1620 Programs from I.C.R., Physics Dept.

I. C. R. #1 D.v.d.H.

Three and Two Dimensional Fourier Summation Program

for Crystal Structure Analysis

with Numerical and Alphanumerical Output

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two errors : page 1, 20

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The program (identification number 043001) is written for the I.B.M. 1620.

Memory: 20,000 digits

Input: Paper tape

Output: a. 12" carriage typewriter

b. 20" carriage typewriter (the latter is not absolutely necessary but allows for more freedom in the format of the output)

c. Tape

Limitations of the Program: See Section I

Timing: See Section I

Cells of the Program:

00029 - 00079	working storage
00100 - 00399	multiplication and addition tables
00402 - 00451	working storage
00452 - 00473	read-area
00474 - 00539	working storage
00540 - 05100	program
05100 - 05999	ccsine and sine table
06000 - 19479	storage for 1st and 2nd summation answers
19495 - 19999	storage for 3rd summation answers
10000 - 13750	initialization program

Hash Total: 67058544165826702962

Duplicating: Use the IBM library program: 1620 Numeric Tape Duplicator/Corrector.

Fourier Example 622909784700595447 26

I. General Theory

The electron density can be evaluated at each point, x, y, z of the unit cell by the formula

$$\rho(x,y,z) = \frac{2}{V} \sum_{h=o}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} A'(hk\ell) \cos 2\pi (hx + ky + \ell z) + B'(hk\ell) \sin 2\pi (hx + ky + \ell z) \qquad (I,1)$$

To calculate a Fourier with this formula proves to be very uneconomical with respect to the computing time involved. In a practical example of a centrosymmetric space group with 2000 Fourier coefficients in which 25 points in the x- and y-direction and 50 points in the z direction have to be calculated, it would take the I.B.M. 1620 about 140 hours to perform the calculations (not including the typing out).

It is possible to rewrite formula I,1 (Lipson and Beevers) in the form:

$$\rho(xyz) = \frac{2}{V} \sum_{\ell=o}^{\infty} \left[\sum_{k=o}^{\infty} \left(\sum_{h=o}^{\infty} A(hk\ell) \cos 2\pi hx + B(hk\ell) \sin 2\pi hx \right) \cos 2\pi ky + \left(\sum_{h=o}^{\infty} F(hk\ell) \cos 2\pi hx + B(hk\ell) \sin 2\pi hx \right) \sin 2\pi ky \right] \cos 2\pi \ell z +$$

$$\left[\sum_{k=o}^{\infty} \left(\sum_{h=o}^{\infty} G(hk\ell) \cos 2\pi hx + C(hk\ell) \sin 2\pi hx \right) \cos 2\pi ky + \left(\sum_{h=o}^{\infty} D(hk\ell) \cos 2\pi hx + H(hk\ell) \sin 2\pi hx \right) \sin 2\pi ky \right] \sin 2\pi \ell z \qquad (I,2)$$

in which:

$$A = F(hk\ell) + F(\bar{h}k\ell) + F(h\bar{k}\ell) + F(hk\bar{\ell}) \qquad I,3$$

$$B = -F(hk\ell) + F(\bar{h}k\ell) + F(h\bar{k}\ell) - F(hk\bar{\ell}) \qquad I,4$$

$$C = -F(hk\ell) + F(\bar{h}k\ell) - F(h\bar{k}\ell) + F(hk\bar{\ell}) \qquad I,5$$

$$D = -F(hk\ell) - F(\bar{h}k\ell) + F(h\bar{k}\ell) + F(hk\bar{\ell}) \qquad I,6$$

In noncentrosymmetric space groups: $F(h_i) = A(h_i)$ and:

$$E = B(hk\ell) - B(\bar{h}k\ell) + B(h\bar{k}\ell) + B(hk\bar{\ell}) \qquad \text{I,7}$$

$$F = B(hk\ell) + B(\bar{h}k\ell) - B(h\bar{k}\ell) + B(hk\bar{\ell}) \qquad \text{I,8}$$

$$G = B(hk\ell) + B(\bar{h}k\ell) + B(h\bar{k}\ell) - B(hk\bar{\ell}) \qquad \text{I,9}$$

$$H = -B(hk\ell) + B(\bar{h}k\ell) + B(h\bar{k}\ell) + B(hk\bar{\ell}) \qquad \text{I,10}$$

A, B,.....H, should include a multiplicity factor.

The form (I,2) cuts the number of arithmetic operations by about a factor of 15. The logic however, and therefore the computer program, becomes more cumbersome and less clear. In fact it cuts the calculation up in three different parts, which are consecutive summations over each of the three axes.

Definition: We call a set of terms, A, B, C,....H, with the same indices h, k and ℓ, an amplitude.

In the first summation over h, sums are made of terms, which have different index h, but the same indices k and ℓ. Pairs of sums are added together as shown in formula I,2.

Definition: Each group of amplitudes for which the indices k and ℓ are the same is called a "group $\langle k\ell \rangle$".

Thus sums are calculated (and pairs of sums) for each group $\langle k\ell \rangle$ and for all needed values of x in the first summation.

The difficulty which occurs will be clarified by an example. We want to make a Fourier synthesis with 1500 amplitudes, which are sorted in 250 groups $\langle k\ell \rangle$. We want to calculate 26 sections on x (values of x). Each group $\langle k\ell \rangle$ gives rise to four sums (formula I,2) for each value of x. The total number of sums is therefore going to be $(250)\cdot(4)\cdot(26) = 26{,}000$ sums. The first possibility is to store all sums inside the computer. In the preceding example that is clearly impossible, and in general one should put severe limitations on the scope of the program.

The second possibility is to store the sums on paper tape, which makes a sort of the sums necessary. A sort with paper tape is however impractical and slow.

The third possibility, which is the one we choose, is to calculate in the first summation stage only for one value of x at a time. In other words to calculate only one section at a time. It is easily possible to store these sums (in the example: (4).(250) = 1000 sums) inside the computer.

The disadvantage of this approach is of course the fact that for each new section the data tape with amplitudes has to be fed in again. Reading paper tape is however much faster than punching data (10 times), which means that this method is (much) more economical in time (for this computer) than calculating the complete first summation all at once.

The calculations and results of the first summation stage are in this case:

$$M(k\ell X) = \sum_{h=c}^{\infty} A(hk\ell) \cos 2\pi hX + E(hk\ell) \sin 2\pi hX \qquad (I,11)$$

$$N(k\ell X) = \sum_{h=c}^{\infty} F(hk\ell) \cos 2\pi hX + B(hk\ell) \sin 2\pi hX \qquad (I,12)$$

$$O(k\ell X) = \sum_{h=o}^{\infty} G(hk\ell) \cos 2\pi hX + C(hk\ell) \sin 2\pi hX \qquad (I,13)$$

$$P(k\ell X) = \sum_{h=o}^{\infty} D(hk\ell) \cos 2\pi hX + H(hk\ell) \sin 2\pi hX \qquad (I,14)$$

in which X is a definite value of x.

These sums are stored with four digits each, while k and ℓ are stored with two digits each, inside the computer. One set of sums (from one group <kℓ>) therefore occupies 20 digits of memory (thus using the variable word length feature of the computer to great avail). They are stored up to memory location 19479. During initialization the program calculates where to store the first set of sums (that is in location 19480 - <kℓ> .20). A value for the total number of groups <kℓ> has thus to be known beforehand.

Definition: <kℓ> = total number of "groups <kℓ>".

Preferably one likes to reuse the storage area occupied by these first summation answers. In what way that is possible is discussed in the next few paragraphs.

The second summation uses the answers of the first summation as amplitudes and performs the following calculations: (See also I,2)

$$R(\ell,X,y) = \sum_{k=o}^{\infty} M(k\ell X) \cos 2\pi\, ky + N(k\ell X) \sin 2\pi\, ky \qquad (I,15)$$

$$S(\ell,X,y) = \sum_{k=o}^{\infty} O(k\ell X) \cos 2\pi\, ky + P(k\ell X) \sin 2\pi\, ky \qquad (I,16)$$

The summations are over k. Sums are made from sets of amplitudes (M,N,O,P) with the same ℓ (X is a definite value and thus for all amplitudes the same). The answers are two sums for each value of y and each value of ℓ.

Definitions:

N_y is the number of points calculated in the y-direction

N_z is the number of points calculated in the z-direction

When ℓ changes the $2\cdot(N_y)$ sums: $R(\ell,X,y)$ and $S(\ell,X,y)$ are stored in memory locations 06000 and up (4-digits each), and the calculation proceeds with the next series of sets of amplitudes.

It appears useful to have all sets of amplitudes (M,N,O,P) with the same value of ℓ stored together. If the sets with ℓ=o are stored in the beginning of the storage area used for first summation answers, and if the ones for ℓ=1 and ℓ=2, etc., follow consecutively, it is possible to use this memory space again for the storage of the second summation answers, because first summation answers, after being used as amplitudes in the second summation, are allowed to be erased.

This procedure is followed and is the main principle of the program, and it enables us to use the memory space between 06000 and 19479 for 1st and 2nd summation answers both.

This does however imply a sorting order on the data tape. It is clear that in the consecutive amplitudes on the data tape the ℓ should change the least (in order to obtain the 1st summation answers in the necessary array) and that the h should

change the most, because the first summation is over h. That is a sorting order $hk\ell$: 0,0,0; 1,0,0; h,0,0; 0,1,0; h,1,0; h,k,0; 0,0,1; 1,0,1; h,0,1; h,k,1; h,k,ℓ. (See also Sections II and IV.)

The third summation calculates:

$$\rho(X,y,z) = \sum_{\ell=0}^{\infty} R(\ell,X,y) \cos 2\pi \ell z + S(\ell,X,y) \sin 2\pi \ell z \qquad (I,17)$$

using the second summation answers as amplitudes.

The procedure of the program is to calculate N_z sums for one value of y (line y = constant) at a time, and the N_z answers are typed or punched out line after line.

The manner in which the memory between locations 06000 and 19479 is used for first and second summation answers indicates the <u>limitations</u> of the <u>program</u>. Neither summation can occupy an area larger than 13480 digits.

For the first summation this means a limitation on the maximum number of groups $\langle k\ell \rangle$ namely:

$$\langle k\ell \rangle_{max} \leq 13480/20 = 674 \qquad (I,18)$$

For the second summation it means a limitation on the maximum value of (= L max) and N_y, namely

$$(N_y \cdot L_{max}) \leq \frac{13480}{8} = 1685 \qquad (I,19)$$

The program will stop and type out ER2, when a <u>momentary</u> overlap occurs of first and second summation answers. That is when an attempt is made to store second summation answers in an area in which first summation answers are stored which are not yet used as amplitudes in the second summation.

It is not felt that the limitations are serious. In some cases the limits might be a few percent smaller. They are only exact when

$$20 \cdot k_{max} = 8 \cdot N_y \qquad (I,20)$$

in each series of ℓ.

The approximate computing times for an example with 1500 amplitudes calculating a section of 25 by 50 points is given below with the main factor determining the computing time in each stage:

		due to:
		no. of amplitudes
Reading	220 sec	
1st summation	71 sec	$\langle k\ell \rangle$
2nd summation	277 sec	$\langle k\ell \rangle \cdot N_y$
3rd summation	480 sec	$\langle k\ell \rangle \cdot N_y \cdot N_z$
Typing	680 sec	$N_y \cdot N_z$

The program can just as well be used for an F^2-synthesis of course.

II. Format of Input and Output

In the preceding section it was supposed that the first summation was over h, the second over k and the third over ℓ, implying the sorting order $h\vec{k}\ell$ and implying sections X = constant.

It is however preferred to have more freedom in arranging the data and three reasons can be named.

a. The ability to make sections in other directions.

b. It might be necessary to sum in another order for instance when a programmed stop occurs (ER2 was mentioned in Section I).

c. Another order of summations might also be preferred in view of the computation time (see timing table in Section I).

For convenience a conversion table is made: Table II, A.

The data tape. Indices are punched with two digits each, terms A-H with four digits each. Each amplitude is followed by a record mark (R.M.). For centro-symmetric space groups one punches only the terms A-D, and the fourth term is followed by a R.M. The first record on the tape has to be an identification (arbitrary number of digits) of the data tape, followed by a R.M. The last record should be any 6-digit number followed by a R.M.

We have written a program (partly checked out), which prepares the data tape (called S.F. - F.S. program). It takes the paper tape output of the structure factor program, sorts the amplitudes in the desired sorting order, combines the structure factor amplitudes to terms (A-H) and arranges the terms according to the sorting order. The synthesis can be brought on absolute scale by including F(000) as term (A), and by multiplying the terms by the factor 2/V beforehand.

The output is either on the typewriter or on the typewriter and paper tape. In general one would use only typewriter output.

Typewriter. The sorting order is equivalent to the order of summation. The first index determines therefore on which axis the sections are. The second index determines the vertical and the third index the horizontal coordinate of the

sections in the typewritten output. The output is preceded by several alphanumeric headings and by one line of numbers, the last being identifications of the specification tape (see Section III), program tape and data tape respectively. The possible choices of the manner in which the answers are typed are described in Section III.

Paper tape. It is possible to punch all density maps out on paper tape together with the typewritten output, thus making a copy of the results on tape. The numerical answers of each section are preceded by the number of the section and each line of answers in the section is preceded by the number denoting the line. Each separate number is followed by a R.M. In the tape output the answers are preceded by the following records: a) identification of the specifications, b) specifications (see Section III), c) identification of the program tape, and d) identification of the data tape.

Projections are calculated as sections. The first index should always be zero (see Table II, A).

