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

I.C.R. #4

Structure Factor Program

and

Least-Squares Sum Maker

for any triclinic, monoclinic and

orthorhombic space group

with an isotropic or anisotropic

temperature factor for each atom separately.

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Contents

The program (identification number 013004) is written for the I.B.M. 1620

Memory: 20,000 digits

Input: Paper tape and typewriter

Output: Paper tape and typewriter

Limitations: See Section III-5 and Section II

Timing: See Table I on following page

Cells of the Program:

00052 - 00079	working storage
00100 - 00399	multiplication and addition tables
00400 - 00499	reading area
00500 - 00560	space group record
00562 - 00589	subroutine
00600 - 00699	general sums
00700 - 00859	working storage
00860 - 06076	program
06076 - 09985	subroutines
10000 - 19999	parameters, trigonometric functions and least-squares sums (packed behind each other)
13000 - 18872	initialization program
Hash total: $6768254290451691767\bar{1}$	This number is checked when the tape is duplicated in our laboratory.

Duplicating: Use the I.B.M. library program: 1620 Numeric Tape Duplicator/Corrector.

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Table I

Timings on problems with 10 atoms.

The calculation time in seconds is given for one reflection.

		Triclinic				Monoclinic				Orthorhombic			
		isotropic		anisotropic		isotropic		anisotropic		isotropic		anisotropic	
		c.	n.c.	c.	n.c.	c.	n.c.	c.	n.c.	c.	n.c.	c.	n.c.
Without Output	Without L.S.	2.1	2.3	2.5	2.7	3.1	3.4	4.2	4.5	5.2	5.6	7.8	8.1
	With L.S.	4.0	4.2	8.5	8.7	5.4	6.3	10.5	11.4	7.5	9.4	15.1	17.0
Short Type	Without L.S.	6.7	8.3	7.0	8.6	7.6	9.1	8.7	10.5	9.8	11.4	12.4	13.9
	With L.S.	8.5	10.2	13.0	14.6	9.9	12.3	15.0	17.4	12.2	15.3	19.7	22.8
Short Type	Without L.S.	8.0	10.4	8.4	10.8	9.1	11.6	10.1	12.6	11.3	13.7	13.7	16.2
Short Tape	With L.S.	9.9	12.4	14.3	16.8	11.4	14.5	16.4	19.5	13.6	17.5	21.0	25.0
Long Type	Without L.S.	12.2	15.7	12.6	16.1	13.3	16.9	15.8	19.4	15.5	18.9	18.0	21.4
Long Tape	With L.S.	14.1	17.7	18.6	22.1	15.6	19.8	22.1	26.3	17.9	22.7	25.3	30.3

c. = centrosymmetric
n.c. = noncentrosymmetric

Section I Introduction

The present program (I.C.R. #4) calculates structure factors and least-squares sums. The sums for a block diagonal matrix are calculated. The final sums can be compiled with possible intermediate sums by the succeeding program: The Processor (I.C.R. #5) (in preparation), which also does the matrix calculations giving the parameter corrections and a new parameter tape. The structure factor output of the present program can also be used for a Fourier calculation (I.C.R. #1), after being sorted and combined by the S.F. - F.S. Sorter (I.C.R. #6) (in preparation).

Section II <u>General Theory</u>

It is possible to distinguish three computational processes by which structure factors are calculated.

1. One can use the "general" formulas, which are listed in the International Tables Volume I. There is one formula for each space group. This approach was used by MacIntyre (1960).

2. It is possible to simplify these "general" formulas to one for each group of reflections separately. These equations are also listed in the International Tables Volume I.

Both these methods are straightforward when isotropic parameters are used for the temperature motion of the atoms, because the symmetry relation of the atoms is included in the expression for the structure factor (1) or achieved by grouping the reflections (2), each group having its own expression for the structure factor. When however anisotropic parameters are used for the temperature motion of the atoms both these methods lose most of their luster because all atoms which are related by rotation axes, screw axes, mirror planes and glide planes have to be dealt with separately (Trueblood 1956), leaving only the center of symmetry relation. Formulas for some monoclinic space groups are given by Rollett and Davis (1955) and for all monoclinic space groups by the author (Thesis, Amsterdam 1960), and for all orthorhombic space groups by Hybl and Marsh (1961).

When anisotropic parameters have to be used routinely, a third method becomes obvious.

3. In this method the contributions of the atoms in the asymmetric unit of the cell are calculated with the basic structure factor equation of P_1 or $P_{\bar{1}}$ while each group of symmetry related atoms is simulated with a set of equivalent indices (sometimes together with a translation vector in the case of a screw axis or a glide plane). Each set of equivalent indices is substituted in the basic formula for P_1 or $P_{\bar{1}}$ and the answers are added to the contributions of the atoms

in the asymmetric unit. This method is used for instance by Cruickshank (1961) and Busing and Levy (1959).

The third method is the one used in this program. There are several reasons for this decision. Contrary to the first methods the calculation is basically the same for all space groups. There are only minor differences for each crystal system. It is also important that calculations with anisotropic parameters are completely straight forward with the last method and definitely less cumbersome than with the first two methods. The most important advantage of the last method is the elegant way with which least-squares sums are made, making the logic of the program easily understandable (see flow charts).

The third method is avoided by most because the calculation is thought to be considerably slower. This however is not true. In general the last method uses more additions while the first two use more multiplications, and it appears that the speeds are quite similar.

The present program follows quite closely the third method as it was described by Cruickshank (1961). With his notation we define

$$A \equiv \sum_r \sum_s A_{rs} \; (= \sum_r A_r)$$

where A_{rs} is the contribution, of the rth atom at its sth equivalent position, to the real part of the structure factor, or similarly A_r is the contribution of the rth atom and its symmetry equivalents. In the same manner B_{rs} and B_r are defined with respect to the imaginary part of the structure factor.

Furthermore any symmetry operation is a combination of a rotation (matrix $\underline{R}$) and a translation (vector $\vec{t}$). The coordinate of an atom equivalent to r can therefore be written as $x_{rs} = \underline{R}\, x_r + \vec{t}$

The argument of the cosine in the expression for A_{rs} is:

$h\, x_{rs} + k\, y_{rs} + \ell\, z_{rs}$, which can thus be written as:

$h\, x_{rs} + k\, y_{rs} + \ell\, z_{rs} = h_s x_r + k_s y_r + \ell_s z_r + ht_x + kt_y + \ell t_z$, where h_s, k_s and ℓ_s are a set of equivalent indices ($h_s = h.\underline{R}$) and $ht_x + kt_y + \ell t_z$ is a quantity which is independent of the particular atom r.

The argument of the exponential in the expression for A_{rs} for an anisotropic atom is

$$h^2 b^{11}_{rs} + hk b^{12}_{rs} + h\ell b^{13}_{rs} + k^2 b^{22}_{rs} + k\ell b^{23}_{rs} + \ell^2 b^{33}_{rs}$$

which can be written as:

$$h_s{}^2 b^{11}_r + h_s k_s b^{12}_r + h_s \ell_s b^{13}_r + k_s{}^2 b^{22}_r + k_s \ell_s b^{23}_r + \ell_s{}^2 b^{33}_r$$

Together they show the relation between equivalent positions and equivalent indices.

The program uses only a diagonal matrix R, and is therefore restricted to triclinic, monoclinic and orthorhombic space groups.

When one has a problem with a space group of higher symmetry one could decrease the symmetry of this space group (for instance by taking out one or more rotation axes) so that the resultant symmetry is orthorhombic, monoclinic or triclinic. In that case one has of course to include the parameters of the atoms of the previously dependent sets as independent parameters into the structure factor calculation made with the lower symmetry.

The expressions with equivalent indices rather than with equivalent positions are used.

For the calculation of a structure factor the relevant equations are thus:

$$|F_c| = \sqrt{A^2 + B^2} \qquad (1)$$

$$A = \sum_r \sum_s A_{rs} \text{ and } B = \sum_r \sum_s B_{rs}$$

$$A_{rs} = f_r \cos 2\pi(h_s x_r + k_s y_r + \ell_s z_r + t_s).$$

$$\exp - (h_s{}^2 b^{11}_r + h_s k_s b^{12}_r + h_s \ell_s b^{13}_r + k_s{}^2 b^{22}_r + k_s \ell_s b^{23}_r + \ell_s{}^2 b^{33}_r) \qquad (2)$$

and

$$B_{rs} = f_r \sin 2\pi(h_s x_r + k_s y_r + \ell_s x_r + t_s). \qquad (3)$$

$$\exp - (h_s{}^2 b^{11}_r + h_s k_s b^{12}_r + h_s \ell_s b^{13}_r + k_s{}^2 b^{22}_r + k_s \ell_s b^{23}_r + \ell_s{}^2 b^{33}_r)$$

For an isotropic atom the exponential is: $\exp - B_r \sin^2\theta/\lambda^2$

The purpose of the least-squares calculation is to minimize $\sum_q w\,(|kF_o| - |F_c|)^2$, where $\sum_q$ is the sum over all reflections, or rather to minimize

$\sum_q w\,(|kF_o| - |F_c| - \Delta|F_c|)^2$, where ΔF_c is the change in F_c as a result of changes in the parameters. By excluding second and higher order expansion terms it is possible to express ΔF_c as:

$$\Delta|F_c| = \sum_{i=1}^{n}\left(\frac{\partial|F_c|}{\partial x_i}\Delta x_i + \frac{\partial|F_c|}{\partial y_i}\Delta y_i + \frac{\partial|F_c|}{\partial z_i}\Delta z_i + \frac{\partial|F_c|}{\partial b_i^{11}}\Delta b_i^{11} + \frac{\partial|F_c|}{\partial b_i^{12}}\Delta b_i^{12} \;\ldots\; + \frac{\partial|F_c|}{\partial b_i^{33}}\Delta b_i^{33}\right)$$

where n is the number of atoms

Using this expansion it is possible to reduce to a set of normal equations by differentiating the function, which has to be minimized, with respect to each change of parameter and in each case summing over all observations, resulting in the matrix

$$\sum_q (|kF_o|-|F_c|)\frac{\partial|F_c|}{\partial x_1} = \sum_{i=1}^{n}\left(\sum_q \Delta x_i \frac{\partial|F_c|}{\partial x_1}\frac{\partial|F_c|}{\partial x_i} + \sum_q \Delta y_i \frac{\partial|F_c|}{\partial x_1}\frac{\partial|F_c|}{\partial_i} + \ldots \sum_q \Delta b_i^{33}\frac{\partial|F_c|}{\partial x_1}\frac{\partial|F_c|}{\partial_i^{33}}\right)$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$\sum_q (|kF_o|-|F_c|)\frac{\partial|F_c|}{\partial b_n^{33}} = \sum_{i=1}^{n}\left(\sum_q \Delta x_i \frac{\partial|F_c|}{\partial b_n^{33}}\frac{\partial|F_c|}{\partial x_i} + \sum_q \Delta y_i \frac{\partial|F_c|}{\partial b_n^{33}}\frac{\partial|F_c|}{\partial y_i} + \ldots \sum_q \Delta b_i^{33}\frac{\partial|F_c|}{\partial b_n^{33}}\frac{\partial|F_c|}{\partial b_i^{33}}\right)$$

$\sum_q$ is the sum over all reflections.

The size of the memory of the computer makes it in general impossible to calculate this full matrix. On the other hand a single diagonal matrix has proven to be erratic at times. The program is primarily written for three dimensional refinement. In that case no overlap will occur between (neighboring) atoms and cross terms of the type

$\frac{\partial|F_c|}{\partial x_i}\frac{\partial|F_c|}{\partial x_j}$, $i \neq j$; and $\frac{\partial|F_c|}{\partial x_i}\frac{\partial|F_c|}{\partial y_j}$ $i \neq j$ etc., are therefore supposed to be negligible. It also accepted that there is no interaction between positional and temperature factor parameters, and that $\frac{\partial|F_c|}{\partial x_i} \frac{\partial|F_c|}{\partial b_j}$, $i = j$, $i \neq j$ are negligible. One is now left with a block diagonal matrix: 3 x 3 matrices for the positional parameters of each atom, 6 x 6 matrices for the anisotropic temperature factor parameters of each atom or 1 x 1 matrices for the isotropic temperature factor parameters of each atom. The two suppositions which are made to reduce the size of the matrix are by no means exactly right (Geller 1961) but this approach has proved its usefulness for three dimensional refinement (Sparks, Prosen, Kruse, Trueblood 1956).

The relevant formulas for making the least-squares sums (matrix and vector terms) are now deduced.

$$|F_c|^2 = A_c^2 + B_c^2 \qquad (4)$$

$$\cos\alpha = \frac{A_c}{|F_c|} \text{ and } \sin\alpha = \frac{B_c}{|F_c|} \qquad (5)$$

Differentiating (4) with respect to any parameter gives:

$$2|F_c| \frac{\partial|F_c|}{\partial P_r} = 2\, A_c \frac{\partial A_c}{\partial P_r} + 2\, B_c \frac{\partial B_c}{\partial P_r}$$

using (5):

$$\frac{\partial|F_c|}{\partial P_r} = \cos\alpha \frac{\partial A_c}{\partial P_r} + \sin\alpha \frac{\partial B_c}{\partial P_r} \qquad (6)$$

(Note that formula 2.10 in Cruickshank (1960) should read $F_c = A \cos\alpha + B \sin\alpha$)

For convenience

$$G_{rs} = A_{rs} \cos\alpha + B_{rs} \sin\alpha \quad \text{and} \quad J_{rs} = B_{rs} \cos\alpha - A_{rs} \sin\alpha \qquad (7)$$

are defined.

There are three types of differential quotients (using expressions (2), (3), (6) and (7)):

$$\frac{\partial |F_c|}{\partial x_r} = \sum_s (-2\pi h_s)\, J_{rs}$$

$$\frac{\partial |F_c|}{\partial b_r^{11}} = -\sum_s (h_s)^2\, G_{rs}$$

$$\frac{\partial |F_c|}{\partial\, 'B_r} = -\frac{\sin^2\theta}{\lambda^2} \sum_s G_{rs}$$

in which x is a positional parameter, b^{11} isan anisotropic temperature factor parameter and 'B is an isotropic temperature factor parameter. Using these differential quotients and the weight, w, and $|kF_o| - |F_c|$, the necessary matrix terms and vector terms are calculated. (A list of these is given in Section IV, 4.)

Note: One has to use $|kF_o| - |F_c|$ instead of $kF_o - F_c$ in the vector terms. And it is for computational <u>convenience</u> <u>only</u> that in centrosymmetric space groups, A_{rs} instead of G_{rs}, and B_{rs} instead of J_{rs} and $kF_o - F_c$ instead of $|kF_o| - |F_c|$ are used to compute the matrix and vector terms in the present program. This is essentially the same as is achieved by Cruickshank (1961) (formulas 2.22 - 2.27) by redefining G_{rs} and J_{rs} so as to include the sign of cos α.

Besides the least-squares sums the program calculates sums from which a correction in the scale factor k and the overall temperature factor $'\overline{B}$ can be calculated.

It is accepted that

$$|kF_o|\,(1 + \Delta K) = |F_c|\,(1 - s^2\, \Delta'\overline{B})$$

in which $s = \sin\theta/\lambda$ ΔK and $\Delta'\overline{B}$ are respectively corrections to the scale factor and overall temperature factor.

The function

$$\sum_q w\, \{(|kF_o| - |F_c|) + |kF_o|\, \Delta K + s^2\, |F_c|\, \Delta'\overline{B}\}^2$$

has to be minimized, giving two normal equations

$$\Delta K \sum_q w\, (|kF_o|)^2 + \Delta'\overline{B} \sum_q w\, s^2\, (|kF_o|)(|F_c|) = -\sum_q w\, (|kF_o|)(|kF_o| - |F_c|)$$

and

$$\Delta K \sum_q w\, s^2\, (|kF_o|)(|F_c|) + \Delta'\overline{B} \sum_q w\, s^4\, (|F_c|)^2 = -\sum_q w\, s^2\, (|F_c|)(|kF_o| - |F_c|)$$

These five sums together with $\sum_q w\,(|kF_o| - |F_c|)$, $\sum_q |kF_o|$, $\sum_q |F_c|$ and $\sum_q |kF_o - F_c|$ are made for all reflections (see Section V, 1c, pg. 38) and will be called general sums.

This routine affords the only coupling between the F_o scale factor and the temperature factors of the structure.

One should take a new scale factor (k') in the following structure factor calculation: $k' = k + k.\Delta K$,

and the individual corrections (from the least-squares sums) $\Delta' B_i$ and Δb_i^{11} should be increased by the difference between $\Delta'\overline{B}$ and the average of all $\Delta' B_i$ and Δb_i^{11} (transformed to principal axes of the vibration ellipsoid and expressed in $A^{\circ 2}$).

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D. W. Cruickshank, Conference Report, Computing Methods and the Phase Problems in X-ray Crystal Analysis. Pergamon Press 1961, p. 32.

S. Geller Acta Cryst. 14, 1026 (1961).

R. A. Sparks, R. J. Prosen, F. M. Kruse, K. N. Trueblood Acta Cryst. 9, 350 (1956).

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Section III Operation, Switch Settings and Messages

1. General

The necessary tapes are the program tape, a parameter tape and a data tape. After reading in the program tape, the initialization of the program is performed, partially by instructions which are requested and typed on the typewriter. During the initialization the parameter tape is read in, or parameters are typed in and the data tape is loaded and read up to the first reflection which has to be calculated. After this the actual program takes over and calculates and puts out the structure factors of reflections as they are read in turn from the data tape. When least-squares sums are made (P.S.1. off) it is possible that one or more series of least-squares sums are punched out intermediately. The last least-squares sums are punched out when the end record (8‡) is sensed and the calculation is finished. It is possible to interrupt the calculation anywhere on the data tape. The inclusion of a structure factor is decided by a logical routine which is a part of the program but which can be changed during the initialization to meet specific purposes. To avoid complications it is better to reload the program when another structure factor calculation has to be carried out.

2. Manual Operation

1. Clear computer. Insert 16 00010 00000; Releass; Start; SCE; Reset.
2. Ready program tape: Insert 36 00000 00300; Release; Start.
3. With the program still partly to be read, the reading will stop:

   Press Start.
4. The first message will be typed out. Follow the typed instructions.

   Always press Release and Start after typing in a number.

3. Switch Settings and Typewriter

Right margin 75 from the left. Tab stops at 20 and 40 from the left.

Parity Switch : Stop

Input/Output Switch : Stop

Overflow Switch : Stop

Program Switch 1

Off: The program will calculate least-squares sums.

On: The program will not calculate least-squares sums.

Program Switch 2

Off: Normal

On: This position should be used when a change has to be made on the data tape. When the switch is on, the next reflection will be typed out before it is calculated; the typewriter will pause to accept information. The corrected form of the reflection (ending with a ǂ) can then be typed in. (See Section III 5a, pg. 22). This setting can also be used to finish a calculation in the middle of the data tape without losing the least-squares sums obtained so far. (See Section III, 4k, pg. 21).

Program Switch 3 and 4 (output switches)

P.S.3 on: P.S.4 on: Short type out and short tape out of structure factors

P.S.3 on: P.S.4 off: Long type out and long tape out of structure factors

P.S.3 off: P.S.4 on: Short type out of structure factors

P.S.3 off: P.S.4 off: No output of structure factors (with P.S.1 off: only L.S. Sums and General Sums; with P.S.1 on: only General Sums) (Least-squares sums are punched on tape only).

4. Messages

This section is an explanation of some of the messages which are typed out. The number in parentheses after each message defines the number of digits required in the information to be typed.

a. Message

"Type in spacegroup number. (3)"

In general the numbering of the International Tables, Volume I is followed and this number should be typed in as a three digit number. It is however essential that the setting of the crystal axes be exactly the same as specified in the Tables. The following additional settings are provided for on the program tape and are given here with their calling number

$P2_1/a$ = 514

$P2_1/n$ = 614

P nam - 562

Only triclinic, monoclinic and orthorhombic spacegroups can be calculated with this program. One can of course treat a higher symmetry by means of an orthorhombic spacegroup.

Thus there is not a rotation matrix and a translation vector for all possible settings. One should however be able to calculate structure factors also in those cases. This can be accomplished by typing in another number (e.g. 999) which is not yet used to define a spacegroup on the actual program tape. In that case the following message is typed out.

"Load additional spacegroup tape. (3)" And at this moment a self-made tape with rotation matrices and translation vectors of the particular setting can be loaded. It is necessary to know what the format of the spacegroup matrices and vectors is, which is explained below by means of three examples. When the spacegroup record which has to be used in the calculation is not the first one on the additional tape then this message will be repeated one or more times. It suffices to press Start after each repeat as long as there is tape which is not yet read.

$P2_1/c$	$P2_1/a$	$Pna2_1$	
014	514	033	
0	0	0	
1	1	1	general identification of a parameter record
6	6	6	
0	5	0	
1	1	3	number of space group
4	4	3	
‡	‡	‡	
1	1	0	1 = centrosymm.; 0 = noncentrosymm.
$\bar{0}$	$\bar{0}$	$\bar{0}$	always the same
2	2	4	1 = triclinic; 2 = monoclinic; 4 = orthorhombic
$\bar{0}$	$\bar{0}$	$\bar{0}$	always the same
$\bar{0}$	$\bar{0}$	$\bar{0}$	always the same
2	2	1	See (i): multiplicity of space group
$\bar{0}$	$\bar{0}$	$\bar{0}$	
1	1	1	first set of equivalent indices (hkℓ)
$\bar{0}$	$\bar{0}$	$\bar{0}$	(diagonal matrix). For instance
1	1	1	for $P2_1/c$: h, k, ℓ
$\bar{0}$	$\bar{0}$	$\bar{0}$	
1	1	1	
$\bar{0}$	$\bar{0}$	$\bar{0}$	
1	1	$\bar{1}$	second set of equivalent indices
$\bar{0}$	$\bar{0}$	$\bar{0}$	(diagonal matrix). For instance
$\bar{1}$	$\bar{1}$	$\bar{1}$	for $P2_1/c$: h, $\bar{k}$, ℓ
$\bar{0}$	$\bar{0}$	$\bar{0}$	
1	1	1	
$\bar{0}$	$\bar{0}$	$\bar{0}$	
0	0	$\bar{1}$	third set of equivalent indices
$\bar{0}$	$\bar{0}$	$\bar{0}$	(diagonal matrix). For instance
0	0	1	for $P2_1/c$: no more equivalent
$\bar{0}$	$\bar{0}$	$\bar{0}$	indices
0	0	1	
$\bar{0}$	$\bar{0}$	$\bar{0}$	
0	0	1	fourth set of equivalent indices
$\bar{0}$	$\bar{0}$	$\bar{0}$	(diagonal matrix). For instance
0	0	$\bar{1}$	for $P2_1/c$: no more equivalent
$\bar{0}$	$\bar{0}$	$\bar{0}$	indices
0	0	1	

$\bar{0}$	$\bar{0}$	$\bar{0}$	
0	0	0	translation belonging to first set of equivalent indices (vector). For instance for $P2_1/c$: + 0, + 0, + 0.
$\bar{0}$	$\bar{0}$	$\bar{0}$	
0	0	0	
$\bar{0}$	$\bar{0}$	$\bar{0}$	
0	0	0	
$\bar{0}$	$\bar{5}$	$\bar{0}$	
0	0	0	translation belonging to second set of equivalent indices (vector). For instance for $P2_1/c$: + 0, + $\frac{1}{2}$, + $\frac{1}{2}$.
$\bar{5}$	$\bar{5}$	$\bar{0}$	
0	0	0	
$\bar{5}$	$\bar{0}$	$\bar{5}$	
0	0	0	
$\bar{0}$	$\bar{0}$	$\bar{5}$	
0	0	0	translations belonging to third set of equivalent indices (vector). For instance for $P2_1/c$: no more equivalent indices
$\bar{0}$	$\bar{0}$	$\bar{5}$	
0	0	0	
$\bar{0}$	$\bar{0}$	$\bar{5}$	
0	0	0	
$\bar{0}$	$\bar{0}$	$\bar{5}$	
0	0	0	translations belonging to fourth set of equivalent indices (vector). For instance for $P2_1/c$: no more equivalent indices
$\bar{0}$	$\bar{0}$	$\bar{5}$	
0	0	0	
$\bar{0}$	$\bar{0}$	$\bar{0}$	
0	0	0	
ǂ	ǂ	ǂ	

(1) Multiplicity factor:

centrosymmetry gives a factor of 2

1-face centering gives a factor of 2

body centering gives a factor of 2

3-face centering gives a factor of 4

Fmmm for instance has a factor of 8 (4 from 3-face centering and 2 from centrosymmetry).

b. There are two possible ways to enter the parameters: from tape and from the typewriter.

