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LOS ALAMOS SCIENTIFIC LABORATORY
LOS ALAMOS of the NEW MEXICO
University of California

An Integrated Series Of
Crystallographic Computer Programs
V. General Least Squares Refinement

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CONTRACT W-7405-ENG. 36

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Printed in USA. Price \$ 4.00. Available from the
Clearinghouse for Federal Scientific
and Technical Information,
National Bureau of Standards,
U. S. Department of Commerce,
Springfield, Virginia

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Report written: September 1964

Report distributed: May 17, 1965

An Integrated Series Of
Crystallographic Computer Programs
V. General Least Squares Refinement

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Abstract

The procedures employed and the computer program used for determining the positions and thermal motions (isotropic and/or anisotropic) of the atoms in a single crystal are described. The basic technique involves an iterative least-squares procedure. A special feature of this program is the inclusion of a secondary-extinction correction as a least-squares parameter. The current report is the fifth of a series encompassing the entire subject of single-crystal analysis.

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Introduction to the Series of Reports

The program described in this report is one of an integrated series of crystallographic computer programs. This series encompasses the entire subject of single-crystal structure analysis and includes programs for such items as:

- (1) crystal orientation for the collection of intensity data
- (2) processing of collected data to allow correction for Lorentz-polarization, absorption, background, and crystal-shape effects
- (3) comparison of processed data over equivalent reflections to ascertain the general validity of the data and to obtain a set of relative F^2 (F has the conventional structure factor meaning.)
- (4) a Fourier series analysis coupled with a plotting routine for obtaining Patterson vector maps and electron density maps of the Fourier and difference Fourier types
- (5) a least-squares procedure for determining the positions and thermal motions (isotropic and/or anisotropic) of the atoms in a single crystal
- (6) various subroutines (two per space group) for the least-squares procedure

(7) miscellaneous procedures employed during and after a structure analysis, e. g., calculation of interatomic distances and angles, of the orientation relationship of thermal ellipsoid axes to the crystallographic axes of the crystal, and of the polyhedral coordination of atoms; and the ordering of calculated and observed structure factors to prepare tables for publication.

Since each of the above items involves many repetitious procedures and calculations, it has been the authors' philosophy to employ computer techniques wherever possible and as early in the process of a structure determination as it is feasible to do so. Following this philosophy greatly reduces manual labor, minimizes clerical errors, and allows the maximum information to be obtained from the data.

Introduction to the Present Report

The basic end product of a crystal structure investigation is the determination of the positions of the atoms in the unit cell. Since experimental data cannot be taken at absolute zero, the thermal movement of the atoms is also of interest.

This report lists the FORTRAN II and FAP programs and describes the iterative least-squares procedure used to determine the positions and thermal motions (isotropic and/or anisotropic) of the atoms in the crystal structure.

The operating deck consists of a general program, GENLES, (with needed subroutines) and two subroutines, FUNCTN and CHANGE, specific for each space group. Once these subroutines have been written for a particular space group they may be used to refine any crystal structure (within certain limits to be described later) that occurs in that space group.

Later reports in this series will list the various FUNCTN and CHANGE subroutines as they become available for the 230 space groups. There is no plan for a systematic or comprehensive writing of these subroutines. It is anticipated that users of GENLES will make available the FUNCTN and CHANGE subroutines they write. In this manner a library of FUNCTN and CHANGE subroutines can be established.

GENLES reads control data from cards in the Monitor deck and basic experimental data, hkl and G from either cards in the Monitor deck or a separate magnetic tape. G may be equal to the structure factor, F , or the structure factor squared, F^2 . An input magnetic tape (LES-7) may have been prepared by our data processing program (LA-3043). An input magnetic tape (LES-5) may also have been prepared by GENLES during a previous run. A LES-5 tape is useful if it is necessary to interrupt the refinement and then start again. The LES-5 tape is thus an intermediate storage tape.

The results of a GENLES refinement are normally written on tape for off-line printing.

The program is normally run through the Monitor system. In addition to tape units A1, A2, A3, B2, and B4 (which are Monitor system tapes) the program requires the use of unit B1. The following is a description of the complete Monitor deck:

* I.D. (Monitor Identification Card)

* XEQ (Monitor Card)

Main Program Binary Cards for GENLES

Subroutine Binary Cards for GENLES

Subroutine Binary Cards for FUNCTN

Subroutine Binary Cards for CHANGE

} from a compilation of
FORTRAN II
and FAP
programs

* DATA (Monitor Card)

Control Cards, etc.

END OF JOB (Monitor Card)

If the user is able to obtain control of the console just prior to or during the time his program is being run by Monitor, then sense switches 1 and 6 are available to exercise some control over the input and output. Prior to the start of the run, depressing sense switch 1 allows the information on the data cards to be read into the computer at the card reader and causes the residual R to be printed on-line. Depressing sense switch 6 causes the value of the residual R, the change in the parameters, and the new parameters themselves to be printed on-line after each cycle.

Mathematical Equations

A general equation relating the observed structure factor F_o , and the calculated structure factor, F_c , for a reflection hkl can be written as

$$|F_o| = \frac{K|F_c|}{\left\{ 1 + g \left[\frac{2(1 + \cos^4 2\theta)}{(1 + \cos^2 2\theta)^2} \right] L_p |F_c|^2 \right\}^{1/2}} \quad (1)$$

where K = scale factor

g = secondary-extinction parameter*

L_p = Lorentz-polarization factor

2θ = diffraction angle for reflection hkl

hkl = Miller indices

The relation between F_c and atoms in the crystal structure is given by

$$F_c = \sum (f_j + \Delta f'_j) T_j \cos \phi_j + i \sum \Delta f''_j T_j \cos \phi_j + i \sum (f_j + \Delta f'_j) T_j \sin \phi_j + i^2 \sum \Delta f''_j T_j \sin \phi_j \quad (2)$$

where f_j = atomic scattering factor for j 'th atom

$\Delta f'_j$ = real portion of anomalous dispersion correction

$\Delta f''_j$ = imaginary portion of anomalous dispersion correction

* Zachariasen, W. H. (1963). Acta Cryst. 16, 1139.

$T_j = \exp(-B_j \sin^2 \theta / \lambda^2)$ for isotropic thermal parameters, and
 $= \exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl)]$ for
 anisotropic thermal parameters

$\phi_j = 2\pi(hx_j + ky_j + lz_j)$, and x_j, y_j, z_j are positional parameters
 for the j 'th atom.

For use in Eq. (1) $|F_c|$ is obtained from Eq. (2) by

$$|F_c| = \left\{ \left[\sum (f_j + \Delta f'_j) T_j \cos \phi_j - \sum \Delta f''_j T_j \sin \phi_j \right]^2 + \left[\sum \Delta f''_j T_j \cos \phi_j + \sum (f_j + \Delta f'_j) T_j \sin \phi_j \right]^2 \right\}^{1/2} \quad (3)$$

Several simplifications of Eqs. (2) and (3) may be accomplished in
 actual applications. For example, if anomalous dispersion is not a
 factor in the crystal structure analysis under consideration, then for
 noncentrosymmetric structures

$$|F_c| = \left\{ \left[\sum f_j T_j \cos \phi_j \right]^2 + \left[\sum f_j T_j \sin \phi_j \right]^2 \right\}^{1/2} \quad (4)$$

and for centrosymmetric structures

$$|F_c| = \left| \sum f_j T_j \cos \phi_j \right| \quad (5)$$

However, if anomalous dispersion is a factor in the crystal
 structure analysis, then for noncentrosymmetric structures

$$|F_c| = \text{Eq. (3)} \quad (6)$$

and for centrosymmetric structures

$$|F_c| = \left\{ \left[\sum (f_j + \Delta f_j') T_j \cos \phi_j \right]^2 + \left[\sum \Delta f_j'' T_j \cos \phi_j \right]^2 \right\}^{1/2} \quad (7)$$

In our illustrative example of the use of this program we choose, for the sake of brevity, to show the application of Eq. (5).

Glossary of Program Terms

Common Storage:

A	Real space unit cell <u>a</u> axis
ASTAR	$\frac{1}{2} \left(\frac{1}{d_{100}} \right)$
B11(35), B22(35), B33(35), B12(35), B13(35), B23(35)	Anisotropic thermal parameters
B1	Real space unit cell <u>b</u> axis
B(70)	Isotropic thermal parameter
BAC/SC	$b^* a^* \cos \gamma^* / 4$
BCC/SA	$b^* c^* \cos \alpha^* / 4$
BIJ(6)	Storage field used for storage of Hollerith output
BSTAR	$\frac{1}{2} \left(\frac{1}{d_{010}} \right)$
C	Real space unit cell <u>c</u> axis
CAC/SB	$c^* a^* \cos \beta^* / 4$
CMAT	Storage field for the coefficient matrix
C/SA	$\cos \alpha$

C O SASR	$\cos \alpha^*$
C O SB	$\cos \beta$
C O SBSR	$\cos \beta^*$
C O SC	$\cos \gamma$
C O SCSR	$\cos \gamma^*$
CSTAR	$\frac{1}{2} \left(\frac{1}{d_{001}} \right)$
DELB11, DELB22, DELB33, DELB12, DELB13, DELB23	Change in the anisotropic thermal parameters
DELB	Change in the isotropic thermal parameter
DELSA	Change in the scale factor
DELX, DELY, DELZ	Change in the positional parameters
DELF	$\Delta F = kF_o - F_c$
DEVB11, DEVB22, DEVB33, DEVB12, DEVB13, DEVB23	Standard deviation of the anisotropic thermal parameters
DEVB	Standard deviation of the isotropic thermal parameter
DEVSCA	Standard deviation of the scale factor
DEVX, DEVY, DEVZ	Standard deviation of the positional parameters
FA	Real portion of F_c
FB	Imaginary portion of F_c
FCALC	Calculated structure factor, for noncentric crystals is equal to $(FA^2 + FB^2)^{\frac{1}{2}}$; for centric crystals is equal to FA.
F O B	Observed value of the structure factor

F ϕ BS	(F ϕ B) ²
F(6)	Storage for six f _i for each reflection hkl
G	Secondary-extinction correction
H1, H2, H3	Miller indices, hkl, used in input
I1, I2, I3	H1, H2, H3, used in output
I4	F ϕ B, used in output
I5	FCALC, used in output
I6	DELF, used in output
I7	FA, used in output
I8	FB, used in output
I9	ALPHA, where tan (ALPHA) = FA/FB
I10	Number of items to be written in output, six (I1 to I6) for centric crystals, nine (I1 to I9) for noncentric crystals
I	General indexing variable
IDB11, IDB22, IDB33, IDB12, IDB13, IDB23, IDB, IDX, IDY, IDZ, IDSC	Row and column index used to identify the specific variable in the correlation matrix
IPCERK	Number of words in memory between top of program storage and bottom of common storage
IR	Number of words used in storing the coefficient matrix
J	Number of different types of atoms
J1(N)	N = 1 to 6; number of atoms of a specific type in the unit cell
J1(7) = J7	Control for location of input data

J1(8) = J8	A variable not used at present
J1(9) = J9	A variable not used at present
J1(10)= J10	A variable not used at present
J1(11)= J11	Control for type of form factor used
J1(12)= J12	Control for type of weighting scheme used
J13	A general indexing variable
J14	A general indexing variable
J15	Control for application of an extinction correction
K(20)	Count of number of reflections having the i'th scale factor
K2	Count of number of reflections included in the least-squares refinement
K3	Count of number of cycles run in the least-squares refinement
L	A general indexing variable
L1	Control for output of structure factor F
L2	Control for output of punched parameter cards
L3	Control for cycle refinement sequence
L4	Control for preparation of an editing tape
L5	A variable not used at present
L6	A variable not used at present
L7	Control for output of the correlation matrix
L8	Control for printed output of reflections for which F_c deviates from F_o by a specified amount
L9	Control for output of a prepared Fourier tape

L10 Control for relative scale on which output is printed
 L11 A variable not used at present
 L12 Control for start of a new job. New job uses same FUNCTN and CHANGE routines and hk_l data tape as old job
 L13 Specification for centric or noncentric output
 L14 Control for inclusion of unobserved reflections in least-squares refinement
 L15 Control for conversion of isotropic to anisotropic thermal parameters
 L16 Control for number of B_i's converted to B_{ij}'s
 L17 Control for use of physically impossible thermal parameters
 L18 Control for interruption of refinement to calculate structure factors only (no least squares are performed)
 L19 A variable not used at present
 L20 A variable not used at present
 M Number of scale factors
 M1 A general indexing variable
 N Number of parameters being varied
 N1 Scale factor index for reflection hk_l
 N2 Control character identification appropriate to the character of F
 N3 Total number of atoms in the asymmetric unit
 NAM(12) Identification of form factor field read off tape R1

NAME(12)	Identification name of the atom
NL1(70)	Number of space group position set in which the i'th atom is placed
NL2(70)	Control for use of anisotropic thermal parameters
NMAX	Largest number of variables that can be processed at any one time
PD(250)	Partial derivative storage field
PR Ø B	Identification of problem name read off tape B1
PR Ø BLM(12)	Identifying name for problem run
Q	Number of reflections minus number of variables, i.e., K2-N
R(250)	Temporary storage
SI	Sense switch 1 indicator
SA(10)	Storage field for sum of weights
SCALE(10)	Scale factors
SDELSQ(10)	Sum of $w(\Delta F)^2$ /scale factor
SINA	$\sin \alpha$
SINASR	$\sin \alpha^*$
SINB	$\sin \beta$
SINBSR	$\sin \beta^*$
SINC	$\sin \gamma$
SQ	$\sin^2 \theta / \lambda^2$
SRH Ø	Sum of $(\Delta F)^2$
SUMDEL	Sum of $ \Delta F $
SUMDSQ	Sum of $SDELSQ(I) * SCALE(I)$, $I = 1$ to M

SUMF OB (10)	Sum of F_o for the i'th scale factor
SUM OB S(10)	Sum of wF_o for the i'th scale factor
SWF	Sum of $w \Delta F $
W	Weight
XRAY	X-ray wavelength
X(I), Y(I), Z(I)	Positional parameters in fractions of the unit cell edges. $I = 35$ if any anisotropic thermal parameters are used, $I = 70$ if only isotropic thermal parameters are used.

Genles:

DELMAX	FL ATF (I8)/100.0
DET	Temporary storage location for B_i during conversion to B_{ij}
DF	Temporary storage for ΔF
DUM	Characterization of tape E1 with regard to identification information
F1	Temporary storage location used in preparing a Fourier input tape
FC	Temporary storage for FCALC
F o	Temporary storage for F o B corrected for extinction
FMAX	Largest value of F o B corrected for extinction
I11	Number of words per record for edit tape
I8TR	A variable in an assigned G o T o statement, i.e., a transfer vector
P	Lorentz-polarization factor multiplied by Zachariasen's correction, i.e.,

$$L_p \left[2 \left\{ \frac{1 + \cos^4 2\theta}{(1 + \cos^2 2\theta)^2} \right\} \right]$$

PF $P \times (FCALC)^2$
 PF1 $(1 + g \text{ PF})^{\frac{1}{2}}$, where g = extinction correction
 PF2 $(PF1)^3$
 PFØ $P \times (FØ)^2$
 SQ1 $\sin^2 \theta$
 XM $10^{\frac{L10}{10}}$, see L control values

Input:

A1 DELTA*S + 1.0, used in form factor table interpolation
 A2 Integral part of A1
 ALPHA Angle α or $\cos \alpha$
 BETA Angle β or $\cos \beta$
 GAMMA Angle γ or $\cos \gamma$
 DELTA $6400./FL/ATF(J11)$, $\sin \theta/\lambda$ interval in form factor table
 S $\sin \theta/\lambda$

Output:

PØS Alpha-numeric character standing for the position set
 ST(6) Ratio of change in a parameter to the standard deviation of the parameter
 SD Temporary storage for sum of $|\Delta F|$

SDW	Temporary storage for sum of $w \Delta F $
SF	Temporary storage for sum of $F\phi B$
SFW	Temporary storage for sum of $w F\phi B $
V	Volume of unit cell
WR	Weighted R factor

Weight:

ZI(6)	Atomic number, Z, divided by the number of atoms with Z as their atomic number
-------	--

Data Cards and/or Tape Description

Data cards for GENLES consist of the following: four cards containing primary control information, a set of atomic parameter cards (with cards containing anisotropic thermal information if this type of analysis is performed), a set of cards containing some auxiliary information, a set of form factor cards, the set of basic experimental data cards, and cards controlling the number of cycles of refinement required along with some output control information.

Primary Control Cards: Four cards required.

Card 1: 72 Hollerith characters for problem identification.

Card 2: In format 7F10.5, I2, the information a, b, c, α , β , γ , λ and control character J15.

a = a axis of the unit cell

b = b axis of the unit cell

c = c axis of the unit cell

α = α angle of the unit cell (may be replaced by $\cos \alpha$)

β = β angle of the unit cell (may be replaced by $\cos \beta$)

γ = γ angle of the unit cell (may be replaced by $\cos \gamma$)

λ = X-ray wavelength used

J15 = a control character governing the application of an extinction correction and its use as a least-squares variable.

J15 = 0, ignored, i.e., no corrections applied;

> 0, an extinction correction will be applied to the data and used as a least-squares variable.

Card 3: In format 12A6 the identification names of the atoms in the unit cell.

Card 4: In format 14I5, I2, the information N, M, J, J1(I) where (I) = 1 to 12.

N = a variable not used at present.

M = number of scale factors employed. For SCO data there is only one scale factor; for Wiessenberg or Precession data, there should be one scale factor for each level of film, etc.

J = number of different types of atoms. J(maximum) equals 6.

If J = -J then a Δf for J different types of atoms will be read from a later card.

J1(1) = number of position sets containing atoms of type 1
J1(2) = number of position sets containing atoms of type 2
J1(3) = number of position sets containing atoms of type 3
J1(4) = number of position sets containing atoms of type 4
J1(5) = number of position sets containing atoms of type 5
J1(6) = number of position sets containing atoms of type 6

The numerical order of atom types should be identical with the order of identification names on Card 3 of Primary Control Cards.

J1(7) Determines the location of experimental structure factor data.

J1(7) = 1, data are located on cards in the on-line card reader
J1(7) = 2, data are located on tape unit B6
J1(7) = 3, data are located on tape unit A6
J1(7) = 4, data are located on tape unit B1
J1(7) = 5, data are located on tape unit B1

Before the start of a normal refinement run, tape unit B1 should contain a blank tape. Prior to the first cycle of refinement the experimental data are transferred to B1. The data for least squares are then read from B1 for each cycle of refinement. If it is necessary to interrupt the refinement, tape B1 should be rewound, unloaded, and saved as a LES-5 tape. To restart the refinement, LES-5 should be remounted on tape unit B1,

and J1(7) should equal 4 or 5.

J1(7) = 6, data are located on cards, but these cards are part of the deck comprising input to Monitor so J1(7) = 6

signifies that the data are on the Monitor input tape A2.

J1(7) = 7, data are located on tape unit A6, to be unloaded after it is read.

J1(7) = 8, data are located on tape unit B6, to be unloaded after it is read.

J1(8) = a variable not used at present

J1(9) = a variable not used at present

J1(10) = a variable not used at present

J1(11) Determines the form of the atomic scattering factor f.

J1(11) = 0, the f curve is approximated by:

$$Ae^{-ax^2} + Be^{-bx^2} + Ce^{-cx^2} + De^{-dx^2} + E,$$

where $x = \sin \theta / \lambda$;

= N, the f curve is approximated by a table of 64

equal intervals from $\sin \theta / \lambda = 0$ to $\sin \theta / \lambda = N/100$.

J1(12) Designates the weighting scheme to be used in the preparation of a LES-5 tape.

J1(12) = 0, the weights written on the LES-5 tape are

equal to the weights contained in the input data;

= 1, the weights written on the LES-5 tape are equal to the weights contained in the input data;

$$\begin{aligned}
&= 2, w = w^{\frac{1}{2}}, \text{ the weights written on the LES-5 tape} \\
&\quad \text{are equal to the square root of the weight con-} \\
&\quad \text{tained on the input data;} \\
&= 3, w = 1/(F_o + 0.02 F_o^2)^{\frac{1}{2}}; \\
&= 4, w = w/(F_o + 0.02 F_o^2)^{\frac{1}{2}}; \\
&= 5, w = (N3/\sum \frac{f_i n_i}{z_i})^{\frac{1}{2}}.
\end{aligned}$$

Two weighting designations are used in the least-squares refinement: either unit weights, or some relative weighting scheme. If J1(12) = 0, unit weights are used. If J1(12) > 0, the weighting scheme originally written on the LES-5 type when it was prepared will be used.

Atomic Parameter Cards: For each atom in a position set, a maximum of two cards is required.

Card 1: Contains the information x, y, z, B, NL1, and NL2, in format
4F10.5, 2I5

x = positional parameter in fractions of the a axis of the
unit cell

y = positional parameter in fractions of the b axis of the
unit cell

z = positional parameter in fractions of the c axis of the
unit cell

B = an isotropic thermal parameter

Nl1 = the space group position set number in which the atom is placed; 1 = a, 2 = b, etc.

Nl2 Designates whether a second card will be read.

= 0, no second card read;

= 1, Card 2 will be read.

NOTE: In space groups containing polar axes, the x and/or y and/or z positions of the first listed atom determine the origin of the unit cell for least-squares purposes. Since these positions are fixed relative to the origin, they are not parameters in the least-squares model. For example, space group #1, P1, has three polar axes. If a crystal belonging to this space group has two atoms located at $x_1y_1z_1$ and $x_2y_2z_2$, then the positions $x_1y_1z_1$ are fixed and no changes in position or standard deviations will be calculated for these positions. The thermal parameter(s) for the atom at $x_1y_1z_1$ and the positional and thermal parameter(s) for the atom at $x_2y_2z_2$ remain variables in the least-squares model, however.

Card 2: Contains the anisotropic thermal parameters B_{11} , B_{22} , B_{33} , B_{12} , B_{13} , and B_{23} , in format 6F10.5

NOTE: If an isotropic thermal analysis is being performed for any particular atom, then that atom does not require a second card. If an anisotropic thermal analysis is being performed for any particular atom, then B for that atom may be 0 (or blank). The

numerical order of the atomic parameter cards should be identical with the order of $J_1(I)$, $I = 1$ to 6 on Card 4 of Primary Control Cards.

Auxiliary Information Cards: These cards contain scale factors and, if used, extinction and imaginary anomalous dispersion corrections.

Card 1: In format 7F10.5 there are M scale factors (See Card 4 of Primary Control Cards)

Card 1a: If more than seven scale factors are employed, the excess are punched in Card 1a, etc., in the same format as Card 1.

Card 2: If $J_{15} > 0$ an extinction correction is placed here in format E10.3

Card 3: If $J < 0$, then J imaginary anomalous dispersion corrections are placed here in format 6F10.5 and are read into SCALE ($I + 14$), $I = 1, J$.

Form Factor Cards: One card is needed for each of J atoms if $J_1(11) = 0$; five cards are needed for each of J atoms if $J_1(11) = N$. If $J_1(11) = 0$, then the card contains ID information, A,a,B,b,C,c,D,d, and E (these are the coefficients of the analytical approximations of the scattering curve) in format A4, A5, 9F7.0. If $J_1(11) = N$, then the cards contain in format 13F5.2 the tabular values of the approximation of the scattering curve. If anomalous dispersion corrections are being used in the calculation of structure factors, the real portion, $\Delta f'$, is applied here. $\Delta f'$ is either added to E or to each point of the tabular curve, depending on the value of $J_1(11)$.

Experimental Data Cards or Tape: One card is required for each experimental hkl reflection. In format 5F5.0, 2I5 each card contains: hkl , F , weight, scale factor appropriate to hkl , and a control character identification appropriate to F .

hkl = Miller indices of the reflection

F = structure factor, or structure factor squared

weight = relative weight assigned to the reflection, hkl

(See control character J1(12) on Card 4 of Primary Control Cards.)

$N1$ = the appropriate scale factor identified with hkl .

For SC0 data there is only one scale factor, and the number punched is 1 regardless of hkl . For Wiessenberg or Precession data the number punched might be 1 for $hk0$ data, 2 for hkl data, 3 for $hk2$ data, etc.

$N2$ = identification appropriate to the character of F .

This is equal to 2 for F^2 and 1 for F .

The reflection 000 is used to detect the end of the data. This reflection is given a scale factor number 1 greater than the number of scale factors (M) used in the calculations; i.e., if there are three scale factors to be varied, then 000 has a scale factor number of 4. The scale factor of 000 subsequently is automatically set equal to 1.0. Thus one can read in the correct value of $F(000)$ and have it used in the output as its true value.

Alternatively, the above information may be transcribed from cards

to magnetic tape and input to the program be accomplished in this manner. For this type of operation J1(7) should equal 2 or 8, and the tape should be mounted on unit B6.

A binary magnetic tape (LES-7) may have been prepared by our data processing program (LA-3043). For this type of operation J1(7) should equal 3 or 7 and the tape should be mounted on unit A6. The data on the LES-7 tape are in binary records containing hkl , F^2 , weight (floating point), scale factor number (fixed point); and $\sin^2 \theta / \lambda^2$ (floating point).