Conversion Table II, A

Sorting order	Terms	Sections or	Vertical coordinate	Horizontal coordinate
Indices	3-Dimensional			
h $\vec{k}$ ℓ	A B C D | E F G H $\neq$	x	y	z
k $\vec{h}$ ℓ	A B D C | F E G H $\neq$	y	x	z
k $\vec{\ell}$ h	A D B C | F G E H $\neq$	y	z	x
h $\vec{\ell}$ k	A C B D | E G F H $\neq$	x	z	y
ℓ $\vec{h}$ k	A C D B | G E F H $\neq$	z	x	y
ℓ $\vec{k}$ h	A D C B | G F E H $\neq$	z	y	x
	Input		Output	
	Projection			
o $\vec{k}$ ℓ	A O O D | O F G O $\neq$	-	y	z
o $\vec{h}$ ℓ	A O O C | O E G O $\neq$	-	x	z
o $\vec{\ell}$ h	A O O C | O G E O $\neq$	-	z	x
o $\vec{\ell}$ k	A C O D | O G F O $\neq$	-	z	y
o $\vec{h}$ k	A C C B | O E F O $\neq$	-	x	y
o $\vec{k}$ h	A C C B | O F E O $\neq$	-	y	x
	Input		Output	

Possible arrangements of the indices on a data tape with their implied sorting order and arrangement of terms, and the format of the typewritten output belonging to it.

III. Operation

a. One can discern the following stages during the operation

1. Loading of the program tape.

2. Tape feeding or typing of the specifications of the summation and the output.

3. Loading of the data tape.

4. Calculating and typing (and taping) of the results of one section.

5. If it was specified in 2. that more than one section had to be calculated: reloading of the data tape and returning to 4. If it was a projection or the last section: halting.

b. Switch settings

Parity : Stop

Input/Output : Stop

Overflow : Stop

Program Switch 1 : On

(When off it will type out all the answers of the first summation in unrounded and unshifted form. Can be used for checking.)

Program Switch 2 : See Section III d, 6, 8.

Program Switch 3 : See Section III d, 8.

Program Switch 4 : See Section III d, 1, 12.

c. Manual Operations

1. Clearing Memory: Insert; Key in : 16 00010 00000; Release; Start.

After clearing: Stop SCE; Reset.

2. Ready Tape Reader with program tape.

3. Loading of program tape : Insert; Key in : 36 00000 00300;

Release; Start.

4. Almost at the end of the program tape the loading will stop :

Press Start.

5. Follow instructions of the messages which are typed out. Always press Release and then Start after typing a specification in.

d. The remainder of this section is an explanation of some of the messages which are typed out. The number in parentheses after each message tells how many digits there are in the number and which have to be typed.

1. Message

"When specs are typed set S.W. 4 off. From tape S.W. 4 on."

In general the specifications of the summation will be typed in. In that case S.W. 4, that is Program Switch 4, should be off. It is however possible to prepare the specifications on tape beforehand. For the preparation of such a tape see Section III d, 12.

2. Message

"Type ident of specs tape now made."

It is necessary to type in a 6-digit number. The number itself is arbitrary but can be useful in a identification scheme.

3. Messages:

"Type 1st sum min."

"Type 1st sum max."

"Type 2nd sum min."

"Type 2nd sum max."

"Type 3rd sum min."

"Type 3rd sum max."

"Type 1st sum delta"

"Type 2nd sum delta"

"Type 3rd sum delta"

These determine the amount of the unit cell to be calculated and the grid spacing.

All are in hundredth of the cell edge. Furthermore:

$$\frac{\text{n th sum max - n th sum min}}{\text{n th delta}} = p, \text{ in which p should be an integer.}$$

The first and the final section are determined respectively by the values of "1st sum min" and "1st sum max." The interval of the sections between the final and the first are determined by "1st sum delta." For a projection the value of "1st sum min" should be typed equal to the value for "1st sum max" and 1st sum delta should be 00.

Similarly the remainder of the values to be typed in determine the part of the sections which needs to be calculated. The allowed range of the values belonging to the first 6 message are from 000 up to 100 and for the last three from 00 up to 98.

Any bloc of the unit cell can be calculated, and it is also possible in the same manner to calculate just one specified point in the unit cell.

4. Messages

"1st sum shift"

"2nd sum shift"

"3rd sum shift"

The program uses a table of cosine and sine values. The table contains 100 values of each and each having four decimal digits after the decimal point. The basic calculation of the Fourier summation is either: $Q_j \cos h_i x_p$ III,1

or: $Q_j \sin h_i x_p$ III,2

The values h_i are integers, and the values x_p always have two decimal digits after the decimal point. Therefore a table of 100 cosine and sine values is sufficient and a straight table look up can be used without interpolation.

The program accepts and works only with fixed decimal numbers, and it is therefore necessary to keep track of the decimal point.

The normal shift after a calculation of the type III,1 or III,2 is four places, due to the four decimal digits of the values in the trigonometric table. Thus typing in 04 for each of the three shift values will keep the decimal point in the answer at the same place as in the terms on the data tape (counted from the right of course).

Normally type 04 for each.

It might happen however that there is an accumulation in a particular sum which gives rise to an overflow (the machine will stop because O-flow is on Stop). One has to restart the calculation by reloading the program tape and changing one of the three shift values (it is of ccurse not necessary to recalculate the sections which are already finished).

It is necessary to consider which shift order has to be changed. There are three possibilities

i. There was a type out: ER. 3. This means an overflow in the 1st summation and therefore "1st sum shift" should now be typed in as 05 instead of 04. If not check I.R. 1 (by putting Display at I.R. 1, and pressing Reset and Display Mar) It should have 02646. If not there is a programming error.

ii. Change 2nd sum shift: from 04 to 05 when the message "Horiz. Indcx" is not yet typed out.

iii. Change 3rd sum shift from 04 to 05 when this message: "Horiz. Index" has been typed out.

It is not likely but indeed possible that an overflow will occur even after a change in one of the shift values is made. The summation in which it happened can again be tied down in the manner described abovc.

On the other hand it is possible that one would like to have the answers with one more digit after the decimal point. This can be achieved most effectively by changing the value of the 1st sum shift from 04 to 03, but can also be done in either of the other summations.

Shift values 02, 03, 04, 05 and 06 can be used in each summation.

5. Message:

"Type in number of answers on a row."

This message will be typed out when P.S. 2 is on. With <u>P.S. 2 on</u> the output will be in <u>numerical form</u>.

With a normal length typewriter carriage it is generally impossible to get all N_z (see Section I) values for one line, y = constant, on one horizontal row. The program is normally set for 16 numerical answers on one row. The first answer on the next row will be a repeat of the last answer on the former row, giving a fairly regular array with multiples $z_{min} + \Delta z$ .15 below each other or the first vertical line of answers.

Thus type in normally: 016. However any other number can be typed in. Typing in 011, will result in listing the answers with multiples $z_{min} + \Delta z$ .10 below each other on the first line.

6. Message

"Output. Type only =1. Tape and type =0."

As was mentioned before, it is possible to make a paper tape copy of the numerical results of the calculation, which may later be used for peak analysis or in the case of a F^2-synthesis, for a superposition procedure. Part of the paper tape output is the specification record, which holds such parameters as were described in Section III d, 3. These summation parameters, determine exactly the array of numbers of the paper tape: general specifications, section identification, line identifications and results.

7. Messages

"Type horiz. spacing"

"Type vert. spacing"

"Type shift spacing"

"Type high limit of peaks"

"Type low limit of peaks"

These messages will be typed out when program switch 2 is off. When P.S. 2 is off the output will be in alphanumerical form.

In order to save the time consumed by plotting manually the numerical answers on the grid of the unit cell, a direct plotting system was devised on an approximate grid.

For this purpose each four digit numerical answer is translated into a one digit alphanumerical answer.

The first three messages. The relative dimensions of the grid can be approached as closely as possible by spacing horizontally (between the one digit answers) and vertically (between the lines). Typing in 00 is interpreted as the normal spacing of the typewriter either horizontally or vertically. Typing 01 will result in one extra space between either the one digit answers or the lines. Similarly 02 will result in two extra spaces etc. An askew cell instead of a rectangular one can be approximated by shifting (0C, C1, or more spaces) the next line with respect to the former one. For a rectangular cell type in 00. For an askew cell type in 01, 02 or more. (The 20" carriage can be very useful in this respect. By changing a few program orders it is possible to shift a line every other line or even less.)

The last two messages. Used as one digit answers are: 41 (=A) up to 79 (=alphanumerical 9). There are thus 39 different answers possible. The characters 50 and 60 are always printed as a space (blank).

If the answers go up to +9999, and down to -9999, one has to type in for the high limit (=H): 09999 and for the low limit (=L): $9999\overline{9}$. It is then necessary to bring all answers in between -9999 and +9999 into the range from 41 to 79, which is of course possible by using a proper scale and base factor (both of which are calculated by the program). In this case an answer P is brought into this range in the program by means of:

$$\frac{P-L}{H-L} \cdot 39 + 41 = \frac{P-(-9999)}{19998} \cdot 39 + 41 \qquad \text{III,3}$$

and sc is any answer $9999 \leq P \leq -9999$.

If the highest answer is 1000 instead of 9999, and the lowest -1000 instead of -9999, only a small part of the possible range should be used in fact only from Q-S, when H was put to +9999 and L put to -9999. In this way all detail in the Fourier might get lost.

It is therefore made possible to type in any high and low limit (with no more than 4 digits). It is not necessary that all the answers fall within the limits. If an answer is outside the limits, the program will insert and type a blank.

8. The use of Program Switch 3.

i. When P.S. 2 is off.

That is in the alphanumerical output. In the direct alphanumerical plotting of a Fourier it is sometimes clarifying to show only the peaks and to suppress the printing of the base level of a Fourier. This can be achieved by setting P.S. 3 on when P.S. 2 is off. The result of this setting is that the printing of all characters below 60 (A up to R) is suppressed and a blank (space) is printed instead. In other words all answers below $(\underline{H+L})$, will not be printed.
2

By proper use of H, L and P.S. 3 one has a great variety of alphanumerical outputs.

When P.S. 3 is on, the character 70 is printed as a zero. When P.S. 3 is off it is transcribed as a space (as are 50 and 60).

These spaces (50,60,70) might possibly be used as contour lines, although we have not had much success with this as yet.

ii. When P.S. 2 is on.

That is in the numeric output. When one does a projection it is sometimes quite impossible to guess what the upper and lower limits are. Of course one might do the projection first numerically, than reload the program and recalculate the projection alphanumerically. It is however possible to repeat only the third summation, without reloading the program.

When program switch 2 and 3 are both set on, the computer will stop after the numerical output is finished and type out the message:

"Set P.S. 2,3. Type alphaspecs."

One has then to set P.S. 2 to off (for alphanumerical output) and P.S. 3 to choice (see Section III c, 7, 8i) and has to type in three 2-digit, one 5-digit, and one 4-digit numbers (with flags over the left-most digits of each number), which are respectively; horizontal space, vertical space, shift space, high limit (H), and low limit (L). See Section III d,7. The last two values H and L are known at this moment. Press Release and then Start and the computer will proceed by plotting this projection again, but now in the desired alphanumerical format.

When it was not a projection but a section the program switches might have to be reset before proceeding with the next section, but not necessarily.

9. Recapitulation of the use of program switches 2 and 3.

i. P.S. 2 off; P.S. 3 off.

Alphanumerical output with 38 characters (A-9).

ii. P.S. 2 off; P.S. 3 on.

Alphanumerical output. Characters /-9 are printed and the characters A-R are transcribed as spaces.

iii. P.S. 2 on; P.S. 3 on.

First numerical output followed by an alphanumerical output (after resetting the switches) of the same projection or section.

iv. P.S. 2 on; P.S. 3 off.

Numerical output.

10. Message

"Type number of groups"

This message requests the typing in of the total number of "groups <kℓ>". The meaning of the term "group <kℓ>" was explained in Section I.

If one erroneously types in this number too small, it will result in error type out; ER 1, which means that the assigned area for the first summation is too small and overflows. The program has to be reloaded in this case. Typing in the number too large does not have immediate repercussions. It can only result in an unnecessary ER 2 type out (momentary overlap of 2nd summation amplitudes and answers; see Section I), because the area assigned by the program to the first summation answers is larger than necessary.

For a projection the number of "groups" is the total number of data.

11. Message

"centrosymm = 1, noncentrosymm = 0"

Essentially all space-groups are dealt with as either P_1 or $P_{\bar{1}}$.

In the first summation only the terms A-D are used when the space-group is centrosymmetric (type in 1), while all terms A-H are used when the space-group is noncentrosymmetric (type in 0). (See also Sections I and II.)

More time is won in the program during the first summation by skipping each term, which is zero.

A loss in time might occur in the 2nd summation for certain space groups, but there is no loss in computing time in the third summation by taking this approach.

12. Message

"Load specification tape"

All the specifications of the summations so far described can be put on a tape with an off-line typewriter and loaded instead of being typed, by setting P.S. 4 on.

The first record on this specification tape should be a 6-digit identification (followed by a record mark).

The next record should be a succession of the following specifications:

1st sum min	3 digits
1st sum max	3 "
2nd sum min	3 "
2nd sum max	3 "
3rd sum min	3 "
3rd sum max	3 "
1st sum delta	2 "
2nd sum delta	2 "
3rd sum delta	2 "
1st sum shift	2 "
2nd sum shift	2 "
3rd sum shift	2 "
horiz. spacing	2 "
vert. spacing	2 "
shift spacing	2 "
high limit	5 "
low limit	4 "
number of groups	4 "
centro/noncentro	1 digit
record mark	1 "

(All but the last two with flags on the left-most digit)

13. Message

"Mcoi"

This is typed out when the calculation is finished.

14. Messages

"Er 1"

"Er 2"

"Er 3"

These messages indicate errors. It will always be necessary to reload the program. Each of them indicate a mistake in planning the calculation, which has to be corrected.

Er 1: The number of "groups <kℓ>" is typed in too small (see Section III d, 10).

Er 2: Momentary overlap of first and second summations answers (see Section III d, 10 and Section I).

Er 3: Overflow in the 1st summation (see Section III d, 4).

15. Tab stops and margin settings.

i. Numerical type out.

With 16 answers on a row the margins should be 86 positions apart.

There should always be tab stops at the 4th and 42nd position from the left margin.

ii. Alphanumerical type out.

The margin will depend on the shape of the grid which is chosen.

There should be a tab stop at the 42nd and 5th position (the last may be changed) from the left margin.

16. More details of the program can be obtained from the flow sheets and program listing. The author would appreciate notification of program errors.

I would like to thank Miss Evelyn Wydro for preparing the program tape and typing this manuscript.

IV. Example

A part of a Fourier projection (001) of the compound 6-azidopurine will be calculated.

