-SECOND(I,1)) * (SECOND(I,2)-SECOND(I,1))
PEAK(I) = (PEAK(I,2)-BACKGND(I)) * FLOAT((-1)** (SCALE(I)+2)*10** ((SCALE(I)-(((-1)*SCALE(I)+3)/2))/2))
TIME(I) = SECOND(I,2) - SECOND(1,2) + 2000.0
LO/EQ
ADD 1 TO I, COMPARE TO N
HIGH
1
35
END OF DO LOOP VARIABLE I
MASS(I) .EQ. MASS(1)
FALSE
TRUE
NREF = NREF + 1
220
ADD 1 TO I, COMPARE TO N
END OF DO LOOP VARIABLE I
K = N
2.11
230
K = I - 1
240
KEEP = K
KOUNT = (NREF+1)/5
JUMP = 0
KOUNT .GE. 2 .AND. MOD(NREF,5) .EQ. 4
JUMP = 5
250
KOUNT .LE. 1
3
04
300
NREF = 0


7
THE FOLLOWING PROGRAM SEGMENT (STATEMENT 200 - STATEMENT 330) INTRODUCES SYNTHETIC FILTEMPS SO THAT THE REFERENCE ISOTOPE CURVE WILL BE FITTED IN SECTIONS OF APPROXIMATELY SIX MEASURED REFERENCE PEAKS PER SECTION (MINIMUM FOUR - MAXIMUM EIGHT).
200
8
J = 1 $ L =
FILTEMP(J) $ M =
L
3.10
210
9
NREF = 0
10
BEGIN DO LOOP
220 I = J, N
SET I = J
11
TRUE
FILTEMP(I) .NE.
L
2
17
230
FALSE
23
BEGIN DO LOOP
260 I = J, K
SET I = J
3.01
24
TRUE
MASS(I) .NE.
MASS(1)
3
01
260
FALSE
25
NREF = NREF + 1
26
TRUE
NREF .GE. 6
3
03
270
FALSE
27
KOUNT
.EQ. 2
TRUE
.AND. JUMP .EQ.
5 .AND. NREF
.GE. 5
3
03
270
FALSE


2.24
260
1
LO/EQ
ADD 1 TO I,
COMPARE TO K
2
24
HIGH
2
END OF DO LOOP
VARIABLE I
2.26
270
3
K = I
2.21
300
4
BEGIN DO LOOP
310 I = J, K
SET I = J
A
310
5
FILTEMP(I) = M
6
LO/EQ
ADD 1 TO I,
COMPARE TO K
HIGH


A
16
INVERT = N + J -
FILTEMP(INVERT+1)
= FILTEMP(INVERT)
MASS(INVERT+1) =
MASS(INVERT)
PEAK(INVERT+1) =
PEAK(INVERT)
320
17
TIME(INVERT+1) =
TIME(INVERT)
18
LO/EQ
ADD 1 TO I,
COMPARE TO N
HIGH
19
END OF DO LOOP
VARIABLE I
20
MASS(J) =
MASS(J-1)
PEAK(J) =
PEAK(J-1)
TIME(J) =
TIME(J-1)
N = N + 1
KEEP = KEEP + 1
K = KEEP


7
END OF DO LOOP
VARIABLE I
8
K .GE. N
TRUE
FALSE
9
J = K + 1 $ L =
FILTEMP(J) $ M =
M + 1
10
KOUNT .LE. 1
TRUE
2
09
210
FALSE
11
KOUNT = KOUNT - 1
12
BEGIN DO LOOP
320 I = J, N
SET I = J
75
13
FITCURV
(FILTEMP,MASS,
N,PEAK,TIME)
14
ANALYZE
(MASS)
15
MEMO
(MASS)
1.03
5
330
21
2.21
250

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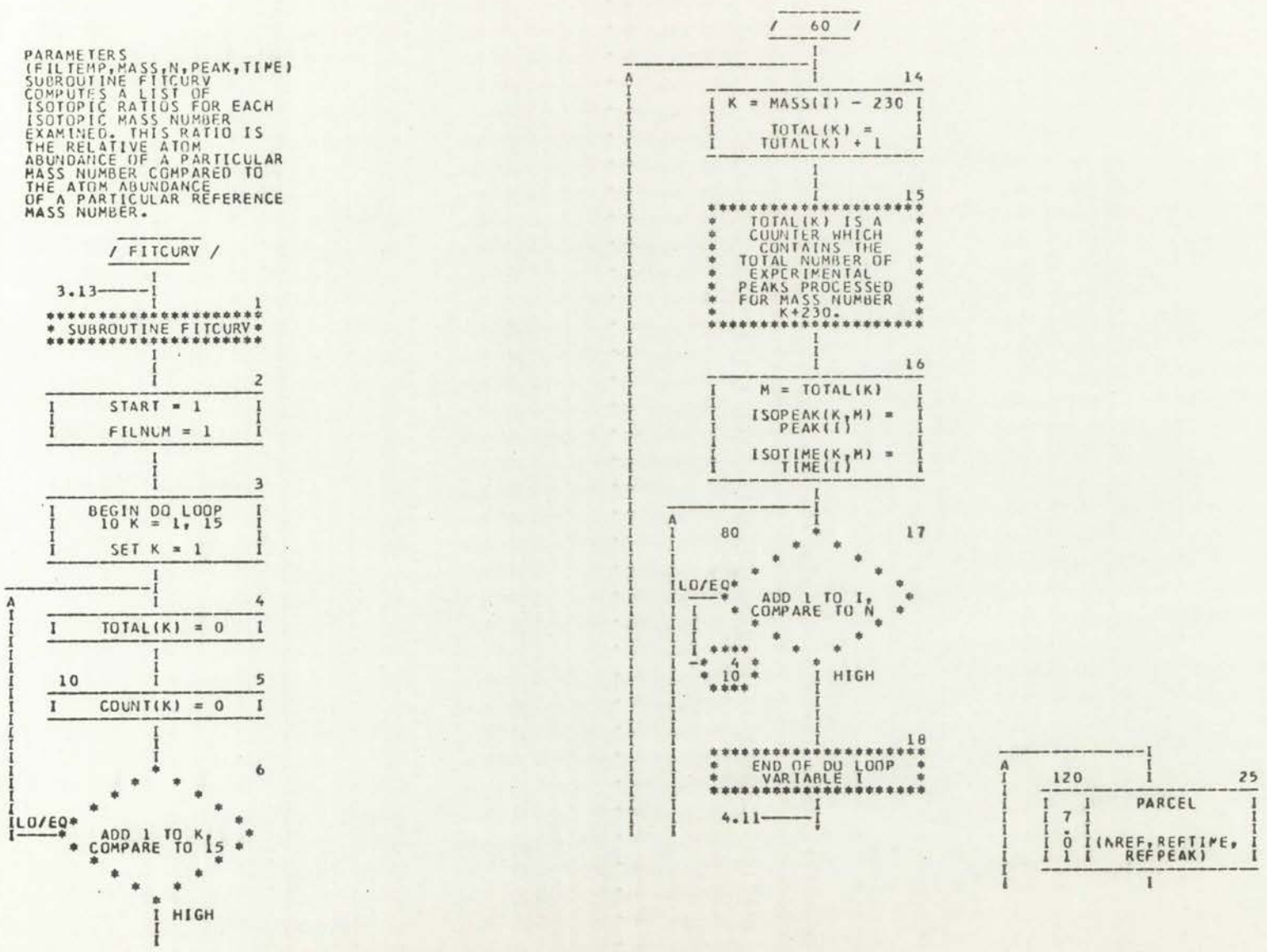
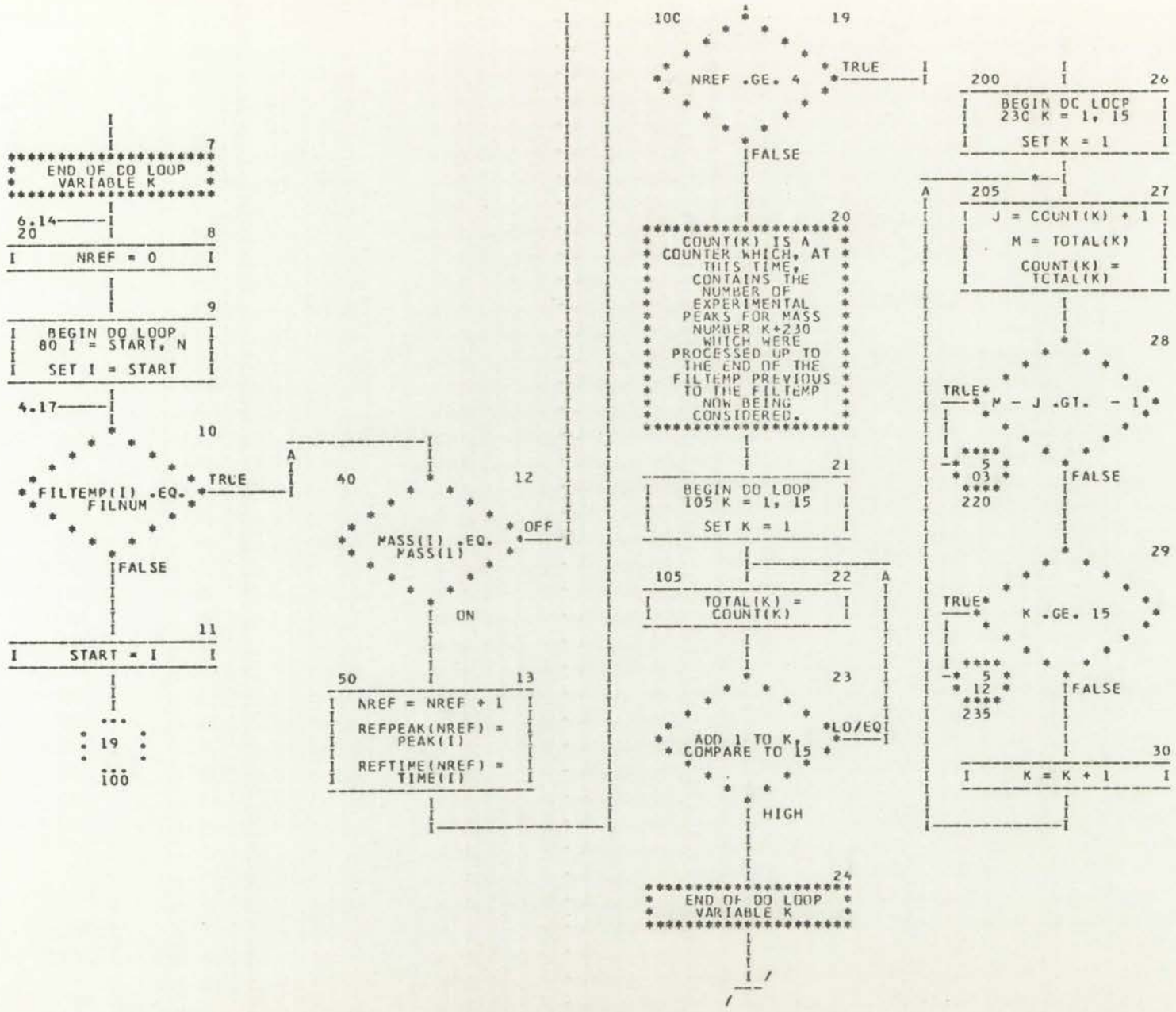
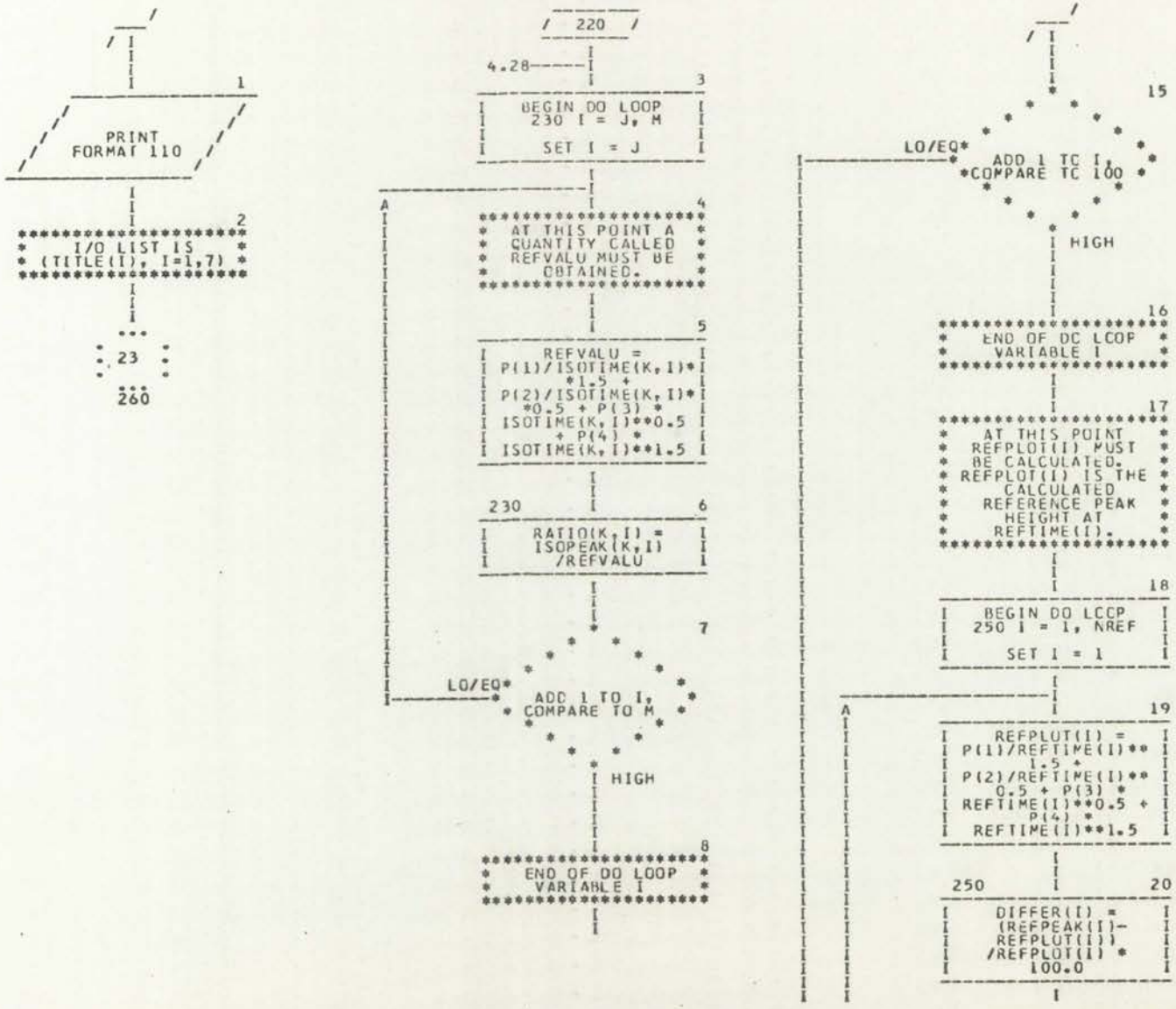
SUBROUTINE FITCURV

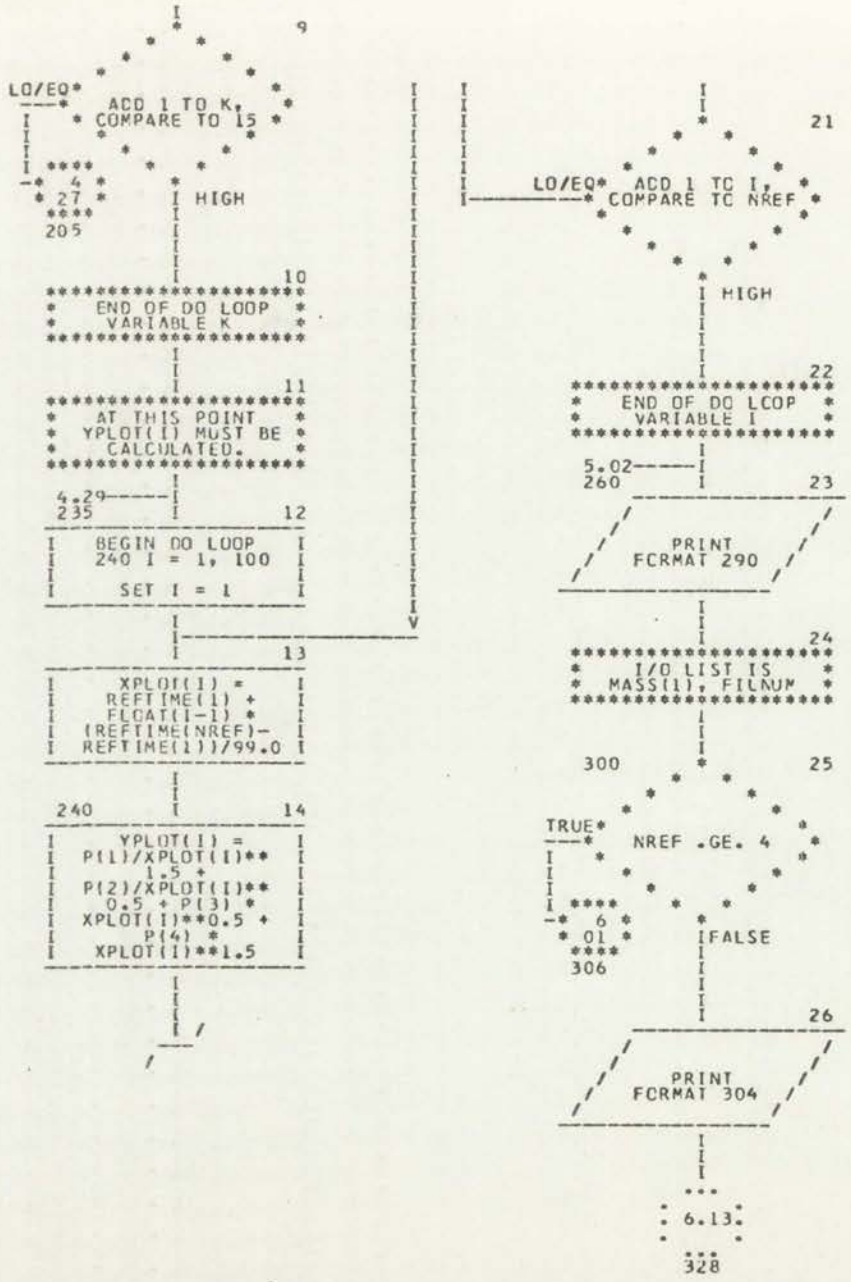
PARAMETERS
(FILTEMP,MASS,N,PEAK,TIME)
SUBROUTINE FITCURV
COMPUTES A LIST OF
ISOTOPIC RATIOS FOR EACH
ISOTOPIC MASS NUMBER
EXAMINED. THIS RATIO IS
THE RELATIVE ATOM
ABUNDANCE OF A PARTICULAR
MASS NUMBER COMPARED TO
THE ATOM ABUNDANCE
OF A PARTICULAR REFERENCE
MASS NUMBER.



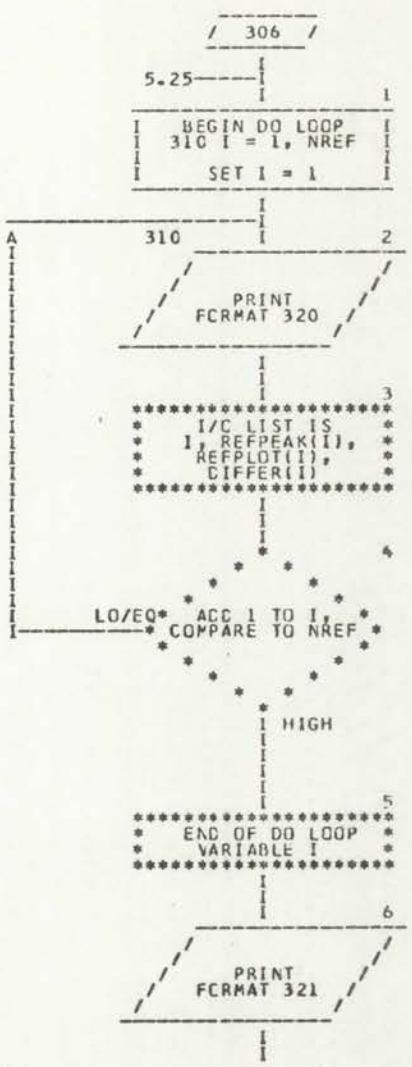

END OF DO LOOP VARIABLE K
7
6.14
20
8
NREF = 0
9
BEGIN DO LOOP
80 I = START, N
SET I = START
4.17
10
FILTEMP(I) .EQ. FILNUM
TRUE
FALSE
11
START = I
19
100
A
40
12
MASS(I) .EQ. MASS(1)
OFF
ON
50
13
NREF = NREF + 1
REFPEAK(NREF) = PEAK(I)
REFTIME(NREF) = TIME(I)
10C
19
NREF .GE. 4
TRUE
FALSE
20
COUNT(K) IS A COUNTER WHICH, AT THIS TIME, CONTAINS THE NUMBER OF EXPERIMENTAL PEAKS FOR MASS NUMBER K+230 WHICH WERE PROCESSED UP TO THE END OF THE FILTEMP PREVIOUS TO THE FILTEMP NOW BEING CONSIDERED.
21
BEGIN DO LOOP
105 K = 1, 15
SET K = 1
105
22
A
TOTAL(K) = COUNT(K)
23
ADD 1 TO K, COMPARE TO 15
LO/EQ
HIGH
24
END OF DO LOOP
VARIABLE K
200
26
BEGIN DO LOOP
230 K = 1, 15
SET K = 1
A
205
27
J = COUNT(K) + 1
M = TOTAL(K)
COUNT(K) = TOTAL(K)
28
TRUE
M - J .GT. - 1
5
03
220
FALSE
29
TRUE
K .GE. 15
5
12
235
FALSE
30
K = K + 1

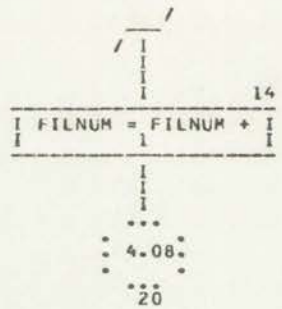
SUBROUTINE FITCURV

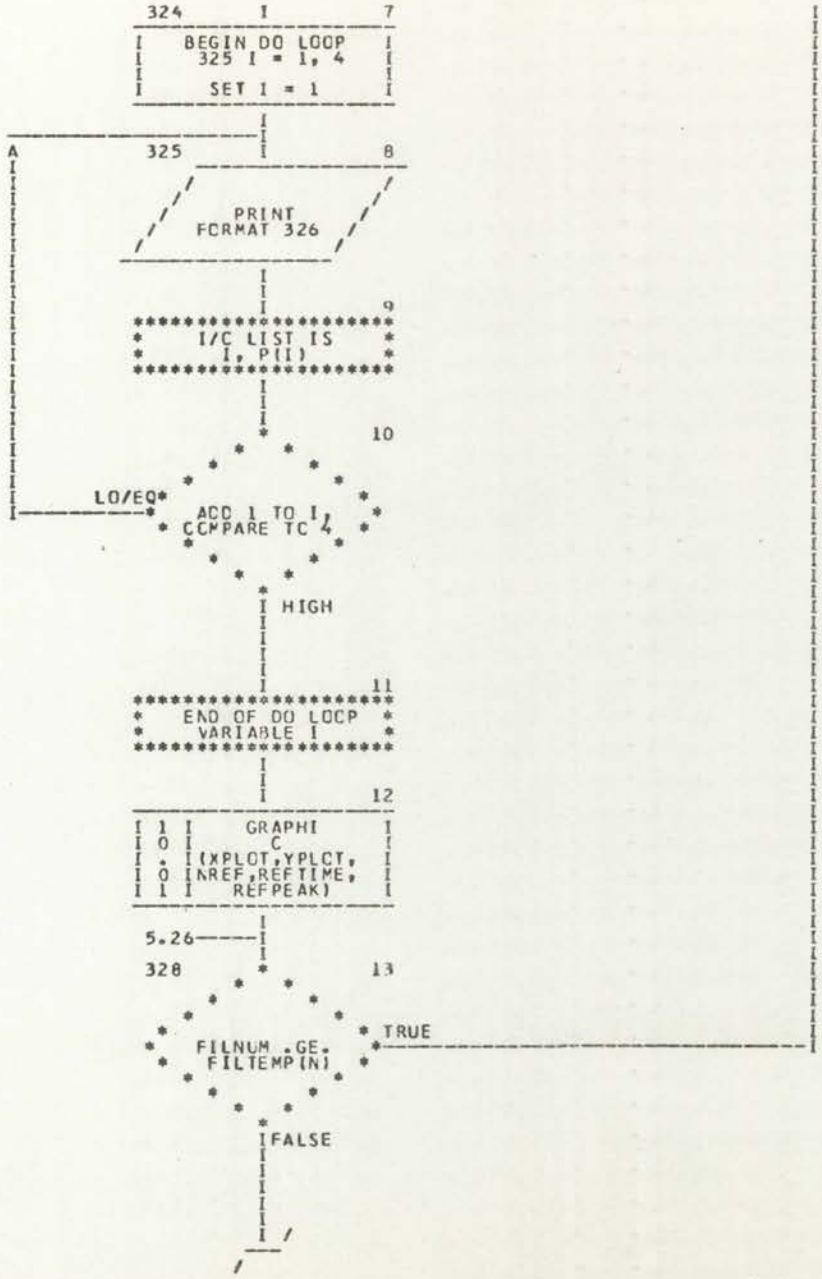



9
LO/EQ*
ADD 1 TO K,
COMPARE TO 15
4
27
205
HIGH
10
END OF DO LOOP
VARIABLE K
11
AT THIS POINT
YPLOT(I) MUST BE
CALCULATED.
4.29
235
12
BEGIN DO LOOP
240 I = 1, 100
SET I = 1
13
XPLOT(I) =
REFTIME(1) +
FLOAT(I-1) *
(REFTIME(NREF)-
REFTIME(1))/99.0
240
14
YPLOT(I) =
P(1)/XPLOT(I)**
1.5 +
P(2)/XPLOT(I)**
0.5 + P(3) *
XPLOT(I)**0.5 +
P(4) *
XPLOT(I)**1.5
21
LO/EQ*
ADD 1 TO I,
COMPARE TO NREF
HIGH
22
END OF DO LOOP
VARIABLE I
5.02
260
23
PRINT
FORMAT 290
24
I/O LIST IS
MASS(1), FILNUM
300
25
TRUE*
NREF .GE. 4
6
01
306
FALSE
26
PRINT
FORMAT 304
6.13
328

SUBROUTINE FITCURV






324
I
7
BEGIN DO LOOP
325 I = 1, 4
SET I = 1
A
325
I
8
PRINT
FORMAT 326
9
I/C LIST IS
I, P(I)
10
LO/EQ
ADD 1 TO I,
COMPARE TO 4
HIGH
11
END OF DO LOOP
VARIABLE I
12
GRAPHI
C
(XPLOT,YPLOT,
NREF,REFTIME,
REFPEAK)
5.26
328
13
TRUE
FILNUM .GE.
FILTEMP(N)
FALSE