Finally, input to the program may also occur through the use of a LES-5 magnetic tape. This tape is prepared by GENLES on tape unit B1 before the first cycle of refinement and contains the following data in binary: hkl , F_o , F_o^2 , relative weight assigned to hkl , scale factor number appropriate to hkl , $\sin^2 \theta / \lambda^2$, and six f's. If it is necessary to interrupt the refinement, LES-5 should be rewound, unloaded, and saved. The refinement may then be restarted with new control and parameter cards and with LES-5 mounted on tape unit B1. For this type of operation J1(7) should equal 4 or 5.

Refinement Cycle Cards: One card is required for each cycle of refinement desired. The card contains the control variables L1 $\rightarrow$ L20 punched in format 20I3. Where the number 1 is designated, it generally means any nonzero integer.

L1 = 0, no operation performed;

= 1, write structure factor, F, on tape unit A3, scaled by

10**L10.

L2 = 0, no operation performed;

= 1, punch parameter cards for further refinement.

L3 = 0, no operation performed, i.e., go to next cycle;

≥ 4, unload B1 and call exit;

= 3, call exit, do not unload B1;

= 2, go to INPUT subroutine (used when an entirely new problem is to be done but the problem still uses the FUNCTN and CHANGE subroutines of the previous job);

= 1, stop at end of current cycle;

≤ -1, select the card reader and load self-loading program.

L4 = 0, no operation performed;

= 1, prepare a binary tape on unit A4 for editing and printing program (to be described in a later report), rewind and unload tape;

= 2, as in 1, but do not unload A4.

L5 = a variable not used at present

L6 = a variable not used at present

L7 = 0, no operation performed;

= 1, write on unit A3 the parameter correlation matrix at the end of the current cycle;

= 2, write the parameter correlation matrix on unit A3 and write unit cell data and the parameter correlation matrix on unit B3 at the end of the current cycle, rewind

and unload B3;

= 3, as in 2, but rewind B3 only; B3 is not unloaded.

L8 = 0, no operation performed;

= L8, will write hk_l , F_o , F_c , etc. on unit A3 if

$$|\Delta F| > (FL/ATF(L8)/100.0) * |F_o| \text{ where } L8 \text{ may be any}$$

number from 1 to 999.

L9 = 0, no operation performed;

= 1, prepare a Fourier input tape on unit B6, rewind at the end of the cycle;

≥ 2 , prepare a Fourier input tape on unit B6, rewind and unload at the end of the cycle.

L10 = N, multiply all F_o , F_c , ΔF in the A3 and A4 output tapes by 10^N

L11 = a variable not used at present

L12 = 0, normal least-squares cycle continued;

= 1, read in new set of parameters.

(a) New problem name, Card 1 of Primary Control Cards

(b) New control card, Card 4 of Primary Control Cards

(c) New parameter cards, Cards 1 and 2 of Atomic

Parameter Cards

Note: Count of refinement cycles is reset to zero, the above cards are read into the program, and essentially a completely new refinement procedure is started.

Ll3 = 0, specifies centric output on units A3, A4, B6;
 = 1, specifies noncentric output on units A3, A4, B6.
 Ll4 = 0, omit unobserved reflections from least-squares
 refinement;
 = 1, include $(-F_o)$, i.e., unobserved reflections in the
 least-squares refinement with $F_oB = -F_oB/2.0$.
 Ll5 = 0, no operation performed;
 = T, starting with the T'th set, convert Ll6 isotropic
 thermal parameter B's to anisotropic (if Ll6 + T > N3
 will convert through N3 only).
 Ll6 = number of B's to convert, if Ll5 > 0.
 Ll7 = 0, only physically plausible thermal parameters are used.
 (Negative isotropic thermal parameters are set to 0.0.
 For anisotropic thermal parameters the 3 x 3 matrix is
 examined. Negative diagonal elements are set to 0.0.
 Off-diagonal elements are examined individually to insure
 that the absolute value of these quantities is less than
 the square root of the diagonal product.);
 = 1, allows negative thermal parameters and other physically
 impossible thermal parameters to be used in the least-
 squares refinement.
 Ll8 = 0, a normal cycle of least squares is performed;
 = 1, suppresses the least-squares iteration.
 Ll9 = a variable not used at present

L20 = a variable not used at present

Output Description

The normal output from GENLES consists of an off-line printout plus any magnetic tapes the user may have prepared. The off-line printout lists the following preliminary information: problem identification, lattice constants and cosine of the angles, the initial positional and thermal parameter for each atom, the initial scale factors, the initial extinction correction (if used), the number of reflections read in, the number of reflections observed, and the number of reflections having a given scale factor identification. Bl tape identification information is also listed and consists of the J1(12) weighting designation number, the problem identification information, and form factor data. If called for, with the appropriate L control character, there may also be listed for each reflection $h, k, l, F_o, F_c, \Delta F, A\text{-PART}, B\text{-PART}$, the phase angle ALPHA in degrees, and/or the correlation matrix of the variable parameters. Then, for each cycle performed are listed four blocks of data. Block A: Problem identification, cycle number, number of reflections used, the conventional residual R, a weighted R (if other than unit weights), the sum of all the deviations squared, the sum of the deviations squared divided by the sum of the weights for each data set with a different scale factor identification, and the standard deviation of the electron

density. Block B: For each scale factor, the factor number, the change from the previous cycle, its standard deviation, its new value, the ratio of its change to its standard deviation, and its parameter identification number. Block C: For each atom, the atom name and number, the space group position set that the atom occupies, the parameter identifications x, y, z, and thermal, the change in each of these parameters, the standard deviation and new value of each parameter, the ratio of the change to the standard deviation for each parameter, and the parameter identification number for each parameter. Block D: The extinction correction (if used) with its change, standard deviation, new value, change/standard deviation, and parameter number.

The various output magnetic tapes: B3, a Fourier input, and an editing and printing tape, are described in detail elsewhere.

As a brief examination of the L control characters will reveal, the user of this program can design a least-squares refinement procedure to meet the peculiarities of virtually any crystal structure analysis within the boundaries of this program.

As a not too outrageous example, consider that on a particular, properly prepared set of data we wish to perform 15 cycles of least-squares refinement.

After two normal cycles of refinement we desire to have the structure factors (calculated with the x, y, z refined positions and thermal parameter of cycle two) written on the output tape and to have the computed factors multiplied by a factor of 100. This is to be

followed by three more normal cycles and then repeated. (Total cycles = 6.)

Starting with the seventh cycle we want to start with (for example) the second set of isotropic thermal parameter B_i 's and convert three sets of B_i 's (sets 2, 3, and 4) to anisotropic parameters. Negative thermal parameters are to be allowed for the next three cycles. Any following sets of isotropic B_i 's will remain isotropic. Three cycles of refinement are required. (Total cycles = 9.)

Beginning with the tenth cycle, we want to perform a refinement with a new set of parameters and to have the structure factors that are calculated from this new set written on the output tape. (Total cycles = 10.) This is to be followed by five cycles of normal refinement. For the fifth cycle of this procedure, we desire that the structure factors be written on the output tape, that parameter cards be punched, that the refinement be stopped after this cycle, that the parameter correlation matrix be written on the output tape, that a Fourier input tape be prepared on unit B6, and that the calculated structure be multiplied by 100.

The package of cycle refinement cards needed to perform the refinement described above is shown in Fig. 1.

34

	DATA SIX-TWELVE CARD
9	
8	
7	
6	
5	
4	
3	
2	
1	
0	
11-X	
12+Y	

Illustrative Example: Input

As an illustrative example of the typical use of this general least-squares program, we consider the refinement for $\text{CuCN}\cdot\text{NH}_3$.^{*} Copper cyanide ammonia is monoclinic with $a = 5.814$, $b = 7.977$, $c = 8.193$, and $\beta = 125.8^\circ$, and belongs in space group $P2_1/c$ (No. 14), with four formula units per unit cell. We assume that a LES-7 input tape is available, that the data were taken using MoK_α X-rays, that $\lambda = 0.7114$, and that an extinction correction will be applied in the refinement. Atomic form factor data are taken from Vol. III of "International Tables for X-ray Crystallography"^{**} and are used in an analytical form. For convenience, a nitrogen form factor is used for the ammonia group. Since the data were obtained on a single-crystal orienter there is only one scale factor. There are four different types of atoms considered: Cu, C, N, and NH_3 . These atoms are all in the same position set which is the general position set e of space group $P2_1/c$. The data input tape is to be located on unit A6 and is to be unloaded after its information is read into the computer.

^{*} Cromer, D. T., Larson, A. C., Roof, R. B., Jr., "The Crystal Structure of $\text{CuCN}\cdot\text{NH}_3$," Acta Cryst. **18** (1965), (in press).

^{**} International Tables for X-ray Crystallography, Vol. III, pg. 201 Kynoch Press (Birmingham) (1962).

The weighting scheme used in the refinement is to be equal to $W(\text{REFINEMENT}) = W(\text{LES-7 Input}) / (F_o + 0.02 F_o^2)^{\frac{1}{2}}$. From a three-dimensional Patterson vector map, we are able to deduce positions for the atoms approximately as follows:

	<u>X</u>	<u>Y</u>	<u>Z</u>
Copper	0.15	0.07	0.15
Nitrogen	0.10	0.25	0.30
Carbon	0.05	0.35	0.35
Ammonia	0.60	0.05	0.30

Anisotropic thermal parameters will be used, and we estimate $B_{11} = 0.03$, $B_{22} = 0.01$, and $B_{33} = 0.02$ for all the atom types. The cross-product terms B_{12} , B_{13} , and B_{23} are initially estimated to be 0.0, and we will let the computer program determine and refine the six parameters of anisotropic thermal motion. We estimate a scale factor to be approximately 2.50 and an extinction coefficient to be approximately 2.50×10^{-6} .

We will perform a total of 10 cycles of refinement, and for the last cycle we wish to write the structure factor F (unscaled) on unit A3, unload unit B1 (containing the LES-5 tape), stop after this cycle, and have the parameter correlation matrix written on unit A3.

The above information is collected on punched cards as outlined in the Data Cards and/or Tape Description section of this report and is illustrated in Fig. 2.

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Fig. 2. Control and Data Cards for the illustrative example.

Illustrative Example: Output

Figure 3 shows the listing of the initial values of the parameters and the results of the first cycle of refinement. It should be noted, for example, that B₃₃ of the N atom wants to become negative and, hence, the cross products B₁₃ and B₂₃ are not physically plausible. At this stage of the refinement these results are of no particular consequence; these parameters are set to 0.0, and the refinement proceeds to the next cycle.

At the end of the fifth cycle, $R = 0.0399$, and the refinement is essentially complete as Δ/σ is typically less than $1/10$, but we allow five more cycles to be run so that the changes in the parameters approach essentially zero and Δ/σ is typically equal to $1/10,000$. Figure 4 lists the results of the last cycle of refinement.

Figure 5 shows the first page of output of the structure factors that are written on tape unit A3. In this example, hkl is listed in terms of increasing $\sin^2\theta$. EDIT, a computer program to be described in a later report, is capable of processing this listing into a more conventional arrangement for publication purposes.

Figure 6 presents the parameter correlation matrix for $\text{CuCN}\cdot\text{NH}_3$. For example, the correlation between parameter No. 29 and parameter No. 15 is 0.033. The maximum correlation occurs between a parameter and itself and is represented by 1.00. A negative correlation signifies that when the value of parameter "a" increases, the value of parameter

LEAST SQUARES REFINEMENT FOR CU CN.NH(3)

LATTICE CONSTANTS ARE A = 5.8140 B = 7.9770 C = 8.1930 CUSA = -0. COSR = -0.58500 COSC = -0.

ATOM	X	Y	Z	B11	B22	B33	B12	B13	B23
COPPER	1	0.150000	0.070000	0.150000	0.030000	0.010000	0.020000	-0.	-0.
NITROGEN	1	0.100000	0.250000	0.300000	0.030000	0.010000	0.020000	-0.	-0.
CARBON	1	0.050000	0.350000	0.350000	0.030000	0.010000	0.020000	-0.	-0.
AMMONIA	1	0.600000	0.050000	0.300000	0.030000	0.010000	0.020000	-0.	-0.

SCALE FACTORS ARE 2.50000

EXTINCTION CORRECTION = 2.500E-06

THERE WERE 542 REFLECTIONS READ IN, OF WHICH 351 WERE OBSERVED

THERE ARE 350 OBSERVED REFLECTIONS WITH SCALE 1

TAPE 5(B1) I. D. INFO J12 WAS 4

LEAST SQUARES REFINEMENT FOR CU CN.NH(3)

FORM FACTOR DATA

CU VOL 3	14.729	5.406	6.726	0.983	2.931	35.968	4.576	-0.	-0.
N VOL 3	3.292	10.426	1.811	28.931	1.348	0.634	0.545	-0.	-0.
C VOL 3	2.794	15.425	1.426	0.754	1.336	41.253	0.441	-0.	-0.
N VOL 3	3.292	10.426	1.811	28.931	1.348	0.634	0.545	-0.	-0.

THIS IS CYCLE NO. 1 IN THIS RUN. 350 REFLECTIONS WERE USED

R = 0.2834 WEIGHTED R = 0.2958 SUM DELSQ = 8.57232E 02 SUM DELSQ/ SUM W = 1.00634E 01 FOR DATA SET WITH SCALE 1
STANDARD DEVIATION OF ELECTRON DENSITY IS 5.509E-01 TIMES THE SQUARE ROOT OF P (THE MULTIPLICITY)

ATOM NAME	NO. POS.	SET PARA.	CHANGE	STD. DEV.	NEW VALUE	DELTA/SIGMA	
SCALE	1		-0.09014662	0.11680464	2.40985337	7.7177E-01	37
COPPER	1	E	X	0.00942632	0.00163095	0.15942632	5.7796E 00
			Y	0.00400113	0.00096013	0.07400113	4.1672E 00
			Z	0.00355701	0.00116085	0.15355701	3.0641E 00
			B11	0.00341964	0.00489543	0.03341964	6.9854E-01
			B22	-0.00228498	0.00167356	0.00771502	1.3653E 00
			B33	-0.00713206	0.00270237	0.01286793	2.6392E 00
			B12	0.00334306	0.00451190	0.00334306	7.4094E-01
			B13	0.03520828	0.00517732	0.03520828	6.8005E 00
			B23	-0.00136375	0.00362215	-0.00136375	3.7650E-01
NITROGEN	1	E	X	-0.00506139	0.01105201	0.09493861	4.5796E-01
			Y	0.00234803	0.00709937	0.25234803	3.3074E-01
			Z	-0.00956244	0.00829884	0.29043755	1.1523E 00
			B11	0.02671835	0.03013142	0.05671835	8.8673E-01
			B22	0.00651739	0.01080840	0.01651739	6.0299E-01
			B33	-0.02183200	0.01574595	0.	1.3865E 00
			B12	-0.01225963	0.03500059	-0.01225963	3.5019E-01
			B13	0.06250285	0.03538342	0.	1.7664E 00
			B23	-0.01410101	0.02291221	0.	6.1544E-01
CARBON	1	E	X	-0.00749823	0.01516105	0.04250177	4.9457E-01
			Y	0.01406872	0.00882521	0.36406872	1.5941E 00
			Z	0.01388598	0.01074724	0.36388598	1.2921E 00
			B11	-0.01059521	0.03802879	0.01940478	2.7861E-01
			B22	0.01547939	0.01242556	0.02547938	1.2458E 00
			B33	-0.02429905	0.02143582	0.	1.1336E 00
			B12	-0.00470786	0.03848264	-0.00470786	1.2234E-01
			B13	-0.00053370	0.04602263	0.	1.1597E-02
			B23	-0.00895481	0.02700955	0.	3.3154E-01
AMMONIA	1	E	X	-0.00718001	0.00984091	0.59281997	7.2961E-01
			Y	-0.00230710	0.00571071	0.04769289	4.0400E-01
			Z	0.01869647	0.00771288	0.31869647	2.4241E 00
			B11	0.00396375	0.02818438	0.03396375	1.4064E-01
			B22	0.01625289	0.01023424	0.02625289	1.5881E 00
			B33	-0.00031515	0.01536751	0.01968484	2.0508E-02
			B12	-0.00052362	0.02615743	-0.00052362	2.0018E-02
			B13	0.03388893	0.03328748	0.03388893	1.0181E 00
			B23	0.00195385	0.01960941	0.00195385	9.9638E-02
EXTINCTION CORRECTION				5.3234E-07	1.6797E-06	3.0323E-06	3.1693E-01

Fig. 3. The listing of the initial values and the results of the first cycle of refinement for the illustrative example.

LEAST SQUARES REFINEMENT FOR CU CN.NH(3)

THIS IS CYCLE NO. 10 IN THIS RUN. 350 REFLECTIONS WERE USED

R = 0.0399 WEIGHTED R = 0.0460 SUM DELSQ = 2.63801E 01 SUM DELSQ/ SUM W = 3.09687E-01 FOR DATA SET WITH SCALE 1
STANDARD DEVIATION OF ELECTRON DENSITY IS 8.635E-02 TIMES THE SQUARE ROOT OF P (THE MULTIPLICITY)

ATOM NAME	NO.	POS.	SET	PARA.	CHANGE	STD. DEV.	NEW VALUE	DELTA/SIGMA	
SCALE	1				0.00000684	0.01507790	2.34640610	4.5402E-04	37
COPPER	1	E	X	0.00000000	0.00024957	0.16044135	7.5517E-06		1
			Y	0.00000000	0.00014396	0.07469328	2.6777E-05		2
			Z	0.00000000	0.00016425	0.15569412	1.8254E-05		3
			B11	-0.00000016	0.00073826	0.03486303	2.2080E-04		4
			B22	-0.00000004	0.00023364	0.00825824	1.6505E-04		5
			B33	-0.00000007	0.00035167	0.01481138	2.0329E-04		6
			B12	-0.00000001	0.00070640	-0.00160649	1.1473E-05		7
			B13	-0.00000012	0.00081007	0.02723429	1.5491E-04		8
			B23	-0.00000001	0.00050733	-0.00452241	2.5983E-05		9
NITROGEN	1	E	X	-0.00000003	0.00159363	0.08168410	2.1220E-05		10
			Y	0.00000001	0.00099808	0.25279787	8.2208E-06		11
			Z	-0.00000001	0.00106455	0.28589550	1.6998E-05		12
			B11	-0.00000013	0.00499881	0.04331497	2.7271E-05		13
			B22	-0.00000005	0.00139356	0.00811426	3.8642E-05		14
			B33	-0.00000004	0.00210083	0.01513266	2.1998E-05		15
			B12	0.00000005	0.00490417	0.00166155	1.1035E-05		16
			B13	-0.00000008	0.00559998	0.03396954	1.5503E-05		17
			B23	0.00000002	0.00306636	-0.00029253	7.9708E-06		18
CARBON	1	E	X	-0.00000006	0.00216772	0.04589629	2.7983E-05		19
			Y	-0.00000000	0.00118486	0.35203747	5.8383E-06		20
			Z	-0.00000005	0.00150833	0.36798503	3.8631E-05		21
			B11	-0.00000015	0.00565625	0.03561281	2.7180E-05		22
			B22	-0.00000008	0.00161444	0.00764814	5.2637E-05		23
			B33	-0.00000007	0.00286360	0.01977010	2.3898E-05		24
			B12	-0.00000015	0.00531577	-0.00189365	2.8437E-05		25
			B13	-0.00000017	0.00711911	0.03625193	2.4882E-05		26
			B23	-0.00000005	0.00383041	-0.00496371	1.4804E-05		27
AMMONIA	1	E	X	0.00000001	0.00150992	0.59456668	6.2356E-06		28
			Y	0.00000000	0.00092153	0.04043234	6.5051E-07		29
			Z	0.00000007	0.00116962	0.32794857	6.4313E-05		30
			B11	-0.00000004	0.00428304	0.02675954	1.1806E-05		31
			B22	-0.00000003	0.00174103	0.01030876	2.0876E-05		32
			B33	-0.00000002	0.00233687	0.01976196	1.0047E-05		33
			B12	0.00000004	0.00388382	0.00146474	9.5978E-06		34
			B13	-0.00000006	0.00533883	0.02252544	1.1631E-05		35
			B23	0.00000001	0.00296826	0.00138476	4.5296E-06		36
EXTINCTION CORRECTION					-3.3346E-10	2.1852E-07	2.9446E-06	1.5260E-03	38

Fig. 4. The results of the last cycle of refinement of the illustrative example.

H	K	L	F0B	FCALC	DEL-F	A-PT	B-PT	ALPHA
0	1	1	47	48	-1			
1	0	0	63	68	-5			
1	1	-1	85	82	3			
1	1	0	48	-49	1			
1	0	-2	50	48	2			
0	2	0	55	50	5			
1	1	-2	27	26	1			
0	2	1	63	-58	-5			
0	0	2	60	-63	4			
1	2	-1	29	-27	-2			
0	1	2	14	-15	1			
1	2	0	9	-6	-3			
1	1	1	6	-9	3			
2	0	-2	43	46	-3			
1	2	-2	66	62	4			
2	1	-2	-5	-1	0			
2	1	-1	54	50	4			
1	1	-3	47	-46	-2			
0	2	2	15	-13	-2			
0	3	1	8	-7	-1			
1	2	1	49	-51	2			
1	3	-1	9	8	1			
2	1	-3	39	41	-2			
2	0	0	12	-11	-1			
2	2	-2	46	49	-3			
1	3	0	56	-55	-1			
2	2	-1	61	-60	-1			
2	1	0	51	-52	0			
1	2	-3	62	60	1			
1	3	-2	63	62	1			
1	0	2	73	-78	5			
0	1	3	60	-58	-2			
2	2	-3	41	42	-1			
1	1	2	10	9	1			
0	3	2	65	-63	-2			
2	2	0	24	-23	-1			
2	0	-4	8	-9	1			
1	3	1	6	-6	1			
0	4	0	12	-11	-1			
1	0	-4	64	-68	4			
2	1	-4	36	37	-1			
2	3	-2	12	-12	0			
0	2	3	9	-8	-2			
2	3	-1	10	11	-1			
3	0	-2	29	29	0			
1	2	2	34	-35	1			
1	1	-4	14	14	-0			
0	4	1	71	-70	-1			
1	3	-3	-5	-5	0			
1	4	-1	7	-6	-0			
3	1	-2	23	-23	0			
3	1	-3	56	57	-2			
2	1	1	63	-64	0			
1	4	0	13	-14	1			
2	3	-3	15	16	-0			
2	2	-4	18	-17	-0			
1	4	-2	17	-17	-0			
3	0	-4	35	35	-0			
1	2	-4	49	-49	-1			
2	3	0	56	-57	1			
3	1	-1	36	-36	0			
3	2	-2	31	31	-0			

Fig. 5. A typical page of the listing of the structure factors for the illustrative example.