The spacegroup was taken as P nam. The actual spacegroup is P $na2_1$, but this does not change the appearance of the projection along the c-axis, which we want to calculate.

In the International Tables, Vol. I, the formulas for the space group P nma are given. In the expression for the electron density therefore the b- and the c-axis should be interchanged, giving on a arbitrary scale (leaving out the parts for ℓ is odd).

$$\rho(xyo) = \sum_{h,k}^{\infty} F(hk\ell) \cos 2\pi hx \cos 2\pi ky \cos 2\pi \ell z \qquad h + k \text{ even}, \ \ell \text{ even}$$

$$- \sum_{h,k}^{\infty} F(hk\ell) \sin 2\pi hx \sin 2\pi ky \cos 2\pi \ell z \qquad h + k \text{ odd}, \ \ell \text{ even} \qquad \text{(IV,1)}$$

This means that for h - k even, $F(hk\ell)$ is equal to the term (A) and for h + k odd, $F(hk\ell)$ is equal to the term B (see formula I,2: cos cos cos → A, sin sin cos → B)

In the output we would like as horizontal coordinate x and as vertical coordinate y. This implies a sorting order okh. According to Table II, A, the data should therefore be punched as follows:

k h A B
00 xx xx xxxxx 00000 00000 xxxxx #, as is shown in the print out of the data tape. Two examples follow. P.S. 4 should be off in both.

a. We want to calculate the projection from y = 0.28 up till y = 0.47, with intervals of .01 and from z = 0.00 up till z = 0.30 with intervals of .02.

The third sum shift order is taken as 05 which is not necessary with respect to overflow, but convenient.

We want an alphanumerical output thus P.S. 2 is off. Horizontally we want one extra space between the answers and vertically no extra space in order to obtain the approximate dimensions of the grid (a = 11.72 A° and b = 17.06 A°). The shift spacing should be zero because it is an orthorhombic space group and the axes are perpendicular.

From a previous calculation of this projection we know that the answers are roughly in between -200 and +800. We want only the peaks and not the base level thus P.S. 3 is on. If we now should put H equal to 00800 and L equal to $02\bar{00}$, we should only print for answers with a numerical value above +300 (see Section III d, 8), and should suppress the printing of quite a large, and possibly important, part of the peak. This can be evaded however by making L lower than -200, for instance: -550. Doing so all answers with a numerical value above +125 are translated into an alphanumerical character and printed, thus plotting a larger part of the peak.

The number of groups is 0194 and this can be checked in the print out of the data tape as being the number of data of the projection.

The messages and results of this first example are shown in figure IV, A.

b. The second example is a numeric print out (P.S. 2 on) of the same part of the projection. The only difference is that now the interval along the y-axis is taken as .02 instead of .01. The value p (explained in Section III d, 3) would then become a non-integer however. This can be corrected by typing in an even instead of an odd value for y max., for instance 0.46. We want only the numeric print out and P.S. 3 should therefore be off.

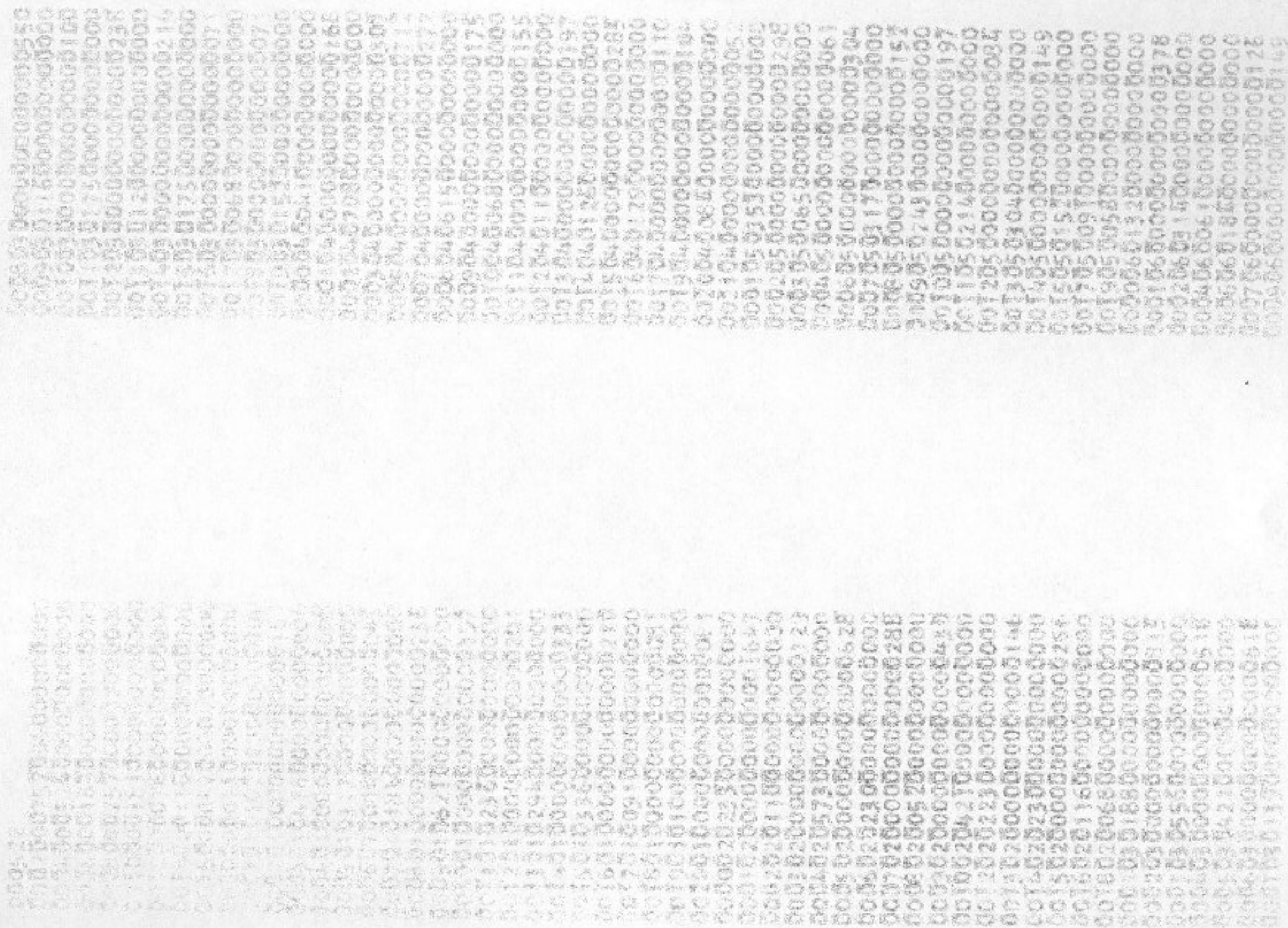
The messages and results of the second example are given in figure IV, B.

```
160001000000
360000000300
SET PROGRAM SWITCHES
WHEN SPECS ARE TYPED SET SW4 OFF.FROM TAPE SW4 ON
TYPE IDENT OF SPECS TAPE NOW MADE(6)        555555
TYPE 1ST SUM MIN.(3)                        000
TYPE 1ST SUM MAX.(3)                        000
TYPE 2ND SUM MIN.(3)                        028
TYPE 2ND SUM MAX.(3)                        047
TYPE 3RD SUM MIN.(3)                        000
TYPE 3RD SUM MAX.(3)                        030
TYPE 1ST SUM DELTA(2)                       00
TYPE 2ND SUM DELTA(2)                       01
TYPE 3RD SUM DELTA(2)                       02
TYPE 1ST SUM SHIFT(2)                       04
TYPE 2ND SUM SHIFT(2)                       04
TYPE 3RD SUM SHIFT(2)                       05
TYPE HORIZ.SPACING(2)                       01
TYPE VERT. SPACING(2)                       00
TYPE SHIFT SPACING(2)                       00
TYPE HIGH LIMIT OF PEAKS(5)                 00800
TYPE LOW LIMIT OF PEAKS(4)                  0550
TYPE NUMBER OF GROUPS(4)                    0194
CENTROSYM=1,NONCENTROSYM=0 (1)              1
MAKE LEADER.SPECS TAPE IS PUNCHED OUT
LOAD DATA TAPE
043001555555000522
XMIN3=.00 XMAX3=0.30 DELTA3=.02


SECTION 000
HORIZ.INDEX3
028                 T U       U V /
029               S Z 1 U   / Y O U
030               U 3 5 Y   S Z 1 V
031               U 3 6 Z / / X Z U
032               S Z 1 W     S U
033                 T U S
034
035                             U W T
036               U T         S O 3 Y
037             T Z 0 U       T 2 6 Z
038             U 2 4 X       S O 2 W
039             U 1 3 X /   /   / U V /
040             / W Y V T V X U /
041                 S / T O 3 Z S
042                     T 1 5 O S
043                     / Y 1 W
044                       T U /
045
046
047
M001
```

EXAMPLE IV , A

```
160001000000
360000000300
SET PROGRAM SWITCHES
WHEN SPECS ARE TYPED SET SW4 OFF.FROM TAPE SW4 ON
TYPE IDENT OF SPECS TAPE NOW MADE(6)          555556
TYPE 1ST SUM MIN.(3)                          000
TYPE 1ST SUM MAX.(3)                          000
TYPE 2ND SUM MIN.(3)                          028
TYPE 2ND SUM MAX.(3)                          046
TYPE 3RD SUM MIN.(3)                          000
TYPE 3RD SUM MAX.(3)                          030
TYPE 1ST SUM DELTA(2)                         00
TYPE 2ND SUM DELTA(2)                         02
TYPE 3RD SUM DELTA(2)                         02
TYPE 1ST SUM SHIFT(2)                         04
TYPE 2ND SUM SHIFT(2)                         04
TYPE 3RD SUM SHIFT(2)                         05
TYPE NUMBER OF GROUPS(4)                      0194
CENTROSYM=1,NONCENTROSYM=0 (1)                1
MAKE LEADER.SPECS TAPE IS PUNCHED OUT
TYPE IN NUMBER OF ANSWERS ON A ROW(3)         011
OUTPUT.TYPE ONLY=1,TAPE AND TYPE=0 (1)        1
LOAD DATA TAPE
043001555556000522
XMIN3=.00 XMAX3=0.30 DELTA3=.02


SECTION 000
HORIZ.INDEX3
028   33   41   95  236  281  127    5   95  283  309  172
      172  19   74  123  154  166
030   44   34  276  592  672  412  138  195  454  525  318
      318  67   59  108  147  157
032   67    4  198  439  518  337  108   73  205  256  133
      133  24   83   94  127  164
034   93   34   31   75   65   44   29    8   17   20   86
      86  104   41   53  122  166
036   34  115  253  242   99    7   39   51   39  194  479
      479 592  398  107   64  124
038   35  282  555  610  373  111   29   22   23  192  471
      471 560  350   81   69  129
040    7  143  334  398  284  217  307  372  274  156  116
      116  75   12   78  109  138
042   92   73   21   16   60  233  511  638  468  186    2
        2  73   90   94  117  138
044  139  137  103   70   38   62  213  267  160   11   65
       65   84  100  138  163  146
046  154  168  150  120  118  111   74   55   78  107  124
     124  140  161  180  173  134
MOO!
```