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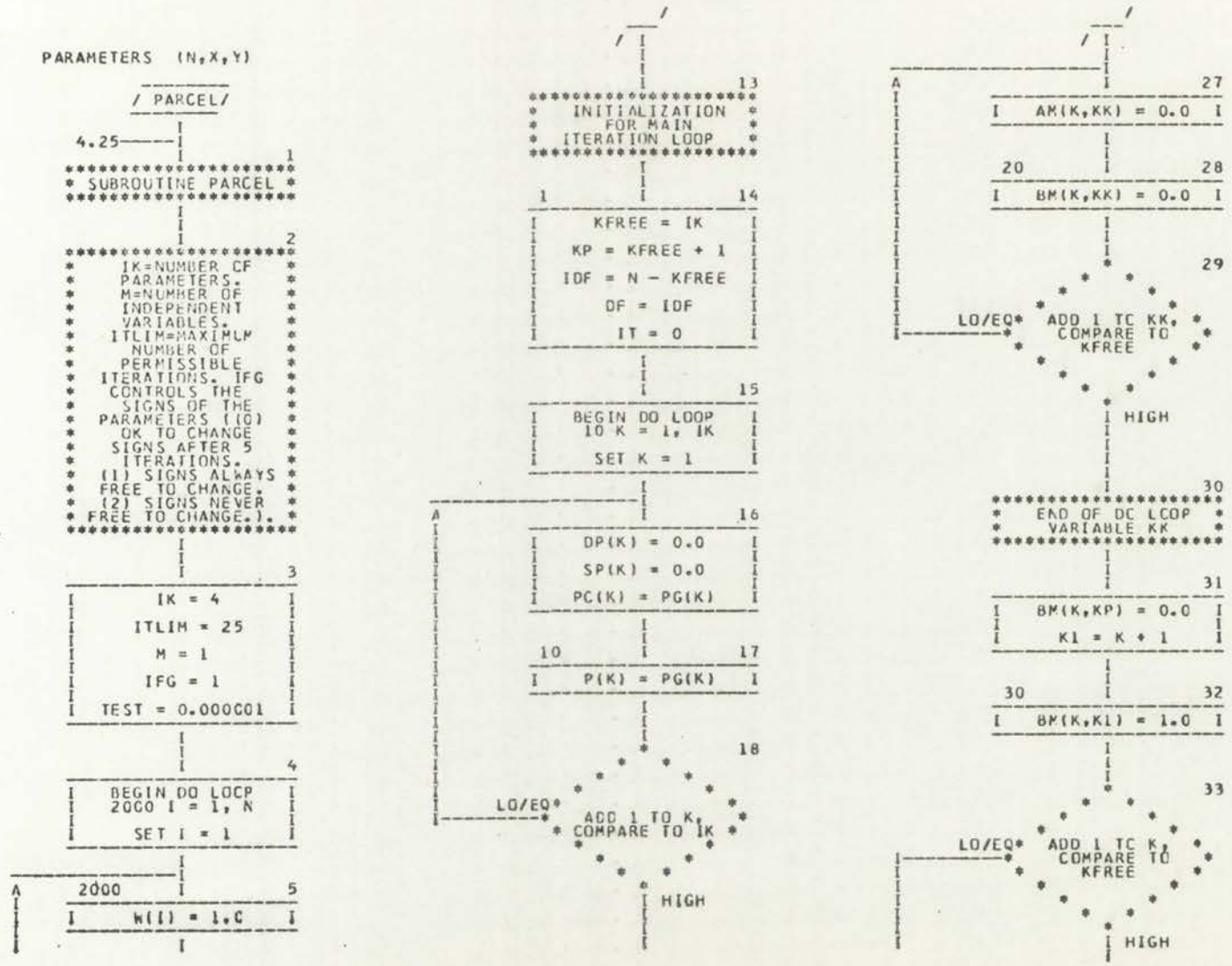
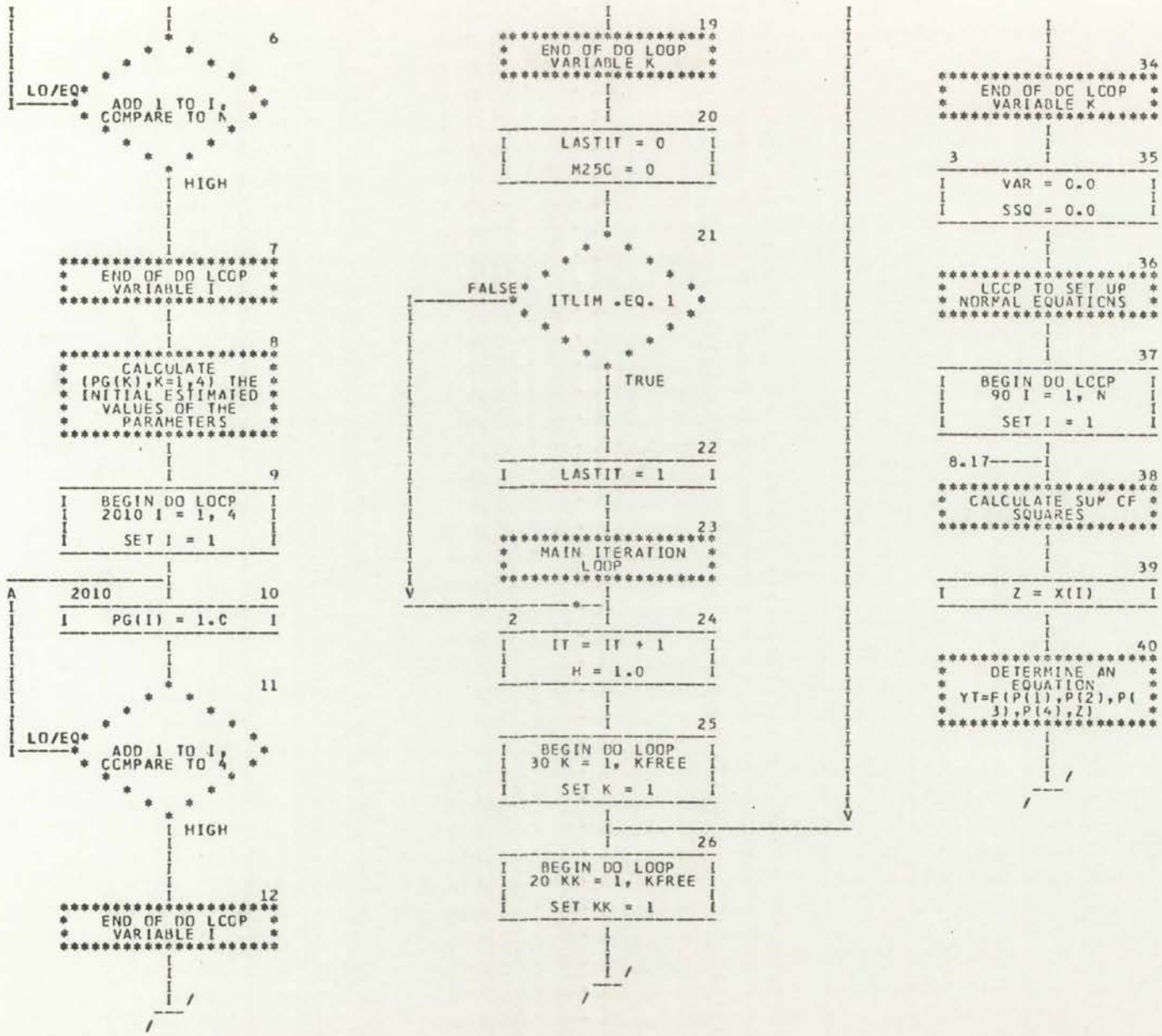
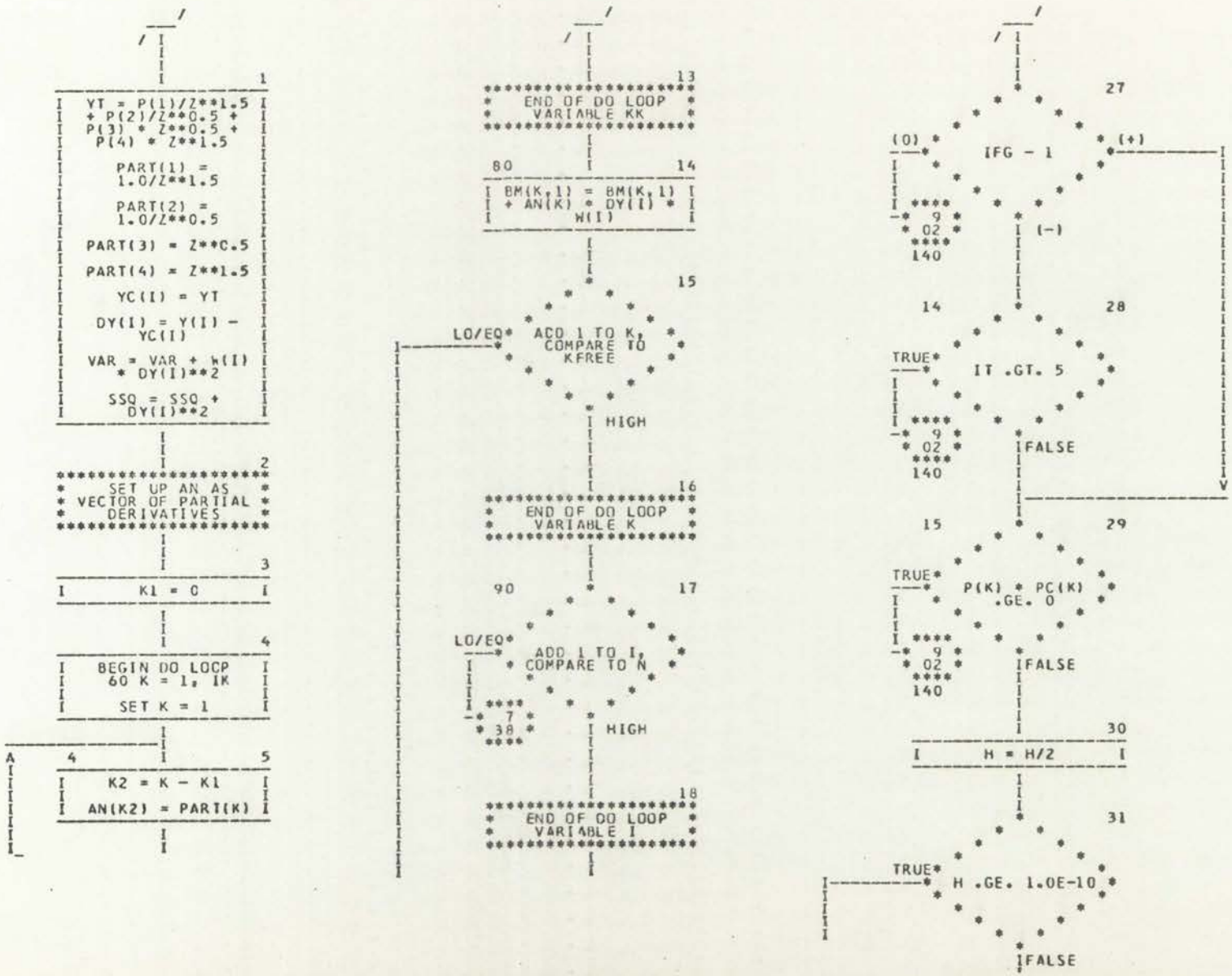
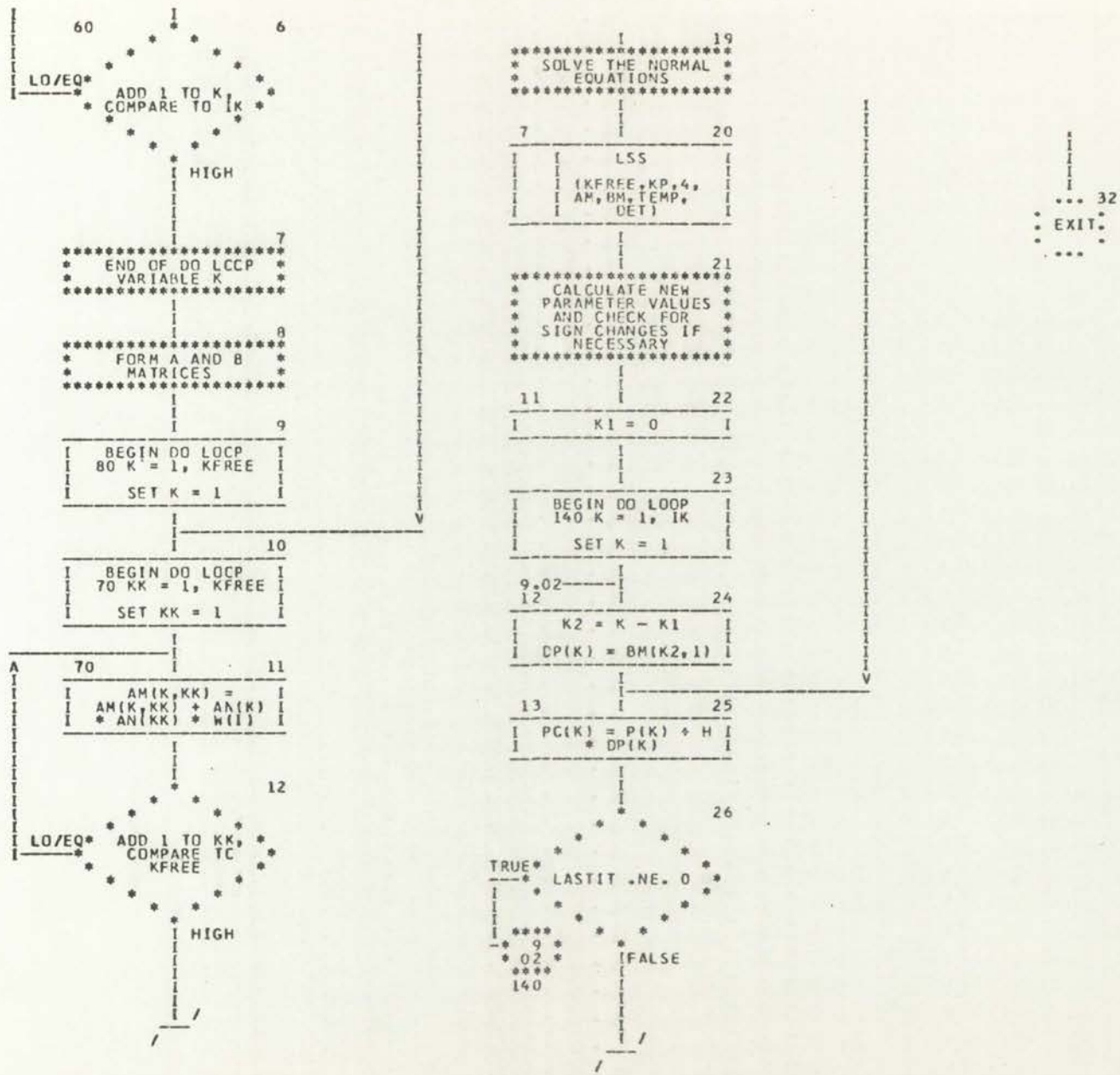
SUBROUTINE PARCEL



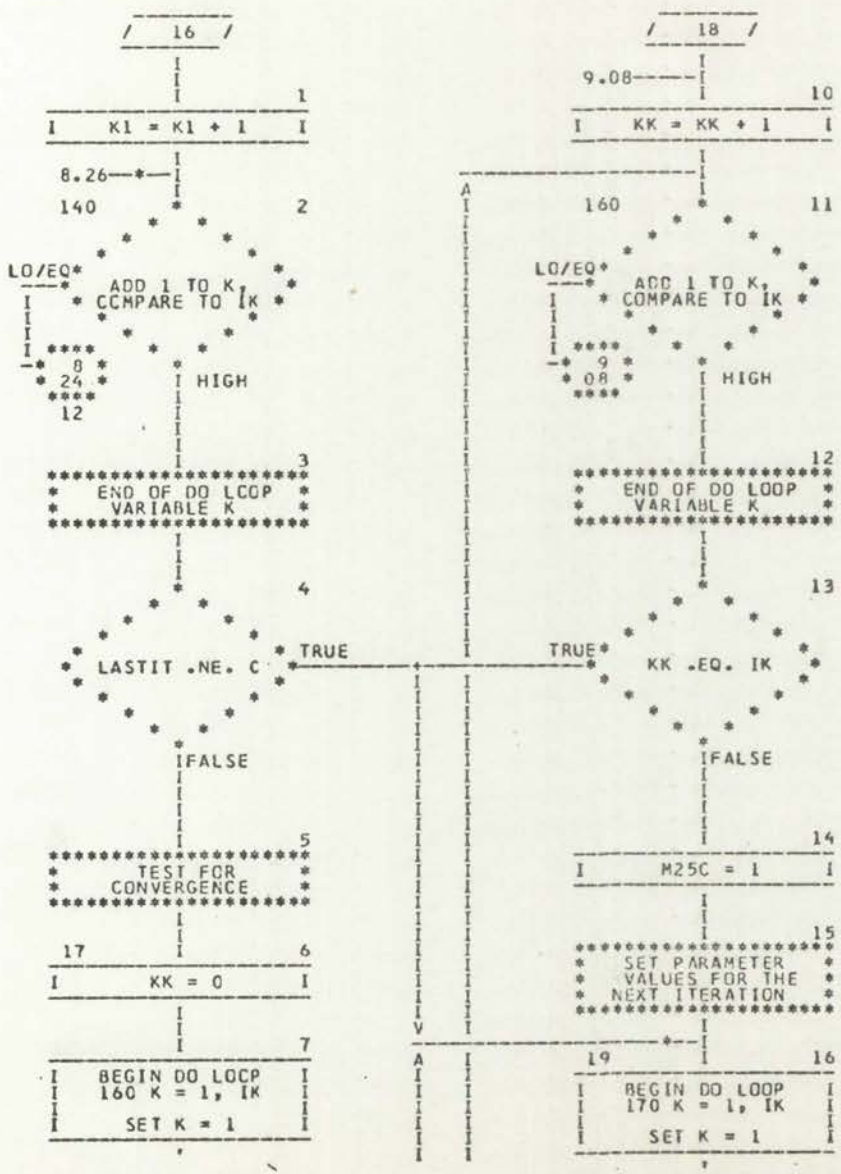

6
LO/EQ*
ADD 1 TO I,
COMPARE TO N
HIGH
7
END OF DO LOOP
VARIABLE I
8
CALCULATE
(PG(K),K=1,4) THE
INITIAL ESTIMATED
VALUES OF THE
PARAMETERS
9
BEGIN DO LOOP
2010 I = 1, 4
SET I = 1
A
2010
10
PG(I) = 1.C
11
LO/EQ*
ADD 1 TO I,
COMPARE TO 4
HIGH
12
END OF DO LOOP
VARIABLE I
19
END OF DO LOOP
VARIABLE K
20
LASTIT = 0
M25C = 0
21
FALSE*
ITLIM .EQ. 1
TRUE
22
LASTIT = 1
23
MAIN ITERATION
LOOP
V
2
24
IT = IT + 1
H = 1.0
25
BEGIN DO LOOP
30 K = 1, KFREE
SET K = 1
26
BEGIN DO LOOP
20 KK = 1, KFREE
SET KK = 1
34
END OF DC LOOP
VARIABLE K
3
35
VAR = 0.0
SSQ = 0.0
36
LOOP TO SET UP
NORMAL EQUATIONS
37
BEGIN DO LOOP
90 I = 1, N
SET I = 1
8.17
38
CALCULATE SUM OF
SQUARES
39
Z = X(I)
40
DETERMINE AN
EQUATION
YT=F(P(1),P(2),P(
3),P(4),Z)

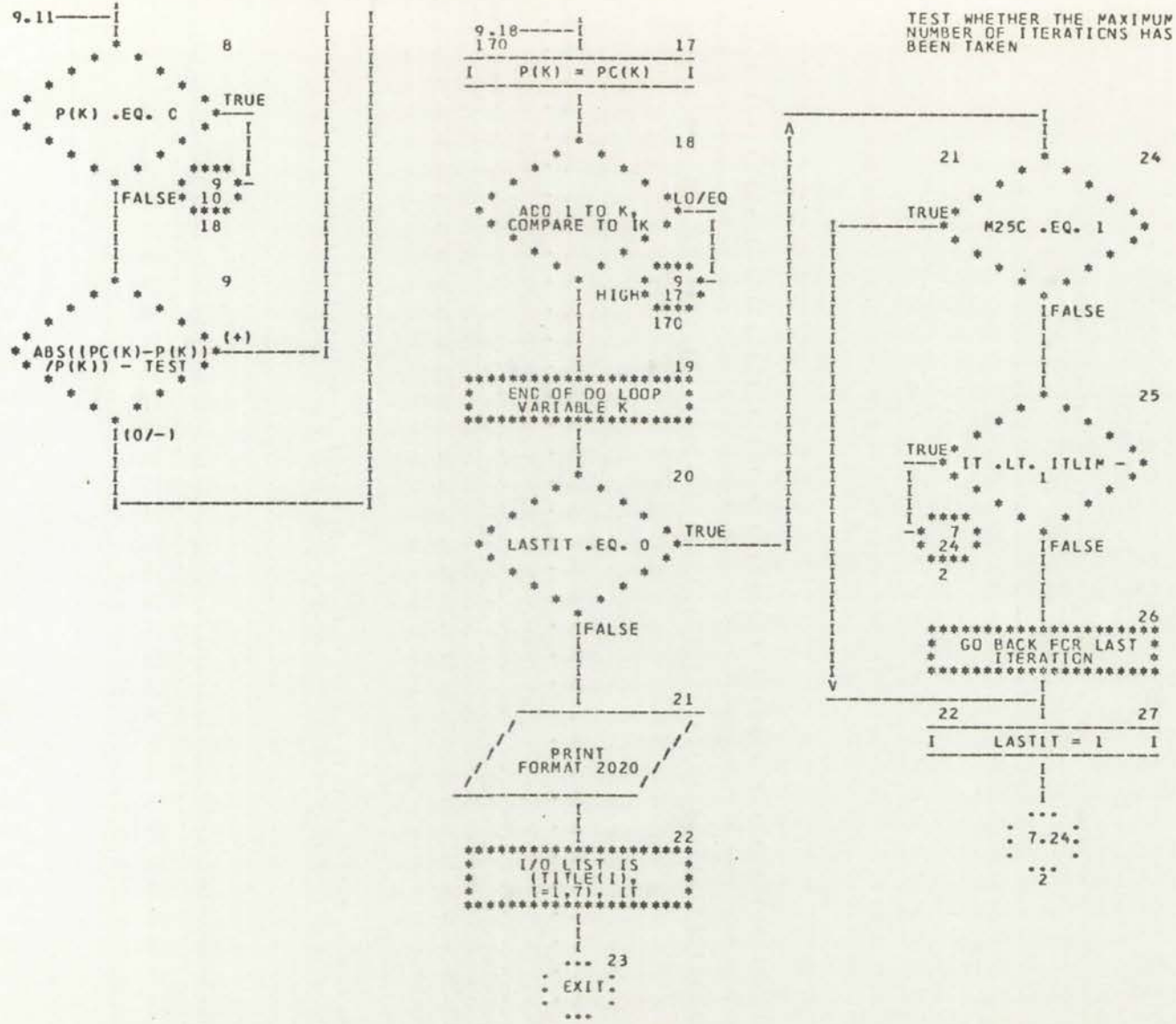
SUBROUTINE PARCEL




60
6
LO/EQ
ADD 1 TO K,
COMPARE TO IK
HIGH
7
END OF DO LOOP
VARIABLE K
8
FORM A AND B
MATRICES
9
BEGIN DO LOOP
80 K = 1, KFREE
SET K = 1
10
BEGIN DO LOOP
70 KK = 1, KFREE
SET KK = 1
A
70
11
AM(K,KK) =
AM(K,KK) + AN(K)
* AN(KK) * W(I)
12
LO/EQ
ADD 1 TO KK,
COMPARE TO
KFREE
HIGH
19
SOLVE THE NORMAL
EQUATIONS
7
20
LSS
(KFREE,KP,4,
AM,BM,TEMP,
DET)
21
CALCULATE NEW
PARAMETER VALUES
AND CHECK FOR
SIGN CHANGES IF
NECESSARY
11
22
K1 = 0
23
BEGIN DO LOOP
140 K = 1, IK
SET K = 1
9.02
12
24
K2 = K - K1
DP(K) = BM(K2,1)
13
25
PC(K) = P(K) + H
* DP(K)
26
TRUE
LASTIT .NE. 0
9
02
140
FALSE
32
EXIT

SUBROUTINE PARCEL




9.11
8
P(K) .EQ. C
TRUE
FALSE
10
9
(+)
ABS((PC(K)-P(K))/P(K)) - TEST
(0/-)
9.18
170
17
P(K) = PC(K)
18
ADD 1 TO K, COMPARE TO IK
LO/EQ
HIGH
17
170
19
END OF DO LOOP VARIABLE K
20
LASTIT .EQ. 0
TRUE
FALSE
21
PRINT FORMAT 2020
22
I/O LIST IS (TITLE(I), I=1,7), IT
23
EXIT
TEST WHETHER THE MAXIMUM NUMBER OF ITERATIONS HAS BEEN TAKEN
21
24
M25C .EQ. 1
TRUE
FALSE
25
IT .LT. ITLIM - 1
TRUE
7
24
2
FALSE
26
GO BACK FOR LAST ITERATION
22
27
LASTIT = 1
7.24
2