Message

RS

"Type a 1 when parameters are to be typed". When no number is typed (or a zero) the message

"Load parameter tape" Reader Start

is typed out, giving the possibility to enter the parameters by means of tape (for format see Section IV, 2, pg. 28). When a 1 is typed two messages will follow

(i) "Type parameter ident (6)"

Any six digit number can be typed, and

(ii) "Type all parameters"

All parameters should now be typed (for format see again Section IV, 2, pg.28). <u>End with a Record Mark (‡)</u>. When an error is made during the typing it is necessary to branch manually to location : 49 13588.

c. Message

"Type length of L.S. Sums (2)"

This is a fixed point program and least-squares sums are made in fields of specified length. To obtain flexibility it is possible to initialize the length of these fields. The possible lengths are 6,7,8 or 9 digits, which is accomplished by typing in respectively 06, 07, 08 or 09.

It is impossible to get an overflow during the actual summing of L.S. terms (see boxes 25, 26, 37 and 38 of flow sheets. Section VII). Just before an overflow can occur all sums, obtained so far, are punched out on tape (our experience is that this will happen on an average once every 300 to 2000 reflections). These and additional sums are compiled by the succeeding program: the Processor (I.C.R. #5).

Concerning flexibility of use of storage (see also Section III, 4d, pg. 16). There is available a certain amount of storage for the least-squares sums. Consequently the number of L.S. sums can be greater when the length of each is smaller. The exact limitations are given in Sections III 5c, d and e, pg. 23, 24. In general we suggest to type in 09.

d. The contributions to the least-squares sums are made and added to the least-squares sums as fixed point numbers to increase the speed of the calculation. To obtain comparable flexibility as with floating point numbers it is possible to set the decimal points in each category of sums during the initialization of the program. The one digit number typed in will be the number of decimal digits after the decimal point in each case.

Messages:	Category	Suggested value to type	Maximum value, which can be typed	Minimum value, which can be typed
"Matrix coordinates (1)"	$w(\frac{\partial\|F\|}{\partial x_i})(\frac{\partial\|F\|}{\partial x_i})$	3	9	q-14
"Vector coordinates (1)"	$w(\|kF_o\|-\|F_c\|)(\frac{\partial\|F\|}{\partial x_i})$	5	7	q-13
"Matrix anisotropic (1)"	$w(\frac{\partial\|F\|}{\partial b_i})(\frac{\partial\|F\|}{\partial b_i})$	1	9	q-14
"Vector anisotropic (1)"	$w(\|kF_o\|-\|F_c\|)(\frac{\partial\|F\|}{\partial b_i})$	3	7	q-13
"Matrix isotropic (1)"	$w(\frac{\partial\|F\|}{\partial 'B_i})(\frac{\partial\|F\|}{\partial 'B_i})$	6	9	q-8
"Vector isotropic (1)"	$w(\|kF_o\|-\|F_c\|)(\frac{\partial\|F\|}{\partial 'B_i})$	6	9	q-10

In this table x_i are positional parameters and b_i and $'B_i$ are anisotropic and respectively isotropic vibrational parameters, and q is the length of one least-squares sum.

By increasing the typed number and therefore increasing the number of decimal digits, one can possibly obtain meaningful sums for hydrogen atoms. Decreasing the number of decimal digits after the decimal point is an absolute necessity when either one of the following <u>error messages</u> is typed out: <u>11</u>, <u>13</u>, <u>16</u>, <u>21</u>, <u>23</u> or <u>26</u>, which pertain to the fact that an overflow has occurred in the calculation of one particular term. Which term that is and therefore which number of decimal digits to decrease is discussed in Section III, 5g, pg. 25.

Finally there is the general suggestion that when the length of the sums is decreased by one it is probably necessary to decrease the number of decimal digits after the decimal point in some or all of the six categories.

c. Part of the program is a logical routine. When the weight is not assigned on the data tape, a weight is calculated in this routine, but the main purpose of this routine is to decide if a reflection should be included in the least-squares calculation. The result of this decision is a part of the output (see Section IV, 3,4, pg. 30 and Section III, 4g, pg. 20) and can therefore be used in the preparation of a Fourier- or difference Fourier data tape.

The routine works such that a reflection is not included when any one of the following conditions is true

$F_o \leq F_o$ min	and $F_c \leq (02.0)\ F_o$ min	(1)
F_o min $< F_c \leq 2\ F_o$ min	and $1.3\ F_c \leq F_o$	(2)
$2\ F_o$ min $< F_c \leq 3\ F_o$ min	and $1.5\ F_c \leq F_o$	(3)
$3\ F_o$ min $< F_c \leq 4\ F_o$ min	and $2.0\ F_c \leq F_o$	(4)
$4\ F_o$ min $< F_c$	and $2.5\ F_c \leq F_o$	(5)
$\lvert F_c \rvert - \lvert F_o \rvert > 0012.5$	and $\sin^2\theta/\lambda^2 < 0.0120$	(6)

The routine is presently set for a value of 2.5 for F_o min. It is however possible to change this as well as the values 1.3, 1.5, 2.0 and 2.5 in the conditions (2), (3), (4) and (5) as well as the values 012.5 and 0.0120 in condition (6) and the value 02.0 in condition (1). The reason for conditions (2), (3), (4) and (5) is obvious. Condition (6) is meant to exclude reflections which are bothered by attenuation (extinction). The use of condition (1) will depend on the fact if one wants to do a Fourier or a difference Fourier. A value of 02.0 seems proper for a difference Fourier as well as for a least-squares calculation but one might want to increase this value to a very high one for the case of a Fourier in order to exclude from this Fourier all reflections which are unobserved.

Message

"Type a '1' to change logical routine." RS

This message is always typed out. When it is required that some of the above conditions be altered a 1 is typed in which case the following five messages are typed out.

(i) Message

"Type in F obs minimum (4)"

A four digit number which should have a value ≥ 001.1 should be typed. As mentioned above the program is presently set for a value 002.5.

(ii) Message

"Type in proportionality constants (4 * 2)"

The values 1.3, 1.5, 2.0 and 2.5 in conditions (2), (3), (4) and (5) can be changed at this moment. An eight digit number should be typed. The first two digits will then replace 1.3, the second two digits 1.5, etc.

(iii) Message

"Type in multiply constant (3)"

A three digit number to replace the value 02.0 in the second part of condition (1), should now be typed.

(iv) Message

"Type in minimal sin sq theta over lambda sq (5)"

The value 0.0120 for $\sin^2\theta/\lambda^2$ in the second part of condition (6) can now be changed. A five digit number should be typed. By typing in 00000 one can essentially inactivate the condition.

(v) Message

"Type in limit of F obs minus F calc. (4)"

At this moment the value 012.5 in the first part of condition (6) can be changed. A four digit number should be typed.

f. It is also possible to make the logical routine ineffective insofar as the decision about the inclusion is concerned. The following message is always typed out.

Message

"Type a 1 to make a choice for each reflection separately."

When a 1 is typed this ineffectiveness is accomplished. With the result that after the calculation and typing of each structure factor, and before the calculation of the contributions to the least-squares sums of this structure factor, the typewriter will be ready and waiting to accept typing. At this moment the F_o and F_c can be compared and a "human" decision can be made. When one wants to include the reflection a 0 (zero) should be typed, and when the reflection should not be included a 1 should be typed. This has then to be done for each reflection.

g. Three considerations are of importance to examplify the possibilities of F_o against F_c comparisons.

(i) The record of each structure factor contains a 5 digit number which is used as the weight (w) of this reflection (see Section IV: Data Tape, pg. 26). When w is any nonzero number then this number is used as the weight of the reflection. When w = 00000 in the record then the weight is calculated by the logical routine (as $(1/F_o)^2$ or $(1/3F_o \text{ min})^2$). Here one can essentially exclude a reflection by having 00001 for the weight. This is however not the normal way to exclude a reflection (see below).

(ii) A decision of the logical routine (see Section III, 4e, pg. 18) can be superseded by one of the code numbers in the structure factor record on the data tape (see Section IV, 1c, pg. 27). A 1 for this code will cause the reflection to be excluded while a 2 will absolutely include the reflection into the least-squares calculation. A 0 will not supersede the decision of the logical routine.

(iii) The procedure described in Section III, 4f, pg. 19 makes it possible to decide for each reflection separately and this will supersede the codes on the data tape as they were described in the previous paragraph. Whatever means are taken, however, the result will be recorded on the output tape (whenever the switch settings are such that there is output on tape) as well as on the output on the typewriter. Code 0 (zero) will designate the fact that the reflection was included while a 1 means that it was not included in the least-squares calculation (see Section IV, Output, pg. 30).

Even when a (difference) Fourier rather than a least-squares calculation is planned (P.S.1 on) it is advantageous to consider these possibilities. The output on tape (P.S.3 on) contains a code (see previous paragraph), which can be used to decide which terms to include in the Fourier. This feature is used in the program which prepares the input data tape for the Fourier from the output tape of the structure factor calculation (I.C.R. #6).

h. Message

"Changes can be made now. Afterwards 4919980."

When no changes have to be made as is in general the case it suffices to press Start. It is however at this moment possible to make manual changes in the program or in the parameter record or to load additional tapes when necessary. After these changes have been made one should press Insert: Type: 49 19980; press Release and Start to proceed with the program.

k. Message

"Type in first reflection to be calculated. (3 * 2)" $\bar{H}H$ $\bar{K}K$ $\bar{L}L$ RS

In a long run it might be necessary to stop in the middle of a data tape. This can be accomplished by setting program switch 2 on (see also Section III, 3, pg. 12). The next reflection which is read from the data tape will be typed out, after which the typewriter waits to accept information. Only when a 8 ǂ is typed will the program punch out the general sums, and least-squares sums which were obtained so far (excluding the last reflection typed out). One can interrupt the calculation as many times as is wanted, because all sums (on tape) will be added together by the next program: the Processor.

It should then however be possible to start the structure factor calculation anywhere on the data tape. After the message is typed out a 6-digit number should be typed being respectively the h, k and ℓ of the first reflection which has to be calculated. Normally this will be the h, k and ℓ of the first reflection on the data tape, but when the calculation was interrupted in the manner which was described in the previous paragraph, one should type in the h, k and ℓ of the reflection which was typed out at the end of the previous run. After pressing Release and Start the program will search for this first reflection.

4. Message

"Seashore"

This message together with the one typed at the beginning, shows that the calculation is finished.

5. Error Messages

a. Stop on Overflow.

If the computer stops on an overflow it is in most cases due to an error in the parameter tape (which then should be remade and the program should be reloaded) or to an error on the data tape. We strongly suggest the use of a small checking program for the data tape before the tape is used in the present program. (See Section V, d).

With respect to an error on the data tape we can distinguish two cases.

(i) The error is known beforehand. In this case one can correct the error easily by putting P.S.2 on, while the program is calculating on the previous reflection. The result is that the erroneous reflection is typed out after which the typewriter pauses. The corrected form of the reflection can then be typed in. Press Release and Start and the program will proceed.

(ii) The error on the data tape is not known beforehand and the program stops on an overflow. Press Reset and Display Mar, with I.R.1, to show the location of the next instruction on the display lights. Consult program listing and flow sheets to find the stage of the calculation. If the program is still in the stage of calculating the structure factor the error can be corrected because this part of the calculation is self initializing. Read out on the typewriter from location 00409. This is the area where each datum is read into and stored. If in error the datum can be corrected by reading into location 00409 from the typewriter. Then branch manually to location 00956: 49 00956. Press Release and Start and the program will proceed.

When this fails reload the program and follow procedure (i) or better still: remake the data tape.

b. Message

"Error in length of parameter tape"

The program can only check on the proper length of the tape. When this message is typed out it is necessary to remake the parameter tape and to reload the program.

c. Message

"Too many atoms. Planning Error."

This message will be typed out when the total area occupied by the parameters and trigonometric functions exceeds 10000 digits. The exact formula is:

$$19 + 18.\ N + 26.\ N_A + 10.\ e.\ N < 10000 \qquad (1)$$

N = number of atoms

N_A = number of anisotropic atoms

e = 1 (triclinic), 2 (monoclinic) or 4 (orthorhombic)

This condition will probably always be obeyed. For a machine with a memory larger than 20K: Press Start; otherwise reload the program and change the manner of calculation.

d. Message

"Planning error. L.S. sum maker."

This message will be typed out when the total area occupied by the parameters, trigonometric functions and least-squares sums exceeds 10000 digits. The exact formula for this condition is:

$$19 + 18.\ N + 26.\ N_A + 10.\ e\ N + q\ \{9\ N_L + 27.\ N_A + 2\ (N_L - N_A)\} < 10000 \qquad (2)$$

N, N_A and e: see Section III 5c

q = length of one least-squares sum

N_L = number of atoms for which least-squares sums are made

This is the key condition for this program. The limitations implied by it are however a function of the crystal system (e) and of q (see Section III, 4c, pg. 16) We will give two examples. Suppose $N = N_L$, a monoclinic space group and q = 6. The condition then reduces to:

$$104\ N + 196\ N_A < 9981 \qquad (3)$$

When working with only isotropic atoms this means $N \leq 95$, and when working with anisotropic atoms only: $N_A \leq 33$.

Or suppose $N = N_L$, an orthorhombic space group and $q = 8$. Condition (2) then reduces to:

$$142 N + 226 N_A < 9981 \quad (4)$$

Meaning either $N \leq 70$ or $N_A \leq 27$, or a mixture obeying (4)

As was pointed out before q can be made smaller sometimes resulting in the necessity to decrease the number of decimal digits after the decimal point in the least-squares sums (see Section III, 4d, pg. 16) and otherwise resulting in more intermediate outputs on tape of least-squares sums.

The feature to have two parameters N and N_L for respectively the number of atoms in the calculation of the structure factor and the number of atoms for which least-squares sums are calculated is mainly meant to include hydrogen in the F_c calculation, but not to take time to refine the parameters of hydrogens. But it is feasible, in a boundary case, that by making $N_L < N$ it will be possible to obey condition (2). In general we feel however that in those cases one is well advised to think about using a bigger and especially about a faster computer than the I.B.M. 1620.

If condition (2) is not obeyed, the program will type out the number of digits by which the capacity of the memory is exceeded. For a 20K machine one has to change the manner of calculation. For a machine with a larger memory than 20K it is possible to proceed with the calculation by pressing Start.

e. When it is planned to use the succeeding program "the Processor" on the results of the present program, it is necessary to check on the limitations of "the Processor."

f. Message

"Err 3"

This message is typed out when an overflow occurs during the multiplication of a trigonometric function with the space group multiplicity, scattering factor and exponential (temperature factor). It is our experience that this condition is mostly due to an error on the data tape, for which the general remark at the beginning of this section is applicable. Otherwise it could only occur when there is a very heavy atom in the structure. The easiest way to circumvent this condition is by changing the space group multiplicity (see Section III, 4a, pg. 12 space group format, reference (i)). The stage where this can be done is when the message: Changes can be made now etc., is typed out. The memory location of the space group multiplicity is 00512. A more difficult and laborious way is to divide all scattering factors on the data tape by a constant factor for all structure factors. When any such change is made the scale factor on the parameter tape has to be adjusted.

g. Messages

"Err 13" "Err 16" and Err 11"

"Err 23" "Err 26" and Err 21"

The length of each least-squares sum is q digits. The contributions to the least-squares sums are calculated in fields of (q-1) digits. When the contribution of a matrix term or a vector term is larger than (q-1) digits either one of the six error messages is typed out:

Err 13 a matrix coordinate contribution

Err 23 is a vector coordinate contribution

Err 16 is a matrix anisotropic parameter contribution

Err 26 is a vector anisotropic parameter contribution

Err 11 is a matrix isotropic parameter contribution

Err 21 is a vector isotropic parameter contribution

In general one only has to decrease the number of decimal digits after the decimal points for that category in which the overflow occurs (see also Section III, 4d, pg. 16), or alternatively to increase the length of all least-squares sums (q). (See Section III, 4c, pg. 16). Reload the program.

Section IV <u>Format</u>

1. <u>Data Tape</u>

Code number	6 digits	xxxxxx
End of line character	1 digit	ǂ
h	2 digits	$\bar{x}$x.
k	2 digits	$\bar{x}$x.
ℓ	2 digits	$\bar{x}$x.
F_o	4 digits	$\bar{x}$xx.x
Sin $^2\theta/\lambda^2$	5 digits	x.xxxx
(a) Code	1 digit	x
(b) Code	1 digit	x
(c) Code	1 digit	x
(d) w (weighing factor)	5 digits	.0xxxxx
(e) f_1 (parameter code: $.\overline{0}0$)	4 digits	xx.xx
f_2 (parameter code: $.\overline{0}4$)	4 digits	$\bar{x}$x.xx
etc.	etc.	etc.
End of line character	1 digit	ǂ
h	2 digits	$\bar{x}$x.
k	2 digits	$\bar{x}$x.
ℓ	2 digits	$\bar{x}$x.
etc.	etc.	etc.
.	.	.
.	.	.
.	.	.
End of line character	1 digit	ǂ
8	1 digit	8
End of line character	1 digit	ǂ

The data tape is thus a succession of records each pertaining to one reflection, while this series of records is preceded by a code record and finished with an end record (8ǂ). The sorting order of the reflections is irrelevant for the present program. The order: h before k before ℓ should always be kept.

Decimal points are not punched and are here only given for convenience.

a. This code is the multiplicity of the reflection.

b. A 1 should be punched when the reflection is not observed, while a 0 (zero) should be punched for an observed reflection.

c. A 0 (zero) should be punched when the logical routine should make the decision about inclusion in the least-squares calculation, a 1 when the reflection should absolutely not be included and a 2 when it should absolutely be included in the least-squares calculation (see also Section III, 4g, pg. 20).

d. This is a five digit number. The zero is not punched and is given for convenience. When the weight is punched as $\bar{0}0000$, the program will assign a weight as follows:

$\frac{1}{F_o^2}$ for $F_o > F_{o\ min}$ and

$\frac{1}{3\ F_{o\ min}^2}$ for $F_o \leq 3\ F_{o\ min}$. (See also Section III, 4g, pg. 20)

e. One should have as many scattering factors as there are types of atoms in the structure. The sequence is essential (see format parameter tape) and should be the same for all reflections. The program assumes that "cold" scattering factors are used.

2. Parameter Tape

Code number		6 digits	xxxxxx
End of line character		1 digit	ǂ
(a) Overall 'B		4 digits	$\bar{x}.xxx$
(b) Number of atoms	(n)	2 digits	$\bar{x}x.$
(c) Number of anisotropic atoms		2 digits	$\bar{x}x.$
(d) Number of isotropic atoms	(m)	2 digits	$\bar{x}x.$
(f) Number of types of atoms		2 digits	$\bar{x}x.$
(e) Number of L.S. atoms	(p)	2 digits	$\bar{x}x.$
(g) Scale factor		5 digits	$\bar{x}.xxxx$
(h) Parameter x_1		4 digits	$.\bar{x}xxx$
Parameter y_1		4 digits	$.\bar{x}xxx$
Parameter z_1		4 digits	$.\bar{x}xxx$
Parameter x_2		4 digits	$.\bar{x}xxx$
etc.		etc.	etc.
(i) Identification I_1		2 digits	$\bar{x}x$
Identification I_2		2 digits	$\bar{x}x$
etc.		etc.	etc.
(k) Parameter b_1^{11}		5 digits	$.\bar{x}xxxx$
Parameter b_1^{12}		5 digits	$.\bar{x}xxxx$
Parameter b_1^{13}		5 digits	$.\bar{x}xxxx$
Parameter b_1^{22}		5 digits	$.\bar{x}xxxx$
Parameter b_1^{23}		5 digits	$.\bar{x}xxxx$
Parameter b_1^{33}		5 digits	$.\bar{x}xxxx$
Parameter b_2^{11}		5 digits	$.\bar{x}xxxx$
etc.		etc.	etc.
(ℓ) Parameter $'B_{n-m}$		4 digits	$\bar{x}.xxx$
Parameter $'B_{n-m+1}$		4 digits	$\bar{x}.xxx$
etc.		etc.	etc.
End of line character		1 digit	ǂ

Decimal points are given for convenience and are not punched.

a. The overall 'B is the average isotropic temperature factor of the structure. This parameter is not used in the present program but in the successive program: The Processor (see also Section I, pg. 3).

b. This should be the number of atoms which are used for calculating the structure factor.

c. and d. The sum of the number of isotropic and anisotropic atoms should be equal to the total number of atoms as described in b.

e. This should be the number of atoms for which least-squares sums are calculated. This number is thus not necessarily the same as the total number of atoms as described in Section IV, 2b, this page. This makes it possible to calculate the correct structure factor but to refine only the parameters of a part of the atoms, for instance to include hydrogens in the structure factor calculation but not in the least-squares calculation (see Section III, 5d, pg. 24). Suppose that the number of atoms is n and the number of L.S. atoms is p, than the atoms for which no least-squares sums are calculated (there are (n-p) of them) should be listed at the end of each parameter area: thus as n-p, n-p+1 ...., n.

f. This should be the total number of scattering factors which are in each record on the data tape.

g. Each F_o is multiplied by this scale factor before they are compared with their F_c.

h., i., k., ℓ. Besides the positional coordinates and temperature factors, there is a group of identifications. An identification can be $\bar{0}0$, $\bar{0}4$, $\bar{0}8$, $\bar{1}2$, etc., and it determines which scattering factor in the record from the data tape should be used, that is respectively the 1st, 2nd, 3rd, 4th etc. It is obvious that the first set of positional parameters corresponds with the first identification and with the first set of temperature factor parameters (anisotropic) or first temperature factor parameter (isotropic). The second set with the second identification and with the second (set) (of) temperature factor parameter(s) and so on. It is also clear that the parameters of all anisotropic atoms precede the parameters of the isotropic ones. (Compare Section IV, 2e, pg. 29, it is thus rather complicated to cut out the least-squares sums for an anisotropic atom. The feature explained in IV, 2c is mainly meant to make it possible to cut out least-squares sums for relatively badly defined atoms like hydrogens which of course are treated as isotropic atoms.) The positional parameters are expressed in tenthousandths of one cycle, the anisotropic parameters are also dimensionless (the anisotropic temperature factor is calculated with the expression: $\exp\ -(b^{11}h^2 + b^{12}hk \ldots . + b^{33}\ell^3))$ and the isotropic parameters are the normal 'B's, expressed in the dimension $Å^2$. The temperature factor should always be physically meaningful, i.e. diminish the geometrical contribution to the structure factor.

3. Output Typewriter

The first output is a line of 24 digits. The first six digits are the identification of the program, the second six the identification of the space group, the third of the parameter tape, and the fourth six digits are the identification of the data tape.

After this line the structure factors are typed out and there is a choice of a short and a long type out (see Section III, 3 and below).

The last ten lines are the ten general sums (see Section I, pg. 10).

$\bar{x}$xxxxxxxx.x	$\Sigma \lvert kF_o - F_c \rvert$
$\bar{x}$xxxxxxxx.x	$\Sigma \lvert kF_o \rvert$
$\bar{x}$xxxxx.xxxx	$\Sigma w (\lvert kF_o \rvert - \lvert F_c \rvert)^2$
$\bar{x}$xxxxx.xxxx	$\Sigma w (\lvert kF_o \rvert)(\lvert kF_c \rvert - \lvert F_c \rvert)$
$\bar{x}$xxxxx.xxxx	$\Sigma w (\lvert kF_o \rvert - \lvert F_c \rvert) \lvert F_c \rvert s^2$
$\bar{x}$xxxxx.xxxx	$\Sigma w (\lvert kF_o \rvert)^2$
$\bar{x}$xxxxx.xxxx	$\Sigma w (\lvert kF_o \rvert)(\lvert F_c \rvert) s^2$
$\bar{x}$xxxxx.xxxx	$\Sigma w (\lvert F_c \rvert)^2 s^4$
$\bar{x}$xxxxxxxxx	The sum in the last 5 digits is the total number of reflections, and the sum in the first 5 digits the number of reflections which was used in the L.S. calculation.
xxxxxxxxx.x	$\Sigma \lvert F_c \rvert$

The decimal points are not typed. The $s^2 = \sin^2\theta/\lambda^2$.

Short typewriter output

xx	h
x	sign of h
space	
xx	k
x	sign of k
space	
xx	ℓ
x	sign of ℓ
space	
xxx.x	kF_o
x	sign of kF_o (always positive)
space	
$\bar{x}$xx.x	F_c
x	sign of F_c
space	

(a) xxx.x	$kF_o - F_c$
x	sign of $kF_o - F_c$
space	
x	Code (= multiplicity; from data tape)
x	Code (0 = observed, 1 = unobserved; from data tape)
(b) x	Code (0 = included in L.S.; 1 = not included in L.S.)
$\bar{x}$.xxxx	$\cos\alpha$ (= A_c/F_c for acentric space groups only)
$\bar{x}$.xxxx	$\sin\alpha$ (= B_c/F_c for acentric space groups only)

<u>Long typewriter output</u>

xx	h
x	sign of h
space	
xx	k
x	sign of k
space	
xx	ℓ
x	sign of ℓ
space	
xxx.x	kF_o
x	sign of kF_o (always positive)
space	
xxx.x	F_c
x	sign of F_c
space	
(a) xxx.x	$kF_o - F_c$
x	sign of $kF_o - F_c$
space	
$\bar{x}$.xxxx	$\sin^2\theta/\lambda^2$

x	Code (= multiplicity; from data tape)
x	Code (0 = observed; 1 = unobserved; from data tape)
(b) x	Code (0 = included in L.S.; 1 = not included in L.S.)
$.\bar{0}xxxxx$	weight (as used in L.S. calculation)
$\bar{x}x.xx$	f_1
$\bar{x}x.xx$	f_2
etc.	
$\bar{x}xx.x$	A_c) for acentric space groups only
$\bar{x}xx.x$	B_c)
$\bar{x}.xxxx$	cos α)
$\bar{x}.xxxx$	sin α)

(a) It is $kF_o - F_c$ for centric space groups and $|kF_o| - |F_c|$ for acentric space group

(b) See also Section III, 4g, pg. 20.