EXAMPLE IV . B



```
END OF PASS I
*
*      THREE DIMENSIONAL FOURIER SUMMATION PROGRAM
*
         DORG 540                                          00540
START2   RCTY                                              00540 34 00000 00102
         WATY  IDENT6                                      00552 39 05047 00100
         TR    402,29                                      00564 31 00402 00029
         H                                                 00576 48 00000 00000
         RNPT  15000                                       00588 36 15000 00300
*
*      INITIALIZATION OF FIRST SUM ANSWER LOCATIONS
*
STARTO   SM    450,1,10                                    00600 12 00450 00001
         MM    450,20,10                                   00612 13 00450 00020
         SF    95                                          00624 32 00095 00000
         S     CONS12,99                                   00636 22 04959 00099
         TF    NEWS12+6,CONS12                             00648 26 01430 04959
         TF    SUMM01+11,CONS12                            00660 26 02181 04959
         SM    CONS12,4,10                                 00672 12 04959 00004
         TF    NEWS15+6,CONS12                             00684 26 01538 04959
         TF    SUMM00+6,CONS12                             00696 26 02140 04959
         SM    CONS12,2,10                                 00708 12 04959 00002
         TF    NEWS14+6,CONS12                             00720 26 01526 04959
         TF    SUMM02+11,CONS12                            00732 26 02265 04959
         AM    CONS12,6,10                                 00744 11 04959 00006
         A     CONS12,99                                   00756 21 04959 00099
         TFM   COUNT9,0,9                                  00768 16 05023 00000
         RCTY                                              00780 34 00000 00102
         WATY  IDENT1                                      00792 39 04937 00100
         TF    IDENT4-1,SECTX                              00804 26 04903 04954
         SPTY                                              00816 34 00000 00101
         WNTY  IDENT4-3                                    00828 38 04901 00100
         BD    NEWS00,TYPTAP                               00840 43 00864 04874
         WNPT  IDENT4-3                                    00852 38 04901 00200
*
*      FIRST SUMMATION.SELECTION OF AMPLITUDES AND ARRANGING
*      OF TRIGONOMETRIC VALUES
*
NEWS00   RNPT  452                                         00864 36 00452 00300
FIRSSM   TF    GROUP2,455,,PAGEB                           00876 26 04961 00455
         TF    GROUP3,457                                  00888 26 04963 00457
         TF    19969,ZERO10                                00900 26 19969 04973
         TF    19979,ZERO10                                00912 26 19979 04973
         TF    19989,ZERO10                                00924 26 19989 04973
         TF    19999,ZERO10                                00936 26 19999 04973
NEWS13   C     455,GROUP2                                  00948 24 00455 04961
         BNZ   NEWS09                                      00960 47 01352 01200
         C     457,GROUP3                                  00972 24 00457 04963
         BNZ   NEWS09                                      00984 47 01352 01200
         M     453,SECTX                                   00996 23 00453 04954
         SF    98                                          01008 32 00098 00000
         TF    ARGUM,99                                    01020 26 04976 00099
         MM    ARGUM,9,10                                  01032 13 04976 00009
         A     NEWS04+11,99                                01044 21 01067 00099
```

```
NEWS04 TR    518,510,,8                          01056 31 00518 05100
       S     NEWS04+11,99                        01068 22 01067 00099
       TR    502,518                             01080 31 00502 00518
       TF    513,509                             01092 26 00513 00509
       TF    517,505                             01104 26 00517 00505
       TF    NEWS53+11,CONS53                    01116 26 01223 04924
       TFM   NEWS52+6,461,9                      01128 16 01194 00461
*
*      FIRST SUMMATION,MULTIPLICATION AND SUMMING
*
NEWS57 TFM   NEWS54+6,19969,7                    01140 16 01230 19969
       TFM   NUMB00,4,10                         01152 16 04984 00004
NEWS55 SM    NUMB00,1,10                         01164 12 04984 00001
NEWS56 BN    NEWS50,,2                           01176 47 01284 01300
NEWS52 CM    461,0,48                            01188 14 00461 00000
       BZ    NEWS51                              01200 46 01236 01200
NEWS53 M     461,505,4                           01212 23 00461 00505
NEWS54 A     19969,99,2                          01224 21 19969 00099
NEWS51 AM    NEWS52+6,4,10                       01236 11 01194 00004
       A     NEWS53+11,CONS02                    01248 21 01223 04982
       AM    NEWS54+6,10,10                      01260 11 01230 00010
       B     NEWS55                              01272 49 01164 00000
NEWS50 SM    NEWS53+11,8,10                      01284 12 01223 00008
       AM    NEWS56+6,36,10                      01296 11 01182 00036
       B     NEWS57                              01308 49 01140 00000
       SM    NEWS56+6,36,10                      01320 12 01182 00036
NEWS58 RNPT  452                                 01332 36 00452 00300
       B     NEWS13                              01344 49 00948 00000
       DORG  *-3                                 01352
*
*      FIRST SUMMATION,ROUNDING AND STORING
*
NEWS09 TFM   NUMB00,4,10                         01352 16 04984 00004
NEWS10 TF    539,19969,7                         01364 26 00539 19969
NEWS20 SF    532                                 01376 32 00532 00000
NEWS21 AM    536,5,10                            01388 11 00536 00005
NEWS22 BNF   NEWS12,539                          01400 44 01424 00539
NEWS24 SF    535                                 01412 32 00535 00000
NEWS12 TF    19467,535,27                        01424 26 19467 00535
NEWS19 BD    NEWS16,531                          01436 43 01690 00531
NEWS17 AM    NEWS10+11,10,10                     01448 11 01375 00010
       AM    NEWS12+6,4,10                       01460 11 01430 00004
       SM    NUMB00,1,10                         01472 12 04984 00001
       BNZ   NEWS10                              01484 47 01364 01200
       SM    NEWS10+11,40,10                     01496 12 01375 00040
       AM    NEWS12+6,4,10                       01508 11 01430 00004
NEWS14 TF    19461,GROUP2,2                      01520 26 19461 04961
NEWS15 TF    19463,GROUP3,2                      01532 26 19463 04963
       BC1   NEWS18                              01544 46 01604 00100
       TF    19957,GROUP2                        01556 26 19957 04961
       TF    19959,GROUP3                        01568 26 19959 04963
       RCTY                                      01580 34 00000 00102
       DNTY  19956                               01592 35 19956 00100
NEWS18 AM    NEWS14+6,20,10                      01604 11 01526 00020
       AM    NEWS15+6,20,10                      01616 11 01538 00020
       AM    COUNT9,1,10                         01628 11 05023 00001
       BNR   FIRSSM,458                          01640 45 00876 00458
       CM    NEWS14+6,19481,7                    01652 14 01526 19481
       BNP   SECIN1                              01664 47 01704 01100
       WATY  INFOM1                              01676 39 05077 00100
       H                                         01688 48 00000 00000
```

```
01690
01690 39 05093 00100
01702 48 00000 00000
01704
```

```
         DORG *-9
NEWS16   WATY INFOM3
         H
         DORG *-9
*
*     INITIALIZATION OF SECOND SUMMATION
*
SECIN1   S     413,410,,PAGE6                01704 22 00413 00410
         TFM   COUNT1,0,9                    01716 16 05031 00000
SECIN8   AM    COUNT1,1,10                   01728 11 05031 00001
         CM    413,0,9                       01740 14 00413 00000
         BZ    SECIN9                        01752 46 01784 01200
         S     413,423                       01764 22 00413 00423
         B     SECIN8                        01776 49 01728 00000
         DORG *-3                            01784
SECIN9   TF    NUMBR2,COUNT1                 01784 26 04900 05031
         MM    NUMBR2,2,10                   01796 13 04900 00002
         TF    CONS05,99                     01808 26 04992 00099
         MM    NUMBR2,8,10                   01820 13 04900 00008
         TF    CONS04,99                     01832 26 05013 00099
         TFM   SECIN3+6,6003,7               01844 16 02054 06003
         TFM   SUBR02+6,6003,7               01856 16 02640 06003
         TF    DELTA,423                     01868 26 05015 00423
         TF    XMINT,410                     01880 26 05018 00410
         TFM   SUBR06+11,NUMBR2,7            01892 16 02381 04900
         TFM   SUBR14+11,4,10                01904 16 02749 00004
         TFM   SUBR13+11,2,10                01916 16 02525 00002
         SM    429,10,10                     01928 12 00429 00010
         CF    429                           01940 33 00429 00000
         TD    SUBR07+6,429                  01952 25 02604 00429
         SM    429,1,10                      01964 12 00429 00001
         TD    SUBR02+11,429                 01976 25 02645 00429
         TD    SUBR19+6,429                  01988 25 02628 00429
         SM    429,3,10                      02000 12 00429 00003
         TD    SUBR11+6,429                  02012 25 02592 00429
         TFM   INDEX3,0,10                   02024 16 05020 00000
*
*     SECOND SUMMATION.PREPARING OF STORAGE FOR NEXT SERIES
*
SECIN4   TF    CLEAR1,CONS05                 02036 26 05028 04992
SECIN3   TFM   6003,0,28                     02048 16 06003 00000
         AM    SECIN3+6,4,10                 02060 11 02054 00004
         SM    CLEAR1,1,10                   02072 12 05028 00001
         BNZ   SECIN3                        02084 47 02048 01200
         C     SECIN3+6,SUMM01+11            02096 24 02054 02181
         BN    SUMM00                        02108 47 02134 01300
         WATY  INFOM2                        02120 39 05085 00100
         H                                   02132 48 00000 00000
         DORG *-9                            02134
*
*     SECOND SUMMATION.SELECTION OF ANPLITUDES
*
SUMM00   C     19463,INDEX3,2                02134 24 T9463 05020
         BNZ   SECIN5                        02146 47 02334 01200
         TFM   NUMB00,4,10                   02158 16 04984 00004
SUMM01   TF    461,19467,57                  02170 26 00461 T9467
         AM    SUMM01+11,4,10                02182 11 02181 00004
         AM    SUMM01+6,4,10                 02194 11 02176 00004
         SM    NUMB00,1,10                   02206 12 04984 00001
         BNZ   SUMM01                        02218 47 02170 01200
```

```
                SM      SUMMO1+6,16,10                  02230 12 02176 00016
                AM      SUMMO1+11,4,10                  02242 11 02181 00004
SUMMO2          BT      SUBRO6,19461,7                  02254 27 02370 19461
                S       SUBRO2+6,CONSO4                 02266 22 02640 05013
                AM      SUMMO +6,20,10                  02278 11 02140 00020
                AM      SUMMO2+11,20,10                 02290 11 02265 00020
                SM      COUNT9,1,10                     02302 12 05023 00001
                BZ      THRINO                          02314 46 02816 01200
                B       SUMMOO                          02326 49 02134 00000
                BORG    *-3                             02334
SECIN5          A       SUBRO2+6,CONSO4                 02334 21 02640 05013
                AM      INDEX3,1,10                     02346 11 05020 00001
                B       ECIN4                           02358 49 02036 00000
*
*       SUBROUTINE,MULTIPLICATION AND SUMMING USED IN SECOND
*       AND THIRD SUMMATION
*
SUBRO6          TF      COUNT1,NUMBR2                   02370 26 05031 04900
                M       SUBRO6-1,DELTA                  02382 23 02369 05015
                SF      98                              02394 32 00098 00000
                TF      ADDIN,99                        02406 26 05033 00099
                M       SUBRO6-1,XMINT                  02418 23 02369 05018
                SF      97                              02430 32 00097 00000
                TF      ARGUM,99                        02442 26 04976 00099
SUBRO4          BD      SUBR10,ARGUM-2                  02454 43 02794 04974
SUBRO9          MM      ARGUM,9,10                      02466 13 04976 00009
                A       SUBRO1+11,99                    02478 21 02501 00099
SUBRO1          TRM     491,5100,7                      02490 31 00491 05100
                S       SUBRO1+11,99                    02502 22 02501 00099
SUBR13          TFM     COUNT2,2,1                      02514 16 05035 00002
                M       494,461                         02526 23 00494 00461
                TF      539,19                          02538 26 00539 00099
                M       498,465                         02550 23 00498 00465
                A       539,99                          02562 21 00539 00099
SUBRO3          CF      532                             02574 33 00532 00000
SUBR11          SF      532                             02586 32 00532 00000
SUBRO7          AM      536,5,10                        02598 11 00536 00005
                BNF     SUBRO2,539                      02610 44 02634 00539
SUBR19          SF      535                             02622 32 00535 00000
SUBRO2          A       6003,535,2                      02634 21 06003 00535
                SM      COUNT2,1,10                     02646 12 05035 00001
                BZ      SUBR14                          02658 46 02738 01200
                AM      SUBRO2+6,4,10                   02670 11 02640 00004
                M       494,469                         02682 23 00494 00469
                TF      539,99                          02694 26 00539 00099
                M       498,473                         02706 23 00498 00473
                A       539,99                          02718 21 00539 00099
                B       SUBR13                          02730 49 02574 00000
                BORG    *-3                             02738
SUBR14          AM      SUBRO2+6,4,10                   02738 11 02640 00004
                SM      COUNT1,1,10                     02750 12 05031 00001
                BZ      SUBRO5                          02762 46 02814 01200
                A       ARGUM,ADDIN                     02774 21 04976 05033
