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Part. II

EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

INELASTIC NEUTRON SCATTERING AND LATTICE DYNAMICS OF METALS IN QUASI-ION APPROXIMATION

by

K. KREBS and K. HÖLZL

1969

Joint Nuclear Research Center
Ispra Establishment - Italy
Reactor Physics Department

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Results are presented for 10 cubic metals. Listings of the pertinent FORTRAN-4 programs are given in Appendix I, II and III.

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ABSTRACT

On the basis of the pseudo-ion model described in Part I, the following lattice dynamical quantities have been calculated :
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KEYWORDS

INELASTIC SCATTERING
NEUTRONS
LATTICES
METALS
IONS
ATOMIC MODELS
FORM FACTOR
PHONONS
DEBYE TEMPERATURE
NUMERICALS
FORTRAN

CONTENTS

INELASTIC NEUTRON SCATTERING
AND LATTICE DYNAMICS OF METALS IN QUASI-ION APPROXIMATION

1. INTRODUCTION *)

This report contains results of lattice dynamical calculations which were made on the basis of the pseudo-ion model [1] described in Part I [2]. The reduction of the experimental inelastic neutron data to pseudo-ion form factors was done by means of a non-linear least square fitting program, called PSAF. Using another program, SKFD, frequency distributions and dynamical structure factors have been computed. These quantities are essential for any calculation of electrical and thermal resistivities or of thermodynamical quantities like specific heats, Debye temperatures or Debye-Waller factors. The computation of the latter quantities is done by a program called CVDWF. Listings of the mentioned FORTRAN-4 programs are given in the Appendix.

2. MODEL

In this passage we recall briefly our model and the underlying assumptions. The interaction energy E(K) between any two lattice particles including 2nd order effects may be written as [3, 4]

$$E(K) = E_{dir}(K) + E_{ind}(K)$$
$$= \frac{4\pi e^2 Z^2}{\Omega_o} \left\{ \frac{G_c^2(K)}{K^2} - \frac{G_{ind}^2(K)}{K^2} \left(1 - \frac{1}{\varepsilon(K)}\right) \right\} \qquad (1)$$

The first term is the direct Coulomb interaction energy between two extended ions with form factors $G_c(K)$, which go to 1 for $K \to 0$. The indirect interaction via the valence electrons is determined by the form factor

$$G_{ind}(K) = G_c(K) - G_{orth}(K) \qquad (2)$$

$G_{orth}(K)$ is the form factor describing orthogonalization effects, for $K \to 0$ it goes to zero, i.e. $G_{orth}(K)$ corresponds to a neutral "charge" distribution.

The dielectric function $\varepsilon(K)$ is given by

$$\varepsilon(K) = 1 + \frac{k_c^2}{K^2} D(t) \quad , \qquad (3)$$

where $k_c^2 = 4k_F/\pi a_o$ and $t = K/2k_F$ (k_F: Fermi wave vector, a_o: Bohr radius).

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*) Manuscript received on 5 May, 1969.

$D(t) = 1$ in the Thomas-Fermi approximation. In the RPA approximation it is given by [5]

$$D(t) = f(t) = \frac{1}{2} + \frac{1 - t^2}{4t^2} \ln \left|\frac{1+t}{1-t}\right| \qquad (4)$$

Including exchange effects we have [3]

$$D(t) = \left(1 - \frac{3t^2}{2 + 6t^2}\right) f(t) \qquad (5)$$

and if we take into account also the fact that the indirect interaction itself is modified by exchange effects [3], we may define an effective dielectric constant using

$$D(t) = \frac{f(t)}{1 - \frac{3}{8}\left(\frac{k_c^2}{k_F}\right)\frac{f(t)}{1+3t^2}} \qquad (6)$$

The corresponding dielectric function will be called $\varepsilon^{*}(K)$.

Equation (1) may be reduced to the following screened interaction between pseudo-ions

$$E(K) = \frac{4\pi e^2 Z^2}{\Omega_o} \frac{G_M^2(K)}{K^2 \varepsilon(K)} \quad , \qquad (7)$$

where the model form factor $G_M(K) = G_{ind}(K)$. This reduction is possible under the following assumptions:

a) the ion cores are small and non-overlapping,

b) the form factors are radially symmetric,

c) the ions behave as rigid particles, i.e. during vibration no moments are excited.

Since (7) is an interaction between extended particles and since it depends explicitly on volume, the validity of the Cauchy relations is not required. $G_{PA}(K) = G_M(K)/\varepsilon(K) \to 0$ for $K \to 0$, thus this quantity characterizes a neutral particle, the so-called pseudo-atom [6]. The pseudo-atom is composed of the bare particle $G(K)$ and the screening cloud $G_{SCL}(K) = - G(K)(1 - 1/\varepsilon(K))$.

If the assumptions a), b) and c) are justified for a certain metal, the potential

$$V(K) = -\frac{4\pi e^2 Z}{\Omega_o} \frac{G_{ind}(K)}{K^2\varepsilon(K)} \qquad (8)$$

with $\varepsilon(K)$ calculated using equation (5) is a valid pseudo-potential, as seen by an electron. Otherwise equation (7) with $D(t)$ from equation (6) should be considered as suitable interpolation formula, which may be used to compute all purely dynamical quantities like phonon frequencies and eigenvectors or the phonon density of states.

For the numerical calculations the following form factor has been assumed

$$G_M(K) = \{ 1 + \sum_{n=1} B_{n+1}\left(\frac{K}{2}\right)^{2n}\} \exp -(B_1 \frac{K}{2})^2 \qquad (9)$$

The parameters B_i are found by non-linear least square fitting to dispersion curves obtained from inelastic neutron scattering experiments.

3. PROGRAMS

Three programs have been written to obtain information on lattice dynamical properties of metals. The basic program is called PSAF, it gives the parameters B_i of the model form factor $G_M(K)$. The program is based on iterative procedures, as discussed by Marquardt [7]. At each step the parameters and the corresponding values for $G(K)$, $V(K)$ and $E(K)$ are calculated. The computation is interrupted when the least square deviations between theoretical and experimental frequencies correspond to the experimental errors of the points of the dispersion curve.

A second program is used to calculate the frequency distribution $g(\nu)$ and the structure factor $S(K)$ using $E(K)$, resp. $G(K)$, with the parameters obtained by PSAF. In order to reduce the computation time for $g(\nu)$ the interpolation procedure of Gilat and Raubenheimer [8] has been adopted. The main importance of $S(K)$ lies in its application to electron scattering problems [9].

The program CVDWF has been written to calculate lattice specific heats, Debye-Waller factors and effective Debye temperatures on the basis of the frequency spectra which are obtained by SKFD.

4. RESULTS

Using the program PSAF we have analyzed the experimental dispersion curves of lithium [10], sodium [11], potassium [12], rubidium [13], copper [14], aluminium [15], lead [16], iron [17], nickel [18] and platinum [19]. The parameters of the form factors, defined in equation (9) are given in Table 1, 2 and 3. With these parameters we have calculated $G(K)$, $G_{SCL}(K)$, $G(K)/\varepsilon^{*}(K)$, $G(K)/\varepsilon(K)$, $V^{*}(K)$ and $V(K)$, results are shown in Figs. 1 - 10. The following Figs. 11 - 20 show the corresponding dispersion curves together with the experimental data on which the fitting processes had been based.

By means of the program SKFD the frequency distribution $g(\nu)$ and the structure factor $S(K)$ for each metal have been computed and are shown in Figs. 21-33. Finally, using program CVDWF and $g(\nu)$ from SKFD the effective Debye temperatures $\Theta_{cal}(T)$ and $\Theta_{2W}(T)$ have been computed, corresponding curves are given in Figs. 34 - 36.

5. CONCLUSION

Programs and results have been presented which are based on the pseudo-ion approximation, proposed in Part I. Our results show that using this approximation one is able to reduce the neutron data to a simple physical model from which it is straightforward to calculate the essential phonon properties of a metal like the phonon density of states, the phonon frequencies and the polarization vectors at arbitrary points in reciprocal space. Results have been obtained for 10 cubic metals.

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TABLE I

Metal (Z)	Li(1)	Na(1)	K(1)	Rb(1)
T ^{o}K	98	90	9	120
B_1	1.30000	1.00000	1.30000	1.30000
B_2	-3.79414	-0,318437	-1.22754	-1.88127
B_3	17.61009	-0.643353	1.43616	-0.18315
B_4	-25.41615	0.045230	-7.61127	-1.95735
B_5	16.65343	0.019116	6.30042	1.21555
B_6	-5.42617		-1.47425	-0.19173
B_7	0.80812			
B_8	-0.00131			
B_9	-0.00788			

TABLE 2

Metal (Z)	Cu(1)	Al(3)	Pb(4)
T °K	300	80	100
B_1	1.30000	0.90000	1.500000
B_2	3.33137	-0.49203	-2.986300
B_3	-17.08360	0.19462	6.597300
B_4	20.16460	-0.16264	-0.734519
B_5	-9.21830	0.00608	-0.625849
B_6	1.53078	-0.00371	1.577600
B_7	0.05365		-0.325560
B_8	-0.05197		-0.118370
B_9			0.025482
B_{10}			0.005343
B_{11}			-0.000271
B_{12}			-0.000196

TABLE 3

Metal (Z)	Fe(2)	Ni(0.54)	Pt(1)
T °K	300	296	300
B_1	1.00000	1.00000	0.85000
B_2	1.75893	-6.14528	-1.23000
B_3	-1.53882	1.98451	0.61388
B_4	1.33014	-2.58300	0.31761
B_5	-0.52898	0.46579	-0.21167
B_6	0.06146	-0.12287	0.03149

