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FIT, A NONLINEAR LEAST-SQUARES FITTING
PROGRAM TO OBTAIN INTERATOMIC FORCE CON-
STANTS FROM OBSERVED PHONON FREQUENCIES

by

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FIT, A NONLINEAR LEAST-SQUARES FITTING PROGRAM TO OBTAIN INTERATOMIC
FORCE CONSTANTS FROM OBSERVED PHONON FREQUENCIES

Thomas Stephen Prevender[†]

ABSTRACT

The computer program described obtains the best-fit interatomic force constants of a material possessing the CsCl structure from its measured phonon dispersion curves. A general Born von Karman force constant model employing interactions up to and including sixth neighbor is used. The program is written in FORTRAN for use with an IBM 360-65 computer.

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1. INTRODUCTION

A nonlinear least-squares fitting program that obtains a set of best-fit force constants from measured phonon dispersion curves is described. The program is written for the particular case of a CsCl lattice but may easily be generalized to other lattice types. The force constant model on which the program is based is a general Born von Karman model. In its present form the program will treat interactions up to and including sixth neighbor. FIT is designed for phonons that have wave vectors in the directions $[0\ 0\ \zeta]$, $[\zeta\ \zeta\ 0]$, $[\zeta\ \zeta\ \zeta]$, or $[\frac{1}{2}\ \frac{1}{2}\ \zeta]$.

The criterion that is used in the program to obtain force constant values is the minimization of the variance ratio, VR, which is defined by

$$VR = \frac{1}{N_D - N_P} \sum_{i=1}^{N_D} \frac{[\nu_C(i) - \nu_O(i)]^2}{[\delta \nu_O(i)]^2} \quad (1)$$

where

- N_D = number of phonons
- N_P = number of fitting parameters
- $\nu_C(i)$ = calculated frequency of the i -th phonon
- $\nu_O(i)$ = measured frequency of the i -th phonon
- $\delta \nu_O(i)$ = uncertainty in the frequency of the i -th phonon

2. PROGRAM DESCRIPTION

The $\nu_C(i)$ are calculated from a set of interatomic force constants that will be referred to as the f_j . A discussion of the derivation of the expressions relating the $\nu_C(i)$ to the f_j has been given elsewhere.^{1,2} To

demonstrate how the program finds a set of best-fit force constants, the effect of a change in the force constants on the variance ratio will be considered. If the set of force constants is changed by the increments Δf_j where in general $\Delta f_1 \neq \Delta f_2 \neq \Delta f_3$ etc., then the new set of force constants will be given by

$$f'_j = f_j + \Delta f_j . \quad (2)$$

The phonon frequencies that may be calculated from the new force constants are

$$v'_c(i) = v_c(i) + \sum_{j=1}^{N_p} \frac{\partial v_c(i)}{\partial f_j} \Delta f_j . \quad (3)$$

If the quantity J_{ij} is defined by

$$J_{ij} = \frac{\partial v_c(i)}{\partial f_j} , \quad (4)$$

then Eq. (3) may be rewritten as

$$v'_c(i) = v_c(i) + \sum_{j=1}^{N_p} J_{ij} \Delta f_j . \quad (5)$$

The new variance ratio for the set of incremented f_j is given by

$$VR' = (N_D - N_p)^{-1} \sum_{i=1}^{N_D} [\delta v_o(i)]^{-2} [v_c(i) + \sum_{j=1}^{N_p} J_{ij} \Delta f_j - v_o(i)]^2 . \quad (6)$$

When Eq. (6) is expanded it becomes

$$\begin{aligned} VR' = & (N_D - N_p)^{-1} \sum_{i=1}^{N_D} [\delta v_o(i)]^{-2} \{ [v_c(i) - v_o(i)]^2 \\ & + 2 \sum_{j=1}^{N_p} [v_c(i) - v_o(i)] J_{ij} \Delta f_j \\ & + \left(\sum_{j=1}^{N_p} J_{ij} \Delta f_j \right) \left(\sum_{k=1}^{N_p} J_{ik} \Delta f_k \right) \} . \end{aligned} \quad (7)$$

