LCR-2, a fortran lattice constant refinement program

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LCR-2, A FORTRAN LATTICE CONSTANT REFINEMENT PROGRAM

by

Donald E. Williams
UNITED STATES ATOMIC ENERGY COMMISSION

Research and Development Report

LCR-2, A FORTRAN
LATTICE CONSTANT REFINEMENT
PROGRAM

by

Donald E. Williams

November, 1964

Ames Laboratory
at
Iowa State University of Science and Technology
F. H. Spedding, Director
Contract W-7405 eng-82
This report is distributed according to the category Chemistry (UC-4) as listed in TID-4500, October 1, 1964.

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Printed in USA. Price $1.00. Available from the

Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.
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IS-1052

LCR-2, A FORTRAN LATTICE CONSTANT
REFINEMENT PROGRAM

Donald E. Williams

ABSTRACT

This report describes a computer program which refines lattice constants for any crystal symmetry by the least squares method. Several types of extrapolation functions are provided, and these functions can be used either singly or in combination. A complete error treatment is made, including covariances between parameters.

MATHEMATICAL METHOD

A residual function, $R$, of the parameters, $p_k$, is defined by the equation $R = \sum w \left[ \Delta(p_k) \right]^2$. This function is minimized by expanding the residuals $\Delta(p_k)$ in a first order Taylor's series about the trial values, setting the partial derivatives of $R$ equal to zero, and solving the resulting set of linear equations for the parameter corrections $\epsilon_k$. The summation is over the observed reflection data, and the weighting factors $w$ are defined by $w = 1/\sigma^2(\Delta)$, where $\sigma(\Delta)$ is the estimated standard deviation of $\Delta$. The linear equations may be written in matrix notation as $C \Delta = q$, where

$$C_{ij} = \sum w \frac{\partial \Delta}{\partial p_i} \frac{\partial \Delta}{\partial p_j} \quad \text{and} \quad q_i = \sum w \frac{\partial \Delta}{\partial p_i}.$$ 

The parameter list defined by this program is the following: the first three parameters are the lengths of the unit cell edges in Å, the second three parameters are the cell angles in degrees, and the last
four parameters are extrapolation function coefficients, to be defined later. Any combination of these ten parameters may be refined by the program.

The residual $\Delta$ is defined by the equation

$$\Delta = (d^*)_2 - 4 \sin^2 \theta/\lambda^2 - 4 \Delta \theta \sin^2 \theta/\lambda^2,$$

$$\Delta \theta = \sum_n K_n f_n(\theta).$$

Thus the systematic error in $\theta$, $\Delta \theta$, is expressed as the sum of contributions from various sources having the functional form $f_n(\theta)$ and coefficient $K_n$.

We now must find expressions for the various derivatives of $d^*$. The quantity $d^*$ may easily be expressed as a function of the reciprocal lattice constants; however, since we have chosen to refine the direct constants, we must express $d^*$ and its derivatives as functions of the direct lattice constants. In terms of the metric tensor $\tilde{g}$, where

$$\tilde{g} = \begin{pmatrix} p_1 p_2 \cos p_6 & p_1 p_3 \cos p_5 \\ p_1 p_3 \cos p_5 & p_2 p_3 \cos p_4 \end{pmatrix}, \quad (d^*)^2 = \mathbf{h} \tilde{g}^{-1} \mathbf{h},$$

$\mathbf{h}$ is the vector of the Miller indices of the reflection.

Although the expressions for the derivatives of $\tilde{g}^{-1}$ with respect to the $p_k$ may be obtained in closed form, they are rather lengthy. This program evaluates these derivatives numerically by incrementing the $p_k$. The increments chosen are $0.005 \text{ Å}$ for the cell edges, and $0.5^\circ$ for the cell angles. The derivatives of $\tilde{g}^{-1}$ need be calculated only once,
since \( \frac{\partial (d^*)^2}{\partial p_k} = \sum_i \sum_j h_i h_j \frac{\partial g_{ij}}{\partial p_k} \). Thus a table may be constructed with the 54 derivatives of each of the elements of \( g^{-1} \) with respect to \( p_k \). Since \( g^{-1} \) is symmetric, only 36 of these are independent.