FIGURE CAPTIONS

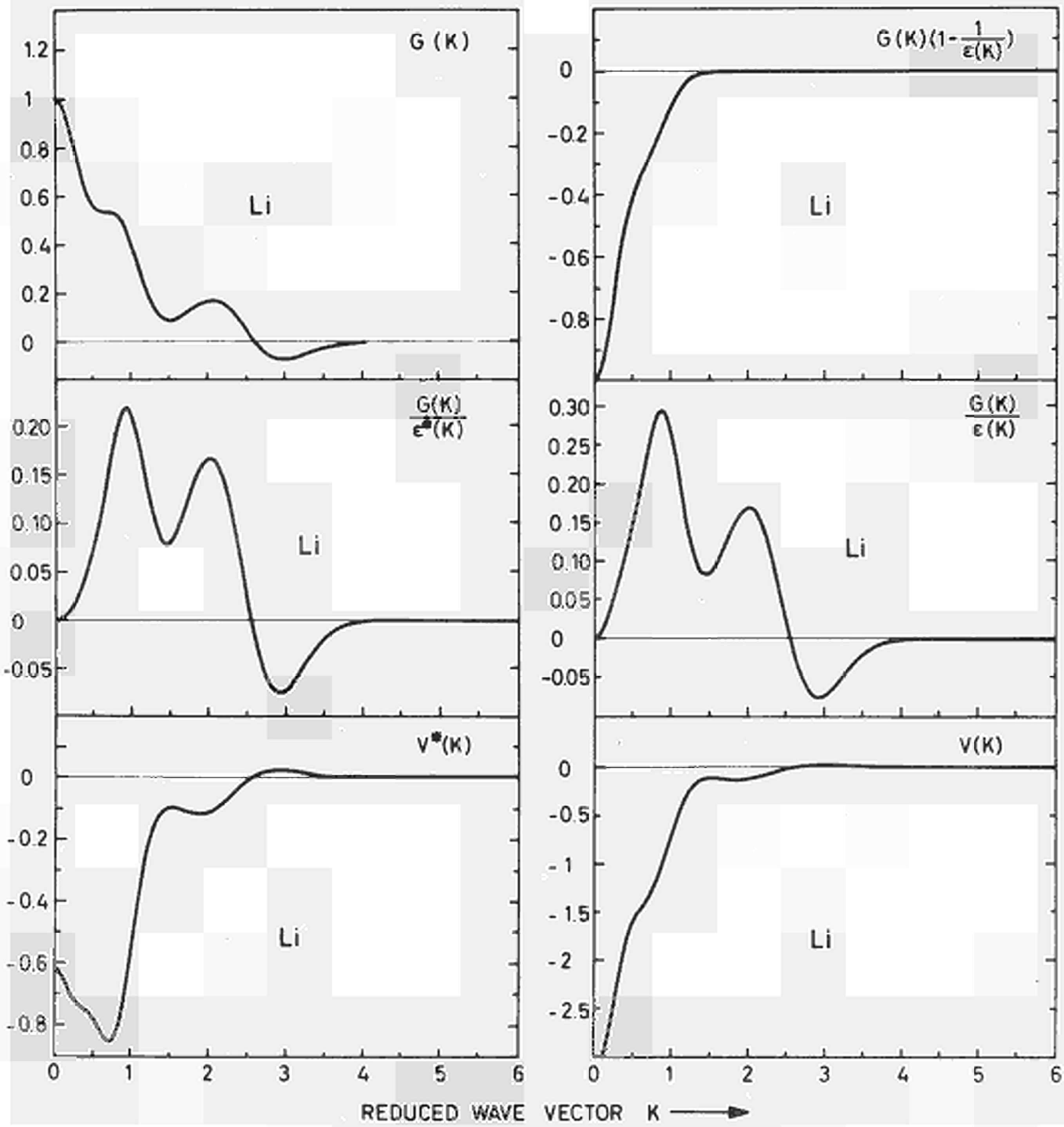
Fig. 1 - 10 Characteristic functions of Li, Na, K, Rb, Cu, Al, Pb, Fe, Ni and Pt

Fig. 11 - 20 Dispersion curves of Li, Na, K, Rb, Cu, Al, Pb, Fe, Ni and Pt

Fig. 21 - 30 Phonon frequency distributions $g(\nu)$ of Li, Na, K,Rb, Cu, Al, Pb, Fe, Ni and Pt

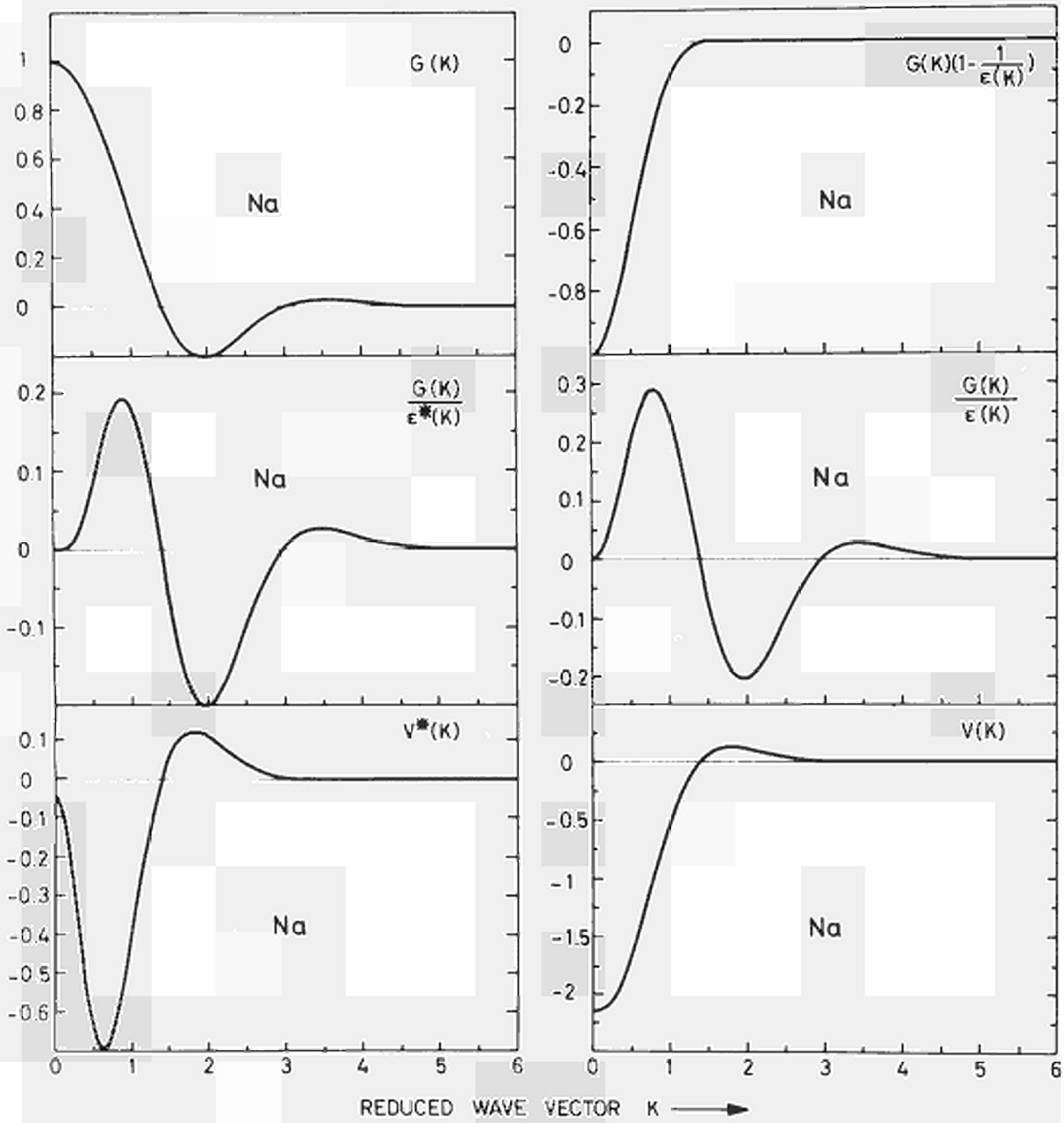
Fig. 31 - 33 Structure factors S(K) of Li, Na, K, Rb, Cu, Al, Pb, Fe, Ni and Pt

Fig. 34 - 36 Debye characteristic temperatures of the lattice specific heat (Θ_c) and of the Debye-Waller factor (Θ_W) for Li, Na, K, Rb, Cu, Al, Rb, Fe, Ni and Pt