LEAST SQUARES REFINEMENT FOR CU CN.NH(3)

THE VALUE OF THE DETERMINANT IS 1.7014E 38

THE POSITIVE DEFINITE CRITERION ARE

1	7.5E 06	2	2.2E 07	3	2.6E 07	4	8.6E 05	5	8.7E 06	6	4.7E 06	7	9.4E 05	8	3.0E 06	9	2.5E 06	10	1.9E 05
11	4.7E 05	12	5.8E 05	13	1.9E 04	14	2.6E 05	15	1.2E 05	16	2.0E 04	17	8.2E 04	18	7.8E 04	19	1.1E 05	20	3.8E 05
21	3.7E 05	22	1.6E 04	23	2.1E 05	24	6.8E 04	25	1.8E 04	26	5.2E 04	27	5.3E 04	28	2.1E 05	29	5.7E 05	30	4.8E 05
31	2.6E 04	32	1.7E 05	33	9.3E 04	34	3.2E 04	35	6.8E 04	36	7.2E 04	37	7.6E 03	38	2.4E 13				
1	1 1.000																		
2	1-0.010	2	2 1.000																
3	1 0.580	3	2-0.032	3	3 1.000														
4	1-0.026	4	2-0.037	4	3-0.009	4	4 1.000												
5	1-0.030	5	2-0.016	5	3-0.012	5	4 0.127	5	5 1.000										
6	1-0.036	6	2-0.034	6	3-0.032	6	4 0.438	6	5 0.138	6	6 1.000								
7	1 0.058	7	2-0.007	7	3 0.025	7	4-0.014	7	5-0.000	7	6-0.032	7	7 1.000						
8	1-0.017	8	2-0.021	8	3-0.023	8	4 0.736	8	5 0.078	8	6 0.743	8	7-0.040	8	8 1.000				
9	1 0.013	9	2 0.020	9	3 0.003	9	4 0.019	9	5-0.063	9	6-0.049	9	7 0.532	9	8-0.021	9	9 1.000		
10	1-0.091	10	2 0.035	10	3-0.013	10	4 0.009	10	5-0.027	10	6-0.042	10	7 0.070	10	8-0.020	10	9 0.044		
10	10 1.000																		
11	1 0.053	11	2-0.016	11	3 0.039	11	4-0.013	11	5 0.003	11	6 0.008	11	7-0.019	11	8-0.014	11	9 0.067		
11	10-0.033	11	11 1.000																
12	1-0.034	12	2 0.016	12	3-0.025	12	4 0.014	12	5 0.022	12	6-0.016	12	7 0.063	12	8-0.013	12	9 0.095		
12	10 0.533	12	11 0.043	12	12 1.000														
13	1-0.015	13	2 0.022	13	3-0.017	13	4 0.056	13	5 0.058	13	6 0.038	13	7-0.036	13	8 0.021	13	9-0.015		
13	10-0.034	13	11-0.047	13	12-0.064	13	13 1.000												
14	1 0.006	14	2-0.054	14	3-0.002	14	4 0.061	14	5 0.040	14	6 0.063	14	7 0.024	14	8 0.059	14	9-0.006		
14	10-0.031	14	11 0.006	14	12-0.032	14	13-0.216	14	14 1.000										
15	1-0.012	15	2 0.023	15	3 0.018	15	4 0.043	15	5 0.059	15	6 0.047	15	7 0.001	15	8 0.029	15	9 0.019		
15	10 0.070	15	11-0.014	15	12 0.066	15	13 0.192	15	14-0.275	15	15 1.000								
16	1-0.061	16	2 0.066	16	3-0.031	16	4-0.021	16	5 0.010	16	6-0.039	16	7 0.002	16	8-0.034	16	9 0.031		
16	10 0.085	16	11-0.138	16	12 0.057	16	13 0.015	16	14 0.024	16	15 0.045	16	16 1.000						
17	1-0.023	17	2 0.005	17	3-0.005	17	4 0.042	17	5 0.060	17	6 0.041	17	7-0.027	17	8 0.020	17	9 0.017		
17	10 0.037	17	11-0.025	17	12-0.013	17	13 0.684	17	14-0.146	17	15 0.700	17	16 0.045	17	17 1.000				
18	1-0.039	18	2 0.012	18	3-0.001	18	4-0.023	18	5-0.018	18	6-0.036	18	7 0.041	18	8-0.024	18	9 0.069		
18	10 0.033	18	11 0.044	18	12 0.094	18	13-0.048	18	14-0.012	18	15-0.002	18	16 0.578	18	17-0.022	18	18 1.000		
19	1-0.068	19	2 0.049	19	3-0.059	19	4-0.016	19	5-0.029	19	6-0.024	19	7-0.127	19	8-0.004	19	9-0.095		
19	10-0.015	19	11-0.107	19	12-0.072	19	13 0.069	19	14 0.004	19	15-0.096	19	16-0.172	19	17-0.042	19	18-0.171		
19	19 1.000																		
20	1 0.013	20	2 0.030	20	3 0.038	20	4-0.040	20	5 0.020	20	6-0.011	20	7 0.019	20	8-0.021	20	9 0.004		
20	10-0.062	20	11 0.121	20	12 0.110	20	13-0.091	20	14-0.110	20	15-0.007	20	16-0.021	20	17-0.105	20	18 0.182		
20	19-0.041	20	20 1.000																
21	1-0.043	21	2-0.041	21	3-0.111	21	4 0.005	21	5-0.018	21	6-0.002	21	7-0.068	21	8 0.005	21	9-0.072		
21	10-0.064	21	11 0.000	21	12 0.025	21	13-0.025	21	14 0.101	21	15-0.127	21	16-0.166	21	17-0.094	21	18-0.123		
21	19 0.625	21	20-0.035	21	21 1.000														
22	1-0.071	22	2-0.072	22	3-0.079	22	4 0.065	22	5 0.022	22	6 0.093	22	7-0.054	22	8 0.084	22	9 0.026		
22	10-0.080	22	11 0.088	22	12 0.060	22	13-0.139	22	14 0.039	22	15-0.084	22	16-0.053	22	17-0.137	22	18 0.063		
22	19-0.061	22	20 0.036	22	21-0.011	22	22 1.000												
23	1-0.015	23	2 0.055	23	3-0.002	23	4 0.048	23	5-0.002	23	6 0.070	23	7-0.074	23	8 0.037	23	9-0.020		
23	10 0.028	23	11 0.019	23	12-0.047	23	13 0.037	23	14 0.192	23	15-0.013	23	16 0.009	23	17 0.084	23	18-0.024		
23	19 0.004	23	20-0.017	23	21 0.019	23	22-0.232	23	23 1.000										

24	1-0.072	24	2-0.056	24	3-0.033	24	4 0.079	24	5 0.043	24	6 0.023	24	7 0.083	24	8 0.061	24	9 0.043
24	10 0.138	24	11-0.029	24	12 0.220	24	13-0.101	24	14-0.008	24	15-0.033	24	16 0.106	24	17-0.112	24	18 0.121
24	19-0.015	24	20 0.027	24	21 0.059	24	22 0.201	24	23-0.225	24	24 1.000						
25	1-0.051	25	2-0.016	25	3-0.013	25	4 0.033	25	5 0.032	25	6-0.014	25	7-0.106	25	8-0.012	25	9-0.041
25	10 0.118	25	11 0.064	25	12 0.105	25	13-0.019	25	14 0.008	25	15 0.142	25	16 0.203	25	17 0.091	25	18 0.140
25	19 0.007	25	20 0.039	25	21-0.013	25	22-0.027	25	23-0.010	25	24-0.002	25	25 1.000				
26	1-0.111	26	2-0.074	26	3-0.076	26	4 0.080	26	5 0.029	26	6 0.077	26	7 0.040	26	8 0.078	26	9 0.052
26	10 0.054	26	11 0.067	26	12 0.193	26	13-0.157	26	14 0.093	26	15-0.090	26	16 0.070	26	17-0.124	26	18 0.136
26	19-0.062	26	20 0.041	26	21 0.014	26	22 0.686	26	23-0.157	26	24 0.698	26	25-0.014	26	26 1.000		
27	1-0.034	27	2 0.007	27	3-0.033	27	4-0.009	27	5-0.041	27	6-0.043	27	7-0.064	27	8-0.029	27	9-0.050
27	10 0.111	27	11-0.118	27	12-0.052	27	13 0.079	27	14-0.026	27	15 0.163	27	16 0.162	27	17 0.169	27	18-0.065
27	19 0.021	27	20-0.087	27	21-0.017	27	22-0.072	27	23-0.043	27	24-0.078	27	25 0.547	27	26-0.082	27	27 1.000
28	1 0.044	28	2 0.012	28	3 0.034	28	4 0.023	28	5-0.013	28	6-0.015	28	7 0.009	28	8 0.002	28	9 0.014
28	10-0.034	28	11 0.038	28	12-0.053	28	13-0.018	28	14-0.019	28	15 0.041	28	16-0.032	28	17 0.014	28	18-0.037
28	19-0.097	28	20-0.006	28	21-0.075	28	22-0.058	28	23 0.020	28	24-0.057	28	25-0.020	28	26-0.076	28	27 0.011
28	28 1.000																
29	1 0.008	29	2-0.029	29	3 0.037	29	4-0.006	29	5 0.043	29	6 0.001	29	7-0.040	29	8-0.010	29	9-0.008
29	10-0.024	29	11 0.043	29	12-0.025	29	13-0.016	29	14-0.064	29	15 0.033	29	16 0.005	29	17 0.019	29	18 0.044
29	19-0.045	29	20-0.064	29	21-0.066	29	22 0.012	29	23-0.011	29	24-0.013	29	25-0.007	29	26-0.001	29	27-0.056
29	28 0.027	29	29 1.000														
30	1 0.026	30	2 0.004	30	3 0.026	30	4 0.020	30	5 0.025	30	6-0.003	30	7 0.015	30	8 0.001	30	9-0.010
30	10-0.046	30	11 0.036	30	12-0.005	30	13-0.006	30	14 0.022	30	15 0.058	30	16-0.030	30	17 0.038	30	18-0.057
30	19-0.067	30	20 0.008	30	21-0.036	30	22-0.067	30	23 0.015	30	24-0.015	30	25 0.018	30	26-0.065	30	27 0.006
30	28 0.529	30	29 0.017	30	30 1.000												
31	1-0.064	31	2 0.026	31	3-0.013	31	4-0.007	31	5 0.057	31	6 0.021	31	7-0.045	31	8-0.014	31	9-0.063
31	10-0.011	31	11 0.006	31	12-0.024	31	13 0.003	31	14 0.003	31	15 0.032	31	16 0.021	31	17 0.010	31	18-0.015
31	19 0.009	31	20-0.008	31	21 0.025	31	22-0.036	31	23 0.014	31	24-0.016	31	25 0.076	31	26-0.026	31	27 0.047
31	28-0.022	31	29-0.015	31	30 0.045	31	31 1.000										
32	1-0.006	32	2-0.063	32	3-0.043	32	4 0.094	32	5-0.000	32	6 0.085	32	7 0.009	32	8 0.075	32	9 0.115
32	10-0.018	32	11-0.008	32	12 0.037	32	13-0.007	32	14 0.037	32	15 0.013	32	16-0.041	32	17 0.005	32	18 0.009
32	19-0.028	32	20 0.039	32	21 0.010	32	22 0.043	32	23 0.098	32	24-0.016	32	25 0.020	32	26 0.025	32	27 0.003
32	28 0.006	32	29-0.101	32	30-0.014	32	31-0.215	32	32 1.000								
33	1 0.046	33	2-0.023	33	3 0.074	33	4 0.021	33	5 0.047	33	6 0.001	33	7-0.000	33	8-0.000	33	9 0.008
33	10-0.016	33	11 0.035	33	12-0.013	33	13 0.027	33	14 0.002	33	15 0.007	33	16 0.008	33	17 0.037	33	18 0.030
33	19 0.025	33	20-0.013	33	21 0.007	33	22-0.015	33	23-0.024	33	24 0.049	33	25 0.012	33	26 0.006	33	27-0.006
33	28 0.044	33	29 0.077	33	30 0.022	33	31 0.091	33	32-0.227	33	33 1.000						
34	1 0.008	34	2-0.036	34	3 0.005	34	4 0.040	34	5 0.022	34	6 0.014	34	7 0.023	34	8 0.030	34	9-0.005
34	10-0.008	34	11-0.018	34	12-0.043	34	13 0.026	34	14-0.041	34	15-0.004	34	16-0.042	34	17 0.015	34	18-0.014
34	19 0.011	34	20 0.018	34	21 0.018	34	22 0.044	34	23-0.049	34	24 0.023	34	25-0.074	34	26 0.031	34	27-0.027
34	28 0.036	34	29-0.058	34	30 0.004	34	31-0.019	34	32 0.008	34	33-0.010	34	34 1.000				
35	1-0.020	35	2 0.009	35	3 0.050	35	4-0.018	35	5 0.043	35	6-0.004	35	7-0.018	35	8-0.012	35	9-0.051
35	10-0.014	35	11 0.025	35	12-0.030	35	13 0.002	35	14 0.004	35	15 0.031	35	16 0.024	35	17 0.002	35	18-0.006
35	19 0.035	35	20-0.010	35	21 0.031	35	22-0.033	35	23-0.003	35	24 0.009	35	25 0.065	35	26-0.008	35	27 0.025
35	28 0.019	35	29 0.021	35	30 0.070	35	31 0.645	35	32-0.182	35	33 0.626	35	34-0.021	35	35 1.000		
36	1 0.012	36	2-0.029	36	3 0.008	36	4 0.015	36	5 0.017	36	6 0.010	36	7-0.011	36	8 0.019	36	9-0.030
36	10-0.060	36	11-0.006	36	12-0.067	36	13 0.031	36	14-0.029	36	15-0.032	36	16-0.015	36	17-0.014	36	18-0.014
36	19 0.036	36	20-0.016	36	21 0.028	36	22 0.036	36	23-0.019	36	24-0.003	36	25-0.042	36	26 0.022	36	27-0.014
36	28 0.007	36	29-0.040	36	30-0.040	36	31-0.023	36	32 0.009	36	33-0.002	36	34 0.507	36	35-0.023	36	36 1.000
37	1 0.054	37	2 0.062	37	3 0.021	37	4-0.554	37	5-0.533	37	6-0.559	37	7-0.013	37	8-0.400	37	9-0.021
37	10 0.032	37	11 0.008	37	12-0.016	37	13-0.090	37	14-0.090	37	15-0.095	37	16 0.031	37	17-0.088	37	18 0.041
37	19 0.055	37	20 0.021	37	21 0.008	37	22-0.070	37	23-0.099	37	24-0.058	37	25-0.032	37	26-0.067	37	27 0.025
37	28 0.007	37	29-0.020	37	30-0.039	37	31-0.065	37	32-0.126	37	33-0.052	37	34-0.015	37	35-0.030	37	36-0.001
37	37 1.000																
38	1-0.060	38	2-0.076	38	3-0.026	38	4 0.369	38	5 0.370	38	6 0.389	38	7 0.029	38	8 0.273	38	9 0.025
38	10-0.058	38	11-0.014	38	12-0.005	38	13 0.019	38	14 0.075	38	15 0.051	38	16-0.049	38	17 0.026	38	18-0.014
38	19-0.101	38	20 0.025	38	21-0.010	38	22 0.035	38	23 0.075	38	24 0.037	38	25-0.008	38	26 0.038	38	27-0.020
38	28-0.035	38	29 0.014	38	30 0.047	38	31 0.077	38	32 0.086	38	33 0.018	38	34 0.013	38	35 0.032	38	36-0.009
38	37-0.747	38	38 1.000														

Fig. 6. Correlation matrix for $\text{CuCN} \cdot \text{NH}_3$.

"b" decreases, and vice-versa. The positive definite criteria listed are defined by Doyle.*

One other item of interest is the time required to run the problem on the computer. Ten cycles of refinement of a 38 x 38 matrix involving 350 data points were performed in 5.43 minutes on an IBM 7094.

Fortran II Listing of Programs

The Fortran II listings of the program GENLES described in this report are shown on the following pages. Several subroutines are called during the operation of GENLES, and these are also listed. UNLOAD and ASIN have been listed in our first report, LA-2974, and are not repeated here. For typical examples of FUNCTN and CHANGE subroutines, see Appendix I.

GENLES	is written in Fortran II				
INPUT	"	"	"	"	"
PARMR	"	"	"	"	"
MATSTP	"	"	"	"	"
WEIGHT	"	"	"	"	"
MATINV	"	"	"	FAP	
IPCDEL	"	"	"	"	

* Doyle, T. C., Inversion of Symmetric Coefficient Matrix of Positive-Definite Quadratic Form, Mathematical Tables and Other Aids to Computation, Vol. XI, No. 58, April 1957, pp. 55-58.

ALPHA	is written in FAP				
UNLOAD	"	"	"	"	"
ASIN	"	"	"	"	"
COS	"	"	"	"	"
OUTPUT	"	"	"	Fortran II	
FUNCTN	"	"	"	"	"
CHANGE	"	"	"	"	"

GENLES is the main program that applies the least-squares concept to the solution of Equation (1). Of the subroutines, INPUT feeds preliminary information and control to GENLES. PARMTR supplies the atomic parameters and other unit cell content information to GENLES. MATSTP sets up the matrix and calls MATINV for its solution. WEIGHT applies various weighting schemes to the experimental data. MATINV inverts the coefficient matrix and computes the changes to be applied to the various parameters. IPCDEL computes the number of cells remaining in the computer memory after a GENLES program utilizing a particular FUNCTN and CHANGE subroutine has been read in. ALPHA converts a position set number to a position set letter character. UNLOAD unloads the various tapes from the tape units. ASIN is an arcsine or arccosine subroutine. COS is a low-accuracy (0.0001) sine or cosine subroutine. OUTPUT prepares the calculations for output from the computer.

FUNCTN is a subroutine that computes FCALC and the partial derivative of FCALC with respect to the various parameters being

considered in a particular space group. The one exception is the extinction correction which, if applied, is general to all space groups and is handled in the GENLES portion of the program. CHANGE computes the changes and standard deviations for each of the parameters of the FUNCTN subroutines and applies the changes to the parameters prior to the start of the next cycle of refinement.

The authors believe that a major advantage of the programming method adopted, i.e., a FUNCTN and CHANGE for each space group, lies in the flexibility with which any structural parameter may be introduced into the least-squares refinement. The most troublesome item in our experience has been insuring that the partial derivatives are correctly formulated.

```

COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),FOB(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(3201),SRHO(11126),
9 SWF(10872),IPCERK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)

DIMENSION I1(1)
DIMENSION PRGB(12),NAM(12)
EQUIVALENCE (CMAT(30),PROB(13),NAM(1))

1 FORMAT (1H 3I3,6I6)
2 FORMAT (47H1 H K L FOB FCALC DEL-F A-PT B-PT ALPHA )
3 FORMAT ( 3F5.0,3F10.3)
4 FORMAT (24I3)
8 FORMAT (12A6)
9 FORMAT (22H-TAPE 5(B1) I. D. INFO10X8HJ12 WAS I2)
10 FORMAT (1H012A6/17H0FORM FACTOR DATA)
11 FORMAT (5H0NONE)
12 FORMAT (1H112A6/1H-6X42H THE FOLLOWING ATOMS WERE MADE ANISOTROPIC
1 /36HO ATOM NAME NO. OLD B NEW B(IJ)S)
13 FORMAT (1H02A6,16F6.2/(13X16F6.2))
14 FORMAT ( 1H02A4,9F8.3)
15 FORMAT (1H 2A6,I3,F7.2,6F10.6)

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IPC BRK = IPCDEL(I)
50 S1 = 0.0
CALL INPUT
XM=1.0
READ TAPE 5, (I1(I), I=1, 6)
WRITE OUTPUT TAPE 9, 9, I6
IF ( XABSF(I1)+XABSF(I2)+XABSF(I3) ) 60, 61, 60
60 DUM=0.0
WRITE OUTPUT TAPE 9, 11
GO TO 70
61 IF ( I4 ) 62, 63, 62
62 READ TAPE 5, NAM, PROB, ((CMAT(I, I1), I1=1, 65), I=1, I5)
GO TO 64
63 READ TAPE 5, NAM, PROB, ((CMAT(I, I1), I1=1, 9), I=1, I5)
64 WRITE OUTPUT TAPE 9, 10, PROB
DUM=1.0
IF ( I4 ) 65, 67, 65
65 DO 66 I=1, I5
66 WRITE OUTPUT TAPE 9, 13, NAM(2*I-1), NAM(2*I), (CMAT(I, I1), I1=1, 65)
GO TO 70
67 WRITE OUTPUT TAPE 9, 14, (NAM(2*I-1), NAM(2*I), (CMAT(I, I1), I1=1, 9), I=
11, I5)
70 REWIND 5
SRHO = 0.0
IR = 10000+IPC BRK
NMAX = (SQRT(FLOATF(IR)*8.0+23.0)-5.0)/2.0
N=NMAX
99 DO 101 I=1, IR
101 CMAT(I)=0.0
IF ( DUM ) 72, 72, 71
71 READ TAPE 5, I
READ TAPE 5, F
72 K2=0
FMAX=0.0
DO 104 I=1, M
SUMQBS(I)=0.0
SUMFQB(I)=0.0
SUMDEL(I)=0.0
SWF(I)=0.0
SA(I)=0.0
104 SDELSQ(I)=0.0
1040 IF ( S1 ) 73, 73, 74
73 READ INPUT TAPE 10, 4, L1, L2, L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13,
1 L14, L15, L16, L17, L18, L19, L20
GO TO 75
74 READ 4, L1, L2, L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15,
1 L16, L17, L18, L19, L20
75 CCNTINUE
XM=10.0**L10
IF ( L12 ) 100, 1047, 100
100 IF ( S1 ) 77, 76, 77
77 READ 8, PROBLM
GO TO 78
76 READ INPUT TAPE 10, 8, PROBLM
78 CCNTINUE
CALL PARMTR
K3=0
1047 IF ( L15 ) 1055, 1055, 1053
1053 I=0
WRITE OUTPUT TAPE 9, 12, PROBLM
I4=0
DO 1059 I1=1, J
I2=J1(I1)
IF ( I2 ) 1059, 1059, 1054

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GEN. LES

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1054 DO 1058 I3=1,I2
      I=I+1
      IF ( I-L15 ) 1058,1056,1056
1056 IF ( N12(I) ) 1057,10571,1058
1057 N12(I)=-N12(I)
      GO TO 10572
10571 N12(I)=1
10572 DET=B(I)
      B11(I)=DET*ASTAR**2
      B22(I)=DET*BSTAR**2
      B33(I)=DET*CSTAR**2
      B12(I)=DET*2.0*ASTAR*BSTAR*COSSCSR
      B13(I)=DET*2.0*ASTAR*CSTAR*COSSBSR
      B23(I)=DET*2.0*BSTAR*CSTAR*COSSASR
      WRITE OUTPUT TAPE 9,15,NAME(2I1-1),NAME(2I1), I3,DET,
      1 B11(I),B22(I),B33(I),B12(I),B13(I),B23(I)
      I4=I4+1
      IF ( I4-L16 ) 1058,1055,1055
1058 CCNTINUE
1059 CONTINUE
1055 IF ( L4 ) 1048,1048,1050
1050 REWIND 4
      WRITE OUTPUT TAPE 4,8,PROBLM
1048 DELMAX = FLOATF(L8)/100.0
      IF ( L9 ) 1021,1052,1021
1021 REWIND 8
      WRITE OUTPUT TAPE 8,8,PROBLM
1052 IF ( L1+L8 ) 103,110,103
103 WRITE OUTPUT TAPE 9,2
110 READ TAPE 5,H1,H2,H3,FCB,FOBS,W,N1,SQ,F
      DO 1101 I=1,N
      R(I) = 0.0
1101 PD(I)=0.0
111 CALL FUNCTN
      FO=FCB
      FC=FCALC
      IF ( SQ ) 200,200,1142
1142 IF ( FCB ) 1150,200,115
1150 IF ( L14 ) 1151,200,1151
1151 FCB=-FCB/2.0
115 IF ( J15 ) 1153,1152,1153
1153 SQ1=SQ*XRAY**2
      P=(1.0+(1.0-2.0*SQ1)**4)/(SQRTF(SQ1-SQ1**2)(1.0+(1.0-2.0*SQ1)**2))
      N=N+1
      PF=P*FCALC**2
      PF1=SQRTF(1.0+G*PF)
      PD(N)=-FCALC**3*P/2.0
      PF2=PF1**3
      DO 1156 I=1,N
1156 PD(I)=PD(I)*PF2
      FCALC=FCALC/PF1
      PFO=P*FCB**2
      FO=FCB/(SQRTF(1.0-G*PFO))
      FMAX=MAX1F(FMAX,PFO)
1152 DELF = SIGNF((FCB-ABSF(FCALC)),FCALC)*SIGNF(1.0,(FCB-ABSF(FCALC)))
      DF = SIGNF((FO-ABSF(FC)),FC)*SIGNF(1.0,(FO-ABSF(FC)))
118 SUMDEL(N1) = SUMDEL(N1)+ABSF(DELF)
      IF ( J12 ) 1180,112,1180
1180 DELF=DELF*W
      SWF(N1)=SWF(N1)+ABSF(DELF)*W
      SA(N1) = SA(N1)+W**2
112 SDELSQ(N1)=SDELSQ(N1)+(DELF/SCALE(N1))**2
1155 K2=K2+1
      SUMFCB(N1)=SUMFCB(N1)+FCB
      SUMOBS(N1)=SUMOBS(N1)+FOBS*W**2
      IF ( L18 ) 1123,1181,1123

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GEN. LES

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1181 IF ( J12 ) 1182,1121,1182
1182 DO 1120 I=1,N
1120 PD(I)=PD(I)*W
1121 SENSE LIGHT 0
      CALL MATSTP
      IF (J12) 1123,1122,1123
1123 DELF = DELF/W
1122 SRHO = SRHO+DF**2
200 IF ( L1 ) 206,201,206
201 IF ( L8 ) 202,205,202
202 IF ( F08 ) 204,203,203
203 IF ( ABSF(DELF)-DELMAX*F08 ) 205,206,206
204 IF ( ABSF(FCALC)+2.0*F08 ) 205,205,206
205 ASSIGN 211 TO L8TR
      IF ( L4 ) 207,300,207
206 ASSIGN 210 TO L8TR
207 I1 = H1
      I2=H2
      I3=H3
      I4 = SIGNF(ABSF(F08)*XM+0.5,F08)
      I5 = SIGNF(ABSF(FCALC)*XM+0.5,FCALC)
      I6 = SIGNF(ABSF(DELF)*XM+0.5,DELF)
      I10 = 6
      I11 = 5
      IF ( L13 ) 208,209,208
208 I9 = MODF(SIGNF(90.0-57.2958*ASINF(FA/FCALC),FB)+360.0,360.0)+0.5
      I8 = SIGNF(ABSF(F8)*XM+0.5,F8)
      I7 = SIGNF(ABSF(FA)*XM+0.5,FA)
      I10 = 9
      I11 = 6
209 GO TO L8TR,(210,211)
210 WRITE OUTPUT TAPE 9,1,(I1(I),I=1,I10)
211 IF ( L4 ) 224,300,224
224 IF ( SQ ) 212,300,212
212 I6 = I9
      WRITE TAPE 4,(I1(I),I=1,I11)
300 IF ( L9 ) 3000,1000,3000
3000 IF ( SQ ) 306,306,301
306 FA = FC
      DF = 0.0
      GO TO 305
301 IF ( F08 ) 1000, 1000, 302
302 IF ( L13 ) 3021,3020,3021
3021 F1=FA
      FA = F0
      FC = F1
      DF = F8
      GO TO 305
3020 FA = SIGNF(F0,FC)
305 WRITE OUTPUT TAPE 8,3,H1,H2,H3,FA,FC,DF
1000 IF ( SQ ) 1399,1399,110
1399 IF ( J15 ) 1398,1401,1398
1398 N=N+1
1401 REWIND 5
      IF ( L9-1 ) 1004,1005,503
1005 END FILE 8
      REWIND 8
      GO TO 1004
503 END FILE 8
      CALL UNLOAD(8)
1004 IF ( L4-1 ) 1001,504,601
504 END FILE 4
      CALL UNLOAD(4)
      GO TO 1001
601 END FILE 4
602 REWIND 4