If the f_j' are the best-fit values, then it is true that

$$\frac{\partial VR'}{\partial f_j'} = 0 \quad (8)$$

It will be assumed that Eq. (8) is approximately true, in which case Eq. (7) becomes, after differentiating

$$0 = \sum_{i=1}^{N_D} [\delta v_0(i)]^{-2} [v_c(i) - v_0(i)] J_{ij} + \sum_{i=1}^{N_D} \sum_{k=1}^{N_p} [\delta v_0(i)]^{-2} J_{ij} (J_{ik} \Delta f_k) \quad (9)$$

This equation may be written in matrix form and solved for the Δf_j to yield

$$\overline{\Delta f} = (\tilde{J}^T \tilde{W} \tilde{J})^{-1} \tilde{J}^T \tilde{W} (\tilde{v}_c - \tilde{v}_0) \quad (10)$$

The quantities in Eq. (9) are defined as

$$\overline{\Delta f} = (\Delta f_1, \Delta f_2, \dots, \Delta f_{N_p})^T \quad (11)$$

$\tilde{J}$ is a matrix, the ii -th element of which was defined in Eq. (4); and $\tilde{W}$ is a diagonal matrix, the ii -th element of which is

$$W_{ii} = [\delta v_0(i)]^{-2} \quad (12)$$

Equation (10) is the expression that is used by FIT to minimize the variance ratio. Starting from an assumed set of force constants that are read into the computer as input data, the program calculates a new set of force constants from Eqs. (10) and (2). It then uses this new set to again

refine the force constants and continues iterating in this manner, refining the force constants with each iteration.

3. INPUT DATA FOR THE PROGRAM

The input data cards are described below, and in addition, by the comment cards in the program.

1st card: M_0 , M_1 , DELTA, NN, ISTOP, ICHECK. FORMAT (3F10.3, 3I5)

M_0 and M_1 are the atomic masses of the atoms located at (000) and ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$)a respectively. The masses are in atomic mass units. DELTA is a parameter such that, if the difference in the variance ratio between two successive iterations is less than DELTA, the program is terminated. NN is the number of force constants read by the computer; NN is also equal to N_p . ISTOP is the maximum number of iterations the program will perform before stopping. ICHECK is a parameter that controls the print-out of information after each iteration. If ICHECK = 1, then, for each iteration the force constants, $v_c(i)$, $[v_c(i) - v_0(i)]$, and $[v_c(i) - v_0(i)] / \delta v_0(i)$ and the variance ratio are printed out. If ICHECK $\neq$ 1, this information is printed out for only the last iteration.

2nd card: MM, XPC. FORMAT (I5, F12.3)

MM is the number of phonons to be read into the computer. XPC is the fractional change that is made in a force constant in order to calculate the J_{ij} . That is, the J_{ij} are calculated from the expression

$$J_{ij} = \frac{v_c(f_1, \dots, f_j + \delta f_j, \dots, f_{N_p})_i - v_c(f_1, \dots, f_{N_p})_i}{\delta f_j} \quad (13)$$

where

$$\delta f_j = XPC - f_j . \quad (14)$$

3rd through 5th card: FF(II). FORMAT (8F10.0)

The FF(II) are the initial assumed values for the interatomic force constants. They are read eight to a card in the order

$$\alpha_1^1, \beta_1^1, \alpha_{10}^2, \alpha_{11}^2, \alpha_{20}^2, \alpha_{21}^2, \alpha_{10}^3, \alpha_{11}^3, \alpha_{30}^3, \alpha_{31}^3, \beta_{30}^3, \beta_{31}^3,$$

$$\alpha_1^4, \alpha_2^4, \beta_1^4, \beta_2^4, \alpha_{10}^5, \alpha_{11}^5, \beta_{10}^5, \beta_{11}^5, \alpha_{10}^6, \alpha_{11}^6, \alpha_{20}^6, \alpha_{21}^6.$$

A description of the notation that is used for the force constants may be found elsewhere.^{1,2}

6th through MM + 6 cards: IDEN(II), VM(II), TOL(II), ZETA(II),
ICRV(II). FORMAT (I5, 3F10.4, I5).