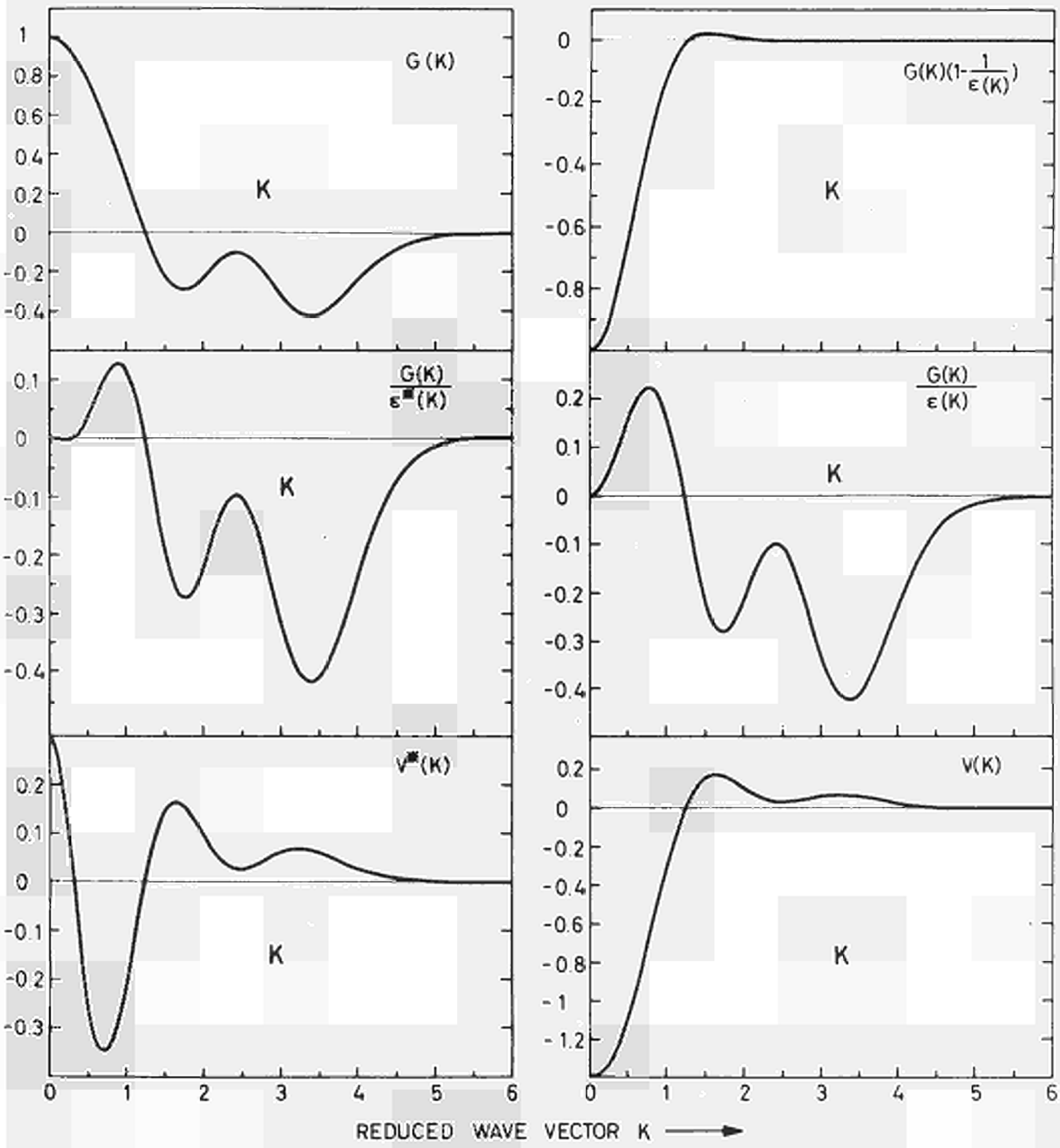
CHARACTERISTIC FUNCTIONS FOR Li

FIG. 1



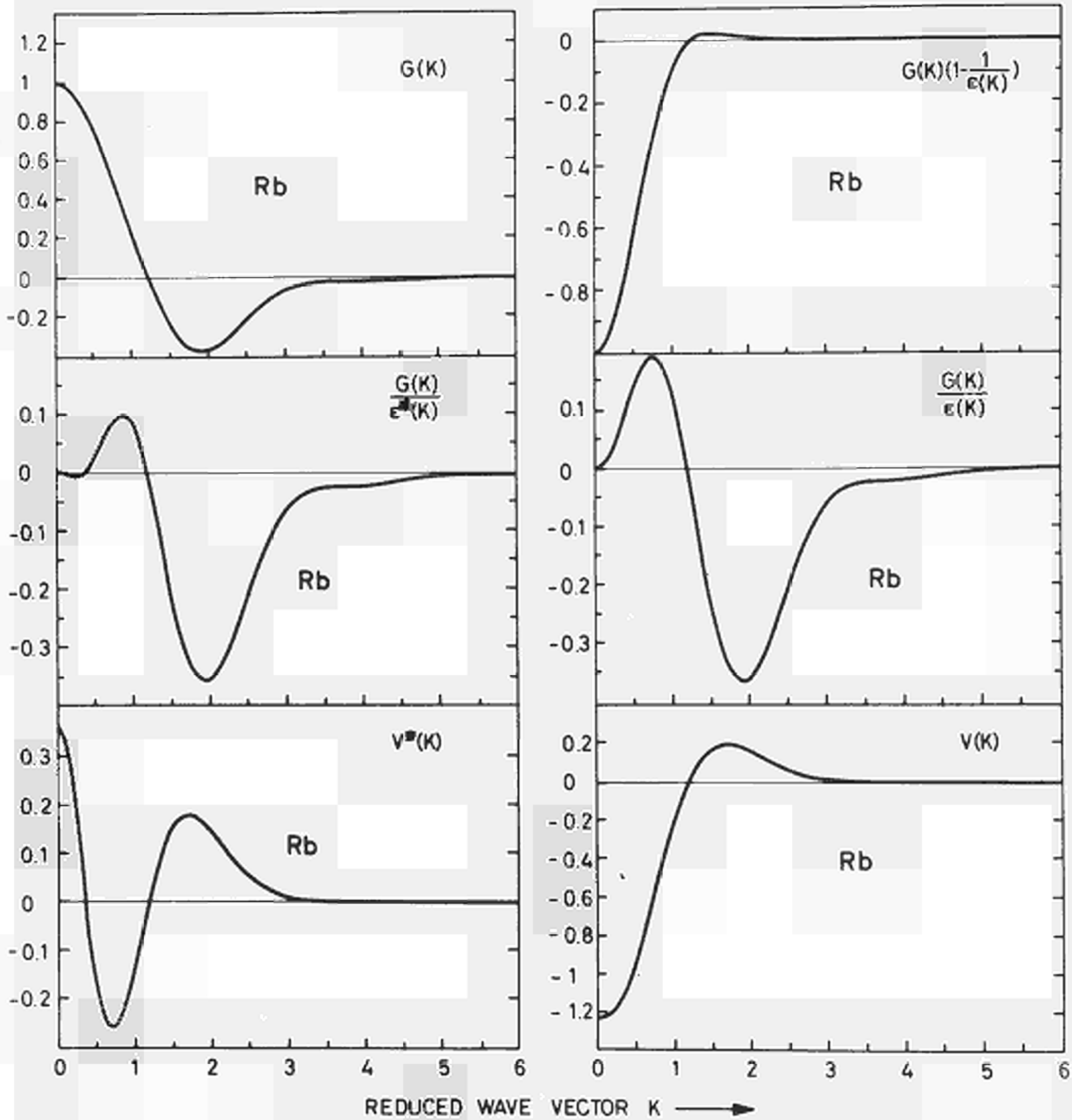
CHARACTERISTIC FUNCTIONS FOR Na

FIG. 2



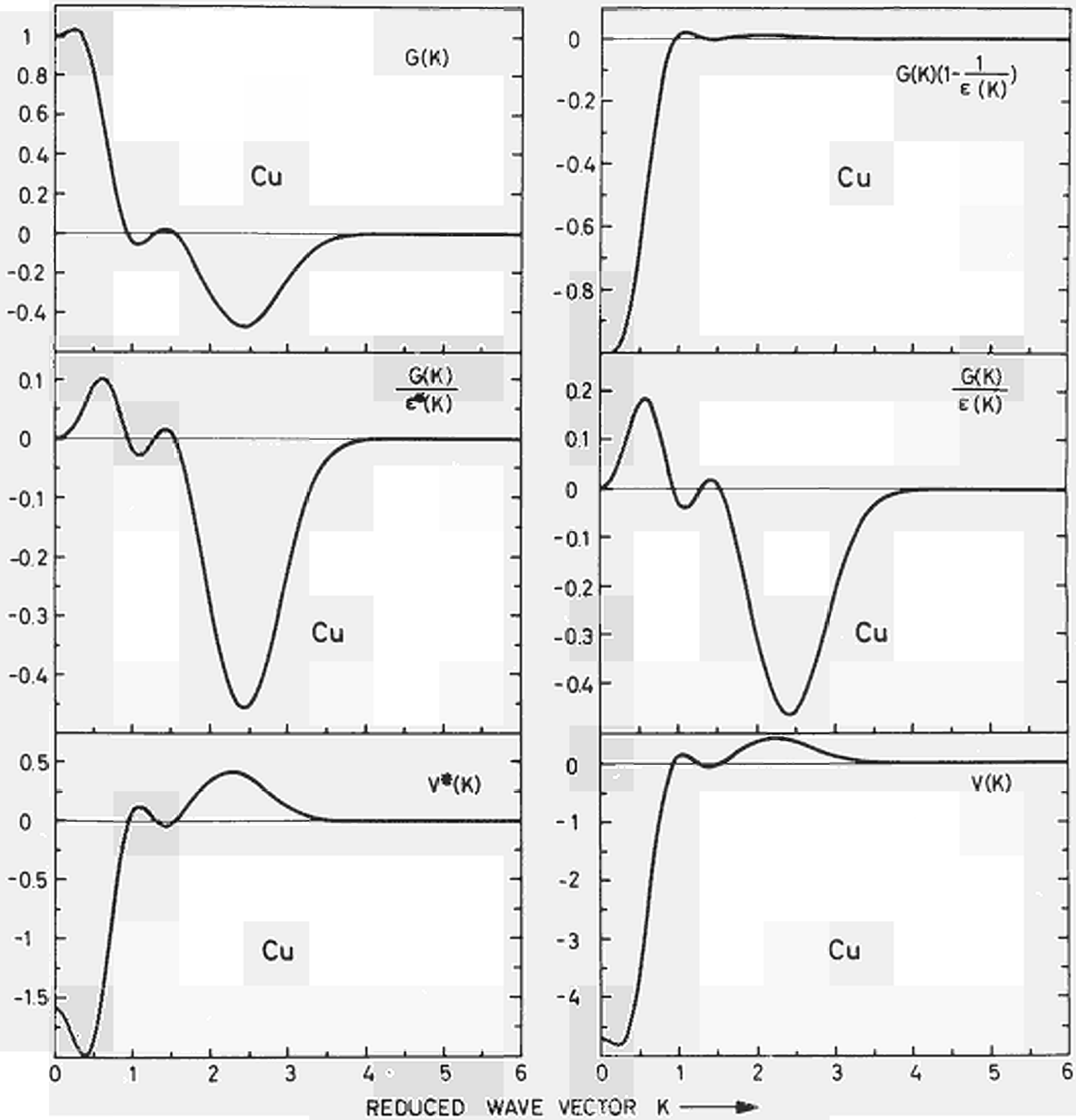
CHARACTERISTIC FUNCTIONS FOR K

FIG 3



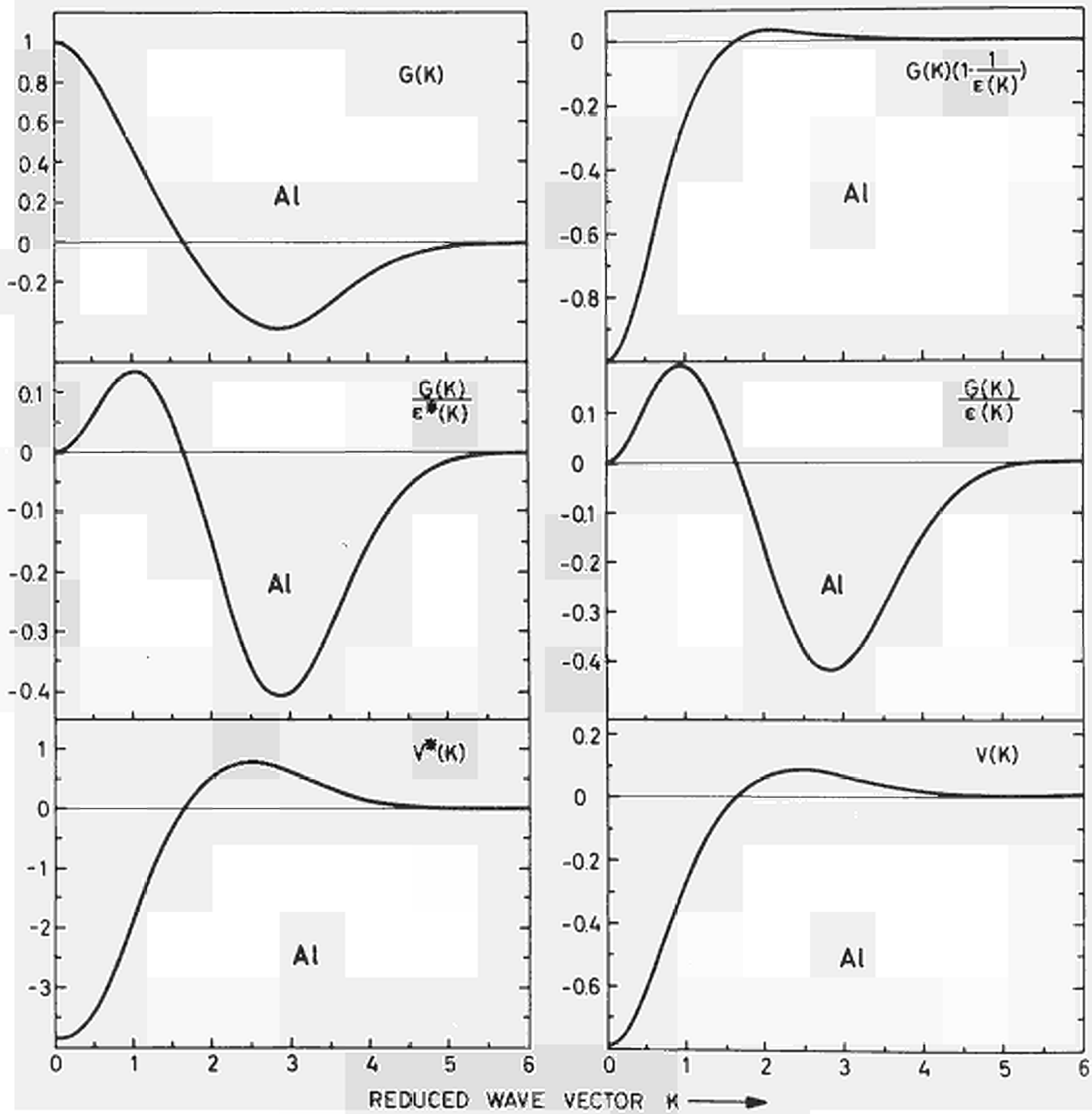