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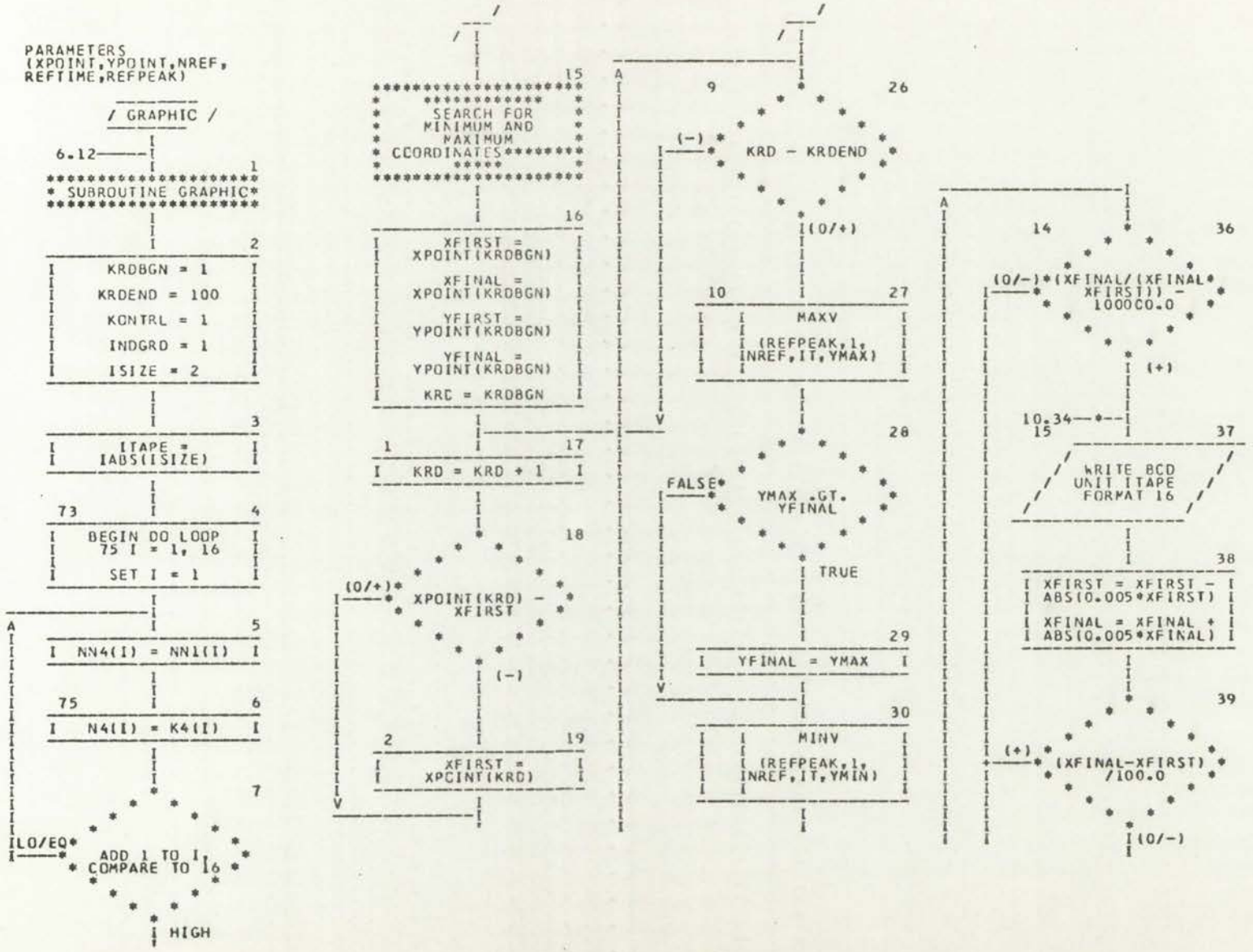
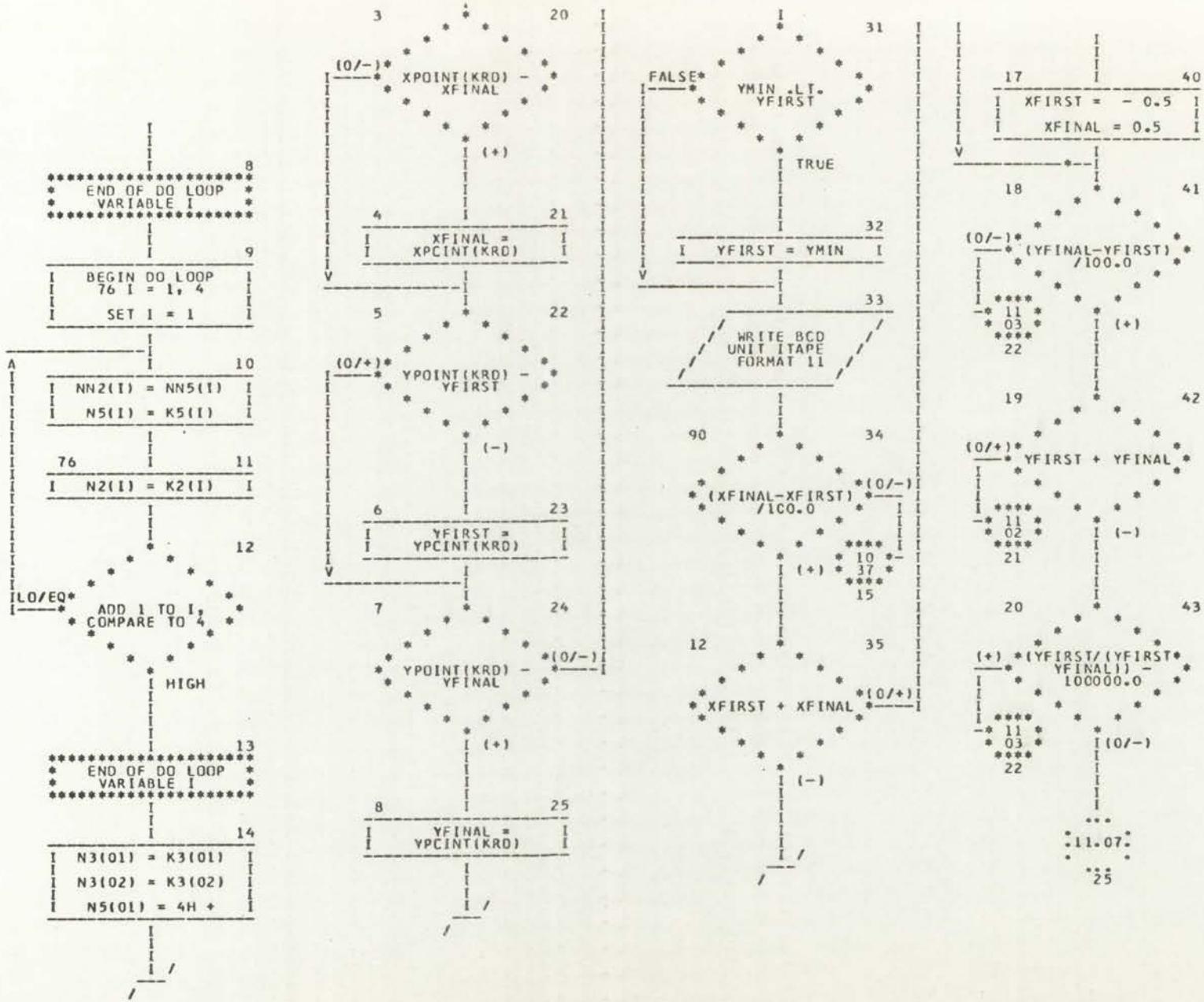
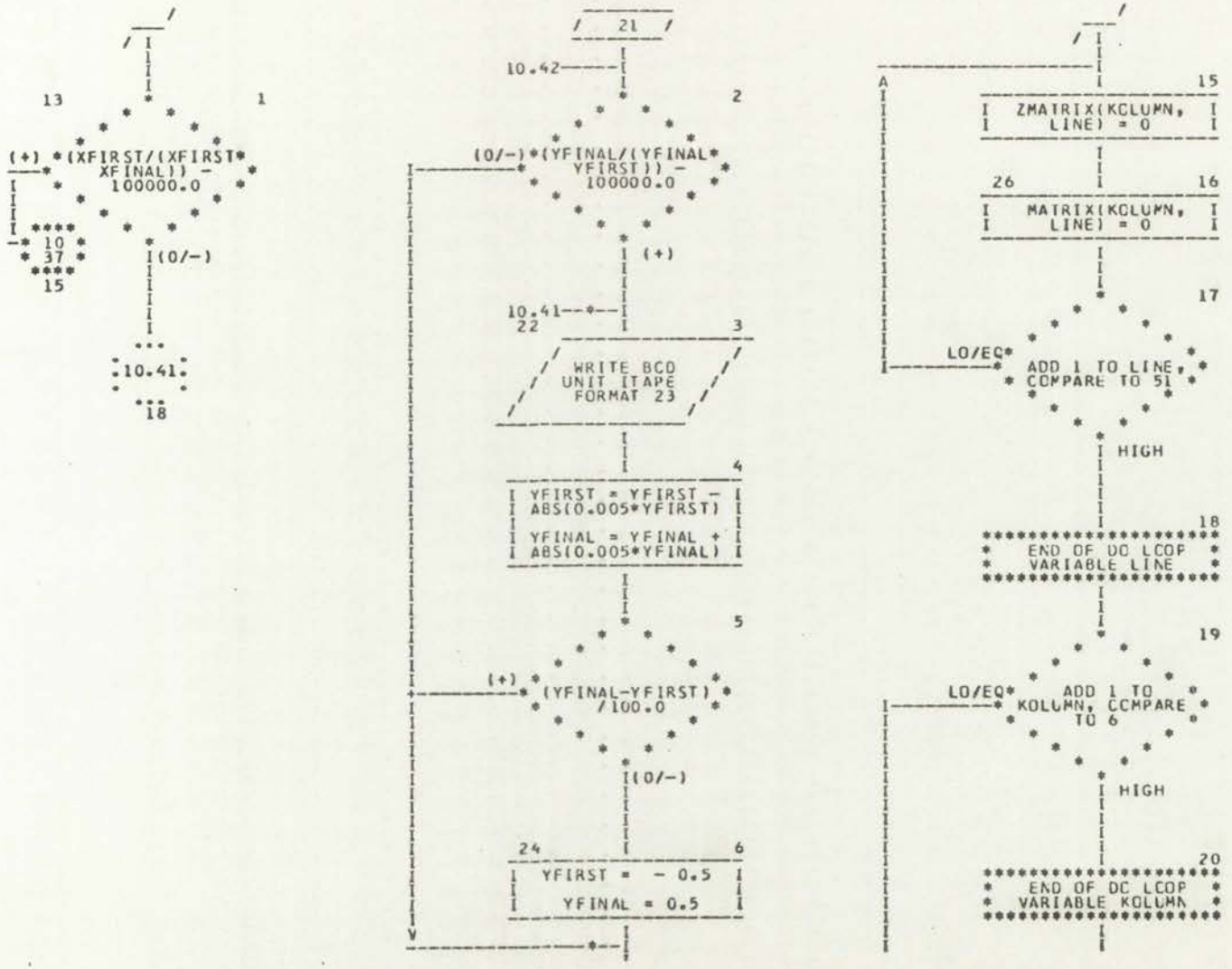
40	12.14
41	12.17
42	13.08
43	13.09
44	13.12
45	13.17
47	14.01
48	14.06
50	14.21
51	15.01
53	15.05
54	15.07
55	15.08
56	15.10
57	15.11
58	15.13
59	16.01
60	16.02
61	16.04
62	16.09
63	16.10
64	16.29
65	16.14
66	16.15
67	16.16
68	16.18
69	16.19
70	16.22
71	16.25
72	16.28
73	10.04
75	10.06
76	10.11
90	10.34
600	11.10
610	13.04

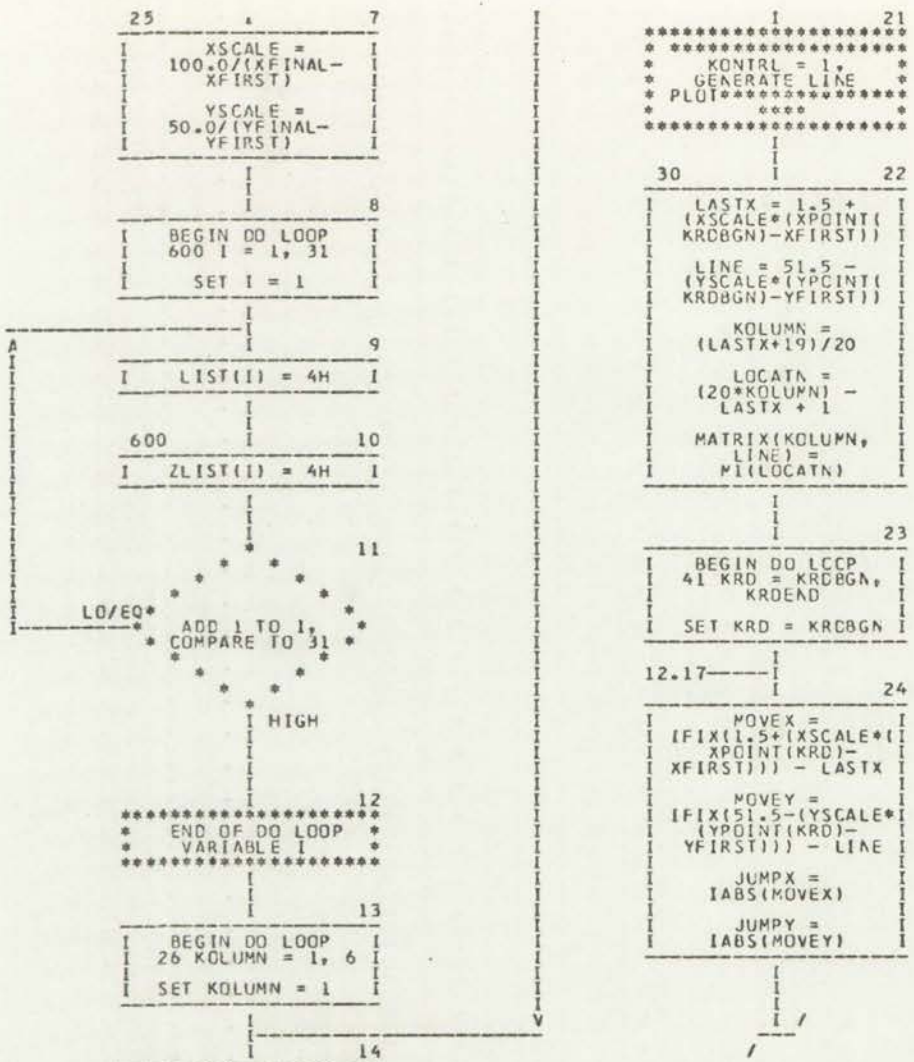
SUBROUTINE GRAPHIC



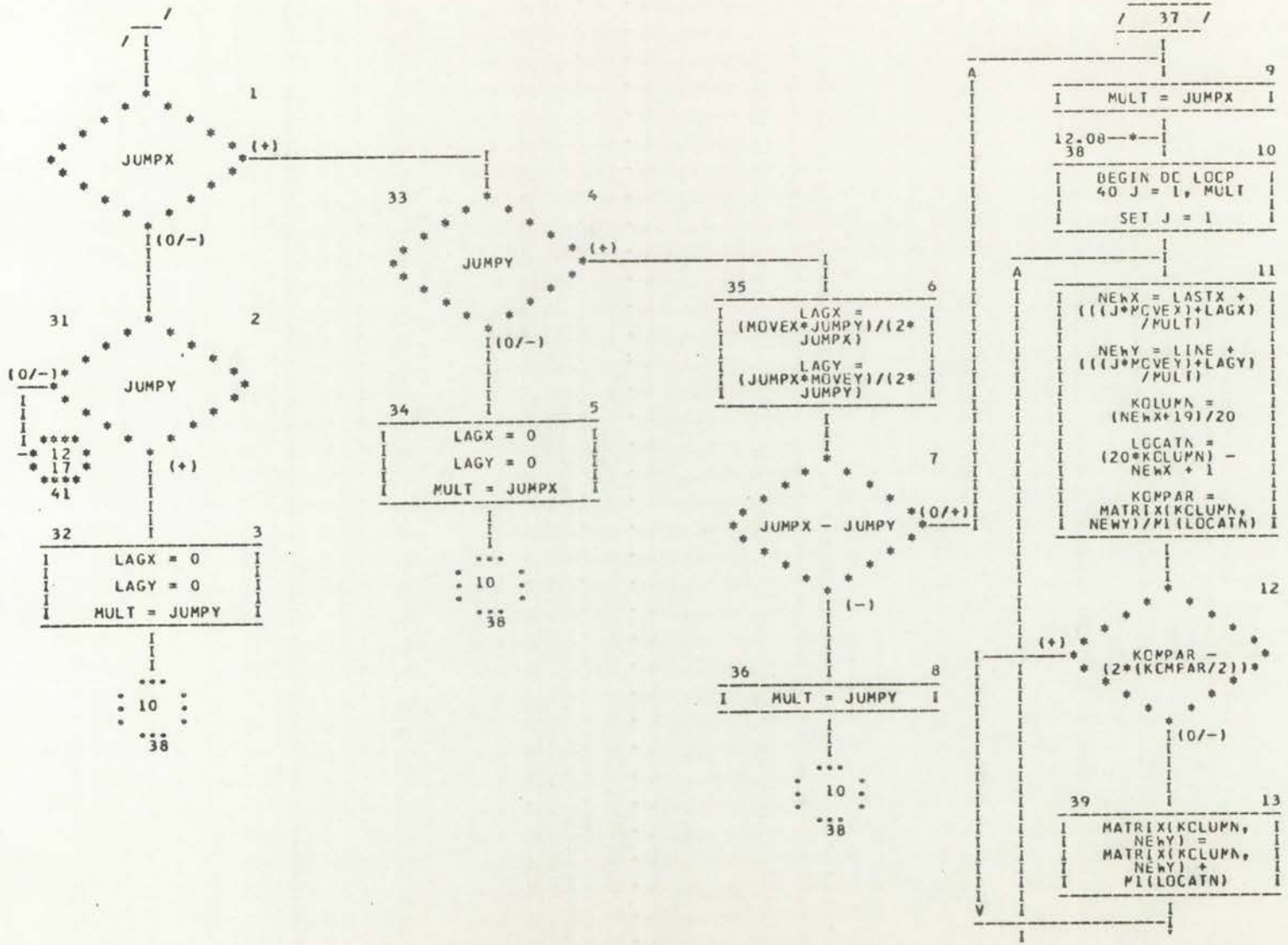

8
END OF DO LOOP
VARIABLE I
9
BEGIN DO LOOP
76 I = 1, 4
SET I = 1
A
10
NN2(I) = NN5(I)
N5(I) = K5(I)
76
11
N2(I) = K2(I)
12
LO/EQ
ADD 1 TO I,
COMPARE TO 4
HIGH
13
END OF DO LOOP
VARIABLE I
14
N3(01) = K3(01)
N3(02) = K3(02)
N5(01) = 4H +
3
20
(0/-)
XPOINT(KRD) -
XFINAL
(+)
4
21
XFINAL =
XPCINT(KRD)
5
22
(0/+)
YPOINT(KRD) -
YFIRST
(-)
6
23
YFIRST =
YPCINT(KRD)
7
24
YPOINT(KRD) -
YFINAL
(+)
8
25
YFINAL =
YPCINT(KRD)
31
FALSE
YMIN .LT.
YFIRST
TRUE
32
YFIRST = YMIN
33
WRITE BCD
UNIT ITAPE
FORMAT 11
90
34
(XFINAL-XFIRST)
/100.0
(0/-)
(+)
10
37
15
12
35
XFIRST + XFINAL
(0/+)
(-)
17
40
XFIRST = - 0.5
XFINAL = 0.5
18
41
(0/-)
(YFINAL-YFIRST)
/100.0
11
03
22
(+)
19
42
(0/+)
YFIRST + YFINAL
11
02
21
(-)
20
43
(+)
(YFIRST/(YFIRST*
YFINAL)) -
100000.0
11
03
22
(0/-)
.11.07.
25

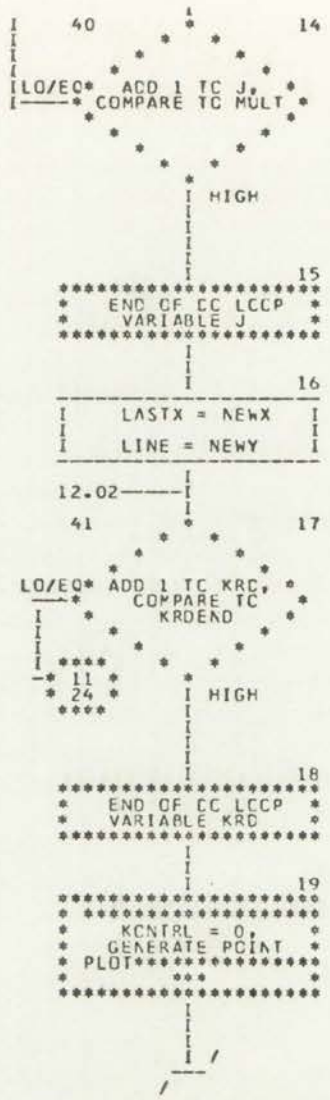
SUBROUTINE GRAPHIC



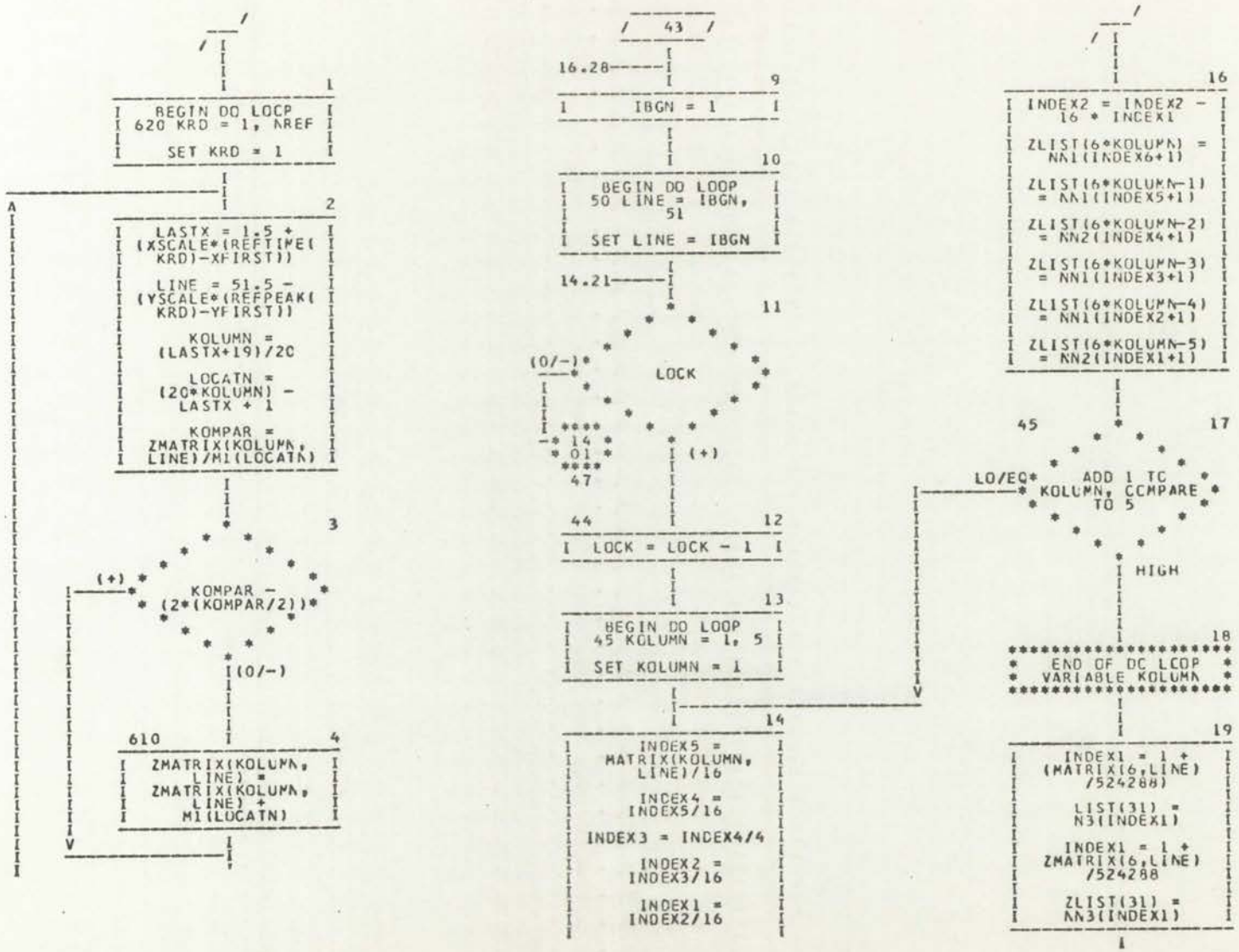

25
7
XSCALE = 100.0/(XFINAL-XFIRST)
YSCALE = 50.0/(YFINAL-YFIRST)
8
BEGIN DO LOOP 600 I = 1, 31
SET I = 1
A
9
LIST(I) = 4H
600
10
ZLIST(I) = 4H
11
LO/EQ
ADD 1 TO I, COMPARE TO 31
HIGH
12
END OF DO LOOP VARIABLE I
13
BEGIN DO LOOP 26 KOLUMN = 1, 6
SET KOLUMN = 1
14
BEGIN DO LOOP 26 LINE = 1, 51
SET LINE = 1
21
KONTRL = 1, GENERATE LINE PLOT
30
22
LASTX = 1.5 + (XSCALE*(XPOINT(KRDBGN)-XFIRST))
LINE = 51.5 - (YSCALE*(YPOINT(KRDBGN)-YFIRST))
KOLUMN = (LASTX+19)/20
LOCATN = (20*KOLUMN) - LASTX + 1
MATRIX(KOLUMN, LINE) = MI(LOCATN)
23
BEGIN DO LOOP 41 KRD = KRDBGN, KRDEND
SET KRD = KRDBGN
12.17
24
MOVEX = IFIX(1.5+(XSCALE*(XPOINT(KRD)-XFIRST))) - LASTX
MOVEY = IFIX(51.5-(YSCALE*(YPOINT(KRD)-YFIRST))) - LINE
JUMPX = IABS(MOVEX)
JUMPY = IABS(MOVEY)

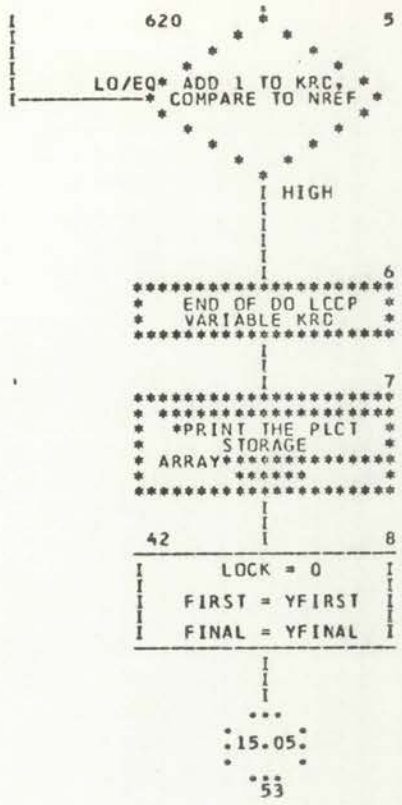
SUBROUTINE GRAPHIC



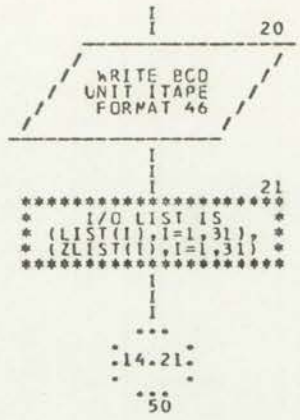

40
14
LO/EQ*
ADD 1 TO J,
COMPARE TO MULT
HIGH
15
END OF DO LOOP
VARIABLE J
16
LASTX = NEWX
LINE = NEWY
12.02
41
17
LO/EQ*
ADD 1 TO KRD,
COMPARE TO
KRDEND
11
24
HIGH
18
END OF DO LOOP
VARIABLE KRD
19
KCNTRL = 0,
GENERATE POINT
PLOT