The derivatives of \( \Delta \) with respect to the extrapolation coefficients \( K_n \) are simply the extrapolation functions \( f_n(\theta) \), multiplied by \( 4 \sin 2\theta/\lambda^2 \).

**EXTRAPOLATION FUNCTIONS**

A discussion of extrapolation functions suitable for typical experimental arrangements is given in the International Tables for X-Ray Crystallography, Vol. II, p. 216 (1959). References to the extensive literature on this subject may also be found there.

Program LCR-2 provides a choice of any combination of the four extrapolation functions listed below. The user may alter the program, if necessary, to change these functions to suit his preference or experimental method.

1. \( \Delta \theta_1 = K_1 \sin 2\theta \). This is equivalent to a linear extrapolation of a plot of \( d \) vs \( \cos^2 \theta \) to \( \theta = 90^\circ \). This function may be used to correct for eccentricity of the sample.

2. \( \Delta \theta_2 = K_2 \cos \theta \). This is equivalent to a linear extrapolation of a plot of \( d \) vs \( \cos \theta \cot \theta \) to \( \theta = 90^\circ \).

3. \( \Delta \theta_3 = K_3 \cos \theta (1/2 + \sin \theta/2\theta) \). This is equivalent to a linear extrapolation of a plot of \( d \) vs \( \frac{1}{2}(\cos^2 \theta/\sin \theta + \cos^2 \theta/\theta) \) to \( \theta = 90^\circ \).

This is the procedure suggested by Nelson and Riley to correct for absorption effects in the sample.
4. $\Delta \theta_4 = K_4$. This is equivalent to a linear extrapolation of a plot of $d$ vs $\cot \theta$ to $\theta = 90^\circ$. This function may be used to correct for a constant calibration error persisting at $2\theta = 180^\circ$. Prior calibration of the experimental apparatus is highly desirable. For example, a substance with accurately known lattice constants, such as Al, may be used for calibration.

It should be noted that these extrapolation functions have a similar mathematical form as $\theta$ approaches $90^\circ$. The lack of orthogonality between these functions will result in a large correlation between the extrapolation coefficients. For this reason, the results obtained with the program when more than one extrapolation coefficient is varied should be cautiously interpreted.

**WEIGHTING FACTORS**

After correction for the systematic error $\Delta \theta$, it is presumed that only random errors in $\theta$ will remain. Assuming the systematic errors are small, the random error in $\Delta$ is given by the equation

$$\sigma(\Delta) = 8 \sigma(\theta) \sin \theta \cos \theta / \lambda^2,$$

and therefore $w = \lambda^4 / 64 \sigma(\theta) \sin^2 \theta \cos^2 \theta$.

The effect of these weighting factors on the final values of the parameters is not negligible, and it is therefore important that they be included.

**INPUT DATA FORMATS**

1. Title card, any alphanumerics in col. 1-70, col. 71-72 blank.

2. Initial lattice constants in angstroms and degrees: FORMAT (6F10.4);
   a, b, c, alpha, beta, and gamma.
3. Control card. Col. 1-10 have parameter selection information for the six lattice constants and the four extrapolation functions; a 1 in the corresponding column includes the parameter in the least squares treatment, otherwise put zero in the column.

Col. 20 has the lattice type code. Triclinic=1, monoclinic=2, orthorhombic=3, tetragonal=4, rhombohedral=5, hexagonal=6, or cubic=7.

Col. 29-30 has the maximum number of least squares cycles desired.

Col. 31-40, 41-50, and 51-60 have damping factors for the shifts in the magnitudes of the lattice constants, the angular constants, and the extrapolation coefficients. These are normally punched 1.0 unless convergence difficulties are encountered.

Col. 69-70 has the number of data cards to be considered.