CHARACTERISTIC FUNCTIONS FOR Rb

FIG. 4



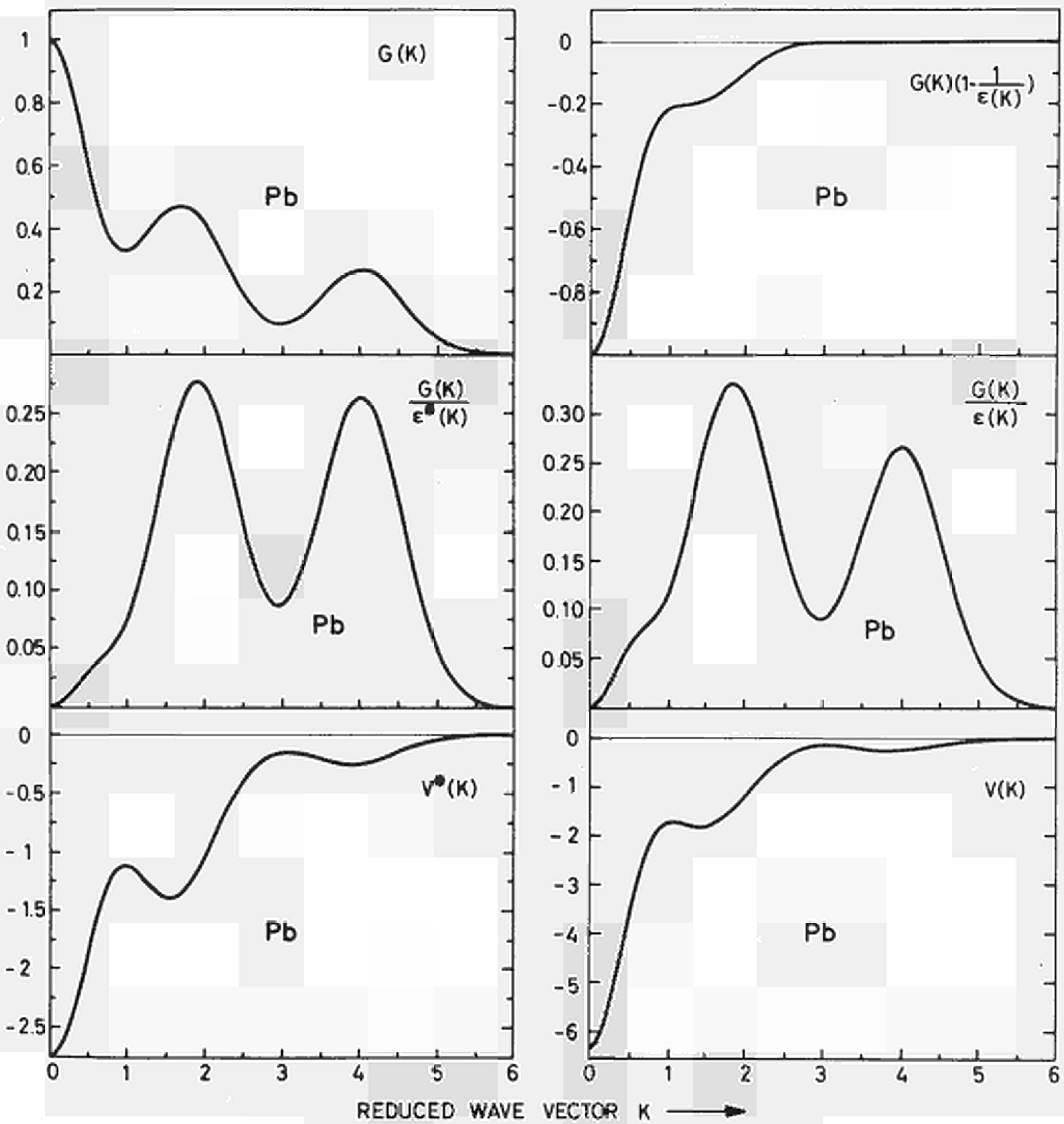
CHARACTERISTIC FUNCTIONS FOR Cu

FIG. 5



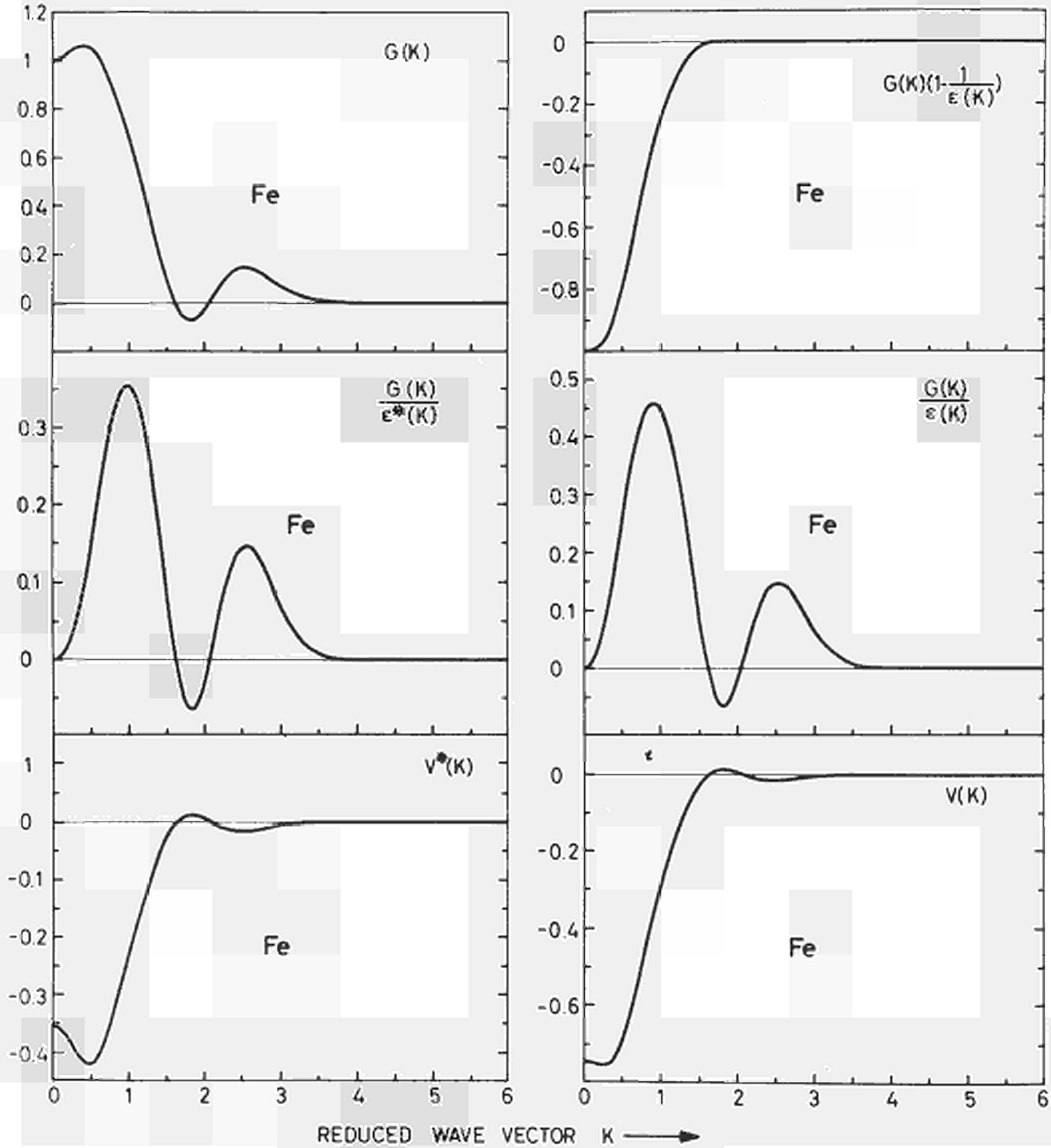
CHARACTERISTIC FUNCTIONS FOR Al

FIG. 6



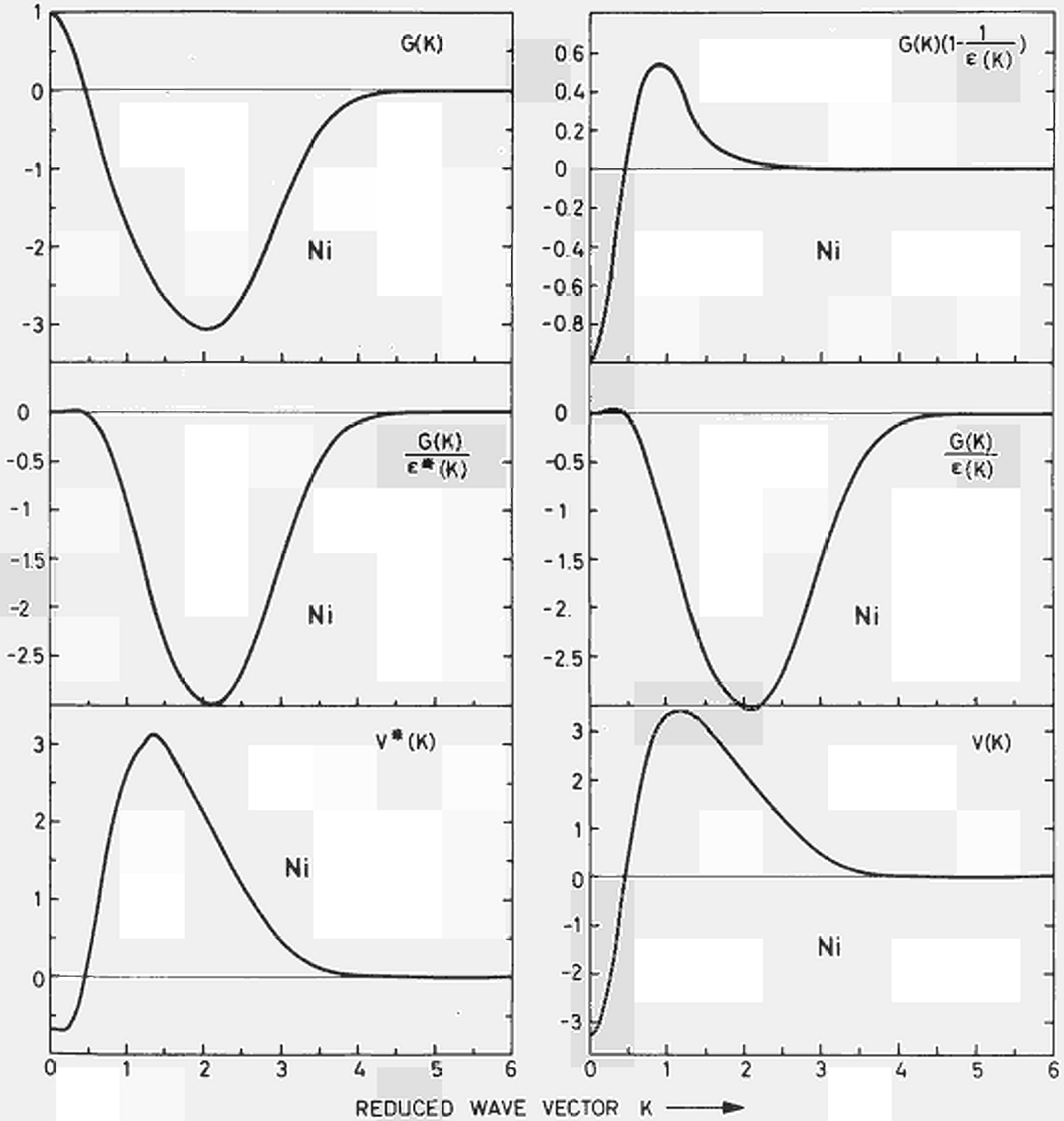