                B       SUBRO4                          02786 49 02454 00000
                BORG    *-3                             02794
SUBR10          TDM     ARGUM-2,0,11                    02794 15 04974 00000
                B       SUBRO9                          02806 49 02466 00000
                BORG    *-3                             02814
SUBRO5          BB                                      02814 42 00000 00000
                BORG    *-9                             02816
```

```
*       INITIALIZATION OF THIRD SUMMATION
*
THRINO  TR    402,29                          02816 31 00402 00029
        S     442,446                         02828 22 00442 00446
        TF    DIVIS1,DIVISC                   02840 26 04998 05004
        TFM   ALPHC1,0,7                      02852 16 05041 00000
THRIN3  AM    ALPHC1,1,10                     02864 11 05041 00001
        S     DIVIS1,442                      02876 22 04998 00442
        BNN   THRIN3                          02888 46 02864 01300
        TFM   SHIFTC,0,9                      02900 16 05044 00000
        TR    19488,WRALPA-3                  02912 31 19488 05005
        TFM   THRI04+11,6003,7                02924 16 03503 06003
        TFM   THRI05+11,6007,7                02936 16 03515 06007
        RCTY                                  02948 34 00000 00102
        WATY  IDENT2                          02960 39 04795 00100
        RCTY                                  02972 34 00000 00102
        S     419,416                         02984 22 00419 00416
        TFM   COUNT1,0,9                      02996 16 05031 00000
THRIN1  AM    COUNT1,1,10                     03008 11 05031 00001
        CM    419,0,9                         03020 14 00419 00000
        BZ    THRIN2                          03032 46 03064 01200
        S     419,425                         03044 22 00419 00425
        B     THRIN1                          03056 49 03008 00000
        DORG  *-3                             03064
THRIN2  TF    NUMBR3,COUNT1                   03064 26 04987 05031
        MM    NUMBR3,5,10                     03076 13 04987 00005
        TF    NUMTH1,99                       03088 26 04890 00099
        TF    NAMPL2,INDEX3                   03100 26 04892 05020
        AM    NAMPL2,1,10                     03112 11 04892 00001
        M     CONS04,NAMPL2                   03124 23 05013 04892
        SF    95                              03136 32 00095 00000
        SM    99,8,10                         03148 12 00099 00008
        TF    NUMTH2,99                       03160 26 04897 00099
        TF    DELTA,425                       03172 26 05015 00425
        TF    XMINT,416                       03184 26 05018 00416
        TFM   SUBR06+11,NUMBR3                03196 16 02381 04987
        TFM   SUBR14+11,5,10                  03208 16 02749 00005
        TFM   SUBR13+11,1,10                  03220 16 02525 00001
        SM    431,10,10                       03232 12 00431 00010
        CF    431                             03244 33 00431 00000
        TD    SUBR07+6,431                    03256 25 02604 00431
        SM    431,1,10                        03268 12 00431 00001
        TD    SUBR02+11,431                   03280 25 02645 00431
        TD    SUBR19+6,431                    03292 25 02628 00431
        SM    431,3,10                        03304 12 00431 00003
        TD    SUBR11+6,431                    03316 25 02592 00431
        TFM   SUBR02+6,20003                  03328 16 02640 20003
THRI00  TFM   19998,0,8                       03340 16 19998 00000
        TF    IDENT4-1,410                    03352 26 04903 00410
*
*       THIRD SUMMATION. PREPARATION OF STORAGE FOR NEXT LINE
*
        TD    19999,400                       03364 25 19999 00400
        TFM   THRI01+6,20000,7                03376 16 03442 20000
        S     THRI01+6,NUMTH1                 03388 22 03442 04890
        TF    COUNT1,NUMBR3                   03400 26 05031 04987
THRI02  SM    COUNT1,1,10                     03412 12 05031 00001
        BZ    THRI03                          03424 46 03468 01200
THRI01  TR    19990,19995,2                   03436 31 19990 19995
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          AM    THR101+6,5,10                    03448 11 03442 00005
          B     THR102                           03460 49 03412 00000
          DORG  *-3                              03468
THR103    TFM   REGIS1,0,10                      03468 16 04909 00000
THR107    S     SUBR02+6,NUMTH1                  03480 22 02640 04890
*
*         THIRD SUMMATION, SELECTION OF AMPLITUDES
*
THR104    TF    461,6003,7                       03492 26 00461 06003
THR105    TF    465,6007,7                       03504 26 00465 06007
THR106    BT    SUBR06,REGIS1                    03516 27 02370 04909
*
*         THIRD SUMMATION, INCREMENTING
*
          A     THR104+11,CONS04                 03528 21 03503 05013
          A     THR105+11,CONS04                 03540 21 03515 05013
          AM    REGIS1,1,10                      03552 11 04909 00001
          C     REGIS1,NAMPL2                    03564 24 04909 04892
          BNZ   THR107                           03576 47 03480 01200
          S     THR104+11,NUMTH2                 03588 22 03503 04897
          S     THR105+11,NUMTH2                 03600 22 03515 04897
          WNTY  IDENT4-3                         03612 38 04901 00100
          BD    THR110,TYPTAP                    03624 43 03648 04874
          WNPT  IDENT4-3                         03636 38 04901 00200
THR110    A     410,423                          03648 21 00410 00423
          SPTY                                   03660 34 00000 00101
          BC2   PRINT2                           03672 46 04236 00200
*
*         ALPHANUMERIC PRINTING, PLOTTING
*
          TBTY                                   03684 34 00000 00108
PRINT1    TFM   COUNSH,0,9                       03696 16 04912 00000
          TFM   PRT011+11,20003,7                03708 16 03823 20003
          S     PRT011+11,NUMTH1                 03720 22 03823 04890
PRT002    C     COUNSH,SHIFTC                    03732 24 04912 05044
          BZ    PRT001                           03744 46 03788 01200
          SPTY                                   03756 34 00000 00101
          AM    COUNSH,1,10                      03768 11 04912 00001
          B     PRT002                           03780 49 03732 00000
          DORG  *-3                              03788
PRT001    A     SHIFTC,437                       03788 21 05044 00437
          TF    COUNT4,NUMBR3                    0380  26 04907 04987
PRT011    TF    MULT01,20003,7                   03812 26 04935 20003
          TDM   MULT01-4,0,11                    03824 15 04931 00000
          CF    MULT01-3                         03836 33 04932 00000
          S     MULT01,446                       03848 22 04935 00446
          M     ALPHC1,MULT01                    03860 23 05041 04935
          BNF   PRT015,99                        03872 44 03904 00099
PRT005    TFM   95,41,1011                       03884 16 00095 00041
          B     PRT004                           03896 49 03952 00000
          DORG  *-3                              03904
PRT015    SF    94                               03904 32 00094 00000
          AM    96,5,10                          03916 11 00096 00005
          CM    95,38,10                         03928 14 00095 00038
          BP    PRT005                           03940 46 03884 01100
PRT004    A     19489,95                         03952 21 19489 00095
          BC3   PRT019                           03964 46 03996 00300
          BD    PRT016,19489                     03976 43 04040 19489
          B     PRT018                           03988 49 04020 00000
          DORG  *-3                              03996
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PRT019 CM    19489,61,10                03996 14 19489 00061
       BNN   PRT016                      04008 46 04040 01300
PRT018 SPTY                             04020 34 00000 00101
       B     PRT017                     04032 49 04052 00000
       DORG  *-3                        04040
PRT016 WATY  19489                      04040 39 19489 00100
PRT017 S     19489,95                   04052 22 19489 00095
       TF    SPACEC,433                 04064 26 04914 00433
PRT014 CM    SPACEC,0,10                04076 14 04914 00000
       BZ    PRT012                     04088 46 04132 01200
       SPTY                            04100 34 00000 00101
       SM    SPACEC,1,10                04112 12 04914 00001
       B     PRT014                     04124 49 04076 00000
       DORG  *-3                        04132
PRT012 AM    PRT011+11,5,10             04132 11 03823 00005
       SM    COUNT4,1,10                04144 12 04907 00001
       BNZ   PRT011                     04156 47 03812 01200
       TF    RETURC,435                 04168 26 04916 00435
PRT013 CM    RETURC,1,1011              04180 14 04916 00001
       BZ    AFTER                      04192 46 04656 01200
       RCTY                            04204 34 00000 00102
       SM    RETURC,1,10                04216 12 04916 00001
       B     PRT013                     04228 49 04180 00000
       DORG  *-3                        04236
*
*      NUMERIC PRINTING
*
PRINT2 TFM   CLEAR1,20000,7             04236 16 05028 20000
       S     CLEAR1,NUMTH1              04248 22 05028 04890
       TFM   PRINC1,0,9                 04260 16 04927 00000
PRT024 TFM   PRINC2,0,9                 04272 16 04930 00000
PRT021 BD    PRT032,TYPTAP              04284 43 04320 04874
       TF    PRT033+6,CLEAR1            04296 26 04314 05028
PRT033 WNPT  20000,,2                   04308 38 20000 00200
PRT032 TF    PRT031+6,CLEAR1            04320 26 04338 05028
PRT031 CF    20000,,2                   04332 33 20000 00000
       TF    PRT022+11,CLEAR1           04344 26 04403 05028
PRT028 TFM   PRT028+9,4,10              04356 16 04365 00004
PRT029 SM    PRT028+9,1,10              04368 12 04365 00001
       BZ    PRT027                     04380 46 04436 01200
PRT022 BD    PR 027,0                   04392 43 04436 00000
       SPTY                            04404 34 00000 00101
       AM    PRT022+11,1,10             04416 11 04403 00001
       B     PRT029                     04428 49 04368 00000
       DORG  *-3                        04436
PRT027 TF    PRT020+6,PRT022+11         04436 26 04454 04403
PRT020 WNTY  20000,,2                   04448 38 20000 00100
       AM    PRINC1,1,10                04460 11 04927 00001
       AM    PRINC2,1,10                04472 11 04930 00001
PRT030 CM    PRINC2,16,9                04484 14 04930 00016
       BNZ   PRT023                     04496 47 04588 01200
       RCTY                            04508 34 00000 00102
       C     PRINC1,NUMBR3              04520 24 04927 04987
       BZ    AFTER                      04532 46 04656 01200
       TFM   PRINC2,0,9                 04544 16 04930 00000
       SM    PRINC1,1,10                04556 12 04927 00001
       TBTY                            04568 34 00000 00108
       B     PRT032                     04580 49 04320 00000
       DORG  *-3                        04588
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PRTO23 AM    CLEAR1,5,10                          04588 11 05028 00005
       C     PRINC1,NUMBR3                        04600 24 04927 04987
       BZ    PRTO26                               04612 46 04644 01200
       RPTY                                       04624 34 00000 00101
       B     PRTO21                               04636 49 04284 00000
       DORG  *-3                                  04644
PRTO26 RCTY                                       04644 34 00000 00102
*
*      THIRD SIMULATION.TEST FOR NEXT LINE
*
AFTER  C     413,IDENT4-1                         04656 24 00413 04903
       BNZ   THRI00                               04668 47 03340 01200
       BNC2  AFTER2                               04680 47 04736 00200
       BNC3  AFTER2                               04692 47 04736 00300
       WATY  MESS05                               04704 39 04821 00100
       RNTY  59                                   04716 36 00059 00100
       B     THRINO                               04728 49 02816 00000
       DORG  *-3                                  04736
*
*      TEST FOR NEXT SECTION
*
AFTER2 C     407,SECTX                            04736 24 00407 04954
       BZ    AFTER3                               04748 46 04780 01200
       A     SECTX,421                            04760 21 04954 00421
       B     START2                               04772 49 00540 00000
       DORG  *-3                                  04780
AFTER3 WATY  IDENT8                               04780 39 04877 00100
       H                                          04792 48 00000 00000
       DORG  *-9                                  04794
IDENT2 DAC   13,HORIZ.INDEX3@                     04795 00013X2 HORIZ.INDEX3‡
MESS05 DAC   27,SET PS2,3.TYPE ALPHASPECS @       04821 00027X2 SET PS2,3.TYPE ALPHASP
‡
 YPTAP DS    1                                    04874 00001
IDENT8 DAC   5,MOOI@                              04877 00005X2 MOOI‡
NUMTH1 DS    5                                    04890 00005
 AMPL2 DS    2                                    04892 00002
NUMTH2 DS    5                                    04897 00005
NUMBR2 DS    3                                    04900 00003
 DENT4 DC    4,000@                               04904 00004   0̄00‡
 OUNT4 DS    3                                    04907 00003
REGIS1 DS    2                                    04909 00002
COUNSH DS    3                                    04912 00003
 PACEC DS    2                                    04914 00002
RETURC DS    2                                    04916 00002
CONS53 DC    8,46100505                           04924 00008   4̄6100505
 RINC1 DS    3                                    04927 00003
 RINC2 DS    3                                    04930 00003
MULTO1 DS    5                                    04935 00005
IDENT1 DAC   8,SECTION@                           04937 00008X2 SECTION‡
 ECTX  DS    3                                    04954 00003
CONS12 DC    5,19467                              04959 00005   1̄9467
GROUP2 DS    2                                    04961 00002
 ROUP3 DS    2                                    04963 00002
ZERO10 DC    10,0                                 04973 00010   0̄000000000
ARGUM  DS    3                                    04976 00003
 ONSO2 DC    6,400004                             04982 00006   4̄00004
 UMBOO DS    2                                    04984 00002
NUMBR3 DS    3                                    04987 00003
CONSO5 DS    5                                    04992 00005