IDEN(II) is an identifying number associated with the II-th phonon. This number may be any integer up to 99999. VM(II) is the measured frequency (in units of 10^{12} Hz) of the II-th phonon. TOL(II) is the uncertainty in the frequency (in units of 10^{12} Hz) of the II-th phonon. ZETA(II) is the wave vector coordinate (ζ) of the II-th phonon. ζ is defined as

$$\zeta = q/q_{MAX} \quad (15)$$

where q is a phonon wave vector, and ICRV(II) is a number that specifies to which branch of the dispersion curves the II-th phonon belongs. The identifying numbers of the various branches are contained in the program listing in Appendix I.

4. ACKNOWLEDGMENTS

The author gratefully acknowledges the programming assistance of J. Crenshaw.

5. REFERENCES

1. G. Gilat and G. Dolling, Phys. Rev. 138, A1053 (1965).
2. T. Prevender, Ph.D. thesis, Iowa State University, Ames, Iowa (1969).

APPENDIX I

PROGRAM LISTING

```
//S1 EXEC FORTG,TIME.GO=2,REGION=128K
//FORT.SYSIN DD *
DOUBLE PRECISION A,B,C,D,E,F,G,H,I,J,K,L,M,N,O,P,Q,R,S,T,MO,M1
DOUBLE PRECISION U,V,X
DOUBLE PRECISION MOM14,PI2MM4,TGL(125),DELNU(125),VNEW(125)
DOUBLE PRECISION JTWV,JTWJL(576),JM,DELTA,F,W,JTW,JTWJ,JTWX(24,24),
1 VM,DELTA,V,FF,AI,AII,AI3,VI,VI2,AM2N4,PI,ZE,WO(125)
DOUBLE PRECISION DCOS,DSQRT
DIMENSION JTW(24,125),JM(125,25),Z(125),JTWJ(24,24)
DIMENSION DELTA,F(25),VM(125),DELTA,V(125),JTWV(24)
DIMENSION FF(25),ZETA(125),ICRV(125),IDEN(125),PCT(125)
EQUIVALENCE (FF(1),A),(FF(2),B),(FF(3),C),(FF(4),D),(FF(5),E),
1 (FF(6),F),(FF(7),G),(FF(8),H),(FF(9),I),(FF(10),J),(FF(11),K
1 (FF(12),L),(FF(13),M),(FF(14),N),(FF(15),O),(FF(16),P),
1 (FF(17),Q),(FF(18),R),(FF(19),S),(FF(20),T),
1 (FF(21),U),(FF(22),V),(FF(23),W),(FF(24),X)
C THIS PROGRAM USES A NON-LINEAR LEAST SQUARES FITTING TECHNIQUE TO
C FIT THE INTERATOMIC FORCE CONSTANTS (UP TO 6TH NEIGHBOR) OF THE
C CSCL STRUCTURE
C MO=MASS OF THE ORIGIN ATOM IN A.M.U.
C M1=MASS OF THE ATOM AT (1,1,1)A/2
C DELTA=DIFFERENCE OF VARIANCE RATIOS BETWEEN ITERATIONS AT WHICH
C THE PROGRAM WILL STOP
C NN=NO. OF FORCE CONSTANTS
C ISTOP=MAXIMUM NO. OF ITERATIONS DESIRED
C ICHECK CONTROLS THE PRINT OUT OF CALCULATED QUANTITIES AFTER EACH ITERATION
READ 1,MO,M1,DELTA,NN,ISTOP,ICHECK
1 FORMAT (3F10.3,3I5)
WRITE (3,1) MO,M1,DELTA,NN,ISTOP,ICHECK
MO=MO/6.02472*1.0E-23
M1=M1/6.02472*1.0E-23
C MM=NO. OF PHONONS
C XPC=FRACTIONAL CHANGE OF FORCE CONSTANTS USED TO CALCULATE DERIVATIVE
READ 2,MM,XPC
2 FORMAT (I5,F12.3)
WRITE (3,2) MM,XPC
C FF(II) ARE THE FORCE CONSTANTS
```

```

      READ 3,(FF(II),II=1,NN)
3  FORMAT (8F10.0)
C  IDEN(II)=IDENTIFICATION NO. OF PHONON
C  VM(II)=FREQUENCY(IN UNITS OF 1.0E12) OF PHONON
C  TOL(II)= ERROR IN PHONON FREQUENCY
C  ZETA(II)= VARIABLE COORDINATE OF PHONON
C  ICRV(II)=IDENTIFICATION NUMBER OF THE BRANCH OF THE DISPERSION CURVES
C  TO WHICH PHONON(II) BELONGS
      READ 4,(IDEN(II),VM(II),TOL(II),ZETA(II),ICRV(II),II=1,MM)
4  FORMAT (I5,3F10.4,I5)
      ICOUNT=0
      VARINT=0.0
      PI=3.14159265358979
      MOM14=4.*MO*M1
      PI2MM4=PI**2*MOM14
      NPLUS=NN+1
      DO 100 II=NPLUS,25
100  FF(II)=0.0
      FF(NPLUS)=0.0
      WRITE (3,5)
5  FORMAT ('      I      OBS.NU(I)      TOL(I)      ZETA(I)      ICR
      1V(I)')
      DO 6 II=1,MM
      VM(II)=VM(II)*1.E+12
      TOL(II)=TOL(II)*1.E+12
6  WRITE (3,7) II,VM(II),TOL(II),ZETA(II),ICRV(II)
7  FORMAT (I5,5X,D10.3,5X,D10.3,5X,F10.2,5X,I5)
      DO 8 II=1,MM
8  WO(II)=1./TOL(II)**2
C  FIRST NEIGHBOR AT (111)
C  SECOND NEIGHBOR AT (200)
C  THIRD NEIGHBOR AT (220)
C  FOURTH NEIGHBOR AT (311)
C  FIFTH NEIGHBOR AT (222)
C  SIXTH NEIGHBOR AT (400)
C  A=ALPHA1-1      S=BETA1-1
C  C=ALPHA10-2      D=ALPHA11-2