```

```

1001 IF ( L18 ) 1304,603,1304
603 CONTINUE
SUMDSQ=0.0
DO 4013 I=1,M
SA(I) = SDELSQ(I)/SA(I)
4013 SUMDSQ=SUMDSQ+SDELSQ(I)*SCALE(I)**2
SENSE LIGHT 1
CALL MATSTP
4023 IF ( L7-1 ) 4022,4022,1010
1010 WRITE TAPE 3,(PD(I),I=1,N)
4022 CALL CHANGE
IF ( J15 ) 4026,4026,4024
4024 G = MIN1F(G+R(N),0.8/FMAX)
4026 IF ( L17 ) 4027,4027,1300
4027 DO 1200 I=1,N3
IF ( B11(I) ) 11001, 1102, 1102
11001 B11(I)=0.0
1102 IF ( N12(I) ) 402,1200,402
402 IF ( B22(I) ) 1103,1104,1104
1103 B22(I)=0.0
1104 IF ( B33(I) ) 1105, 1106, 1106
1105 B33(I)=0.0
1106 IF ( B11(I)*B22(I)-B12(I)**2/4.0 ) 1107, 1108, 1108
1107 B12(I)=0.0
1108 IF ( B11(I)*B33(I)-B13(I)**2/4.0 ) 1109,11010,11010
1109 B13(I)=0.0
11010 IF ( B22(I)*B33(I)-B23(I)**2/4.0 ) 11011,1200,1200
11011 B23(I)=0.0
1200 CONTINUE
1300 CONTINUE
IF ( L7-1 ) 1304,1304,1301
1301 CONTINUE
WRITE TAPE 3,A,B1,C,COSA,COSB,COSC,J,(J1(I),I=1,J),NAME,N3
DO 1305 I = 1,N3
WRITE TAPE 3, X(I),Y(I),Z(I),B11(I),B22(I),B33(I),B12(I),B13(I),
1 B23(I),N12(I),IDX(I),IDY(I),IDZ(I),IDB11(I),IDB22(I),IDB33(I),
2 IDB12(I),IDB13(I),IDB23(I)
1305 CONTINUE
WRITE TAPE 3,M,J15
WRITE TAPE 3,(SCALE(I),IDSC(I),I=1,M)
IF (J15)1307,1307,1306
1306 WRITE TAPE 3, G,N
1307 CONTINUE
END FILE 3
IF ( L7-2 ) 1303,1303,1302
1302 CONTINUE
REWIND 3
GO TO 1304
1303 CONTINUE
CALL UNLOAD (3)
1304 CONTINUE
CALL OUTPUT
IF ( L3-1 ) 99,97,98
95 READ TAPE 5,N
CALL UNLOAD (5)
96 CALL EXIT
97 PAUSE 7777
GO TO 99
98 IF ( L3-3 ) 50,96,95
END(1,1,0,0,0,1,1,1,C,1,0,C,C,0,0)

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SUBROUTINE INPUT
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEVB(1101),
3 DEVB11(1101),DEVB22(1201),DEVB33(1301),DEVB12(1401),DEVB13(1501),
4 DEVB23(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F0B(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 CDSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 CUSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),ACCSA(11094),CACOSB(11095),BACUSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S(11125),
8B1J(3201),SRHO(11126),
9 SWF(10872),IPCERK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132)
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEVB(1),DEVB11(1),DEVB22(1),
7 DEVB33(1),DEVB12(1),DEVB13(1),DEVB23(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
1 FORMAT (12A6)
2 FORMAT (1X,A5,11A6)
3 FORMAT (35H DATA LOCATION GIVEN INCORRECTLY AS15/1H1)
4 FORMAT ( 19HOSCALE FACTORS ARE 10F10.5)
5 FORMAT (5F5.0,5I5)
6 FORMAT (7F10.5)
7 FORMAT (7E10.3)
8 FORMAT (7F10.5,12)
9 FORMAT (13F5.2)
10 FORMAT (11HOTHER WERE15,30H REFLECTIONS READ IN, OF WHICH15,
1 14H WERE OBSERVED)
11 FORMAT (10HOTHER ARE15,32H OBSERVED REFLECTIONS WITH SCALE13)
12 FORMAT ( 24H0EXTINCTION CORRECTION =1PE10.3)
13 FORMAT ( 33H0DELTA F DOUBLE PRIME CORRECTIONS/
1 (1H 2A6,F6.3))
22 FORMAT (A4,A5,9F7.0)
SENSE LIGHT 0
REWIND 5
IF ( SENSE SWITCH 1 ) 30,31

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30 S1=1.0
100 READ 1,PROBLM
    READ 8,A,B1,C,ALPHA,BETA,GAMMA,XRAY,J15
    READ 1,(NAME(I),I=1,12)
    GO TO 32
31 READ INPUT TAPE 10,1,PROBLM
    READ INPUT TAPE 10,8,A,B1,C,ALPHA,BETA,GAMMA,XRAY,J15
    READ INPUT TAPE 10,1,(NAME(I),I=1,12)
32 CONTINUE
    K3=0
    IF ( ALPHA-1.0 ) 101,101,102
101 COSA=ALPHA
    GO TO 103
102 COSA=COS1F(ALPHA/360.0)
103 IF ( BETA-1.0 ) 104,104,105
104 COSB=BETA
    GO TO 1050
105 COSB=COS1F(BETA/360.0)
1050 IF ( GAMMA-1.0 ) 1051,1051,1052
1051 COSC=GAMMA
    GO TO 1053
1052 COSC=COS1F(GAMMA/360.0)
1053 SINA=SQRTF(1.0-COSA**2)
    SINB=SQRTF(1.0-COSB**2)
    SINC=SQRTF(1.0-COSC**2)
    COSASR=(COSB*COSC-COSA)/(SINB*SINC)
    COSBSR=(COSA*COSC-COSB)/(SINA*SINC)
    COSCSR=(COSA*COSB-COSC)/(SINA*SINB)
    SINASR=SQRTF(1.0-COSASR**2)
    SINBSR=SQRTF(1.0-COSBSR**2)
    ASTAR=0.5/(A*SINC*SINBSR)
    BSTAR=0.5/(B1*SINC*SINASR)
    CSTAR=0.5/(C*SINA*SINBSR)
    BCCOSA=BSSTAR*CSSTAR*CCSASR*2.0
    CACOSB=CSTAR*ASTAR*COSBSR*2.0
    BACOSC=BSSTAR*ASTAR*COSCSR*2.0
    CALL PARMTR
    M=M
    IF ( J7-9 ) 106,1060,1060
1060 IF(S1)33,33,34
    33 WRITE OUTPUT TAPE 9,3,J7
    CALL EXIT
    34 PRINT 3,J7
    PAUSE
    GO TO 100
106 IF ( J11 ) 1054,1055,1054
1054 DELTA=J11
    DELTA=6400./DELTA
1055 J7=J1(7)
    IF(S1)35,35,36
    35 READ INPUT TAPE 10,6,(SCALE(I),I=1,M)
    GO TO 37
    36 CONTINUE
    READ 6,(SCALE(I),I=1,M)
    37 CONTINUE
    WRITE OUTPUT TAPE 9,4,(SCALE(I),I=1,M)
    IF ( J15 ) 202,202,200
200 IF(S1)38,38,39
    38 READ INPUT TAPE 10,7,G
    GO TO 40
    39 READ 7,G
    40 CONTINUE
    WRITE OUTPUT TAPE 9,12,G
    IF ( XRAY ) 201,201,202
201 XRAY=0.7114
202 IF ( J ) 203,203,204

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INPUT
INPUT

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203 IF(S1)41,41,42
41 READ INPUT TAPE 10,6,(SCALE(I+14),I=1,J)
GO TO 43
42 READ 6,(SCALE(I+14),I=1,J)
43 CONTINUE
WRITE OUTPUT TAPE 9,13,(NAME(21-1),NAME(21),SCALE(I+14),I=1,J)
204 SCALE(M+1)=1.0
GO TO (1063,1061,1062,30000,30000,1063,1062,1061),J7
1061 REWIND 8
GO TO 1063
1062 REWIND 7
1063 DO 107 I=1,J
IF ( J11 ) 1064,1064,1065
1064 IF(S1)44,44,45
44 READ INPUT TAPE 10,22,PD(I),R(I),(CMAT(I,I1),I1=1,9)
GO TO 107
45 READ 22,PD(I),R(I),(CMAT(I,I1),I1=1,9)
GO TO 107
1065 IF(S1)46,46,47
46 READ INPUT TAPE 10,9,(CMAT(I,I1),I1=1,65)
GO TO 107
47 READ 9,(CMAT(I,I1),I1=1,65)
107 CCNTINUE
DO 108 I=1,M
SUMFOB(I)=0.0
SUMOBS(I)=0.0
108 K(I)=0
K1=0
I=0
WRITE TAPE 5,I,I,I,J11,J,J12
IF ( J11 ) 1090,1090,109
109 WRITE TAPE 5,NAME,PROBLM,((CMAT(I1,I2),I2=1,65),I1=1,J)
GO TO 110
1090 WRITE TAPE 5,(PD(I),R(I),I=1,6),PROBLM,((CMAT(I,I1),I1=1,9),I=1,6)
110 I=I+1
GO TO (111,112,130,30000,30000,131,130,112),J7
131 READ INPUT TAPE 10,5,H1,H2,H3,FOBS,W,N1,N2
GO TO 113
130 READ TAPE 7,H1,H2,H3,FOBS,W,N1,SQ
GO TO 115
111 READ 5,H1,H2,H3,FOBS,W,N1,N2
GO TO 113
112 READ INPUT TAPE 8,5,H1,H2,H3,FOBS,W,N1,N2
113 SQ=(H1*ASTAR)**2+(H2*BSTAR)**2+(H3*CSTAR)**2
1+H1*H2*BACCSC+H1*H3*CACOSB+H2*H3*BCCOSA
IF ( N2 - 1 ) 115, 116, 115
115 IF ( FOBS )117,118,118
116 FOB=FOBS
FOBS=ABSF(FOB)*FOB
GO TO 119
117 FOB=-SQRTF(FOBS)
GO TO 119
118 FOB=SQRTF(FOBS)
119 CCNTINUE
DO 1240 I1=1,J
IF ( J11 ) 1230,124,1230
1230 S=SQRTF(SQ)
A1=DELTA*S+1.0
M1=A1
A2=M1
F(I1)=CMAT(I1,M1)+(CMAT(I1,M1+1)-CMAT(I1,M1))*(A1-A2)
GO TO 1240
124 F(I1) = CMAT(I1,9)
DO 60 I2=1,7,2
60 F(I1) = F(I1)+CMAT(I1,I2)*EXPF(-SQ*CMAT(I1,I2+1))
1240 CONTINUE

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      CALL WEIGHT
      IF ( SQ ) 205,205,126
205 N1=M+1
126 CONTINUE
      IF ( N1 ) 120,120,121
120 N1=1
121 IF ( FOR ) 123,123,122
122 K(N1)=K(N1)+1
      K1=K1+1
123 CONTINUE
      WRITE TAPE 5,H1,H2,H3,FOB,FOBS,W,N1,SQ,F
      IF ( SQ ) 127,127,110
127 END FILE 5
      REWIND 5
      WRITE OUTPUT TAPE 9, 10, I,K1
      IF ( S1 ) 49,49,48
48 CONTINUE
      PRINT 10,I,K1
49 CONTINUE
      Q=K1-N
      WRITE OUTPUT TAPE 9,11,(K(1),I,I=1,M)
      GO TO (30000,128,129,30000,30000,30000,1290,1280),J7
128 REWIND 8
      GO TO 30000
129 REWIND 7
30000 RETURN
1290 CALL UNLOAD (7)
      GO TO 30000
1280 CALL UNLOAD (8)
      GO TO 30000
      END(1,1,0,0,0,1,1,1,0,1,0,0,0,0,0)

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INPUT

PARMTR

2/08/65

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SUBROUTINE PARMTR
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOR(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),FOB(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
COMMON00
COMMON01
COMMON02
COMMON03
COMMON04
COMMON05
COMMON06
COMMON07
COMMON08
COMMON09
COMMON10
COMMON11
COMMON12
COMMON13
COMMON14
COMMON15
COMMON16
COMMON17
COMMON18
COMMON19
COMMON20
COMMON21
COMMON22

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2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096), COMMON23
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101), COMMON24
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105), L4(11106), L5(11107)COMMON25
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113), COMMON26
6L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),COMMON27
7L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125), COMMON28
8UIJ(3201),SRHO(11126), COMMON29
9 SWF(10872),IPCERK(11127),K3(11130),DEVX(3001),DEVY(3101)) COMMON30
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132)COMMON31
1),K2(11133),NMAX(11134)) COMMON32
DIMENSION CMAT(100,100), B(90),X(45), COMMON33
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45), COMMON34
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20), COMMON35
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6), COMMON36
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),COMMON37
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1), COMMON38
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEVB(1),DEVB11(1),DEVB22(1), COMMON39
7 DEVB33(1),DEVB12(1),DEVB13(1),DEVB23(1),DEVSCA(1),PD(1), COMMON40
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1), COMMON41
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1) COMMON42
DIMENSION SWF(20) COMMON43
1 FORMAT (1H12A6)
6 FORMAT (7F10.5)
7 FORMAT (14I5,12)
8 FORMAT (4F10.5,2I5)
19 FORMAT (26H LATTICE CONSTANTS ARE A =F8.4,4H B =F8.4,4H C =F8.4,7H
1 COSA =F8.5,7H COSB =F8.5,7H COSC =F8.5/1H06X4HATOM9X1HX9X1HY9X1HZ
28X3HB117X3HB227X3HB337X3HB127X3HB137X3HB23)
20 FORMAT (A7,A6,I3,9F10.6)
21 FORMAT (1H )
IF(S1)35,35,36
35 READ INPUT TAPE 10,7,N,M,J,(J1(I),I=1,12)
GO TO 37
36 CONTINUE
READ 7,N,M,J,(J1(I),I=1,12)
37 CONTINUE
N3=0
DO 100 I=1,J
100 N3=N3+XABSF(J1(I))
DO 106 I=1,N3
IF(S1)30,30,31
30 READ INPUT TAPE 10,8,X(I),Y(I),Z(I),B(I),N11(I),N12(I)
GO TO 32
31 CONTINUE
READ 8,X(I),Y(I),Z(I),B(I),N11(I),N12(I)
32 CONTINUE
IF ( N12(I) ) 106,106,1066
1066 IF(S1)33,33,34
33 READ INPUT TAPE 10,6,B11(I),B22(I),B33(I),B12(I),B13(I),B23(I)
GO TO 106
34 READ 6,B11(I),B22(I),B33(I),B12(I),B13(I),B23(I)
106 CONTINUE
I2=0
WRITE OUTPUT TAPE 9,1,PROBLM
WRITE OUTPUT TAPE 9,19,A,B1,C,COSA,COSB,COSC
DO 1061 I=1,J
J13=J1(I)
IF ( J13 ) 1062,1061,1062
1062 WRITE OUTPUT TAPE 9,21
DO 1060 I1=1,J13
I2=I2+1
1060 WRITE OUTPUT TAPE 9,20,NAME(2*I-1),NAME(2*I),I1,X(I2),
1 Y(I2),Z(I2),B(I2),B22(I2),B33(I2),B12(I2),B13(I2),B23(I2)
1061 CONTINUE
RETURN
END(1,1,0,0,0,1,1,1,0,1,0,0,0,0,0)

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PRMT RED
PRMT RED
PRMT RED

SUBROUTINE MATSTP

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COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(1201),SRHO(11126),
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)

5 FORMAT (1H112A6/33H0THE VALUE OF THE DETERMINANT IS IPE12.4
1 //36H0THE POSITIVE DEFINITE CRITERION ARE /(10(I4,1PE8.1)))
7 FORMAT (1H /(9(I4,I3,F6.3)))

IF (SENSE LIGHT 1) 2,1
1 IF(N-NMAX)3,3,4
2 CONTINUE
CALL MATINV(CMAT(IR),PD(500),N)
1099 Q=K2-N
IF (L7-1) 400,401,412
412 REWIND 3
WRITE TAPE 3,PROBLM,N
401 WRITE OUTPUT TAPE 9,5,PROBLM,CMAT(1),(I,CMAT(I+1),I=1,N)
I5=N+N+1
I2=I5
I4=I2
DO 1008 I=1,N

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```

      I2=I2+1
      I3=I5
      DO 1007 I1=1,I
      I3=I3+I1
      I4=I4+1
1007 PD(I1)=CMAT(I4)/SQRTF(CMAT(I2)*CMAT(I3))
      IF ( L7-1 ) 1009,1008,1009
1009 WRITE TAPE 3,(PD(I1),I1=1,I)
1008 WRITE OUTPUT TAPE 9,7,(I,I1,PD(I1),I1=1,I)
      400 I1=2N+1
      I2=N+1
      DO 1100 I=1,N
      I1=I1+1
      I2=I2+1
      PD(I)=SQRTF(CMAT(I1)*SUMDSQ/Q)
1100 R(I)=CMAT(I2)
      GO TO 51
      3 CONTINUE
1122 IR=N+1
      DO 120 I=1,N
      IR=IR+1
120 CMAT(IR)=CMAT(IR)+DELF*PD(I)
      DO 121 I=1,N
      DO 121 I1=1,I
      IR=IR+1
121 CMAT(IR)=CMAT(IR)+PD(I)*PD(I1)
      GO TO 51
      4 L18=1
      51 RETURN
      END(1,1,0,0,0,1,1,1,0,1,0,0,0,0,0)

```

WEIGHT TO HANDLE SEVERAL CASES

2/08/65

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SUBROUTINE WEIGHT
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1 J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),R1(11078),C(11079),COSA(11080),COSH(11081),
9 CUSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 CUSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BC,COSA(11094),CACOSB(11095),BACOSC(11096),
COMMON00
COMMON01
COMMON02
COMMON03
COMMON04
COMMON05
COMMON06
COMMON07
COMMON08
COMMON09
COMMON10
COMMON11
COMMON12
COMMON13
COMMON14
COMMON15
COMMON16
COMMON17
COMMON18
COMMON19
COMMON20
COMMON21
COMMON22
COMMON23