 IVIS1 DS    6                                    04998 000 6
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DIVISC DC    6,3[illegible]000                    05004 00006    $80000
WRALPA DC    4,41[illegible]@                     05008 00004    410‡
CONS04 DS    5                                    05013 00005
DELTA  DS    2                                    05015 00002
XMINT  DS    3                                    05018 00003
INDEX3 DS    2                                    05020 00002
COUNT9 DS    3                                    05023 00003
CLEAR1 DS    5                                    05028 00005
COUNT1 DS    3                                    05031 00003
ADDIN  DS    2                                    05033 00002
COUNT2 DS    2                                    05035 00002
ALPHC1 DS    6                                    05041 00006
SHIFTC DS    3                                    05044 00003
IDENT6 DAC   15,LOAD DATA TAPE@                   05047 00015X2 LOAD DATA TAPE‡
INFOM1 DAC   4,ER1@                               05077 00004X2 ER1‡
INFOM2 DAC   4,ER2@                               05085 00004X2 ER2‡
INFOM3 DAC   4,ER3@                               05093 00 04X2 ER3‡
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*
*       THE REMAINDER OF THE PROGRAM IS USED ONLY ONCE FOR LOADING AND
*       INITIALIZATION PURPOSES,AND IS ERASED DURING THE CALCULATION
*       BY THE ANSWERS OF THE FIRST AND SECOND SUMMATION
*
        DORG 10000                                              10000
*
*       LOADING OF COS AND SIN TABLE
*
        TFM   COUNT8,100,9                                      10000 16 13730 00T00
        TFM   PREP04+6,5100,7                                   10012 16 10030 05100
PREP04  RMPT 5100                                               10024 36 05100 00300
        AM    PREP04+6,9,10                                     10036 11 10030 00009
        SM    COUNT8,1,10                                       10048 12 13730 00001
        BNZ   PREP04                                            10060 47 10024 01200
*
*       GENERAL INITIALIZATION OF THE PROGRAM AND PREPARATION OF
*       THE SPECIFICATIONS OF THE CALCULATION
*
PREP00  RCTY                                                    10072 34 00000 00102
        WATY MESS75                                             10084 39 13579 00100
        H                                                       10096 48 00000 00000
        TDM   TYPTAP,1                                          10108 15 04874 00001
        RCTY                                                    10120 34 00000 00102
        WATY MESS69                                             10132 39 13127 00100
        H                                                       10144 48 00000 00000
        BC4   PREP01                                            10156 46 11488 00400
        RCTY                                                    10168 34 00000 00102
        WATY MESS70                                             10180 39 13227 00100
        TBTY                                                    10192 34 00000 00108
        RNTY  IDENT9-6                                          10204 36 13738 00100
        SF    IDENT9-6                                          10216 32 13738 00000
        RCTY                                                    10228 34 00000 00102
        WATY MESS50                                             10240 39 12257 00100
        TBTY                                                    10252 34 00000 00108
        RNTY  402                                               10264 36 00402 00100
        SF    402                                               10276 32 00402 00000
        TF    SECTX,404                                         10288 26 04954 00404
        RCTY                                                    10300 34 00000 00102
        WATY MESS51                                             10312 39 12299 00100
        TBTY                                                    10324 34 00000 00108
        RNTY  405                                               10336 36 00405 00100
        SF    405                                               10348 32 00405 00000
        RCTY                                                    10360 34 00000 00102
        WATY MESS52                                             10372 39 12341 00100
        TBTY                                                    10384 34 00000 00108
        RNTY  408                                               10396 36 00408 00100
        SF    4                                                 10408 32 00408 00 00
        RCTY                                                    10420 34 00000 00102
        WATY MESS53                                             10432 39 12383 00100
        TBTY                                                    10444 34 00000 00108
        RNTY  411                                               10456 36 00411 00100
        SF    411                                               10468 32 00411 00000
        RCTY                                                    10480 34 00000 00102
        WATY MESS54                                             10492 39 12425 00100
        TBTY                                                    10504 34 00000 00108
        RNTY  414                                               10516 36 00414 00100
        SF    414                                               10528 32 00414 00000
        RCTY                                                    10540 34 00000 00102
        WATY MESS55                                             10552 39 12467 00100
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TBTY
RNTY 417
SF   417
RCTY
WATY MESS56
TBTY
RNTY 420
SF   420
RCTY
WATY MESS57
TBTY
RNTY 422
SF   422
RCTY
WATY MESS58
TBTY
RNTY 424
SF   424
RCTY
WATY MESS59
TBTY
RNTY 426
SF   426
RCTY
WATY MESS60
TBTY
RNTY 428
SF   428
RCTY
WATY MESS61
TBTY
RNTY 430
SF   430
TFM  4[illegible]2,10[illegible]00,7
TFM  4[illegible]1,1000,811
BC2  PREPOS
RCTY
WATY MESS62
TBTY
RNTY 432
SF   432
RCTY
WATY MESS63
TBTY
RNTY 434
SF   434
RCTY
WATY MESS64
TBTY
RNTY 436
SF   436
RCTY
WATY MESS65
TBTY
RNTY 438
SF   438
RCTY
WATY MESS66
TBTY
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10564 34 00000 00106
10576 36 00417 00100
10588 32 00417 00000
10600 34 00000 00102
10612 39 12509 00100
10624 34 00000 00106
10636 36 00420 00100
10648 32 00420 00000
10660 34 00000 00102
10672 39 12553 00100
10684 34 00000 00106
10696 36 00422 00100
10708 32 00422 00000
10720 34 00000 00102
10732 39 12597 00100
10744 34 00000 00106
10756 36 00424 00100
10768 32 00424 00000
10780 34 00000 00102
10792 39 12641 00100
10804 34 00000 00106
10816 36 00426 00100
10828 32 00426 00000
10840 34 00000 00102
10852 39 12685 00100
10864 34 00000 00106
10876 36 00428 00100
10888 32 00428 00000
10900 34 00000 00102
10912 39 12729 00100
10924 34 00000 00106
10936 36 00430 00100
10948 32 00430 00000
10960 16 00442 T0000
10972 16 00446 0T000
10984 46 11296 00200
10996 34 00000 00102
11008 39 12773 00100
11020 34 00000 00106
11032 36 00432 00100
11044 32 00432 00000
11056 34 00000 00102
11068 39 12817 00100
11080 34 00000 00106
11092 36 00434 00100
11104 32 00434 00000
11116 34 00000 00102
11128 39 12861 00100
11140 34 00000 00106
11152 36 00436 00100
11164 32 00436 00000
11176 34 00000 00102
11188 39 12905 00100
11200 34 00000 00106
11212 36 00438 00100
11224 32 00438 00000
11236 34 00000 00102
11248 39 12961 00100
11260 34 00000 00106
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         RNTY  443
         SF    443
PREP05   RCTY
         WATY  MESS67
         TBTY
         RNTY  447
         SF    447
         RCTY
         WATY  MESS68
         TBTY
         RNTY  451
         RCTY
         WATY  MESS71
         H
         WNPT  IDENT9-6
         TD    452,400
         WNPT  402
         B     PREP02
PREP01   BNC2  PREP10
         TFM   442,10000,7
         TFM   446,1000,8
PREP10   RCTY
         WATY  MESS72
         H
         RNPT  IDENT9-6
         RNPT  402
         TF    SECTX,404
PREP02   BNC2  PREP06
         RCTY
         WATY  MESS74
         TBTY
         RNTY  PRT030+9
         SF    PRT030+9
         RCTY
         WATY  MESS73
         TBTY
         RNTY  TYPTAP
         BD    PREP06,TYPTAP
         BNC4  PREP06
         RCTY
         WATY  MESS76
         H
         WNPT  IDENT9-6
         WNPT  402
PREP06   SM    427,10,10
         CF    427
         TD    NEWS21+6,427
         SM    427,1,10
         TD    NEWS24+6,427
         TD    NEWS12+11,427
         SM    427,3,10
         TD    NEWS20+6,427
         SM    427,1,10
         TD    NEWS19+11,427
         BD    PREP03,451
         B     PREP07
PREP03   TF    NEWS56+11,INWS07+11
PREP07   TD    IDENT3+32*2-4,425
         TD    IDENT3+32*2-6,424
         TD    IDENT3+32*2-26,419
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11272 36 00443 00100
11284 32 00443 00000
11296 34 00000 00102
11308 39 13015 00100
11320 34 00000 00108
11332 36 00447 00100
11344 32 00447 00000
11356 34 00000 00102
11368 39 13065 00100
11380 34 00000 00108
11392 36 00451 00100
11404 34 00000 00102
11416 39 13301 00100
11428 46 00000 00000
11440 38 13738 00200
11452 25 00452 00400
11464 38 00402 00200
11476 49 11596 00000
11488 47 11524 00200
11500 16 00442 T0000
11512 16 00446 0T000
11524 34 00000 00102
11536 39 13377 00100
11548 48 00000 00000
11560 36 13738 00300
11572 36 00402 00300
11584 26 04954 00404
11596 47 11800 00200
11608 34 00000 00102
11620 39 13503 00100
11632 34 00000 00108
11644 36 04493 00100
11656 32 04493 00000
11668 34 00000 00102
11680 39 13425 00100
11692 34 00000 00108
11704 36 04874 00100
11716 43 11800 04874
11728 47 11800 00400
11740 34 00000 00102
11752 39 13621 00100
11764 48 00000 00000
11776 38 13738 00200
11788 38 00402 00200
11800 12 00427 000T0
11812 33 00427 00000
11824 25 01394 00427
11836 12 00427 00001
11848 25 01418 00427
11860 25 01435 00427
11872 12 00427 00003
11884 25 01382 00427
11896 12 00427 00001
11908 25 01447 00427
11920 43 11944 00451
11932 49 11956 00000
11944 25 01187 13727
11956 25 13713 00425
11968 25 13711 00424
11980 25 13691 00419
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        TD    IDENT3+32*2-28,418                    11992 25 13689 00418
        TD    IDENT3+32*2-32,417                    12004 25 13685 00417
        TD    IDENT3+32*2-48,416                    12016 25 13669 00416
        TD    IDENT3+32*2-50,415                    12028 25 13667 00415
        TR    29,402                                12040 31 00029 00402
        RCTY                                        12052 34 00000 00102
        WATY  IDENT6                                12064 39 05047 00100
        H                                           12076 48 00000 00000
        RNPT  15000                                 12088 36 15000 00300
        RCTY                                        12100 34 00000 00102
        WNTY  IDENT7-6                              12112 38 13731 00100
        WNTY  IDENT9-6                              12124 38 13738 010
        WNTY  15000                                 12136 38 15000 00100
        BD    PREP11,TYPTAP                         12148 43 12184 04874
        WNPT  IDENT7-6                              12160 38 13731 00200
        WNPT  15000                                 12172 38 15000 00200
PREP11  RCTY                                        12184 34 00000 00102
        WATY  IDENT3                                12196 39 13653 00100
        RCTY                                        12208 34 00000 00102
        RCTY                                        12220 34 00000 00102
        TD    19959,400                             12232 25 19959 00400
        B     START0                                12244 49 00600 00000
MESS50  DAC   21,TYPE 1ST SUM MIN.(3)@              12257 00021X2 TYPE 1ST SUM MIN.(3)$
MESS51  DAC   21,TYPE 1ST SUM MAX.(3)@              12299 00021X2 TYPE 1ST SUM MAX.(3)$
 ESS52  DAC   21,TYPE 2ND SUM MIN.(3)@              12341 00021X2 TYPE 2ND SUM MIN.(3)$
MESS53  DAC   21,TYPE 2ND SUM MAX.(3)@              12383 00021X2 TYPE 2ND SUM MAX.(3)$
MESS54  DAC   21,TYPE 3RD SUM MIN.(3)@              12425 00021X2 TYPE 3RD SUM MIN.(3)$
 ESS55  DAC   21,TYPE 3RD SUM MAX.(3)@              12467 00021X2 TYPE 3RD SUM MAX.(3)$
 ESS56  DAC   22,TYPE 1ST SUM DELTA(2)@             12509 00022X2 TYPE 1ST SUM DELTA(2)$
MESS57  DAC   22,TYPE 2ND SUM DELTA(2)@             12553 00022X2 TYPE 2ND SUM DELTA(2)$
MESS58  DAC   22,TYPE 3RD SUM DELTA(2)@             12597 00022X2 TYPE 3RD SUM DELTA(2)$
 ESS59  DAC   22,TYPE 1ST SUM SHIFT(2)@             12641 00022X2 TYPE 1ST SUM SHIFT(2)$
MESS60  DAC   22,TYPE 2ND SUM SHIFT(2)@             12685 00022X2 TYPE 2ND SUM SHIFT(2)$
MESS61  DAC   22,TYPE 3RD SUM SHIFT(2)@             12729 00022X2 TYPE 3RD SUM SHIFT(2)$
 ESS62  DAC   22,TYPE HORIZ.SPACING(2)@             12773 00022X2 TYPE HORIZ.SPACING(2)$
 ESS63  DAC   22,TYPE VERT. SPACING(2)@             12817 00022X2 TYPE VERT. SPACING(2)$
MESS64  DAC   22,TYPE SHIFT SPACING(2)@             12861 00022X2 TYPE SHIFT SPACING(2)$
 ESS65  DAC   28,TYPE HIGH LIMIT OF PEAKS(5)@
 2905 00028X2 TYPE HIGH LIMIT OF PEAKS(5)$
MESS66  DAC   27,TYPE LOW LIMIT OF PEAKS(4)@       12961 00027X2 TYPE LOW LIMIT OF PEAK
)$
 ESS67  DAC   25,TYPE NUMBER OF GROUPS(4)@         13015 00025X2 TYPE NUMBER OF GROUPS(
 ESS68  DAC   31,CENTROSYM=1,NONCENTROSYM=0 (1)@
13065 00031X2 CENTROSYM=1,NONCENTROSYM=0 (1)$
 ESS69  DAC   50,WHEN SPECS ARE TYPED SET SW4 OFF.FROM TAPE SW4 ON@
 3127 00050X2 WHEN SPECS ARE TYPED SET SW4 OFF.FROM TAPE SW4 ON$
MESS70  DAC   37,TYPE IDENT OF SPECS TAPE NOW MADE(6)@
 3227 00037X2 TYPE IDENT OF SPECS TAPE NOW MADE(6)$
 ESS71  DAC   38,MAKE LEADER.SPECS TAPE IS PUNCHED OUT@
 3301 00038X2 MAKE LEADER.SPECS TAPE IS PUNCHED OUT$
MESS72  DAC   24,LOAD SPECIFICATION TAPE@          13377 00024X2 LOAD SPECIFICATION TAP
 ESS73  DAC   39,OUTPUT.TYPE ONLY=1.TAPE AND TYPE=0 (1)@
 3425 00039X2 OUTPUT.TYPE ONLY=1.TAPE AND TYPE=0 (1)$
MESS74  DAC   38,TYPE IN NUMBER OF ANSWERS ON A ROW(3)@
 3503 00038X2 TYPE IN NUMBER OF ANSWERS ON A ROW(3)$
 ESS75  DAC   21,SET PROGRAM SWITCHES@              13579 00021X2 SET PROGRAM SWITCHES$
MESS76  DAC   16,MAKE TAPELEADER@                   13621 00016X2 MAKE TAPELEADER$
```
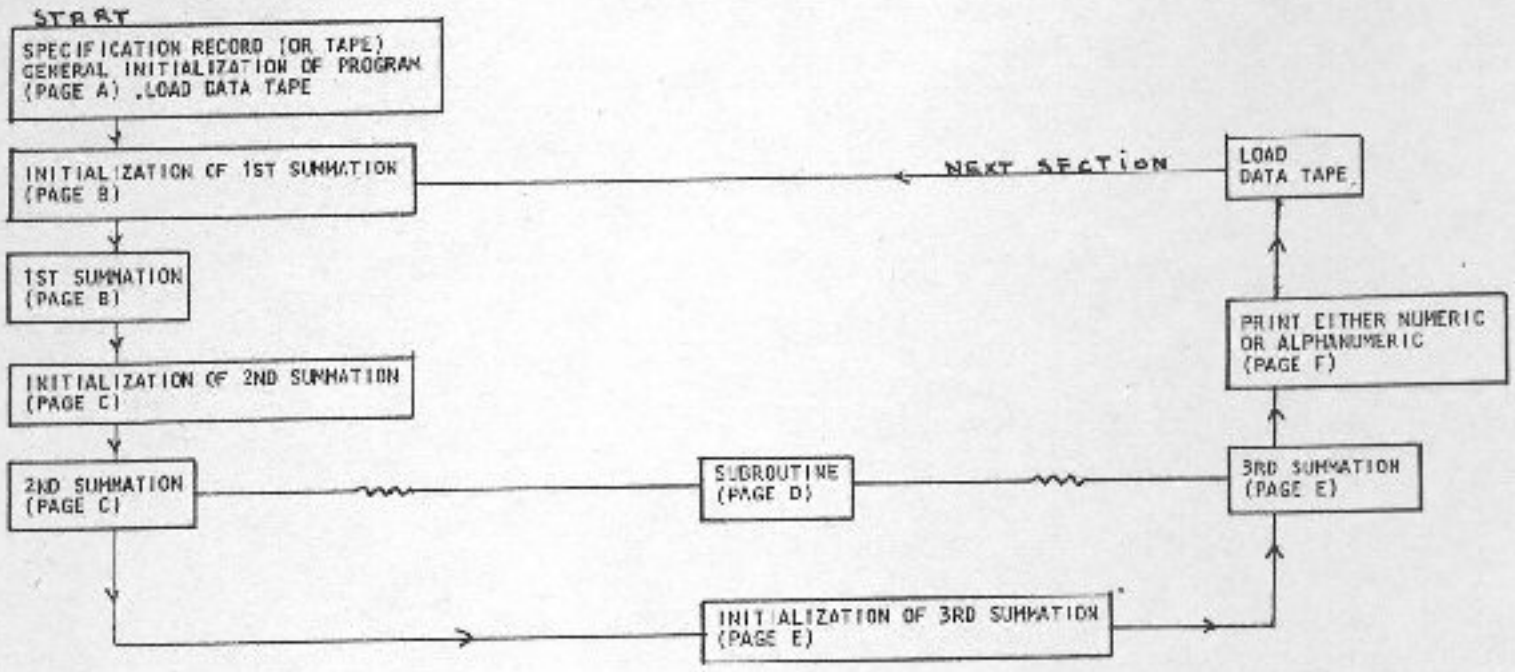
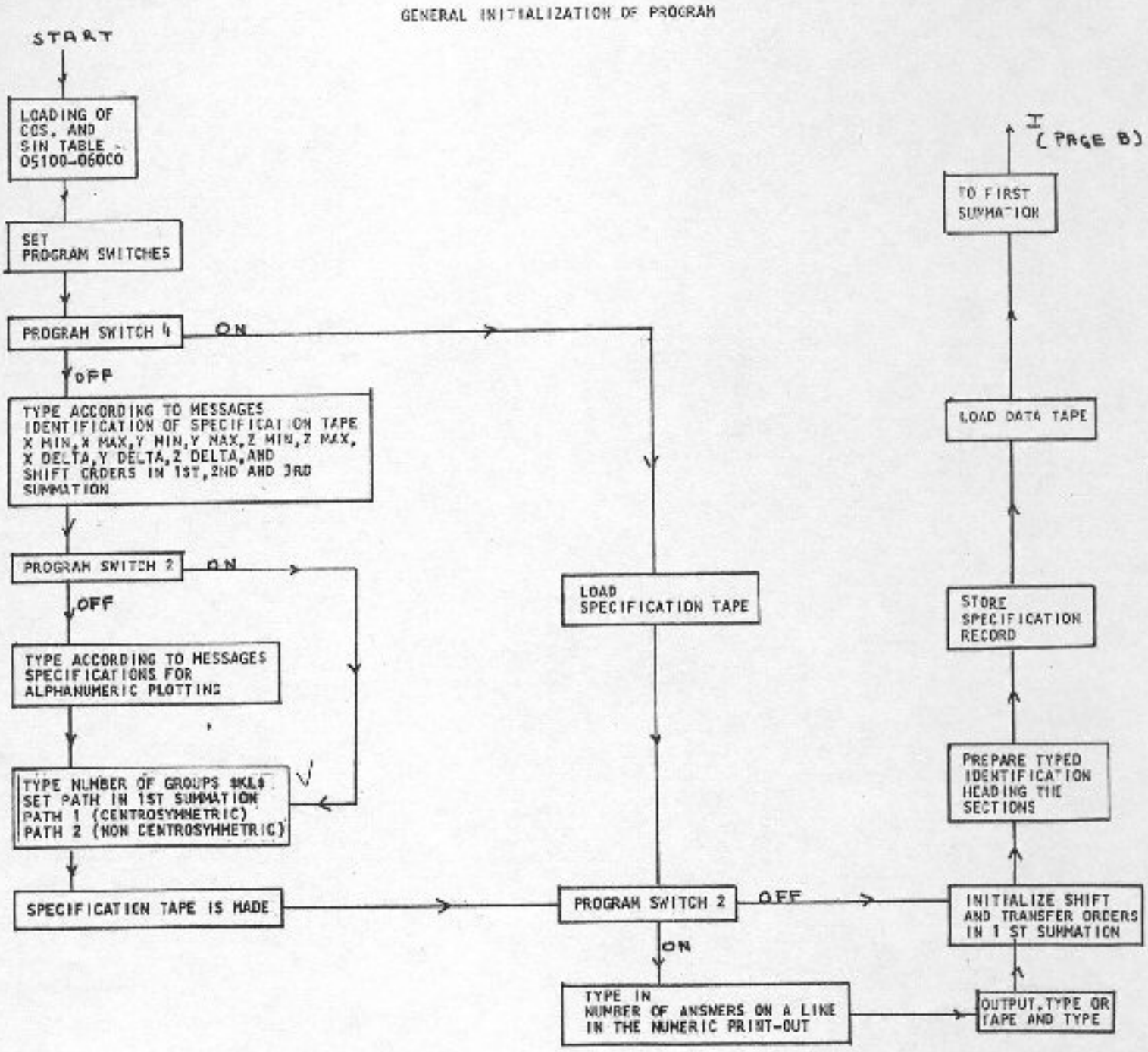

```
IDENT3 DAC  32,XMIN3=.00 XMAX3=0.00 DELTA3=.00@
13653 00032X2 XMIN3=.00 XMAX3=0.00 DELTA3=.0 ‡
INWS07 BN   NEWS58,,2                                  13716 47 Ø1332 01300
COUNT8 DS   3                                          13730 00003
IDENT7 DC   7,043001@                                  13737 00007   Ø43001‡
IDENT9 DC   7,00 000@                                  13744 00007   Ø00000‡
       DEND 10000                                      10000
END OF PASSII
```