```



```

C   G=ALPHA10-3      H=ALPHA11-3      I=ALPHA30-3      J=ALPHA31-3
C   K=BETA30-3       L=BETA31-3
C   M=ALPHA1-4        N=ALPHA2-4        O=BETA1-4        P=BETA2-4
C   Q=ALPHA10-5       R=ALPHA11-5       S=BETA10-5       T=BETA11-5
C   U=ALPHA10-6       V=ALPHA11-6       W=ALPHA20-6       X=ALPHA21-6
9   WRITE (3,10) ICOUNT
10  FORMAT (1H0,38HFORCE CONSTANTS FOR ITERATIO NUMBER ,I3)
    DO 11 II=1,MM
11  Z(II)=WO(II)
    WRITE (3,12) FF
12  FORMAT(5D15.6)
    WRITE (3,13)
13  FORMAT ('OTHESE ARE THE NEGATIVE CALCULATED FREQUENCIES')
    WRITE (3,14)
14  FORMAT(' CURVE NO.   II      JJ  NU(II,JJ)**2      AI      AII
1      A13')
    DO 15 JJ=1,NN
15  DELTAF(JJ)=FF(JJ)*XPC
    DELTAF(NPLUS)=0.0
    DO 16 II=1,MM
    ZE = ZETA(II)
    ICURVE = ICRV(II)
    DO 17 JJ=1,NPLUS
    TF=FF(JJ)
    FF (JJ)=FF(JJ)+DELTAF(JJ)
    AM2N4=4.*(A+M+2.*N)
    GO TO (18,18,19,19,20,20,21,21,22,22,23,23,24,24,25,25,26,27),
1    ICURVE
18  CONTINUE
    AI=MO*((AM2N4)+(D+4.*H+4.*R)*(1.-DCOS(2.*PI*ZE)))
    I+MO*(V*(1.-DCOS(4.*PI*ZE)))
    AII=M1*(AM2N4+(C+4.*G+4.*Q)*(1.-DCOS(2.*PI*ZE)))
    I+M1*(U*(1.-DCOS(4.*PI*ZE)))
    A13=((4.*A+8.*N)*DCOS(PI*ZE)+4.*M*DCOS(3.*PI*ZE))*2*MGM14
    VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
    VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
    IF (ICURVE.EQ. 1) JM(II,JJ)=VI

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```

C CURVE 1 IS LO (001)
  IF (ICURVE.EQ. 2) JM(II,JJ)=VI2
C CURVE 2 IS LA (001)
  GO TO 28
19 CONTINUE
  AI=MO*(AM2N4+(F+2.*H+2.*J+4.*R)*(1.-DCOS(2.*PI*ZE)))
  1+MO*(X*(1.-DCOS(4.*PI*ZE)))
  AII=M1*(AM2N4+(E+2.*G+2.*I+4.*Q)*(1.-DCOS(2.*PI*ZE)))
  1+M1*(W*(1.-DCOS(4.*PI*ZE)))
  A13=((4.*(A+M+N)*DCOS(PI*ZE)+4.*N*DCOS(3.*PI*ZE))**2)*MOM14
  VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
  VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
  IF (ICURVE.EQ. 3) JM(II,JJ)=VI
C CURVE 3 IS TO (001)
  IF (ICURVE.EQ. 4) JM(II,JJ)=VI2
C CURVE 4 IS TA (001)
  GO TO 28
20 CONTINUE
  AI=MO*(AM2N4+(D+2.*F+3.*R-2.*T)*(1.-DCOS(2.*PI*ZE))
  1+(2.*H+J+2.*L)*(1.-DCOS(4.*PI*ZE)))+(R+2.*T)*(1.-DCOS(6.*PI*ZE)))
  2+MO*((V+2.*X)*(1.-DCOS(4.*PI*ZE)))
  AII=M1*(AM2N4+(C+2.*E+3.*Q-2.*S)*(1.-DCOS(2.*PI*ZE))
  1+(2.*G+I+2.*K)*(1.-DCOS(4.*PI*ZE)))+(Q+2.*S)*(1.-DCOS(6.*PI*ZE)))
  2+M1*((U+2.*W)*(1.-DCOS(4.*PI*ZE)))
  A13=((3.*A-2.*B+M+2.*N+2.*O-4.*P)*DCOS(PI*ZE)+(A+2.*B+2.*M+4.*N
  1-4.*O)*DCOS(3.*PI*ZE)+(M+2.*N+2.*O+4.*P)*DCOS(5.*PI*ZE))**2)*MOM14
  VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
  VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
  IF (ICURVE.EQ. 5) JM(II,JJ)=VI
C CURVE 5 IS LO (111)
  IF (ICURVE.EQ. 6) JM(II,JJ)=VI2
C CURVE 6 IS LA (111)
  GO TO 28
21 CONTINUE
  AI=MO*(AM2N4+(D+2.*F+3.*R+T)*(1.-DCOS(2.*PI*ZE)))+(2.*H
  1+J-L)*(1.-DCOS(4.*PI*ZE)))+(R-T)*(1.-DCOS(6.*PI*ZE)))
  2+MO*((V+2.*X)*(1.-DCOS(4.*PI*ZE)))