SUBROUTINE GRAPHIC

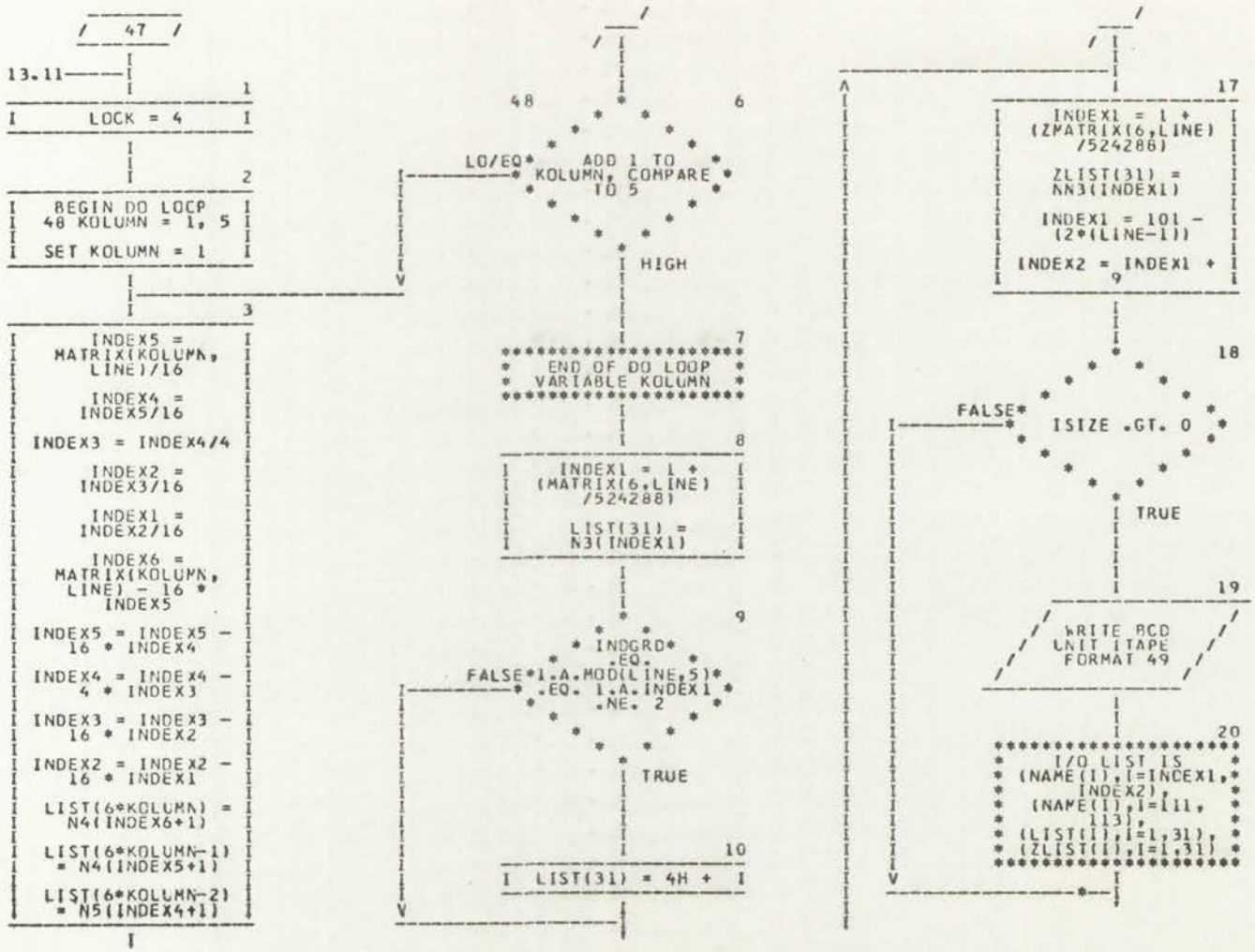


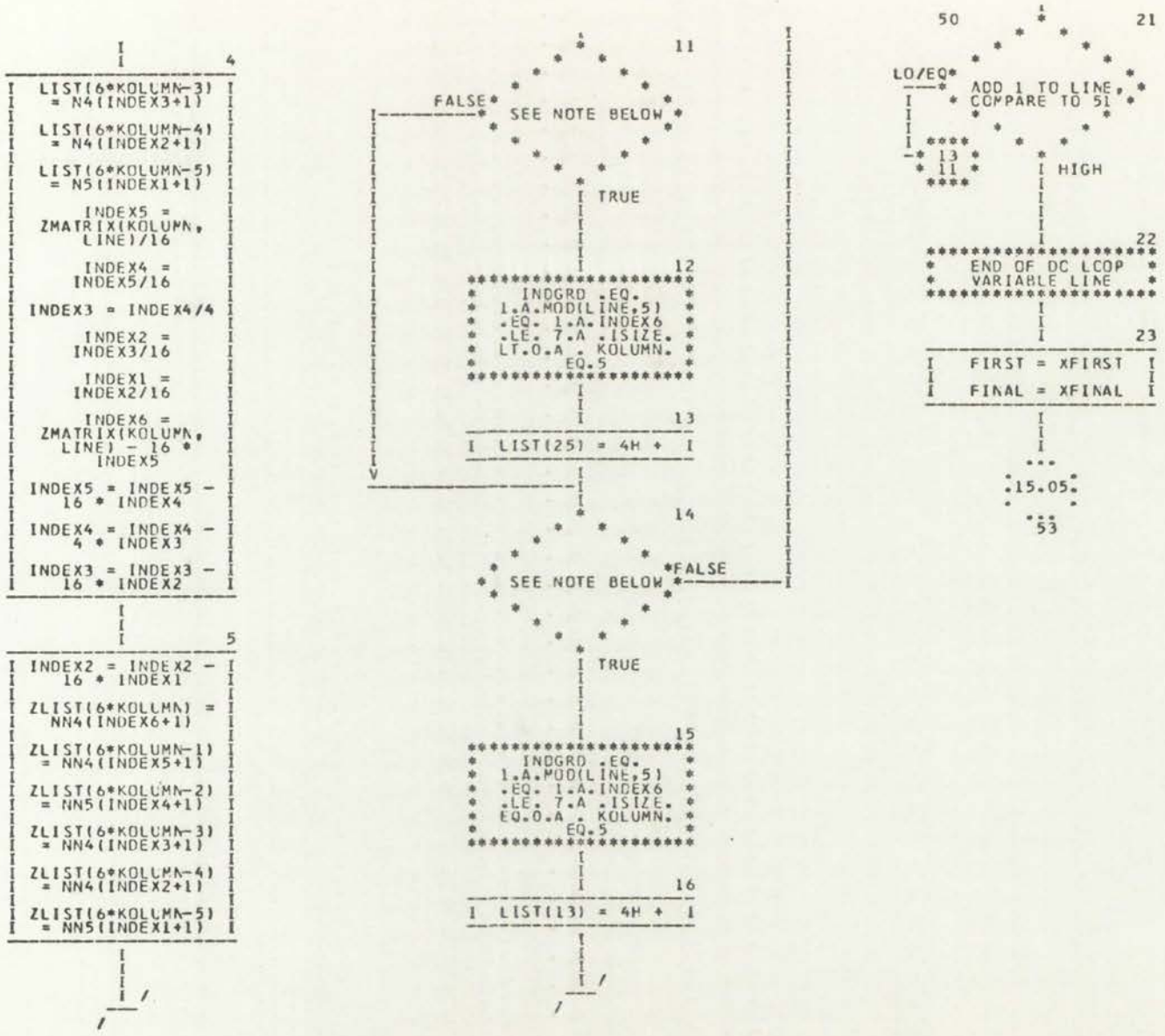

620
5
LO/EQ* ADD 1 TO KRC, *
* COMPARE TO NREF *
HIGH
6
END OF DO LOOP
VARIABLE KRC
7
*PRINT THE PLOT
STORAGE
ARRAY
42
8
LOCK = 0
FIRST = YFIRST
FINAL = YFINAL
.15.05.
53


INDEX6 = MATRIX(KOLUMN, LINE) - 16 * INDEX5
INDEX5 = INDEX5 - 16 * INDEX4
INDEX4 = INDEX4 - 4 * INDEX3
INDEX3 = INDEX3 - 16 * INDEX2
INDEX2 = INDEX2 - 16 * INDEX1
LIST(6*KOLUMN) = N1(INDEX6+1)
LIST(6*KOLUMN-1) = N1(INDEX5+1)
LIST(6*KOLUMN-2) = N2(INDEX4+1)
15
LIST(6*KOLUMN-3) = N1(INDEX3+1)
LIST(6*KOLUMN-4) = N1(INDEX2+1)
LIST(6*KOLUMN-5) = N2(INDEX1+1)
INDEX5 = ZMATRIX(KOLUMN, LINE)/16
INDEX4 = INDEX5/16
INDEX3 = INDEX4/4
INDEX2 = INDEX3/16
INDEX1 = INDEX2/16
INDEX6 = ZMATRIX(KOLUMN, LINE) - 16 * INDEX5
INDEX5 = INDEX5 - 16 * INDEX4
INDEX4 = INDEX4 - 4 * INDEX3
INDEX3 = INDEX3 - 16 * INDEX2

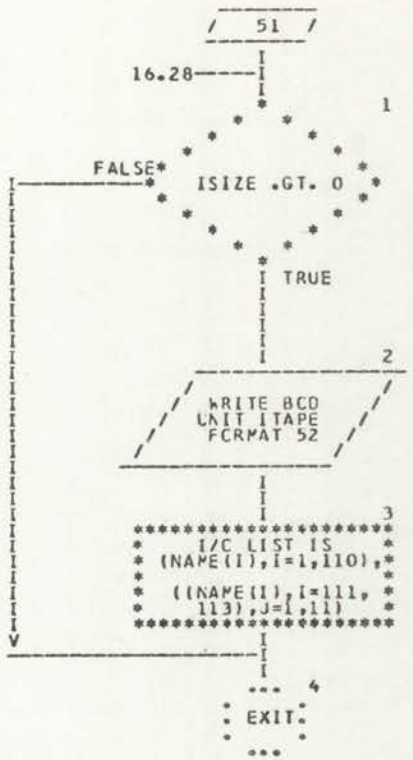

20
WRITE BCD UNIT ITAPE FORMAT 46
21
I/O LIST IS
(LIST(I),I=1,31),
(ZLIST(I),I=1,31)
.14.21.
50

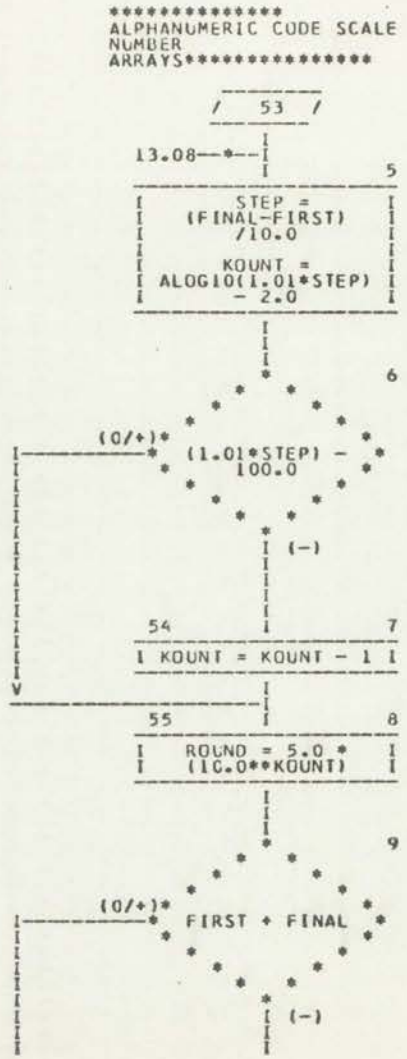
SUBROUTINE GRAPHIC

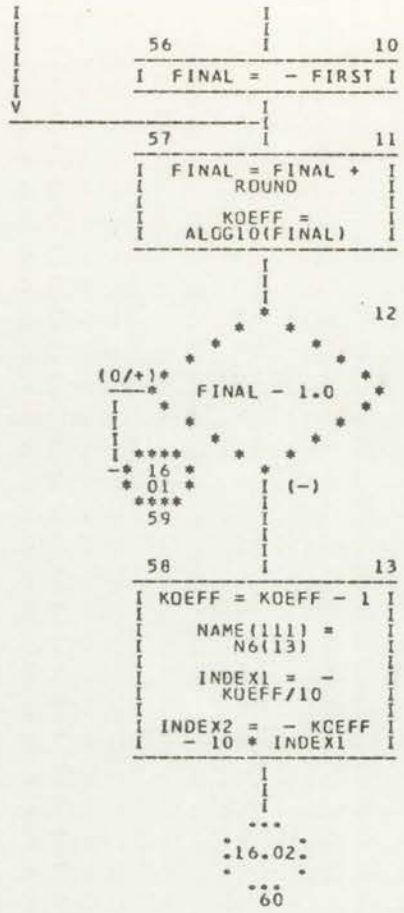



4
LIST(6*KOLUMN-3) = N4(INDEX3+1)
LIST(6*KOLUMN-4) = N4(INDEX2+1)
LIST(6*KOLUMN-5) = N5(INDEX1+1)
INDEX5 = ZMATRIX(KOLUMN, LINE)/16
INDEX4 = INDEX5/16
INDEX3 = INDEX4/4
INDEX2 = INDEX3/16
INDEX1 = INDEX2/16
INDEX6 = ZMATRIX(KOLUMN, LINE) - 16 * INDEX5
INDEX5 = INDEX5 - 16 * INDEX4
INDEX4 = INDEX4 - 4 * INDEX3
INDEX3 = INDEX3 - 16 * INDEX2
5
INDEX2 = INDEX2 - 16 * INDEX1
ZLIST(6*KOLUMN) = NN4(INDEX6+1)
ZLIST(6*KOLUMN-1) = NN4(INDEX5+1)
ZLIST(6*KOLUMN-2) = NN5(INDEX4+1)
ZLIST(6*KOLUMN-3) = NN4(INDEX3+1)
ZLIST(6*KOLUMN-4) = NN4(INDEX2+1)
ZLIST(6*KOLUMN-5) = NN5(INDEX1+1)
11
FALSE
SEE NOTE BELOW
TRUE
12
INDGRD .EQ. 1.A.MOD(LINE,5) .EQ. 1.A.INDEX6 .LE. 7.A .ISIZE. LT.0.A . KOLUMN. EQ.5
13
LIST(25) = 4H +
14
SEE NOTE BELOW
FALSE
TRUE
15
INDGRD .EQ. 1.A.MOD(LINE,5) .EQ. 1.A.INDEX6 .LE. 7.A .ISIZE. EQ.0.A . KOLUMN. EQ.5
16
LIST(13) = 4H +
50
21
LO/EQ
ADD 1 TO LINE, COMPARE TO 51
13
11
HIGH
22
END OF DC LOOP VARIABLE LINE
23
FIRST = XFIRST
FINAL = XFINAL
.15.05.
53

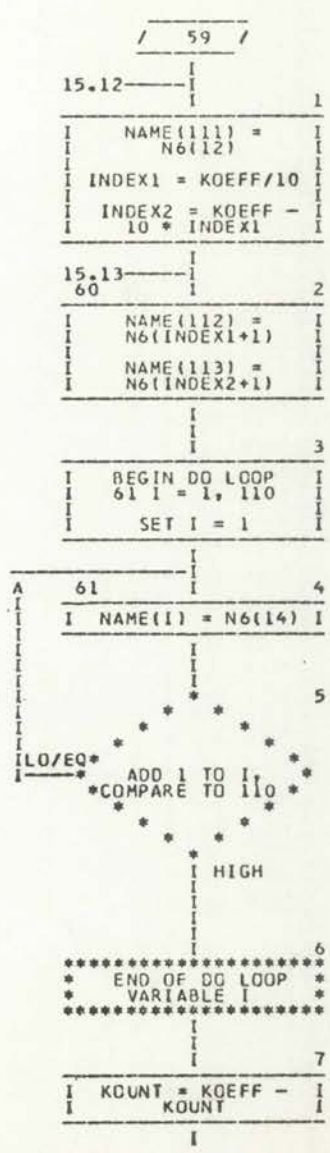
SUBROUTINE GRAPHIC

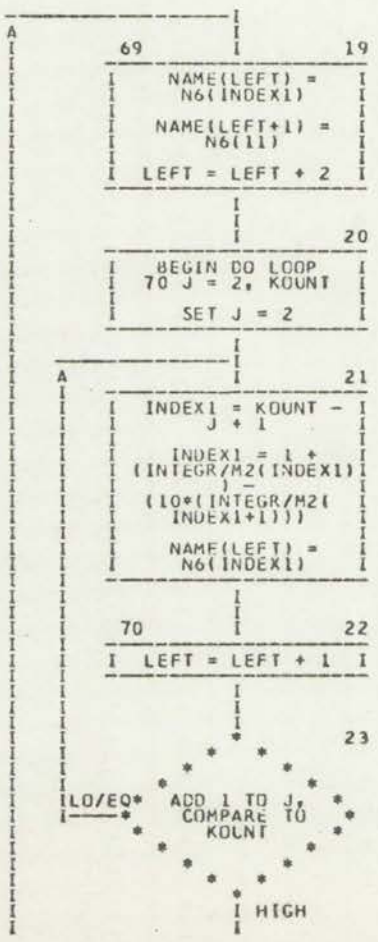


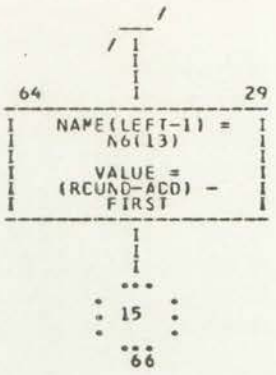


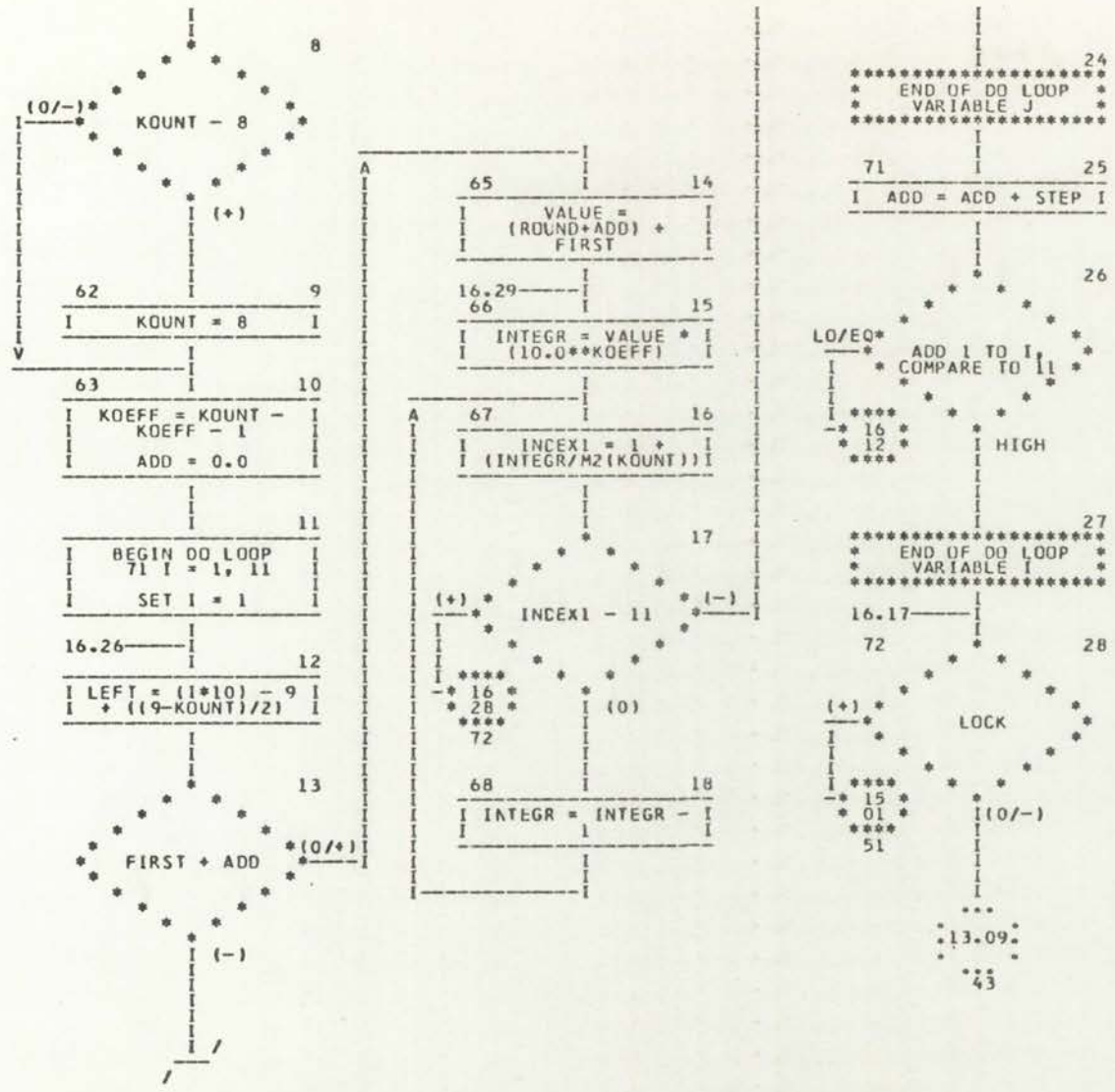

56
10
FINAL = - FIRST
57
11
FINAL = FINAL +
ROUND
KOEFF =
ALOG10(FINAL)
12
(0/+)
FINAL - 1.0
16
01
59
(-)
58
13
KOEFF = KOEFF - 1
NAME(111) =
N6(13)
INDEX1 = -
KOEFF/10
INDEX2 = - KOEFF
- 10 * INDEX1
16.02
60

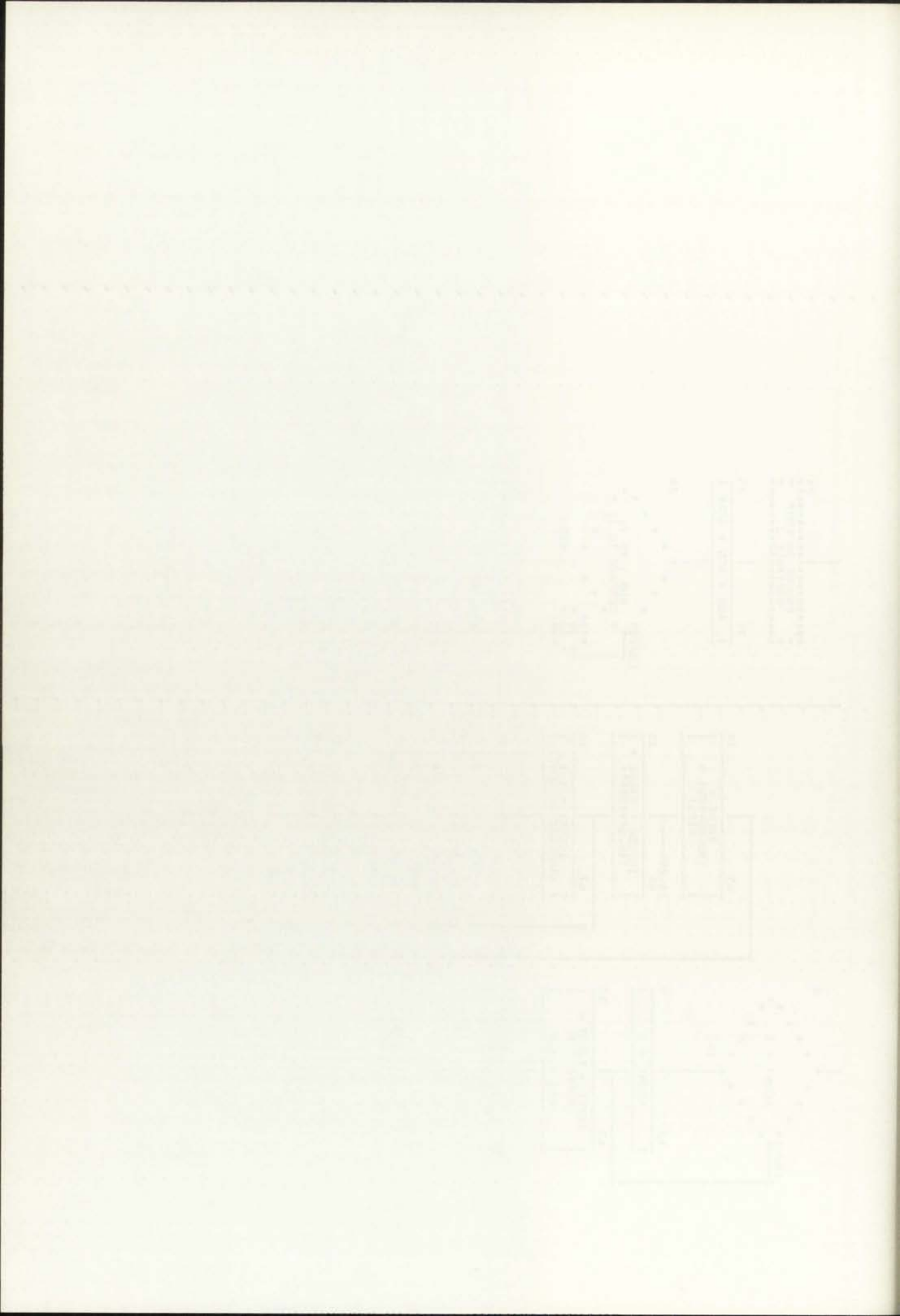
SUBROUTINE GRAPHIC








8
(0/-)
KOUNT - 8
(+)
62
9
KOUNT = 8
63
10
KOEFF = KOUNT - KOEFF - 1
ADD = 0.0
11
BEGIN DO LOOP 71 I = 1, 11
SET I = 1
16.26
12
LEFT = (I*10) - 9 + ((9-KOUNT)/2)
13
(0/+)
FIRST + ADD
(-)
A
65
14
VALUE = (ROUND+ADD) + FIRST
16.29
66
15
INTEGR = VALUE * (10.0**KOEFF)
A
67
16
INCEX1 = 1 + (INTEGR/M2(KOUNT))
17
(+)
(-)
INCEX1 - 11
16
28
72
(0)
68
18
INTEGR = INTEGR -
24
END OF DO LOOP VARIABLE J
71
25
ADD = ACD + STEP I
26
LO/EQ
ADD 1 TO I, COMPARE TO 11
16
12
HIGH
27
END OF DO LOOP VARIABLE I
16.17
72
28
(+)
LOCK
15
01
51
(0/-)
13.09
43