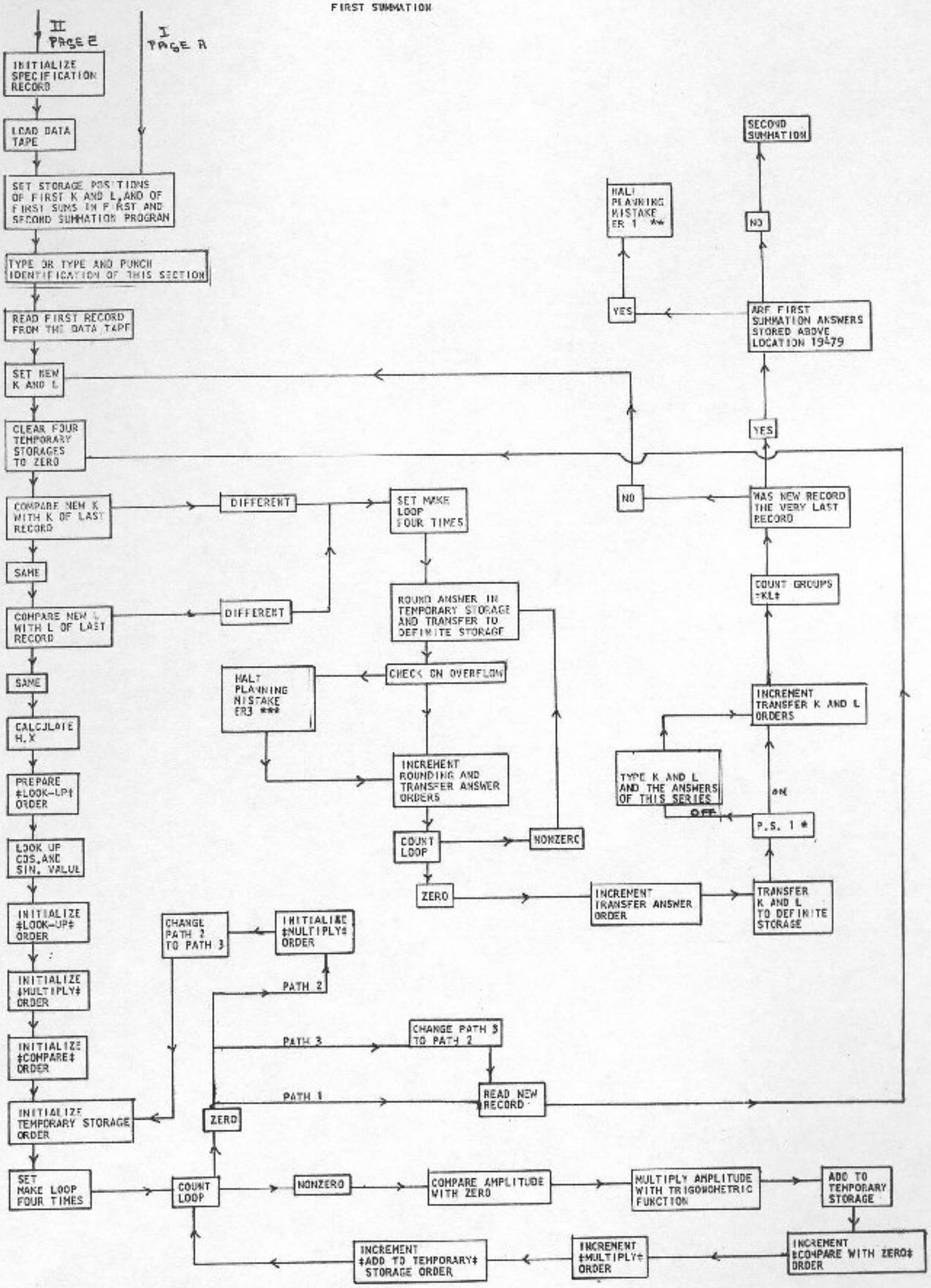
(INDEX TO FLOW SHEETS)