```

```

      AII=M1*(AM2N4+(C+2.*E+3.*Q+S)*(1.-DCOS(2.*PI*ZE)))+(2.*G+I-K)
1  *(1.-DCOS(4.*PI*ZE)))+(Q-S)*(1.-DCOS(6.*PI*ZE)))
2+M1*((U+2.*W)*(1.-DCOS(4.*PI*ZE)))
      A13=((3.*A+B+M+2.*N-O+2.*P)*DCOS(PI*ZE)+(A-B+2.*M+4.*N+2.*O)
1*DCOS(3.*PI*ZE)+(M+2.*N-O-2.*P)*DCOS(5.*PI*ZE))*2*MOM14
      VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
      VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
      IF (ICURVE.EQ. 7) JM(II,JJ)=VI
C CURVE 7 IS TO (111)
      IF (ICURVE.EQ. 8) JM(II,JJ)=VI2
C CURVE 8 IS TA (111)
      GO TO 28
22 CONTINUE
      AI=MO*((AM2N4)+(D+F+2.*H+2.*J)*(1.-DCOS(2.*PI*ZE)))+(H+L+2.*R+2.
1*T)*(1.-DCOS(4.*PI*ZE)))
2+MO*((V+X)*(1.-DCOS(4.*PI*ZE)))
      AII=M1*(AM2N4+(C+E+2.*G+2.*I)*(1.-DCOS(2.*PI*ZE)))+(G+K+2.*Q+2.*S)*
1(1.-DCOS(4.*PI*ZE)))
2+M1*((U+W)*(1.-DCOS(4.*PI*ZE)))
      A13=(A-B+N-O+(A+B+M+2.*N+O-2.*P)*DCOS(2.*PI*ZE)+(M+N+2.*P)*DCOS(4.
1*PI*ZE))*2*MOM14*4.
      VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
      VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
      IF (ICURVE.EQ. 9) JM(II,JJ)=VI
C CURVE 9 IS LO (110)
      IF (ICURVE.EQ.10) JM(II,JJ)=VI2
C CURVE 10 IS LA (110)
      GO TO 28
23 CONTINUE
      AI=MO*(AM2N4+(2.*F+4.*H)*(1.-DCOS(2.*PI*ZE)))+(J+2.*R)*
1(1.-DCOS(4.*PI*ZE)))
2+MO*(2.*X*(1.-DCOS(4.*PI*ZE)))
      AII=M1*(AM2N4+(2.*E+4.*G)*(1.-DCOS(2.*PI*ZE)))+(I+2.*Q)*(1.-DCOS(4.
1*PI*ZE)))
2+M1*(2.*W*(1.-DCOS(4.*PI*ZE)))
      A13=((A+M)+(A+M+2.*N)*(DCOS(2.*PI*ZE))+2.*N*DCOS(4.*PI*ZE))*2*4.*
1 MOM14