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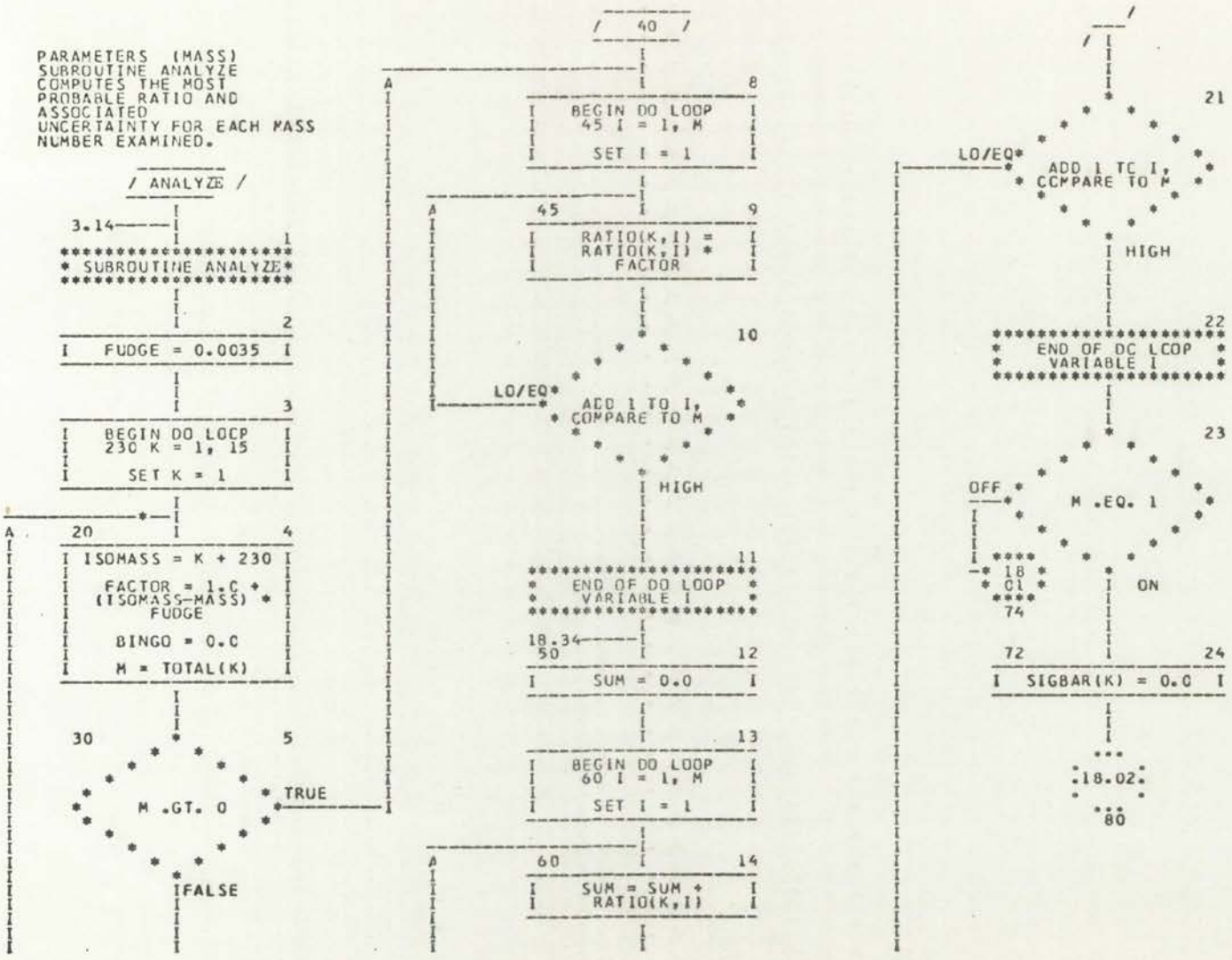
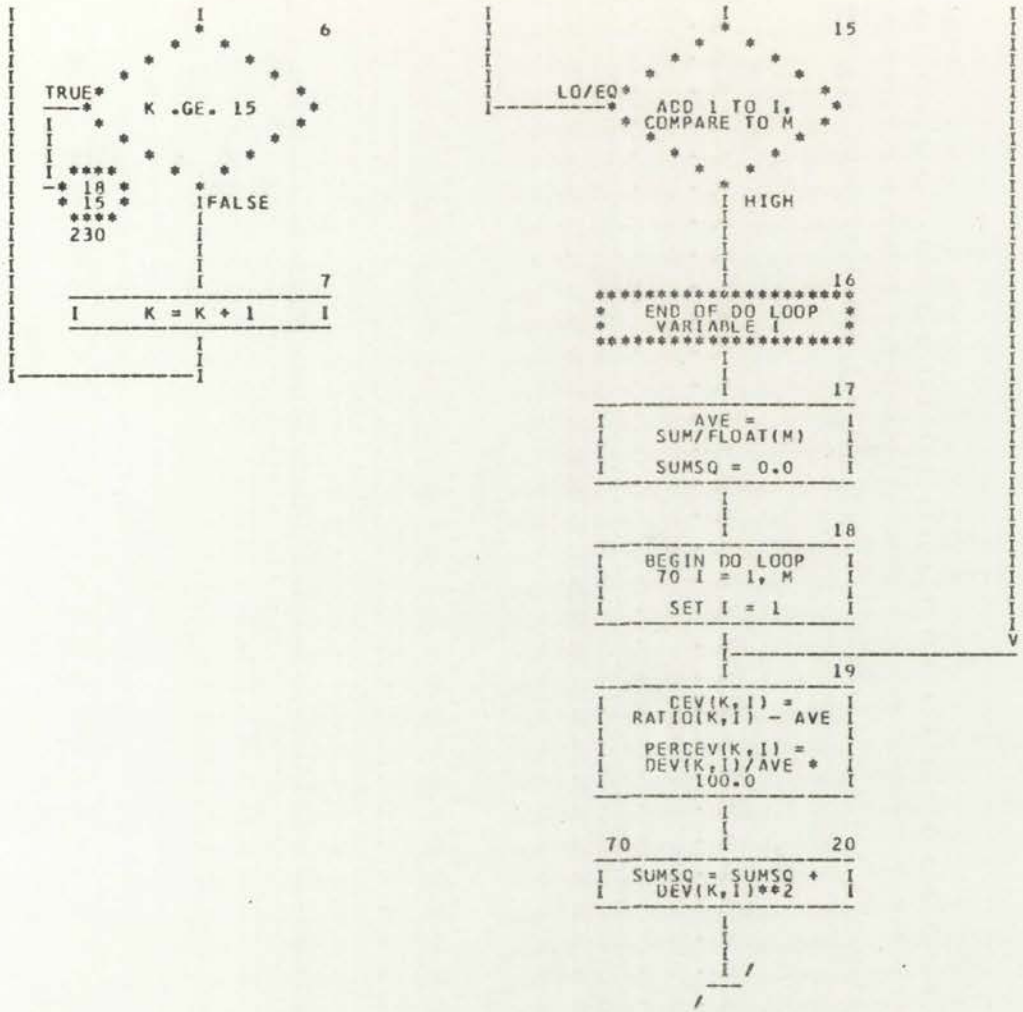
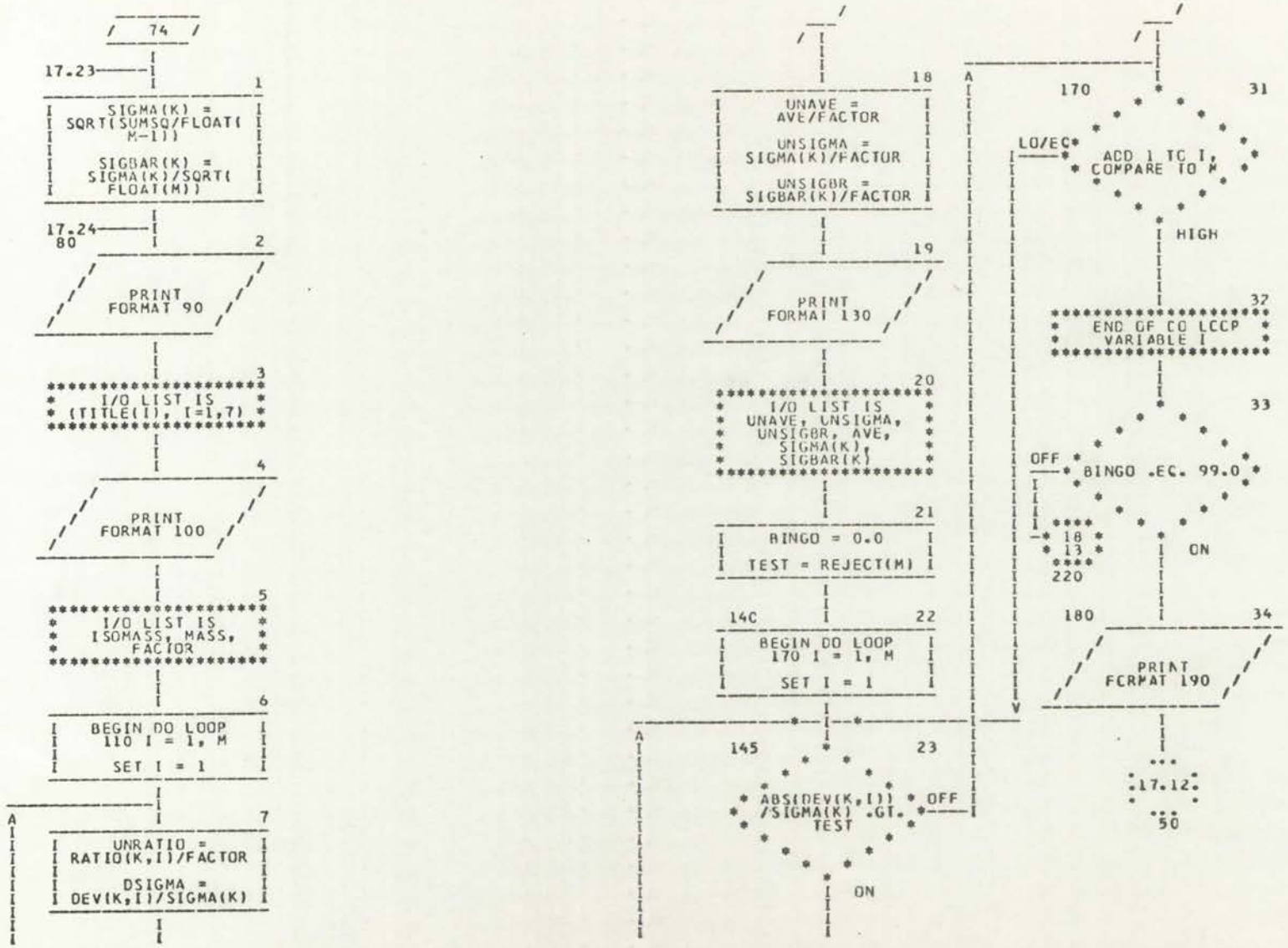
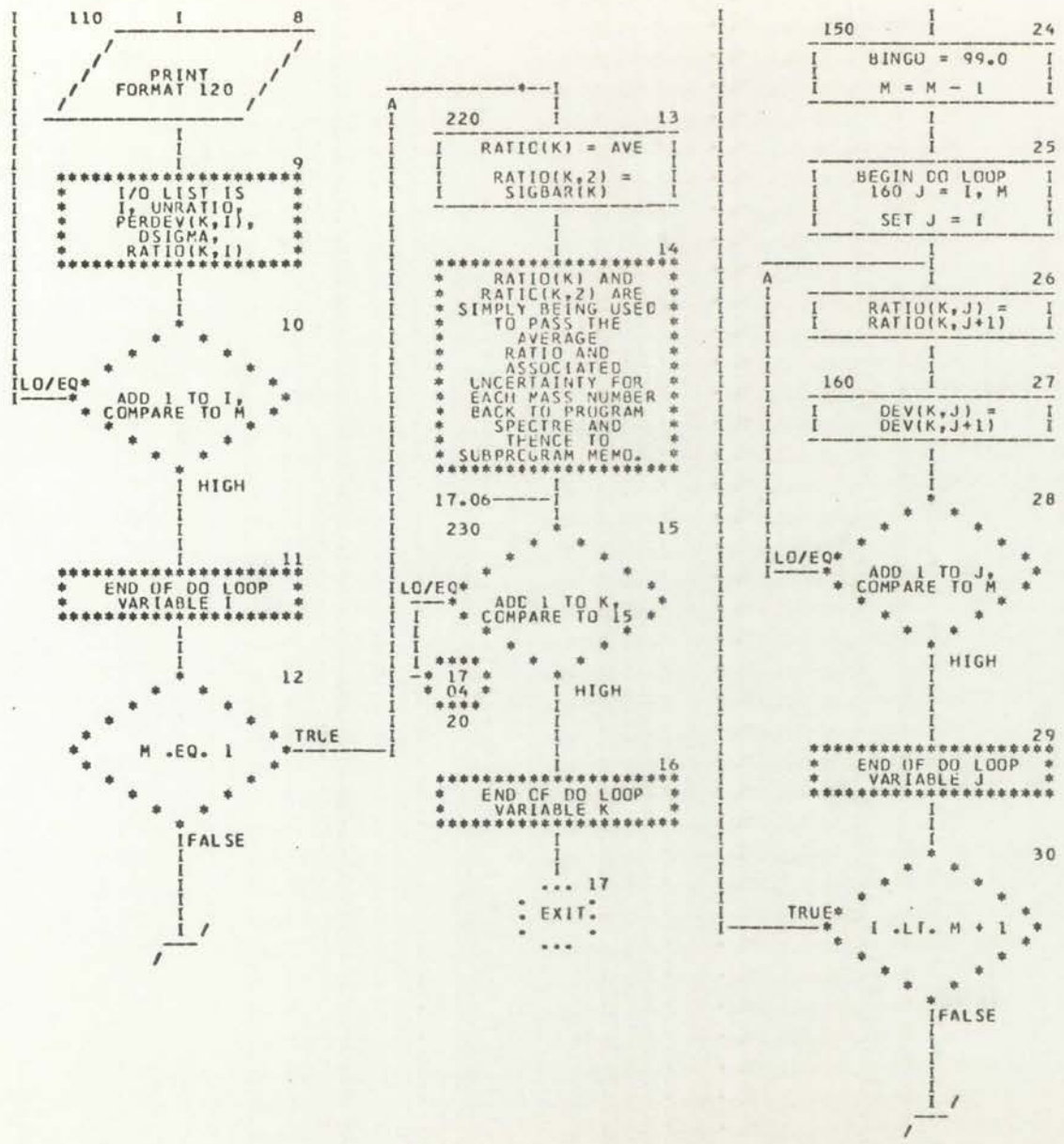
SUBROLTINE ANALYZE




6
TRUE
K .GE. 15
FALSE
230
7
K = K + 1
15
LO/EQ
ADD 1 TO I,
COMPARE TO M
HIGH
16
END OF DO LOOP
VARIABLE I
17
AVE =
SUM/FLOAT(M)
SUMSQ = 0.0
18
BEGIN DO LOOP
70 I = 1, M
SET I = 1
19
DEV(K,I) =
RATIO(K,I) - AVE
PERCEV(K,I) =
DEV(K,I)/AVE *
100.0
70
20
SUMSQ = SUMSQ +
DEV(K,I)**2

SUBROUTINE ANALYZE




110
8
PRINT FORMAT 120
9
I/O LIST IS I, UNRATIO, PERDEV(K,I), DSIGMA, RATIO(K,I)
10
LO/EQ
ADD 1 TO I, COMPARE TO M
HIGH
11
END OF DO LOOP VARIABLE I
12
M .EQ. 1
TRUE
FALSE
A
220
13
RATIO(K) = AVE
RATIO(K,2) = SIGBAR(K)
14
RATIO(K) AND RATIO(K,2) ARE SIMPLY BEING USED TO PASS THE AVERAGE RATIO AND ASSOCIATED UNCERTAINTY FOR EACH MASS NUMBER BACK TO PROGRAM SPECTRE AND THENCE TO SUBPROGRAM MEMO.
17.06
230
15
LO/EQ
ADD 1 TO K, COMPARE TO 15
17
04
20
HIGH
16
END OF DO LOOP VARIABLE K
... 17
EXIT.
150
24
BINGO = 99.0
M = M - 1
25
BEGIN DO LOOP 160 J = I, M
SET J = I
A
26
RATIO(K,J) = RATIO(K,J+1)
160
27
DEV(K,J) = DEV(K,J+1)
28
LO/EQ
ADD 1 TO J, COMPARE TO M
HIGH
29
END OF DO LOOP VARIABLE J
30
TRUE
I .LT. M + 1
FALSE

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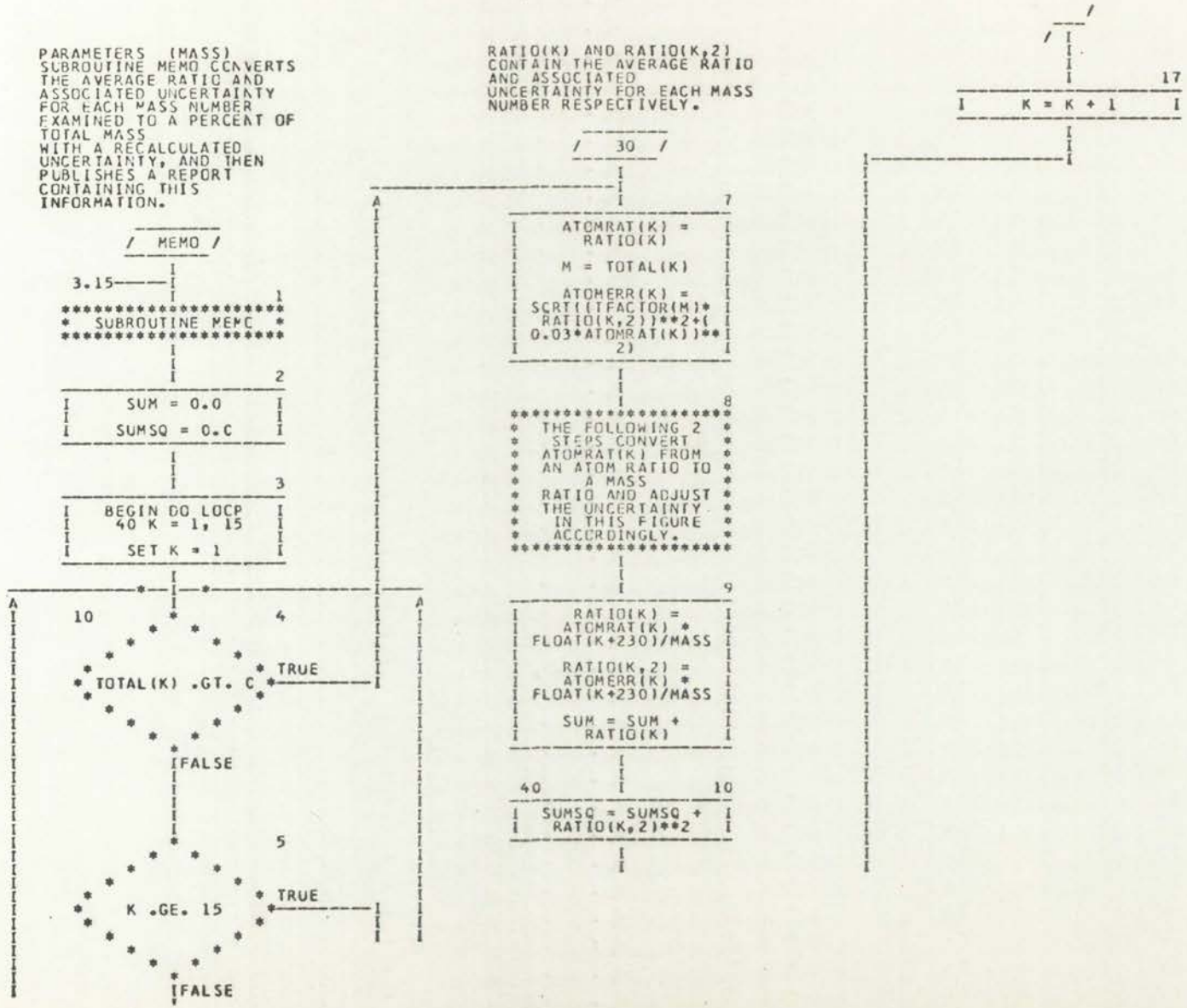
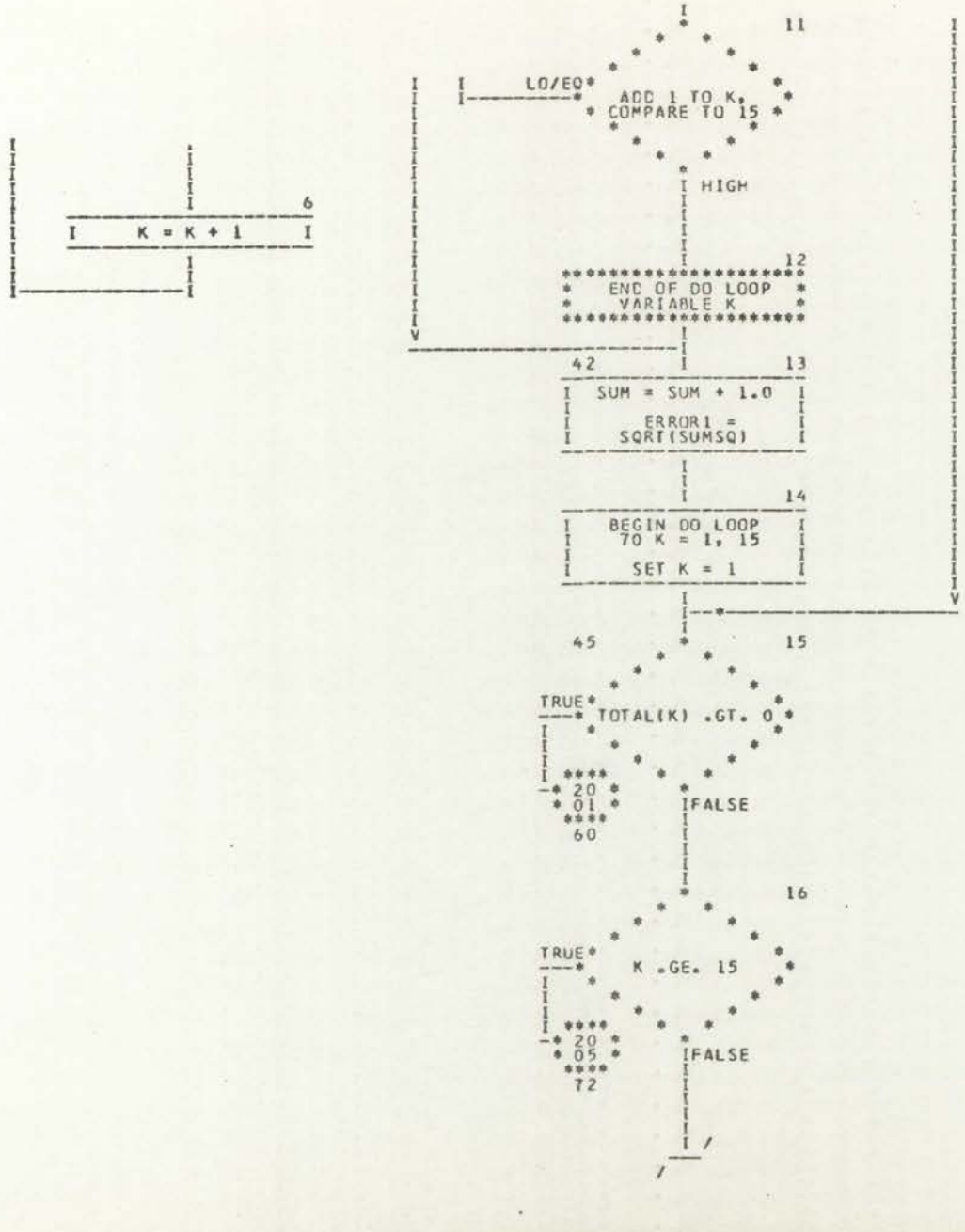
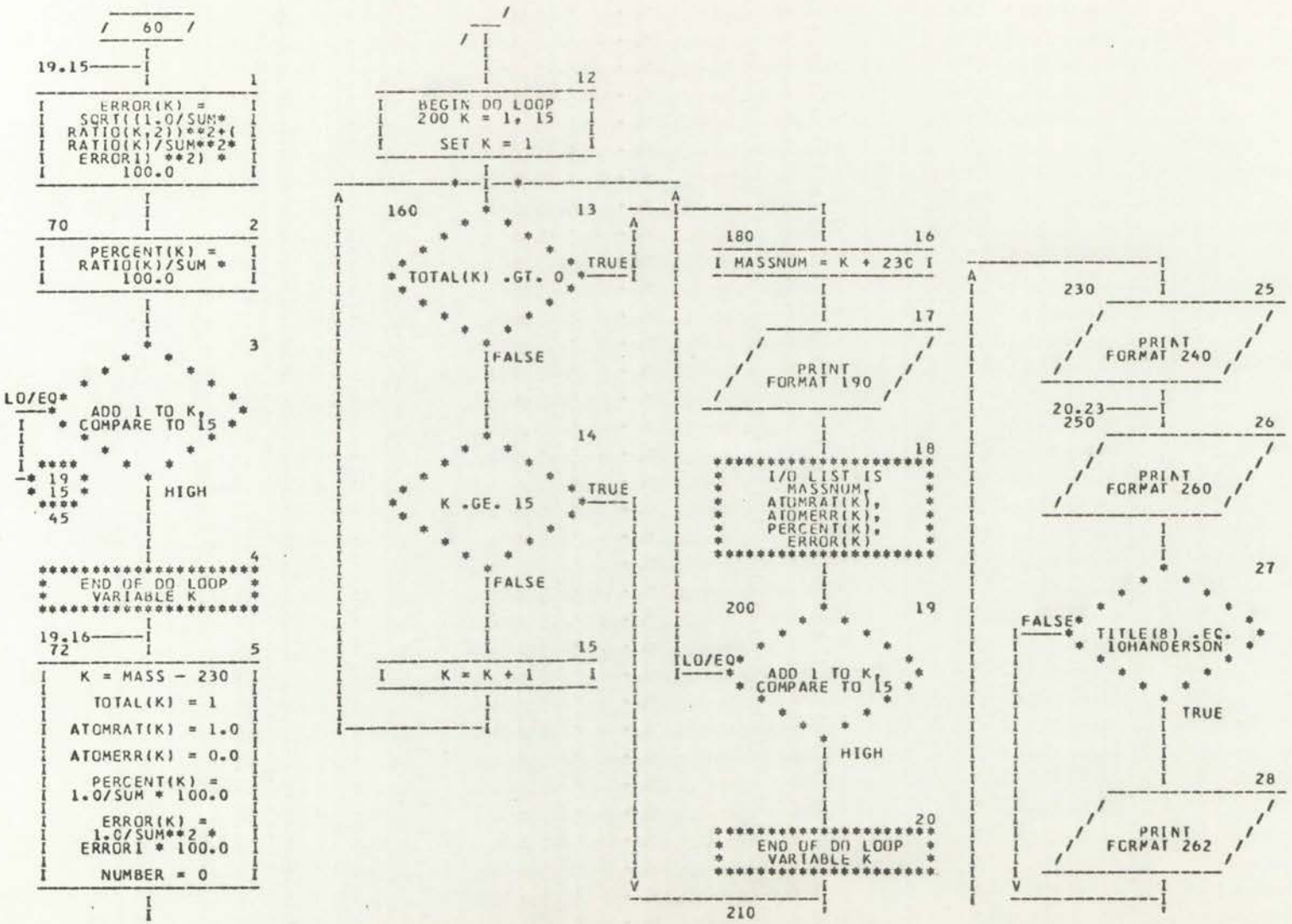
SUBROUTINE MEMO

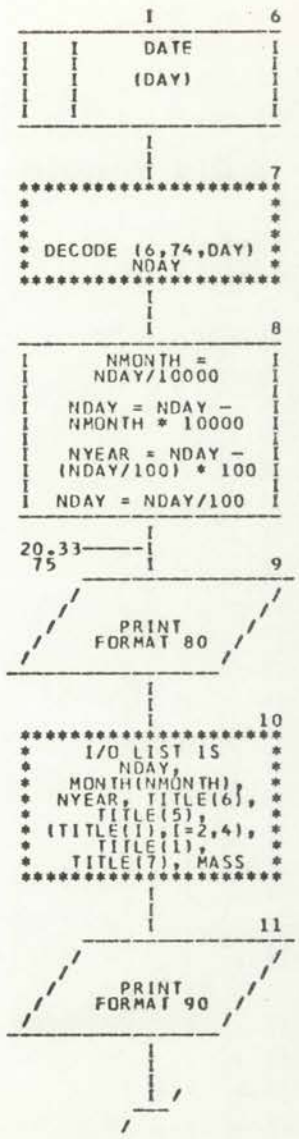
PARAMETERS (MASS)
SUBROUTINE MEMO CONVERTS THE AVERAGE RATIO AND ASSOCIATED UNCERTAINTY FOR EACH MASS NUMBER EXAMINED TO A PERCENT OF TOTAL MASS WITH A RECALCULATED UNCERTAINTY, AND THEN PUBLISHES A REPORT CONTAINING THIS INFORMATION.