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3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),      COMMON24
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105), L4(11106), L5(11107)COMMON25
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),  COMMON26
6L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),COMMON27
7L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),  COMMON28
88IJ(3201),SRHO(11126),      COMMON29
9 SWF(10872),IPCRK(11127),K3(11130),DEVX(3001),DEVY(3101)      COMMON30
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132)COMMON31
1),K2(11133),NMAX(11134))      COMMON32
DIMENSION CMAT(100,100),      B(90),X(45),      COMMON33
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),  COMMON34
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),      COMMON35
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),      COMMON36
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),COMMON37
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),  COMMON38
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),  COMMON39
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PU(1),      COMMON40
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),      COMMON41
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)      COMMON42
DIMENSION SWF(20)      COMMON43
DIMENSION ZI(6)
IF ( J12 ) 100,100,1
1 GO TO (100,2,3,4,5),J12
2 W=SQRTF(W)
100 RETURN
3 W=1.0/(SQRTF(FOB+0.02*FOBS))
GO TO 100
4 W=W/(SQRTF(FOB+0.02*FOBS))
GO TO 100
5 IF ( SENSE LIGHT 1 ) 53,50
50 IF ( J11 ) 51,52,51
51 DO 510 I=1,J
510 ZI(I)=CMAT(I)/(FLOATF(J1(I)))
GO TO 53
52 DO 520 I=1,J
520 ZI(I)=(CMAT(I,1)+CMAT(I,3)+CMAT(I,5)+CMAT(I,7)+CMAT(I,9))/(FLOATF(
1J1(I)))
53 SENSE LIGHT 1
W=0.0
DO 54 I=1,J
54 W=W+F(I)/ZI(I)
W=FLOATF(N3)/W
GO TO 100
END(1,1,0,0,0,1,1,1,0,1,0,0,0,0,0)

```

MATINV FAP VERSION OF LAS884 COMPATABLE TO FORTRAN
PREPROCESSOR UPDATE PROGRAM

2/08/65

AMAVO SXD COMMON+0000,1

ST A

0002 SOURCE ORDER ERROR

LDQ* 3,4

CH 0004 SOURCE ORDER ERROR

RQL 18

CH 10004 SOURCE ORDER ERROR

XCA

CH 0007 SOURCE ORDER ERROR

STO COMMON+3

CH 0010 SOURCE ORDER ERROR

CLA 1,4

FWAG

CH 0029 SOURCE ORDER ERROR

BMAV1 FDP ,4

CH 0102 SOURCE ORDER ERROR

BMAV2-FDP ,4

CH 0122 SOURCE ORDER ERROR

DMAV1 FDP ,2

CH 0216 SOURCE ORDER ERROR

TRA 4,4

CH 0264 SOURCE ORDER ERROR

COMMON BSS 13

CH 0262 SOURCE ORDER ERROR

69

		00000	ENTRY MATINV
		00000	ENTRY AMAVO
00000	-0634 00 1 0041C	AMAVO SXD COMMON+0000,1	
00001	-0634 00 2 00411	SXD COMMON+0001,2	
00002	0560 60 4 00003	LDQ* 3,4	
00003	-0773 00 0 00022	RQL 18	
00004	-0600 00 0 00421	STQ COMMON+0009,0	
00005	0200 00 0 00421	MPY COMMON+0009,0	
00006	0131 00 0 00000	XCA	
00007	0400 00 0 00421	ADD COMMON+0009,0	
00010	0771 00 0 00001	ARS 0001,0	
00011	0601 00 0 00413	STU COMMON+3	
00012	0500 00 4 00002	CLA 2,4	
00013	0601 00 0 00417	STO COMMON+0007,0	
00014	0400 00 0 00421	ADD COMMON+0009,0	
00015	0621 00 0 00102	STA AMAV1,0	
00016	0621 00 0 00134	STA AMAV2,0	
00017	0621 00 0 00166	STA AMAV3,0	
00020	0621 00 0 00173	STA AMAV4,0	
00021	0621 00 0 00330	STA AMAV5,0	
00022	0621 00 0 00375	STA AMAV6,0	
00023	0400 00 0 00421	ADD COMMON+0009,0	
00024	0621 00 0 00135	STA AMAV7,0	
00025	0621 00 0 00144	STA AMAV8,0	
00026	0621 00 0 00145	STA BMAV1,0	
00027	0621 00 0 00167	STA BMAV2,0	

ST A
ST B

N
N SQUARED INTO AC
N BY N +1
1/2N.N+1 TO AC

FWAD

DN FWAD N

D2N

S884
S884
0002
0003
CH 0004
CH 10004
0005
0006
CH 0007
0008
0009
CH 0010
CH 0011
0012
0013
0014
0015
0016
0017
0018
0019
0020
0021
0022
0023
0024

00030	0621	00	0	00172	STA BMAV3,0		0025
00031	0621	00	0	00326	STA BMAV4,0		0026
00032	0621	00	0	00360	STA BMAV5,0		0027
00033	0621	00	0	00376	STA BMAV6,0		0028
00034	0500	00	4	00001	CLA 1,4	FWAG	CH 0029
00035	0761	00	0	00000	NOP		CH 0030
00036	0400	00	0	00413	ADD COMMON+0003,0	G1/2N.N+1	0031
00037	0621	00	0	00101	STA BMAV7,0		0032
00040	0621	00	0	00146	STA BMAV8,0		0033
00041	0621	00	0	00174	STA CMAV1,0		0034
00042	0621	00	0	00207	STA CMAV2,0		0035
00043	0621	00	0	00212	STA CMAV3,0		0036
00044	0621	00	0	00272	STA CMAV4,0		0037
00045	0621	00	0	00334	STA CMAV5,0		0038
00046	0400	00	0	00421	ADD COMMON+0009,0	G1 2N N PL 3	0039
00047	0621	00	0	00357	STA CMAV6,0		0040
00050	0621	00	0	00402	STA CMAV7,0		0041
00051	0400	00	0	00421	ADD COMMON+0009,0	G1/2N.N+5	0042
00052	0621	00	0	00210	STA CMAV8,0		0043
00053	0621	00	0	00327	STA DMAV1,0		0044
00054	0621	00	0	00351	STA DMAV2,0		0045
00055	0621	00	0	00353	STA DMAV3,0		0046
00056	-0634	00	4	00414	SXD COMMON+0004,4	STORE C	0047
00057	0502	00	0	00116	CLS DMAV4,0	-1	0048
00060	0601	00	0	00416	STO COMMON+0006,0	-1 INITIALS J2	0049
00061	0534	00	4	00421	LXA COMMON+0009,4	N INITIALS C2	0050
00062	0500	00	0	00416	CLA COMMON+0006,0	J2	0051
00063	0400	00	0	00116	ADD DMAV4,0	J2+1	0052
00064	0601	00	0	00416	STO COMMON+0006,0	INTO J2	0053
00065	0601	00	0	00422	STO COMMON+0010,0	J2 INITIALS J1	0054
00066	0601	00	0	00423	STO COMMON+0011,0	J1 STAR EQUALS J1	0055
00067	0500	00	0	00117	CLA DMAV5,0	T12 TR TO 95	0056
00070	0601	00	0	00132	STO DMAV6,0	T12 INTO T1	0057
00071	0500	00	0	00126	CLA DMAV7,0	T37 TR TO 114	0058
00072	0601	00	0	00137	STO DMAV8,0	T37 INTO T3	0059
00073	-0634	00	4	00412	HMAV1 SXD COMMON+0002,4	STORE C2	0060
00074	0534	00	2	00421	IMAV7 LXA COMMON+0009,2	Q1 N INITIALS B1	0061
00075	0534	00	4	00421	LXA COMMON+0009,4	C1	0062
00076	0500	00	0	00413	CLA COMMON+0003,0	1/2N.N+1	0063
00077	0402	00	0	00422	SUB COMMON+0010,0	1/2N.N+1 - J1	0064
00100	0734	00	1	00000	PAX ,1	INITs A1	0065
00101	0500	00	1	00000	BMAV7 CLA ,1	31 SETS G1/2N.N+1	0066
00102	0601	00	4	00000	AMAV1 STO ,4	12 SETS DN	0067
00103	0500	00	0	00423	CLA COMMON+0011,0	J1 STAR	0068
00104	-0100	00	0	00106	TNZ EMAV1,0		0069
00105	-0634	00	1	00413	SXD COMMON+0003,1	STORE A1 FOR DIAG G	0070
00106	0402	00	0	00116	EMAV1 SUB DMAV4,0	J1-1	0071
00107	0601	00	0	00423	STO COMMON+0011,0	J1-1 INTO J1 STAR	0072
00110	-0120	00	0	00127	TMI EMAV2,0	J1 NEG	0073
00111	-2 00001	2	00112	00112	TXN EMAV3,2,0001	B1 PAGE 3	0074
00112	-0634	00	2	00113	EMAV3 SXD EMAV4,2		0075
00113	2 00000	1	00130	00130	EMAV4 TIX EMAV5,1	77 SETS B1 A NEVER B	0076
00114	+201400000000				HMAV2 DEC +0.10000000000E+01	FLT 1	0077

00115 0000 00 0 00000 IMAV2 HTR ,0
00116 0000 00 0 00001 DMAV4 HTR 0001,0
00117 0020 00 0 00133 DMAV5 TRA EMAV6,0
00120 0020 00 0 00161 GMAV4 TRA EMAV7,0
00121 0020 00 0 00255 IMAV1 TRA EMAV8,0
00122 0020 00 0 00320 IMAV8 TRA FMAV1,0
00123 0020 00 0 00372 JMAV4 TRA FMAV2,0
00124 0020 00 0 00245 HMAV5 TRA FMAV3,0
00125 0020 00 0 00313 IMAV6 TRA FMAV4,0
00126 0020 00 0 00154 DMAV7 TRA FMAV5,0
00127 -2 00001 1 00131 EMAV2 TNX FMAV6,1,0001
00130 2 00001 4 00101 EMAV5 TIX BMAV7,4,0001
00131 -0534 00 4 00412 FMAV6 LXD COMMON+0002,4
00132 0420 00 0 00000 DMAV6 HPR ,0
00133 0534 00 2 00421 EMAV6 LXA COMMON+0009,2
00134 0500 00 2 00000 AMAV2 CLA ,2
00135 0601 00 2 00000 AMAV7 STO ,2
00136 2 00001 2 00134 TIX AMAV2,2,0001
00137 0420 00 0 00000 DMAV8 HPR ,0
00140 -0534 00 1 00424 GMAV8 LXD COMMON+0012,1
00141 2 00001 1 00142 TIX FMAV7,1,0001
00142 -0534 00 2 00412 FMAV7 LXD COMMON+0002,2
00143 2 00001 2 00144 TIX AMAV8,2,0001
00144 0502 00 2 00000 AMAV8 CLS ,2
00145 0241 00 4 00000 BMAV1 FDP ,4
00146 -0600 00 1 00000 BMAV8 STQ ,1
00147 2 00001 1 00150 TIX FMAV8,1,0001
00150 2 00001 2 00144 FMAV8 TIX AMAV8,2,0001
00151 2 00001 4 00152 TIX GMAV1,4,0001
00152 3 00001 4 00062 GMAV1 TXH GMAV2,4,0001
00153 0020 00 0 00205 TRA GMAV3,0
00154 0500 00 0 00120 FMAV5 CLA GMAV4,0
00155 0601 00 0 00132 STO DMAV6,0
00156 -0534 00 2 00413 LXD COMMON+0003,2
00157 -0634 00 2 00424 SXD COMMON+0012,2
00160 0020 00 0 00200 TRA GMAV5,0
00161 0500 00 0 00421 EMAV7 CLA COMMON+0009,0
00162 0402 00 0 00422 SUB COMMON+0010,0
00163 0734 00 2 00000 PAX ,2
00164 -0534 00 4 00412 LXD COMMON+0002,4
00165 -0534 00 1 00413 LXD COMMON+0003,1
00166 0502 00 4 00000 AMAV3 CLS ,4
00167 0241 00 4 00000 BMAV2 FDP ,4
00170 -0600 00 0 00415 STQ COMMON+0005,0
00171 0560 00 0 00415 GMAV7 LDQ COMMON+0005,0
00172 0260 00 2 00000 BMAV3 FMP ,2
00173 0300 00 2 00000 AMAV4 FAD ,2
00174 0601 00 1 00000 CMAV1 STO ,1
00175 -2 00001 2 00177 TNX GMAV6,2,0001
00176 2 00001 1 00171 TIX GMAV7,1,0001
00177 -2 00001 1 00140 GMAV6 TNX GMAV8,1,0001
00200 0500 00 0 00422 GMAV5 CLA COMMON+0010,0
00201 0400 00 0 00116 ADD DMAV4,0

0 0078
1 0079
T12 0080
T14 0081
T16 0082
T17 0083
T18 0084
T32 0085
T33 0086
T37 0087
A1 PAGE 3 0088
C1 0089
UNSTORE C2 OR C4 0090
T1 58 103 154 161 191 0091
T12 TAR N INITS B21 0092
13 SETS DN 0093
19 SETS D2N 0094
B21 GR 1 0095
T3 60 185 0096
1ST PASS DIAG AD INA2 0097
A2 PAGE 3 A2 NEVER 1 0098
C2 INITIALS B22 0099
B22 NEVER 1 0100
20 SETS D2N 0101
CH 0102
32 SETS G1/2N.N+1 0103
A2 NEVER 1 0104
B22 PAGE 3 0105
C2 PAGE 2 NEVER 1 0106
EXIT FROM FORM A2JK 0107
T14 TR TO 117 0108
T14 INTO T1 0109
DIAG AD 1ST PASS 0110
0111
0112
0113
T14 TARGET N 0114
N-J1 0115
NIJ1 INITIALS B23 P2 0116
UNSTORE C2 0117
DIAG ADDRESS INITS A2 0118
14 SETS DN 0119
CH 0122
ST QUNT 0121
0122
23 SETS D2N B23 0123
15 SETS DN B23 0124
33 SETS G1/2N.N+1 0125
B23 PAGE 2 0126
A2 NEVER 1 0127
A2 0128
J1 0129
J1+1 0130

00202	0601	00	0	00422	STO COMMON+0010,0
00203	0601	00	0	00423	STO COMMON+0011,0
00204	0020	00	0	00073	TRA HMAV1,0
00205	0534	00	4	00421	GMAV3 LXA COMMON+0009,4
00206	0534	00	1	00413	LXA COMMON+0003,1
00207	0500	00	1	00000	CMAV2 CLA ,1
00210	0601	00	4	00000	CMAV8 STO ,4
00211	0500	00	0	00114	CLA HMAV2,0
00212	0601	00	1	00000	CMAV3 STO ,1
00213	-0634	00	4	00214	SXD HMAV3,4
00214	-2	00000	1	00216	HMAV3 TNX HMAV4,1
00215	2	00001	4	00207	TIX CMAV2,4,0001
00216	0500	00	0	00124	HMAV4 CLA HMAV5,0
00217	0601	00	0	00137	STO DMAV8,0
00220	0500	00	0	00421	CLA COMMON+0009,0
00221	0400	00	0	00116	ADD DMAV4,0
00222	0621	00	0	00416	STA COMMON+0006,0
00223	0500	00	0	00416	IMAV5 CLA COMMON+0006,0
00224	0402	00	0	00116	SUB DMAV4,0
00225	0601	00	0	00416	STO COMMON+0006,0
00226	0402	00	0	00116	SUB DMAV4,0
00227	0734	00	4	00000	PAX ,4
00230	-2	00001	4	00275	TNX HMAV6,4,0001
00231	0500	00	0	00417	CLA COMMON+0007,0
00232	0400	00	0	00416	ADD COMMON+0006,0
00233	0621	00	0	00264	STA HMAV7,0
00234	0400	00	0	00421	ADD COMMON+0009,0
00235	0621	00	0	00265	STA HMAV8,0
00236	0500	00	0	00117	IMAV4 CLA DMAV5,0
00237	0601	00	0	00132	STO DMAV6,0
00240	0500	00	0	00416	CLA COMMON+0006,0
00241	0402	00	0	00116	SUB DMAV4,0
00242	0601	00	0	00422	STO COMMON+0010,0
00243	0601	00	0	00423	STO COMMON+0011,0
00244	0020	00	0	00073	TRA HMAV1,0
00245	0500	00	0	00121	FMAV3 CLA IMAV1,0
00246	0601	00	0	00132	STO DMAV6,0
00247	0500	00	0	00412	CLA COMMON+0002,0
00250	0771	00	0	00022	ARS 0018,0
00251	0402	00	0	00116	SUB DMAV4,0
00252	0601	00	0	00422	STO COMMON+0010,0
00253	0601	00	0	00423	STO COMMON+0011,0
00254	0020	00	0	00073	TRA HMAV1,0
00255	0502	00	0	00412	EMAV8 CLS COMMON+0002,0
00256	0771	00	0	00022	ARS 0018,0
00257	0400	00	0	00416	ADD COMMON+0006,0
00260	0734	00	2	00000	PAX ,2
00261	-0534	00	1	00413	LXD COMMON+0003,1
00262	0500	00	0	00115	CLA IMAV2,0
00263	0601	00	0	00415	STO COMMON+0005,0
00264	0560	00	2	00000	HMAV7 LDQ ,2
00265	0260	00	2	00000	HMAV8 FMP ,2
00266	0300	00	0	00415	FAD COMMON+0005,0

J1+1 INTO J1	0131
J1 STAR	0132
	0133
N INITS C3 ENT	0134
1/2N.N+1 INITIALS A3	0135
34 SETS G1/2N.N+1 A3	0136
42 SETS G1/2N.N+5 C3	0137
FLOATING 1	0138
35 SETS G1/2N.N+1 A3	0139
C3 TO DEC	0140
A3 135 SETS EX 1 DIAG	0141
C3	0142
T32 TR TO 160	0143
T32 INTO T3	0144
N	0145
N+1	0146
N+1 INITIALS J3	0147
J3	0148
J3-1	0149
J3-1 INTO J3	0150
J3-1	0151
J3-1 INITIALS C4	0152
	0153
DO	0154
DJ3	0155
DJ3	0156
DJ3+N	0157
	0158
T12 TR TO 95	0159
T12 INTO T1	0160
J3	0161
J3-1	0162
J3 MIN 1 INTO J3	0163
J1 STAR	0164
	0165
T16 TR TO 167 T32TAR	0166
T16	0167
C4 TO AC DEC	0168
C4 TO AC AD	0169
C4-1	0170
C4 MINUS 1 INTO J1	0171
C4 MIN 1 TO J1 STAR	0172
	0173
MINUS C4 TO AC DEC	0174
-C4 TO AC AD	0175
J3-C4 TO AC AD	0176
J3-C4 INITIALS B4	0177
A1 INITIALS A4	0178
0	0179
0 INITIALS 1-5	0180
150 SETS DJ3 84	0181
151 SETS DN+J3 84	0182
SUM	0183


```

00354 0534 00 2 00421      LXA COMMON+0009,2
00355 0500 00 0 00123      CLA JMAV4,0
00356 0601 00 0 00132      STO DMAV6,0
00357 0500 00 2 00000      CMAV6 CLA ,2
00360 0601 00 2 00000      BMAV5 STO ,2
00361 2 00001 2 00357      TIX CMAV6,2,0001
00362 0534 00 4 00421      LXA COMMON+0009,4
00363 0502 00 0 00116      CLS DMAV4,0
00364 0601 00 0 00422      STO COMMON+0010,0
00365 0500 00 0 00422      JMAV5 CLA COMMON+0010,0
00366 0400 00 0 00116      ADD DMAV4,0
00367 0601 00 0 00422      STO COMMON+0010,0
00370 0601 00 0 00423      STO COMMON+0011,0
00371 0020 00 0 00073      TRA HMAV1,0
00372 0534 00 2 00421      FMAV2 LXA COMMON+0009,2
00373 0500 00 0 00115      CLA IMAV2,0
00374 0601 00 0 00415      STO COMMON+0005,0
00375 0560 00 2 00000      AMAV6 LDQ ,2
00376 0260 00 2 00000      BMAV6 FMP ,2
00377 0300 00 0 00415      FAD COMMON+0005,0
00400 0601 00 0 00415      STO COMMON+0005,0
00401 2 00001 2 00375      TIX AMAV6,2,0001
00402 0601 00 4 00000      CMAV7 STO ,4
00403 2 00001 4 00365      TIX JMAV5,4,0001
00404 -0534 00 1 00410      LXD COMMON+0000,1
00405 -0534 00 2 00411      LXD COMMON+0001,2
00406 -0534 00 4 00414      LXD COMMON+0004,4
00407 0020 00 4 00004      TRA 4,4
00410      COMMON BSS 13
      MATINV SYN AMAVO
      END

```

```

N INITIALS B71      0237
T18 TR TO 23M      0238
T18 INTO T1        0239
39 SETS G1/2N.N+3  0240
25 SETS D2N        0241
      0242
N INITIALS C72      0243
-1                  0244
-1 INITIALS J1      0245
J1                  0246
J1+1                0247
J1+1 INTO J1        0248
      J1 STAR      0249
      0250
N INITIALS B72      0251
0                    0252
0 INITIALS SUM      0253
17 SETS DN B72      0254
26 SETS D2N        0255
FORM AJIR INV BR = XJ 0256
SUM                  0257
B72                  0258
40 SETS G1/2N.N+3 C72 0259
C72                  0260
RESTGRE A           0261
      B           0262
      C           0263
CH 0264
CH 0262
$884

```

MATINV FAP VERSION OF LAS884 COMPATABLE TO FORTRAN
POST PROCESSOR ASSEMBLY DATA

2/08/65

425 IS THE FIRST LOCATION NOT USED BY THIS PROGRAM

REFERENCES TO DEFINED SYMBOLS

0	AMAV0	0, 425
102	AMAV1	15
134	AMAV2	16, 136
166	AMAV3	17
173	AMAV4	20
330	AMAV5	21
375	AMAV6	22, 401
135	AMAV7	24
144	AMAV8	25, 143, 150
145	BMAV1	26
167	BMAV2	27
172	BMAV3	30


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121 IMAV1 245
115 IMAV2 262, 320, 373
271 IMAV3 270
236 IMAV4 273
223 IMAV5 274
125 IMAV6 275
74 IMAV7 312, 317, 345
122 IMAV8 313
346 JMAV1 335
303 JMAV2 344
350 JMAV3 352
123 JMAV4 355
365 JMAV5 403
410 COMMON 0, 1, 4, 5, 7, 11, 13, 14, 23, 36, 46, 51, 56, 60, 61, 62, 64
        65, 66, 73, 74, 75, 76, 77, 103, 105, 107, 131, 133, 140, 142, 156, 157, 161
        162, 164, 165, 170, 171, 200, 202, 203, 205, 206, 220, 222, 223, 225, 231, 232, 234
        240, 242, 243, 247, 252, 253, 255, 257, 261, 263, 266, 267, 277, 300, 302, 305, 307
        310, 311, 315, 316, 321, 322, 323, 325, 331, 332, 336, 337, 341, 342, 343, 346, 354
        362, 364, 365, 367, 370, 372, 374, 377, 400, 404, 405, 406
0 MATINV 0, 425

```

NO ERROR IN ABOVE ASSEMBLY.

402 LINES OUTPUT.

110401

2/08/65

PROGRAM TO MAKE ALL STORAGE USABLE

SST

BINARY CARD NO. PCDELTA0		ENTRY	IPCDEL
00000			
BINARY CARD NO. PCDELTA1			
00000	0500 00 0 00015	IPCDEL CLA	=077777000000
00001	-0320 00 0 03733	ANA	(PCBK)
00002	0601 00 0 00012	STO	TOP
00003	0500 00 0 00013	CLA	=077777
00004	-0320 00 0 03733	ANA	(PCBK)
00005	0767 00 0 00022	ALS	18
00006	0402 00 0 00012	SUB	TOP
00007	0760 00 0 00003	SSP	
00010	0400 00 0 00014	ADD	=01000000
00011	0020 00 4 00002	TRA	2.4
00012	+000000000000	TOP DEC	0.0
		END	

LITERALS

00013	000000077777
00014	000001000000
00015	077777000000

POST PROCESSOR ASSEMBLY DATA

16 IS THE FIRST LOCATION NOT USED BY THIS PROGRAM

REFERENCES TO DEFINED SYMBOLS

12	TOP	2, 6
73600	BUTTOP	
3734	BOTTOM	
3732	DATEBX	
2	FINTAP	
3730	FLAGBX	
0	IPCDEL	0
1	LIBTAP	
3731	LINECT	
7	MBNTAP	
10	MCHTAP	
5	MINFAP	
6	MLSTAP	
3	SINTAP	
11	SNPTAP	
122	SYSACC	
114	SYSCEM	
155	SYSCK1	
156	SYSCK2	
120	SYSCLR	
144	SYSCLR	
102	SYSCLR	
124	SYSCLD	
101	SYSCLD	
115	SYSCLD	
77777	SYSCLD	
132	SYSGET	
117	SYSIDR	
151	SYSINI	
152	SYSIN2	
116	SYSIOX	
133	SYSJOB	
104	SYSKEY	

140 SYSLB1
 141 SYSLB2
 142 SYSLB3
 143 SYSLB4
 121 SYSLDR
 3720 SYSORG
 147 SYSOU1
 150 SYSOU2
 146 SYSPCH
 123 SYSPID
 106 SYSPDS
 153 SYSPPI
 154 SYSPPI2
 145 SYSPRT
 103 SYSRET
 113 SYSRPT
 126 SYSSLD
 105 SYSSWS
 1 SYSTAP
 127 SYSTCH
 100 SYSTRA
 131 SYSTWT
 111 SYSUAV
 110 SYSUBC
 112 SYSUCW
 107 SYSUNI
 157 SYSUT1
 160 SYSUT2
 161 SYSUT3
 162 SYSUT4
 4 TINTAP
 77677 TOPMEM
 702 (ACTIV
 703 (ACTVX
 720 (BCD5R
 721 (BCD5X
 10000 (CHKU)
 741 (CHPSW
 724 (CHXAC
 750 (CHXSP
 717 (CKWAT
 746 (COMMD
 736 (COMMM
 722 (CVPRT
 73662 (DATE)
 716 (DECVA
 715 (DECVD
 73645 (DGLD)
 73603 (DIAG)
 710 (ENHSW
 73665 (ENDS)
 732 (ETTXI
 743 (FDAMT
 73660 (FGBX)
 747 (IBCDZ
 740 (IOXS1
 73667 (LBLD)
 73652 (LIBT)
 73661 (LNCT)
 73600 (LOAD)
 73666 (LUOR)
 737 (LTPOS
 73644 (MECL)
 73664 (MSLN)
 704 (NDATA
 705 (NDSLX

712 (PAUSE
 711 (PAWSX
 3733 (PCBK) 1, 4
 73651 (PGCT)
 73614 (PNCH)
 73611 (PRNT)
 706 (PROUT)
 707 (PUNCH)
 40014 (RBEC)
 40004 (RBEP)
 40010 (RBNC)
 40000 (RBNP)
 727 (RCHXI)
 726 (RCTXI)
 40016 (RDEC)
 40006 (RDEP)
 40012 (RDNC)
 40002 (RDNP)
 73622 (REST)
 73672 (SCHU)
 744 (SDCXI)
 73643 (SECL)
 20010 (SKBC)
 20000 (SKBP)
 20012 (SKDC)
 20002 (SKDP)
 1000 (SNAP)
 73663 (SNCT)
 73617 (STAT)
 745 (STCXI)
 73626 (STDN)
 723 (STOPD)
 713 (STOPX)
 10003 (SUAV)
 10002 (SUNV)
 714 (SYMUN)
 73606 (TAPE)
 730 (TCOXI)
 733 (TEFXI)
 4000 (TPER)
 735 (TRAPS)
 734 (TRAPX)
 731 (TRCXI)
 742 (TRPSW)
 725 (URRXI)
 40011 (WBNC)
 40001 (WBNP)
 40013 (WDNC)
 40003 (WDNP)
 40015 (WEFC)
 40005 (WEFP)
 40031 (WROW)

NO ERROR IN ABOVE ASSEMBLY.

192 LINES OUTPUT.

110424

ALPHA

2/08/65

			ENTRY	ALPHA
00000	0760 00 0 00000	00000	ALPHA CHS	
00001	0400 00 0 00022	00002	ADD	NINE
00002	0100 00 0 00004	00003	TZE	A
00003	-0120 00 0 00006	00004	TMI	B
00004	0400 00 0 00024	00005	ADD	A1
00005	0020 00 0 00021	00006	TRA	G
00006	0400 00 0 00022	00007	ADD	NINE
00007	0100 00 0 00011	00010	TZE	C
00010	-0120 00 0 00013	00011	TMI	D
00011	0400 00 0 00025	00012	ADD	A1+1
00012	0020 00 0 00021	00013	TRA	G
00013	0400 00 0 00023	00014	ADD	NINE+1
00014	0100 00 0 00016	00015	TZE	E
00015	-0120 00 0 00020	00016	TMI	F
00016	0400 00 0 00026	00017	ADD	A1+2
00017	0020 00 0 00021	00020	TRA	G
00020	0500 00 0 00027	00021	F CLA	A1+3
00021	0020 00 4 00001	00022	G TRA	1,4
00022	+000011000000	00023	NINE DEC	9817,8817
00023	+000010000000	00024	A1 HCI	4, I R Z ALPHA
00024	606031606060	00025		
00025	606051606060	00026		
00026	606071606060	00027		
00027	214347302160			

END

POST PROCESSOR ASSEMBLY DATA

30 IS THE FIRST LOCATION NOT USED BY THIS PROGRAM

REFERENCES TO DEFINED SYMBOLS

4	A	2		
6	B	3		
11	C	7		
13	D	10		
16	E	14		
20	F	15		
21	G	5,	12,	17
24	A1	4,	11,	16,
22	NINE	1,	6,	13
0	ALPHA	0		

NO ERROR IN ABOVE ASSEMBLY.

48 LINES OUTPUT.

110448

2/08/65

			00001	ENTRY SIN1	
			00000	ENTRY COS1	
00000	0300	00 0	00054	COS1 FAD A0051,0	
00001	0560	00 0	00055	SIN1 LDQ A0052,0	
00002	0601	00 0	00056	STO A0053,0	MF74003
00003	0760	00 0	00003	SSP ,0	MF74004
00004	0040	00 0	00045	TLQ A0054,0	MF74005
00005	0402	00 0	00052	SUB A0055,0	MF74006
00006	-0120	00 0	00030	TMI A0056,0	MF74007
00007	0400	00 0	00052	ADD A0055,0	MF74008
00010	-0300	00 0	00055	UFA A0052,0	MF74009
00011	-0600	00 0	00057	STQ A0057,0	MF74010
00012	0765	00 0	00002	LRS 0002,0	MF74011
00013	-0754	00 0	00002	B0054 PXD 0002,0	MF74012
00014	-0773	00 0	00001	RQL 0001,0	MF74013
00015	-0600	00 0	00060	STQ A0058,0	MF74014
00016	0763	00 0	00001	LLS 0001,0	MF74015
00017	0100	00 0	00021	TZE B0051,0	MF74016
00020	0500	00 0	00054	CLA A0051,0	MF74017
00021	-0302	00 0	00057	B0051 UFS A0057,0	MF74018
00022	0560	00 0	00060	LDQ A0058,0	MF74019
00023	0763	00 0	00000	LLS ,0	MF74020
00024	0560	00 0	00056	LDQ A0053,0	MF74021
00025	0162	00 0	00027	TQP B0052,0	MF74022
00026	0760	00 0	00002	CHS ,0	MF74023
00027	0601	00 0	00056	B0052 STO A0053,0	MF74024
00030	0560	00 0	00056	A0056 LDQ A0053,0	MF74025
00031	0260	00 0	00056	FMP A0053,0	MF74026
00032	0601	00 0	00057	STO A0057,0	MF74027
00033	0560	00 0	00047	LDQ B0053,0	MF74028
00034	-0634	00 4	00060	SXD A0058,4	MF74029
00035	0534	00 4	00013	LXA B0054,4	MF74030
00036	0260	00 0	00057	B0055 FMP A0057,0	MF74031
00037	0300	00 4	00052	FAD A0055,4	MF74032
00040	0765	00 0	00043	LRS 0035,0	MF74033
00041	2 00001	4 00036		TIX B0055,4,0001	MF74034
00042	0260	00 0	00056	FMP A0053,0	MF74035
00043	-0534	00 4	00060	LXD A0058,4	MF74036
00044	0020	00 4	00001	TRA 0001,4	MF74037
00045	0500	00 0	00053	A0054 CLA B0056,0	MF74038
00046	0020	00 4	00001	TRA 0001,4	MF74039
00047	+207451644256			B0053 DEC +7.44552448000E+01	MF74040
00050	-206511252531			B0057 DEC -4.11666688000E+01	MF74041
00051	+203622051264			H0058 DEC +6.28251200000E+00	MF74042
00052	+176000000000			A0055 OCT 176000000000	MF74043
00053	+201000000000			B0056 OCT 201000000000	MF74044
00054	+177400000000			A0051 DEC +2.50000000000E-01	MF74045
00055	+231000000000			A0052 OCT 231000000000	MF74046
00056	0000	00 0	00000	A0053 HTR ,0	MF74047
00057	0000	00 0	00000	A0057 HTR ,0	MF74048
00060	0000	00 0	00000	A0058 HTR ,0	MF74049
				END	MF74

POST PROCESSOR ASSEMBLY DATA

61 IS THE FIRST LOCATION NOT USED BY THIS PROGRAM

REFERENCES TO DEFINED SYMBOLS

0	COS1	0	
1	SIN1	0	
54	A0051	0,	20
55	A0052	1,	10
56	A0053	2,	24, 27, 30, 31, 42
45	A0054	4	

52	A0055	5,	7,	37
30	A0056	6,		
57	A0057	11,	21,	32, 36
60	A0058	15,	22,	34, 43
21	B0051	17		
27	B0052	25		
47	B0053	33		
13	B0054	35		
36	B0055	41		
53	B0056	45		
50	B0057			
51	B0058			

NO ERROR IN ABOVE ASSEMBLY.