```

```

      VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
      VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
      IF (ICURVE.EQ.11) JM(II,JJ)=VI
C   CURVE 11 IS T1G (110)
      IF (ICURVE.EQ.12) JM(II,JJ)=VI2
C   CURVE 12 IS T1A (110)
      GO TO 28
24  CONTINUE
      AI=MO*(AM2N4+(D+F+2.*H+2.*J)*(1.-DCOS(2.*PI*ZE))+(H-L+2.*R-2.*T)*
1   (1.-DCOS(4.*PI*ZE)))
      2+MO*((V+X)*(1.-DCOS(4.*PI*ZE)))
      AII=M1*(AM2N4+(C+E+2.*G+2.*I)*(1.-DCOS(2.*PI*ZE))+(G-K+2.*Q-2.*S)
1   (1.-DCOS(4.*PI*ZE)))
      2+M1*((U+W)*(1.-DCOS(4.*PI*ZE)))
      A13=((A+N+B+O)+(A-B+M+2.*N-O+2.*P)*(DCOS(2.*PI*ZE))+(M+N-2.*P)*(DC
1   OS(4.*PI*ZE)))*2*4.*MOM14
      VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
      VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
      IF (ICURVE.EQ.13) JM(II,JJ)=VI
C   CURVE 13 IS T2O (110)
      IF (ICURVE.EQ.14) JM(II,JJ)=VI2
C   CURVE 14 IS T2A (110)
      GO TO 28
25  CONTINUE
      AI=MO*(2.*(2.*A+2.*M+4.*N+D+2.*H+F+2.*J)+(F-2.*H-2.*J+4.*R)*(1.-
1   DCOS(2.*PI*ZE)))
      2+MO*(X*(1.-DCOS(4.*PI*ZE)))
      AII=M1*(2.*(2.*A+2.*M+4.*N+C+2.*G+E+2.*I)+(E-2.*G-2.*I+4.*Q)*(1.-
1   DCOS(2.*PI*ZE)))
      2+M1*(W*(1.-DCOS(4.*PI*ZE)))
      A13=((2.*P-B)*(DCOS(PI*ZE))-O*DCOS(3.*PI*ZE))*2*16.*MOM14
      VI=(AI+AII+DSQRT((AI-AII)**2+A13))/PI2MM4
      VI2=(AI+AII-DSQRT((AI-AII)**2+A13))/PI2MM4
      IF (ICURVE.EQ.15) JM(II,JJ)=VI
C   CURVE 15 IS PIO (.5,.5,Z)
      IF (ICURVE.EQ.16) JM(II,JJ)=VI2
C   CURVE 16 IS PIA (.5,.5,Z)

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        GO TO 28
26 CONTINUE
    VI=(4.*(A+M+2.*N+F+2.*H)+(D-4.*H+4.*R)*(1.-DCOS(2.*PI*ZE)))/(2.*
    1PI**2*M1)
    2+(V*(1.-DCOS(4.*PI*ZE)))/(2.*PI**2*M1)
    JM(II,JJ)=VI
C CURVE 17 IS DELO (.5,.5,Z)
    GO TO 28
27 CONTINUE
    VI=(4.*(A+M+2.*N+E+2.*G)+(C-4.*G+4.*Q)*(1.-DCOS(2.*PI*ZE)))/(2.*
    1PI**2*M0)