4. Output Paper Tape

The first three records on the paper tape are the 24 digit identification (see Section IV, 3, pg. 30), a copy of the parameter tape and a 14 digit record of specifications concerning the length and decimal points of the least-squares sums.

After these records, structure factor answers are punched. There are two possible formats of the punched structure factors (see also Section III, 3).

(i) The <u>short tape output</u> is the same as the short type out, but for the fact that spaces are left out and the signs are always on the right most digit of each number.

(ii) The <u>long tape output</u> has in addition to short tape output, the $\sin^2\theta/\lambda^2$ directly before the three codes and the weight, as used in the calculation, directly after the three codes.

These structure factors are mixed with intermediate least-squares sums when least-squares sums are calculated. Least-squares sums are namely punched out during the calculation just before they can overflow. The array is recognizable by the presence or non-presence of preceding records of the sort 8‡ and 78‡. Structure factors are not preceded by such a record. Intermediate L.S. sums (all of which are punched as separate records) are preceded by 8‡; the last L.S. sums are preceded by 78‡. Directly after the last L.S. sums the general sums are punched as ten 10-digit records.

The decimal points of the least-squares and the length of a sum are set during the initialization of the program. The matrix terms of the coordinate sums should be multiplied by $4\pi^2$ and the vector terms of the coordinate sums by 2π before further use.

The array of the least-squares sums is an obvious one and given below.

$w\left(\frac{\partial F}{\partial x_1}\right)\left(\frac{\partial F}{\partial x_1}\right)$; $w\left(\frac{\partial F}{\partial x_1}\right)\left(\frac{\partial F}{\partial y_1}\right)$; $w\left(\frac{\partial F}{\partial x_1}\right)\left(\frac{\partial F}{\partial z_1}\right)$; $w\left(\frac{\partial F}{\partial y_1}\right)\left(\frac{\partial F}{\partial y_1}\right)$;

$w\left(\frac{\partial F}{\partial y_1}\right)\left(\frac{\partial F}{\partial z_1}\right)$; $w\left(\frac{\partial F}{\partial z_1}\right)\left(\frac{\partial F}{\partial z_1}\right)$; $w\,(kF_o - F_c)\left(\frac{\partial F}{\partial x_1}\right)$; $w\,(kF_o - F_c)\left(\frac{\partial F}{\partial y_1}\right)$;

$w\,(kF_o - F_c)\left(\frac{\partial F}{\partial z_1}\right)$; $w\left(\frac{\partial F}{\partial x_2}\right)\left(\frac{\partial F}{\partial x_2}\right)$ etc.......

$w\left(\frac{\partial F}{\partial b_1^{11}}\right)\left(\frac{\partial F}{\partial b_1^{11}}\right)$; $w\left(\frac{\partial F}{\partial b_1^{11}}\right)\left(\frac{\partial F}{\partial b_1^{12}}\right)$; $w\left(\frac{\partial F}{\partial b_1^{11}}\right)\left(\frac{\partial F}{\partial b_1^{13}}\right)$; $w\left(\frac{\partial F}{\partial b_1^{11}}\right)\left(\frac{\partial F}{\partial b_1^{22}}\right)$;

$w\left(\frac{\partial F}{\partial b_1^{11}}\right)\left(\frac{\partial F}{\partial b_1^{23}}\right)$; $w\left(\frac{\partial F}{\partial b_1^{11}}\right)\left(\frac{\partial F}{\partial b_1^{33}}\right)$; $w\left(\frac{\partial F}{\partial b_1^{22}}\right)\left(\frac{\partial F}{\partial b_1^{22}}\right)$; .....; $w\left(\frac{\partial F}{\partial b_1^{33}}\right)\left(\frac{\partial F}{\partial b_1^{33}}\right)$;

$w\,(kF_o - F_c)\left(\frac{\partial F}{\partial b_1^{11}}\right)$; .....; $w\,(kF_o - F_c)\left(\frac{\partial F}{\partial b_1^{33}}\right)$; $w\left(\frac{\partial F}{\partial b_2^{11}}\right)\left(\frac{\partial F}{\partial b_2^{11}}\right)$ etc.......

$w\left(\frac{\partial F}{\partial B_{n-m}}\right)\left(\frac{\partial F}{\partial B_{n-m}}\right)$; $w\,(kF_o - F_c)\left(\frac{\partial F}{\partial B_{n-m}}\right)$; $w\left(\frac{\partial F}{\partial B_{n-m+1}}\right)\left(\frac{\partial F}{\partial B_{n-m+1}}\right)$;

etc. . . . . ; $w\,(kF_o - F_c)\left(\frac{\partial F}{\partial B_n}\right)$;

Each sum is followed by a record mark ‡.

Section V

1. Additional Information

a. Card program

It is believed that the present program is fairly easily changed to a card program. All read and write orders of the paper tape will therefore be discussed. The orders in 13060, 13108, 13156, 13228 and 13252 deal with the reading of the identifications of the space groups and of the space groups itself. It is suggested to have one card for each space group, on it is punched: the identification, R.M., space group record, R.M.; and to have those cards behind the program cards.

The order in

13060	INIT 01	RNPT	SPACEL-6

should be replaced by two orders:

	INIT 01	RNCD	19010
		TR	SPACEL-6, 19010

The order in

13108	RNPT	19010

can be deleted

The order in

13156	INIT 00	RNPT	507

should become

	INIT 00	TR	507, 19017

The order in

13228	RNPT	SPACEL-6

should be replaced by two orders:

	RNCD	19010
	TR	SPACEL-6, 19010

and the order in

13252	RNPT	507

should be replaced by:

	TR	507, 19017

The orders in 13504 and 13516 deal with the reading of parameters from tape. Because it is also possible to type parameters in rather than reading them from tape, this would not necessarily pose a problem. When parameters are preferably read from cards we suggest that the identification be punched on the first card and the parameters on the card(s) following with a record mark behind the identification and behind the very last digit of the parameters, and then to replace the order in

13504 RNPT 19006

with RNCD 19006 and the order in

13516 RNPT 10000

with a small loop:

```
            TFM    INIT 70+6, 10000
INIT 70     RNCD   10000
            AM     INIT 70+6, 80,10
            BNLC   INIT 70
```

The order in 16684 reads the identification of the data tape. It is suggested to have this on a single card in front of the deck of data cards with a record mark behind the identification. The order in

16660 RNPT 19012

can then be changed to: RNCD 19012

The order in

16696 WNPT 18994

Writes all the identifications: program, space group, parameters and data, and can be changed to: WNCD 18994

The order in

16708 INIT 15 RNPT 19051

is part of a loop which searches for the first reflection on the data tape which has to be calculated. We suggest one piece of data (one reflection) on one card, with a record mark after the last scattering factor, then this order can be changed to:

INIT 15 RNCD 19051

The order in

```
16804                               WNPT    10000
```

records the parameters. This order should be changed to a loop

```
                                    TFM     INIT 80+6, 10000
                         INIT 08    WNCD    10000
                                    SM      PARALT, 80,10
                                    BP      INIT 08
```

The order in

```
16816                               WNPT    SUMLET-1
```

can be changed to WNCD SUMLET-1

Only the first 15 columns on the card will be meaningful. They record the specifications of the least-squares calculation.

In the main program each paper tape order can be changed directly to a card order. This is necessary because only 14 digits are left for program space.

The order in

```
00944                    START 6    RNPT    409
```

reads each piece of data in and can be changed to

```
                         START 6    RNCD    409
```

when there is indeed one reflection on one card. The last card of the data deck should have 8ǂ. The area up to 00500 is available for reading.

The orders in

```
04136                    OUTP 61    WNPT    401
```

and

```
04228                               WNPT    401
```

punch the result of the structure factor calculation (for different switch settings respectively) and can be changed to

```
                         OUTP 61    WNCD    401
and
                                    WNCD    401
```

Only the information before the record mark on the output cards is meaningful.

The orders in

05372 CHSM 02 WNPT 399

and

05500 FINAL 0 WNPT 398

punch preceding records making it possible to recognize that the following output is least-squares sums (see Section IV, Output Tape) and can be changed to

CHSM 02 WNCD 399

and

FINAL 0 WNCD 398

resulting in cards with a record mark in the second respectively third columns.

The order in

05492 CHSM 51 WNPT GENSUM,,2

punches one least-squares sum at a time and can be changed to

CHSM 51 WNCD GENSUM,,2

resulting in as many output cards as there are least-squares sums. Similarly the order in

05640 WNPT GENSUM-9

punches one general sum at a time and can be changed to

WNCD GENSUM-9

resulting in ten output cards.

In both cases, only the information on the card before the record mark is meaningful.

b. Atoms at special positions

Atoms with one or more fixed coordinates cause no problems in triclinic, monoclinic and orthorhombic space groups. It is however necessary to scale the scattering factor on the data tape down by a factor.

c. General Sums

In calculating the general sums which are needed in the 2 x 2 matrix for $\overline{B}$ and k, there might be some advantage in using only those reflections which were used in the least-squares calculation in order to minimize the same sum: $\Sigma\, w\, (|kF_o| - |F_c|)^2$. On the other hand only the absolute values are compared in the 2 x 2 matrix for k and $\bar{B}$ while in the least-squares calculation the phases of F_c are involved in obtaining the best agreement between $|F_c|$ and $|kF_o|$. A certain number of reflections unacceptable for the use in the least-squares calculation on the ground that the phases can not adequately be determined, are acceptable for those general sums where only agreement between $|kF_o|$ and $|F_c|$ is important. Similarly one could prefer to use only observed reflections for those general sums.

In the present program all reflections are included in those general sums. It is possible to change the program with a "patch". The beginning of the routine calculating the products of $(|kF_o| - |F_c|)$, $|kF_o|$, and $|F_c|\, s^2$, and the summing of the products is in location 03560. An unobserved reflection is at that moment recognized by a "1" in 00425, and a logically unacceptable reflection by a "1" in 00426.

2. Example

The example given is not too realistic but might be of help.

Parameter tape. The average temperature factor is not used in this program ($\overline{0}000$); the structure has four atoms ($\overline{0}4$) of which one ($\overline{0}1$) has anisotropic temperature factors and three ($\overline{0}2$) have isotropic temperature factors; there are four ($\overline{0}4$) different scattering factors on the data tape, and least-squares sums will only be calculated for the first three atoms ($\overline{0}3$). The F_o scale factor is 1.100. The coordinate parameters x, y, z of the first, i.e. anisotropic atom are respectively: .1180, .0200 and.1650; the coordinates x, y, z of the second atom are respectively: .3300, .1150 and .1600, etc. The scattering factor of the anisotropic atom is the fourth ($\overline{1}2$) on the data tape. The scattering factor of the second atom is third ($\overline{0}8$), of the third atom second ($\overline{0}4$), and of the fourth atom first ($\overline{0}0$), on the data tape. The six temperature factors of the first atom are .02000, -.00100 .... .07500. The temperature factor of the second atom is 2.300 Å^2.

SECTION V.1

CHECKING PROGRAM FOR DATA TAPE.LOAD ADDITION AND MULTIPLICATION TABLE FIRST.THEN LOAD THE FOLLOWING PROGRAM.

```
01000  36 00401 00300
01012  46 01036 00300
01024  38 00401 00200
01036  36 00401 00300
01048  45 01096 00402
01060  46 01084 00300
01072  38 00401 00200
01084  48 00000 00000
01096  16 01119 0̄1568
01108  26 01131 0̄1568
01120  44 01492 00401
01132  11 01119 000̄5
01144  14 01119 0̄1598
01156  47 01108 01200
01168  16 01191 0̄1598
01180  26 01203 0̄1598
01192  44 01216 0̄0408
01204  49 01492 00000
01216  11 01191 000̄5
01228  14 01191 0̄1663
01240  47 01180 01200
01252  16 01275 0̄0424
01264  44 01492 0̄0424
01276  11 01275 000̄1
01288  16 01297 000̄3
01300  26 01323 01275
01312  44 01336 0̄0425
01324  49 01492 00000
01336  11 01275 000̄1
01348  12 01297 000̄1
01360  47 01300 01200
01372  26 01395 01275
01384  45 01264 00428
01396  46 01432 00100
01408  34 00000 00102
01420  38 00401 00100
01432  46 01456 00200
01444  48 00000 00000
01456  46 01480 00300
01468  38 00401 00200
01480  49 01036 00000
01492  34 00000 00102
01504  34 00000 00108
01516  38 00401 00100
01528  34 00000 00102
01540  36 00401 00100
01552  49 01048 00000
01564  0̄04010̄04030̄04050̄04070̄04110̄04190̄04080̄04090̄04120̄04130̄04140̄0415
       0̄04160̄04170̄04180̄04200̄04210̄04220̄0423‡
```

P.S.1	OFF	EACH REFLECTION IS TYPED.
P.S.1	ON	NO TYPE OUT.
P.S.2	OFF	PROGRAM STOPS AFTER EACH REFLECTION IS CHECKED.
P.S.2	ON	PROGRAM DOES NOT STOP.
P.S.3	OFF	NEW (CORRECTED) DATA TAPE IS PUNCHED.
P.S.3	ON	NO PUNCH OUT.

Data tape. There are five reflections on the data tape. The first reflection (113) has an F_o of 13.1 and a sin $^2\theta/\lambda^2$ of .0871. The weight (from experimental observation) is .003592, after which the four scattering factors for this reflection follow: .26, 2.58, 4.17 and 11.10.

Running of the example. The space group is $P2_12_12_1$ (019). Program switch 1 off (for least-squares sums), 2 off, 3 and 4 on (to obtain a short type out and a short tape out). The parameters are on tape. The logical routine wants to be changed, and a choice about inclusion of the reflection into the least-squares sums should be made by the logical routine of the program. The first reflection on the data tape is thus (113) → (010103).

Typewriter output. The reflection (113) has an $F_c = \sqrt{A_c^2 + B_c^2}$ of 14.3, and was included into the least-squares calculation. The cos α = -.9930 etc. The sum of $|F_o - F_c|$ is 32.7; $\Sigma\ |kF_c|$ = 92.0 etc.

Paper tape output. The first record are identifications, the second is a copy of the parameters, the third are the least-squares specifications. The next five records are copies of the calculated structure factors. The record 78+ means that the (last) least-squares sums will follow. The first 9 of these are the 6 matrix terms and 3 vector terms of the 3 x 3 matrix for the coordinates of the first atom. The next 9 records are those for the second atom. The next 9 for the coordinates of the third atom. The next 27 records are the 21 matrix and 6 vector terms of the 6 x 6 matrix for anisotropic vibrations of the first atom. The next 2 records are the 1 matrix and 1 vector term of the isotropic vibration of the second atom, and the next 2 those for the third atom. The remaining 10 records are the general sums.

I would like to thank Miss Evelyn Wydro for preparing the program source tape and for typing this manuscript and I would like to thank Mrs. Jean Minkin for typing the flow sheets.

May 18, 1962

EXAMPLE ... COPY OF THE PARAMETER TAPE

```
123456 ≠
000004810310403110001180020016503300115016000200165013002000 ...
20000010000400019000020000750023000240003000≠
```

COPY OF THE DATA TAPE

```
258369 ≠
0101030131008718000359200260258041711130 ≠
0102030134009148000208200250252040711092 ≠
0103030239009868001335400230243039211065 ≠
0104030099010878000049400210233037211029 ≠
0105030234012178000012000180222035009990 ≠
8 ≠
```

RUNNING OF THE EXAMPLE

```
160001000000
360000000300
TYPE IN SPACEGROUP NUMBER (3)                      019
SET PROGRAM SWITCHES
TYPE A 1 WHEN PARAMETERS ARE TO BE TYPED
LOAD PARAMETER TAPE
TYPE LENGTH OF L.S.SUMS (2)                        09
PREPARATION OF DECIMAL POINTS IN L.S.SUMS.
SEE WRITE UP FOR SUGGESTIONS
MATRIX COORDINATES(1)                              3
VECTOR COORDINATES(1)                              5
MATRIX ANISOTROPIC(1)                              1
VECTOR ANISOTROPIC(1)                              1
MATRIX ISOTROPIC(1)                                6
VECTOR ISOTROPIC(1)                                6
TYPE A 1 TO CHANG/ LOGICAL ROUTINE 1
TYPE IN F OBS. MINIMUM(4)                          0035
TYPE IN PROPORTIONALITY CONSTANTS(4*2)             13152020
TYPE IN MULTIPLY CONSTANT(3)                       050
TYPE IN MINIMAL SINSQ THETA OVER LAMDASQ(5)        00000
TYPE IN LIMIT OF F OBS. MINUS F CALC.(4)           0120
TYPE A 1 TO MAKE CHOICE FOR EACH REFLECTION SEPARATELY
CHANGES CAN BE MADE NOW.AFTERWARDS 4019980
LOAD DATA TAPE
TYPE IN FIRST REFLECTION TO BE CALCULATED(3*2) 010103
0130040160191234568369
AND THEY ALL WENT TO THE

01  01  03  0144  [illegible]  0001   00009930001185
01  02  03  0147  [illegible]  0067-  00009935001299
01  03  03  0263  [illegible]  0165   00010000000918
01  04  03  0109  0071  0038   00009859001690
01  05  03  0257  [illegible]  0116   00010000000705
```

```
0̄000000327
0̄000000920
0̄000292798
0̄000466796
0̄000017807
0̄000845561
0̄000037255
0̄000001861
0̄000400005
0̄000000607
SEASHORE
```