82 LINES OUTPUT.

110472

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SUBROUTINE OUTPUT
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IOZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSH(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMOSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8BIJ(3201),SRHO(11126),
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132)
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IOZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1))
DIMENSION SWF(20)
DIMENSION BIJ(9),ST(6)
1 FORMAT (1H112A6)
2 FORMAT (6F10.7,I5)
3 FORMAT (1H02A6,I3,3XA6,3XA1,3F14.8,1PE18.4,I10,/(28XA1,0P3F14.8,1P
1E18.4,I10))
4 FORMAT ( ,28X1H83F14.8,1PE18.4,I10)
5 FORMAT ( ,26XA3,0P3F14.8,1PE18.4,I10)
6 FORMAT (7F10.5)
7 FORMAT (22HOEXTINCTION CORRECTION 7X3(3X1PE11.4),E18.4,I10)
8 FORMAT (4F10.7,2I5,I15)
9 FORMAT (1P7E10.3)
10 FORMAT (42H STANDARD DEVIATION OF ELECTRON DENSITY IS 1PE12.3,
1 46H TIMES THE SQUARE ROOT OF P (THE MULTIPLICITY) )
11 FORMAT (12A6)
12 FORMAT (A7,A6,I7)
13 FORMAT (4F10.7,I5)
14 FORMAT (18HOTHIS IS CYCLE NO.13,13H IN THIS RUN.15,22H REFLECTIONS
1 WERE USED/1H )
15 FORMAT (3H R=F10.5,27H SUM OF RESIDUALS SQUARED =1PE12.5,

```

OUTPUT

```

1 24H FOR DATA SET WITH SCALE I3)
16 FORMAT (12H OVERALL R =F10.5,27H SUM OF RESIDUALS SQUARED =F12.2) OUTPUT
17 FORMAT (70H0 ATOM NAME NO. POS. SET PARA. CHANGE STD. DE
1V. NEW VALUE7X11HDELTA/SIGMA)
18 FORMAT (1H06X5HSCALEI4,13X0P3F14.8,1PE18.4,I10)
19 FORMAT (4H R =F8.4,13H WEIGHTED R =F8.4, OUTPUT
1 12H SUM DELSQ =1PE12.5,19H SUM. DELSQ/ SUM W =E12.5,
2 24H FOR DATA SET WITH SCALE I3) OUTPUT
20 FORMAT (13H0 OVERALL R =F8.4,13H WEIGHTED R =F8.4, OUTPUT
1 27H SUM OF RESIDUALS SQUARED =1PE12.5) OUTPUT
21 FORMAT (1H1)
22 FORMAT (1H$4F10.7,2I5,I15)
23 FORMAT (1H$6F10.7,I5)
24 FORMAT (1H$7F10.5)
25 FORMAT (1H$1PE10.3)
26 FORMAT (1H$12A6)
27 FORMAT (2H$ 2A6,I7)
28 FORMAT (1H012A6)
BIJ(1) = 3HB11
BIJ(2) = 3HB22
BIJ(3) = 3HB33
BIJ(4) = 3HB12
BIJ(5) = 3HB13
BIJ(6) = 3HB23
BIJ(7) = 1HX
BIJ(8) = 1HY
BIJ(9) = 1HZ
K3=K3+1
IF (S1)30,30,31
30 IF (SENSE SWITCH 6 ) 31,32
31 PRINT 28,PROBLM
PRINT 14,K3,K2
32 CONTINUE
WRITE OUTPUT TAPE 9,1,PROBLM
WRITE OUTPUT TAPE 9,14,K3,K2
10000 SD=0.0
SF=0.0
SDW=0.0
SFW=0.0
DO 10001 I=1,M
R=SUMDEL(I)/(SUMFOR(I))
ST(I)=ABSF(DELSCA(I)/DEVSCA(I))
IF ( J12 ) 300,300,1100
300 IF ( S1 ) 34,34,33
33 PRINT 15,R,SDELSQ(I),I
34 CONTINUE
WRITE OUTPUT TAPE 9,15,R,SDELSQ(I),I
GO TO 1101
1100 WR=SWF(I)/SUMOBS(I)
IF ( S1 ) 36,36,35
35 CONTINUE
PRINT 19,R,WR,SDELSQ(I),SA(I),I
36 CONTINUE
WRITE OUTPUT TAPE 9,19,R,WR,SDELSQ(I),SA(I),I
SDW=SDW+SWF(I)
SFW=SFW+SUMOBS(I)
1101 SD=SD+SUMDEL(I)
10001 SF=SF+SUMFOR(I)
IF ( M-1 ) 10003, 10003, 10002
10002 R=SD/SF
IF ( J12 ) 301,301,1102
301 IF ( S1 ) 38,38,37
37 PRINT 16,R,SUMDSQ
38 CONTINUE
WRITE OUTPUT TAPE 9,16,R,SUMDSQ
10003 V = A*B1*C*SINASR*SINB*SINC

```

```

      SRHO=SQRTF(SRHO)/V
      WRITE OUTPUT TAPE 9,10,SRHO
      IF ( S1 ) 40,40,39
39  CONTINUE
      PRINT 10,SRHO
40  CONTINUE
      N4 = 3*M+8
      WRITE OUTPUT TAPE 9,17
      WRITE OUTPUT TAPE 9,18,(I,DELSCA(I),DEVSCA(I),SCALE(I),
1  ST(I),IDSC(I),I=1,M)
      IF(L18)302,302,100
302 IF ( SENSE SWITCH 6 ) 101,102
101 PRINT 17
      PRINT 18,(I,DELSCA(I),DEVSCA(I),SCALE(I),ST(I),IDSC(I),I=1,M)
102 I2=0
      DO 11111 I = 1,J
        J13=J1(I)
        IF ( J13 ) 11111,11111,50
50  DO 11000 I1=1,J13
        I2=I2+1
        IF ( N12(I2) ) 110,110,111
111 IF ( N4-49 ) 112,112,207
110 IF ( N4-54 ) 112,112,207
207 WRITE OUTPUT TAPE 9,1,PROBLEM
      WRITE OUTPUT TAPE 9,17
      N4=3
112 N4=N4+4
      POS=ALPHAF( N11(I2) )
      ST(1)=ABSF(DELV(I2)/DEVX(I2))
      ST(2)=ABSF(DELY(I2)/DEVY(I2))
      ST(3)=ABSF(DELV(I2)/DEVZ(I2))
      WRITE OUTPUT TAPE 9,3,NAME(2I-1),NAME(2I),I1,POS,BIJ(7),DELV(I2),
1  DEVX(I2),X(I2),ST(1),IDV(I2),BIJ(8),DELY(I2),DEVY(I2),Y(I2),ST(2)
2  ,IDY(I2),BIJ(9),DELV(I2),DEVZ(I2),Z(I2),ST(3),IDZ(I2)
      IF ( SENSE SWITCH 6 ) 200,201
200 CONTINUE
      PRINT 3,NAME(2I-1),NAME(2I),I1,POS,BIJ(7),DELV(I2),
1  DEVX(I2),X(I2),ST(1),IDV(I2),BIJ(8),DELY(I2),DEVY(I2),Y(I2),ST(2)
2  ,IDY(I2),BIJ(9),DELV(I2),DEVZ(I2),Z(I2),ST(3),IDZ(I2)
201 IF ( N12(I2) ) 202,202,204
202 N4=N4+1
      ST(1)=ABSF(DELB(I2)/DEV8(I2))
      WRITE OUTPUT TAPE 9,4,DELB(I2),DEV8(I2),B(I2),ST(1),IDB(I2)
      IF ( SENSE SWITCH 6 )203,11000
203 PRINT 4,DELB(I2),DEV8(I2),B(I2),ST(1),IDB(I2)
      GO TO 11000
204 N4=N4+6
      ST(1)=ABSF(DELB11(I2)/DEV811(I2))
      ST(2)=ABSF(DELB22(I2)/DEV822(I2))
      ST(3)=ABSF(DELB33(I2)/DEV833(I2))
      ST(4)=ABSF(DELB12(I2)/DEV812(I2))
      ST(5)=ABSF(DELB13(I2)/DEV813(I2))
      ST(6)=ABSF(DELB23(I2)/DEV823(I2))
      WRITE OUTPUT TAPE 9,5
1  ,BIJ(1),DELB11(I2),DEV811(I2),B11(I2),ST(1),IDB11(I2)
2  ,BIJ(2),DELB22(I2),DEV822(I2),B22(I2),ST(2),IDB22(I2)
3  ,BIJ(3),DELB33(I2),DEV833(I2),B33(I2),ST(3),IDB33(I2)
4  ,BIJ(4),DELB12(I2),DEV812(I2),B12(I2),ST(4),IDB12(I2)
5  ,BIJ(5),DELB13(I2),DEV813(I2),B13(I2),ST(5),IDB13(I2)
6  ,BIJ(6),DELB23(I2),DEV823(I2),B23(I2),ST(6),IDB23(I2)
      IF ( SENSE SWITCH 6 )205,11000
205 CONTINUE
      PRINT 5
1  ,BIJ(1),DELB11(I2),DEV811(I2),B11(I2),ST(1),IDB11(I2)
2  ,BIJ(2),DELB22(I2),DEV822(I2),B22(I2),ST(2),IDB22(I2)
3  ,BIJ(3),DELB33(I2),DEV833(I2),B33(I2),ST(3),IDB33(I2)

```



```

      4 ,B1J(4),DELB12(I2),DEV812(I2),B12(I2),ST(4),IDB12(I2)
      5 ,B1J(5),DELB13(I2),DEV813(I2),B13(I2),ST(5),IDB13(I2)
      6 ,B1J(6),DELB23(I2),DEV823(I2),B23(I2),ST(6),IDB23(I2)
11000 CONTINUE
11111 CONTINUE
      ST(1)=ABSF(R(N)/PD(N))
      IF ( J15 ) 11002,11002,11001
11001 WRITE OUTPUT TAPE 9,7,R(N),PD(N),G ,ST(1),N
      IF ( S1 ) 44,44,43
      43 CONTINUE
      PRINT              7,R(N),PD(N),G ,ST(1),N
      44 CONTINUE
11002 IF ( SENSE SWITCH 6 ) 208,400
      208 PRINT 21
      400 IF(L2)12000,100,12000
12000 IF(S1)81,81,52
      81 WRITE OUTPUT TAPE 9,26,PROBLM
      52 DO 12001 I=1,N3
      IF(S1)53,53,54
      53 WRITE OUTPUT TAPE 9,22,X(I),Y(I),Z(I),B(I),N11(I),N12(I),I
      GO TO 55
      54 CONTINUE
      PUNCH 8,X(I),Y(I),Z(I),B(I),N11(I),N12(I),I
      55 CONTINUE
      IF ( N12(I) )12001,12001,1200
1200 IF(S1)56,56,57
      56 WRITE OUTPUT TAPE 9,23,B11(I),B22(I),B33(I),B12(I),B13(I),B23(I),I
      GO TO 12001
      57 PUNCH 2,B11(I),B22(I),B33(I),B12(I),B13(I),B23(I),I
12001 CONTINUE
      500 IF(S1)58,58,59
      58 WRITE OUTPUT TAPE 9,24,(SCALE(I),I=1,M)
      GO TO 60
      59 PUNCH 6,(SCALE(I),I=1,M)
      60 CONTINUE
      IF(J15)100,100,501
      501 IF(S1)61,61,62
      61 WRITE OUTPUT TAPE 9,25,G
      GO TO 100
      62 PUNCH 9,G
      100 IF ( L3 ) 402,1001,1001
1001 RETURN
1102 WR=SDW/SFW
      IF ( S1 ) 42,42,41
      41 CONTINUE
      PRINT 20,R,WR,SUMDSQ
      42 CONTINUE
      WRITE OUTPUT TAPE 9,20,R,WR,SUMDSQ
      GO TO 10003
      402 CONTINUE
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

```

OUTPUT

OUTPUT

OUTPUT
OUTPUT

APPENDIX I

Fortran II listings for FUNCTN and CHANGE subroutines for the space groups

No. 1	P1
2	$\bar{P}1$
4	$P2_1$
7	Pc
11	$P2_1/m$
13	$P2/c$
14	$P2_1/c$
15	$C2/c$

covering the triclinic and approximately half the monoclinic system are given on the following pages. These subroutines were written by various persons at various times. Therefore, while each subroutine does its proper job, certain symbols and definitions do not enjoy consistent use throughout. An understanding of the procedures performed by a particular FUNCTN/CHANGE subroutine requires a thorough study of the particular subroutine in conjunction with a knowledge of the position sets and the symmetry of the anisotropic thermal motions.

The subroutines for all the space groups listed are capable of performing the normal least-squares analysis on all position sets while utilizing isotropic/anisotropic thermal motions. In addition,

space group, C2/c, (No. 15) has been modified to allow the use of anomalous dispersion corrections in the calculation of structure factors. The program for space group C2/c does not process the anomalous dispersion corrections as least-squares variables. This procedure illustrates one aspect of Eq. (7). With respect to this equation, the imaginary portion of the dispersion correction for a centrosymmetric structure is placed in the B portion of the equation of a noncentrosymmetric structure. This type of modification is illustrated in the Fortran II listing for space group C2/c starting at statement 1000 + 1 and continuing through statement 1006.

It might be noted that all derivatives in these examples are slightly incorrect in that they should all be multiplied by the scale factor. For our (Los Alamos) purposes this is not a significant error in that we use only one scale factor, and, hence, this term can be cancelled out in all terms, or omitted. This was done to save a small amount of computer time, which seemed important for the original IBM-704 programs.

```

SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEVH11(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFUB(10862),SUMOBS(10882),K(10902),SDELSQ(10922),
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085),
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(3201),SRHO(11126),
9 SWF(10872),IPCERK(11127),K3(11130),DEVX(3001),DEVY(3101),
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132),
1),K2(11133),NMAX(11134),
DIMENSION CMAT(100,100), B(90),X(45),
1 E11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
DIMENSION PA(1),PB(1)
EQUIVALENCE (PA,PD),(R,PB)
FUB=FUB*SCALE(N1)
DELF=0.0
FCALC=0.0
SENSE LIGHT 1
I2=1
I3=1
FA=0.0
FB=0.0
DO 200 I=1,J
J13=J1(1)
DO 200 I1=1,J13
I4=N12(I2)
IF (I4) I01,I01,I00
101 T=EXP(-B(I2)*SQ)*F(I)
GO TO 110
100 T=EXP(-(H1**2*B11(I2)+H2**2*B22(I2)+H3**2*B33(I2)
+H1*H2*B12(I2)+H1*H3*B13(I2)+H2*H3*B23(I2)))*F(I)
110 ARG1=H1*X(I2)+H2*Y(I2)+H3*Z(I2)
AF=COS1F(ARG1)*T
BF=SIN1F(ARG1)*T
AA=6.2831853*AF
AB=-6.2831853*BF
IF (SENSE LIGHT 1) I15,I16
COMMON00
COMMON01
COMMON02
COMMON03
COMMON04
COMMON05
COMMON06
COMMON07
COMMON08
COMMON09
COMMON10
COMMON11
COMMON12
COMMON13
COMMON14
COMMON15
COMMON16
COMMON17
COMMON18
COMMON19
COMMON20
COMMON21
COMMON22
COMMON23
COMMON24
COMMON25
COMMON26
COMMON27
COMMON28
COMMON29
COMMON30
COMMON31
COMMON32
COMMON33
COMMON34
COMMON35
COMMON36
COMMON37
COMMON38
COMMON39
COMMON40
COMMON41
COMMON42
COMMON43

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116 PA(I3 )=H1*AB
    PA(I3+1)=H2*AB
    PA(I3+2)=H3*AB
    PB(I3 )=H1*AA
    PB(I3+1)=H2*AA
    PB(I3+2)=H3*AA
    I3=I3+3
119 IF (I4)120,120,121
120 PA(I3)=-AF*SQ
    PB(I3)=-BF*SQ
    I3=I3+1
    GO TO 150
121 PA(I3)=-H1**2*AF
    PA(I3+1)=-H2**2*AF
    PA(I3+2)=-H3**2*AF
    PA(I3+3)=-H1*H2*AF
    PA(I3+4)=-H1*H3*AF
    PA(I3+5)=-H2*H3*AF
    PB(I3)=-H1**2*BF
    PB(I3+1)=-H2**2*BF
    PB(I3+2)=-H3**2*BF
    PB(I3+3)=-H1*H2*BF
    PB(I3+4)=-H1*H3*BF
    PB(I3+5)=-H2*H3*BF
    I3=I3+6
    GO TO 150
150 FA=FA+AF
    FB=FB+BF
200 I2=I2+1
    N=I3+M-1
    FCALC=SQRTF(FA**2+FB**2)
    I3=I3-1
    DO 210 I=1,I3
210 PD(I)=(FA*PA(I)+FB*PB(I))/FCALC
    I3=I3+N1
    PD(I3)=-FCALC/SCALE(N1)
    RETURN
    END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

```

```

SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501), COMMON00
COMMON1
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501), COMMON02
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101), COMMON03
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),COMMON04
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001), COMMON05
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401), COMMON06
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801), COMMON07
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816), COMMON08
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836), COMMON09
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922)) COMMON10
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957), COMMON11
1J7(10951),J8(10951), COMMON12
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),COMMON13
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051), COMMON14
4 N1(11052),N2(11053),N3(11054),F0B(11055),W(11056),N1(11057), COMMON15
5 SQ(11058),N1(11059),N2(11060),N3(11061),I(11062),I1(11072), COMMON16
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066), COMMON17
7 I8(11065),I9(11064),I10(11063),J1(11073),L(11074),M(11075), COMMON18
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081), COMMON19
9 COSC(11082),ASTAR(11083),HSTAR(11084),CSTAR(11085)) COMMON20
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087), COMMON21
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR COMMON22
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACCOSC(11096), COMMON23
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101), COMMON24
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)COMMON25
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113), COMMON26
6L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),COMMON27
7L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125), COMMON28
8B1J(3201),SRHO(11126), COMMON29
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101)) COMMON30
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132)COMMON31
1),K2(11133),NMAX(11134)) COMMON32
DIMENSION CMAT(100,100), B(90),X(45), COMMON33
1 B11(1),B22(45),Y(45),B33(45),Z(45),H12(45),N11(45),B13(45), COMMON34
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20), COMMON35
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6), COMMON36
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),COMMON37
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1), COMMON38
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1), COMMON39
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1), COMMON40
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1), COMMON41
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1) COMMON42
DIMENSION SWF(20) COMMON43
11=1
SENSE LIGHT 1
DO 200 I=1,N3
IF (SENSE LIGHT 1)98,97
98 DELX(I)=0.0
DELY(I)=0.0
DELZ(I)=0.0
DEVX(I)=0.0
DEVY(I)=0.0
DEVZ(I)=0.0
IDX(I) = 0
IDY(I) = 0
IDZ(I) = 0
GO TO 99
97 DELX(I)=R(I1 )
DELY(I)=R(I1+1)
DELZ(I)=R(I1+2)
DEVX(I)=PD(I1 )
DEVY(I)=PD(I1+1)
DEVZ(I)=PD(I1+2)
X(I)=X(I)+DELX(I)
Y(I)=Y(I)+DELY(I)
Z(I)=Z(I)+DELZ(I)
IDX(I) = I1
IDY(I) = I1+1

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```

      IDZ(I) = I1+2
      I1=I1+3
99  IF ( N12(I) ) 100,100,101
100 DELB(I)=R(I1)
      DEV8(I)=PD(I1)
      ID8(I) = I1
      I1=I1+1
      B(I)=B(I)+DELB(I)
      GO TO 200
101 DELB11(I)=R(I1)
      DELB22(I)=R(I1+1)
      DELB33(I)=R(I1+2)
      DELB12(I)=R(I1+3)
      DELB13(I)=R(I1+4)
      DELB23(I)=R(I1+5)
      DEV811(I)=PD(I1)
      DEV822(I)=PD(I1+1)
      DEV833(I)=PD(I1+2)
      DEV812(I)=PD(I1+3)
      DEV813(I)=PD(I1+4)
      DEV823(I)=PD(I1+5)
      ID811(I) = I1
      ID822(I) = I1+1
      ID833(I) = I1+2
      ID812(I) = I1+3
      ID813(I) = I1+4
      ID823(I) = I1+5
      I1=I1+6
      B11(I)=B11(I)+DELB11(I)
      B22(I)=B22(I)+DELB22(I)
      B33(I)=B33(I)+DELB33(I)
      B12(I)=B12(I)+DELB12(I)
      B13(I)=B13(I)+DELB13(I)
      B23(I)=B23(I)+DELB23(I)
200 CONTINUE
      DO 300 I=1,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=R(I1)
      IDSC(I) = I1
      IF ( SCALE(I)+DELSCA(I) ) 201,201,202
201 SCALE(I)=SCALE(I)/(1.0-DELSCA(I)/SCALE(I))
      GO TO 300
202 SCALE(I)=SCALE(I)+DELSCA(I)
300 I1=I1+1
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEVX(1101),
3 DEVB11(1101),DEVB22(1201),DEVB33(1301),DEVB12(1401),DEVB13(1501),
4 DEVB23(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),FOB(11055),W(11056),N1(11057),
5 S0(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCUSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(3201),SRHO(11126),
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEVB(1),DEVB11(1),DEVB22(1),
7 DEVB33(1),DEVB12(1),DEVB13(1),DEVB23(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1))
DIMENSION SWF(20)
FOB=FOB*SCALE(N1)
DELF=0.0
FCALC=0.0
I3=1
I2=1
DO 201 I=1,J
J13=J1(I)
DO 201 I1=1,J13
I4=N11(I3)
I5=N12(I3)
IF(I5)100,100,101
100 T=EXPF(-B(I3)*SQ)
GO TO 102
101 T=EXPF(-(H1**2*B11(I3)+H2**2*B22(I3)+H3**2*B33(I3)
1+H1*H2*B12(I3)+H1*H3*B13(I3)+H2*H3*B23(I3)))
102 GO TO (110,120,130,140,150,160,170,180,190),I4
110 FA=F(I)*T
111 IF(I5)112,112,113
112 PD(I2)=-SQ*FA
I2=I2+1
GO TO 200
113 PD(I2)=-H1**2*FA
PD(I2+1)=-H2**2*FA
PD(I2+2)=-H3**2*FA
PD(I2+3)=-H1*H2*FA