CHARACTERISTIC FUNCTIONS FOR Pb

FIG. 7



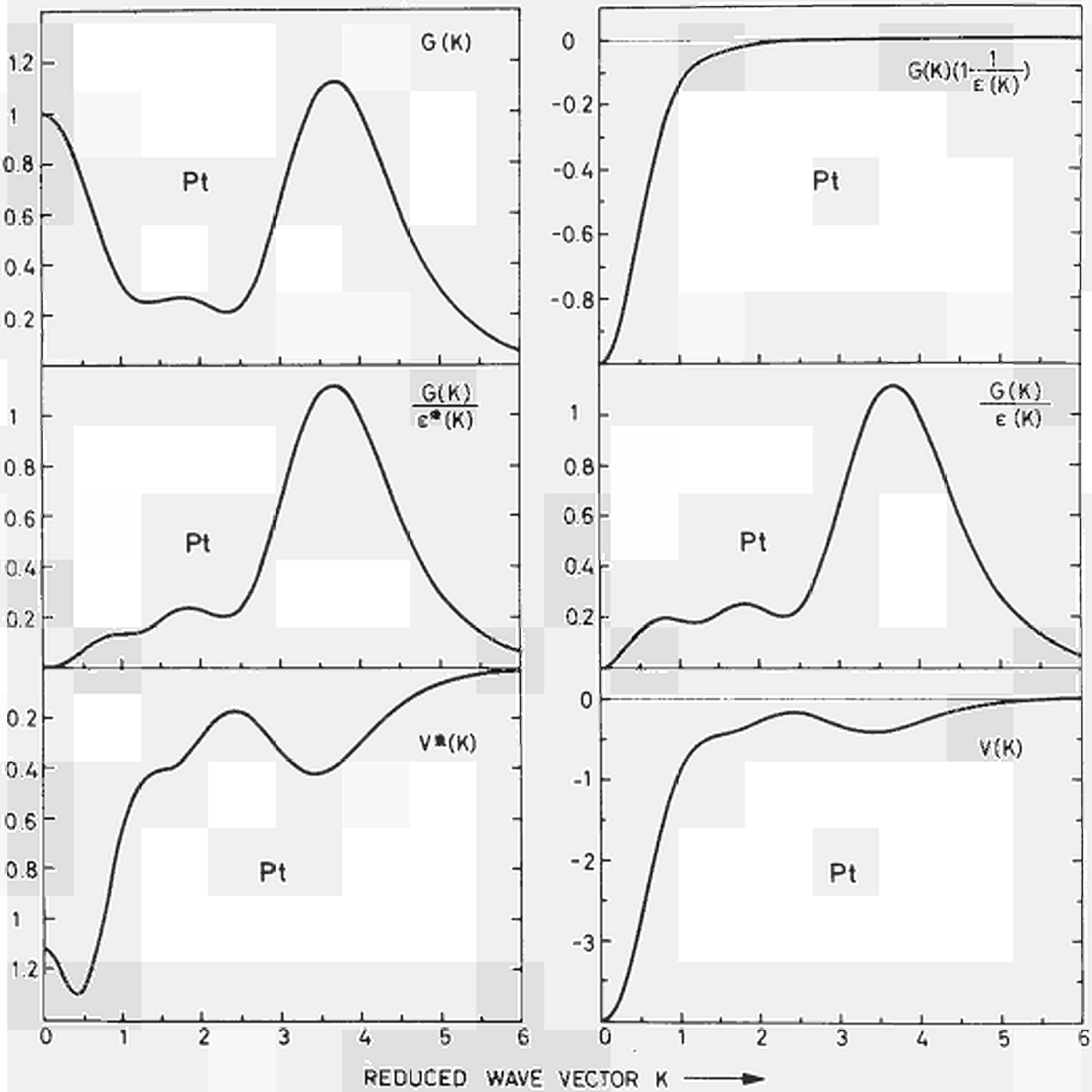
CHARACTERISTIC FUNCTIONS FOR Fe

FIG. 8



CHARACTERISTIC FUNCTIONS FOR Ni

FIG. 9



CHARACTERISTIC FUNCTIONS FOR Pt

FIG. 10

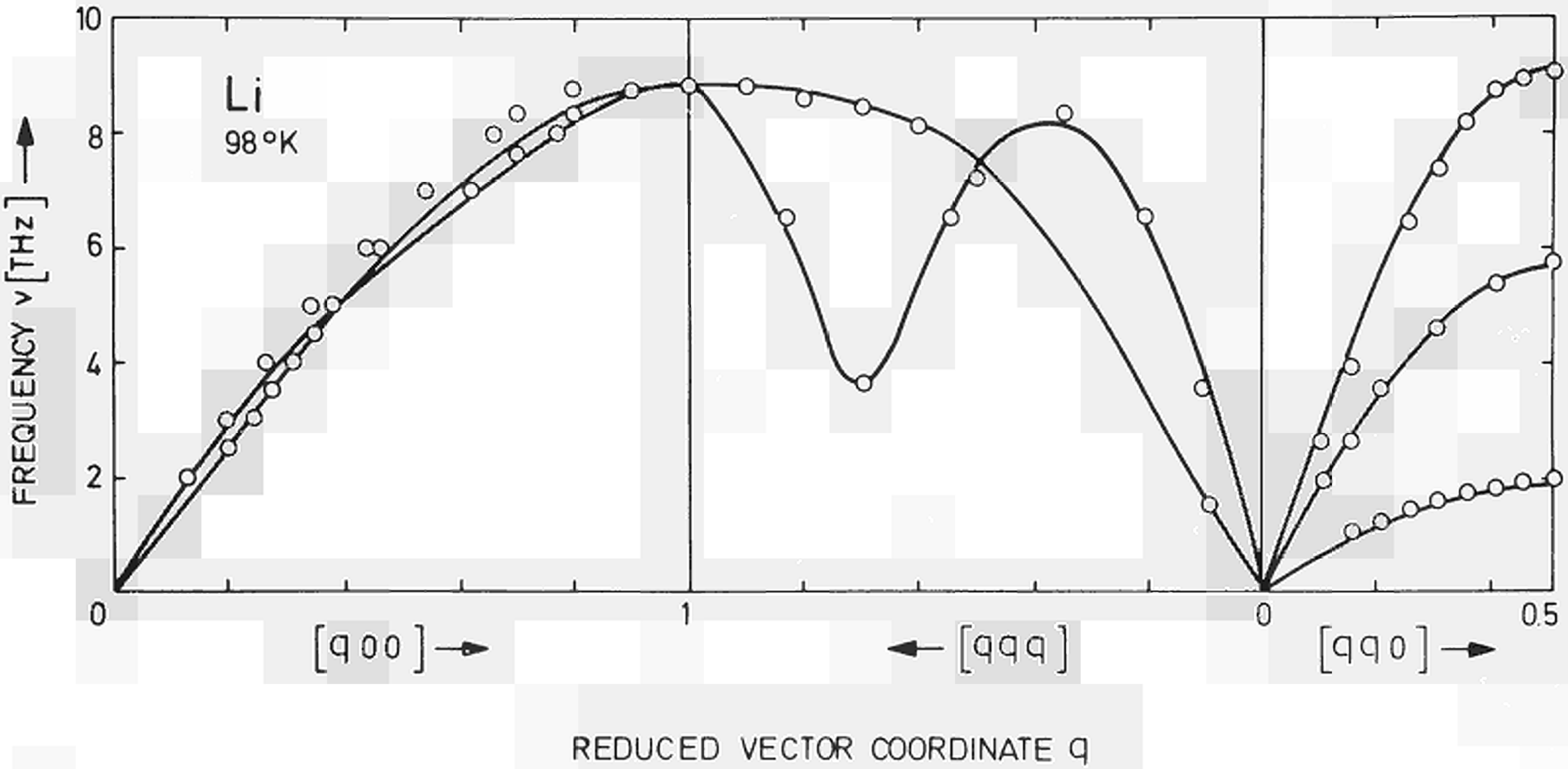
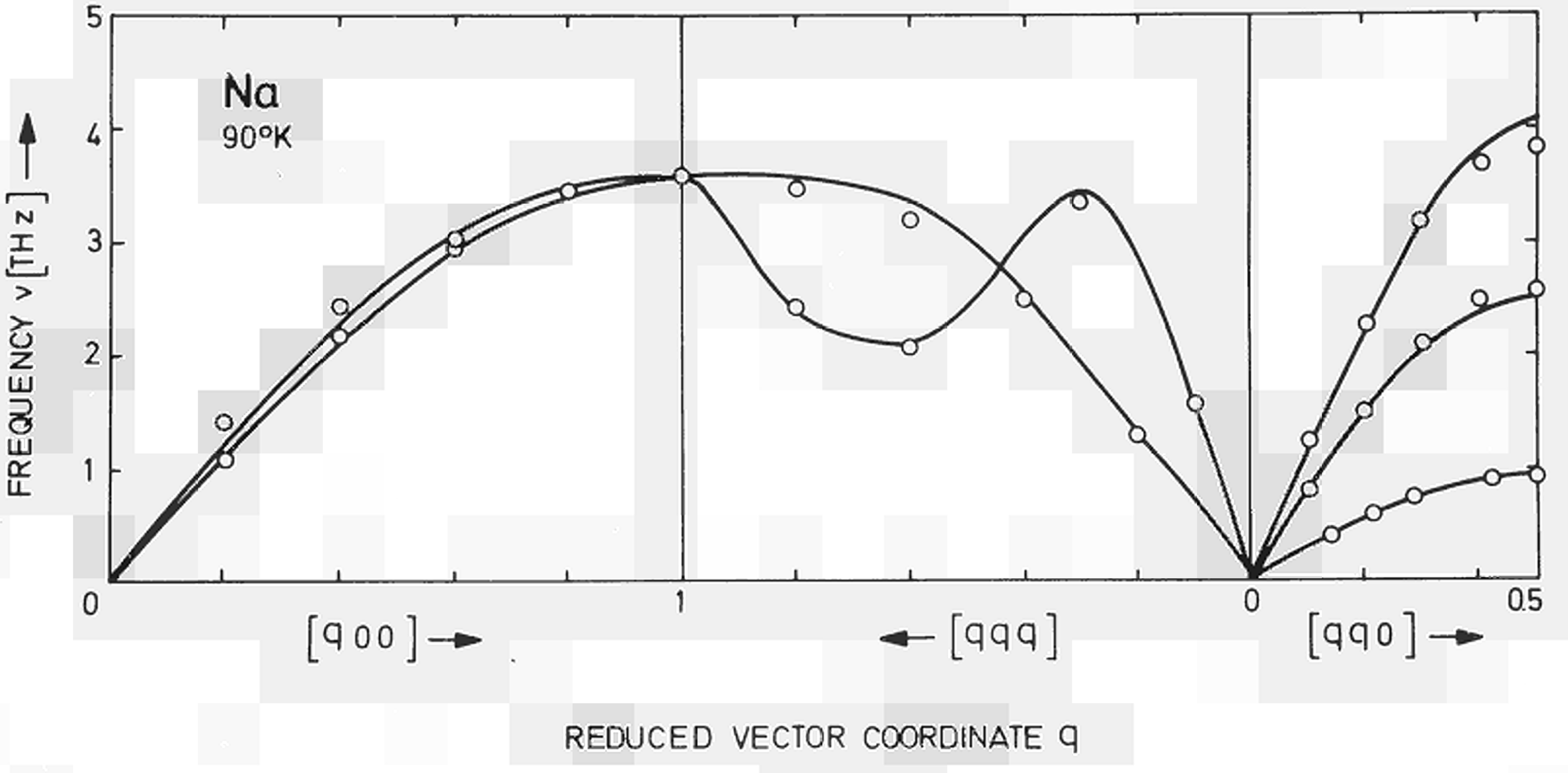