COPY OF THE OUTPUT TAPE

```
0̄130040160̄19123456258369≠
0̄0000̄40̄10̄30̄40̄31̄10001̄1800̄2001̄6503̄3001̄1501̄6000̄2001̄6501̄3002̄0002̄4000̄1001̄20̄804
0̄0̄2000̄0̄0100̄0̄4000̄1900̄0̄2000̄75002̄3002̄4003̄000≠
0̄90̄30̄50̄10̄10̄60̄6≠
0̄10̄10̄30̄1440̄1430̄0018000̄9930̄0̄1189̄≠
0̄10̄20̄30̄1470̄1540̄0078000̄99350̄1299̄≠
0̄10̄30̄30̄2630̄0980̄16580̄01̄0000̄0̄0918̄≠
0̄10̄40̄30̄1090̄0711̄0038800̄98590̄1690̄≠
0̄10̄50̄30̄2570̄1410̄1168001̄0000̄0̄0709≠
78≠
0̄00006407≠
0̄00003393≠
0̄00000167≠
0̄00017269≠
0̄00002827≠
0̄00000615≠
0̄00007923≠
0̄00007951̄≠
0̄00003785≠
0̄00002590≠
0̄00001252≠
0̄00000760≠
0̄00006683≠
0̄00000578≠
0̄00000933≠
0̄00011413≠
0̄00072165≠
0̄00000433≠
0̄00000560≠
0̄00000090≠
0̄00000129≠
0̄00001399≠
0̄00001045≠
0̄00001806≠
0̄00013160̄≠
0̄00016931≠
0̄00003452≠
0̄00000072≠
0̄00000031̄≠
0̄00000009≠
0̄00000104≠
0̄00000024≠
0̄00000669≠
0̄00000200≠
0̄00000030̄≠

0̄00000227̄≠
0̄00000017̄≠
0̄00000297̄≠
0̄00000004≠
0̄00000031≠
0̄00000004≠
0̄00000095≠
0̄00000645≠
0̄00000035≠
0̄00000948≠
0̄00000009≠
0̄00000223≠
0̄00006048≠
0̄00000000≠
0̄00000004≠
0̄00000000≠
0̄00000030̄≠
0̄00000001̄≠
0̄00000014̄≠
0̄00023098≠
0̄00003249≠
0̄00002588≠
0̄00002641̄≠
0̄000000327≠
0̄000000920≠
0̄000292798≠
0̄000466796≠
0̄000017807≠
0̄000845561≠
0̄000037255≠
0̄000001861≠
0̄000400005≠
0̄000000607≠
```

```
*                         SECTION VI                         *
*                                                            *
* PROGRAM LISTING OF THE STRUCTURE FACTOR PROGRAM AND        *
* LEAST-SQUARES SUM MAKER                                    *
*                                                            *
       DORG 860                                    00860
* CLEAR L.S. SUMS TO ZERO *
START1 TFM  COUNTA,0                               00860 16 05819 00000
START2 TFM  START3+6,0                             00872 16 00890 00000
START3 TF   0,0                                    00884 26 00000 00000
START4 AM   START3+6,0                             00896 11 00890 00000
       SM   COUNTA,1,10                            00908 12 05819 00001
       BNZ  START3                                 00920 47 00884 01200
START5 B    START7                                 00932 49 00956 00000
* READ DATA             *
START6 RNPT 409                                    00944 36 00409 00300
START7 BNC2 START8                                 00956 47 01016 00200
       WNTY 409                                    00968 38 00409 00100
       RCTY                                        00980 34 00000 00102
       RNTY 409                                    00992 36 00409 00100
       RCTY                                        01004 34 00000 00102
START8 TFM  START5+1,41,10                         01016 16 00933 00041
* CHECK ON FINAL RECORD*
       BNR  ROTR00,410                             01028 45 01048 00410
       B    FINAL0                                 01040 49 05560 00000
       DORG *-3                                    01048
* CALCULATION OF EQUIVALENT INDICES,AND SCALARS*
ROTR00 TF   COUNTA,509                             01048 26 05819 00509
       TFM  ROTR01+6,514,7                         01060 16 01150 00514
       TFM  ROTR03+6,735,7                         01072 16 01174 00735
       TFM  ROTR06+6,703,7                         01084 16 01294 00703
       TFM  ROTR04+11,538,7                        01096 16 01203 00538
ROTR07 TFM  ROTR01+11,410,7                        01108 16 01155 00410
ROTR05 TFM  ROTR05+9,3,10                          01120 16 01129 00003
       TFM  ROTR02+11,0,8                          01132 16 01167 00000
ROTR01 M    514,410                                01144 23 00514 00410
ROTR02 SF   98                                     01156 32 00098 00000
ROTR03 TF   735,99                                 01168 26 00735 00099
       TF   ROTR04+6,ROTR01+11                     01180 26 01198 01155
ROTR04 M    410,538                                01192 23 00410 00538
       A    ROTR02+11,99                           01204 21 01167 00099
       AM   ROTR01+6,2,10                          01216 11 01150 00002
       AM   ROTR01+11,2,10                         01228 11 01155 00002
       AM   ROTR03+6,2,10                          01240 11 01174 00002
       AM   ROTR04+11,2,10                         01252 11 01203 00002
       SM   ROTR05+9,1,10                          01264 12 01129 00001
       BNZ  ROTR01                                 01276 47 01144 01200
ROTR06 TF   703,ROTR02+11                          01288 26 00703 01167
       AM   ROTR06+6,4,10                          01300 11 01294 00004
       SM   COUNTA,1,10                            01312 12 05819 00001
       BNZ  ROTR07                                 01324 47 01108 01200
* COMBINATIONS H.H,H.K,H.L,K.K,ETC.*
COHK00 TF   COUNTA,509                             01336 26 05819 00509
       TFM  COHK02+6,761,7                         01348 16 01426 00761
       TFM  COHK01+11,735,7                        01360 16 01419 00735
```

```
       TFM  COHK03+11,741,7                  01372 16 01467 00741
COHK05 TF   COHK06+11,COHK03+11              01384 26 01503 01467
COHK04 TF   COHK01+6,COHK01+11               01396 26 01414 01419
COHK01 M    735,735                          01408 23 00735 00735
COHK02 TF   761,99                           01420 26 00761 00099
       AM   COHK02+6,4,10                    01432 11 01426 00004
       AM   COHK01+6,2,10                    01444 11 01414 00002
COHK03 CM   COHK01+6,741,7                   01456 14 01414 00741
       BNZ  COHK01                           01468 47 01408 01200
       AM   COHK01+11,2,10                   01480 11 01419 00002
COHK06 CM   COHK01+11,741,7                  01492 14 01419 00741
       BNZ  COHK04                           01504 47 01396 01200
       AM   COHK03+11,6,10                   01516 11 01467 00006
       SM   COUNTA,1,10                      01528 12 05819 00001
       BNZ  COHK05                           01540 47 01384 01200
* CALCULATION OF THE COS AND SIN FOR ALL ATOMS AND EQUIVALENT REFLECTIONS*
TRIG00 TFM  TRIG11+6,0,7                     01552 16 01954 00000
TRIG01 TFM  TRIG12+6,0,7                     01564 16 01966 00000
       TFM  TRIG03+11,10022,7                01576 16 01647 10022
       TF   COUNTA,10005                     01588 26 05819 10005
TRIG14 TFM  TRIG03+6,410,7                   01600 16 01642 00410
       TFM  TRIG04+6,721,7                   01612 16 01654 00721
TRIG02 TFM  TRIG02+9,3,10                    01624 16 01633 00003
TRIG03 M    412,10022                        01636 23 00412 10022
TRIG04 TF   721,99                           01648 26 00721 00099
       AM   TRIG03+6,2,10                    01660 11 01642 00002
       AM   TRIG03+11,4,10                   01672 11 01647 00004
       AM   TRIG04+6,6,10                    01684 11 01654 00006
       SM   TRIG02+9,1,10                    01696 12 01633 00001
       BNZ  TRIG03                           01708 47 01636 01200
TRIG05 TF   TRIG02+9,509                     01720 26 01633 00509
       TFM  TRIG10+6,703,7                   01732 16 01894 00703
       TFM  TRIG07+11,514,7                  01744 16 01815 00514
TRIG13 TF   STOR00,ZEROCL-8                  01756 26 05841 05825
       TFM  TRIG08+11,721,7                  01768 16 01839 00721
TRIG06 TFM  TRIG06+9,3,10                    01780 16 01789 00003
TRIG09 TFM  TRIG08+1,21,10                   01792 16 01829 00021
TRIG07 BNF  TRIG08,514                       01804 44 01828 00514
       TFM  TRIG08+1,22,10                   01816 16 01829 00022
TRIG08 A    STOR00,721                       01828 21 05841 00721
       AM   TRIG07+11,2,10                   01840 11 01815 00002
       AM   TRIG08+11,6,10                   01852 11 01839 00006
       SM   TRIG06+9,1,10                    01864 12 01789 00001
       BNZ  TRIG09                           01876 47 01792 01200
TRIG10 MM   703,100,9                        01888 13 00703 00100
       A    99,STOR00                        01900 21 00099 05841
       AM   TRIG10+6,4,10                    01912 11 01894 00004
       SF   96                               01924 32 00096 00000
       BT   COSROU,99                        01936 27 07002 00099
TRIG11 TF   0,COSANS                         01948 26 00000 07552
TRIG12 TF   0,SINANS                         01960 26 00000 07557
       AM   TRIG11+6,10,10                   01972 11 01954 00010
       AM   TRIG12+6,10,10                   01984 11 01966 00010
       SM   TRIG02+9,1,10                    01996 12 01633 00001
       BNZ  TRIG13                           02008 47 01756 01200
       SM   COUNTA,1,10                      02020 12 05819 00001
       BNZ  TRIG14                           02032 47 01600 01200
* MULTIPLICATION OF ALL COS AND SIN BY EXPONENTIAL(TEMPERATURE FACTOR)*
* MULTIPLICITY FACTOR AND SCATTERING FACTOR*
EXMU00 TF   COUNTA-2,10007                   02044 26 05817 10007
       TF   COUNTA,10009                     02056 26 05819 10009
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EXMU09 TFM  EXMU08+11,0,7           02068 16 02415 00000
EXMU01 TFM  EXMU06+6,0,7            02080 16 02266 00000
EXMU02 TFM  EXMU03+11,0,7           02092 16 02127 00000
EXMU14 TFM  EXMU04+6,435,7          02104 16 02206 00435
EXMU03 A    EXMU04+6,0              02116 21 02206 00000
       AM   EXMU03+11,2,10          02128 11 02127 00002
       TF   COUNTB,509              02140 26 05867 00509
       CM   COUNTA-2,0,10           02152 14 05817 00000
       BZ   EXMU13                  02164 46 02660 01200
       TFM  EXMU16+1,41,10          02176 16 02537 00041
       TFM  EXMU06+11,761,7         02188 16 02271 00761
EXMU04 M    435,512                 02200 23 00435 00512
       SF   95                      02212 32 00095 00000
       TF   STOR00,99               02224 26 05841 00099
EXMU05 TFM  EXMU05+9,6,10           02236 16 02245 00006
       TF   STOR01,ZEROCL-5         02248 26 05851 05828
EXMU06 M    0,761                   02260 23 00000 00761
       A    STOR01,99               02272 21 05851 00099
       AM   EXMU06+6,5,10           02284 11 02266 00005
       AM   EXMU06+11,4,10          02296 11 02271 00004
       SM   EXMU05+9,1,10           02308 12 02245 00001
       BNZ  EXMU06                  02320 47 02260 01200
       SF   STOR01-5                02332 32 05846 00000
       BT   EXPROU,STOR01           02344 27 08094 05851
EXMU07 TFM  EXMU07+9,2,10           02356 16 02365 00002
EXMU12 M    EXPANS,STOR00           02368 23 08457 05841
       AM   96,5,10                 02380 11 00096 00005
       TF   STOR01,95               02392 26 05851 00095
EXMU08 M    STOR01,0                02404 23 05851 00000
       AM   95,5,10                 02416 11 00095 00005
       BNF  EXMU10,99               02428 44 02452 00099
       SF   94                      02440 32 00094 00000
EXMU10 SF   90                      02452 32 00090 00000
       BD   ERROR3,89               02464 43 05790 00089
       TF   EXMU11+6,EXMU08+11      02476 26 02494 02415
EXMU11 TF   0,94                    02488 26 00000 00094
       AM   EXMU08+11,5,10          02500 11 02415 00005
       SM   EXMU07+9,1,10           02512 12 02365 00001
       BNZ  EXMU12                  02524 47 02368 01200
EXMU16 NOP  EXMU17                  02536 41 02616 00000
       SM   EXMU06+6,30,10          02548 12 02266 00030
       SM   COUNTB,1,10             02560 12 05867 00001
       BNZ  EXMU05                  02572 47 02236 01200
       AM   EXMU06+6,30,10          02584 11 02266 00030
       SM   COUNTA-2,1,10           02596 12 05817 00001
       B    EXMU14                  02608 49 02104 00000
       DORG *-3                     02616
EXMU17 SM   COUNTB,1,10             02616 12 05867 00001
       BNZ  EXMU07                  02628 47 02356 01200
       SM   COUNTA,1,10             02640 12 05819 00001
       B    EXMU14                  02652 49 02104 00000
       DORG *-3                     02660
EXMU13 CM   COUNTA,0,10             02660 14 05819 00000
       BZ   SFSM00                  02672 46 02824 01200
       TF   EXMU18+6,EXMU04+6       02684 26 02702 02206
EXMU18 M    435,512                 02696 23 00435 00512
       SF   95                      02708 32 00095 00000
       TF   STOR00,99               02720 26 05841 00099
       TFM  EXMU16+1,49,10          02732 16 02537 00049
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        TF    EXMU15+11,EXMU06+6              02744 26 02779 02266
        SM    EXMU15+11,1,10                  02756 12 02779 00001
EXMU15  M     423,0                           02768 23 00423 00000
        SF    92                              02780 32 00092 00000
        AM    EXMU06+6,4,10                   02792 11 02266 00004
        BT    EXPROU,97                       02804 27 08094 00097
        B     EXMU07                          02816 49 02356 00000
        DORG  *-3                             02824
* SUMMING OF THE CONTRIBUTIONS FROM ALL ATOMS AND EQUIVALENT*
* REFLECTIONS TO THE STRUCTURE FACTOR*
SFSM00  TFM   SFSM01+11,0,7                   02824 16 02895 00000
        TFM   SFSM03+1,41,10                  02836 16 02981 00041
        M     509,10005                       02848 23 00509 10005
SFSM07  TF    COUNTA,99                       02860 26 05819 00099
        TF    STORO1,ZEROCL-7                 02872 26 05851 05826
SFSM01  A     STORO1,0                        02884 21 05851 00000
        AM    SFSM01+11,10,10                 02896 11 02895 00010
        SM    COUNTA,1,10                     02908 12 05819 00001
        BNZ   SFSM01                          02920 47 02884 01200
        AM    STORO1-1,5,10                   02932 11 05850 00005
        SF    STORO1-5                        02944 32 05846 00000
        BNF   SFSM03,STORO1                   02956 44 02980 05851
        SF    STORO1-2                        02968 32 05849 00000
SFSM03  NOP   SFSM04                          02980 41 03084 00000
SFSM02  TF    SINSQD,423                      02992 26 05872 00423
        TD    419,400                         03004 25 00419 00400
        TR    401,409                         03016 31 00401 00409
        TF    414,STORO1-2                    03028 26 00414 05849
        BD    SFSM05,507                      03040 43 03300 00507
        TFM   SFSM03+1,49,10                  03052 16 02981 00049
SFSM06  TFM   SFSM01+11,0,7                   03064 16 02895 00000
        B     SFSM07                          03076 49 02860 00000
        DORG  *-3                             03084
* FOR ACENTRIC SPACEGROUPS ONLY.CALCULATION OF F FROM A AND B.*
* AND CALCULATION OF PHASE ANGLES*
SFSM04  TF    STORO1-6,414                    03084 26 05845 00414
        M     STORO1-6,STORO1-6               03096 23 05845 05845
        TF    STORO2,ZEROCL-4                 03108 26 05865 05829
        A     STORO2,99                       03120 21 05865 00099
        M     STORO1-2,STORO1-2               03132 23 05849 05849
        A     STORO2,99                       03144 21 05865 00099
        BT    SQUROU,STORO2                   03156 27 08904 05865
        SF    SQUROU-4                        03168 32 08900 00000
        TF    414,SQUROU-1                    03180 26 00414 08903
        TF    GOZINT-5,414                    03192 26 08565 00414
        BT    GOZINT,STORO1-6                 03204 27 08570 05845
        SF    GOZANS-4                        03216 32 00048 00000
        TF    STORO2-11,GOZANS                03228 26 05854 00052
        BT    GOZINT,STORO1-2                 03240 27 08570 05849
        SF    GOZANS-4                        03252 32 00048 00000
        TF    STORO2-6,GOZANS                 03264 26 05859 00052
        TD    STORO2-5,400                    03276 25 05860 00400
SFSM08  TR    0,STORO1-9                      03288 31 00000 05842
* SCALING OF FO.SUMS FO,FC,AND FO MINUS FC.*
SFSM05  M     410,10018                       03300 23 0010  10018
        AM    96,5,10                         03312 11 00096 00005
        SF    92                              03324 32 00092 00000
        TF    410,95                          03336 26 00410 00095
        TF    GENSUM-12,95                    03348 26 05998 00095
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        TF    GENSUM-6,95                          03360 26 06004 00095
        TF    SFSM09+11,414                        03372 26 03395 00414
SFSM09  CF    SFSM09+11                            03384 33 03395 00000
        A     699,SFSM09+11                        03396 21 00699 03395
        AM    689,1,10                             03408 11 00689 00001
        A     619,95                               03420 21 00619 00095
        S     GENSUM-12,SFSM09+11                  03432 22 05998 03395
        BNF   SFSM10,414                           03444 44 03468 00414
        SF    95                                   03456 32 00095 00000
SFSM10  S     95,414                               0348  22 00095 00414
        TF    418,95                               03480 26 00418 00095
        CF    95                                   03492 33 00095 00000
        A     609,95                               03504 21 00609 00095
        M     414,SINSQD                           03516 23 00414 05872
        AM    96,5,10                              03528 11 00096 00005
        TF    GENSUM,95                            03540 26 06010 00095
* TO LOGICAL ROUTINE         *
        B     LOGROU                               03552 49 09154 00000
        DORG  *-3                                  03560
* CONTRIBUTIONS TO GENERAL SUMS*
SFSM15  TFM   SFSM11+11,GENSUM-12                  03560 16 03607 05998
        TFM   SFSM12+6,629,7                       03572 16 03686 00629
SFSM14  TF    SFSM11+6,SFSM11+11                   03584 26 03602 03607
SFSM11  M     GENSUM-12,GENSUM-12                  03596 23 05998 05998
        TF    GENSUM-18,99                         03608 26 05992 00099
        M     GENSUM-18,WEIGHT                     03620 23 05992 06017
        AM    96,5,10                              03632 11 00096 00005
        BNF   SFSM13,99                            03644 44 03668 00099
        SF    95                                   03656 32 00095 00000
SFSM13  SF    86                                   03668 32 00086 00000
SFSM12  A     629,95                               03680 21 00629 00095
        AM    SFSM11+6,6,10                        03692 11 03602 00006
        AM    SFSM12+6,10,10                       03704 11 03686 00010
        CM    SFSM11+6,GENSUM+6                    03716 14 03602 06016
        BNE   SFSM11                               03728 47 03596 01200
        AM    SFSM11+11,6,10                       03740 11 03607 00006
        CM    SFSM11+11,GENSUM+6                   03752 14 03607 06016
        BNE   SFSM14                               03764 47 03584 01200
* OUTPUT ROUTINE.FOUR CHOICES BY P.S.3 AND P.S. 4*
OUTP00  BC3   OUTP01                               03776 46 03800 00300
        BNC4  OUTP05                               03788 47 04252 00400
OUTP01  TR    96,BLANK-1                           03800 31 00096 06060
        TFM   TYPT00+6,95                          03812 16 00570 00095
        TFM   TYPT01+11,418                        03824 16 03859 00418
TYPT99  TFM   TYPT02+11,00,10                      03836 16 03883 00000
TYPT01  BNF   TYPT02,418                           03848 44 03872 00418
        TFM   TYPT02+11,20,10                      03860 16 03883 00020
TYPT02  BTM   TYPT00,00,10                         03872 17 00564 00000
        TF    TYPT03+11,TYPT01+11                  03884 26 03907 03859
TYPT03  TD    TYPT04+11,418                        03896 25 03919 00418
TYPT04  BTM   TYPT00,70,10                         03908 17 00564 00070
TYPT08  SM    TYPT01+11,1,10                       03920 12 03859 00001
        TF    TYPT05+11,TYPT01+11                  03932 26 03955 03859
TYPT05  TD    TYPT06+11,418                        03944 25 03967 00418
TYPT06  BTM   TYPT00,70,10                         03956 17 00564 00070
        TF    TYPT07+11,TYPT01+11                  03968 26 03991 03859
TYPT07  BNF   TYPT08,418                           03980 44 03920 00418
        BTM   TYPT00,00,10                         03992 17 00564 00000
        SM    TYPT01+11,1,10                       04004 12 03859 00001
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        CM    TYPT01+11,400                         04016 14 03859 00400
        BNE   TYPT99                                04028 47 03836 01200
        WATY  39                                    04040 39 00039 00100
OUTP09  NOP   LOGR13                                04052 41 09882 00000
OUTP12  TF    423,SINSQD                            04064 26 00423 05872
        BC4   OUTP60                                04076 46 04156 00400
        WNTY  419                                   04088 38 00419 00100
        TD    432,400                               04100 25 00432 00400
        BD    OUTP61,507                            04112 43 04136 00507
        TR    432,STOR01-1                          04124 31 00432 05850
OUTP61  WNPT  401                                   04136 38 00401 00200
        B     OUTP04                                04148 49 04240 00000
        DORG  *-3                                   04156
OUTP60  TD    427,400                               04156 25 00427 00400
        BD    OUTP62,507                            04168 43 04192 00507
        TR    427,STOR01-1                          04180 31 00427 05850
OUTP62  WNTY  424                                   04192 38 00424 00100
        BNC3  OUTP04                                04204 47 04240 00300
        TR    419,424                               04216 31 00419 00424
        WNPT  401                                   04228 38 00401 00200
OUTP04  RCTY                                        04240 34 00000 00102
OUTP05  NOP   START6                                04252 41 00944 00000
        BC1   START6                                04264 46 00944 00100
*                                                   *
* LEAST-SQUARES SUM MAKER                           *
*                                                   *
        AM    684,1,10                              04276 11 00684 00001
        BD    COOR00,507                            04288 43 04636 00507
* FOR ACENTRIC SPACE GROUPS ONLY.MAKE G(RS) AND J(RS)*
        M     10013,509                             04300 23 10013 00509
        TF    COUNTA,99                             04312 26 05819 00099
LSCF01  TFM   LSCF04+6,0                            04324 16 04414 00000
LSCF02  TFM   LSCF02+9,2,10                         04336 16 04345 00002
        TFM   LSCF06+6,GENSUM-15                    04348 16 04474 05995
        TF    LSCF08+6,LSCF04+6                     04360 26 04594 04414
LSCF07  TF    LSCF09+6,LSCF04+6                     04372 26 04606 04414
LSCF03  TFM   LSCF03+9,2,10                         04384 16 04393 00002
        TFM   LSCF04+11,STOR02-11                   04396 16 04419 05854
LSCF04  M     0,0                                   04408 23 00000 00000
        AM    96,5,10                               04420 11 00096 00005
        BNF   LSCF05,99                             04432 44 04456 00099
        SF    95                                    04444 32 00095 00000
LSCF05  SF    91                                    04456 32 00091 00000
LSCF06  TF    0,95                                  04468 26 00000 00095
        AM    LSCF04+11,5,10                        04480 11 04419 00005
        AM    LSCF06+6,5,10                         04492 11 04474 00005
        SM    LSCF03+9,1,10                         04504 12 04393 00001
        BNZ   LSCF04                                04516 47 04408 01200
        AM    LSCF04+6,5,10                         04528 11 04414 00005
        SM    LSCF02+9,1,10                         04540 12 04345 00001
        BNZ   LSCF07                                04552 47 04372 01200
        A     GENSUM-15,GENSUM                      04564 21 05995 06010
        S     GENSUM-5,GENSUM-10                    04576 22 06005 06000
LSCF08  TF    0,GENSUM-15                           04588 26 00000 05995
LSCF09  TF    0,GENSUM-5                            04600 26 00000 06005
        SM    COUNTA,1,10                           04612 12 05819 00001
        BNZ   LSCF02                                04624 47 04336 01200
* INITIALIZATION OF SUBROUTINE WHICH CALCULATES CONTRIBUTIONS*
* TO L.S. SUMS*
COOR00  TFM   LSSM09+6,0                            04636 16 06706 00000
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       TFM  LSSM00+11,3,10                      04648 16 05087 00003
       TFM  LSSM14+11,735                       04660 16 05111 00735
COOR09 TFM  LSSM03+6,0                          04672 16 05154 00000
       MM   509,6,10                            04684 13 00509 00006
       SM   99,2,10                             04696 12 00099 00002
       TF   LSSM15+11,99                        04708 26 05231 00099
       TFM  LSSM16+11,6,10                      04720 16 05195 00006
* INITIALIZATION OF L.S. SUBROUTINE FOR COORDINATE PARAMETERS SUMS*
COOR01 TFM  LSSM19+6,0                          04732 16 05658 00000
COOR02 TFM  LSSM20+6,0                          04744 16 05682 00000
COOR03 TFM  LSSM08+11,0                         04756 16 05699 00000
COOR04 TFM  LSSM09+11,0                         04768 16 05711 00000
COOR05 TFM  LSSM21+6,0                          04780 16 05850 00000
COOR06 TFM  LSSM22+6,0                          04792 16 05874 00000
COOR07 TFM  LSSM12+11,0                         04804 16 05891 00000
COOR08 TFM  LSSM13+11,0                         04816 16 05915 00000
       BT   LSSM00,10013                        04828 27 05076 10013
COOR10 TFM  LSSM03+6,0                          04840 16 05154 00000
       CM   10007,0,10                          04852 14 10007 00000
       BZ   COOR20                              04864 46 05056 01200
       TFM  LSSM00+11,6,10                      04876 16 05087 00006
       TFM  LSSM14+11,761                       04888 16 05111 00761
       MM   509,24,10                           04900 13 00509 00024
       SM   99,4,10                             04912 12 00099 00004
       TF   LSSM15+11,99                        04924 26 05231 00099
       TFM  LSSM16+11,24,10                     04936 16 05195 00024
* INITIALIZATION OF L.S. SUBROUTINE FOR ANISOTROPIC PARAMETER SUMS*
COOR11 TFM  LSSM19+6,0                          04948 16 05658 00000
COOR12 TFM  LSSM20+6,0                          04960 16 05682 00000
COOR13 TFM  LSSM08+11,0                         04972 16 05699 00000
COOR14 TFM  LSSM09+11,0                         04984 16 05711 00000
COOR15 TFM  LSSM21+6,0                          04996 16 05850 00000
COOR16 TFM  LSSM22+6,0                          05008 16 05874 00000
COOR17 TFM  LSSM12+11,0                         05020 16 05891 00000
COOR18 TFM  LSSM13+11,0                         05032 16 05915 00000
       BT   LSSM00,10007                        05044 27 05076 10007
COOR20 TF   STOR00,10013                        05056 26 05841 10013
       S    STOR00,10007                        05068 22 05841 10007
       BZ   CHSM09                              05080 46 05248 01200
       TFM  LSSM00+11,1,10                      05092 16 05087 00001
       TFM  LSSM14+11,SINSQD-1                  05104 16 05111 05871
       TFM  LSSM15+11,0,8                       05116 16 05231 00000
       TFM  LSSM16+11,0,10                      05128 16 05195 00000
* INITIALIZATION OF L.S. SUBROUTINE FOR ISOTROPIC PARAMETER SUMS*
COOR21 TFM  LSSM19+6,0                          05140 16 05658 00000
COOR22 TFM  LSSM20+6,0                          05152 16 05682 00000
COOR23 TFM  LSSM08+11,0                         05164 16 05699 00000
COOR24 TFM  LSSM09+11,0                         05176 16 05711 00000
COOR25 TFM  LSSM21+6,0                          05188 16 05850 00000
COOR26 TFM  LSSM22+6,0                          05200 16 05874 00000
COOR27 TFM  LSSM12+11,0                         05212 16 05891 00000
COOR28 TFM  LSSM13+11,0                         05224 16 05915 00000
       BT   LSSM00,STOR00                       05236 27 05076 05841
* CHECKING SIZE OF L.S. SUMS*
CHSM09 TF   CHSM10+11,LSSM09+6                  05248 26 05283 05706
CHSM11 SM   CHSM10+11,0,10                      05260 12 05283 00000
CHSM10 BD   CHSM12,0                            05272 43 05328 00000
CHSM13 SM   CHSM10+11,0                         05284 12 05283 00000
CHSM14 CM   CHSM10+11,0                         05296 14 05283 00000
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       BNZ   CHSM10                     05308 47 05272 01200
       B     START6                     05320 49 00944 00000
       DORG  *-3                        05328
CHSM12 TF    CHSM00+11,LSSM09+6         05328 26 05363 06705
CHSM01 SM    CHSM00+11,0,10             05340 12 05363 00000
CHSM00 TF    STOR00,0                   05352 26 05841 00000
       CM    STOR00,89,10               05364 14 05841 00089
       BP    CHSM02                     05376 46 05432 01100
CHSM03 SM    CHSM00+11,0                05388 12 05363 00000
CHSM04 CM    CHSM00+11,0                05400 14 05363 00000
       BNE   CHSM00                     05412 47 05352 01200
       B     START6                     05424 49 00944 00000
       DORG  *-3                        05432
* PUNCHING OF L.S. SUMS WHEN FIRST TWO DIGITS OF ANY SUM IS LARGER THAN 89*
CHSM02 WNPT  399                        05432 38 00399 00200
       RCTY                             05444 34 00000 00102
CHSM52 TFM   COUNTA,0                   05456 16 05819 00000
CHSM53 TFM   CHSM50+11,0                05468 16 05491 00000
CHSM50 TF    GENSUM,0                   05480 26 06010 00000
CHSM51 WNPT  GENSUM,,2                  05492 38 06010 00200
CHSM54 AM    CHSM50+11,0                05504 11 05491 00000
       SM    COUNTA,1,10                05516 12 05819 00001
       BNZ   CHSM50                     05528 47 05480 01200
       BNR   START1,410                 05540 45 00860 00410
       B     FINAL2                     05552 49 05592 00000
       DORG  *-3                        05560
FINAL0 WNPT  398                        05560 38 00398 00200
       BC1   FINAL2                     05572 46 05592 00100
       B     CHSM52                     05584 49 05456 00000
       DORG  *-3                        05592
FINAL2 TFM   FINAL3+11,609              05592 16 05615 00609
FINAL3 TF    GENSUM,609                 05604 26 06010 00609
       RCTY                             05616 34 00000 00102
       WNTY  GENSUM-9                   05628 38 06001 00100
       WNPT  GENSUM-9                   05640 38 06001 00200
       AM    FINAL3+11,10,10            05652 11 05615 00010
       CM    FINAL3+11,709              05664 14 05615 00709
       BNZ   FINAL3                     05676 47 05604 01200
       RCTY                             05688 34 00000 00102
       WATY  THEEN1                     05700 39 06043 00100
* ROUTINE FROM FINAL0 IS INITIATED BY LAST RECORD ON DATA TAPE *
* PUNCHED WERE FINAL SET OF L.S. SUMS AND OUTPUT OF GENERAL SUMS*
       H                                05712 48 00000 00000
       DORG  *-9                        05714
* ERROR ROUTINES     *
ERROR0 RCTY                             05714 34 00000 00102
       TD    ERRORA+8,LSSM00+11         05726 25 06027 06087
       WATY  ERRORA                     05738 39 06019 00100
       H                                05750 48 00000 00000
       DORG  *-9                        05752
ERROR1 RCTY                             05752 34 00000 00102
       TD    ERRORB+8,LSSM00+11         05764 25 06039 06087
       WATY  ERRORB                     05776 39 06031 00100
       H                                05788 48 00000 00000
       DORG  *-9                        05790
ERROR3 RCTY                             05790 34 00000 00102
       WATY  ERRORD                     05802 39 06065 00100
       H                                05814 48 00000 00000
       DORG  *-9                        05816
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* CONSTANTS, SYMBOLS AND MESSAGES*
COUNTA DS    4                          05819 00004
ZEROCL DC    14,0                       05833 00014    00000000000000
STOR00 DS    8                          05841 00008
STOR01 DS    10                         05851 00010
STOR02 DS    14                         05865 00014
COUNTB DS    2                          05867 00002
SINSQD DS    5                          05872 00005
LSSSUM DS    60                         05932 00060
GENSUM DS    78                         06010 00078
       DC    1,@                        06011 00001    *
WEIGHT DS    6                          06017 00006
ERRORA DAC   6,ERR10@                   06019 00006X2 ERR10*
ERRORB DAC   6,ERR20@                   06031 00006X2 ERR20*
THEEN1 DAC   9,SEASHORE@                06043 00009X2 SEASHORE*
BLANK  DAC   2, @                       06061 00002X2  *
ERRORD DAC   5,ERR3@                    06065 00005X2 ERR3*
       NOP                              06074 41 00000 00000
       DORG  *-9                        06076
```