Control card is FORMAT (10I1, 2I10, 3F10.2, I10).

4. Data cards, FORMAT (6F10.0). These contain h, k, t, two theta, estimated error in two theta, and the wave length.

Any number of sets of data may be processed without reloading the program. Each data set consists of items 1 to 4 above.

5. Stopper card, any alphanumerics in col. 1-70, 1 in col. 72.
START  ACOUNTA0015  D.WILLIAMS  
COMPILE  RUN  FORTRAN  LIST  
LCR-2  LATTICE  CONSTANT  REFINEMENT  D.WILLIAMS  APRIL 1964  
INPUT  IS  AS  FOLLOWS  
TITLE  CARD,  FORMAT(14A5,12)  
INITIAL  LATTICE  CONSTANTS  IN  ANGSTROMS  AND  DEGREES,  FORMAT(6F10.4)  
CONTROL  CARD,  FORMAT((IC11,2110,3F10.2,1IC)  
COL.  1-10  HAS  PARAMETER  SELECTION  INFORMATION  FOR  THE  SIX  LATTICE  
CONSTANTS  AND  FOUR  EXTRAPOLATION  FUNCTIONS,  1=SELECT,  0=CC  NCT  
SELECT  
COL.  11-20  HAS  LATTICE  TYPE  CODE  
1=TRICLINIC  
2=MONOCLINIC  
3=CENTERED  
4=TETRAGONAL  
5=RHOMBOHEDRAL  
6=HEXAGONAL  
7=CUBIC  
COL.  21-30  HAS  NUMBER  OF  LEAST  SQUARES  CYCLES  DESIRED  
COL.  31-40  HAS  DAMPING  FACTOR  FOR  TRANSLATIONAL  CONSTANT  SHIFTS  
COL.  41-50  HAS  DAMPING  FACTOR  FOR  ANGULAR  CONSTANT  SHIFTS  
COL.  51-60  HAS  DAMPING  FACTOR  FOR  EXTRAPOLATION  CONSTANTS  
COL.  61-70  HAS  NUMBER  OF  DATA  CARDS  TO  BE  CONSIDERED  
DATA  CARDS,  FORMAT(6F10.1),  H,  K,  L,  THETA,  ESTIMATED  ERROR  IN  
TWO  THETA,  WAVE  LENGTH  
STEPS  PER  CARD,  FORMAT(14A5,12),  +1  IN  CCL.  71-72  
EXTRAPOLATION  FUNCTIONS  
1.  DELTA  THETA=K1*SIN(2.0*THETA)  
2.  DELTA  THETA=K2*COS(THETA)  
3.  NELSON-RILEY,  DELTA  THETA=K3*COS(THETA)*(0.5+SIN(THETA)/(2.0* 
THETA))  
4.  DELTA  THETA=K4  
DIMENSION  TITLE(14),  ALAT(10),ISEL(10),XH(3,500),THETA(50),  
1  ERROR(50),  ROW(10),  CC(3,3,6),  ALINC(6),  ALDEL(6),  DP(10),  
2  ANORM(65),  AVEC(10),  WAVE(50),  CORR(10),  SCEV(10),  ALCUT(10)  