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        PD(I2+4)=-H1*H3*FA
        PD(I2+5)=-H2*H3*FA
        I2=I2+6
        GO TO 200
120 IF(MODF(H3,2.0))121,110,121
121 FA=-F(I)*T
        GO TO 111
130 IF(MODF(H2,2.0))121,110,121
140 IF(MODF(H1,2.0))121,110,121
150 IF(MODF((H1+H2),2.0))121,110,121
160 IF(MODF((H1+H3),2.0))121,110,121
170 IF(MODF((H2+H3),2.0))121,110,121
180 IF(MODF((H1+H2+H3),2.0))121,110,121
190 ARG1=H1*X(I3)+H2*Y(I3)+H3*Z(I3)
        CX1=COS1F(ARG1)
        SX1=-SIN1F(ARG1)*12.5663706*F(I)*T
        FA=2.0*F(I)*T*CX1
        PD(I2)=H1*SX1
        PD(I2+1)=H2*SX1
        PD(I2+2)=H3*SX1
        I2=I2+3
        GO TO 111
200 FCALC=FCALC+FA
201 I3=I3+1
        N=I2+M-1
        I2=I2+N1-1
        PD(I2)=-FCALC/SCALE(N1)
        RETURN
END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501), COMMON00
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501), COMMON01
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101), COMMON02
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),COMMON03
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001), COMMON04
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401), COMMON05
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801), COMMON06
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816), COMMON07
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836), COMMON08
9 F(10842),SUMF08(10862),SUM08S(10882),K(10902),SDELSQ(10922) COMMON09
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957), COMMON10
1J7(10951),J8(10951), COMMON11
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),COMMON12
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051), COMMON13
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057), COMMON14
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072), COMMON15
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066), COMMON16
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075), COMMON17
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSH(11081), COMMON18
9 CUSC(11082),ASTAR(11083),HSTAR(11084),CSTAR(11085) COMMON19
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087), COMMON20
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR COMMON21
2 (11092),SINBSR(11093),HCCUSA(11094),CACOSB(11095),BACOSC(11096), COMMON22
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101), COMMON23
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)COMMON24
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113), COMMON25
6,L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),COMMON26
7,L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125), COMMON27
8H1J(3201),SRHO(11126), COMMON28
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101) COMMON29
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F08S(11131),IR(11132)COMMON30
1),K2(11133),NMAX(11134) COMMON31
2 DIMENSION CMAT(100,100), H(90),X(45), COMMON32
3 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),B13(45), COMMON33
4 N12(45),B23(45),SCALE(20),F(6),SUMF08(20),SUM08S(20), COMMON34
5 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6), COMMON35
6 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),COMMON36
7 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1), COMMON37
8 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1), COMMON38
9 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1), COMMON39
R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1), COMMON40
IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1) COMMON41
DIMENSION SWF(20) COMMON42
I1=1 COMMON43
DO 200 I=1,N3
I2=N11(I)
I3=N12(I)
GO TO (110,110,110,110,110,110,110,110,120),I2
110 DELX(I)=0.0
DELY(I)=0.0
DELZ(I)=0.0
DEVX(I)=0.0
DEVY(I)=0.0
DEVZ(I)=0.0
IOX(I) = 0
IOY(I) = 0
IOZ(I) = 0
111 DELB(I)=R(I1)
DEV8(I)=PD(I1)
B(I)=B(I)+DELB(I)
IDB(I) = I1
I1=I1+1
IF ( I3 ) 200,200,112
120 DELX(I)=R(I1 )
DELY(I)=R(I1+1)
DELZ(I)=R(I1+2)
DEVX(I)=PD(I1 )
DEVY(I)=PD(I1+1)

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DEVZ(I)=PD(I1+2)
X(I)=X(I)+DELX(I)
Y(I)=Y(I)+DELY(I)
Z(I)=Z(I)+DELZ(I)
IDX(I) = I1
IDY(I) = I1+1
IOZ(I) = I1+2
I1=I1+3
GO TO 111
112 DELB22(I)=R(I1 )
DELB33(I)=R(I1+1)
DELB12(I)=R(I1+2)
DELB13(I)=R(I1+3)
DELB23(I)=R(I1+4)
DEVB22(I)=PD(I1 )
DEVB33(I)=PD(I1+1)
DEVB12(I)=PD(I1+2)
DEVB13(I)=PD(I1+3)
DEVB23(I)=PD(I1+4)
B22(I)=B22(I)+DELB22(I)
B33(I)=B33(I)+DELB33(I)
B12(I)=B12(I)+DELB12(I)
B13(I)=B13(I)+DELB13(I)
B23(I)=B23(I)+DELB23(I)
IDB22(I) = I1
IDB33(I) = I1+1
IDB12(I) = I1+2
IDB13(I) = I1+3
IDB23(I) = I1+4
I1=I1+5
200 CONTINUE
DO 205 I=1,M
DELSA(I)=R(I1)
DEVSA(I)=PD(I1)
IDSC(I) = I1
IF(SCALE(I)+DELSA(I))201,201,202
201 SCALE(I)=SCALE(I)/(1.0-DELSA(I)/SCALE(I))
GO TO 205
202 SCALE(I)=SCALE(I)+DELSA(I)
205 I1=I1+1
RETURN
END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),R(10781),B11(10781),H22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J1(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),CUSB(11081),
9 COSC(11082),ASTAR(11083),HSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMOSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(3201),SRHO(11126),
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), R(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
DIMENSION PA(1),PB(1)
EQUIVALENCE (PA,PD),(R,PB)
FA=0.0
FB=0.0
DELF=0.0
FCALC=0.0
F0B=F0B*SCALE(N1)
I2=1
I3=1
DO 200 I=1,J
I4=J1(1)
DO 200 I1=1,I4
X1=H1*X(I2)+H2*Y(I2)+H3*Z(I2)
X2=-H1*X(I2)+H2*(Y(I2)+0.5)-H3*Z(I2)
IF ( N12(I2) ) 100,101,100
100 H11=H1*(H1*B11(I2)+H3*B13(I2))+H2*H2*B22(I2)+H3*H3*B33(I2)
H12=H1*H2*B12(I2)+H2*H3*B23(I2)
T1=EXP(-H11-H12)
T2=EXP(-H11+H12)
GO TO 102
101 T1=EXP(-SQ*B(I2))
T2=T1
102 CX1=COS1F(X1)*T1
CX2=COS1F(X2)*T2
SX1=SIN1F(X1)*T1

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SX2=SIN1F(X2)*T2
AF=F(I)*(CX1+CX2)
BF=F(I)*(SX1+SX2)
IF ( N12(I2) ) 150,105,105
105 CONTINUE
PF=+6.283185305*F(I)
PA(I3)=-PF*H1*(SX1-SX2)
PB(I3)=PF*H1*(CX1-CX2)
PA(I3+1)=-PF*H2*(SX1+SX2)
PB(I3+1)=PF*H2*(CX1+CX2)
PA(I3+2)=-PF*H3*(SX1-SX2)
PB(I3+2)=PF*H3*(CX1-CX2)
IF ( N12(I2) ) 104,103,104
104 PA(I3+3)=-AF*H1*H1
PB(I3+3)=-BF*H1*H1
PA(I3+4)=-AF*H2*H2
PB(I3+4)=-BF*H2*H2
PA(I3+5)=-AF*H3*H3
PB(I3+5)=-BF*H3*H3
PA(I3+6)=-H1*H2*F(I)*(CX1-CX2)
PB(I3+6)=-H1*H2*F(I)*(SX1-SX2)
PA(I3+7)=-H1*H3*AF
PB(I3+7)=-H1*H3*BF
PA(I3+8)=-H2*H3*F(I)*(CX1-CX2)
PB(I3+8)=-H2*H3*F(I)*(SX1-SX2)
I3=I3+9
GO TO 150
103 PA(I3+3)=-SQ*AF
PB(I3+3)=-SQ*BF
I3=I3+4
150 FA=FA+AF
FB=FB+BF
200 I2=I2+1
N=I3+M-2
FCALC=SQRTF(FA**2+FB**2)
I3=I3-1
DO 210 I=1,I3
210 PD(I)=(FA*PA(I)+FB*PB(I))/FCALC
IF ( N1-1 ) 220,220,230
220 PD(2)=-FCALC/SCALE(N1)
GO TO 300
230 I3=I3+N1-1
PD(I3)=-FCALC/SCALE(N1)
300 CONTINUE
400 RETURN
END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV6(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMF08(10862),SUMOBS(10882),K(10902),SDELSQ(10922)
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),CUSA(11080),CUSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085)
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCUSA(11094),CACOSH(11095),BACUSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMOSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6,L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7,L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8BIJ(11201),SRHO(11126),
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101)
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132)
1),K2(11133),NMAX(11134)
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N1(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMF08(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
YU=Y(1)
I1=1
DO 200 I=1,N3
IF ( N12(I) ) 104,105,105
104 DELX(I) = 0.0
DELY(I) = 0.0
DELZ(I) = 0.0
DELB(I) = 0.0
DEVX(I) = 0.0
DEVY(I) = 0.0
DEVZ(I) = 0.0
DEV8(I) = 0.0
IDX(I) = 0
IDY(I) = 0
IDZ(I) = 0
IDB(I) = 0
GO TO 200
105 CONTINUE
DELX(I)=R(I1 )
DELY(I)=R(I1+1)
DELZ(I)=R(I1+2)
DELB(I)=R(I1+3)
DEVX(I)=PD(I1 )
DEVY(I)=PD(I1+1)
DEVZ(I)=PD(I1+2)

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      DEVB(I)=PD(I1+3)
103 X(I)=X(I)+DELX(I)
      Y(I)=Y(I)+DELY(I)
      Z(I)=Z(I)+DELZ(I)
      B(I)=B(I)+DELB(I)
      IDX(I) = I1
      IDY(I) = I1+1
      IDZ(I) = I1+2
      IDB(I) = I1+3
      IF ( N12(I) ) 102,102,100
100 DELB22(I)=R(I1+4)
      DELB33(I)=R(I1+5)
      DELB12(I)=R(I1+6)
      DELB13(I)=R(I1+7)
      DELB23(I)=R(I1+8)
      DEVB22(I)=PD(I1+4)
      DEVB33(I)=PD(I1+5)
      DEVB12(I)=PD(I1+6)
      DEVB13(I)=PD(I1+7)
      DEVB23(I)=PD(I1+8)
      B22(I)=B22(I)+DELB22(I)
      B33(I)=B33(I)+DELB33(I)
      B12(I)=B12(I)+DELB12(I)
      B13(I)=B13(I)+DELB13(I)
      B23(I)=B23(I)+DELB23(I)
      IDB22(I) = I1+4
      IDB33(I) = I1+5
      IDB12(I) = I1+6
      IDB13(I) = I1+7
      IDB23(I) = I1+8
      I1=I1+9
      GO TO 200
102 I1=I1+4
200 CONTINUE
      Y(I)=Y0
      DELSCA(I)=DELY(I)
      DEVSCA(I)=DEVY(I)
      DELY(I)=0.0
      DEVY(I)=0.0
      IDSC(I) = IDY(I)
      IDY(I) = 0
      IF ( M-1 ) 300,300,204
204 DO 210 I=2,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=PD(I1)
      IDSC(I) = I1
210 I1=I1+1
300 DO 301 I = 1,M
      IF ( SCALE(I)+DELSCA(I) ) 205,205,206
205 SCALE(I)=SCALE(I)/(1.0-DELSCA(I)/SCALE(I))
      GO TO 301
206 SCALE(I)=SCALE(I)+DELSCA(I)
301 CONTINUE
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F0B(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(3201),SRHO(11126),
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100),
2 B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELB(1),DELY(1),DELZ(1),DELB11(1),
5 DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1))
DIMENSION SWF(20)
DIMENSION PA(1),PB(1)
EQUIVALENCE (PA,PD),(R,PB)
F0B=FOB*SCALE(N1)
FA=0.0
FB=0.0
FCALC=0.0
DELF=0.0
I2=1
I3=1
SENSE LIGHT 1
C TEST SENSE LIGHT 1 TO DROP X AND Z PARAMETERS ATOM 1
DO 200 I=1,J
J13=J1(I)
DO 200 I1=1,J13
IF (N12(I2))100,101,100
100 T3=H1*(H1*B11(I2)+H3*B13(I2))+H2*H2*B22(I2)+H3*H3*B33(I2)
T4=H2*(H1*B12(I2)+H3*B23(I2))
T1=EXP(-T3-T4)
T2=EXP(-T3+T4)
GO TO 102
101 T1=EXP(-SQ*B(I2))
T2=T1
102 X1=H1*X(I2)+H2*Y(I2)+H3*Z(I2)
X2=H1*X(I2)-H2*Y(I2)+H3*(Z(I2)+0.5)
CX1=COS1F(X1)*T1
COMMON00
COMMON01
COMMON02
COMMON03
COMMON04
COMMON05
COMMON06
COMMON07
COMMON08
COMMON09
COMMON10
COMMON11
COMMON12
COMMON13
COMMON14
COMMON15
COMMON16
COMMON17
COMMON18
COMMON19
COMMON20
COMMON21
COMMON22
COMMON23
COMMON24
COMMON25
COMMON26
COMMON27
COMMON28
COMMON29
COMMON30
COMMON31
COMMON32
COMMON33
COMMON34
COMMON35
COMMON36
COMMON37
COMMON38
COMMON39
COMMON40
COMMON41
COMMON42
COMMON43

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CX2=COS1F(X2)*T2
SX1=SIN1F(X1)*T1
SX2=SIN1F(X2)*T2
AF=F(1)*(CX1+CX2)
BF=F(1)*(SX1+SX2)
PF=6.283185305*F(1)
IF (SENSE LIGHT 1)115,116
C TEST FOR FIRST ATOM
115 PA(I3)=-PF*H2*(SX1-SX2)
PB(I3)=PF*H2*(CX1-CX2)
I3=I3+1
GO TO 117
116 PA(I3)=-PF*H1*(SX1+SX2)
PB(I3)=PF*H1*(CX1+CX2)
PA(I3+1)=-PF*H2*(SX1-SX2)
PB(I3+1)=PF*H2*(CX1-CX2)
PA(I3+2)=-PF*H3*(SX1+SX2)
PB(I3+2)=PF*H3*(CX1+CX2)
I3=I3+3
117 IF ( N12(I2) )119,118,119
118 PA(I3)=-SQ*AF
PB(I3)=-SQ*BF
I3=I3+1
GO TO 150
119 PA(I3)=-AF*H1*H1
PB(I3)=-BF*H1*H1
PA(I3+1)=-AF*H2*H2
PB(I3+1)=-BF*H2*H2
PA(I3+2)=-AF*H3*H3
PB(I3+2)=-BF*H3*H3
PA(I3+3)=-F(1)*H1*H2*(CX1-CX2)
PB(I3+3)=-F(1)*H1*H2*(SX1-SX2)
PA(I3+4)=-AF*H1*H3
PB(I3+4)=-BF*H1*H3
PA(I3+5)=-F(1)*H2*H3*(CX1-CX2)
PB(I3+5)=-F(1)*H2*H3*(SX1-SX2)
I3=I3+6
150 FA=FA+AF
FB=FB+BF
200 I2=I2+1
N=I3+M-1
FCALC=SQRTF(FA**2+FB**2)
I3=I3-1
DO 210 I=1,I3
210 PD(I)=(FA*PA(I)+FB*PB(I))/FCALC
I3=I3+N1
PD(I3)=-FCALC/SCALE(N1)
RETURN
END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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2/08/65

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDH12(2501),IDH13(2601),IDH23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),R(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),FOB(11055),W(11056),N1(11057),
5 S0(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 CUSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),CUSASR(11086),COSBSR(11087),
1 CUSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASK
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 H1J(13201),SRHO(11126),
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FUBS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDH12(1),IDH13(1),IDH23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
SENSE LIGHT 1
I1=1
DO 200 I=1,N3
IF (SENSE LIGHT 1)97,98
97 DELX(I)=0.0
DELY(I)=R(I1)
DELZ(I)=0.0
DEVX(I)=0.0
DEVY(I)=PD(I1)
DEVZ(I)=0.0
Y(I)=Y(I)+DELY(I)
IDX(I)=0
IDY(I)=I1
IDZ(I)=0
DELB(I)=R(I1+1)
DEV8(I)=PD(I1+1)
B(I)=B(I)+DELB(I)
IDB(I)=I1+1
I1=I1+2
GO TO 99
98 DELX(I)=R(I1)
DELY(I)=R(I1+1)
DELZ(I)=R(I1+2)
DELB(I)=R(I1+3)
DEVX(I)=PD(I1)

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      DEVY(I)=PD(I1+1)
      DEVZ(I)=PD(I1+2)
      DEVB(I)=PD(I1+3)
      IDX(I)=I1
      IDY(I)=I1+1
      IDZ(I)=I1+2
      IDB(I)=I1+3
      X(I)=X(I)+DELX(I)
      Y(I)=Y(I)+DELY(I)
      Z(I)=Z(I)+DELZ(I)
      B(I)=B(I)+DELB(I)
      I1=I1+4
99  IF ( N12(I) )101,200,101
101 DELB22(I)=R(I1)
      DELB33(I)=R(I1+1)
      DELB12(I)=R(I1+2)
      DELB13(I)=R(I1+3)
      DELB23(I)=R(I1+4)
      DEVB22(I)=PD(I1)
      DEVB33(I)=PD(I1+1)
      DEVB12(I)=PD(I1+2)
      DEVB13(I)=PD(I1+3)
      DEVB23(I)=PD(I1+4)
      IDB22(I)=I1
      IDB33(I)=I1+1
      IDB12(I)=I1+2
      IDB13(I)=I1+3
      IDB23(I)=I1+4
      B22(I)=B22(I)+DELB22(I)
      B33(I)=B33(I)+DELB33(I)
      B12(I)=B12(I)+DELB12(I)
      B13(I)=B13(I)+DELB13(I)
      B23(I)=B23(I)+DELB23(I)
      I1=I1+5
200 CONTINUE
      DO 300 I=1,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=PD(I1)
      IOSCA(I)=I1
      IF (SCALE(I)+DELSCA(I))201,201,202
201 SCALE(I)=SCALE(I)/(1.0-DELSCA(I)/SCALE(I))
      GO TO 300
202 SCALE(I)=SCALE(I)+DELSCA(I)
300 I1=I1+1
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501), COMMON00
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501), COMMON01
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101), COMMON02
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),COMMON03
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001), COMMON04
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401), COMMON05
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801), COMMON06
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816), COMMON07
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836), COMMON08
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922) COMMON09
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957), COMMON10
1J7(10951),J8(10951), COMMON11
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),COMMON12
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051), COMMON13
4 H1(11052),H2(11053),H3(11054),F0B(11055),W(11056),N1(11057), COMMON14
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072), COMMON15
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066), COMMON16
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075), COMMON17
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081), COMMON18
9 COSC(11082),ASTAR(11083),HSTAR(11084),CSTAR(11085) COMMON19
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087), COMMON20
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR COMMON21
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096), COMMON22
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101), COMMON23
4 SUMOSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)COMMON24
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113), COMMON25
6,L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),COMMON26
7,L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125), COMMON27
8B1J(3201),SRHO(11126), COMMON28
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101) COMMON29
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132)COMMON30
1),K2(11133),NMAX(11134) COMMON31
2 DIMENSION CMAT(100,100), B(90),X(45), COMMON32
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45), COMMON33
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20), COMMON34
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6), COMMON35
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),COMMON36
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1), COMMON37
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1), COMMON38
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1), COMMON39
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1), COMMON40
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1) COMMON41
DIMENSION SWF(20) COMMON42
FCALC=0.0 COMMON43
H25=H2*0.5
F0B=F0B*SCALE(N1)
DELF=0.0
I2=1
I3=1
DO 1001 I=1,J
I4=J1(I)
DO 1001 I1=1,I4
I5=N11(I2)
IF ( N12(I2) ) 1,1,2
1 T1=EXP(-B(I2)*SQ)*F(I)
T2=T1
GO TO 3
2 H1B=(H1*B11(I2)+H3*B13(I2))*H1+H2**2*B22(I2)+H3**2*B33(I2)
H2B=H2*(H1*B12(I2)+H3*B23(I2))
T1=EXP(-(H1B+H2B))*F(I)
T2=EXP(-(H1B-H2B))*F(I)
3 GO TO ( 100,200,300,400,500,600 ),15
100 C1=T1
C2=COS1F(H25)*T2
101 AF=C1+C2
IF ( N12(I2) ) 102,102,103
102 PD(I3)=-SQ*AF
I3=I3+1

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GO TO 1000
103 PD(I3) =-H1**2*AF
PD(I3+1)=-H2**2*AF
PD(I3+2)=-H3**2*AF
PD(I3+3)=-H1*H2*(C1-C2)
PD(I3+4)=-H1*H3*AF
PD(I3+5)=-H2*H3*(C1-C2)
I3=I3+6
GO TO 1000
200 C1=COS1F(H1/2.0)*T1
C2=COS1F((H1+H2)/2.0)*T2
GO TO 101
300 C1=COS1F(H3/2.0)*T1
C2=COS1F((H2+H3)/2.0)*T2
GO TO 101
400 C1=COS1F((H1+H3)/2.0)*T1
C2=COS1F((H1+H2+H3)/2.0)*T2
GO TO 101
500 CX=H1*X(I2)+H2/4.0+H3*Z(I2)
SX=SIN1F(CX)*T1
AF=2.0*COS1F(CX)*T1
PD(I3) =-12.5663706*H1*SX
PD(I3+1)=-12.5663706*H3*SX
I3=I3+2
IF ( N12(I2) ) 102,102,501
501 PD(I3) =-H1**2*AF
PD(I3+1)=-H2**2*AF
PD(I3+2)=-H3**2*AF
PD(I3+3)=-H1*H3*AF
I3=I3+4
GO TO 1000
600 HX=H1*X(I2)
HY=H2*Y(I2)
HZ=H3*Z(I2)
CX=HX+HY+HZ
CY=HX-HY+HZ+H25
C1=COS1F(CX)*T1*2.0
C2=COS1F(CY)*T2*2.0
S =SIN1F(CX)*T1*2.0
S2=SIN1F(CY)*T2*2.0
PD(I3) =-6.28318531*H1*(S +S2)
PD(I3+1)=-6.28318531*H2*(S -S2)
PD(I3+2)=-6.28318531*H3*(S +S2)
I3=I3+3
GO TO 101
1000 I2=I2+1
1001 FCALC=FCALC+AF
N=I3-1+M
I3=I3+N1-1
PD(I3)=-FCALC/SCALE(N1)
RETURN
END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),ID8(2201),ID811(2201),ID822(2301),ID833(2401),
6 ID812(2501),ID813(2601),ID823(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 S0(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(11201),SRHO(11126),
9 SWF(10872),PCBRK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FUBS(11131),IR(11132)
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),ID811(1),ID822(1),ID833(1),
9 ID812(1),ID813(1),ID823(1),ID8(1),IDSC(1)
DIMENSION SWF(20)
I1=1
DO 1000 I=1,N3
I2=N11(I)
SENSE LIGHT 0
GU TO (100,100,100,100,500,600),I2
100 DELX(I)=0.0
DELY(I)=0.0
DELZ(I)=0.0
DEVX(I)=0.0
DEVY(I)=0.0
DEVZ(I)=0.0
IDX(I) = 0
IDY(I) = 0
IDZ(I) = 0
104 DELB11(I)=R(I1)
DEV811(I)=PD(I1)
B11(I)=DELB11(I)+B11(I)
IDB11(I) = I1
I1=I1+1
IF ( N12(I) ) 900,900,101
101 DELB22(I)=R(I1)
DELB33(I)=R(I1+1)
DEV822(I)=PD(I1)
DEV833(I)=PD(I1+1)
B22(I)=B22(I)+DELB22(I)

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      B33(I)=B33(I)+DEL833(I)
      I0822(I) = I1
      I0833(I) = I1+1
      I1=I1+2
      IF ( SENSE LIGHT 1 ) 102,103
102  DEL813(I)=R(I1)
      DEV813(I)=PD(I1)
      U13(I)=B13(I)+DEL813(I)
      I0813(I) = I1
      I1=I1+1
      GO TO 900
103  DEL812(I)=R(I1)
      DEL813(I)=R(I1+1)
      DEL823(I)=R(I1+2)
      DEV812(I)=PD(I1)
      DEV813(I)=PD(I1+1)
      DEV823(I)=PD(I1+2)
      B12(I)=DEL812(I)+B12(I)
      B13(I)=DEL813(I)+B13(I)
      B23(I)=DEL823(I)+B23(I)
      I0812(I) = I1
      I0813(I) = I1+1
      I0823(I) = I1+2
      I1=I1+3
      GO TO 900
500  DELX(I)=R(I1)
      DELZ(I)=R(I1+1)
      DEVX(I)=PD(I1)
      DEVZ(I)=PD(I1+1)
      DELY(I)=0.0
      DEVY(I)=0.0
      I0X(I) = I1
      I0Y(I) = 0
      I0Z(I) = I1+1
      I1=I1+2
      DEL812(I)=0.0
      DEL823(I)=0.0
      DEV812(I)=0.0
      DEV823(I)=0.0
      I0812(I) = 0
      I0823(I) = 0
      B23(I)=0.0
      B12(I)=0.0
      SENSE LIGHT 1
      GO TO 104
600  DELX(I)=R(I1)
      DELY(I)=R(I1+1)
      DELZ(I)=R(I1+2)
      DEVX(I)=PD(I1)
      DEVY(I)=PD(I1+1)
      DEVZ(I)=PD(I1+2)
      I0X(I) = I1
      I0Y(I) = I1+1
      I0Z(I) = I1+2
      I1=I1+3
      GO TO 104
900  X(I)=X(I)+DELX(I)
      Y(I)=Y(I)+DELY(I)
1000 Z(I)=Z(I)+DELZ(I)
      DO 205 I=1,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=PD(I1)
      I0SC(I) = I1
      IF (SCALE(I)+DELSCA(I))201,201,202
201  SCALE(I)=SCALE(I)/(1.0-DELSCA(I))/SCALE(I)
      GO TO 205
202  SCALE(I)=SCALE(I)+DELSCA(I)
205  I1=I1+1
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501), COMMON00
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501), COMMON01
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101), COMMON02
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501), COMMON03
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001), COMMON04
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401), COMMON05
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801), COMMON06
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816), COMMON07
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836), COMMON08
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922) COMMON09
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957), COMMON10
1J7(10951),J8(10951), COMMON11
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944), COMMON12
3 J15(10943),N11(111204),N12(111027),PROBLM(11039),NAME(11051), COMMON13
4 H1(11052),H2(11053),H3(11054),F0B(11055),W(11056),N1(11057), COMMON14
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072), COMMON15
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066), COMMON16
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075), COMMON17
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081), COMMON18
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085), COMMON19
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087), COMMON20
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR COMMON21
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096), COMMON22
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101), COMMON23
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107), COMMON24
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113), COMMON25
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119), COMMON26
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),ST(11125), COMMON27
8 B1J(3201),SRHO(11126), COMMON28
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101), COMMON29
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132), COMMON30
1),K2(11133),NMAX(11134), COMMON31
2 DIMENSION CMAT(100,100), B(90),X(45), COMMON32
3 1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45), COMMON33
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20), COMMON34
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6), COMMON35
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1), COMMON36
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1), COMMON37
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1), COMMON38
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1), COMMON39
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1), COMMON40
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1) COMMON41
2 DIMENSION SWF(20) COMMON42
FCALC=0.0
DELF=0.0
F0B=F0B*SCALE(N1)
I2=1
I3=1
DO 200 I=1,J
J13=J1(1)
DO 200 I1=1,J13
SENSE LIGHT 0
I4=N11(12)
IF ( N12(I2) ) 100,101,100
101 T1=EXP(-SQ*B(I2))
T2=T1
GO TO 102
100 T3=H1*(H1*H11(I2)+H3*B13(I2))+H2**2*B22(I2)+H3**2*B33(I2)
T4=H2*(H1*B12(I2)+H3*B23(I2))
GO TO ( 1000,1000,1000,1001,1001,1000 ) ,I4
1000 T1=EXP(-T3-T4)
T2=EXP(-T3+T4)
GO TO 102
1001 T1=EXP(-T3)
T2=T1
102 GO TO ( 103,104,105,106,107,108,109 ) ,I4
103 ARG1=0.0
ARG2=H3/2.0