Li
98 °K
FREQUENCY ν [THz] →
10
8
6
4
2
0
1
0
0.5
[q 0 0] →
← [q q q]
[q q 0] →
REDUCED VECTOR COORDINATE q

FIG. 11



Na
90°K
FREQUENCY ν [THz] →
5
4
3
2
1
0
1
0
0.5
[q00] →
← [qqq]
[qq0] →
REDUCED VECTOR COORDINATE q

FIG. 12

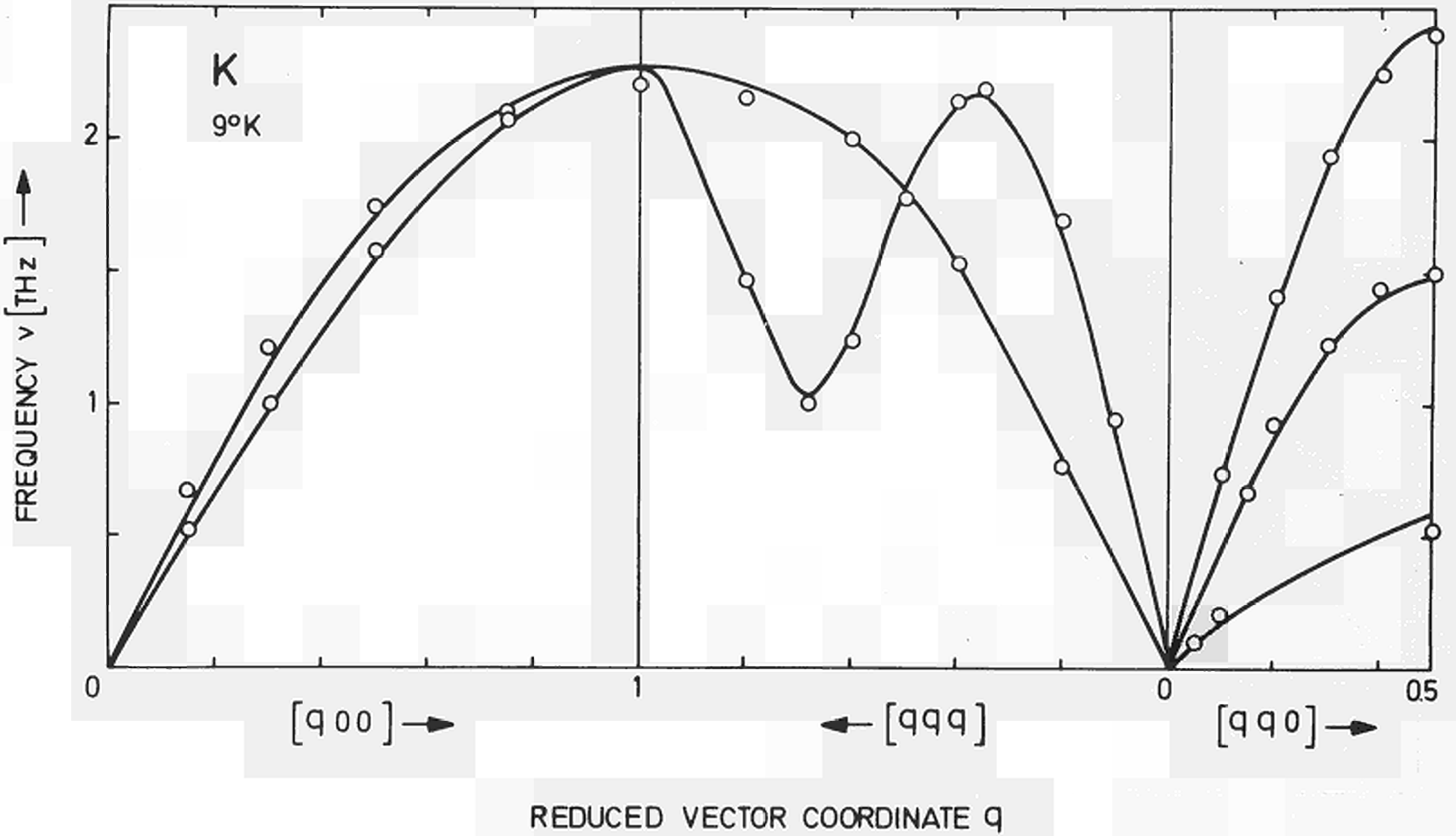
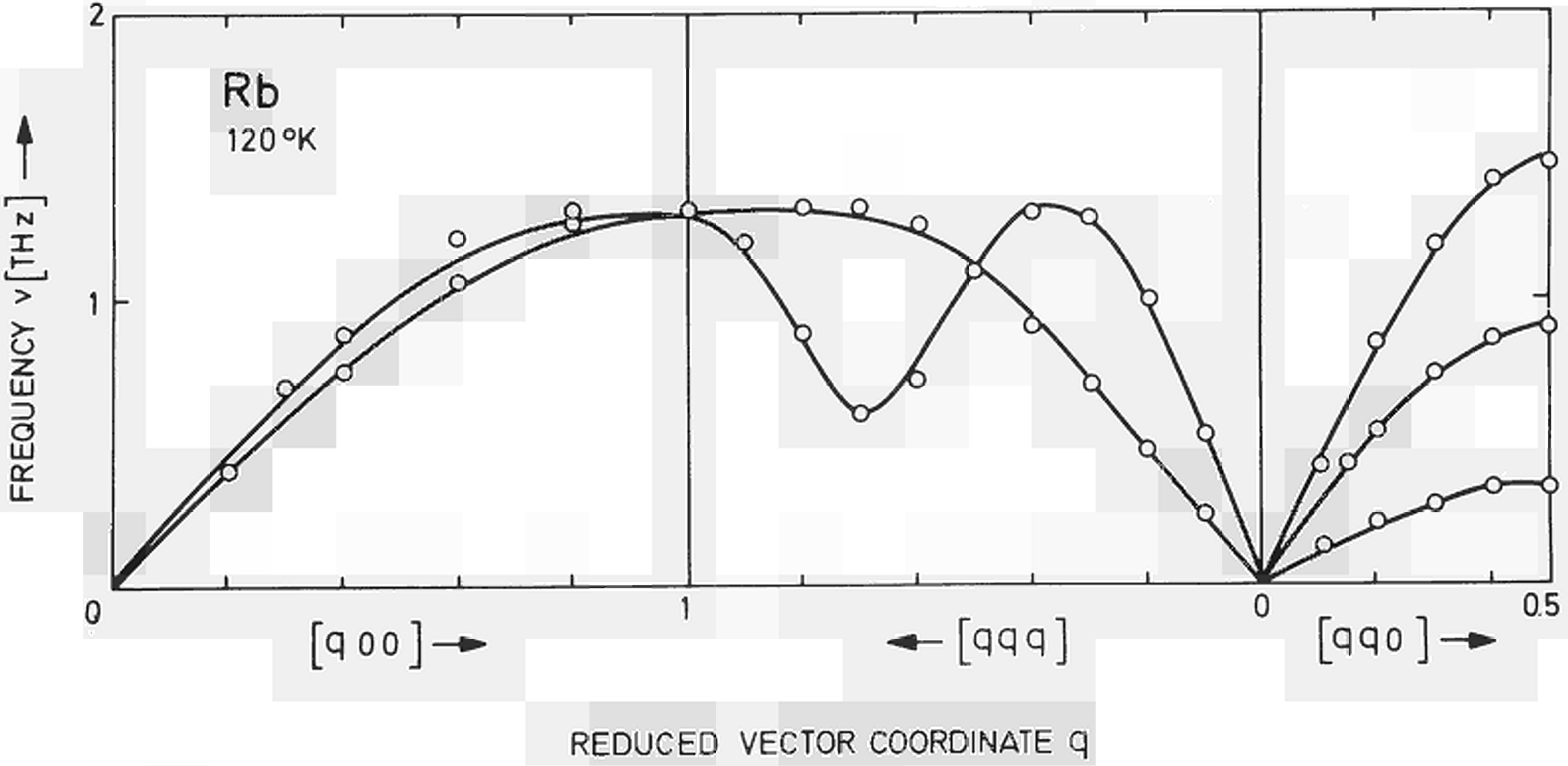
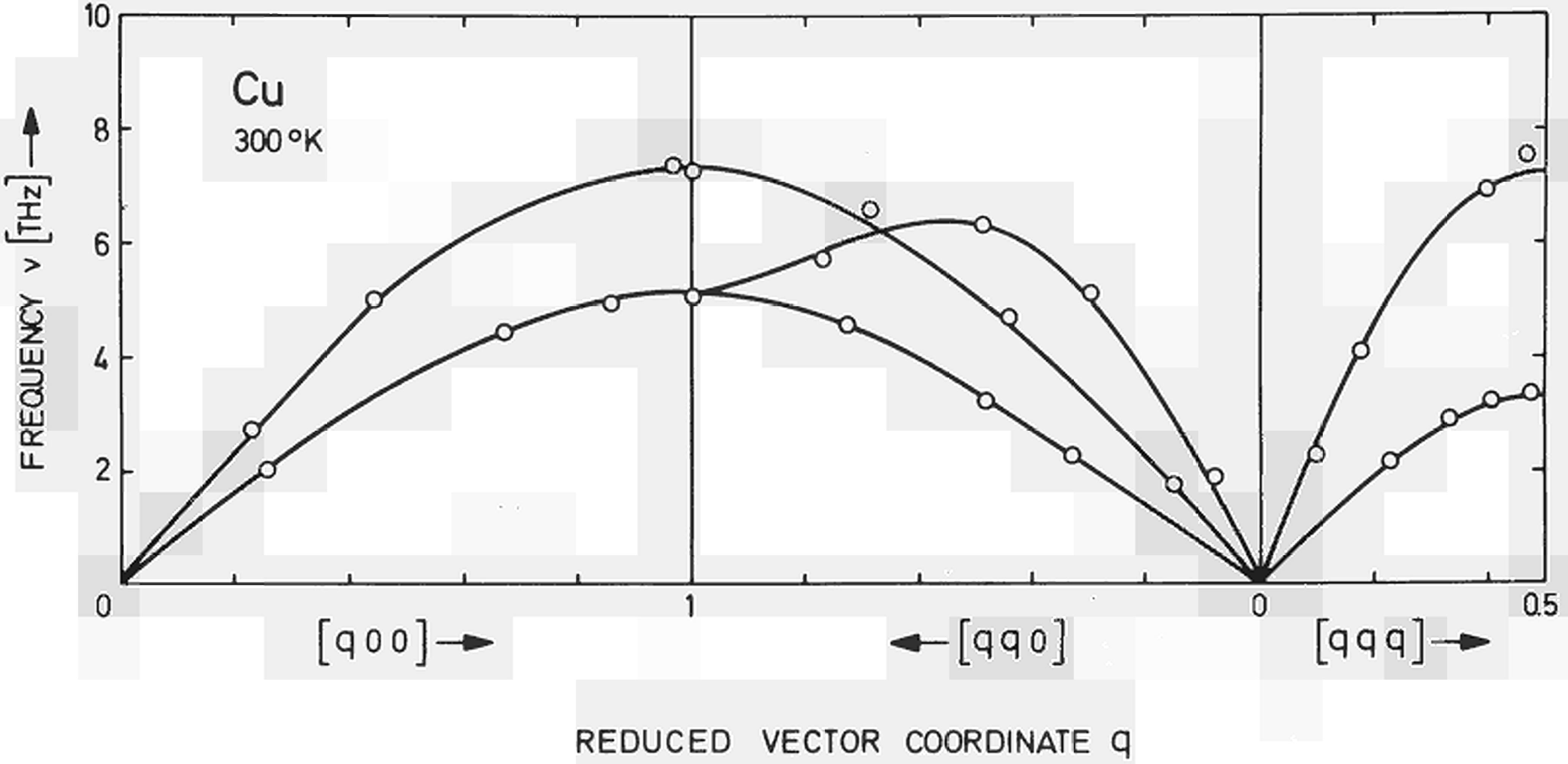