GENERAL INITIALIZATION OF PROGRAM



FIRST SUMMATION



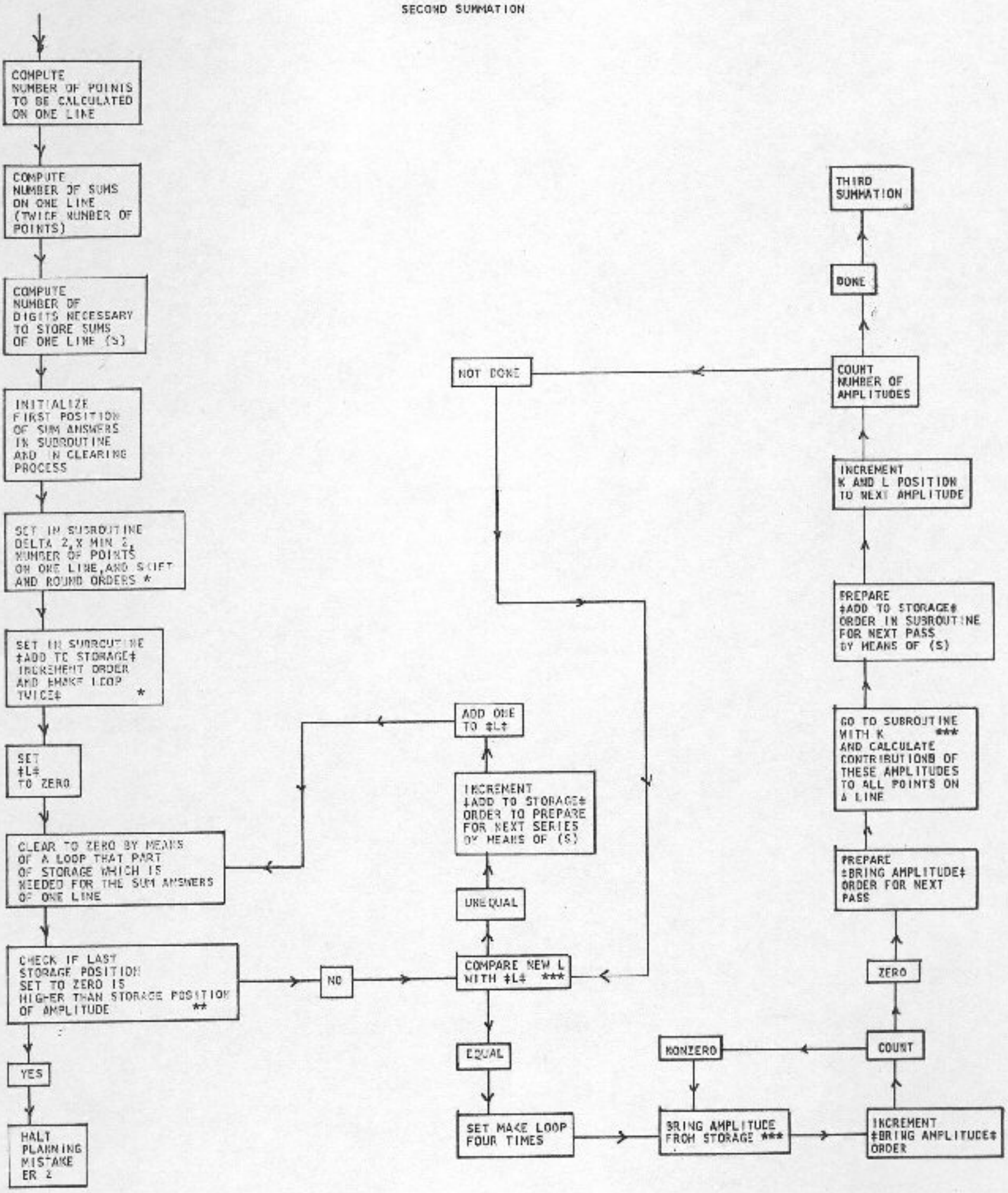
B

* PROGRAM SWITCH

** ‡NUMBER OF GROUPS‡ IN SPECIFICATION RECORD IS TOO SMALL.

*** SHIFT ORDERS IN THE 1ST SUMMATION SHOULD BE INCREASED.

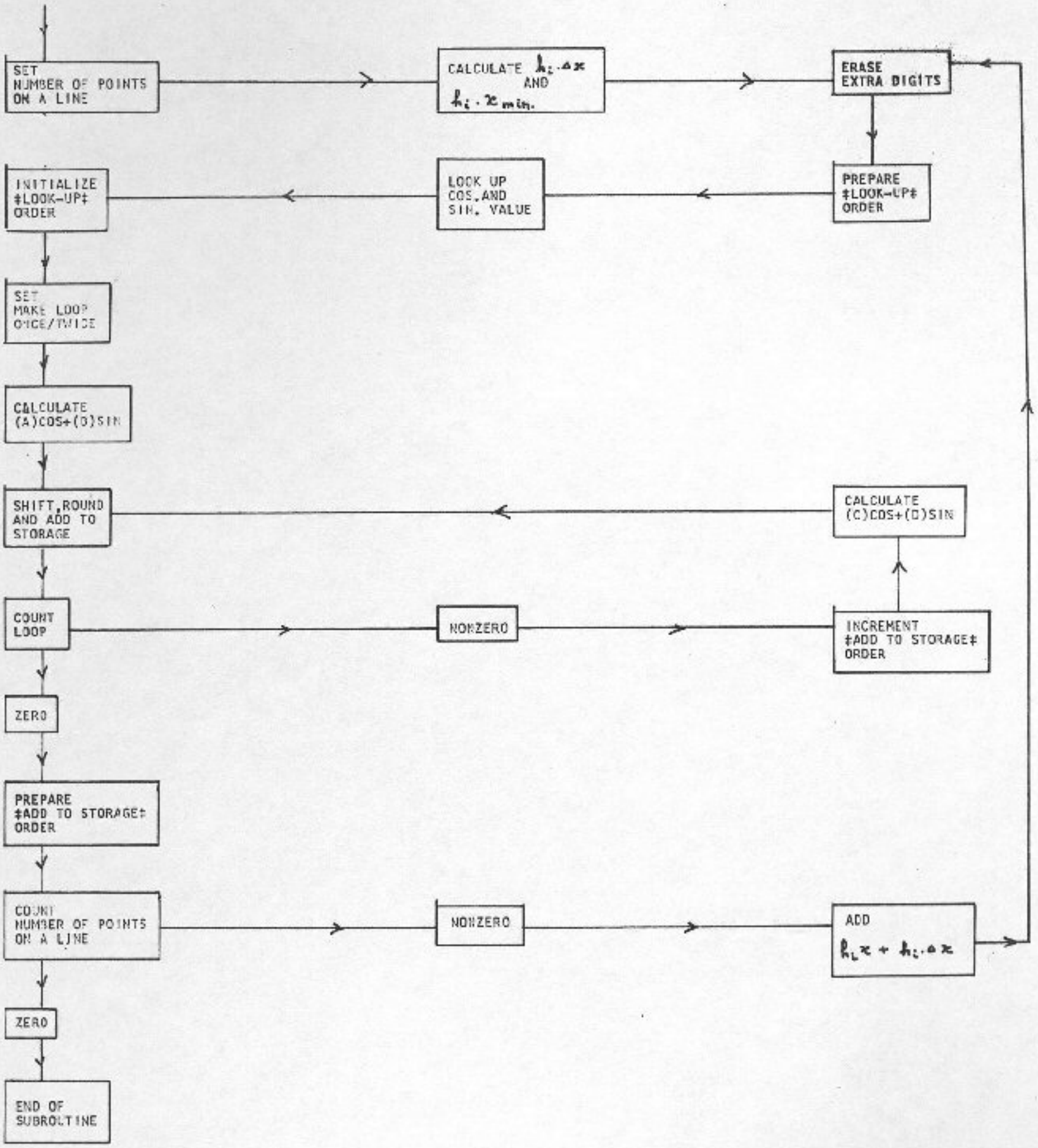
SECOND SUMMATION



* SEE SUBROUTINE
** THIS IS A CHECK TO SEE IF THERE IS A MOMENTARY OVERLAP OF FIRST AND SECOND SUMMATION (AMPLITUDES-SUM ANSWERS).
THE FIRST SUMMATION ANSWERS (HERE AMPLITUDES) ARE USED SERIALLY WHILE THE SECOND SUM ANSWERS ARE STORED SERIALLY.
THE SECOND SUM ANSWERS ARE STORED FROM POSITION 0500D - LP, WHILE THE FIRST SUM ANSWERS ARE STORED UP TO LOCATION 19479.
***THE POSITIONS OF K AND L, AND OF FIRST AMPLITUDE ARE INITIALIZED DURING THE FIRST SUMMATION.

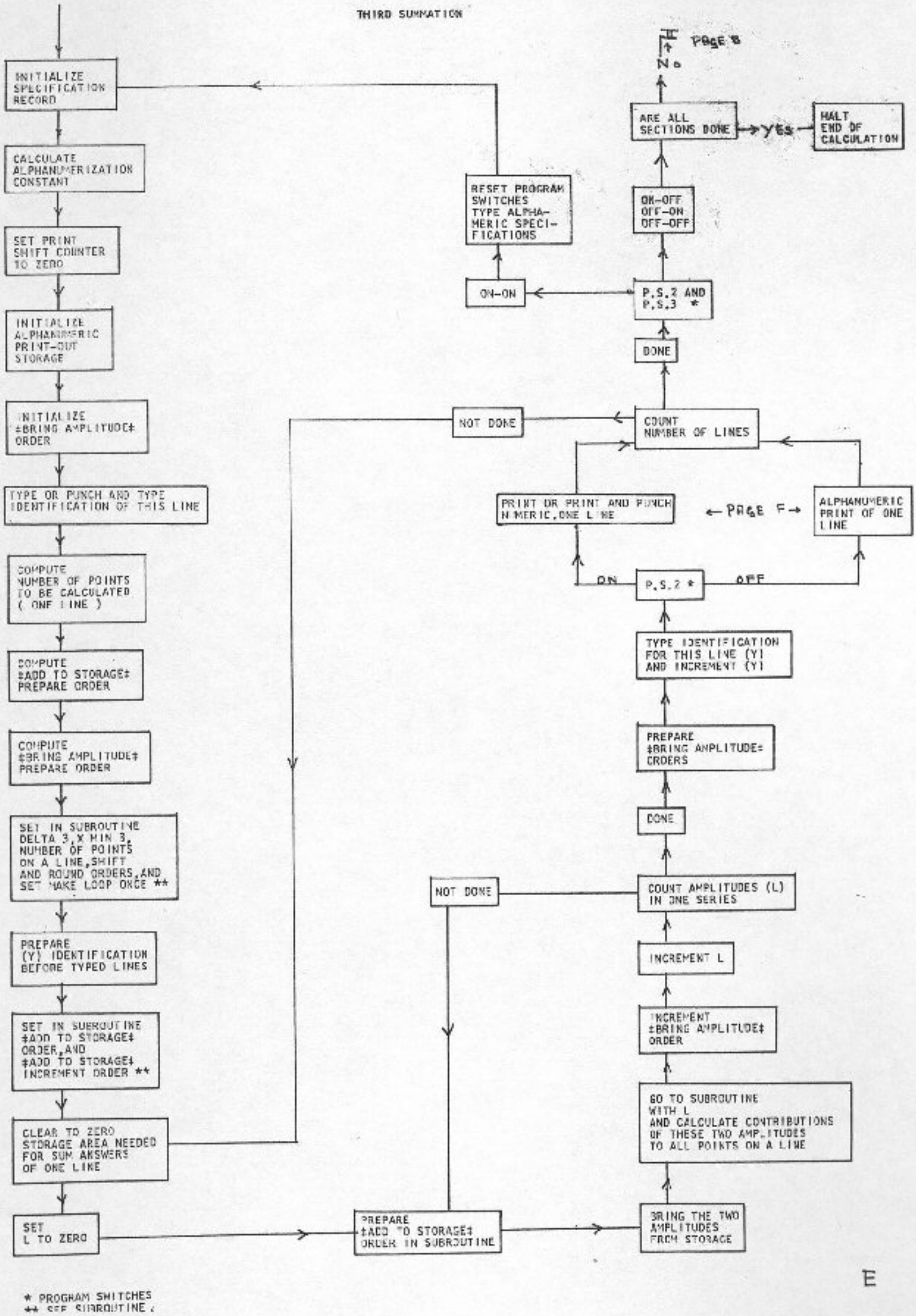
C

SUBROUTINE



D

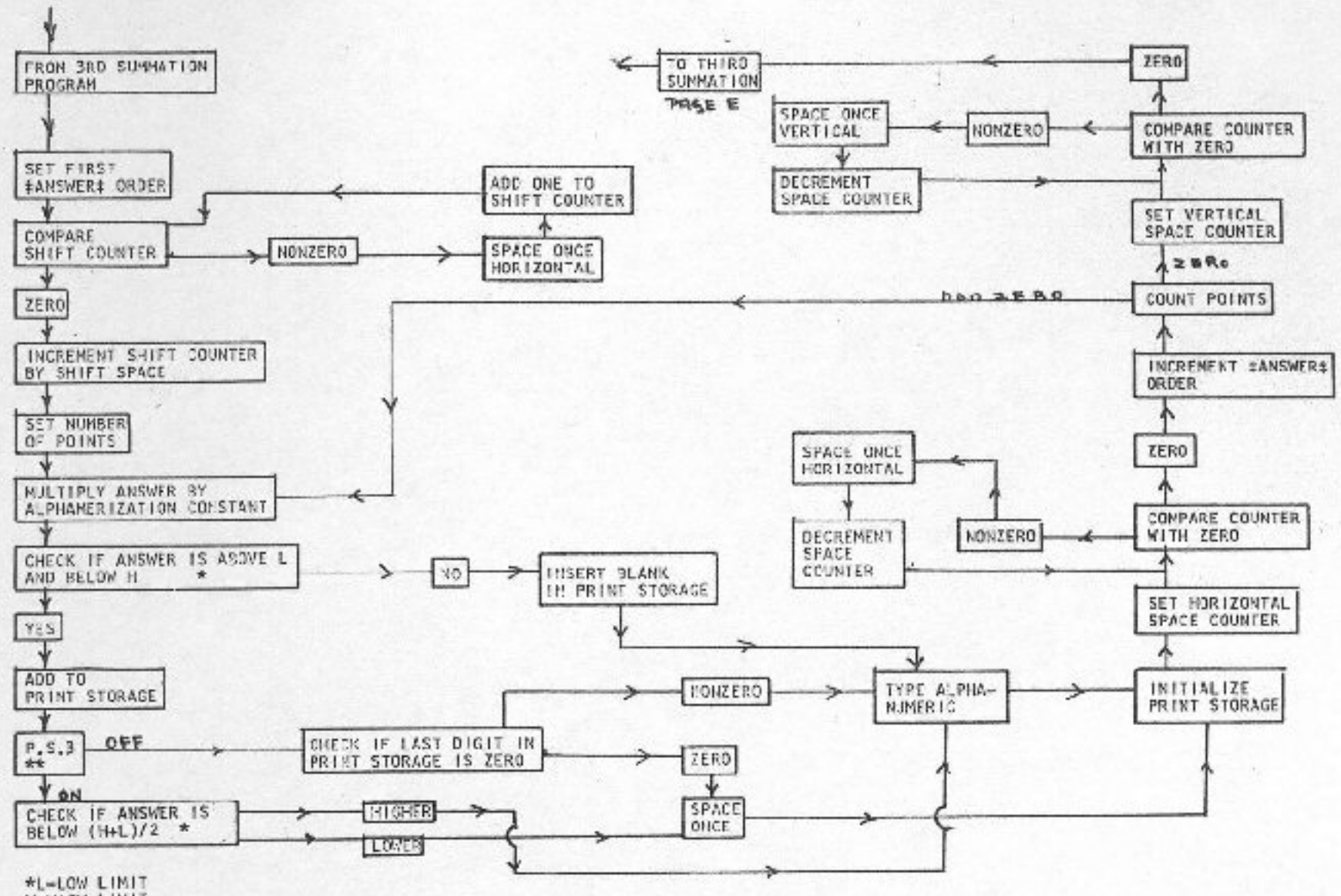
THIRD SUMMATION



* PROGRAM SWITCHES
** SEE SUBROUTINE

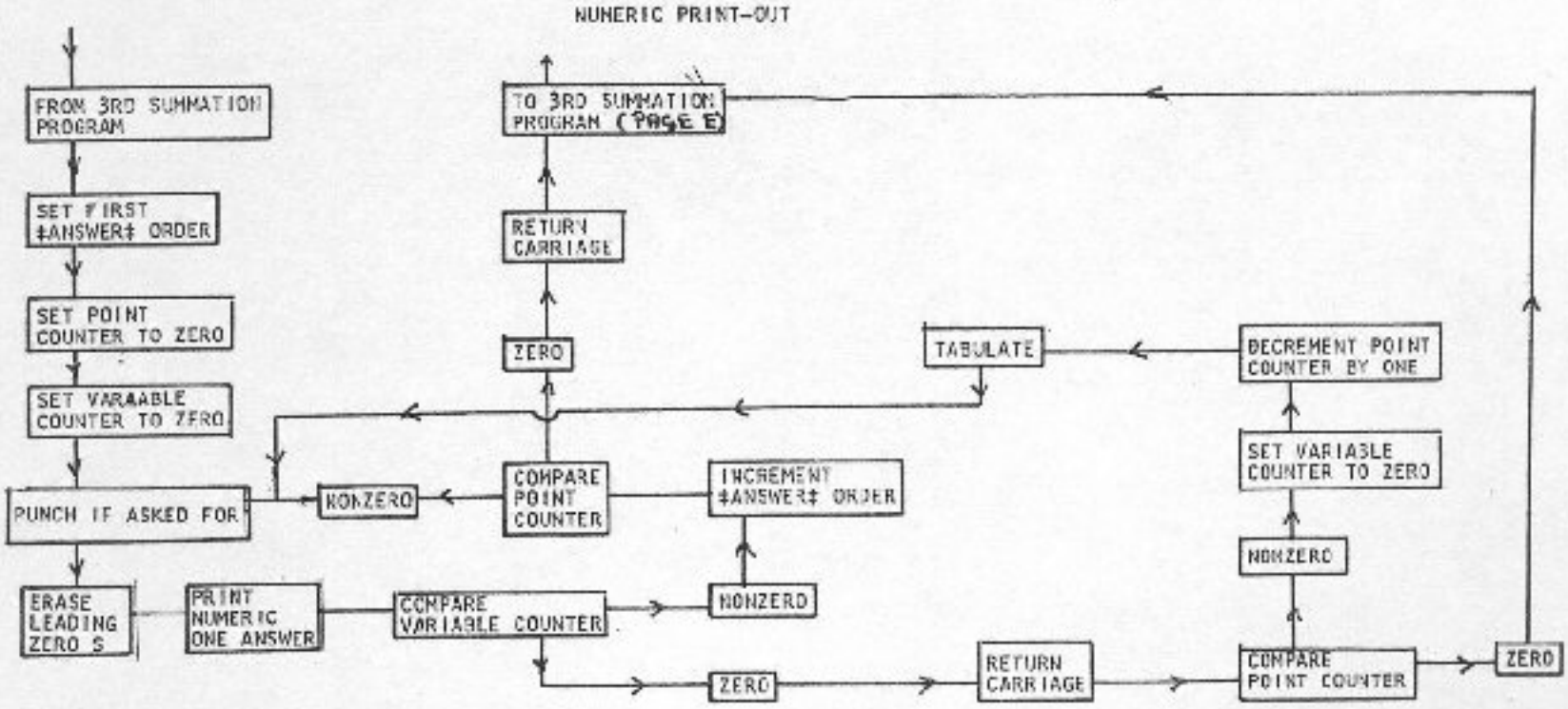
E

ALPHANUMERIC PRINT-OUT



*L=LOW LIMIT
H=HIGH LIMIT
** P.S.=PROGRAM SWITCH

NUMERIC PRINT-OUT



F