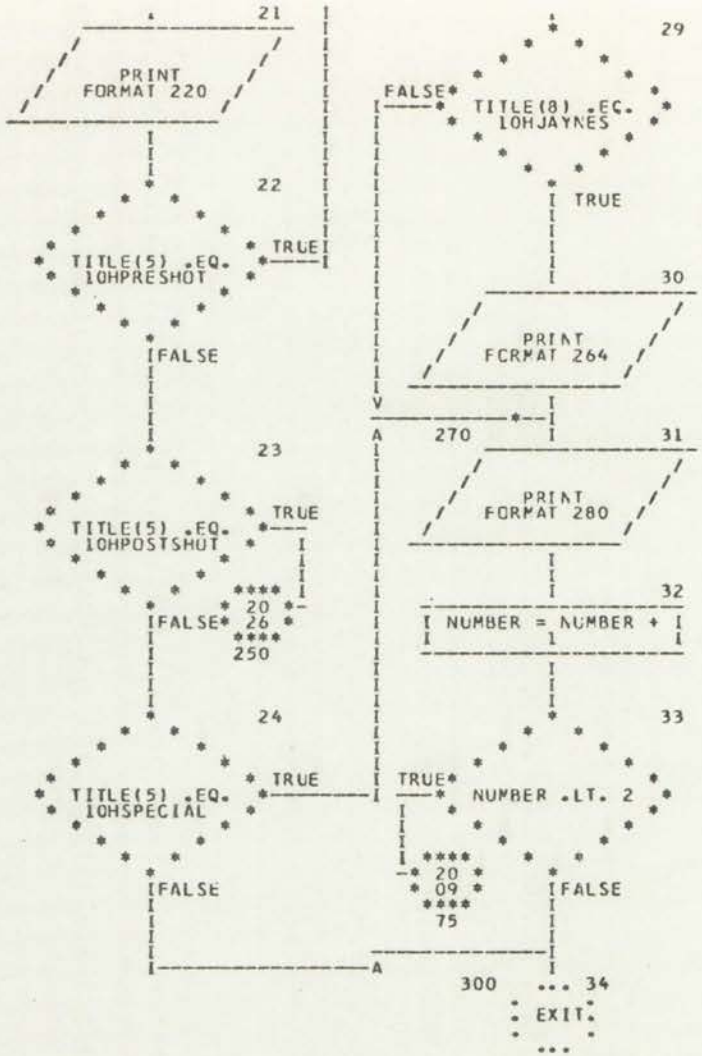



11
LO/EQ
ADD 1 TO K,
COMPARE TO 15
HIGH
6
K = K + 1
12
END OF DO LOOP
VARIABLE K
42
13
SUM = SUM + 1.0
ERROR1 =
SQRT(SUMSQ)
14
BEGIN DO LOOP
70 K = 1, 15
SET K = 1
45
15
TRUE
TOTAL(K) .GT. 0
20
01
60
FALSE
16
TRUE
K .GE. 15
20
05
72
FALSE

SUBROUTINE MEMO




6
DATE
(DAY)
7
DECODE (6,74,DAY)
NDAY
8
NMONTH =
NDAY/10000
NDAY = NDAY -
NMONTH * 10000
NYEAR = NDAY -
(NDAY/100) * 100
NDAY = NDAY/100
20,33
75
9
PRINT
FORMAT 80
10
I/O LIST IS
NDAY,
MONTH(NMONTH),
NYEAR, TITLE(6),
TITLE(5),
(TITLE(I),I=2,4),
TITLE(1),
TITLE(7), MASS
11
PRINT
FORMAT 90


21
PRINT
FORMAT 220
22
TITLE(5) .EQ.
10HPRESHOT
TRUE
FALSE
23
TITLE(5) .EQ.
10HPOSTSHOT
TRUE
FALSE
20
26
250
24
TITLE(5) .EQ.
10HSPECIAL
TRUE
FALSE
29
TITLE(8) .EQ.
10HJAYNES
FALSE
TRUE
30
PRINT
FORMAT 264
270
31
PRINT
FORMAT 280
32
NUMBER = NUMBER + 1
33
NUMBER .LT. 2
TRUE
FALSE
20
09
75
300
34
EXIT