K
9°K
FREQUENCY ν [THz] →
2
1
0
1
0
0.5
[q00] →
← [qqq]
[qq0] →
REDUCED VECTOR COORDINATE q

FIG. 13



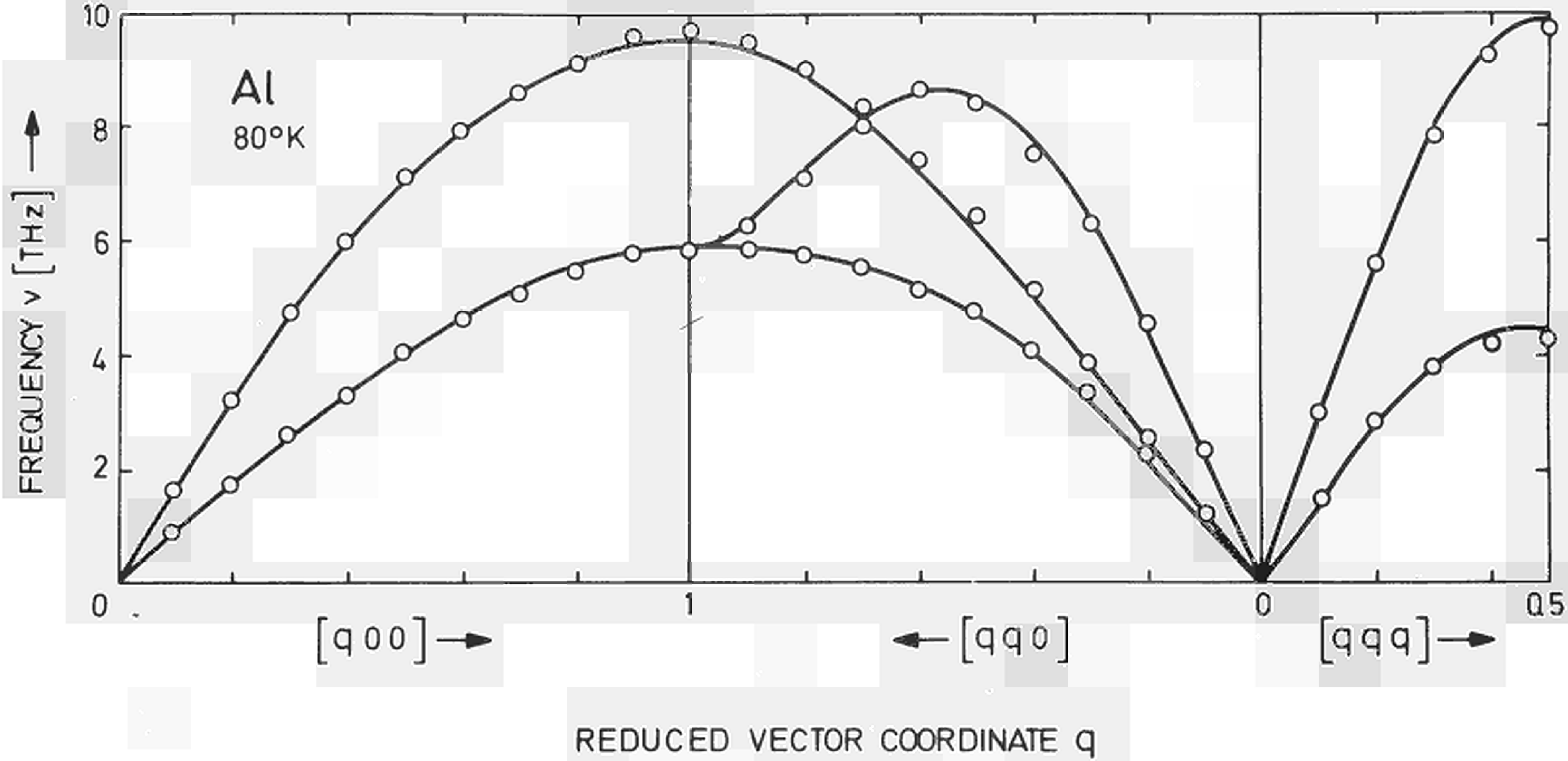
Rb
120 °K
FREQUENCY ν [THz] →
2
1
0
1
0
0.5
[q 0 0] →
← [q q q]
[q q 0] →
REDUCED VECTOR COORDINATE q

FIG. 14



Cu
300 °K
FREQUENCY ν [THz] →
10
8
6
4
2
0
1
0
0.5
[q 0 0] →
← [q q 0]
[q q q] →
REDUCED VECTOR COORDINATE q

FIG. 15



Al
80°K
FREQUENCY ν [THz] →
10
8
6
4
2
0
1
0
0.5
[q 0 0] →
← [q q 0]
[q q q] →
REDUCED VECTOR COORDINATE q