99  READ  101,  (TITLE(I),  I=1,14),  KEY  
101  FORMAT(14A5,12)  
100  PRINT  102,  (TITLE(I),  I=1,14)  
102  FORMAT((1C14A5)  
READ  103,  (ALAT(I),  I=1,6)  
103  FORMAT(6F10.4)  
PRINT  104,  (ALAT(I),  I=1,6)  
104  FORMAT(1H030H  INITIAL  LATTICE  CONSTANTS  
1  /1H02A=F8.4,4H  B=F8.4,4H  C=F8.4,  
2  8H  ALPHA=F6.2,7H  BETA=F6.2,8H  GAMMA=F6.2)  
READ  105,  (ISEL(I),I=1,10),  LCCDE,  NC,  CPM,  CPA,  DP,  NDATA  
105  FORMAT(10I1,7I1C,3F10.2,110)  
PRINT  106,  (ISEL(I),I=1,10),  NC,  CPM,  CPA,  DP,  NDATA  
106  FORMAT((1HC  0MISEL(I)=10I1,5H  NG=12,6H  DPM=F4.2,  
1  6H  CPA=F4.2,6H  DP=F4.2,8H  NDATA=I4)  
GO  TO  (126,132,123,129,128,130,121),LCCDE  
121  PRINT  115  
115  FORMAT((1HC15H  CUBIC  LATTICE)  
GO  TO  135  
128  PRINT  116  
116  FORMAT((1HC25H  RHCMBOHEDRAL  LATTICE)  
GO  TO  135  
129  PRINT  117
117 FORMAT (1HC20H TETRAGONAL LATTICE)
GO TO 135
130 PRINT 118
118 FORMAT (1HC20H HEXAGONAL LATTICE )
GO TO 135
123 PRINT 119
119 FORMAT (1HC25H RHOHMBOIC LATTICE )
GO TO 135
132 PRINT 120
120 FORMAT (1HC20H MONOCLINIC LATTICE)
GO TO 135
126 PRINT 134
134 FORMAT (1HC20H TRICLINIC LATTICE )
135 CONTINUE
READ 107, ((XH(J,I),J=1,3),THETA(I),ERRCR(I), WAVE(I), I=1, NDATA)
107 FORMAT (6F10.0)
CO 108 I=7, 10
108 ALAT(I)=0.0
NV=0
CO 111 I=1, 10
111 NV=NV+ISEL(I)
AP=NV*(NV+3)/2
AN=NV+1
CO 113 I=1, 3
ALCEL(I)=0.005
ALAT(I+3)=ALAT(I+3)/57.29580
113 ALCEL(I+3)=0.5/57.29580
IC=1
C START REFINEMENT CYCLES
176 IF (IC-NC) 1176, 1176, 97
1176 CO 109 I=1, 10
109 AVEC(I)=0.0
CO 110 I=1, NP
110 ANOR(I)=0.0
RSLM=0.0
C OBTAIN DC MATRIX, UPPER TRIANGULAR PORTION, DOUBLED OFF-DIAGONALS
CO 136 I=1, 3
CO 136 J=1, 3
CIJO=CIJ(I,J,ALAT)
CO 136 K=1, 6
CC(I,J,K)=C*0
CO 137 L=1, 6
137 ALINC(L)=ALAT(L)
IF (ISEL(K)) 136, 136, 206
206 ALINC(K)=ALAT(K)+ALDEL(K)
C SET SYMMETRY RELATED PARAMETERS