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      GO TO 120
104 ARG1=(H1+H2)/2.0
      ARG2=(H1+H2+H3)/2.0
      GO TO 120
105 ARG1=H2/2.0
      ARG2=(H2+H3)/2.0
      GO TO 120
106 ARG1=H1/2.0
      ARG2=(H1+H3)/2.0
      GO TO 120
107 ARG1=H2*Y(I2)+H3/4.0
      ARG2=-ARG1
      GO TO 120
108 ARG1=H1/2.0+H2*Y(I2)+H3/4.0
      ARG2=-ARG1
109 X1=H1*X(I2)+H3*Z(I2)
      X2=H2*Y(I2)
      ARG1=X1+X2
      ARG2=X1-X2+H3/2.0
120 CX1=T1*COS1F(ARG1)
      CX2=T2*COS1F(ARG2)
      SX1=T1*SIN1F(ARG1)
      SX2=T2*SIN1F(ARG2)
      AF=F(I)*(CX1+CX2)
      IF (I4-7)122,121,121
121 AF=AF*2.0
122 PF=-F(I)*12.56637
      GO TO ( 140,140,140,140,131,131,132 ) ,I4
132 PD(I3 )=H1*PF*(SX1+SX2)
      PD(I3+1)=H2*PF*(SX1-SX2)
      PD(I3+2)=H3*PF*(SX1+SX2)
      I3=I3+3
      GO TO 140
131 PD(I3 )=-H2*6.283185*F(I)*(SX1-SX2)
      I3=I3+1
      GO TO 140
140 IF ( N12(I2) ) 141,142,141
142 PD(I3)=-SQ*AF
      I3=I3+1
      GO TO 150
141 PD(I3 )=-H1**2*AF
      PD(I3+1)=-H2**2*AF
      PD(I3+2)=-H3**2*AF
      GO TO ( 143,143,143,143,144,144,145 ) ,I4
144 PD(I3+3)=-H1*H3*AF
      I3=I3+4
      GO TO 150
143 T5=1.0
      GO TO 147
145 T5=2.0
      GO TO 147
147 PD(I3+3)=-H1*H2*T5*F(I)*(CX1-CX2)
      PD(I3+4)=-H1*H3*AF
      PD(I3+5)=-H2*H3*T5*F(I)*(CX1-CX2)
      I3=I3+6
      GO TO 150
150 FCALC=FCALC+AF
200 I2=I2+1
      N=I3+M-1
      I3=I3+N1-1
      PD(I3)=-FCALC/SCALE(N1)
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501), COMMON00
COMMON01
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501), COMMON02
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101), COMMON03
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),COMMON04
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001), COMMON05
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401), COMMON06
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801), COMMON07
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816), COMMON08
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836), COMMON09
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922)) COMMON10
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957), COMMON11
J7(10951),J8(10951), COMMON12
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),COMMON13
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051), COMMON14
4 H1(11052),H2(11053),H3(11054),FOB(11055),W(11056),N1(11057), COMMON15
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072), COMMON16
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066), COMMON17
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075), COMMON18
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081), COMMON19
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085)) COMMON20
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087), COMMON21
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR COMMON22
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096), COMMON23
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101), COMMON24
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)COMMON25
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113), COMMON26
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),COMMON27
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125), COMMON28
8 B1J(3201),SRHO(11126), COMMON29
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101)) COMMON30
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132)COMMON31
1),K2(11133),NMAX(11134)) COMMON32
DIMENSION CMAT(100,100), B(90),X(45), COMMON33
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45), COMMON34
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20), COMMON35
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6), COMMON36
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),COMMON37
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1), COMMON38
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1), COMMON39
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1), COMMON40
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1), COMMON41
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1) COMMON42
DIMENSION SWF(20) COMMON43
I1=1
DO 200 I=1,N3
I2=N11(I)
GO TO (103,103,103,103,102,102,101),I2
101 DELX(I)=R(I1)
DELY(I)=R(I1+1)
DELZ(I)=R(I1+2)
DEVX(I)=PD(I1)
DEVY(I)=PD(I1+1)
DEVZ(I)=PD(I1+2)
X(I)=X(I)+DELX(I)
Y(I)=Y(I)+DELY(I)
Z(I)=Z(I)+DELZ(I)
IDX(I) = I1
IDY(I) = I1+1
IDZ(I) = I1+2
I1=I1+3
104 IF ( N12(I) ) 110,120,110
102 DELX(I)=0.0
DELY(I)=R(I1)
DELZ(I)=0.0
DEVX(I)=0.0
DEVY(I)=PD(I1)
DEVZ(I)=0.0
Y(I)=Y(I)+DELY(I)

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```

      IDX(I) = 0
      IDY(I) = 11
      IDZ(I) = 0
      I1=I1+1
      GO TO 104
103  DELX(I)=0.0
      DELY(I)=0.0
      DELZ(I)=0.0
      DEVX(I)=0.0
      DEVY(I)=0.0
      DEVZ(I)=0.0
      IDX(I) = 0
      IDY(I) = 0
      IDZ(I) = 0
      GO TO 104
120  DELB(I)=R(I1)
      DEVB(I)=PD(I1)
      B(I)=B(I)+DELB(I)
      IDH(I) = 11
      I1=I1+1
      GO TO 200
110  DELH11(I)=R(I1 )
      DELB22(I)=R(I1+1)
      DELB33(I)=R(I1+2)
      DEVB11(I)=PD(I1 )
      DEVB22(I)=PD(I1+1)
      DEVB33(I)=PD(I1+2)
      B11(I)=B11(I)+DELB11(I)
      B22(I)=B22(I)+DELB22(I)
      B33(I)=B33(I)+DELB33(I)
      IDB11(I) = 11
      IDB22(I) = 11+1
      IDB33(I) = 11+2
      I1=I1+3
      GO TO (140,140,140,140,150,150,140),I2
140  DELB12(I)=R(I1 )
      DELB13(I)=R(I1+1)
      DELB23(I)=R(I1+2)
      DEVB12(I)=PD(I1 )
      DEVB13(I)=PD(I1+1)
      DEVB23(I)=PD(I1+2)
      B12(I)=B12(I)+DELB12(I)
      B13(I)=B13(I)+DELB13(I)
      B23(I)=B23(I)+DELB23(I)
      IDB12(I) = 11
      IDB13(I) = 11+1
      IDB23(I) = 11+2
      I1=I1+3
      GO TO 200
150  DELB12(I)=0.0
      DELB13(I)=R(I1)
      DELB23(I)=0.0
      DEVB12(I)=0.0
      DEVB13(I)=PD(I1)
      DEVB23(I)=0.0
      B13(I)=B13(I)+DELB13(I)
      IDB12(I) = 0
      IDB13(I) = 11
      IDB23(I) = 0
      I1=I1+1
200  CONTINUE
      DO 300 I=1,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=PD(I1)
      IDSC(I) = 11
      IF ( SCALE(I)+DELSCA(I) ) 201,201,202
201  SCALE(I)=SCALE(I)/(1.0-DELSCA(I)/SCALE(I))
      GO TO 300
202  SCALE(I)=SCALE(I)+DELSCA(I)
300  I1=I1+1
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEVB(1101),
3 DEVB11(1101),DEVB22(1201),DEVB33(1301),DEVB12(1401),DEVB13(1501),
4 DEVB23(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922)
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N1(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085)
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(13201),SRHO(11126),
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),FOBS(11131),IR(11132)
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEVB(1),DEVB11(1),DEVB22(1),
7 DEVB33(1),DEVB12(1),DEVB13(1),DEVB23(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
FCALC=0.0
DELF=0.0
FOB=FOB*SCALE(N1)
I2=1
I3=1
DO 200 I=1,J
J13=J1(I)
DO 200 I1=1,J13
FAC = F(I)
X1 = X(I2)*H1+Z(I2)*H3
X2=H2*Y(I2)
X3=X1+X2
X4=X1-X2+(H2+H3)/2.0
IF ( N12(I2) ) 101,101,100
100 T4=H2*H1*B12(I2)+H2*H3*B23(I2)
T3=H1*(B11(I2)*H1+B13(I2)*H3)+H2**2*B22(I2)+H3**2*B33(I2)
T1=EXP(-T3-T4)
T2=EXP(-T3+T4)
GO TO 102
101 T1=EXP(-SQ*B(I2))
T2=T1
102 SX1=SIN1F(X3)*T1
SX2=SIN1F(X4)*T2
T1 = T1*COS1F(X3)
T2=COS1F(X4)*T2
COMMON00
COMMON01
COMMON02
COMMON03
COMMON04
COMMON05
COMMON06
COMMON07
COMMON08
COMMON09
COMMON10
COMMON11
COMMON12
COMMON13
COMMON14
COMMON15
COMMON16
COMMON17
COMMON18
COMMON19
COMMON20
COMMON21
COMMON22
COMMON23
COMMON24
COMMON25
COMMON26
COMMON27
COMMON28
COMMON29
COMMON30
COMMON31
COMMON32
COMMON33
COMMON34
COMMON35
COMMON36
COMMON37
COMMON38
COMMON39
COMMON40
COMMON41
COMMON42
COMMON43

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      IF ( N11(I2)-5 ) 110,150,150
110 FAC = FAC/2.0
150 AF = FAC*2.0*(T1+T2)
      IF ( N11(I2)-5 ) 160,151,151
151 PF = -FAC*12.56637
      PD(I3 )=H1*PF*(SX1+SX2)
      PD(I3+1)=H2*PF*(SX1-SX2)
      PD(I3+2)=H3*PF*(SX1+SX2)
      I3=I3+3
160 IF ( N12(I2) ) 170,170,161
161 PD(I3 )=-H1**2*AF
      PD(I3+1)=-H2**2*AF
      PD(I3+2)=-H3**2*AF
      PD(I3+3) = -H1*H2*FAC*(T1-T2)*2.0
      PD(I3+4)=-H1*H3*AF
      PD(I3+5) = -H2*H3*FAC*(T1-T2)*2.0
165 I3=I3+6
      GO TO 190
170 PD(I3)=-SQ*AF
      I3=I3+1
190 FCALC=FCALC+AF
200 I2=I2+1
      N=N1-M-1
      I3=I3+N1-1
      PD(I3)=-FCALC/SCALE(N1)
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F0B(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASK
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSB(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMOSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6,L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7,L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8B1J(3201),SRHO(11126),
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132),
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
I1=1
DO 200 I=1,N3
I2=N11(I)
GU TO (102,102,102,102,101),I2
101 DELX(I)=R(I1)
DELY(I)=R(I1+1)
DELZ(I)=R(I1+2)
DEVX(I)=PD(I1)
DEVY(I)=PD(I1+1)
DEVZ(I)=PD(I1+2)
X(I)=X(I)+DELX(I)
Y(I)=Y(I)+DELY(I)
Z(I)=Z(I)+DELZ(I)
IDX(I) = I1
IDY(I) = I1+1
IDZ(I) = I1+2
I1=I1+3
104 DELB(I)=R(I1)
DEV8(I)= PD(I1)
B(I)=B(I)+DELB(I)
IDB(I) = I1
I1=I1+1
103 IF ( N12(I) ) 200,200,105
102 DELX(I)=0.0
DELY(I)=0.0

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      DELZ(I)=0.0
      DEVX(I)=0.0
      DEVY(I)=0.0
      DEVZ(I)=0.0
      IDX(I) = 0
      IDY(I) = 0
      IDZ(I) = 0
      GO TO 104
105  DELB22(I)=R(I1 )
      DELB33(I)=R(I1+1)
      DELB12(I)=R(I1+2)
      DELB13(I)=R(I1+3)
      DELB23(I)=R(I1+4)
      DEVB22(I)=PD(I1 )
      DEVB33(I)=PD(I1+1)
      DEVB12(I)=PD(I1+2)
      DEVB13(I)=PD(I1+3)
      DEVB23(I)=PD(I1+4)
      IDB22(I) = I1
      IDB33(I) = I1+1
      IDB12(I) = I1+2
      IDB13(I) = I1+3
      IDB23(I) = I1+4
      I1=I1+5
      B22(I)=B22(I)+DELB22(I)
      B33(I)=B33(I)+DELB33(I)
      B12(I)=B12(I)+DELB12(I)
      B13(I)=B13(I)+DELB13(I)
      B23(I)=B23(I)+DELB23(I)
200  CONTINUE
      DO 300 I=1,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=PD(I1)
      IDSC (I) = I1
      IF ( SCALE(I)+DELSCA(I) ) 201,201,202
201  SCALE(I)=SCALE(I)/(1.0-DELSCA(I)/SCALE(I))
      GO TO 300
202  SCALE(I)=SCALE(I)+DELSCA(I)
300  I1=I1+1
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE FUNCTN
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEVB11(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F08(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J1(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSR(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMDSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107),
5 L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6 L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7 L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S1(11125),
8 B1J(3201),SRHO(11126),
9 SWF(10872),IPCBRK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F08(11131),IR(11132)
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),R12(45),N11(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
FB=0.0
I7=2
FCALC=0.0
F08=F08*SCALE(N1)
DELF=0.0
H35=H3*0.5
I2=1
I3=1
DO 1001 I=1,J
FAC=F(1)*2.0
I4=J1(I)
DO 1001 I1=1,I4
I5=N11(I2)
IF ( N12(I2) ) 1,1,2
1 T1=EXP(-B(I2)*SQ)*FAC
T2=T1
GO TO 3
2 H1B=(H1*B11(I2)+H3*B13(I2))*H1+H2**2*B22(I2)+H3**2*B33(I2)
H2B=H2*(H1*B12(I2)+H3*B23(I2))
T1=EXP(-H1B+H2B)*FAC
T2=EXP(-H1B-H2B)*FAC
3 GO TO ( 100,200,300,400,500,600 ),I5
100 C1=COS1F(0.0)*T1
C2=COS1F(H35)*T2
101 AF=C1+C2

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      IF ( N12(I2) ) 102,102,103
102 PD(I3)=-SQ*AF
   I3=I3+1
   GO TO 1000
103 PD(I3) =-H1**2*AF
   PD(I3+1)=-H2**2*AF
   PD(I3+2)=-H3**2*AF
   PD(I3+3)=-H1*H2*(C1-C2)
   PD(I3+4)=-H1*H3*AF
   PD(I3+5)=-H2*H3*(C1-C2)
   I3=I3+6
   GO TO 1000
200 C1=COS1F(H2*0.5)*T1
   C2=COS1F((H2+H3)*0.5)*T2
   GO TO 101
300 C1=COS1F((H1+H2)*0.25)*T1
   C2=COS1F((-H1+H2)*0.25+H35)*T2
   GO TO 101
400 C1=COS1F((H1+H2)*0.25+H35)*T1
   C2=COS1F((-H1+H2)*0.25)*T2
   GO TO 101
500 CX=H2*Y(I2)+H3*0.25
   SX=SIN1F(CX)*T1
   AF=2.0*COS1F(CX)*T1
   PD(I3)=-12.56637061*H2*SX
   I3=I3+1
      IF ( N12(I2) ) 102,102,501
501 PD(I3) =-H1**2*AF
   PD(I3+1)=-H2**2*AF
   PD(I3+2)=-H3**2*AF
   PD(I3+3)=-H1*H3*AF
   I3=I3+4
   GO TO 1000
600 HX=H1*X(I2)
   HY=H2*Y(I2)
   HZ=H3*Z(I2)
   CX=HX+HY+HZ
   CY=HX-HY+HZ+H35
   C1=COS1F(CX)*T1*2.0
   C2=COS1F(CY)*T2*2.0
   S =SIN1F(CX)*T1*2.0
   S2=SIN1F(CY)*T2*2.0
   PD(I3) =-6.28318531*H1*(S +S2)
   PD(I3+1)=-6.28318531*H2*(S -S2)
   PD(I3+2)=-6.28318531*H3*(S +S2)
   I3=I3+3
   GO TO 101
1000 I2=I2+1
      IF(J) 1004,1001,1001
1004 CONTINUE
   BF=AF*SCALE(I+14)/F(I)
   FB=FB+BF
   DO1002 I6=17, I3
1002 R(I6-1)=PD(I6-1)*SCALE(I+14)/F(I)
   I7=I3+1
1001 FCALC=FCALC+AF
   N=I3+M-1
   I3=I3-1
      IF (J) 1005,1006,1006
1005 CONTINUE
   FA=FCALC
   FCALC=SQRTF(FA**2+FB**2)
   DO1003 I=1, I3
1003 PD(I)=(FA*PD(I)+FB*R(I))/FCALC
1006 CONTINUE
   I3=I3+N1
   PD(I3)=-FCALC/SCALE(N1)
   RETURN
END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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SUBROUTINE CHANGE
COMMON X,N1,IR,J12,N
EQUIVALENCE (CMAT(10001), R(10251),PD(10501),
1 DELX(101),DELY(201),DELZ(301),DELB(401),DELB11(401),DELB22(501),
2 DELB33(601),DELB12(701),DELB13(801),DELB23(901),DEV8(1101),
3 DEV811(1101),DEV822(1201),DEV833(1301),DEV812(1401),DEV813(1501),
4 DEV823(1601),DELSA(1701),DEVSCA(1801),IDX(1901),IDY(2001),
5 IDZ(2101),IDB(2201),IDB11(2201),IDB22(2301),IDB33(2401),
6 IDB12(2501),IDB13(2601),IDB23(2701),IDSC(2801),
7 X(10571),Y(10641),Z(10711),B(10781),B11(10781),B22(10816),
8 B33(10536),B12(10606),B13(10676),B23(10746),SCALE(10836),
9 F(10842),SUMFOB(10862),SUMOBS(10882),K(10902),SDELSQ(10922))
EQUIVALENCE (CMAT(10001),SUMDEL(10942),J1(10957),
1J7(10951),J8(10951),
2 J9(10949),J10(10948),J11(10947),J12(10946),J13(10945),J14(10944),
3 J15(10943),N11(11204),N12(11027),PROBLM(11039),NAME(11051),
4 H1(11052),H2(11053),H3(11054),F0B(11055),W(11056),N1(11057),
5 SQ(11058),N(11059),N2(11060),N3(11061),I(11062),I1(11072),
6 I2(11071),I3(11070),I4(11069),I5(11068),I6(11067),I7(11066),
7 I8(11065),I9(11064),I10(11063),J(11073),L(11074),M(11075),
8 M1(11076),A(11077),B1(11078),C(11079),COSA(11080),COSB(11081),
9 COSC(11082),ASTAR(11083),BSTAR(11084),CSTAR(11085))
EQUIVALENCE (CMAT(10001),COSASR(11086),COSBSR(11087),
1 COSCSR(11088),SINA(11089),SINB(11090),SINC(11091),SINASR
2 (11092),SINBSR(11093),BCCOSA(11094),CACOSR(11095),BACOSC(11096),
3 FCALC(11097),DELF(11098),FA(11099),FB(11100),XRAY(11101),
4 SUMOSQ(11102),L1(11103),L2(11104),L3(11105),L4(11106),L5(11107)
5,L6(11108),L7(11109),L8(11110),L9(11111),L10(11112),L11(11113),
6,L12(11114),L13(11115),L14(11116),L15(11117),L16(11118),L17(11119),
7,L18(11120),L19(11121),L20(11122),Q(11123),G(11124),S(11125),
8BIJ(3201),SRHO(11126),
9 SWF(10872),IPC8RK(11127),K3(11130),DEVX(3001),DEVY(3101))
EQUIVALENCE (CMAT(10001),DEVZ(2901),SA(10852),F0BS(11131),IR(11132)
1),K2(11133),NMAX(11134))
DIMENSION CMAT(100,100), B(90),X(45),
1 B11(1),B22(45),Y(45),B33(45),Z(45),B12(45),B13(45),
2 N12(45),B23(45),SCALE(20),F(6),SUMFOB(20),SUMOBS(20),
3 K(20),SDELSQ(20),SUMDEL(20),J1(1),SA(6),
4 PROBLM(12),NAME(12),DELX(1),DELY(1),DELZ(1),DELB(1),
5 DELB11(1),DELB22(1),DELB33(1),DELB12(1),DELB13(1),DELB23(1),
6 DELSCA(1),DEVX(1),DEVY(1),DEVZ(1),DEV8(1),DEV811(1),DEV822(1),
7 DEV833(1),DEV812(1),DEV813(1),DEV823(1),DEVSCA(1),PD(1),
8 R(1),IDX(1),IDY(1),IDZ(1),IDB11(1),IDB22(1),IDB33(1),
9 IDB12(1),IDB13(1),IDB23(1),IDB(1),IDSC(1)
DIMENSION SWF(20)
I1=1
DO 1000 I=1,N3
I2=N11(I)
SENSE LIGHT 0
GO TO (100,100,100,100,500,600),I2
100 DELX(I)=0.0
DELY(I)=0.0
DELZ(I)=0.0
DEVX(I)=0.0
DEVY(I)=0.0
DEVZ(I)=0.0
IDX(I) = 0
IDY(I) = 0
IDZ(I) = 0
104 DELB11(I)=R(I1)
DEV811(I)=PD(I1)
B11(I)=DELB11(I)+B11(I)
IDB11(I) = I1
I1=I1+1
IF ( N12(I) ) 900,900,101
101 DELB22(I)=R(I1)
DELB33(I)=R(I1+1)
DEV822(I)=PD(I1)
DEV833(I)=PD(I1+1)
B22(I)=B22(I)+DELB22(I)

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      B33(I)=B33(I)+DEL833(I)
      ID822(I) = I1
      ID833(I) = I1+1
      I1=I1+2
      IF ( SENSE LIGHT 1 ) 102,103
102  DEL813(I)=R(I1)
      DEV813(I)=PD(I1)
      B13(I)=B13(I)+DEL813(I)
      ID813(I) = I1
      I1=I1+1
      GO TO 900
103  DEL812(I)=R(I1)
      DEL813(I)=R(I1+1)
      DEL823(I)=R(I1+2)
      DEV812(I)=PD(I1)
      DEV813(I)=PD(I1+1)
      DEV823(I)=PD(I1+2)
      B12(I)=DEL812(I)+B12(I)
      B13(I)=DEL813(I)+B13(I)
      B23(I)=DEL823(I)+B23(I)
      ID812(I) = I1
      ID813(I) = I1+1
      ID823(I) = I1+2
      I1=I1+3
      GO TO 900
500  DELY(I)=R(I1)
      DEVY(I)=PD(I1)
      DELX(I)=0.0
      DEVX(I)=0.0
      DELZ(I)=0.0
      DEVZ(I)=0.0
      IDX(I) = 0
      IDY(I) = I1
      IDZ(I) = 0
      I1=I1+1
      DEL812(I)=0.0
      DEL823(I)=0.0
      DEV812(I)=0.0
      DEV823(I)=0.0
      B23(I)=0.0
      B12(I)=0.0
      ID823(I) = 0
      ID812(I) = 0
      SENSE LIGHT 1
      GO TO 104
600  DELX(I)=R(I1)
      DELY(I)=R(I1+1)
      DELZ(I)=R(I1+2)
      DEVX(I)=PD(I1)
      DEVY(I)=PD(I1+1)
      DEVZ(I)=PD(I1+2)
      IDX(I) = I1
      IDY(I) = I1+1
      IDZ(I) = I1+2
      I1=I1+3
      GO TO 104
900  X(I)=X(I)+DELX(I)
      Y(I)=Y(I)+DELY(I)
1000 Z(I)=Z(I)+DELZ(I)
      DO 205 I=1,M
      DELSCA(I)=R(I1)
      DEVSCA(I)=PD(I1)
      IDSC(I) = I1
      IF (SCALE(I)+DELSCA(I))201,201,202
201  SCALE(I)=SCALE(I)/(1.0-DELSCA(I)/SCALE(I))
      GO TO 205
202  SCALE(I)=SCALE(I)+DELSCA(I)
205  I1=I1+1
      RETURN
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

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