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*                                             *
*        SUBROUTINES                          *
*                                             *
* SUBROUTINE WHICH CALCULATES CONTRIBUTIONS TO L.S. SUMS*
LSSM00 TFM  LSSM00+9,3,10                     06076 16 06085 00003
       TFM  LSSM06+6,GENSUM-65                06088 16 06502 05945
LSSM14 TFM  LSSM03+11,0                       06100 16 06159 00000
       TFM  LSSM02+6,LSSSUM-50                06112 16 06442 05882
LSSM01 TF   COUNTA,509                        06124 26 05819 00509
       TF   STORO1,ZEROCL-4                   06136 26 05851 05829
* CALCULATION OF DIFFERENTIAL QUOTIENT.MULTIPLICATION BY WEIGHT*
LSSM03 M    0,0                               06148 23 00000 00000
       S    STORO1,99                         06160 22 05851 00099
       AM   LSSM03+6,10,10                    06172 11 06154 00010
LSSM16 AM   LSSM03+11,6,10                    06184 11 06159 00006
       SM   COUNTA,1,10                       06196 12 05819 00001
       BNZ  LSSM03                            06208 47 06148 01200
LSSM15 SM   LSSM03+11,0,8                     06220 12 06159 00000
       S    LSSM03+6,510                      06232 22 06154 00510
       BD   LSSM02,STORO1-9                   06244 43 06436 05842
       SF   STORO1-8                          06256 32 05843 00000
       BD   LSSM02,STORO1-8                   06268 43 06436 05843
       SF   STORO1-7                          06280 32 05844 00000
       BD   LSSM02,STORO1-7                   06292 43 06436 05844
       SF   STORO1-6                          06304 32 05845 00000
       BD   LSSM02,STORO1-6                   06316 43 06436 05845
       SF   STORO1-5                          06328 32 05846 00000
       BD   LSSM02,STORO1-5                   06340 43 06436 05846
       SF   STORO1-4                          06352 32 05847 00000
       BD   LSSM02,STORO1-4                   06364 43 06436 05847
       SF   STORO1-3                          06376 32 05848 00000
       BD   LSSM02,STORO1-3                   06388 43 06436 05848
       SF   STORO1-2                          06400 32 05849 00000
       BD   LSSM02,STORO1-2                   06412 43 06436 05849
       SF   STORO1-1                          06424 32 05850 00000
LSSM02 TF   LSSSUM-50,STORO1                  06436 26 05882 05851
       M    STORO1,WEIGHT                     06448 23 05851 06017
       AM   97,5,10                           06460 11 00097 00005
       BNF  LSSM06,99                         06472 44 06496 00099
       SF   96                                06484 32 00096 00000
LSSM06 TF   GENSUM-65,96                      06496 26 05945 00096
       AM   LSSM02+6,10,10                    06508 11 06442 00010
       AM   LSSM06+6,13,10                    06520 11 06502 00013
       SM   LSSM00+9,1,10                     06532 12 06085 00001
       BNZ  LSSM01                            06544 47 06124 01200
       A    LSSM03+6,510                      06556 21 06154 00510
* CALCULATION OF MATRIX TERMS AND SUMMING*
       TF   COUNTA-2,LSSM00+11                06568 26 05817 06087
       TFM  LSSM10+11,LSSSUM-50               06580 16 06615 05882
       TFM  LSSM07+6,GENSUM-65                06592 16 06646 05945
LSSM10 TFM  LSSM07+11,LSSSUM-50               06604 16 06651 05882
       TF   COUNTA,COUNTA-2                   06616 26 05819 05817
LSSM30 TFM  79,0,9                            06628 16 00079 00000
LSSM07 M    GENSUM-65,LSSSUM-50               06640 23 05945 05882
LSSM19 SF   0                                 06652 32 00000 00000
       BNF  LSSM08,99                         06664 44 06688 00099
LSSM20 SF   0                                 06676 32 00000 00000
LSSM08 BD   ERRORO,0                          06688 43 05714 00000
LSSM09 A    0,0                               06700 21 00000 00000
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LSSM17 AM   LSSM09+6,0                        06712 11 06706 00000
       AM   LSSM07+11,10,10                   06724 11 06651 00010
       SM   COUNTA,1,10                       06736 12 05819 00001
       BNZ  LSSM30                            06748 47 06628 01200
       AM   LSSM07+6,13,10                    06760 11 06546 00013
       AM   LSSM10+11,10,10                   06772 11 06615 00010
       SM   COUNTA-2,1,10                     06784 12 05817 00001
       BNZ  LSSM10                            06796 47 06604 01200
* CALCULATION OF VECTOR TERMS AND SUMMING*
       TF   COUNTA,LSSM00+11                  06808 26 05819 06087
       TFM  LSSM11+6,GENSUM-65                06820 16 06838 05945
LSSM11 M    GENSUM-65,418                     06832 23 05945 00418
LSSM21 SF   0                                 06844 32 00000 00000
       BNF  LSSM12,99                         06856 44 06880 00099
LSSM22 SF   0                                 06868 32 00000 00000
LSSM12 BD   ERROR1,0                          06880 43 05752 00000
       TF   LSSM13+6,LSSM09+6                 06892 26 06910 06706
LSSM13 A    0,0                               06904 21 00000 00000
LSSM18 AM   LSSM09+6,0                        06916 11 06706 00000
       AM   LSSM11+6,13,10                    06928 11 06838 00013
       SM   COUNTA,1,10                       06940 12 05819 00001
       BNZ  LSSM11                            06952 47 06832 01200
       SM   LSSM00-1,1,10                     06964 12 06075 00001
       BNZ  LSSM00                            06976 47 06076 01200
       BB                                     06988 42 00000 00000
       DORG *-9                               06990
* COSINE AND SINE ROUTINE*
       NOP                                    06990 41 00000 00000
COSROU TFM  COSR07+11,CTABL1                  07002 16 07493 07962
       TFM  COSR09+11,CTABL1+125              07014 16 07549 08087
       TF   STCS00,COSRND                     07026 26 07917 07910
       TF   COSROU-6,COSROU-1                 07038 26 06996 07001
       CF   COSROU-1                          07050 33 07001 00000
       TFM  STCS01,10000,7                    07062 16 07924 10000
       S    STCS01,COSROU-1                   07074 22 07924 07001
       SF   COSROU-2                          07086 32 07000 00000
       CM   COSROU-1,50,10                    07098 14 07001 00050
       TFM  COSR16+1,21,10                    07110 16 07879 00021
       BNP  COSR01                            07122 47 07170 01100
       TF   COSROU-1,STCS01                   07134 26 07001 07924
       SF   COSROU-2                          07146 32 07000 00000
       TFM  COSR16+1,22,10                    07158 16 07879 00022
COSR01 M    COSROU-1,CTCS00                   07170 23 07001 07945
       TF   STCS01,97                         07182 26 07924 00097
       M    COSROU-1,COSROU-1                 07194 23 07001 07001
       TF   STCS02,99                         07206 26 07938 00099
       MM   STCS02,1974,8                     07218 13 07938 01974
       S    STCS00,95                         07230 22 07917 00095
       CM   COSROU-3,49,10                    07242 14 06999 00049
       BNP  COSR03                            07254 47 07366 01100
       CM   COSROU-3,74,10                    07266 14 06999 0007
       BNP  COSR02                            07278 47 07334 01100
       TFM  QUADRT,10,10                      07290 16 07947 00010
       SF   COSROU-3                          07302 32 06999 00000
       AM   COSROU-3,50,10                    07314 11 06999 00050
       B    COSR04                            07326 49 07414 00000
       DORG *-3                               07334
COSR02 TFM  QUADRT,0,10                       07334 16 07947 00000
       SM   COSROU-3,50,10                    07346 12 06999 00050
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       B    COSR06                             07358 49 07446 00000
       DORG *-3                                07366
COSR03 CM   COSROU-3,24,10                     07366 14 06999 00024
       BNP  COSR05                             07378 47 07434 01100
       TFM  QUADRT,1,10                        07390 16 07947 00001
       SF   COSROU-3                           07402 32 06999 00000
COSR04 AM   COSROU-3,50,10                     07414 11 06999 00050
       B    COSR06                             07426 49 07446 00000
       DORG *-3                                07434
COSR05 TFM  QUADRT,11,10                       07434 16 07947 00011
COSR06 MM   COSROU-3,5,10                      07446 13 06999 00005
       A    COSR07+11,99                       07458 21 07493 00099
       S    COSR09+11,99                       07470 22 07649 00099
COSR07 M    STCS00-1,0,7                       07482 23 07916 00000
       TF   STCS02,95                          07494 26 07938 00095
       TF   COSR17+11,COSR07+11                07506 26 07529 07493
COSR17 M    STCS01,0,7                         07518 23 07924 00000
       TF   STCS03,94                          07530 26 07931 00094
       BD   COSR08,QUADRT-1                    07542 43 07578 07946
       SF   STCS02                             07554 32 07938 00000
       SF   STCS03                             07566 32 07931 00000
COSR08 TFM  COSR10+1,21,10                     07578 16 07651 00021
       TFM  COSR12+1,22,10                     07590 16 07687 00022
       BD   COSR09,QUADRT                      07602 43 07638 07947
       TFM  COSR10+1,22,10                     07614 16 07651 00022
       TFM  COSR12+1,21,10                     07626 16 07687 00021
COSR09 M    STCS00-1,0                         07638 23 07916 00000
COSR10 A    STCS03,95                          07650 21 07931 00095
       TF   COSR11+11,COSR09+11                07662 26 07685 07649
COSR11 M    STCS01,0                           07674 23 07924 00000
COSR12 S    STCS02,94                          07686 22 07938 00094
       AM   STCS02,5,10                        07698 11 07938 00005
       BNF  COSR13,STCS02                      07710 44 07746 07938
       SM   STCS02,10,10                       07722 12 07938 00010
       SF   STCS02-1                           07734 32 07937 00000
COSR13 SF   STCS02-5                           07746 32 07933 00000
       AM   STCS03,5,10                        07758 11 07931 00005
       BNF  COSR14,STCS03                      07770 44 07806 07931
       SM   STCS03,10,10                       07782 12 07931 00010
       SF   STCS03-1                           07794 32 07930 00000
COSR14 SF   STCS03-5                           07806 32 07926 00000
       BNF  COSR15,COSROU-6                    07818 44 07866 06996
       TFM  STCS00,0,7                         07830 16 07917 00000
       S    STCS00,STCS03-1                    07842 22 07917 07930
       TF   STCS03-1,STCS00                    07854 26 07930 07917
COSR15 TFM  SINANS,0,7                         07866 16 07957 00000
COSR16 A    SINANS,STCS03-1                    07878 21 07957 07930
       TF   COSANS,STCS02-1                    07890 26 07952 07937
       BB                                      07902 42 00000 00000
       DORG *-9                                07904
COSRND DC   7,1000005                          07910 00007    1000005
STCS00 DS   7                                  07917 00007
STCS01 DS   7                                  07924 00007
STCS03 DS   7                                  07931 00007
STCS02 DS   7                                  07938 00007
CTCS00 DC   7,62825                            07945 00007    0062825
QUADRT DS   2                                  07947 00002
COSANS DS   5                                  07952 00005
SINANS DS   5                                  07957 00005
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CTABL1  DC    5,99999                        07962 00005     99999
        DC    5,99803                        07967 00005     99803
        DC    5,99211                        07972 00005     99211
        DC    5,98229                        07977 00005     98229
        DC    5,96858                        07982 00005     96858
        DC    5,95106                        07987 00005     95106
        DC    5,92978                        07992 00005     92978
        DC    5,90483                        07997 00005     90483
        DC    5,87631                        08002 00005     87631
        DC    5,84433                        08007 00005     84433
        DC    5,80902                        08012 00005     80902
        DC    5,77051                        08017 00005     77051
        DC    5,72897                        08022 00005     72897
        DC    5,68455                        08027 00005     68455
        DC    5,63742                        08032 00005     63742
        DC    5,58779                        08037 00005     58779
        DC    5,53583                        08042 00005     53583
        DC    5,48175                        08047 00005     48175
        DC    5,42578                        08052 00005     42578
        DC    5,36812                        08057 00005     36812
        DC    5,30902                        08062 00005     30902
        DC    5,24869                        08067 00005     24869
        DC    5,18738                        08072 00005     18738
        DC    5,12533                        08077 00005     12533
        DC    5,06279                        08082 00005     06279
        DC    5,00000                        08087 00005     00000
* EXPONENTIAL ROUTINE*
        NOP                                  08088 41 00000 00000
        DORG  *-5                            08094
EXPROU  C     ZEROEX,EXPROU-1                08094 24 08433 08093
        BE    EXPRO4                         08106 46 08402 01200
        TF    STEX00,CSEX00                  08118 26 08447 08440
        SF    EXPROU-4                       08130 32 08090 00000
        S     STEX00-1,EXPROU-1              08142 22 08446 00093
        M     EXPROU-1,EXPROU-1              08154 23 08093 08093
        TF    STEX01,96                      08166 26 08452 00096
        MM    STEX01,5,10                    08178 13 08452 00005
        A     STEX00,97                      08190 21 08447 00097
        M     EXPROU-1,STEX01                08202 23 08093 08452
        TF    STEX01,95                      08214 26 08452 00095
        MM    STEX01,167,9                   08226 13 08452 00167
        S     STEX00,94                      08238 22 08447 00094
        TFM   EXPRO1+11,EXTBL1+5             08250 16 08345 08467
        TFM   EXPRO2+11,EXTBL1               08262 16 08369 08462
        CF    EXPROU-6                       08274 33 08088 00000
        TD    EXPRO5+11,EXPROU-5             08286 25 08321 08089
        TD    EXPRO6+11,EXPROU-6             08298 25 08333 08088
EXPRO5  AM    EXPRO1+10,0,10                 08310 11 08344 00000
EXPRO6  AM    EXPRO2+10,0,10                 08322 11 08368 00000
EXPRO1  M     STEX00,EXTBL1+5                08334 23 08447 08467
        TF    STEX00,94                      08346 26 08447 00094
EXPRO2  M     STEX00,EXTBL1                  08358 23 08447 08462
        AM    94,5,10                        08370 11 00094 00005
        SF    89                             08382 32 00089 00000
        B     EXPRO3                         08394 49 08414 00000
        DORG  *-3                            08402
EXPRO4  TF    93,EXTBL1                      08402 26 00093 08462
EXPRO3  TF    EXPANS,93                      08414 26 08457 00093
        BB                                   08426 42 00000 00000
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        DORG *-9                               08428
ZEROEX  DC   6,0                               08433 00006    000000
CSEXOO  DC   7,1000000                         08440 00007    1000000
STEXOO  DS   7                                 08447 00007
STEXO1  DS   5                                 08452 00005
EXPANS  DS   5                                 08457 00005
EXTBL1  DC   5,99999                           08462 00005    99999
        DC   5,99999                           08467 00005    99999
        DC   5,36788                           08472 00005    36788
        DC   5,90484                           08477 00005    90484
        DC   5,13534                           08482 00005    13534
        DC   5,81874                           08487 00005    81874
        DC   5,04979                           08492 00005    04979
        DC   5,74082                           08497 00005    74082
        DC   5,01832                           08502 00005    01832
        DC   5,67032                           08507 00005    67032
        DC   5,00674                           08512 00005    00674
        DC   5,60653                           08517 00005    60653
        DC   5,00248                           08522 00005    00248
        DC   5,54882                           08527 00005    54882
        DC   5,00091                           08532 00005    00091
        DC   5,49658                           08537 00005    49658
        DC   5,00034                           08542 00005    00034
        DC   5,44933                           08547 00005    44933
        DC   5,00012                           08552 00005    00012
        DC   5,40657                           08557 00005    40657
* DIVIDE ROUTINE*
        NOP                                    08558 41 00000 00000
GOZINT  TF   GOZBEE,GOZINT-5                   08570 26 08891 08565
        CF   GOZBEE                            08582 33 08891 00000
        CM   GOZBEE,0,8                        08594 14 08891 00000
        BE   GOZIN3                            08606 46 08856 01200
        TF   GOZADJ,GOZUN1                     08618 26 00072 08887
        S    GOZADJ-1,GOZBEE                   08630 22 00071 08891
        TF   ZINTER,GOZADJ-1                   08642 26 00079 00071
        S    GOZADJ,ZINTER                     08654 22 00072 00079
        TD   GOZARE+1,400                      08666 25 00064 00400
        TF   GOZARE,GOZERS                     08678 26 00063 08879
        TF   GOZARE-10,GOZERS                  08690 26 00053 08879
        A    GOZARE,GOZINT-1                   08702 21 00063 08569
        CF   GOZARE                            08714 33 00063 00000
GOZIN1  BD   GOZIN2,GOZANS+3                   08726 43 08758 00055
        A    GOZARE-3,ZINTER                   08738 21 00060 00079
        B    GOZIN1                            08750 49 08726 00000
        DORG *-3                               08758
GOZIN2  TR   GOZHFT,GOZHFT+1                   08758 31 00045 00046
        TDM  GOZARE,0                          08770 15 00063 00000
        S    GOZARE-3,GOZADJ                   08782 22 00060 00072
        BNF  GOZIN1,GOZHFT                     08794 44 08726 00045
        AM   GOZANS+1,5,10                     08806 11 00053 00005
        M    GOZINT-1,GOZINT-5                 08818 23 08569 08565
        BNF  GOZIN4,99                         08830 44 08854 00099
        SF   GOZANS                            08842 32 00052 00000
GOZIN4  BB                                     08854 42 00000 00000
        DORG *-9                               08856
GOZIN3  TF   GOZANS,GOZERS-2                   08856 26 00052 08877
        BB                                     08868 42 00000 00000
        DORG *-9                               08870
GOZERS  DC   10,0                              08879 00010    0000000000
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GOZUN1 DC    8,10000000                                  08887 00008    T0000000
GOZBEE DS    4                                           08891 00004
ZINTER DS    ,79                                         00079 00000
GOZADJ DS    ,72                                         00072 00000
GOZARE DS    ,63                                         00063 00000
GOZANS DS    ,52                                         00052 00000
GOZHFT DS    ,45                                         00045 00000
* SQUARE ROOT ROUTINE*
       NOP                                               08892 41 00000 00000
SQUROU C     SQUROU-1,GOZERS                             08904 24 08903 08879
       BE    SQURO5                                      08916 46 09124 01200
       TF    PLUGOO,SQUARO                               08928 26 09142 09152
       TFM   SQURO1+11,PLUGOO                            08940 16 08975 09142
       MM    SQUROU-1,5,10                               08952 13 08903 00005
SQURO1 S     99,PLUGOO                                   08964 22 00099 09142
       BNN   SQURO3                                      08976 46 09068 01300
       TF    SQURO2+11,SQURO1+11                         08988 26 09011 08975
SQURO2 A     99,0                                        09000 21 00099 00000
       SM    PLUGOO-5,45,10                              09012 12 09137 00045
       TR    PLUGOO-16,PLUGOO-15                         09024 31 09126 09127
       SM    SQURO1+11,2,10                              09036 12 08975 00002
       BNR   SQURO1,PLUGOO-4                             09048 45 08964 09138
       B     SQURO4                                      09060 49 09088 00000
       DORG  *-3                                         09068
SQURO3 AM    PLUGOO-7,1,10                               09068 11 09135 00001
       B     SQURO1                                      09080 49 08964 00000
       DORG  *-3                                         09088
SQURO4 AM    PLUGOO-8,5,10                               09088 11 09134 00005
       SF    PLUGOO-12                                   09100 32 09130 00000
       TF    SQUROU-1,PLUGOO-9                           09112 26 08903 09133
SQURO5 BB                                                09124 42 00000 00000
       DORG  *-9                                         09126
PLUGOO DS    17                                          09142 00017
       DC    1,@                                         09143 00001    ‡
SQUARO DC    9,5000000                                   09152 00009    005000000
* LOGICAL ROUTINE*
LOGROU MM    LOGFMN,3,10                                 09154 13 09953 00003
       SF    96                                          09166 32 00096 00000
       TF    LOGFM3,99                                   09178 26 09972 00099
       S     99,LOGFMN                                   09190 22 00099 09953
       TF    LOGFM2,99                                   09202 26 09960 00099
       TFM   OUTPO5+1,41,10                              09214 16 04253 00041
       CM    431,0,7                                     09226 14 00431 00000
       BE    LOGRO1                                      09238 46 09270 01200
       TF    WEIGHT,431                                  09250 26 06017 00431
       B     LOGRO4                                      09262 49 09386 00000
       DORG  *-3                                         09270
LOGRO1 C     410,LOGFM3                                  09270 24 00410 09972
       BP    LOGRO2                                      09282 46 09314 01100
       TF    GOZINT-5,LOGFM3                             09294 26 08565 09972
       B     LOGRO3                                      09306 49 09326 00000
       DORG  *-3                                         09314
LOGRO2 TF    GOZINT-5,410                                09314 26 08565 00410
LOGRO3 BTM   GOZINT,10,8                                 09326 17 08570 00010
       SF    GOZANS-3                                    09338 32 00049 00000
       M     GOZANS,GOZANS                               09350 23 00052 00052
       SF    93                                          09362 32 00093 00000
       TF    WEIGHT,97                                   09374 26 06017 00097
LOGRO4 TF    431,WEIGHT                                  09386 26 00431 06017
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       TD    LOGR14+11,424          09398 25 09421 00424
LOGR14 MM    431,0,10               09410 13 00431 00000
       SF    94                     09422 32 00094 00000
       TF    WEIGHT,99              09434 26 06017 00099
       BD    LOGR12,426             09446 43 09838 00426
       TF    LOGFCL,414             09458 26 09976 00414
       CF    LOGFCL                 09470 33 09976 00000
       C     410,LOGFMN             09482 24 00410 09953
       BNN   LOGR05                 09494 46 09542 01300
       M     LOGFMN,LOGMPL          09506 23 09953 09956
       C     98,LOGFCL              09518 24 00098 09976
       BNN   LOGR11                 09530 47 09802 01300
LOGR05 TFM   LOGR06+11,LOGAAA-6     09542 16 09613 09962
       TF    LOGR07+11,LOGFM2       09554 26 09589 09960
LOGR08 TFM   LOGR08+9,3,10          09566 16 09575 00003
LOGR07 CM    410,LOGFM2             09578 14 00410 09960
       BNN   LOGR09                 09590 46 09638 01300
LOGR06 M     LOGFCL,LOGAAA-6        09602 23 09976 09962
       C     98,410                 09614 24 00098 00410
       BN    LOGR11                 09626 47 09802 01300
LOGR09 A     LOGR07+11,LOGFMN       09638 21 09589 09953
       AM    LOGR06+11,2,10         09650 11 09613 00002
       SM    LOGR08+9,1,10          09662 12 09575 00001
       BNZ   LOGR07                 09674 47 09578 01200
       M     LOGFCL,LOGAAA          09686 23 09976 09968
       C     98,410                 09698 24 00098 00410
       BN    LOGR11                 09710 47 09802 01300
       C     SINSQD,LOGSIN          09722 24 05872 09981
       BP    LOGR10                 09734 46 09782 01100
       S     LOGFCL,410             09746 22 09976 00410
       C     LOGFCL,LOGDIF          09758 24 09976 09985
       BP    LOGR11                 09770 46 09802 01100
LOGR10 TDM   426,0                  09782 15 00426 00000
       B     SFSM15                 09794 49 03560 00000
       DORG  *-3                    09802
LOGR11 TDM   426,1                  09802 15 00426 00001
       TFM   OUTP05+1,49,10         09814 16 04253 00049
       B     SFSM15,,10             09826 49 03560 00000
LOGR12 TD    LOGR12-1,426           09838 25 09837 00426
       CM    LOGR12-1,1,10          09850 14 09837 00001
       BE    LOGR11                 09862 46 09802 01200
       B     LOGR10                 09874 49 09782 00000
       DORG  *-3                    09882
LOGR13 RNTY  426                    09882 36 00426 00100
       SPTY                         09894 34 00000 00101
       TFM   OUTP05+1,49,10         09906 16 04253 00049
       BD    OUTP12,426             09918 43 04064 00426
       TFM   OUTP05+1,41,10         09930 16 04253 00041
       B     OUTP12                 09942 49 04064 00000
       DORG  *-3                    09950
LOGFMN DC    4,25                   09953 00004    0025
LOGMPL DC    3,20                   09956 00003    020
LOGFM2 DS    4                      09960 00004
       DC    2,13                   09962 00002    13
       DC    2,15                   09964 00002    15
       DC    2,20                   09966 00002    20
LOGAAA DC    2,25                   09968 00002    25
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LOGFM3 DS    4                                     09972 00004
LOGFCL DS    4                                     09976 00004
LOGSIN DC    5,120                                 09981 00005    00120
LOGDIF DC    4,125                                 09985 00004    0125
* SUBROUTINE FOR TYPOUT*
       DORG 562                                    00562
       NOP                                         00562 41 00000 00000
       DORG *-9                                    00564
TYPT00 TF    95,TYPT00-1                           00564 26 00095 00563
       SM    TYPT00+6,2,10                         00576 12 00570 00002
       BB                                          00588 42 00000 00000
       DORG *-9                                    00590
```

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*                                                                     *
* INITIALIZATION OF STRUCTURE FACTOR-L.S. SUM MAKER PROGRAM*
*                                                                     *
       DORG 13000                               13000
* CHOICE OF SPACE GROUP*
       RCTY                                     13000 34 00000 00102
       WATY MESS01                              13012 39 17019 00100