GO TO (201,201,201,202,203,202,205), LCCDE
202 ALINC(2)=ALINC(1)
GO TO 201
203 ALINC(5)=ALINC(4)
ALINC(6)=ALINC(4)
205 ALINC(3)=ALINC(1)
GO TO 202
201 CC(I,J,K)=(CIJ(I,J,ALAT)-CIJO)/ALDEL(K)
136 CONTINUE
C START LCP THROUGH REFLECTION DATA
CO 141 M=1, NDATA
DELTA=0.0
CO 143 I=1, 3
CO 143 J=1, 3
143 DELTA=DELTA+CIJ(I,J,ALAT)*XH(I,M)*XH(J,J)
C CALCULATE DERIVATIVES OF DELTA WITH RESPECT TO LATTICE PARAMETERS
CO 142 K=1, 6
CP(K)=0.0
CO 142 I=1, 3
CO 142 J=1, 3
142 CP(K)+DP(K)*OC(I,J,K)*XH(I,M)*XH(J,M)
WTHE=THETA(M)*114.3916C
WS2TH=SINF(2.0*WTHE)
WSTH=SINF(WTHE)
WCTH=CCSF(WTHE)
WAV2=WAVE(M)*WAVE(M)
FLAMB=4.0/WAV2
WDELTH= ALAT(7)*WS2TH+ ALAT(8)*WCTH + ALAT(9)*WCTH*
1 (0.5+WS2TH/(2.0*WTHE))+ALAT(10)
CELTA=CELTA-FLAM8*WS2TH+WCTH*WS2TH
CP(7)=-WS2TH*WS2TH*FLAMB
CP(8)=-WS2TH*WCTH*FLAMB
CP(9)=-WS2TH*WCTH*(0.5+WS2TH/(2.0*WTHE))*FLAMB
CP(10)=-WS2TH*FLAMB
WATE=WAV2/(ERROR(M)*WS2TH)
CO 144 I=1, 10
144 CP(I)=CP(I)*WATE
CELTA=CELTA*WATE
C ADE TERMS TO MATRIX
RSUM=RSUM+CELTA*CELTA
KK=NV
K=0
CO 145 I=1, 10
IF (ISEL(I)) 145, 145, 146
145 J=1, 10
IF (ISEL(J)) 147, 147, 148
148 KK=KK+1
ANORM(KK)=ANORM(KK)+DP(I)*DP(J)
147 CONTINUE
K=K+1
AVEC(K)=AVEC(K)-CELTA*DP(I)
145 CONTINUE
141 CONTINUE
CALL SYMLIN(ANCRM,NV,AVEC,NG)
IF (NG) 152, 151, 152
152 PRINT 150
150 FORMAT (10H035H NORMAL EQUATIONS ARE SINGULAR )
GO TO 99
151 =RSUM/(FLCATF(NDATA)-FLCATF(NV))
CO 161 I=NAN, NP
161 ANCRM[I]=ANORM[I]*h
CO 153 I=1, 10
IF (ISEL(I)) 154, 154, 153
154 CORR(I)=0.0
SDEV(I)=0.0
153 CONTINUE
K=0
CO 155 I=1, 3
IF (ISEL(I)) 155, 155, 156
156 K=K+1
ALAT(I)=ALAT(I)+ANCRM(K)*DPM
CORR(I)=ANCRM(K)*DPM
KK=K*NV+K*(K-1)/2
SDEV(I)=SQRTF(ANCRM(KK))
155 ALCUT(I)=ALAT(I)
CO 157 I=4, 6
IF (ISEL(I)) 157, 157, 158
158 K=K+1
CORR(I) = ANCRM(K) * DPA * 57.295800
ALAT(I) = ALAT(I) + ANCRM(K) * DPA
KK = K * (NV + 1) - K * (K - 1) / 2
SDEV(I) = 57.295800 * SQRTF(ANORM(KK))