APPENDIX E

COMPLETE LISTING OF PROGRAM SPECTRE

This source listing was produced on September 4, 1970 at the Central Computer Facility at LASL. An actual data deck was included and the program was compiled and executed at the same time to ensure proper performance. The output of the program was correct in all respects establishing the completeness and accuracy of this listing. The resultant output appears in Appendix F.

```
      PROGRAM SPECTRE (INPUT,TAPE 10=INPUT,OUTPUT,TAPE 2=OUTPUT)
C PROGRAM SPECTRE PRODUCES A SET OF ISOTOPE WEIGHT PERCENTAGES PRESENT
C IN A SINGLE MASS SPECTROMETER SAMPLE.
      INTEGER FILTEMP(100),SCALE(100),MASS(100),TOTAL(15)
      REAL HOUR(100,3),MINUTE(100,3),SECOND(100,3),SUMTIME(100,3),
     C PEAK(100,3),BACKGND(100),TIME(100),RATIO(15,50),P(4)
      COMMON TITLE(8),RATIO,TOTAL,P
      EQUIVALENCE (HOUR,BACKGND),(MINUTE,TIME)
    5 READ 8, TITLE
    8 FORMAT (8A10)
      IF (EOF,10) 80,10
   10 PRINT 12, (TITLE(I), I=1,7),(TITLE(I),I=1,7)
   12 FORMAT (1H12XA10,2X3A10,2XA10,2XA10,2XA10,5X11H* SPECTRE *)
      PRINT 14, (TITLE(I),I=1,7)
   14 FORMAT (1H12XA10,2X3A10,2XA10,2XA10,2XA10,5X11H* SPECTRE *//
     C X2X11HINPUT DATA:///
     C X2X67HFILTEMP CODE, SCALE FACTOR, MASS NUMBER (FOLLOWED BY 3 DATA
     C POINTS)/
     C X2X55HHOUR:MINUTE:SECOND, INTEGRATION TIME (SEC), PEAK HEIGHT)
      DO 40 I=1,100
      READ 20, FILTEMP(I),SCALE(I),MASS(I)
   20 FORMAT (I1,I2,I3)
      IF (FILTEMP(I).EQ.9.AND.SCALE(I).EQ.99) GO TO 50
   40 READ 45, (HOUR(I,J),MINUTE(I,J),SECOND(I,J),SUMTIME(I,J),
     C PEAK(I,J),J=1,3)
   45 FORMAT (F1,2F2,F3,F6)
   50 N=I-1
      K=N/4
      DO 52 I=1,K
      KA=K+I $ KB=2*K+I $ KC=3*K+I
   52 PRINT 54, I,FILTEMP(I),SCALE(I),MASS(I),
     C KA,FILTEMP(KA),SCALE(KA),MASS(KA),
     C KB,FILTEMP(KB),SCALE(KB),MASS(KB),
     C KC,FILTEMP(KC),SCALE(KC),MASS(KC),
     C (HOUR(I,J),MINUTE(I,J),SECOND(I,J),SUMTIME(I,J),PEAK(I,J),
     C HOUR(KA,J),MINUTE(KA,J),SECOND(KA,J),SUMTIME(KA,J),PEAK(KA,J),
     C HOUR(KB,J),MINUTE(KB,J),SECOND(KB,J),SUMTIME(KB,J),PEAK(KB,J),
     C HOUR(KC,J),MINUTE(KC,J),SECOND(KC,J),SUMTIME(KC,J),PEAK(KC,J),
     C J=1,3)
   54 FORMAT (1HO2XI2,1H.2XI1,2XI2,2XI3,15XI2,1H.2XI1,2XI2,2XI3,
     C         15XI2,1H.2XI1,2XI2,2XI3,15XI2,1H.2XI1,2XI2,2XI3/
     C (X4XF1,1HOF2,1HOF2,2XF3,2XF6,10XF1,1HOF2,1HOF2,2XF3,2XF6,
     C  10XF1,1HOF2,1HOF2,2XF3,2XF6,10XF1,1HOF2,1HOF2,2XF3,2XF6))
      K=4*K+1
      IF (N.LT.K) GO TO 58
      DO 55 I=K,N
   55 PRINT 56, I,FILTEMP(I),SCALE(I),MASS(I),(HOUR(I,J),MINUTE(I,J),
     C SECOND(I,J),SUMTIME(I,J),PEAK(I,J),J=1,3)
   56 FORMAT (1HO92XI2,1H.2XI1,2XI2,2XI3/(X94XF1,1HOF2,1HOF2,2XF3,2XF6))
   58 DO 70 I=1,N
      DO 60 J=1,3
      SECOND(I,J)=HOUR(I,J)*3600.0+MINUTE(I,J)*60.0+SECOND(I,J)
     C -SUMTIME(I,J)/2.0
   60 PEAK(I,J)=PEAK(I,J)/SUMTIME(I,J)
      BACKGND(I)=PEAK(I,1)+(PEAK(I,3)-PEAK(I,1))/(SECOND(I,3)
     C -SECOND(I,1))*(SECOND(I,2)-SECOND(I,1))
      PEAK(I)=(PEAK(I,2)-BACKGND(I))*FLOAT(((-1)**SCALE(I)+2)*10**
     C ((SCALE(I)-(((-1)**SCALE(I)+3)/2))/2))
```

```
   70 TIME(I)=SECOND(I,2)-SECOND(1,2)+2000.0
C THE FOLLOWING PROGRAM SEGMENT (STATEMENT 200 - STATEMENT 330)
C INTRODUCES SYNTHETIC FILTEMPS SO THAT THE REFERENCE ISOTOPE CURVE WILL
C BE FITTED IN SECTIONS OF APPROXIMATELY SIX MEASURED REFERENCE PEAKS
C PER SECTION (MINIMUM FOUR - MAXIMUM EIGHT).
  200 J=1 $ L=FILTEMP(J) $ M=1
  210 NREF=0
      DO 220 I=J,N
      IF (FILTEMP(I).NE.L) GO TO 230
      IF (MASS(I).EQ.MASS(1)) NREF=NREF+1
  220 CONTINUE
      K=N
      GO TO 240
  230 K=I-1
  240 KEEP=K
      KOUNT=(NREF+1)/5
      JUMP=0
      IF (KOUNT.GE.2.AND.MOD(NREF,5).EQ.4) JUMP=5
  250 IF (KOUNT.LE.1) GO TO 300
      NREF=0
      DO 260 I=J,K
      IF (MASS(I).NE.MASS(1)) GO TO 260
      NREF=NREF+1
      IF (NREF.GE.6) GO TO 270
      IF (KOUNT.EQ.2.AND.JUMP.EQ.5.AND.NREF.GE.5) GO TO 270
  260 CONTINUE
  270 K=I
  300 DO 310 I=J,K
  310 FILTEMP(I)=M
      IF (K.GE.N) GO TO 75
      J=K+1 $ L=FILTEMP(J) $ M=M+1
      IF (KOUNT.LE.1) GO TO 210
      KOUNT=KOUNT-1
      DO 320 I=J,N
      INVERT=N+J-I
      FILTEMP(INVERT+1)=FILTEMP(INVERT)
      MASS(INVERT+1)=MASS(INVERT)
      PEAK(INVERT+1)=PEAK(INVERT)
  320 TIME(INVERT+1)=TIME(INVERT)
      MASS(J)=MASS(J-1)
      PEAK(J)=PEAK(J-1)
      TIME(J)=TIME(J-1)
      N=N+1
      KEEP=KEEP+1
      K=KEEP
  330 GO TO 250
   75 CALL FITCURV (FILTEMP,MASS,N,PEAK,TIME)
      CALL ANALYZE (MASS)
      CALL MEMO (MASS)
      GO TO 5
   80 STOP
      END
```

```
      SUBROUTINE FITCURV (FILTEMP,MASS,N,PEAK,TIME)
C SUBROUTINE FITCURV COMPUTES A LIST OF ISOTOPIC RATIOS FOR EACH
C ISOTOPIC MASS NUMBER EXAMINED.  THIS RATIO IS THE RELATIVE ATOM
C ABUNDANCE OF A PARTICULAR MASS NUMBER COMPARED TO THE ATOM ABUNDANCE
C OF A PARTICULAR REFERENCE MASS NUMBER.
      INTEGER FILTEMP(100),MASS(100),START,FILNUM,TOTAL(15),COUNT(15)
      REAL PEAK(100),TIME(100),REFPEAK(50),REFTIME(50),ISOPEAK(15,50),
     C ISOTIME(15,50),RATIO(15,50),XPLOT(100),YPLOT(100),XLABEL(9),
     C YLABEL(9),REFPLOT(50),DIFFER(50),X(50),Y(50),P(4)
      COMMON TITLE(8),RATIO,TOTAL,P
      EQUIVALENCE (ISOPEAK,RATIO)
      START=1
      FILNUM=1
      DO 10 K=1,15
      TOTAL(K)=0
   10 COUNT(K)=0
   20 NREF=0
      DO 80 I=START,N
      IF (FILTEMP(I).EQ.FILNUM) GO TO 40
      START=I
      GO TO 100
   40 IF (MASS(I).EQ.MASS(1)) 50,60
   50 NREF=NREF+1
      REFPEAK(NREF)=PEAK(I)
      REFTIME(NREF)=TIME(I)
      GO TO 80
   60 K=MASS(I)-230
      TOTAL(K)=TOTAL(K)+1
C TOTAL(K) IS A COUNTER WHICH CONTAINS THE TOTAL NUMBER OF EXPERIMENTAL
C PEAKS PROCESSED FOR MASS NUMBER K+230.
      M=TOTAL(K)
      ISOPEAK(K,M)=PEAK(I)
      ISOTIME(K,M)=TIME(I)
   80 CONTINUE
  100 IF (NREF.GE.4) GO TO 120
C COUNT(K) IS A COUNTER WHICH, AT THIS TIME, CONTAINS THE NUMBER OF
C EXPERIMENTAL PEAKS FOR MASS NUMBER K+230 WHICH WERE PROCESSED UP TO
C THE END OF THE FILTEMP PREVIOUS TO THE FILTEMP NOW BEING CONSIDERED.
      DO 105 K=1,15
  105 TOTAL(K)=COUNT(K)
      PRINT 110, (TITLE(I), I=1,7)
  110 FORMAT (1H1 2X A10,2X 3A10,2X A10,2X A10,2X A10,5X 11H* SPECTRE */// )
      GO TO 260
  120 CALL PARCEL (NREF,REFTIME,REFPEAK)
  200 DO 230 K=1,15
  205 J=COUNT(K)+1
      M=TOTAL(K)
      COUNT(K)=TOTAL(K)
      IF (M-J.GT.-1) GO TO 220
      IF (K.GE.15) GO TO 235
      K=K+1
      GO TO 205
  220 DO 230 I=J,M
C AT THIS POINT A QUANTITY CALLED REFVALU MUST BE OBTAINED.
      REFVALU=P(1)/ISOTIME(K,I)**1.5+P(2)/ISOTIME(K,I)**0.5
     C +P(3)*ISOTIME(K,I)**0.5+P(4)*ISOTIME(K,I)**1.5
  230 RATIO(K,I)=ISOPEAK(K,I)/REFVALU
C AT THIS POINT YPLOT(I) MUST BE CALCULATED.
```

```
  235 DO 240 I=1,100
      XPLOT(I)=REFTIME(1)+FLOAT(I-1)*(REFTIME(NREF)-REFTIME(1))/99.0
  240 YPLOT(I)=P(1)/XPLOT(I)**1.5+P(2)/XPLOT(I)**0.5
     C +P(3)*XPLOT(I)**0.5+P(4)*XPLOT(I)**1.5
C AT THIS POINT REFPLOT(I) MUST BE CALCULATED.
C REFPLOT(I) IS THE CALCULATED REFERENCE PEAK HEIGHT AT REFTIME(I).
      DO 250 I=1,NREF
      REFPLOT(I)=P(1)/REFTIME(I)**1.5+P(2)/REFTIME(I)**0.5
     C +P(3)*REFTIME(I)**0.5+P(4)*REFTIME(I)**1.5
  250 DIFFER(I)=(REFPEAK(I)-REFPLOT(I))/REFPLOT(I)*100.0
  260 PRINT 290, MASS(1),FILNUM
  290 FORMAT (X20X22HREFERENCE MASS NUMBER I3,8X9HFILTEMP (I1,1H)//
     C X5X82HMEASURED REFERENCE PEAK          CALCULATED REFERENCE PEAK
     C      PERCENT DIFFERENCE//)
  300 IF (NREF.GE.4) GO TO 306
      PRINT 304
  304 FORMAT (X77H***** LESS THAN FOUR REFERENCE PEAKS WERE MEASURED AT
     CTHIS FILTEMP, THEREFORE/
     C X74H***** A REFERENCE CURVE HAS NOT BEEN CALCULATED AND ALL DATA
     CTAKEN AT THIS/
     C X31H***** FILTEMP HAS BEEN IGNORED.//)
      GO TO 328
  306 DO 310 I=1,NREF
  310 PRINT 320, I,REFPEAK(I),REFPLOT(I),DIFFER(I)
  320 FORMAT (XI2,1H.2XF18.1,13XF18.1,15XF10.2)
      PRINT 321
  321 FORMAT(4(/)X100HTHE FUNCTION BEING FITTED IS:  REFERENCE VALUE=P(1
     C)/T**1.5 + P(2)/T**0.5 + P(3)*T**0.5 + P(4)*T**1.5///)
  324 DO 325 I=1,4
  325 PRINT 326, I,P(I)
  326 FORMAT (X5X2HP(I1,2H):1XE20.10)
      CALL GRAPHIC (XPLOT,YPLOT,NREF,REFTIME,REFPEAK)
  328 IF (FILNUM.GE.FILTEMP(N)) GO TO 340
      FILNUM=FILNUM+1
      GO TO 20
  340 RETURN
      END
```

```
      SUBROUTINE PARCEL (N,X,Y)
      INTEGER TOTAL(15)
      REAL RATIO(15,50),X(50),Y(50),PG(4),W(50),DP(4),SP(4),PC(4),P(4),
     C AM(4,4),BM(4,5),YC(50),DY(50),AN(4),PART(4)
      COMMON TITLE(8),RATIO,TOTAL,P
C IK=NUMBER OF PARAMETERS.  M=NUMBER OF INDEPENDENT VARIABLES.
C ITLIM=MAXIMUM NUMBER OF PERMISSIBLE ITERATIONS.  IFG CONTROLS THE
C SIGNS OF THE PARAMETERS ((0) OK TO CHANGE SIGNS AFTER 5 ITERATIONS.
C (1) SIGNS ALWAYS FREE TO CHANGE.  (2) SIGNS NEVER FREE TO CHANGE.).
      IK=4
      ITLIM=25
      M=1
      IFG=1
      TEST=0.000001
      DO 2000 I=1,N
 2000 W(I)=1.0
C CALCULATE (PG(K),K=1,4) THE INITIAL ESTIMATED VALUES OF THE PARAMETERS
      DO 2010 I=1,4
 2010 PG(I)=1.0
C INITIALIZATION FOR MAIN ITERATION LOOP
    1 KFREE=IK
      KP=KFREE+1
      IDF=N-KFREE
      DF=IDF
      IT=0
      DO 10 K=1,IK
      DP(K)=0.0
      SP(K)=0.0
      PC(K)=PG(K)
   10 P(K)=PG(K)
      LASTIT=0
      M25C=0
      IF (ITLIM.EQ.1) LASTIT=1
C MAIN ITERATION LOOP
    2 IT=IT+1
      H=1.0
      DO 30 K=1,KFREE
      DO 20 KK=1,KFREE
      AM(K,KK)=0.0
   20 BM(K,KK)=0.0
      BM(K,KP)=0.0
      K1=K+1
   30 BM(K,K1)=1.0
    3 VAR=0.0
      SSQ=0.0
C LOOP TO SET UP NORMAL EQUATIONS
      DO 90 I=1,N
C CALCULATE SUM OF SQUARES
      Z=X(I)
C DETERMINE AN EQUATION YT=F(P(1),P(2),P(3),P(4),Z)
      YT=P(1)/Z**1.5+P(2)/Z**0.5+P(3)*Z**0.5+P(4)*Z**1.5
      PART(1)=1.0/Z**1.5
      PART(2)=1.0/Z**0.5
      PART(3)=Z**0.5
      PART(4)=Z**1.5
      YC(I)=YT
      DY(I)=Y(I)-YC(I)
      VAR=VAR+W(I)*DY(I)**2
```

```
      SSQ=SSQ+DY(I)**2
C SET UP AN AS VECTOR OF PARTIAL DERIVATIVES
      K1=0
      DO 60 K=1,IK
    4 K2=K-K1
      AN(K2)=PART(K)
   60 CONTINUE
C FORM A AND B MATRICES
      DO 80 K=1,KFREE
      DO 70 KK=1,KFREE
   70 AM(K,KK)=AM(K,KK)+AN(K)*AN(KK)*W(I)
   80 BM(K,1)=BM(K,1)+AN(K)*DY(I)*W(I)
   90 CONTINUE
C SOLVE THE NORMAL EQUATIONS
    7 CALL LSS (KFREE,KP,4,AM,BM,TEMP,DET)
C CALCULATE NEW PARAMETER VALUES AND CHECK FOR SIGN CHANGES IF NECESSARY
   11 K1=0
      DO 140 K=1,IK
   12 K2=K-K1
      DP(K)=BM(K2,1)
   13 PC(K)=P(K)+H*DP(K)
      IF(LASTIT.NE.0)GOTO140
      IF(IFG-1)14,140,15
   14 IF(IT.GT.5)GOTO140
   15 IF(P(K)*PC(K).GE.0)GOTO140
      H=H/2
      IF(H.GE.1.0E-10)GOTO13
      RETURN
   16 K1=K1+1
  140 CONTINUE
      IF(LASTIT.NE.0)GOTO19
C TEST FOR CONVERGENCE
   17 KK=0
      DO 160 K=1,IK
      IF(P(K).EQ.0)GOTO18
      IF(ABS((PC(K)-P(K))/P(K))-TEST)160,160,19
   18 KK=KK+1
  160 CONTINUE
      IF(KK.EQ.IK)GOTO19
      M25C=1
C SET PARAMETER VALUES FOR THE NEXT ITERATION
   19 DO 170 K=1,IK
  170 P(K)=PC(K)
      IF(LASTIT.EQ.0)GOTO21
      PRINT 2020, (TITLE(I), I=1,7),IT
 2020 FORMAT (1H12XA10,2X3A10,2XA10,2XA10,2XA10,5X11H* SPECTRE *////
     C X2X38HTHE NUMBER OF ITERATIONS REQUIRED WAS I2/)
      RETURN
C TEST WHETHER THE MAXIMUM NUMBER OF ITERATIONS HAS BEEN TAKEN
   21 IF(M25C.EQ.1)GOTO22
      IF(IT.LT.ITLIM-1)GOTO2
C GO BACK FOR LAST ITERATION
   22 LASTIT=1
      GOTO2
      END
```

```
      SUBROUTINE GRAPHIC (XPOINT,YPOINT,NREF,REFTIME,REFPEAK)
      INTEGER ZMATRIX(6,51),ZLIST(31)
      DIMENSION NAME(113),MATRIX(6,51),LIST(31),XPOINT(100),
     C YPOINT(100),REFTIME(50),REFPEAK(50)
      DIMENSION M1(20),M2(8),N1(16),N2(4),N3(2),N4(16),N5(4),N6(14)
     C ,K2(4),K3(2),K4(16),K5(4),L2(4),L3(2),L4(16),L5(4),NN1(16),
     C NN2(4),NN3(2),NN4(16),NN5(4)
      KRDBGN=1
      KRDEND=100
      KCNTRL=1
      INCGRD=1
      ISIZE=2
      DATA M1(01),M1(02),M1(03),M1(04),M1(05),M1(06),M1(07),M1(08),
     1     M1(09),M1(10),M1(11),M1(12),M1(13),M1(14),M1(15),M1(16),
     2     M1(17),M1(18),M1(19),M1(20)/     1,     2,     4,     8,
     3         16,    32,    64,   128,   256,   512,  1024,  2048,
     4       4096,  8192, 16384, 32768, 65536,131072,262144,524288/
      DATA M2(01),M2(02),M2(03),M2(04),M2(05),M2(06),M2(07),M2(08)/
     1          1, 10, 100, 1000, 10000, 100000, 1000000, 10000000/
      DATA N1(01),N1(02),N1(03),N1(04),N1(05),N1(06),N1(07),N1(08),
     1     N1(09),N1(10),N1(11),N1(12),N1(13),N1(14),N1(15),N1(16)/
     C 4H    ,4H   .,4H  . ,4H  ..,4H .  ,4H . .,4H .. ,4H ...,
     C 4H.   ,4H.  .,4H. . ,4H. ..,4H..  ,4H.. .,4H... ,4H..../
      DATA NN1(01),NN1(02),NN1(03),NN1(04),NN1(05),NN1(06),NN1(07),
     C NN1(08),NN1(09),NN1(10),NN1(11),NN1(12),NN1(13),NN1(14),
     C NN1(15),NN1(16)/
     C 4H    ,4H   0,4H  0 ,4H  00,4H 0  ,4H 0 0,4H 00 ,4H 000,
     C 4H0   ,4H0  0,4H0 0 ,4H0 00,4H00  ,4H00 0,4H000 ,4H0000/
      DATA NN3(01),NN3(02)/4H    ,4H0   /
      DATA K2(01),K2(02),K2(03),K2(04)/4H    ,4H .  ,4H.   ,4H..  /
      DATA K3(01),K3(02)/4H    ,4H.   /
      DATA K4(01),K4(02),K4(03),K4(04),K4(05),K4(06),K4(07),K4(08)  ,
     1     K4(09),K4(10),K4(11),K4(12),K4(13),K4(14),K4(15),K4(16)/
     C 4H    ,4H   .,4H  . ,4H  ..,4H .  ,4H . .,4H .. ,4H ...,
     C 4H.   ,4H.  .,4H. . ,4H. ..,4H..  ,4H.. .,4H... ,4H..../
      DATA K5(01),K5(02),K5(03),K5(04)/4H    ,4H .  ,4H.   ,4H..  /
      DATA NN5(01),NN5(02),NN5(03),NN5(04)/4H    ,4H 0  ,4H0   ,4H00  /
      DATA N6(01),N6(02),N6(03),N6(04),N6(05),N6(06),N6(07),N6(08),
     1     N6(09),N6(10),N6(11),N6(12),N6(13),N6(14)/4H0   ,4H1   ,
     2     4H2   ,4H3   ,4H4   ,4H5   ,4H6   ,4H7   ,4H8   ,4H9   ,
     3     4H.   ,4H+   ,4H-   ,4H    /
      ITAPE=IABS(ISIZE)
   73 DO 75 I=1,16
      NN4(I)=NN1(I)
   75 N4(I)=K4(I)
      DO 76 I=1,4
      NN2(I)=NN5(I)
      N5(I)=K5(I)
   76 N2(I)=K2(I)
      N3(01)=K3(01)
      N3(02)=K3(02)
      N5(01)=4H+
C     ************SEARCH FOR MINIMUM AND MAXIMUM COORDINATES************
      XFIRST=XPOINT(KRDBGN)
      XFINAL=XPOINT(KRDBGN)
      YFIRST=YPOINT(KRDBGN)
      YFINAL=YPOINT(KRDBGN)
      KRD=KRDBGN
```

```
    1 KRD=KRD+1
      IF(XPOINT(KRD)-XFIRST)2,3,3
    2 XFIRST=XPOINT(KRD)
    3 IF(XPOINT(KRD)-XFINAL)5,5,4
    4 XFINAL=XPOINT(KRD)
    5 IF(YPOINT(KRD)-YFIRST)6,7,7
    6 YFIRST=YPOINT(KRD)
    7 IF(YPOINT(KRD)-YFINAL)9,9,8
    8 YFINAL=YPOINT(KRD)
    9 IF(KRD-KRDEND)1,10,10
   10 CALL MAXV (REFPEAK,1,NREF,IT,YMAX)
      IF (YMAX.GT.YFINAL) YFINAL=YMAX
      CALL MINV (REFPEAK,1,NREF,IT,YMIN)
      IF (YMIN.LT.YFIRST) YFIRST=YMIN
      WRITE(ITAPE,11)
   11 FORMAT(1H1)
   90 IF((XFINAL-XFIRST)/100.0)15,15,12
   12 IF(XFIRST+XFINAL)13,14,14
   13 IF((XFIRST/(XFIRST-XFINAL))-100000.0)18,18,15
   14 IF((XFINAL/(XFINAL-XFIRST))-100000.0)18,18,15
   15 WRITE(ITAPE,16)
   16 FORMAT(16X,51HPLOT ERROR, ZERO XPOINT HORIZONTAL COORDINATE RANGE)
      XFIRST=XFIRST-ABS(0.005*XFIRST)
      XFINAL=XFINAL+ABS(0.005*XFINAL)
      IF((XFINAL-XFIRST)/100.0)17,17,18
   17 XFIRST=-0.5
      XFINAL=0.5
   18 IF((YFINAL-YFIRST)/100.0)22,22,19
   19 IF(YFIRST+YFINAL)20,21,21
   20 IF((YFIRST/(YFIRST-YFINAL))-100000.0)25,25,22
   21 IF((YFINAL/(YFINAL-YFIRST))-100000.0)25,25,22
   22 WRITE(ITAPE,23)
   23 FORMAT(16X,51HPLOT ERROR, ZERO YPOINT VERTICAL COORDINATE RANGE  )
      YFIRST=YFIRST-ABS(0.005*YFIRST)
      YFINAL=YFINAL+ABS(0.005*YFINAL)
      IF((YFINAL-YFIRST)/100.0)24,24,25
   24 YFIRST=-0.5
      YFINAL=0.5
   25 XSCALE=100.0/(XFINAL-XFIRST)
      YSCALE=50.0/(YFINAL-YFIRST)
      DO 600 I=1,31
      LIST(I)=4H
  600 ZLIST(I)=4H
      DO 26 KOLUMN=1,6
      DO 26 LINE=1,51
      ZMATRIX(KOLUMN,LINE)=0
   26 MATRIX(KOLUMN,LINE)=0
C     ******************KONTRL = 1, GENERATE LINE PLOT******************
   30 LASTX=1.5+(XSCALE*(XPOINT(KRDBGN)-XFIRST))
      LINE=51.5-(YSCALE*(YPOINT(KRDBGN)-YFIRST))
      KOLUMN=(LASTX+19)/20
      LOCATN=(20*KOLUMN)-LASTX+1
      MATRIX(KOLUMN,LINE)=M1(LOCATN)
      DO 41 KRD=KRDBGN,KRDEND
      MOVEX=IFIX(1.5+(XSCALE*(XPOINT(KRD)-XFIRST)))-LASTX
      MOVEY=IFIX(51.5-(YSCALE*(YPOINT(KRD)-YFIRST)))-LINE
      JUMPX=IABS(MOVEX)
      JUMPY=IABS(MOVEY)
```

```
      IF(JUMPX)31,31,33
   31 IF(JUMPY)41,41,32
   32 LAGX=0
      LAGY=0
      MULT=JUMPY
      GO TO 38
   33 IF(JUMPY)34,34,35
   34 LAGX=0
      LAGY=0
      MULT=JUMPX
      GO TO 38
   35 LAGX=(MOVEX*JUMPY)/(2*JUMPX)
      LAGY=(JUMPX*MOVEY)/(2*JUMPY)
      IF(JUMPX-JUMPY)36,37,37
   36 MULT=JUMPY
      GO TO 38
   37 MULT=JUMPX
   38 DO 40 J=1,MULT
      NEWX=LASTX+(((J*MOVEX)+LAGX)/MULT)
      NEWY=LINE+(((J*MOVEY)+LAGY)/MULT)
      KOLUMN=(NEWX+19)/20
      LOCATN=(20*KOLUMN)-NEWX+1
      KOMPAR=MATRIX(KOLUMN,NEWY)/M1(LOCATN)
      IF(KOMPAR-(2*(KOMPAR/2)))39,39,40
   39 MATRIX(KOLUMN,NEWY)=MATRIX(KOLUMN,NEWY)+M1(LOCATN)
   40 CONTINUE
      LASTX=NEWX
      LINE=NEWY
   41 CONTINUE
C     ******************KONTRL = 0, GENERATE POINT PLOT*****************
      DO 620 KRD=1,NREF
      LASTX=1.5+(XSCALE*(REFTIME(KRD)-XFIRST))
      LINE=51.5-(YSCALE*(REFPEAK(KRD)-YFIRST))
      KOLUMN=(LASTX+19)/20
      LOCATN=(20*KOLUMN)-LASTX+1
      KOMPAR=ZMATRIX(KOLUMN,LINE)/M1(LOCATN)
      IF (KOMPAR-(2*(KOMPAR/2))) 610,610,620
  610 ZMATRIX(KOLUMN,LINE)=ZMATRIX(KOLUMN,LINE)+M1(LOCATN)
  620 CONTINUE
C     ******************PRINT THE PLOT STORAGE ARRAY*******************
   42 LOCK=0
      FIRST=YFIRST
      FINAL=YFINAL
      GO TO 53
   43 IBGN=1
      DO 50 LINE=IBGN,51
      IF(LOCK)47,47,44
   44 LOCK=LOCK-1
      DO 45 KOLUMN=1,5
      INDEX5=MATRIX(KOLUMN,LINE)/16
      INDEX4=INDEX5/16
      INDEX3=INDEX4/4
      INDEX2=INDEX3/16
      INDEX1=INDEX2/16
      INDEX6=MATRIX(KOLUMN,LINE)-16*INDEX5
      INDEX5=INDEX5-16*INDEX4
      INDEX4=INDEX4-4*INDEX3
      INDEX3=INDEX3-16*INDEX2
```

```
      INDEX2=INDEX2-16*INDEX1
      LIST(6*KOLUMN)   =N1(INDEX6+1)
      LIST(6*KOLUMN-1)=N1(INDEX5+1)
      LIST(6*KOLUMN-2)=N2(INDEX4+1)
      LIST(6*KOLUMN-3)=N1(INDEX3+1)
      LIST(6*KOLUMN-4)=N1(INDEX2+1)
      LIST(6*KOLUMN-5)=N2(INDEX1+1)
      INDEX5=ZMATRIX(KOLUMN,LINE)/16
      INDEX4=INDEX5/16
      INDEX3=INDEX4/4
      INDEX2=INDEX3/16
      INDEX1=INDEX2/16
      INDEX6=ZMATRIX(KOLUMN,LINE)-16*INDEX5
      INDEX5=INDEX5-16*INDEX4
      INDEX4=INDEX4-4*INDEX3
      INDEX3=INDEX3-16*INDEX2
      INDEX2=INDEX2-16*INDEX1
      ZLIST(6*KOLUMN)=NN1(INDEX6+1)
      ZLIST(6*KOLUMN-1)=NN1(INDEX5+1)
      ZLIST(6*KOLUMN-2)=NN2(INDEX4+1)
      ZLIST(6*KOLUMN-3)=NN1(INDEX3+1)
      ZLIST(6*KOLUMN-4)=NN1(INDEX2+1)
      ZLIST(6*KOLUMN-5)=NN2(INDEX1+1)
   45 CONTINUE
      INDEX1=1+(MATRIX(6,LINE)/524288)
      LIST(31)=N3(INDEX1)
      INDEX1=1+ZMATRIX(6,LINE)/524288
      ZLIST(31)=NN3(INDEX1)
      WRITE(ITAPE,46)(LIST(I),I=1,31),(ZLIST(I),I=1,31)
   46 FORMAT (1H+15X10(A2,2A4),A1/X15X10(A2,2A4),A1)
      GO TO 50
   47 LOCK=4
      DO 48 KOLUMN=1,5
      INDEX5=MATRIX(KOLUMN,LINE)/16
      INDEX4=INDEX5/16
      INDEX3=INDEX4/4
      INDEX2=INDEX3/16
      INDEX1=INDEX2/16
      INDEX6=MATRIX(KOLUMN,LINE)-16*INDEX5
      INDEX5=INDEX5-16*INDEX4
      INDEX4=INDEX4-4*INDEX3
      INDEX3=INDEX3-16*INDEX2
      INDEX2=INDEX2-16*INDEX1
      LIST(6*KOLUMN)   =N4(INDEX6+1)
      LIST(6*KOLUMN-1)=N4(INDEX5+1)
      LIST(6*KOLUMN-2)=N5(INDEX4+1)
      LIST(6*KOLUMN-3)=N4(INDEX3+1)
      LIST(6*KOLUMN-4)=N4(INDEX2+1)
      LIST(6*KOLUMN-5)=N5(INDEX1+1)
      INDEX5=ZMATRIX(KOLUMN,LINE)/16
      INDEX4=INDEX5/16
      INDEX3=INDEX4/4
      INDEX2=INDEX3/16
      INDEX1=INDEX2/16
      INDEX6=ZMATRIX(KOLUMN,LINE)-16*INDEX5
      INDEX5=INDEX5-16*INDEX4
      INDEX4=INDEX4-4*INDEX3
      INDEX3=INDEX3-16*INDEX2
```

```
      INDEX2=INDEX2-16*INDEX1
      ZLIST(6*KOLUMN)=NN4(INDEX6+1)
      ZLIST(6*KOLUMN-1)=NN4(INDEX5+1)
      ZLIST(6*KOLUMN-2)=NN5(INDEX4+1)
      ZLIST(6*KOLUMN-3)=NN4(INDEX3+1)
      ZLIST(6*KOLUMN-4)=NN4(INDEX2+1)
      ZLIST(6*KOLUMN-5)=NN5(INDEX1+1)
   48 CONTINUE
      INDEX1=1+(MATRIX(6,LINE)/524288)
      LIST(31)=N3(INDEX1)
      IF(INDGRD.EQ.1.A.MOD(LINE,5).EQ.1.A.INDEX1.NE.2) LIST(31)=4H+
      IF(INDGRD.EQ.1.A.MOD(LINE,5).EQ.1.A.INDEX6.LE.7.A.ISIZE.LT.0.A.
     1KOLUMN.EQ.5) LIST(25)=4H+
      IF(INDGRD.EQ.1.A.MOD(LINE,5).EQ.1.A.INDEX6.LE.7.A.ISIZE.EQ.0.A.
     1KOLUMN.EQ.5) LIST(13)=4H+
      INDEX1=1+(ZMATRIX(6,LINE)/524288)
      ZLIST(31)=NN3(INDEX1)
      INDEX1=101-(2*(LINE-1))
      INDEX2=INDEX1+9
      IF (ISIZE.GT.0)
     1WRITE(ITAPE,49)(NAME(I),I=INDEX1,INDEX2),(NAME(I),I=111,113),
     2 (LIST(I),I=1,31),(ZLIST(I),I=1,31)
   49 FORMAT (1H+10A1,1HE3A1,1X10(A2,2A4),A1/X15X10(A2,2A4),A1)
   50 CONTINUE
      FIRST=XFIRST
      FINAL=XFINAL
      GO TO 53
   51 IF (ISIZE.GT.0)
     1WRITE(ITAPE,52)(NAME(I),I=1,110),((NAME(I),I=111,113),J=1,11)
   52 FORMAT(1HO,11X,110A1/9X,11(6X,1HE,3A1))
      RETURN
C
C     **************ALPHANUMERIC CODE SCALE NUMBER ARRAYS****************
   53 STEP=(FINAL-FIRST)/10.0
      KOUNT=ALOG10(1.01*STEP)-2.0
      IF((1.01*STEP)-100.0)54,55,55
   54 KOUNT=KOUNT-1
   55 ROUND=5.0*(10.0**KOUNT)
      IF(FIRST+FINAL)56,57,57
   56 FINAL=-FIRST
   57 FINAL=FINAL+ROUND
      KOEFF=ALOG10(FINAL)
      IF(FINAL-1.0)58,59,59
   58 KOEFF=KOEFF-1
      NAME(111)=N6(13)
      INDEX1=-KOEFF/10
      INDEX2=-KOEFF-10*INDEX1
      GO TO 60
   59 NAME(111)=N6(12)
      INDEX1=KOEFF/10
      INDEX2=KOEFF-10*INDEX1
   60 NAME(112)=N6(INDEX1+1)
      NAME(113)=N6(INDEX2+1)
      DO 61 I=1,110
   61 NAME(I)=N6(14)
      KOUNT=KOEFF-KOUNT
      IF(KOUNT-8)63,63,62
   62 KOUNT=8
```

```
63 KOEFF=KOUNT-KOEFF-1
   ADD=0.0
   DO 71 I=1,11
   LEFT=(I*10)-9+((9-KOUNT)/2)
   IF(FIRST+ADD)64,65,65
64 NAME(LEFT-1)=N6(13)
   VALUE=(ROUND-ADD)-FIRST
   GO TO 66
65 VALUE=(ROUND+ADD)+FIRST
66 INTEGR=VALUE*(10.0**KOEFF)
67 INDEX1=1+(INTEGR/M2(KOUNT))
   IF(INDEX1-11)69,68,72
68 INTEGR=INTEGR-1
   GO TO 67
69 NAME(LEFT)=N6(INDEX1)
   NAME(LEFT+1)=N6(11)
   LEFT=LEFT+2
   DO 70 J=2,KOUNT
   INDEX1=KOUNT-J+1
   INDEX1=1+(INTEGR/M2(INDEX1))-(10*(INTEGR/M2(INDEX1+1)))
   NAME(LEFT)=N6(INDEX1)
70 LEFT=LEFT+1
71 ADD=ADD+STEP
72 IF(LOCK)43,43,51
   END
```

```
      SUBROUTINE ANALYZE (MASS)
C SUBROUTINE ANALYZE COMPUTES THE MOST PROBABLE RATIO AND ASSOCIATED
C UNCERTAINTY FOR EACH MASS NUMBER EXAMINED.
      INTEGER TOTAL(15)
      REAL RATIO(15,50),DEV(15,50),SIGMA(15),SIGBAR(15),REJECT(20),P(4),
     C PERDEV(15,50)
      COMMON TITLE(8),RATIO,TOTAL,P
      FUDGE=0.0035
      DATA (REJECT(I),I=1,20)/1.15,1.15,1.15,1.46,1.67,1.82,1.94,2.03,
     C 2.11,2.18,2.23,2.29,2.33,2.37,2.41,2.44,2.47,2.50,2.53,2.56/
      DO 230 K=1,15
   20 ISOMASS=K+230
      FACTOR=1.0+(ISOMASS-MASS)*FUDGE
      BINGO=0.0
      M=TOTAL(K)
   30 IF (M.GT.0) GO TO 40
      IF (K.GE.15) GO TO 230
      K=K+1
      GO TO 20
   40 DO 45 I=1,M
   45 RATIO(K,I)=RATIO(K,I)*FACTOR
   50 SUM=0.0
      DO 60 I=1,M
   60 SUM=SUM+RATIO(K,I)
      AVE=SUM/FLOAT(M)
      SUMSQ=0.0
      DO 70 I=1,M
      DEV(K,I)=RATIO(K,I)-AVE
      PERDEV(K,I)=DEV(K,I)/AVE*100.0
   70 SUMSQ=SUMSQ+DEV(K,I)**2
      IF (M.EQ.1) 72,74
   72 SIGBAR(K)=0.0
      GO TO 80
   74 SIGMA(K)=SQRT(SUMSQ/FLOAT(M-1))
      SIGBAR(K)=SIGMA(K)/SQRT(FLOAT(M))
   80 PRINT 90, (TITLE(I), I=1,7)
   90 FORMAT (1H1 2XA10,2X3A10,2XA10,2XA10,2XA10,5X11H* SPECTRE */////)
      PRINT 100, ISOMASS,MASS,FACTOR
  100 FORMAT (X2X20HISOTOPE MASS NUMBER I3//
     C X2X22HREFERENCE MASS NUMBER I3//
     C X2X18HCORRECTION FACTOR F7.5///
     C X2X80HMEASUREMENT NO.    UNCORRECTED RATIO          DEVIATION
     C      CORRECTED RATIO/
     C X42X19H(PERCENT)   (SIGMA)///)
      DO 110 I=1,M
      UNRATIO=RATIO(K,I)/FACTOR
      DSIGMA=DEV(K,I)/SIGMA(K)
  110 PRINT 120, I,UNRATIO,PERDEV(K,I),DSIGMA,RATIO(K,I)
  120 FORMAT (X2XI2,1H.16XF10.5,12XF6.2,5XF6.2,6XF10.5)
      IF (M.EQ.1) GO TO 220
      UNAVE=AVE/FACTOR
      UNSIGMA=SIGMA(K)/FACTOR
      UNSIGBR=SIGBAR(K)/FACTOR
      PRINT 130, UNAVE,UNSIGMA,UNSIGBR,AVE,SIGMA(K),SIGBAR(K)
  130 FORMAT (//X2X52HTHE UNCORRECTED AVERAGE RATIO=
     C  F14.8/
     C X2X52HSTANDARD DEVIATION IN AN UNCORRECTED SINGLE RATIO=  F14.8/
     C X2X52HSTANDARD DEVIATION IN THE UNCORRECTED AVERAGE RATIO=F14.8//
```

```
     C X2X52HTHE CORRECTED AVERAGE RATIO=                                F14.8/
     C X2X52HSTANDARD DEVIATION IN A CORRECTED SINGLE RATIO=             F14.8/
     C X2X52HSTANDARD DEVIATION IN THE CORRECTED AVERAGE RATIO=          F14.8//
     C /)
      BINGO=0.0
      TEST=REJECT(M)
  140 DO 170 I=1,M
  145 IF (ABS(DEV(K,I))/SIGMA(K).GT.TEST) 150,170
  150 BINGO=99.0
      M=M-1
      DO 160 J=I,M
      RATIO(K,J)=RATIO(K,J+1)
  160 DEV(K,J)=DEV(K,J+1)
      IF (I.LT.M+1) GO TO 145
  170 CONTINUE
      IF (BINGO.EQ.99.0) 180,220
  180 PRINT 190
  190 FORMAT (X70H  *****  THE FOREGOING TABLE CONTAINS ONE OR MCRE RATI
     COS WHICH DEVIATE/
     C X77H  *****  UNACCEPTABLY FROM THE AVERAGE.  A RECOMPUTATION WITH
     COUT THESE RATIOS/
     C X17H  *****  FOLLOWS:////)
      GO TO 50
  220 RATIO(K)=AVE
      RATIO(K,2)=SIGBAR(K)
C RATIO(K) AND RATIO(K,2) ARE SIMPLY BEING USED TO PASS THE AVERAGE
C RATIO AND ASSOCIATED UNCERTAINTY FOR EACH MASS NUMBER BACK TO PROGRAM
C SPECTRE AND THENCE TO SUBPROGRAM MEMO.
  230 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE MEMO (MASS)
C SUBROUTINE MEMO CONVERTS THE AVERAGE RATIO AND ASSOCIATED UNCERTAINTY
C FOR EACH MASS NUMBER EXAMINED TO A PERCENT OF TOTAL MASS
C WITH A RECALCULATED UNCERTAINTY, AND THEN PUBLISHES A REPORT
C CONTAINING THIS INFORMATION.
      INTEGER TOTAL(15),MONTH(12)
      REAL RATIO(15,50),ATOMRAT(15),ATOMERR(15),PERCENT(15),ERROR(15),
     C P(4),TFACTOR(20)
      COMMON TITLE(8),RATIO,TOTAL,P
      EQUIVALENCE (RATIO,PERCENT)
      SUM=0.0
      SUMSQ=0.0
      DATA (TFACTOR(I),I=1,20)/1.00,12.7,4.30,3.18,2.78,2.57,2.45,2.36,
     C 2.31,2.26,2.23,2.20,2.18,2.16,2.14,2.13,2.12,2.11,2.10,2.09/
      DO 40 K=1,15
   10 IF (TOTAL(K).GT.0) GO TO 30
      IF (K.GE.15) GO TO 42
      K=K+1
      GO TO 10
C RATIO(K) AND RATIO(K,2) CONTAIN THE AVERAGE RATIO AND ASSOCIATED
C UNCERTAINTY FOR EACH MASS NUMBER RESPECTIVELY.
   30 ATOMRAT(K)=RATIO(K)
      M=TOTAL(K)
      ATOMERR(K)=SQRT((TFACTOR(M)*RATIO(K,2))**2+(0.03*ATOMRAT(K))**2)
C THE FOLLOWING 2 STEPS CONVERT ATOMRAT(K) FROM AN ATOM RATIO TO A MASS
C RATIO AND ADJUST THE UNCERTAINTY IN THIS FIGURE ACCORDINGLY.
      RATIO(K)=ATOMRAT(K)*FLOAT(K+230)/MASS
      RATIO(K,2)=ATOMERR(K)*FLOAT(K+230)/MASS
      SUM=SUM+RATIO(K)
   40 SUMSQ=SUMSQ+RATIO(K,2)**2
   42 SUM=SUM+1.0
      ERROR1=SQRT(SUMSQ)
      DO 70 K=1,15
   45 IF (TOTAL(K).GT.0) GO TO 60
      IF (K.GE.15) GO TO 72
      K=K+1
      GO TO 45
   60 ERROR(K)=SQRT((1.0/SUM*RATIO(K,2))**2+(RATIO(K)/SUM**2*ERROR1)
     C **2)*100.0
   70 PERCENT(K)=RATIO(K)/SUM*100.0
   72 K=MASS-230
      TOTAL(K)=1
      ATOMRAT(K)=1.0
      ATOMERR(K)=0.0
      PERCENT(K)=1.0/SUM*100.0
      ERROR(K)=1.0/SUM**2*ERROR1*100.0
      NUMBER=0
      CALL DATE (DAY)
      DECODE (6,74,DAY) NDAY
   74 FORMAT (I6)
      NMONTH=NDAY/10000
      NDAY=NDAY-NMONTH*10000
      NYEAR=NDAY-(NDAY/100)*100
      NDAY=NDAY/100
      DATA (MONTH(I),I=1,12)/3HJAN,3HFEB,3HMAR,3HAPR,3HMAY,3HJUN,3HJUL,
     C 3HAUG,3HSEP,3HOCT,3HNOV,3HDEC/
   75 PRINT 80, NDAY,MONTH(NMONTH),NYEAR,TITLE(6),TITLE(5),
     C (TITLE(I),I=2,4),TITLE(1),TITLE(7),MASS
```

```
 80 FORMAT (1H1,44X,32HLOS ALAMOS SCIENTIFIC LABORATORY/
   C X48X24HUNIVERSITY OF CALIFORNIA/
   C X46X28HLOS ALAMOS, NEW MEXICO 87544///
   C X31X17HOFFICE MEMORANDUM,50X,11H* SPECTRE *///
   C X2X22HTO      :  DISTRIBUTION,24X,6HDATE: I2,1XA3,1XI2//
   C X2X24HFROM    :  R. M. TISINGER//
   C X2X38HSUBJECT:  MASS SPECTROMETER ANALYSIS (A10,1XA10,9X1H)/
   C X39X32H(SAMPLE SERIAL NUMBER          )//
   C X39X1H(3A10,1H)/
   C X2X8HSYMBOL : 4(/)
   C X15X55HAN ANALYSIS OF THE SAMPLE DESCRIBED ABOVE WAS COMPLETED/
   C X10X3HON A9,41H.  THIS ANALYSIS WAS PERFORMED USING THE A10/
   C X10X64HMASS SPECTROMETER.  RESULTS ARE TABULATED BELOW WITH UNCER
   CTAINTY/
   C X10X60HEXPRESSED AT THE NINETY-FIVE PERCENT CONFIDENCE LEVEL.  AT
   COM/
   C X10X64HRATIO IS THE NUMERICAL RATIO OF THE NUMBER OF ATOMS OF SPE
   CCIFIED/
   C X10X50HMASS NUMBER TO THE NUMBER OF ATOMS OF MASS NUMBER I3,1H.
   C ///)
     PRINT 90
 90 FORMAT (X10X60HMASS NUMBER        ATOM RATIO                    WEIGH
   CT PERCENT//)
     DO 200 K=1,15
160  IF (TOTAL(K).GT.0) GO TO 180
     IF (K.GE.15) GO TO 210
     K=K+1
     GO TO 160
180  MASSNUM=K+230
     PRINT 190, MASSNUM,ATOMRAT(K),ATOMERR(K),PERCENT(K),ERROR(K)
190  FORMAT (X10XI3,6XF11.5,4H +- F8.5,11XF7.4,4H +- F7.4/)
200  CONTINUE
210  PRINT 220
220  FORMAT (4(/)X48X14HR. M. TISINGER/
   C X48X9HGROUP W-7 /
   C X10X13HDISTRIBUTION:/)
     IF (TITLE(5).EQ.10HPRESHOT    ) GO TO 230
     IF (TITLE(5).EQ.10HPOSTSHOT   ) GO TO 250
     IF (TITLE(5).EQ.10HSPECIAL    ) GO TO 270
     GO TO 300
230  PRINT 240
240  FORMAT (X15X22H  W- 1  J. J. WECHSLER)
250  PRINT 260
260  FORMAT (X15X17H  W- 4  R. CANADA/
   C X15X34H  J-11  E. G. HANTEL / G. A. COWAN)
     IF (TITLE(8).EQ.10HANDERSON   ) PRINT 262
262  FORMAT (X15X22HCMB-11  J. W. ANDERSON)
     IF (TITLE(8).EQ.10HJAYNES     ) PRINT 264
264  FORMAT (X15X20HCMB- 6  G. E. JAYNES)
270  PRINT 280
280  FORMAT (X15X22H  W- 7  W. H. CHAMBERS/
   C X15X22H  W- 7  R. M. TISINGER)
     NUMBER=NUMBER+1
     IF (NUMBER.LT.2) GO TO 75
300  RETURN
     END
```

APPENDIX F

OUTPUT

The output pages contained in this Appendix are representitive of the results regularly obtained with program SPECTRE. This particular output was produced on September 4, 1970 using an actual data deck during a computer run made for the purpose of generating the listing for Appendix E. The sample material was obtained from a supply of National Bureau of Standards' Standard Reference Material U-930 (NBS-930). The isotopic composition of NBS-930 has been carefully measured and the atom and weight percentage figures published by the National Bureau of Standards are stated in Figure 16. Figure 16 is located on page 139 for ease in comparison with the corresponding experimental figures on page 138.