       TBTY                                     13024 34 00000 00108
       RNTY SPACEG-2                            13036 36 16926 00100
       SF   SPACEG-2                            13048 32 16926 00000
INIT01 RNPT SPACEL-6                            13060 36 16929 00300
       SF   SPACEL-3                            13072 32 16932 00000
       C    SPACEG,SPACEL-1                     13084 24 16928 16934
       BE   INIT00                              13096 46 13156 01200
       RNPT 19010                               13108 36 19010 00300
INIT03 CM   SPACEL-1,74,9                       13120 14 16934 00074
       BNE  INIT01                              13132 47 13060 01200
       B    INIT53                              13144 49 13300 00000
INIT00 RNPT 507                                 13156 36 00507 00300
       TR   19000,SPACEL-6                      13168 31 19000 16929
       B    INIT03                              13180 49 13120 00000
INIT52 RCTY                                     13192 34 00000 00102
       WATY MESS29                              13204 39 18759 00100
       H                                        13216 48 00000 00000
       RNPT SPACEL-6                            13228 36 16929 00300
       SF   SPACEL-3                            13240 32 16932 00000
       RNPT 507                                 13252 36 00507 00300
       C    SPACEG,SPACEL-1                     13264 24 16928 16934
       BNE  INIT53                              13276 47 13300 01200
       TR   19000,SPACEL-6                      13288 31 19000 16929
INIT53 BNR  INIT52,19006                        13300 45 13192 19006
       TFM  INIT04+6,609                        13312 16 13342 00609
* CLEARING TO ZERO OF GENERAL SUM AREA*
       TFM  COUNTA,10,10                        13324 16 05819 00010
INIT04 TF   609,ZEROCL-4                        13336 26 00609 05829
       AM   INIT04+6,10,10                      13348 11 13342 00010
       SM   COUNTA,1,10                         13360 12 05819 00001
       BNZ  INIT04                              13372 47 13336 01200
       RCTY                                     13384 34 00000 00102
       WATY MESS02                              13396 39 17079 00100
       H                                        13408 48 00000 00000
       RCTY                                     13420 34 00000 00102
       WATY MESS31                              13432 39 18521 00100
       RNTY PARCHK                              13444 36 16925 00100
       BD   INIT54,PARCHK                       13456 43 13540 16925
       RCTY                                     13468 34 00000 00102
* LOADING OF PARAMETERS*
       WATY MESS03                              13480 39 17121 00100
       H                                        13492 48 00000 00000
       RNPT 19006                               13504 36 19006 00300
       RNPT 10000                               13516 36 10000 00300
       B    INIT55                              13528 49 13636 00000
INIT54 RCTY                                     13540 34 00000 00102
       WATY MESS32                              13552 39 18603 00100
       SPTY                                     13564 34 00000 00101
       RNTY 19006                               13576 36 19006 00100
       RCTY                                     13588 34 00000 00102
       WATY MESS33                              13600 39 18651 00100
       RCTY                                     13612 34 00000 00102
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      RNTY 10000                               13624 36 10000 00100
INIT55 MM  10005,14,10                         13636 13 10005 000Ī4
      TF   PARALT,99                           13648 26 16939 00099
      TFM  COORLT,10023,7                      13660 16 16954 Ī0023
      A    COORLT,99                           13672 21 16954 00099
      MM   10007,30,10                         13684 13 10007 000Ī0
      A    PARALT,99                           13696 21 16939 00099
      MM   10009,4,10                          13708 13 10009 0000Ī
      A    PARALT,99                           13720 21 16939 00099
      AM   PARALT,20,8                         13732 11 16939 0Ī020
      TFM  INIT61+11,9999,7                    13744 16 13779 Ī9999
      A    INIT61+11,PARALT                    13756 21 13779 16939
INIT61 BNR INIT60,0                            13768 45 13792 00000
      B    INIT62                              13780 49 13828 00000
INIT60 RCTY                                    13792 34 00000 00102
      WATY MESS34                              13804 39 18691 00100
      H                                        13816 48 00000 00000
INIT62 TFM FIRCOS,10004,7                      13828 16 16944 Ī0004
* INITIALIZATION OF FIRST COS AND SIN LOCATION AND OF LOCATIONS *
* PARAMETERS*
      A    FIRCOS,PARALT                       13840 21 16944 16939
      TF   FIRSIN,FIRCOS                       13852 26 16949 16944
      AM   FIRSIN,5,10                         13864 11 16949 0000Ī
      TF   TRIG00+11,FIRCOS                    13876 26 01563 16944
      TF   TRIG01+11,FIRSIN                    13888 26 01575 16949
      TF   EXMU09+11,FIRCOS                    13900 26 02079 16944
      TF   SFSM00+11,FIRCOS                    13912 26 02835 16944
      TF   SFSM06+11,FIRSIN                    13924 26 03075 16949
      TF   LSCF01+11,FIRCOS                    13936 26 04335 16944
      TF   COOR09+11,FIRSIN                    13948 26 04683 16949
      TF   COOR10+11,FIRCOS                    13960 26 04851 16944
      TF   EXMU01+11,COORLT                    13972 26 02091 16954
      MM   10005,12,9                          13984 13 10005 000Ī2
      AM   99,10020,7                          13996 11 00099 Ī0020
      TF   EXMU02+11,99                        14008 26 02103 00099
      TFM  RECDLT,432,7                        14020 16 16959 Ī0432
      MM   10011,4,10                          14032 13 10011 0000Ī
      A    RECDLT,99                           14044 21 16959 00099
      TF   SFSM08+6,RECDLT                     14056 26 03294 16959
* CHECK SIZE OF COMPUTATION*
      TF   FIRLSM,FIRCOS                       14068 26 16964 16944
      MM   10005,10,10                         14080 13 10005 000Ī0
      TF   MOMENT,99                           14092 26 16969 00099
      M    MOMENT,509                          14104 23 16969 00509
      SF   95                                  14116 32 00095 00000
      A    FIRLSM,9                            112   21 16964 00099
      SM   FIRLSM,5,10                         14140 12 16964 0000Ī
      CM   FIRLSM,20000,7                      14152 14 16964 Ī0000
      BNP  INIT05                              14164 47 14212 01100
      RCTY                                     14176 34 00000 00102
      WATY MESS04                              14188 39 17161 00100
      H                                        14200 48 00000 00000
INIT05 BC1 INIT06                              14212 46 15964 00100
* FOR L.S. SUM MAKER ONLY*
      RCTY                                     14224 34 00000 00102
      WATY MESS05                              14236 39 17221 00100
      TBTY                                     14248 34 00000 00108
      RNTY SUMLEN-1                            14260 36 16992 00100
      SF   SUMLEN-1                            14272 32 16992 00000
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        TF    SUMLET,SUMLEN                                 14284 26 17002 16993
        TDM   SUMLEN-1,1,11                                 14296 15 16992 00001
        CM    SUMLEN,19,10                                  14308 14 16993 00019
        BNE   INIT07                                        14320 47 14344 01200
        AM    SUMLEN,1,10                                   14332 11 16993 00001
INIT07  B     INIT09                                        14344 49 14452 00000
INIT10  CF    CHSCND                                        14356 33 16974 00000
        RCTY                                                14368 34 00000 00102
        WATY  MESS08                                        14380 39 17277 00100
        WNTY  CHSCND-4                                      14392 38 16970 00100
        SPTY                                                14404 34 00000 00101
        WATY  MESS09                                        14416 39 17299 00100
        H                                                   14428 48 00000 00000
        B     INIT11                                        14440 49 14608 00000
* CHECK IF THE PRESENT PROGRAM CAN HANDLE THE CALCULATION*
INIT09  MM    10013,11,10                                   14452 13 10013 00011
        TF    MOMENT,99                                     14464 26 16969 00099
        MM    10007,25,10                                   14476 13 10007 00025
        A     MOMENT,99                                     14488 21 16969 00099
        M     MOMENT,SUMLET                                 14500 23 16969 17002
        SF    95                                            14512 32 00095 00000
        TFM   CHSCND,19999,7                                14524 16 16974 19999
        S     CHSCND,FIRLSM                                 14536 22 16974 16964
        S     CHSCND,99                                     14548 22 16974 00099
        BNN   INIT11                                        14560 46 14608 01300
        RCTY                                                14572 34 00000 00102
        WATY  MESS10                                        14584 39 17313 00100
        B     INIT10                                        14596 49 14356 00000
* INITIALIZATION OF L.S. SUM MAKER*
INIT11  TF    FIRLST,FIRLSM                                 14608 26 17000 16964
        A     FIRLST,SUMLET                                 14620 21 17000 17002
        TF    START1+11,MOMENT                              14632 26 00871 16969
        TF    CHSM52+11,MOMENT                              14644 26 05467 16969
        TF    CHSM53+11,FIRLST                              14656 26 05479 17000
        TF    CHSM54+11,SUMLET                              14668 26 05515 17002
        S     CHSM51+6,SUMLET                               14680 22 05498 17002
        AM    CHSM51+6,1,10                                 14692 11 05498 00001
        TF    START2+11,FIRLST                              14704 26 00883 17000
        TF    START4+11,SUMLET                              14716 26 00907 17002
        TFM   CHSCND,ZEROCL-14                              14728 16 16974 05819
        A     CHSCND,SUMLET                                 14740 21 16974 17002
        TF    START3+11,CHSCND                              14752 26 00895 16974
        TF    COOROO+11,FIRLST                              14764 26 04647 17000
        TF    LSSM17+11,SUMLET                              14776 26 06723 17002
        TF    LSSM18+11,SUMLET                              14788 26 06927 17002
        MM    SUMLET,2,10                                   14800 13 17002 00002
        SM    99,1,10                                       14812 12 00099 00001
        TF    CHSM11+11,99                                  14824 26 05271 00099
        SM    99,1,10                                       14836 12 00099 00001
        TF    CHSM01+11,99                                  14848 26 05351 00099
        TF    CHSM03+11,SUMLET                              14860 26 05399 17002
        TF    CHSM13+11,SUMLET                              14872 26 05295 17002
        TF    99,FIRLSM                                     14884 26 00099 16964
        S     99,SUMLET                                     14896 22 00099 17002
        AM    99,1,10                                       14908 11 00099 00001
        TF    CHSM14+11,99                                  14920 26 05307 00099
        AM    99,1,10                                       14932 11 00099 00001
        TF    CHSM04+11,99                                  14944 26 05411 00099
        RCTY                                                14956 34 00000 00102
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        WATY MESS11                          14968 39 17371 00100
        RCTY                                 14980 34 00000 00102
        WATY MESS12                          14992 39 17457 00100
        RCTY                                 15004 34 00000 00102
        WATY MESS13                          15016 39 17515 00100
        TBTY                                 15028 34 00000 00108
        RNTY CORMAT                          15040 36 17004 00100
        TFM  FLAGST,90,10                    15052 16 16995 00090
        A    FLAGST,CORMAT                   15064 21 16995 17004
        TF   COOR02+11,FLAGST                15076 26 04755 16995
        TF   COOR04+11,FLAGST                15088 26 04779 16995
        S    FLAGST,SUMLET                   15100 22 16995 17002
        AM   FLAGST,1,10                     15112 11 16995 00001
        TF   COOR03+11,FLAGST                15124 26 04767 16995
        AM   FLAGST,1,10                     15136 11 16995 00001
        TF   COOR01+11,FLAGST                15148 26 04743 16995
        RCTY                                 15160 34 00000 00102
        WATY MESS14                          15172 39 17559 00100
        TBTY                                 15184 34 00000 00108
        RNTY CORVEC                          15196 36 17006 00100
        TFM  FLAGST,92,10                    15208 16 16995 00092
        A    FLAGST,CORVEC                   15220 21 16995 17006
        TF   COOR06+11,FLAGST                15232 26 04803 16995
        TF   COOR08+11,FLAGST                15244 26 04827 16995
        S    FLAGST,SUMLET                   15256 22 16995 17002
        AM   FLAGST,1,10                     15268 11 16995 00001
        TF   COOR07+11,FLAGST                15280 26 04815 16995
        AM   FLAGST,1,10                     15292 11 16995 00001
        TF   COOR05+11,FLAGST                15304 26 04791 16995
        CM   10007,0,10                      15316 14 10007 00000
        BE   INIT17                          15328 46 15652 01200
        RCTY                                 15340 34 00000 00102
        WATY MESS15                          15352 39 17603 00100
        TBTY                                 15364 34 00000 00108
        RNTY ANIMAT                          15376 36 17008 00100
        TFM  FLAGST,90,10                    15388 16 16995 00090
        A    FLAGST,ANIMAT                   15400 21 16995 17008
        TF   COOR12+11,FLAGST                15412 26 04971 16995
        TF   COOR14+11,FLAGST                15424 26 04995 16995
        S    FLAGST,SUMLET                   15436 22 16995 17002
        AM   FLAGST,1,10                     15448 11 16995 00001
        TF   COOR13+11,FLAGST                15460 26 04983 16995
        AM   FLAGST,1,10                     15472 11 16995 00001
        TF   COOR11+11,FLAGST                15484 26 04959 16995
        RCTY                                 15496 34 00000 00102
        WATY MESS16                          15508 39 17647 00100
        TBTY                                 15520 34 00000 00108
        RNTY ANIVEC                          15532 36 17010 00100
        TFM  FLAGST,92,10                    15544 16 16995 00092
        A    FLAGST,ANIVEC                   15556 21 16995 17010
        TF   COOR16+11,FLAGST                15568 26 05019 16995
        TF   COOR18+11,FLAGST                15580 26 05043 16995
        S    FLAGST,SUMLET                   15592 22 16995 17002
        AM   FLAGST,1,10                     15604 11 16995 00001
        TF   COOR17+11,FLAGST                15616 26 05031 16995
        AM   FLAGST,1,10                     15628 11 16995 00001
        TF   COOR15+11,FLAGST                15640 26 05007 16995
INIT17  RCTY                                 15652 34 00000 00102
        WATY MESS17                          15664 39 17691 00100
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       TBTY                                         15676 34 00000 00108
       RNTY ISOMAT                                  15688 36 17012 00100
       TFM  FLAGST,84,10                            15700 16 16995 00084
       A    FLAGST,ISOMAT                           15712 21 16995 17012
       TF   COOR22+11,FLAGST                        15724 26 05163 16995
       TF   COOR24+11,FLAGST                        15736 26 05187 16995
       S    FLAGST,SUMLET                           15748 22 16995 17002
       AM   FLAGST,1,10                             15760 11 16995 00001
       TF   COOR23+11,FLAGST                        15772 26 05175 16995
       AM   FLAGST,1,10                             15784 11 16995 00001
       TF   COOR21+11,FLAGST                        15796 26 05151 16995
       RCTY                                         15808 34 00000 00102
       WATY MESS18                                  15820 39 17731 00100
       TBTY                                         15832 34 00000 00108
       RNTY ISOVEC                                  15844 36 17014 00100
       TFM  FLAGST,89,10                            15856 16 16995 00089
       A    FLAGST,ISOVEC                           15868 21 16995 17014
       TF   COOR26+11,FLAGST                        15880 26 05211 16995
       TF   COOR28+11,FLAGST                        15892 26 05235 16995
       S    FLAGST,SUMLET                           15904 22 16995 17002
       AM   FLAGST,1,10                             15916 11 16995 00001
       TF   COOR27+11,FLAGST                        15928 26 05223 16995
       AM   FLAGST,1,10                             15940 11 16995 00001
       TF   COOR25+11,FLAGST                        15952 26 05199 16995
* POSSIBLE CHANGE OF LOGICAL ROUTINE*
INIT06 RCTY                                         15964 34 00000 00102
       TDM  LOGCHG,0                                15976 15 17016 00000
       WATY MESS19                                  15988 39 17771 00100
       SPTY                                         16000 34 00000 00101
       RNTY LOGCHG                                  16012 36 17016 00100
       BD   INIT12,LOGCHG                           16024 43 16048 17016
       B    INIT13                                  16036 49 16384 00000
INIT12 RCTY                                         16048 34 00000 00102
       WATY MESS20                                  16060 39 17841 00100
       TBTY                                         16072 34 00000 00108
       RNTY LOGFMN-3                                16084 36 09950 00100
       SF   LOGFMN-3                                16096 32 09950 00000
       RCTY                                         16108 34 00000 00102
       WATY MESS21                                  16120 39 17893 00100
       TBTY                                         16132 34 00000 00108
       RNTY LOGAAA-7                                16144 36 09961 00100
       SF   LOGAAA-7                                16156 32 09961 00000
       SF   LOGAAA-5                                16168 32 09963 00000
       SF   LOGAAA-3                                16180 32 09965 00000
       SF   LOGAAA-1                                16192 32 09967 00000
       RCTY                                         16204 34 00000 00102
       WATY MESS30                                  16216 39 18463 00100
       TBTY                                         16228 34 00000 00108
       RNTY LOGMPL-2                                16240 36 09954 00100
       SF   LOGMPL-2                                16252 32 09954 00000
       RCTY                                         16264 34 00000 00102
       WATY MESS22                                  16276 39 17971 00100
       TBTY                                         16288 34 00000 00108
       RNTY LOGSIN-4                                16300 36 09977 00100
       SF   LOGSIN-4                                16312 32 09977 00000
       RCTY                                         16324 34 00000 00102
       WATY MESS23                                  16336 39 18059 00100
       TBTY                                         16348 34 00000 00108
       RNTY LOGDIF-3                                16360 36 09982 00100
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       SF   LOGDIF-3                             16372 32 09982 00000
INIT13 TFM  OUTP09+1,41,10                       16384 16 04053 00041
       TDM  OWNCHC,0                             16396 15 16924 00000
       RCTY                                      16408 34 00000 00102
       WATY MESS27                               16420 39 18351 00100
       WATY MESS28                               16432 39 18399 00100
       SPTY                                      16444 34 00000 00101
       RNTY OWNCHC                               16456 36 16924 00100
       BD   INIT20,OWNCHC                        16468 43 16492 16924
       B    INIT21                               16480 49 16504 00000
INIT20 TFM  OUTP09+1,49,10                       16492 16 04053 00049
INIT21 RCTY                                      16504 34 00000 00102
       WATY MESS24                               16516 39 18141 00100
       H                                         16528 48 00000 00000
INIT14 RCTY                                      16540 34 00000 00102
       WATY MESS25                               16552 39 18227 00100
* SEARCH ON DATA TAPE FOR REFLECTION TO BE CALCULATED FIRST*
       H                                         16564 48 00000 00000
       RCTY                                      16576 34 00000 00102
       WATY MESS26                               16588 39 18257 00100
       SPTY                                      16600 34 00000 00101
       RNTY FIRRFL-5                             16612 36 16976 00100
       SF   FIRRFL-5                             16624 32 16976 00000
       SF   FIRRFL-3                             16636 32 16978 00000
       SF   FIRRFL-1                             16648 32 16980 00000
       RNPT 19012                                16660 36 19012 00300
       RCTY                                      16672 34 00000 00102
       WNTY 18994                                16684 38 18994 00100
       WNPT 18994                                16696 38 18994 00200
INIT15 RNPT 19051                                16708 36 19051 00300
       C    19052,FIRRFL-4                       16720 24 19052 16977
       BNE  INIT15                               16732 47 16708 01200
       C    19054,FIRRFL-2                       16744 24 19054 16979
       BNE  INIT15                               16756 47 16708 01200
       C    19056,FIRRFL                         16768 24 19056 16981
       BNE  INIT15                               16780 47 16708 01200
       TR   409,19051                            16792 31 00409 19051
       WNPT 10000                                16804 38 10000 00200
       WNPT SUMLET-1                             16816 38 17001 00200
       RCTY                                      16828 34 00000 00102
       WATY MESS35                               16840 39 18823 00100
       RCTY                                      16852 34 00000 00102
       RCTY                                      16864 34 00000 00102
       TFM  START5+1,49,10                       16876 16 00933 00049
       BC1  INIT16                               16888 46 16912 00100
       B    START1                               16900 49 00860 00000
INIT16 B    START7                               16912 49 00956 00000
* SYMBOLS,CONSTANTS AND MESSAGES OF INITIALIZATION PROGRAM*
OWNCHC DC   1,0                                  16924 00001   0
PARCHK DC   1,0                                  16925 00001   0
SPACEG DS   3                                    16928 00003
IDENTP DC   6,013004,18999                       18999 00006   013004
SPACEL DS   7                                    16935 00007
PARALT DS   4                                    16939 00004
FIRCOS DS   5                                    16944 00005
FIRSIN DS   5                                    16949 00005
COORLT DS   5                                    16954 00005
RECOLT DS   5                                    16959 00005
FIRLSM DS   5                                    16964 00005
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MOMENT DS   5                                              16969 00005
CHSCND DS   5                                              16974 00005
       DC   1,@                                            16975 00001   ‡
FIRRFL DC   6,0                                            16981 00006   0̄00000
PROCFT DC   5,10000                                        16986 00005   1̄0000
PROCSD DC   5,10000                                        16991 00005   1̄0000
SUMLEN DS   2                                              16993 00002
FLAGST DS   2                                              16995 00002
FIRLST DS   5                                              17000 00005
SUMLET DC   2,0                                            17002 00002   0̄0
CORMAT DC   2,0                                            17004 00002   0̄0
CORVEC DC   2,0                                            17006 00002   0̄0
ANIMAT DC   2,0                                            17008 00002   0̄0
ANIVEC DC   2,0                                            17010 00002   0̄0
ISOMAT DC   2,0                                            17012 00002   0̄0
ISOVEC DC   2,0                                            17014 00002   0̄0
       DC   1,@                                            17015 00001   ‡
LOGCHG DC   1,0                                            17016 00001   0̄
MESS01 DAC  30,TYPE IN SPACEGROUP NUMBER (3)@                            17019 00030X2
E IN SPACEGROUP NUMBER (3)‡
MESS02 DAC  21,SET PROGRAM SWITCHES@             17079 00021X2 SET PROGRAM SWITCHES‡
MESS03 DAC  20,LOAD PARAMETER TAPE@              17121 00020X2 LOAD PARAMETER TAPE‡
MESS04 DAC  30,TOO MANY ATOMS.PLANNING ERROR@                            17161 00030X2
 MANY ATOMS.PLANNING ERROR‡
MESS05 DAC  28,TYPE LENGTH OF L.S.SUMS (2)@                              17221 00028X2
E LENGTH OF L.S.SUMS (2)‡
MESS08 DAC  11,EXCESS OF @                       17277 00011X2 EXCESS OF ‡
MESS09 DAC  7,DIGITS@                            17299 00007X2 DIGITS‡
MESS10 DAC  29,PLANNING ERROR.L.S.SUM MAKER@                             17313 00029X2
NING ERROR.L.S.SUM MAKER‡
MESS11 DAC  43,PREPARATION OF DECIMAL POINTS IN L.S.SUMS.@               17371 00043X2
PARATION OF DECIMAL POINTS IN L.S.SUMS.‡
MESS12 DAC  29,SEE WRITE UP FOR SUGGESTIONS@                             17457 00029X2
 WRITE UP FOR SUGGESTIONS‡
MESS13 DAC  22,MATRIX COORDINATES(1)@            17515 00022X2 MATRIX COORDINATES(1)
MESS14 DAC  22,VECTOR COORDINATES(1)@            17559 00022X2 VECTOR COORDINATES(1)
MESS15 DAC  22,MATRIX ANISOTROPIC(1)@            17603 00022X2 MATRIX ANISOTROPIC(1)
MESS16 DAC  22,VECTOR ANISOTROPIC(1)@            17647 00022X2 VECTOR ANISOTROPIC(1)
MESS17 DAC  20,MATRIX ISOTROPIC(1)@              17691 00020X2 MATRIX ISOTROPIC(1)‡
MESS18 DAC  20,VECTOR ISOTROPIC(1)@              17731 00020X2 VECTOR ISOTROPIC(1)‡
MESS19 DAC  35,TYPE A 1 TO CHANGE LOGICAL ROUTINE@                       17771 00035X2
E A 1 TO CHANGE LOGICAL ROUTINE‡
MESS20 DAC  26,TYPE IN F OBS. MINIMUM(4)@  17841 00026X2 TYPE IN F OBS. MINIMU
4)‡
MESS21 DAC  39,TYPE IN PROPORTIONALITY CONSTANTS(4*2)@                   17893 00039X2
E IN PROPORTIONALITY CONSTANTS(4*2)‡
MESS22 DAC  44,TYPE IN MINIMAL SINSQ THETA OVER LAMDASQ(5)@              17971 00044X2
E IN MINIMAL SINSQ THETA OVER LAMDASQ(5)‡
MESS23 DAC  41,TYPE IN LIMIT OF F OBS. MINUS F CALC.(4)@                 18059 00041X2
E IN LIMIT OF F OBS. MINUS F CALC.(4)‡
MESS24 DAC  43,CHANGES CAN BE MADE NOW.AFTERWARDS 4919980@               18141 00043X2
NGES CAN BE MADE NOW.AFTERWARDS 4919980‡
MESS25 DAC  15,LOAD DATA TAPE@                   18227 00015X2 LOAD DATA TAPE‡
MESS26 DAC  47,TYPE IN FIRST REFLECTION TO BE CALCULATED(3*2)@  18257 00047X2
 IN FIRST REFLECTION TO BE CALCULATED(3*2)‡
MESS27 DAC  24,TYPE A 1 TO MAKE CHOICE@    18351 00024X2 TYPE A 1 TO MAKE CHOI
‡
```