157
ALCLT(I) = ALAT(I) * 57.295800
DO 159 I = 7, 10
IF (ISEL(I)) 159, 159, 160
160
K = K + 1
CORR(I) = ANCRM(K) * DPK * 57.295800
ALAT(I) = ALAT(I) + ANCRM(K) * DPK
KK = K * (NV + 1) - K * (K - 1) / 2
SDEV(I) = 57.295800 * SQRTF(ANORM(KK))

159
ALCLT(I) = ALAT(I) * 57.295800
C SET SYMMETRY RELATED PARAMETERS
GO TO (1201, 12C1, 1201, 1202, 1203, 1202, 12C5), LCCDE

1202
ALAT(2) = ALAT(1)
ALCLT(2) = ALCLT(1)
GO TC 1201
1203
ALAT(5) = ALAT(4)
ALCLT(5) = ALCLT(4)
ALAT(6) = ALAT(4)
ALCLT(6) = ALCLT(4)
1205
ALAT(3) = ALAT(1)
ALAT(3) = ALAT(1)
GO TC 1202
1201 CONTINUE
C OUTPUT RESULTS FOR CYCLE IN ANGSTROMS AND DEGREES
PRINT 166, IC
166 FORMAT (1C5, 5HCYCLE I3, 32H A B C
1 40H ALPHA BETA GAMMA K(1)
2 39H K(2) K(3) K(4) RSLM/(indata-NV))
PRINT 170, (ICRRR(I), I = 1, IC)
170 FORMAT (1HC10HCHANGE 3F10.4, 3F10.3, 4F08.4)
PRINT 171, (ALCUT(I), I = 1, IC)
171 FORMAT (1HC10HNEw VALUE 3F10.4, 3F10.3, 4F08.4, E15.5)
PRINT 172, (SDEV(I), I = 1, 10)
172 FORMAT (1HC10HESC 3F10.4, 3F10.3, 4F08.4)
C TEST FOR END OF REFINEMENT
K = C
GO 501
501 IC = IC + 1
IF (ISEL(I)) 501, 501, 502
502
K = K + 1
KK = K * (NV + 1) - K * (K - 1) / 2
IF ((ABS(ANORM(K)) / SQRTF(ANORM(KK))) - C) 501, 503, 503
501 CONTINUE
GO TC 97
503 IC = IC + 1
GO TO 176
C TERMINATE REFINEMENT
97 IF (NC) 14C1, 14C1, 1197
1197 PRINT 301, (ANCRM(I), I = NAN, NP)
301 FORMAT (1H0 50H VARIANCE-COVARIANCE MATRIX IN ANGSTROMS AND RADI
1 5HANS /((1HO7E15.6))
CO 302 K = 1, NV
KK = K * (NV + 1) - K * (K - 1) / 2
302 SDEV(K) = C / SQRTF(ANORM(KK))
PRINT 303
303 FORMAT (1H0 20H CORRELATION MATRIX)
KK = NAN
CO 304 I = 1, NV
CO 305 J = 1, NV
305 RDH(J) = 0.0
DIMENSION ALAT(6)
COSA=COSF(ALAT(4))
COSB=COSF(ALAT(5))
COSC=COSF(ALAT(6))
DET=1.0/(1.0-COSA*COSA-COSB*COSB-COSC*COSC+2.0*COSA*COSB*COSC)
GO TO (7,8,6,1)
7 GO TO (1,2,3,1, J)
8 GO TO (9,4,5, J)
1 CIJ=DET*(1.0-COSA*COSA)/(ALAT(1)*ALAT(1))
GO TO 9
2 CIJ=DET*(CCSA*COSB-COSC)*2.0/(ALAT(1)*ALAT(2))
GO TO 9
3 CIJ=DET*(CCSA*COSC-COSB)*2.0/(ALAT(1)*ALAT(3))
GO TO 9
4 CIJ=DET*(1.0-CCS*COSB)/(ALAT(2)*ALAT(2))
GO TO 9
5 CIJ=DET*(CCS*COSC-COSC)*2.0/(ALAT(2)*ALAT(3))
GO TO 9
6 CIJ=DET*(1.0-CCSC*COSC)/(ALAT(3)*ALAT(3))
RETURN
END
SYMMETRIC LINEAR EQUATION SOLVER USING SYMINV

SUBROUTINE SYMLINE(AM, NV, VEC, ISING)

DIMENSION AM(9869), VEC(139)

CALL SYMINV(AM, NV, ISING)

IF (ISING) 99, 2, 99

2 CO 3 I=1, NV

3 AM(I)=0.0

4 J=1, NV

5 IJMUL=I*NV+J-(I*(I-1))/2

6 GO TO 4

7 AM(I)=AM(I)+AM(IJMUL)*VEC(J)

8 CONTINUE

99 RETURN

END

END

INVERT POSITIVE DEFINITE SYMMETRIC MATRIX OF ORDER NV D.WILLIAMS

MATRIX IS STORED AS FOLLOWS

MATRIX ELEMENTS BY ROWS, GIVING ONLY UPPER TRIANGULAR PART

A TOTAL OF NV*(NV+1)/2 STORAGE CELLS IS REQUIRED

LOCATION AM(NV+1) IS STARTING ADDRESS OF MATRIX

NG=0 IS NORMAL RETURN, NG=1 IS RETURN FOR SINGULAR MATRIX

INVERSE MATRIX IS RETURNED TO SAME LOCATION I.E. AM(NV+1)