    2+(U*(1.-DCOS(4.*PI*ZE)))/(2.*PI**2*M0)
    JM(II,JJ)=VI
C CURVE 18 IS DELA (.5,.5,Z)
28 FF(JJ)=TF
    IF (JM(II,JJ).GE.0) GO TO 17
    JM(II,JJ)=-JM(II,JJ)
    IF (JJ-NPLUS) 17,29,29
29 WRITE (3,30) ICURVE,II,JJ,JM(II,JJ),AI,AII,A13
30 FORMAT ( 17,I8,I7,4D14.6)
17 CONTINUE
16 CONTINUE
    DO 31 II=1,MM
    DO 31 JJ=1,NPLUS
31 JM(II,JJ)=DSQRT(JM(II,JJ))
    DO 32 II=1,MM
    DO 33 JJ=1,NN
    IF (DELTAF(JJ)) 34,35,34
35 JM(II,JJ)=0.
    GO TO 33
34 JM(II,JJ)=(JM(II,JJ)-JM(II,NPLUS))/DELTAF(JJ)
33 CONTINUE
32 CONTINUE
    IF (ICHECK.NE.1) GO TO 36
    WRITE (3,37)
37 FORMAT ('OTHESE ARE THE CALCULATED FREQUENCIES USING THE INITIAL
    1FORCE CONSTANTS')

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WRITE (3,38) (II,JM(II,NPLUS),II=1,MM)
38 FORMAT (5(I8,2X,D13.6))
WRITE (3,39)
39 FORMAT ('OHERE ARE NU(CALC.)-NU(OBS.)')
36 DO 40 II=1,MM
DELNU(II)=0.0
40 DELNU(II)=DELNU(II)+JM(II,NPLUS)-VM(II)
IF (ICHECK.NE.1) GO TO 41
WRITE (3,38) (II,DELNU(II),II=1,MM)
WRITE (3,42)
42 FORMAT ('OHERE ARE (NU(CALC)-NU(OBS.))/NU(OBS.)')
DO 43 II=1,MM
PCT(II)=0.0
43 PCT(II)=DELNU(II)/VM(II)
WRITE (3,38) (II,PCT(II),II=1,MM)
41 QINT=0.0
VARI=0.0
DO 44 II=1,MM
44 QINT=QINT+Z(II)*((DELNU(II)**2)
IZZ=NN
VARI=VARI+QINT/(MM-IZZ)
IF(ICHECK.EQ.1) GO TO 45
IF(ABS(VARI-VARINT).LT.DELTA) GO TO 46
VARINT=VARI
IZZ = 1
DO 47 JJ=1,NN
DO 48 II=1,MM
IF (JM(II,JJ).NE.0.) GO TO 49
48 CONTINUE
GO TO 47
49 DO 50 II=1,MM
50 JM (II,IZZ)=JM(II,JJ)
IZZ=IZZ+1
47 CONTINUE
IZZ=IZZ-1
DO 51 II=1,NN
DO 52 JJ=1,MM

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      DELTAV(JJ)=0
52  JTW(II,JJ)=0
      DO 53 JJ=1,NN
53  JTWX(II,JJ)=0.
51  CONTINUE
      DO 54 II=1,IZZ
      DO 54 JJ=1,MM
54  JTW(II,JJ) = JM(JJ,II)*Z(JJ)
      DO 55 II=1,IZZ
      DO 55 JJ=1,IZZ
      DO 55 KK= 1,MM
55  JTWX(II,JJ)=JTWX(II,JJ)+JTW(II,KK)*JM(KK,JJ)
      KK=1
      DO 56 JJ = 1,IZZ
      DO 56 II=1,IZZ