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MESS28 DAC  32, FOR EACH REFLECTION SEPARATELY@                 18399 00032X2  F
R EACH REFLECTION SEPARATELY$
MESS30 DAC  29,TYPE IN MULTIPLY CONSTANT(3)@                    18463 00029X2 TY
E IN MULTIPLY CONSTANT(3)$
MESS31 DAC  41,TYPE A 1 WHEN PARAMETERS ARE TO BE TYPED@        18521 00041X2 TY
E A 1 WHEN PARAMETERS ARE TO BE TYPED$
MESS32 DAC  24,TYPE PARAMETER IDENT(6)@    18603 00024X2 TYPE PARAMETER IDENT(6
$
MESS33 DAC  20,TYPE ALL PARAMETERS@        18651 00020X2 TYPE ALL PARAMETERS$
MESS34 DAC  34,ERROR IN LENGTH OF PARAMETER TAPE@               18691 00034X2 ER
OR IN LENGTH OF PARAMETER TAPE$
MESS29 DAC  32,LOAD ADDITIONAL SPACEGROUP TAPE@                 18759 00032X2 LO
D ADDITIONAL SPACEGROUP TAPE$
MESS35 DAC  25,AND THEY ALL WENT TO THE@   18823 00025X2 AND THEY ALL WENT TO TH
$
       DORG 19980                          19980
       B    INIT14                         19980 49 16540 00000
       DEND 13000                          13000
END OF PASSII
```

THE SPACE GROUP TAPE WHICH IS AT THE END OF THE PROGRAM TAPE