The following output pages are complete and in the order produced. The first and last pages (title and letter report) are included only once, whereas they were actually printed twice. The letter report is the real product of program SPECTRE, and is disseminated according to the indicated distribution. The other output pages are reviewed to ensure that measurements were consistant and that nothing untoward occurred. These pages, along with a copy of the letter report, are then filed for record purposes.

TABLE 3. A Sequential Listing of Output Sections

Sequence Number	Section Name	Pages (inclusive)	Use
1.	Title page	126	for identification after filing
2.	Input data	127 - 128	to establish a permanent record
3.	Reference curves and calculations[1]	129 - 134	for verifying that smooth well-fitted curves have been found
4.	Isotope measurement data	135 - 137	to allow an examination of the data for each isotope
5.	Letter report	138	for immediate distribution

[1]Reference curves are plotted with reference peak height in arbitrary units along the vertical axis and time in seconds along the horizontal axis.

INPUT DATA:

FILTEMP CODE, SCALE FACTOR, MASS NUMBER (FOLLOWED BY 3 DATA POINTS)
HOUR:MINUTE:SECOND, INTEGRATION TIME (SEC), PEAK HEIGHT

1.	1	7	235		10.	1	4	238		19.	1	2	236		28.	1	2	234	
0	2	28	10	605	0	12	38	10	3988	0	22	54	10	40466	0	32	28	10	41368
0	2	50	10	37909	0	13	10	10	25832	0	23	12	10	46184	0	33	2	10	69546
0	3	22	10	111	0	13	26	10	4005	0	23	26	10	40449	0	33	24	10	41355
2.	1	4	238		11.	1	6	235		20.	1	6	235		29.	1	6	235	
0	3	40	10	4052	0	13	46	10	371	0	23	44	10	374	0	33	44	10	382
0	4	20	10	61814	0	14	18	10	35428	0	24	12	10	26985	0	34	12	10	23042
0	4	38	10	4039	0	14	36	10	376	0	24	28	10	382	0	34	30	10	384
3.	1	4	238		12.	1	4	238		21.	1	2	236		30.	1	5	235	
0	4	56	10	4000	0	14	54	10	4002	0	24	52	10	40697	0	34	48	10	1199
0	5	36	10	51900	0	15	22	10	22843	0	25	20	10	46552	0	35	18	10	68300
0	5	52	10	4010	0	15	38	10	4007	0	25	38	10	40728	0	35	40	10	1202
4.	1	7	235		13.	1	4	238		22.	1	2	236		31.	1	2	234	
0	6	16	10	95	0	15	56	10	3993	0	25	56	10	40696	0	36	4	10	41429
0	6	42	10	21988	0	16	18	10	21898	0	26	18	10	46548	0	36	42	10	65957
0	6	58	10	101	0	16	34	10	4000	0	26	34	10	40697	0	36	58	10	41626
5.	1	6	235		14.	1	6	235		23.	1	6	235		32.	1	2	234	
0	7	16	10	374	0	16	52	10	370	0	26	52	10	375	0	37	16	10	41413
0	7	38	10	65707	0	17	22	10	31965	0	27	20	10	26286	0	37	46	10	65248
0	8	0	10	380	0	17	40	10	376	0	27	36	10	380	0	38	10	10	41426
6.	1	4	238		15.	1	2	236		24.	1	2	236		33.	1	5	235	
0	8	22	10	3988	0	18	0	10	40361	0	27	56	10	40972	0	38	30	10	1201
0	8	50	10	36467	0	18	46	10	46868	0	28	20	10	46469	0	38	56	10	57472
0	9	6	10	4022	0	19	4	10	40345	0	28	36	10	40988	0	39	16	10	1205
7.	1	4	238		16.	1	2	236		25.	1	2	236		34.	1	2	234	
0	9	24	10	3985	0	19	22	10	40352	0	28	54	10	40978	0	39	34	10	41504
0	9	48	10	33178	0	19	50	10	46491	0	29	16	10	46606	0	40	6	10	61936
0	10	10	10	3996	0	20	10	10	40236	0	29	32	10	40791	0	40	24	10	41480
8.	1	6	235		17.	1	6	235		26.	1	6	235		35.	1	2	234	
0	10	32	10	370	0	20	32	10	371	0	29	52	10	372	0	40	42	10	41527
0	10	58	10	46052	0	21	10	10	28284	0	30	22	10	25319	0	41	4	10	60731
0	11	18	10	383	0	21	26	10	376	0	30	40	10	381	0	41	24	10	41510
9.	1	4	238		18.	1	2	236		27.	1	2	234		36.	1	5	235	
0	11	36	10	4000	0	21	46	10	40443	0	31	0	10	41297	0	41	42	10	1204
0	12	4	10	27735	0	22	16	10	46331	0	31	50	10	70073	0	42	36	10	45469
0	12	20	10	4536	0	22	36	10	40398	0	32	10	10	41441	0	42	56	10	1212

```
37.  1   2  234
  0 43 14   10   41668
  0 43 38   10   57507
  0 43 58   10   41623

38.  1   2  234
  0 44 16   10   41639
  0 44 40   10   56195
  0 44 58   10   41644

39.  1   5  235
  0 45 16   10    1203
  0 45 42   10   37590
  0 46 10   10    1209
```

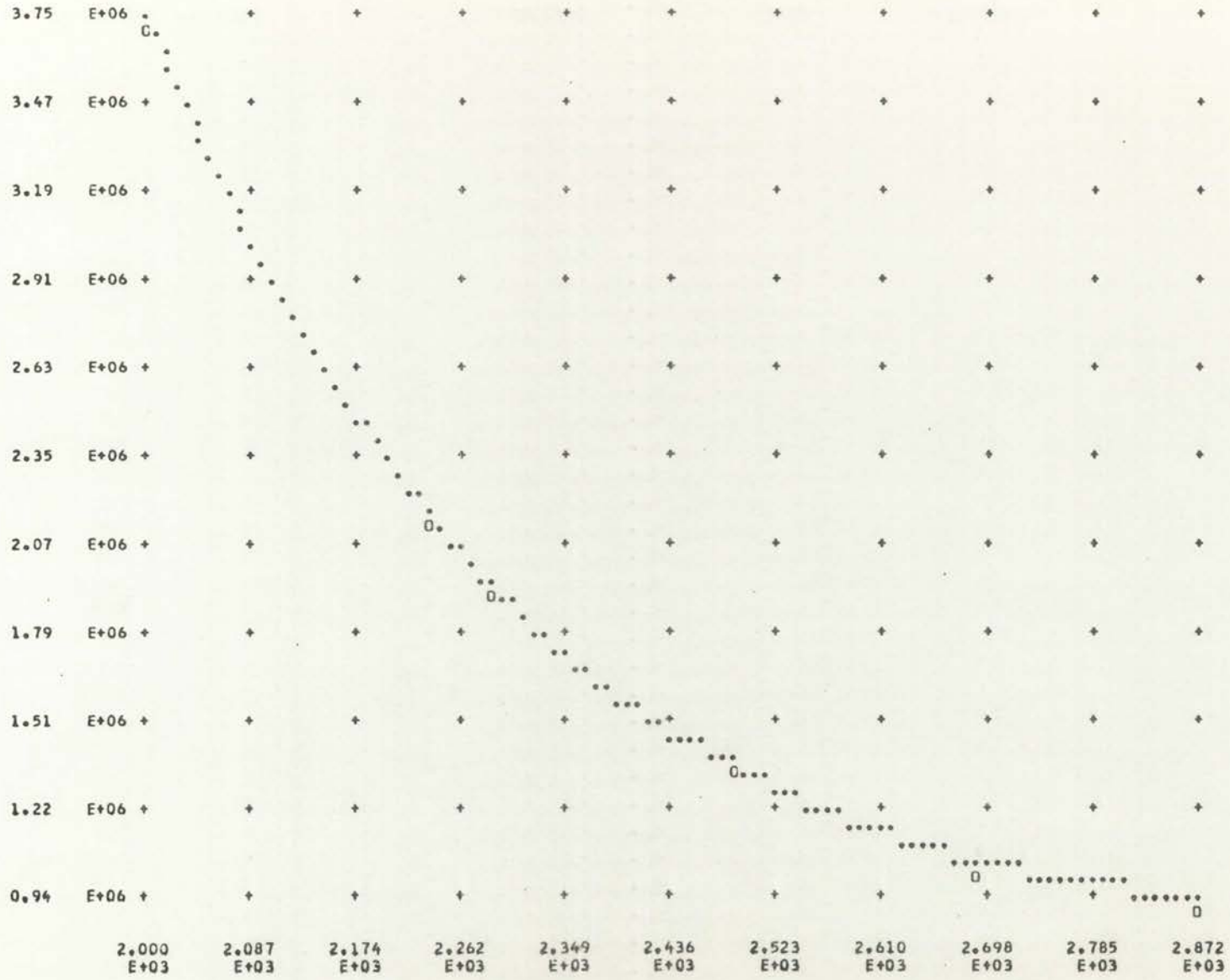
THE NUMBER OF ITERATIONS REQUIRED WAS 3

REFERENCE MASS NUMBER 235 FILTEMP (1)

	MEASURED REFERENCE PEAK	CALCULATED REFERENCE PEAK	PERCENT DIFFERENCE
1.	3750525.9	3749031.3	.04
2.	2188928.6	2198967.3	-.46
3.	1959900.0	1954699.3	.27
4.	1370239.6	1359482.4	.79
5.	1051614.0	1062733.5	-1.05
6.	947737.5	944031.8	.39

THE FUNCTION BEING FITTED IS: REFERENCE VALUE=P(1)/T**1.5 + P(2)/T**0.5 + P(3)*T**0.5 + P(4)*T**1.5

P(1): .4549562729E+13
P(2): -.4198884319E+10
P(3): .1316134667E+07
P(4): -.1351261508E+03


3.75 E+06
3.47 E+06
3.19 E+06
2.91 E+06
2.63 E+06
2.35 E+06
2.07 E+06
1.79 E+06
1.51 E+06
1.22 E+06
0.94 E+06
2.000 E+03
2.087 E+03
2.174 E+03
2.262 E+03
2.349 E+03
2.436 E+03
2.523 E+03
2.610 E+03
2.698 E+03
2.785 E+03
2.872 E+03

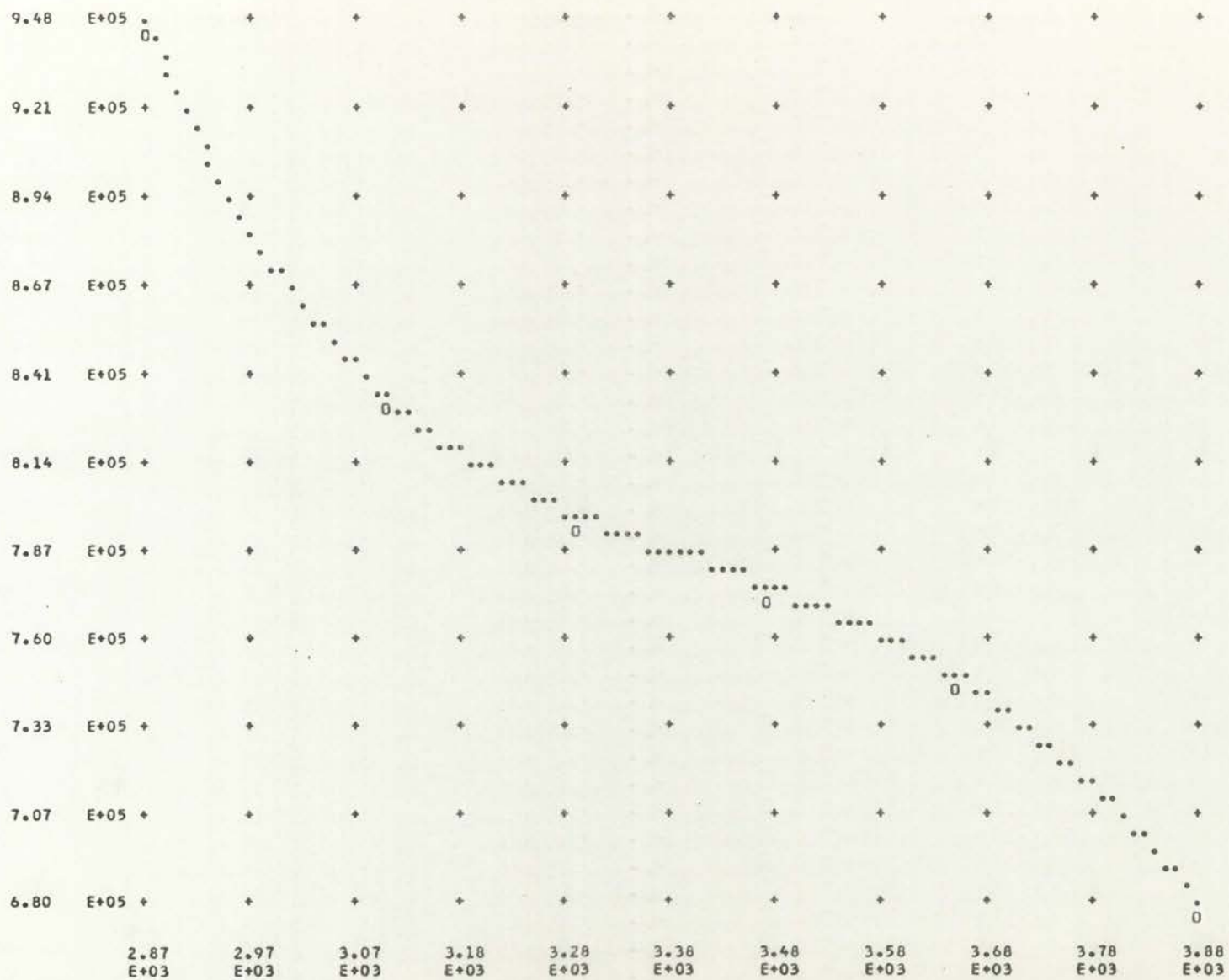
THE NUMBER OF ITERATIONS REQUIRED WAS 3

REFERENCE MASS NUMBER 235 FILTEMP (2)

	MEASURED REFERENCE PEAK	CALCULATED REFERENCE PEAK	PERCENT DIFFERENCE
1.	947737.5	947923.4	-.02
2.	837284.4	836342.2	.11
3.	798177.3	799541.3	-.17
4.	777234.5	776673.8	.07
5.	748241.2	748074.8	.02
6.	679763.5	679883.1	-.02

THE FUNCTION BEING FITTED IS: REFERENCE VALUE=P(1)/T**1.5 + P(2)/T**0.5 + P(3)*T**0.5 + P(4)*T**1.5

P(1): .4166503420E+13
P(2): -.3647590149E+10
P(3): .1091309507E+07
P(4): -.1074856525E+03


9.48 E+05
9.21 E+05
8.94 E+05
8.67 E+05
8.41 E+05
8.14 E+05
7.87 E+05
7.60 E+05
7.33 E+05
7.07 E+05
6.80 E+05
2.87 E+03
2.97 E+03
3.07 E+03
3.18 E+03
3.28 E+03
3.38 E+03
3.48 E+03
3.58 E+03
3.68 E+03
3.78 E+03
3.88 E+03

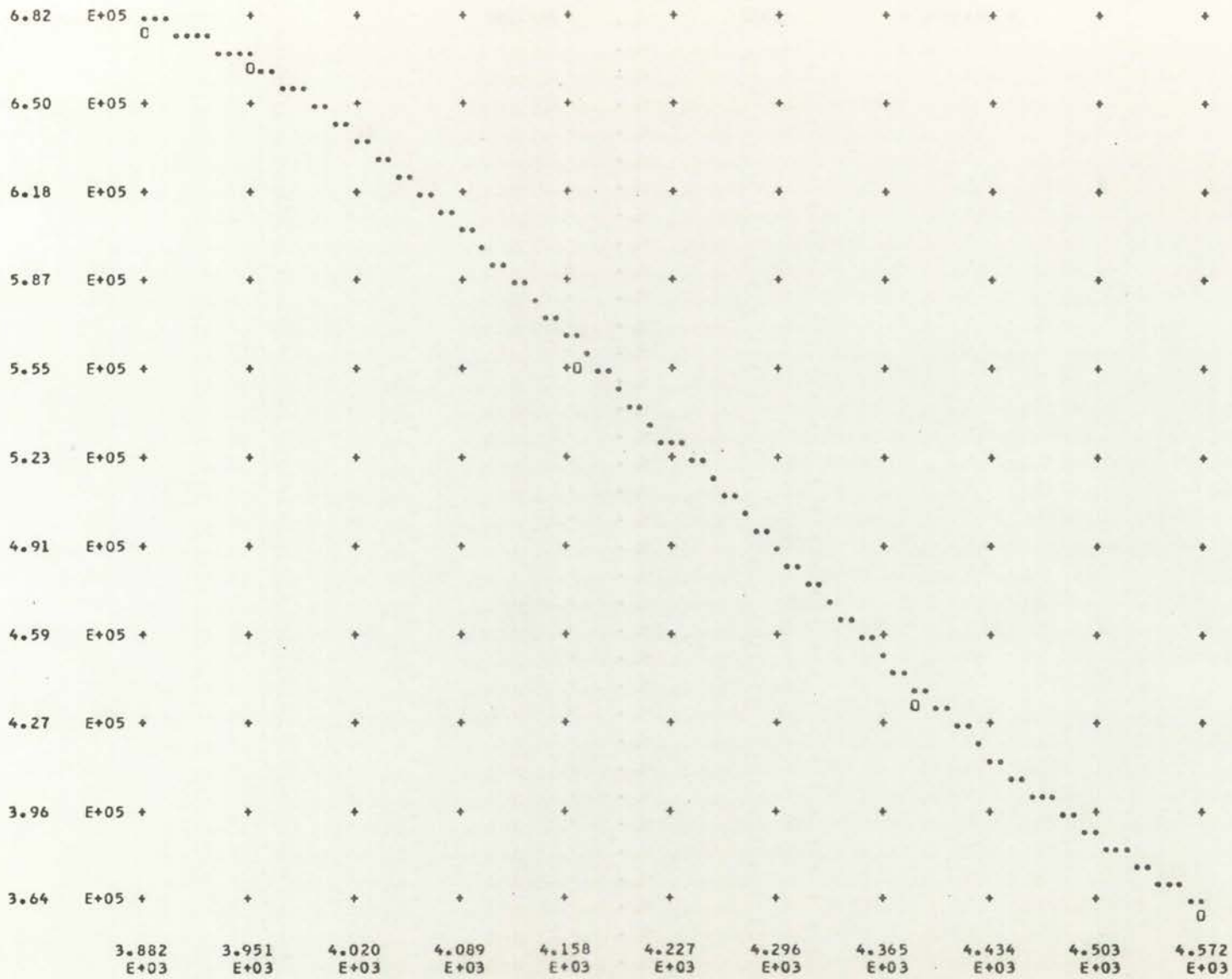
THE NUMBER OF ITERATIONS REQUIRED WAS 4

REFERENCE MASS NUMBER 235 FILTEMP (3)

	MEASURED REFERENCE PEAK	CALCULATED REFERENCE PEAK	PERCENT DIFFERENCE
1.	679763.5	681931.3	-.32
2.	670992.7	667307.3	.55
3.	562687.4	565528.1	-.50
4.	442591.6	440713.0	.43
5.	363841.1	364396.6	-.15

THE FUNCTION BEING FITTED IS: REFERENCE VALUE=P(1)/T**1.5 + P(2)/T**0.5 + P(3)*T**0.5 + P(4)*T**1.5

P(1): -.2153389068E+14
P(2): .1535957577E+11
P(3): -.3601515619E+07
P(4): .2794379427E+03


6.82 E+05
6.50 E+05
6.18 E+05
5.87 E+05
5.55 E+05
5.23 E+05
4.91 E+05
4.59 E+05
4.27 E+05
3.96 E+05
3.64 E+05
3.882 E+03
3.951 E+03
4.020 E+03
4.089 E+03
4.158 E+03
4.227 E+03
4.296 E+03
4.365 E+03
4.434 E+03
4.503 E+03
4.572 E+03

ISOTOPE MASS NUMBER 234

REFERENCE MASS NUMBER 235

CORRECTION FACTOR .99650

MEASUREMENT NO.	UNCORRECTED RATIO	DEVIATION (PERCENT)	DEVIATION (SIGMA)	CORRECTED RATIO
1.	.01183	1.17	.68	.01179
2.	.01198	2.51	1.45	.01194
3.	.01152	-1.50	-.87	.01147
4.	.01183	1.23	.71	.01179
5.	.01169	-.03	-.02	.01165
6.	.01173	.38	.22	.01169
7.	.01159	-.83	-.48	.01155
8.	.01135	-2.93	-1.70	.01131

THE UNCORRECTED AVERAGE RATIO= .01169008
STANDARD DEVIATION IN AN UNCORRECTED SINGLE RATIO= .00020152
STANDARD DEVIATION IN THE UNCORRECTED AVERAGE RATIO= .00007125

THE CORRECTED AVERAGE RATIO= .01164916
STANDARD DEVIATION IN A CORRECTED SINGLE RATIO= .00020081
STANDARD DEVIATION IN THE CORRECTED AVERAGE RATIO= .00007100

ISOTOPE MASS NUMBER 236

REFERENCE MASS NUMBER 235

CORRECTION FACTOR 1.00350

MEASUREMENT NO.	UNCORRECTED RATIO	DEVIATION (PERCENT)	DEVIATION (SIGMA)	CORRECTED RATIO
1.	.00219	.02	.01	.00219
2.	.00215	-1.43	-.64	.00216
3.	.00216	-.97	-.43	.00217
4.	.00212	-2.82	-1.26	.00213
5.	.00221	1.28	.57	.00222
6.	.00224	2.42	1.08	.00225
7.	.00214	-2.05	-.91	.00215
8.	.00226	3.55	1.58	.00227

THE UNCORRECTED AVERAGE RATIO= .00218604
STANDARD DEVIATION IN AN UNCORRECTED SINGLE RATIO= .00004905
STANDARD DEVIATION IN THE UNCORRECTED AVERAGE RATIO= .00001734

THE CORRECTED AVERAGE RATIO= .00219369
STANDARD DEVIATION IN A CORRECTED SINGLE RATIO= .00004922
STANDARD DEVIATION IN THE CORRECTED AVERAGE RATIO= .00001740

ISOTOPE MASS NUMBER 238

REFERENCE MASS NUMBER 235

CORRECTION FACTOR 1.01050

MEASUREMENT NO.	UNCORRECTED RATIO	DEVIATION (PERCENT)	DEVIATION (SIGMA)	CORRECTED RATIO
1.	.05724	.86	.59	.05784
2.	.05650	-.45	-.31	.05709
3.	.05742	1.18	.81	.05803
4.	.05739	1.12	.77	.05799
5.	.05679	.06	.04	.05739
6.	.05750	1.32	.91	.05811
7.	.05602	-1.30	-.89	.05661
8.	.05517	-2.80	-1.92	.05575

THE UNCORRECTED AVERAGE RATIO= .05675377
STANDARD DEVIATION IN AN UNCORRECTED SINGLE RATIO= .00082675
STANDARD DEVIATION IN THE UNCORRECTED AVERAGE RATIO= .00029230

THE CORRECTED AVERAGE RATIO= .05734969
STANDARD DEVIATION IN A CORRECTED SINGLE RATIO= .00083543
STANDARD DEVIATION IN THE CORRECTED AVERAGE RATIO= .00029537

LOS ALAMOS SCIENTIFIC LABORATORY
UNIVERSITY OF CALIFORNIA
LOS ALAMOS, NEW MEXICO 87544

OFFICE MEMORANDUM

TO : DISTRIBUTION DATE: 4 SEP 70

FROM : R. M. TISINGER

SUBJECT: MASS SPECTROMETER ANALYSIS (SPECIAL)
(SAMPLE SERIAL NUMBER)
(NBS-930)

SYMBOL :

AN ANALYSIS OF THE SAMPLE DESCRIBED ABOVE WAS COMPLETED ON 31 AUG 70. THIS ANALYSIS WAS PERFORMED USING THE AVCO MASS SPECTROMETER. RESULTS ARE TABULATED BELOW WITH UNCERTAINTY EXPRESSED AT THE NINETY-FIVE PERCENT CONFIDENCE LEVEL. ATOM RATIO IS THE NUMERICAL RATIO OF THE NUMBER OF ATOMS OF SPECIFIED MASS NUMBER TO THE NUMBER OF ATOMS OF MASS NUMBER 235.

MASS NUMBER	ATOM RATIO	WEIGHT PERCENT
234	.01165 +- .00039	1.0822 +- .0361
235	1.00000 +- 0.00000	93.2936 +- .1672
236	.00219 +- .00008	.2055 +- .0073
238	.05735 +- .00186	5.4187 +- .1757

R. M. TISINGER
GROUP W-7

DISTRIBUTION:

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W- 7 R. M. TISINGER

U. S. Department of Commerce
John T. Connor, Secretary
National Bureau of Standards
A. V. Astin, Director

Certificate of Analysis

Standard Reference Material U-930

Uranium Isotopic Standard

	^{234}U	^{235}U	^{236}U	^{238}U
Atom percent	1.0812	93.336	0.2027	5.380
	±0.0020	±0.010	±.0006	±0.005
Weight percent	1.0759	93.276	.2034	5.445

The material consists of highly purified oxide, U_3O_8. The atomic weight of the material is calculated to be 235.197, using the nuclidic masses 234.0409; 235.0439; 236.0457; and 238.0508.

The values for ^{234}U and ^{236}U are calculated from measurements at the National Bureau of Standards. The samples were spiked with high-purity ^{233}U to approximate the ^{234}U concentration, the ratios ^{233}U to ^{234}U and ^{233}U to ^{236}U were measured on a triple-filament equipped surface ionization mass spectrometer with d-c amplifier circuits.

The values for ^{235}U and ^{238}U are derived from measurements made at the National Bureau of Standards, at Union Carbide Nuclear Co., Oak Ridge, Tenn., and at Goodyear Atomic Corp., Portsmouth, Ohio, each laboratory's value being given equal weight. Values obtained at NBS are the result of direct measurement of the ^{235}U to ^{238}U ratio using triple filament thermal ionization. The observed ratios were corrected for mass discrimination effects by determining the system bias from measurements on standards U-500 and U-900. Experience at NBS has shown, through intercomparison of the standards, and synthetic mixtures at the 10-, 50-, and 90-percent ^{235}U level prepared from high-purity ^{235}U and ^{238}U isotopes, that a constant bias for a given procedure can be maintained over the range of 5- to 95-percent ^{235}U. Values from Union Carbide and Goodyear Atomic are based on direct determinations of the ^{238}U concentration by oxide dilution and UF_6 analysis, and then the ratio calculated using the NBS values for ^{234}U and ^{236}U, and the ^{235}U value obtained by difference.

The limits indicated for the isotopic concentrations are at least as large as the 95-percent confidence level for a single determination. The ^{235}U to ^{238}U ratio for this standard, 17.349, is known to at least 0.1 percent; at the same time the pooled variance for the calibration system is significantly smaller.

Mass spectrometry measurements at NBS were made by Ernest L. Garner and William R. Shields on solutions prepared by Lawrence A. Machlan and Martha S. Richmond.

WASHINGTON, D.C. 20234
February 11, 1966

W. Wayne Meinke, Chief
Office of Standard Reference Materials

(This certificate supersedes certificate of 12-1-58)

FIGURE 16. The provisional Certificate of Analysis for the NBS-930 uranium isotopic standard.

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