METHOD-BUSING AND LEVY, COMM. ACM, AUGUST 1962

SUBROUTINE SYMINV(AM, NV, NG)

DIMENSION AM(9869)

DIAGONALIZE

CO 24 I=1, NV

10 I=I*NV-(I*(I-1))/2

II=I+1

LI=(I-1)*NV+I-((I-1)*(I-2))/2

AM(LI)=FLOATF(I)

BIGAJJ=0.0

CO 2 J=I, NV

JJ=J*NV+J-(J*(J-1))/2

IF (ABSF(AM(JJ))-BIGAJJ) 22, 2, 3

3 BIGAJJ=ABSF(AM(JJ))

AM(LI)=FLOATF(J)

2 CONTINUE

CALL AINTCHIAM(NV, I, IO, II, LI)

RESUME DIAGONALIZE

20 IF(AM(II)) 22, 22, 21

21 NG=1

GO TO 62

22 AM(II)=1.0/AM(II)

10 I=I-1

IQ=I-1*NV-((I-1)*(I-2))/2

II=I+1

IF(I-I*NV) 28, 28, 29

28 CO 23 K=I, NV

IK=I+K

IKC=IQO+K
23 AM(IKQ) = AM(I)*AM(IK)
   CO 24 J=I, NV
   JQ=J*NV-(J*(J-1))/2
   IJ=10+J
   CO 24 K=J, NV
   JK=JO*K
   IK=IQ*K
   CO 24 AM(JK)=AM(JK)+AM(IK)*AM(IJ)
   C RESTORE
   29 I=NV-1
   55 IO=I*NV-(I*(I-1))/2
   II=IO+I
   LI=(I-1)*NV+I-((I-1)*(I-2))/2
   II=I+1
   GO 5C J=I1, NV
   IJ=IO+J

   50 AM(IJ)=0.0
   IQ=(I-1)*NV-((I-1)*(I-2))/2
   CO 52 J=I1, NV
   JO=J*NV-(J*(J-1))/2
   IJ=10+J
   IJQ=IQ*K+J
   CO 30 K=J, NV
   IK=IO*K
   JK=JO*K
   AM(IK)=AM(IK)+AM(IJ)*AM(JK)
   IF (J-K) 53, 30, 53
   53 IK=IQ*K
   AM(IJ)=AM(IJ)+AM(IK)*AM(JK)
   30 CONTINUE
   52 AM(II)=AM(II)+AM(IJ)*AM(IJ)
   C INTERCHANGE
   CALL AINTCH(AI,NV,II,IO,II,LI)
   I=I-1
   IF (I) 61, 61, 55
   61 NG=0
   62 RETURN
END

C INTERCHANGE subroutine for SYMINV
SUBROUTINE AINTCH(AI,NV,II,IO,II,LI).
DIMENSION AM(9869)
10 LI=XINTF(AI(LI))
   IF(LI-I) 15, 16, 15
15 LI=IO+LI
   LIO=LI*NV-(LI*(LI-1))/2
   CO 11 J=I, NV
   IJ=10+J
   WORK=AM(IJ)
   IF(LI-J) 13, 13, 12
12 JLI=J*NV+LI-((J-J-1))/2
   AM(IJ)=AM(JLI)
   AM(JLI)*WORK
   GO TO 11
13 LLI=LIO+J
   AM(IJ)=AM(LIJ)
   AM(LIJ)=WORK
11 CONTINUE
\texttt{\textbackslash Work}=\texttt{AM(II)} \\
\texttt{AM(II)}=\texttt{AM(IL)} \\
\texttt{AM(IL)}=\texttt{WORK} \\
\texttt{16 \textbackslash RETURN} \\
\texttt{ENC} \\
\texttt{END} \\
\texttt{ACCNTAOG15 \textbackslash amp;D.WILLIAMS2}