```
016001≠00100101010101000000000000000000000000000000000000000000≠
016002≠10100201010101000000000000000000000000000000000000000000≠
016003≠00200101010101010100000000000000000000000000000000000000≠
016004≠00200101010101010100000000000000000000500000000000000000≠
016005≠00200201010101010100000000000000000000000000000000000000≠
016006≠00200101010101010100000000000000000000000000000000000000≠
016007≠00200101010101010100000000000000000000050000000000000000≠
016008≠00200201010101010100000000000000000000000000000000000000≠
016009≠00200201010101010100000000000000000000050000000000000000≠
016010≠10200201010101010100000000000000000000030000000000000000≠
016011≠10200201010101010100000000000000000000500000000000000000≠
016012≠10200401010101010100000000000000000000000000000000000000≠
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016038≠00400201010101010101010101010101000000000000000000000000≠
016039≠00400201010101010101010101010101000000000000005000005000≠
016040≠00400201010101010101010101010101000000000000005000005000≠
```

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016041≠00400201010101010101010101010101000000000000505000505000≠
016042≠00400401010101010101010101010101000000000000000000000000≠
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016045≠00400201010101010101010101010101000000000000000050000050≠
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```
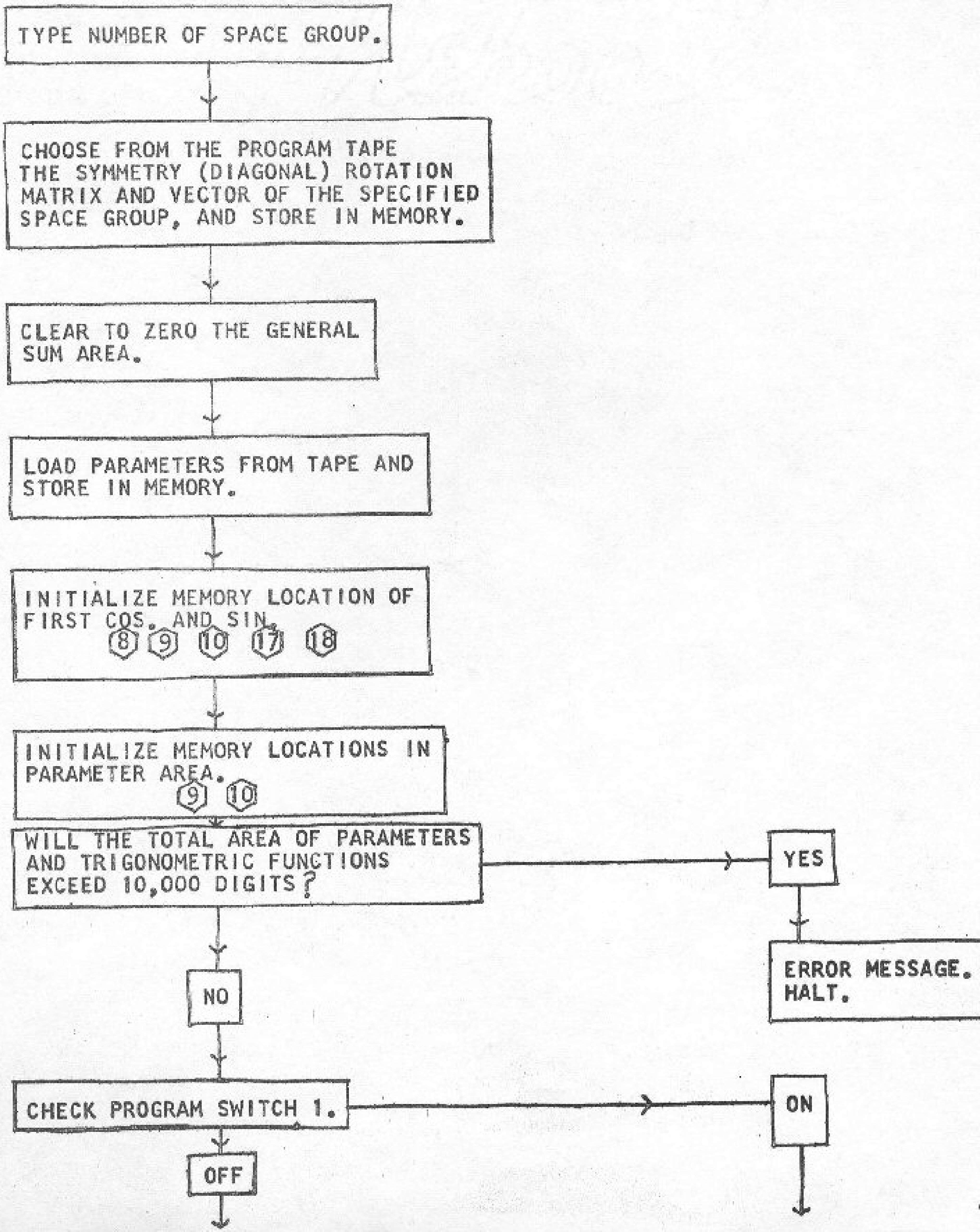
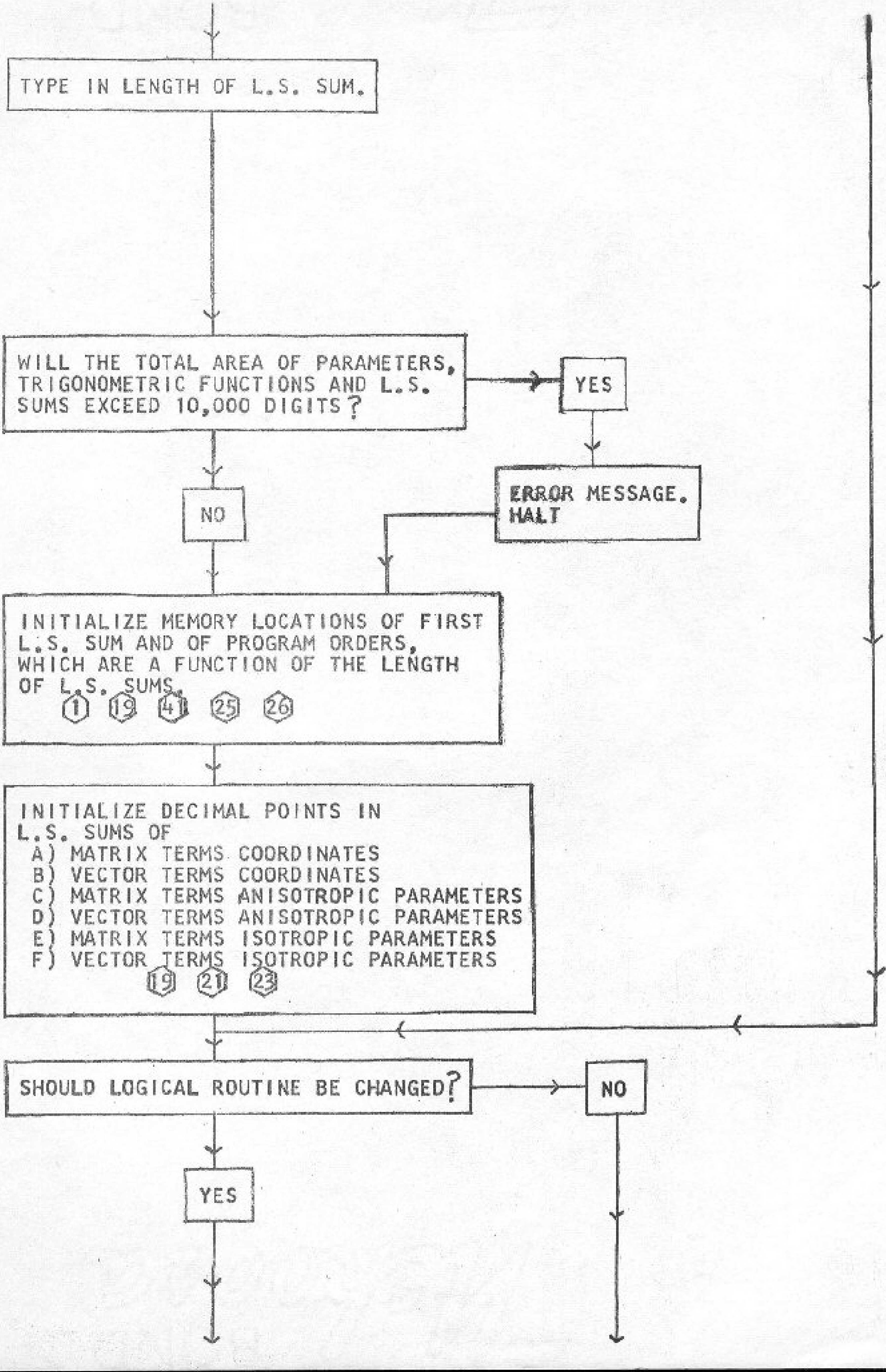
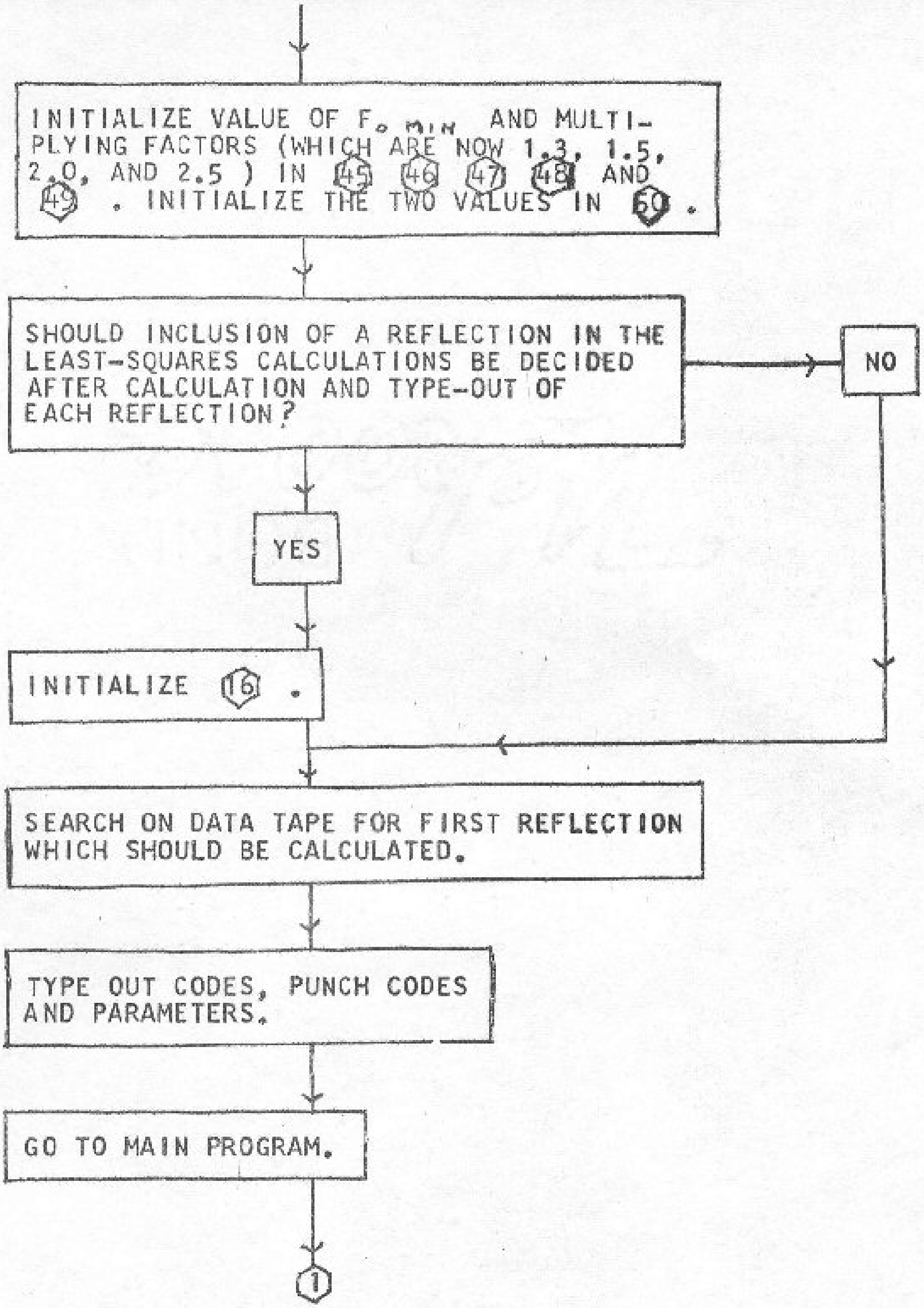

* SECTION VII *

INITIALIZATION PROGRAM

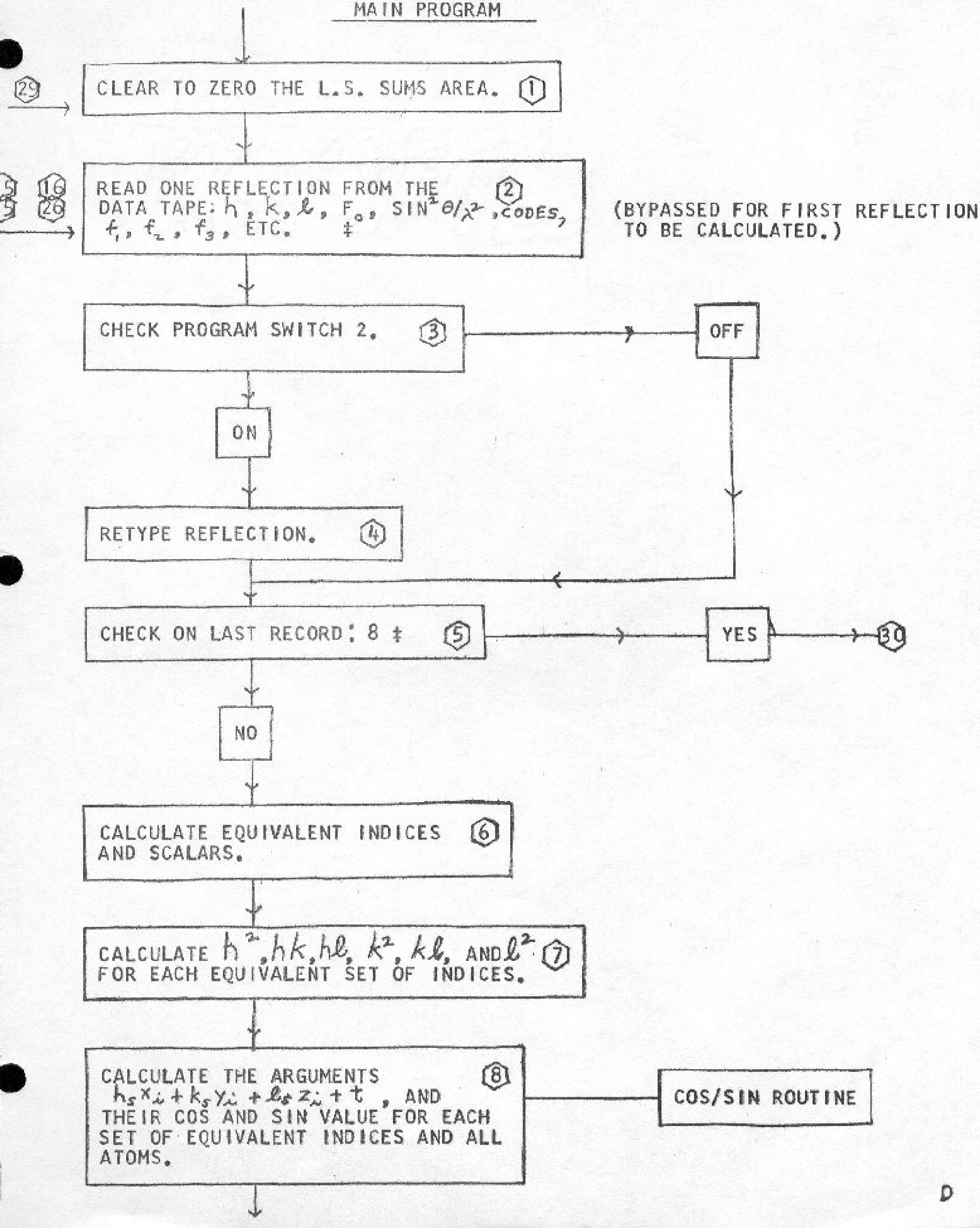




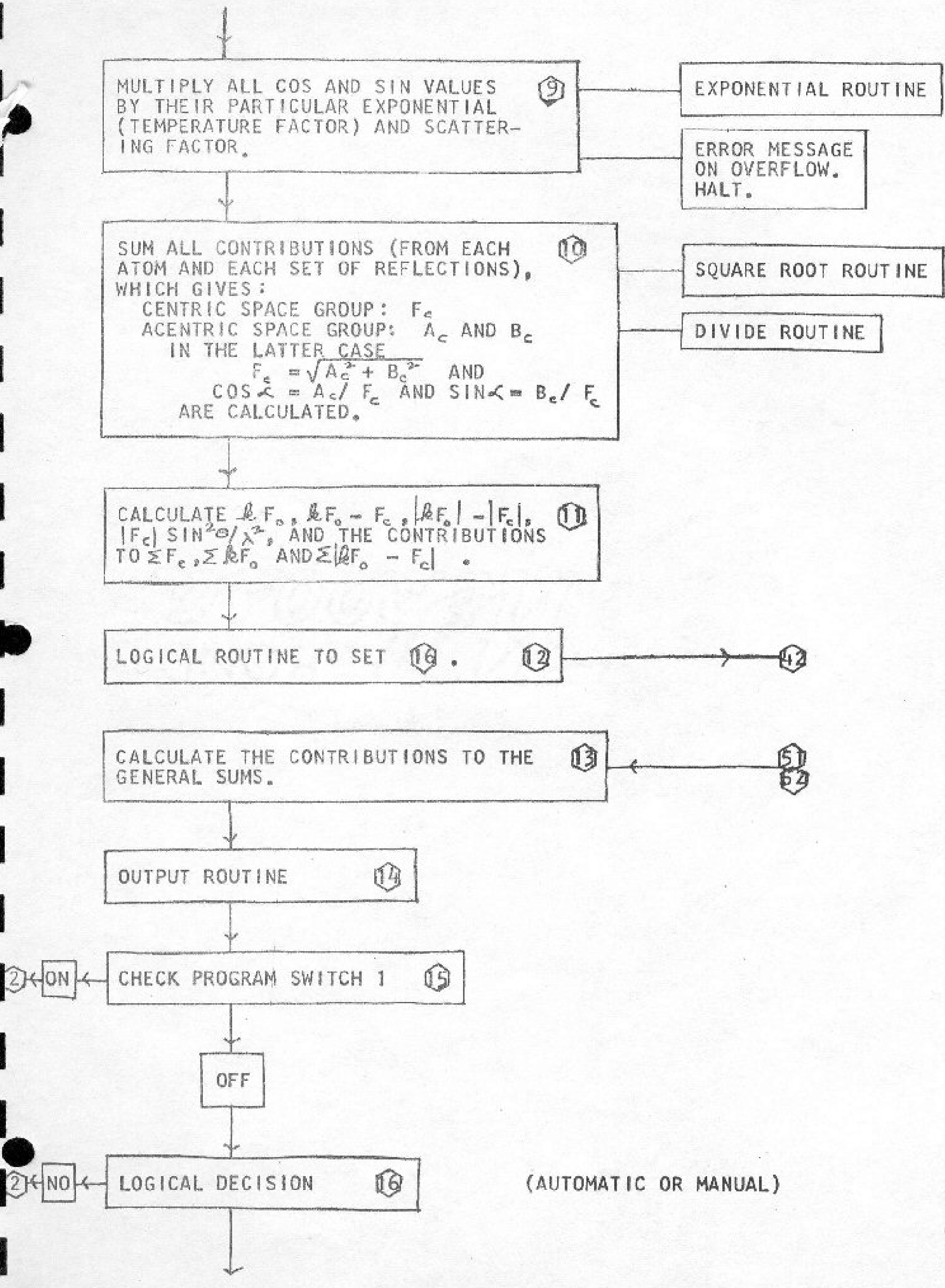
TYPE IN LENGTH OF L.S. SUM.
WILL THE TOTAL AREA OF PARAMETERS, TRIGONOMETRIC FUNCTIONS AND L.S. SUMS EXCEED 10,000 DIGITS?
YES
ERROR MESSAGE. HALT
NO
INITIALIZE MEMORY LOCATIONS OF FIRST L.S. SUM AND OF PROGRAM ORDERS, WHICH ARE A FUNCTION OF THE LENGTH OF L.S. SUMS.
1 19 41 25 26
INITIALIZE DECIMAL POINTS IN L.S. SUMS OF
A) MATRIX TERMS COORDINATES
B) VECTOR TERMS COORDINATES
C) MATRIX TERMS ANISOTROPIC PARAMETERS
D) VECTOR TERMS ANISOTROPIC PARAMETERS
E) MATRIX TERMS ISOTROPIC PARAMETERS
F) VECTOR TERMS ISOTROPIC PARAMETERS
19 21 23
SHOULD LOGICAL ROUTINE BE CHANGED?
NO
YES


INITIALIZE VALUE OF $F_{o\,min}$ AND MULTIPLYING FACTORS (WHICH ARE NOW 1.3, 1.5, 2.0, AND 2.5) IN 45 46 47 48 AND 49 . INITIALIZE THE TWO VALUES IN 50 .
SHOULD INCLUSION OF A REFLECTION IN THE LEAST-SQUARES CALCULATIONS BE DECIDED AFTER CALCULATION AND TYPE-OUT OF EACH REFLECTION?
NO
YES
INITIALIZE 16 .
SEARCH ON DATA TAPE FOR FIRST REFLECTION WHICH SHOULD BE CALCULATED.
TYPE OUT CODES, PUNCH CODES AND PARAMETERS.
GO TO MAIN PROGRAM.
1

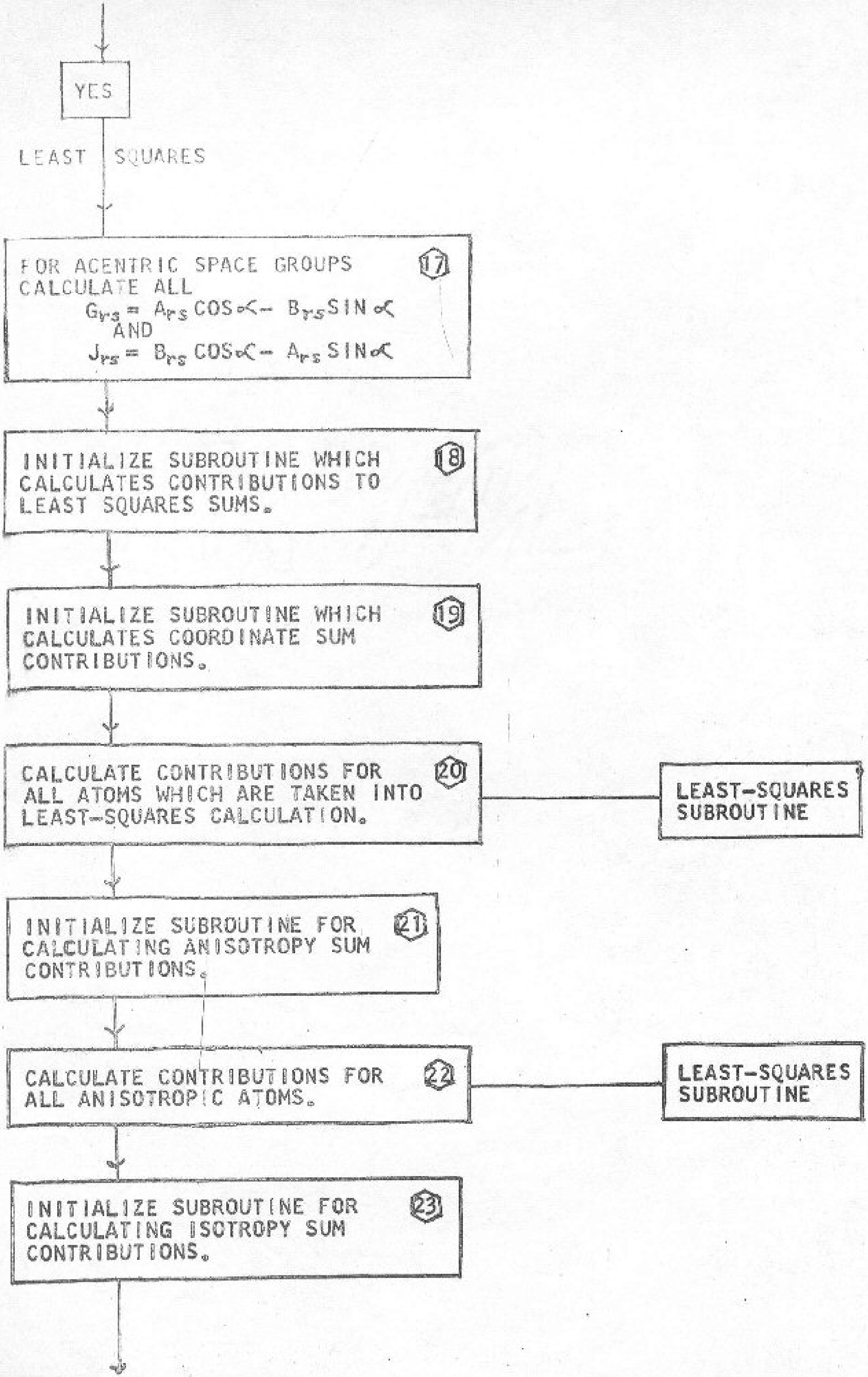
MAIN PROGRAM



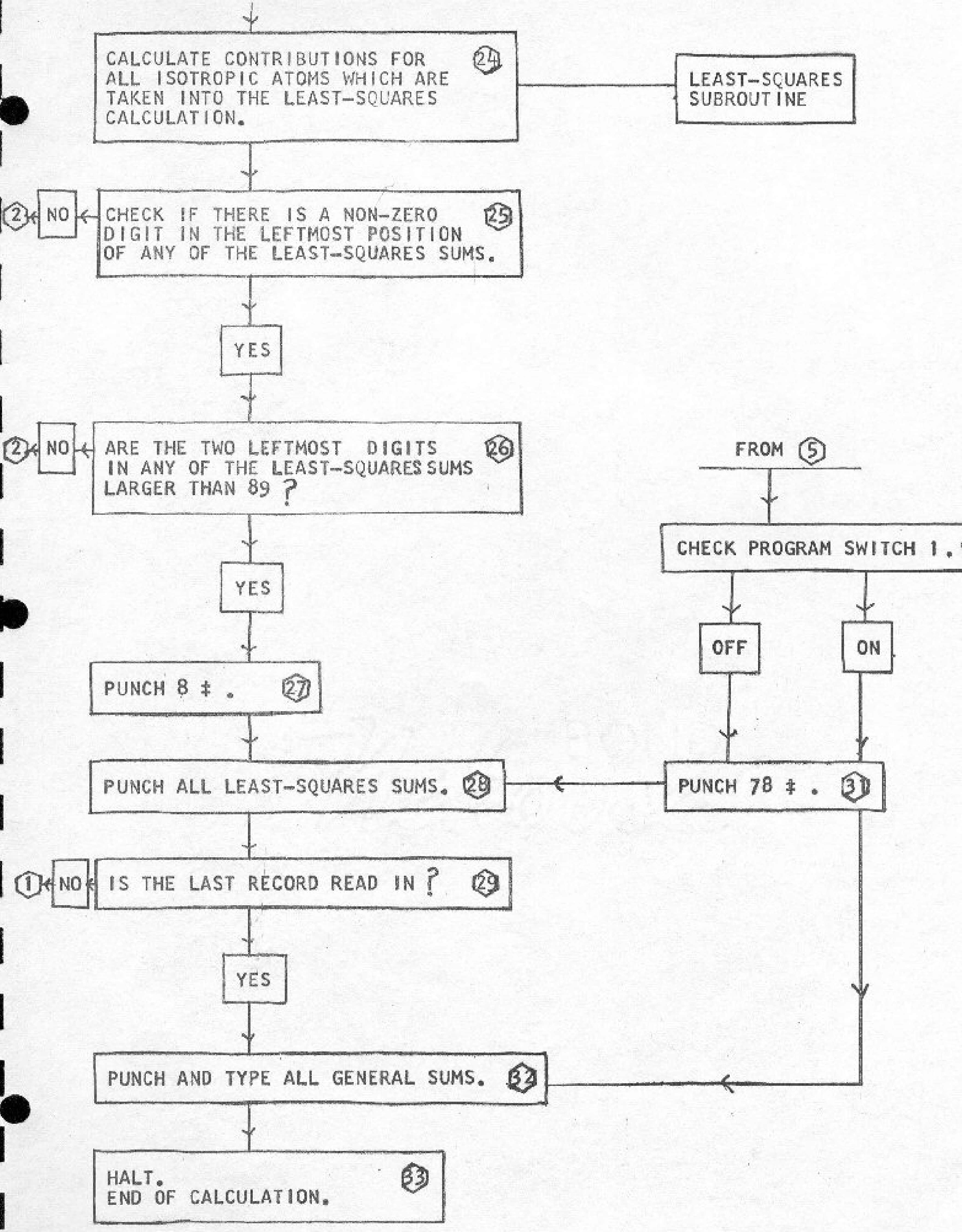
D


MULTIPLY ALL COS AND SIN VALUES BY THEIR PARTICULAR EXPONENTIAL (TEMPERATURE FACTOR) AND SCATTERING FACTOR.
9
EXPONENTIAL ROUTINE
ERROR MESSAGE ON OVERFLOW. HALT.
SUM ALL CONTRIBUTIONS (FROM EACH ATOM AND EACH SET OF REFLECTIONS), WHICH GIVES:
CENTRIC SPACE GROUP: F_c
ACENTRIC SPACE GROUP: A_c AND B_c
IN THE LATTER CASE
$F_c = \sqrt{A_c^2 + B_c^2}$ AND
$\cos\alpha = A_c / F_c$ AND $\sin\alpha = B_c / F_c$
ARE CALCULATED.
10
SQUARE ROOT ROUTINE
DIVIDE ROUTINE
CALCULATE kF_o, $kF_o - F_c$, $|kF_o| - |F_c|$, $|F_c| \sin^2\theta/\lambda^2$, AND THE CONTRIBUTIONS TO ΣF_c, ΣkF_o AND $\Sigma |kF_o - F_c|$.
11
LOGICAL ROUTINE TO SET 16.
12
42
CALCULATE THE CONTRIBUTIONS TO THE GENERAL SUMS.
13
51
62
OUTPUT ROUTINE
14
2
ON
CHECK PROGRAM SWITCH 1
15
OFF
2
NO
LOGICAL DECISION
16
(AUTOMATIC OR MANUAL)

E

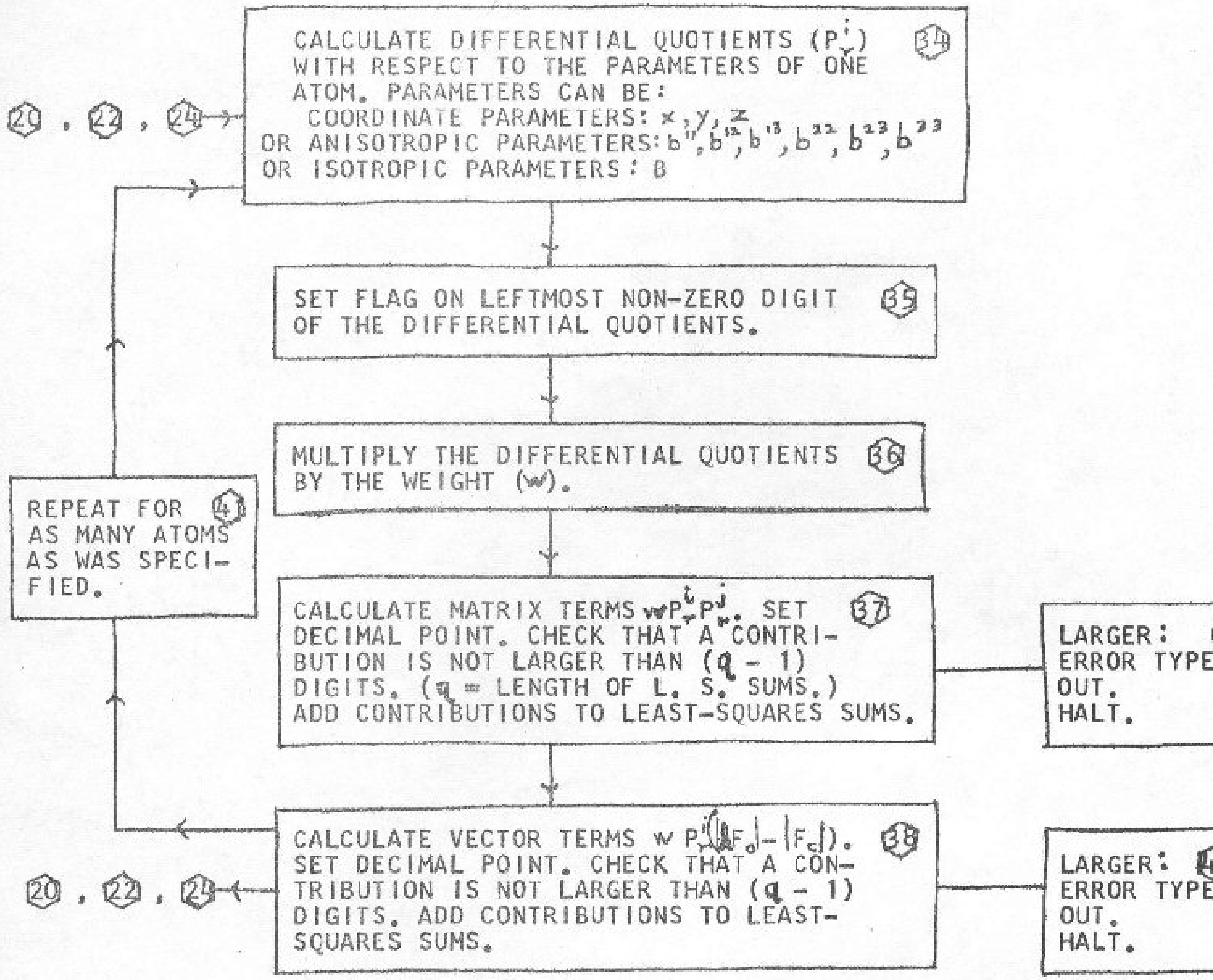

YES
LEAST SQUARES
FOR ACENTRIC SPACE GROUPS CALCULATE ALL
$G_{rs} = A_{rs} \cos\alpha - B_{rs} \sin\alpha$
AND
$J_{rs} = B_{rs} \cos\alpha - A_{rs} \sin\alpha$
17
INITIALIZE SUBROUTINE WHICH CALCULATES CONTRIBUTIONS TO LEAST SQUARES SUMS.
18
INITIALIZE SUBROUTINE WHICH CALCULATES COORDINATE SUM CONTRIBUTIONS.
19
CALCULATE CONTRIBUTIONS FOR ALL ATOMS WHICH ARE TAKEN INTO LEAST-SQUARES CALCULATION.
20
LEAST-SQUARES SUBROUTINE
INITIALIZE SUBROUTINE FOR CALCULATING ANISOTROPY SUM CONTRIBUTIONS.
21
CALCULATE CONTRIBUTIONS FOR ALL ANISOTROPIC ATOMS.
22
LEAST-SQUARES SUBROUTINE
INITIALIZE SUBROUTINE FOR CALCULATING ISOTROPY SUM CONTRIBUTIONS.
23

F

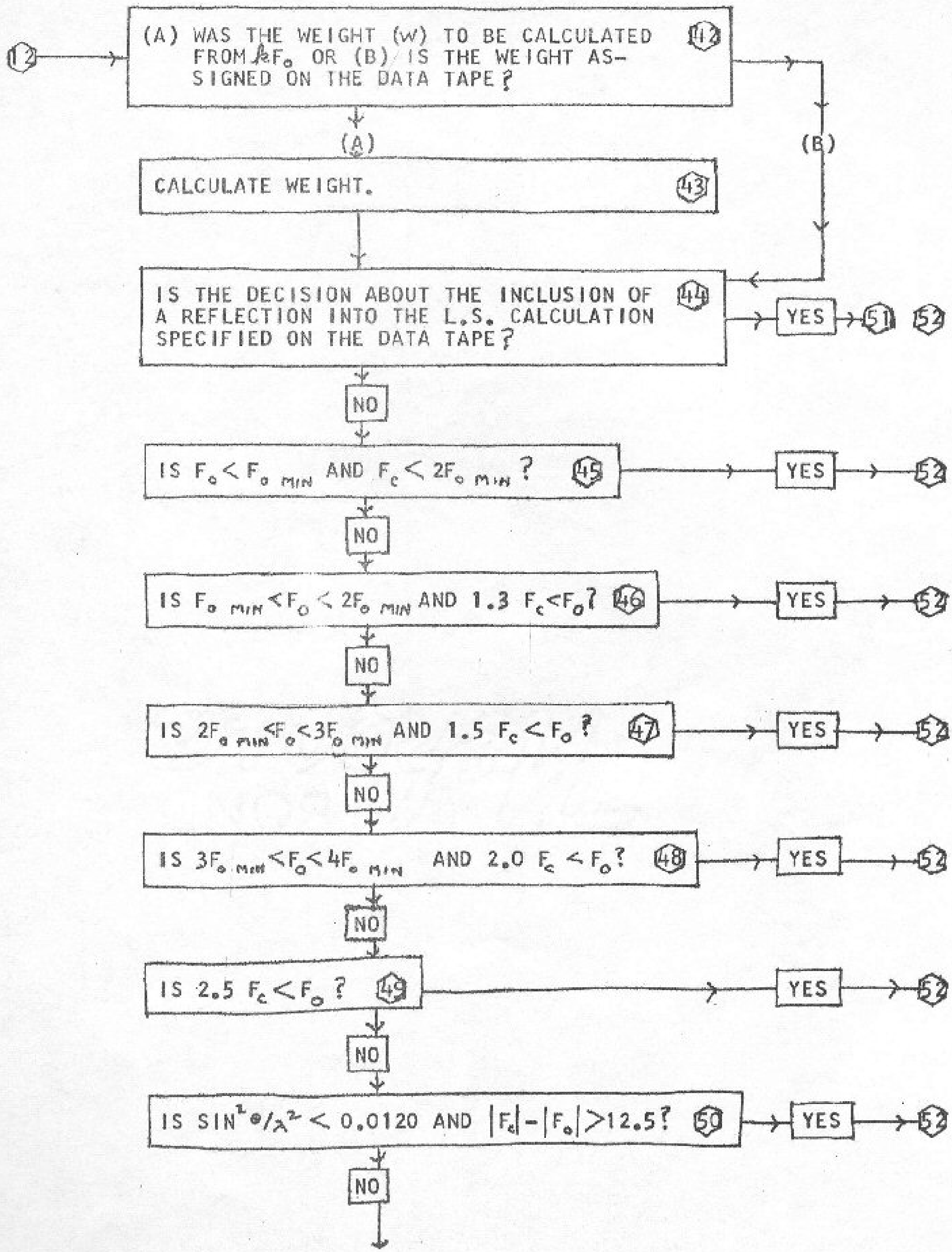

CALCULATE CONTRIBUTIONS FOR ALL ISOTROPIC ATOMS WHICH ARE TAKEN INTO THE LEAST-SQUARES CALCULATION. 24
LEAST-SQUARES SUBROUTINE
CHECK IF THERE IS A NON-ZERO DIGIT IN THE LEFTMOST POSITION OF ANY OF THE LEAST-SQUARES SUMS. 25
NO
2
YES
ARE THE TWO LEFTMOST DIGITS IN ANY OF THE LEAST-SQUARES SUMS LARGER THAN 89 ? 26
NO
2
YES
PUNCH 8 ‡ . 27
FROM 5
CHECK PROGRAM SWITCH 1.
OFF
ON
PUNCH ALL LEAST-SQUARES SUMS. 28
PUNCH 78 ‡ . 31
IS THE LAST RECORD READ IN ? 29
NO
1
YES
PUNCH AND TYPE ALL GENERAL SUMS. 32
HALT.
END OF CALCULATION. 33

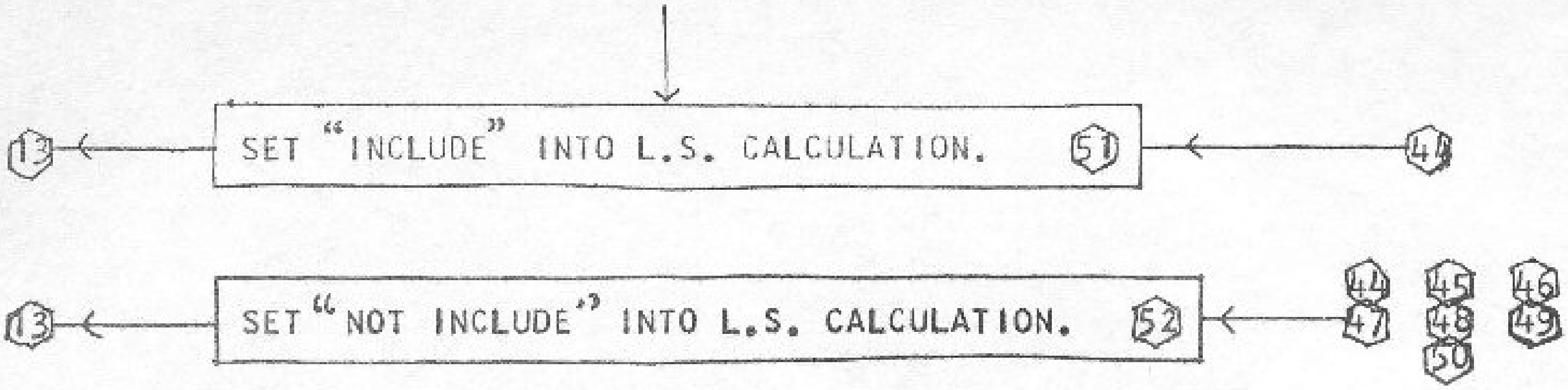
LEAST-SQUARES SUBROUTINE

A ROUTINE WHICH CALCULATES CONTRIBUTIONS TO LEAST-SQUARES SUMS



LOGICAL ROUTINE





SET "INCLUDE" INTO L.S. CALCULATION.
51
13
SET "NOT INCLUDE" INTO L.S. CALCULATION.
52
13
44
45
46
47
48
49
50

OUTPUT ROUTINE

P.S. 3 ON P.S. 4 ON	SHORT TYPE-OUT AND SHORT TAPE-OUT
P.S. 3 ON P.S. 4 OFF	LONG TYPE-OUT AND LONG TAPE-OUT
P.S. 3 OFF P.S. 4 ON	SHORT TAPE-OUT
P.S. 3 OFF P.S. 4 OFF	NO TYPE-OUT OR TAPE-OUT

FOR EXPLANATION OF THE WORDS "SHORT TYPE-OUT" AND "LONG TYPE-OUT" SEE SECTION ON FORMAT.

COSINE AND SINE ROUTINE

THIS ROUTINE COMBINES A TABLE LOOK-UP AND AN ARITHMETIC CALCULATION. THE PRINCIPLE IS:

$$\mathrm{COS}.abcd = \mathrm{COS}.ab\,\mathrm{COS}.00cd - \mathrm{SIN}.ab\,\mathrm{SIN}.00cd$$

AND

$$\mathrm{SIN}.abcd = \mathrm{SIN}.ab\,\mathrm{COS}.00cd + \mathrm{COS}.ab\,\mathrm{SIN}.00cd$$

THE VALUE .ab IS REDUCED TO THE FIRST QUADRANT (BETWEEN .00 AND .25) AND THE VALUES OF COS.ab AND SIN.ab ARE FOUND IN A TABLE OF 26 ENTRIES STORED IN MEMORY.

THE VALUE OF .00cd CAN BE REDUCED TO THE RANGE BETWEEN .0000 AND .0050. THE VALUES OF COS.00cd AND SIN.00cd ARE THEN CALCULATED BY MEANS OF

$$\mathrm{COS}.00cd = 1 - 19.74\,(.00cd)^2 \quad \text{AND} \quad \mathrm{SIN}.00cd = 6.2825\,(.00cd)\ .$$

THE ANSWERS OF COS.abcd AND SIN.abcd ARE CORRECT TO 1 IN THE FIFTH DECIMAL DIGIT.

EXPONENTIAL ROUTINE

THIS ROUTINE IS ALSO A COMBINATION OF A TABLE LOOK-UP AND AN ARITHMETIC CALCULATION. THE PRINCIPLE IS;

$$\mathrm{EXP} - a.bcde = (\mathrm{EXP} - a)\ \mathrm{EXP}\,(-0.b)\ \mathrm{EXP}\,(-0.0cde)$$

(EXP −a) AND (EXP −0.b) ARE LOOKED UP IN 10 ENTRY TABLES STORED IN MEMORY.

THE VALUE OF EXP (−0.0cde) IS CALCULATED ARITHMETICALLY:

$$1 - 0.0cde + 1/2\,(0.0cde)^2 - 1/6\,(0.0cde)^3\ .$$

THE ANSWER OF EXP (-a.bcde) IS ACCURATE TO 1 IN THE FIFTH DECIMAL DIGIT.

DIVIDE ROUTINE

THIS SUBROUTINE IS BASED ON THE SAME PRINCIPLE AS THE DIVIDE SUB-ROUTINE IN THE FORTRAN SYSTEM. (SEE I.B.M. 1620 TECHNICAL MEMO NO. 50, MAY 1, 1961.)

SQUARE ROOT ROUTINE

THIS ROUTINE IS TAKEN FROM A FRIDEN CALCULATOR MANUAL, 1959 . THE PROCEDURE IS BASED ON THE METHOD OF ODD NUMBERS.

L