      JTWJL(KK)=JTWX(II,JJ)
56  KK=KK+1
      DO 57 II=1,24
      DELTAF(II)=0
57  JTWV(II)=0.
      DO 58 JJ = 1,IZZ
      DO 58 II = 1,MM
58  JTWV(JJ)=JTWV(JJ)+JTW(JJ,II)*DELNU(II)
      EPS=1.E-15
      IER=0
      CALL DGELG (JTWV,JTWJL,IZZ,1,EPS,IER)
      WRITE (3,2) IER
      DO 59 JJ = 1,IZZ
59  DELTAF (JJ)=JTWV(JJ)
      DO 60 JJ=1,MM
      DO 60 II = 1,IZZ
60  DELTAV(JJ) = DELTAV(JJ)+JM(JJ,II)*DELTAF(II)
      DO 61 II=1,MM
      VNEW(II)=0.0
61  VNEW(II)=VNEW(II)+VM(II)+DELTAV(II)
      QPRIME = 0.
      VARF=0.0

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```

DC 62 II=1,MM
62 QPRIME=QPRIME+Z(II)*((JM(II,NPLUS)+DELTAV(II)-VM(II))**2)
VARF=QPRIME/(MM-IZZ)
WRITE (3,63)
63 FORMAT ('HERE ARE THE CALCULATED FORCE CONSTANTS CHANGES')
WRITE (3,64) (DELTAF(II),II=1,NN)
64 FORMAT (10(2X,D10.4))
WRITE (3,64)
WRITE (3,65) VARI,VARF,ICOUNT
65 FORMAT ('0INITIAL VAR. RATIO      FINAL VAR. RATIO      I'/2(6X,E14.
14),7X,I3)
ICOUNT=ICOUNT+1
IF(ICOUNT.GT.ISTOP) GO TO 45
DO 66 II=1,24
IF (DELTAF(II)) 67,66,68
67 IF(DELTAF(II)+1000.0) 69,66,66
69 DELTAF(II)=-1000.0
GO TO 66
68 IF(DELTAF(II)-1000.0) 66,66,70
70 DELTAF(II)=1000.0
66 CONTINUE
FF(1)=FF(1)-DELTAF(1)
FF(2)=FF(2)-DELTAF(2)
FF(3)=FF(3)-DELTAF(3)
FF(4)=FF(4)-DELTAF(4)
FF(5)=FF(5)-DELTAF(5)
FF(6)=FF(6)-DELTAF(6)
FF(7)=FF(7)-DELTAF(7)
FF(8)=FF(8)-DELTAF(8)
FF(9)=FF(9)-DELTAF(9)
FF(10)=FF(10)-DELTAF(10)
FF(11)=FF(11)-DELTAF(11)
FF(12)=FF(12)-DELTAF(12)
FF(13)=FF(13)-DELTAF(13)
FF(14)=FF(14)-DELTAF(14)
FF(15)=FF(15)-DELTAF(15)
FF(16)=FF(16)-DELTAF(16)

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FF(17)=FF(17)-DELTA(17)
FF(18)=FF(18)-DELTA(18)
FF(19)=FF(19)-DELTA(19)
FF(20)=FF(20)-DELTA(20)
FF(21)=FF(21)-DELTA(21)
FF(22)=FF(22)-DELTA(22)
FF(23)=FF(23)-DELTA(23)
FF(24)=FF(24)-DELTA(24)
WRITE (3,64) (DELTA(II),II=1,NN)
GO TO 9
46 ICHECK=1
GO TO 9
45 CONTINUE
END
```