FIG. 16

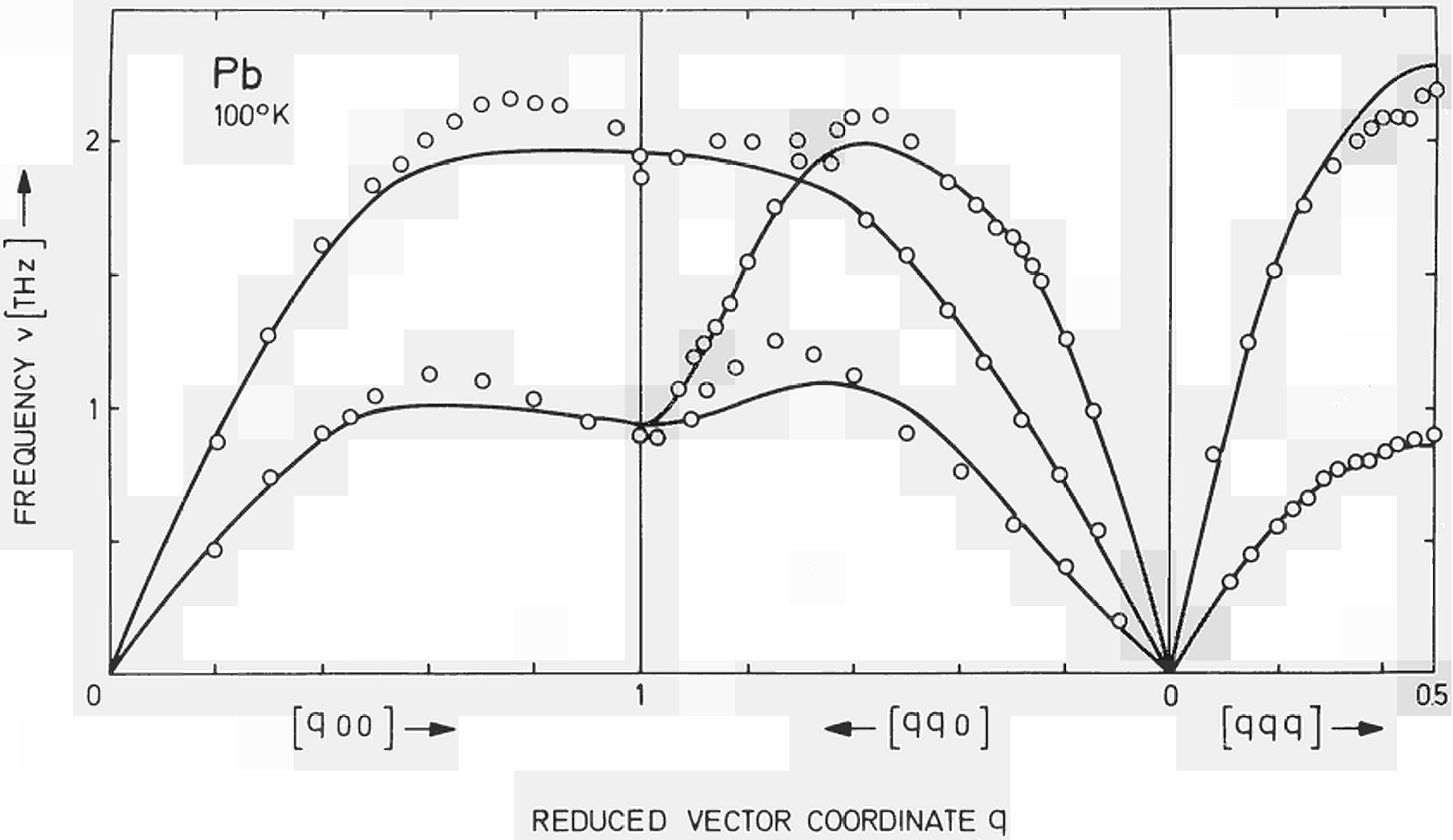

Pb
100°K
FREQUENCY ν [THz] →
2
1
0
1
0
0.5
[q00] →
← [qq0]
[qqq] →
REDUCED VECTOR COORDINATE q

FIG. 17

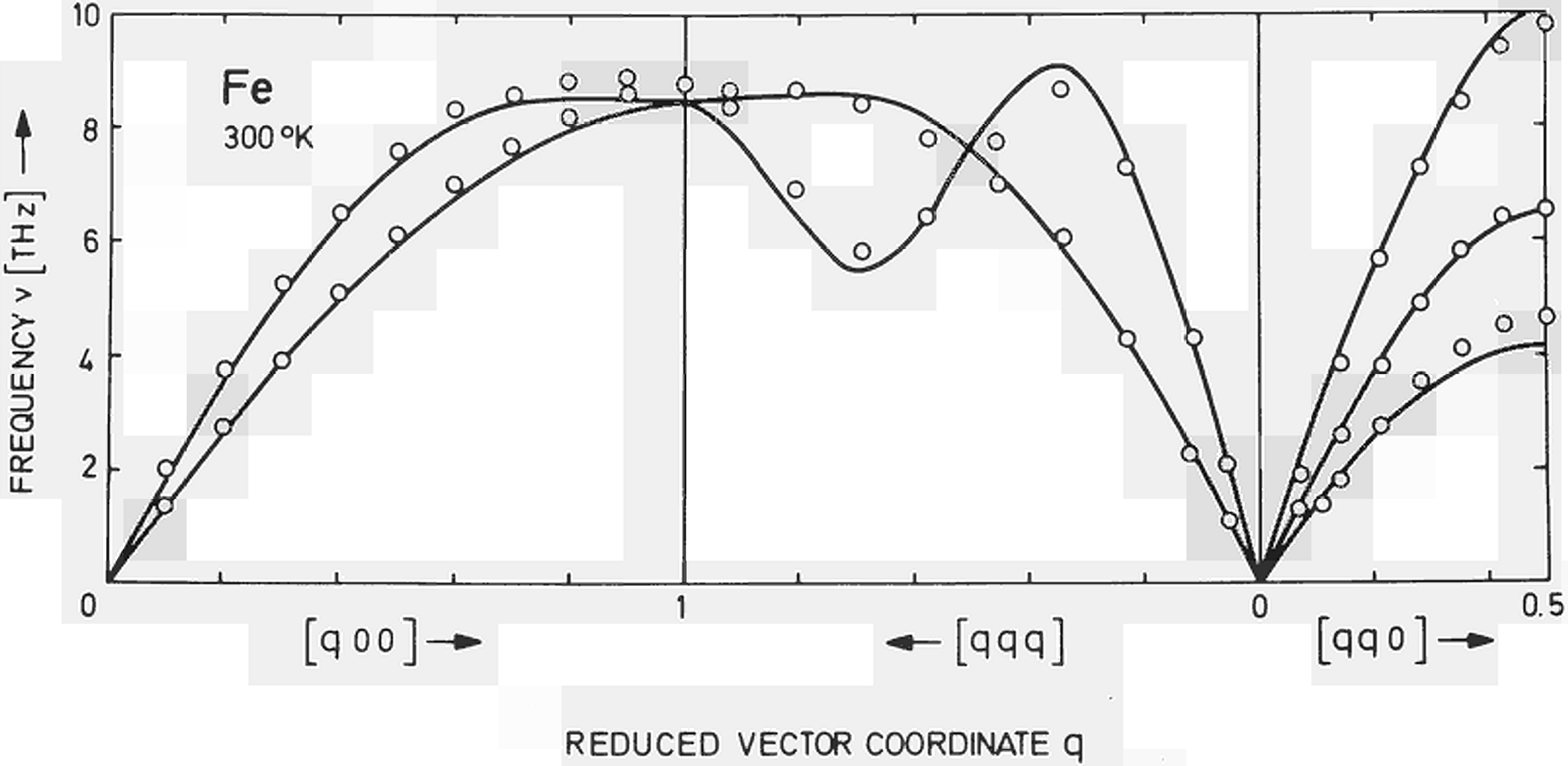

Fe
300 °K
FREQUENCY ν [THz] →
10
8
6
4
2
0
1
0
0.5
[q 0 0] →
← [q q q]
[q q 0] →
REDUCED VECTOR COORDINATE q

FIG. 18

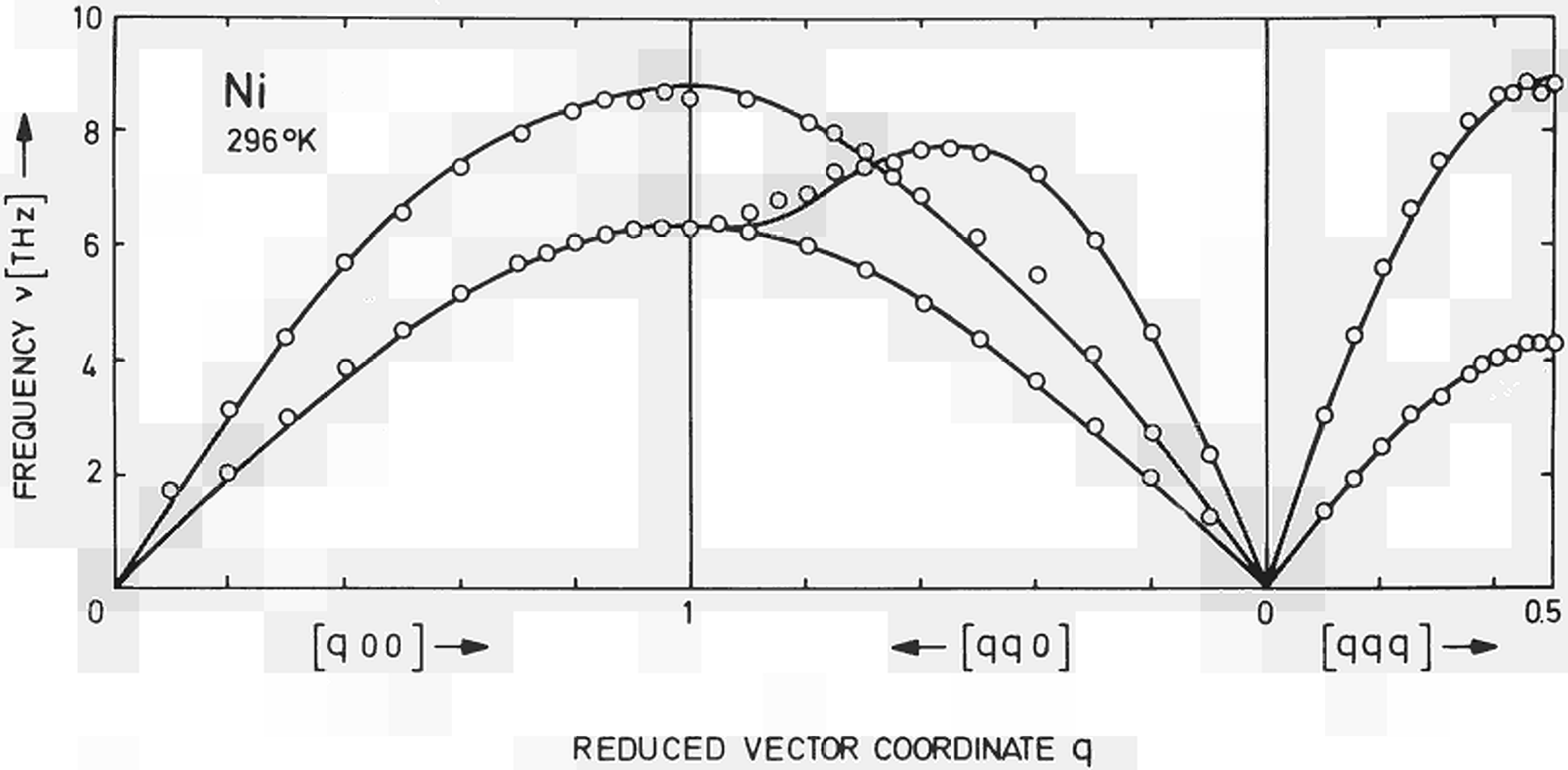

Ni
296 °K
FREQUENCY ν [THz]
10
8
6
4
2
0
1
0
0.5
[q 0 0]
[q q 0]
[q q q]
REDUCED VECTOR COORDINATE q

FIG. 19

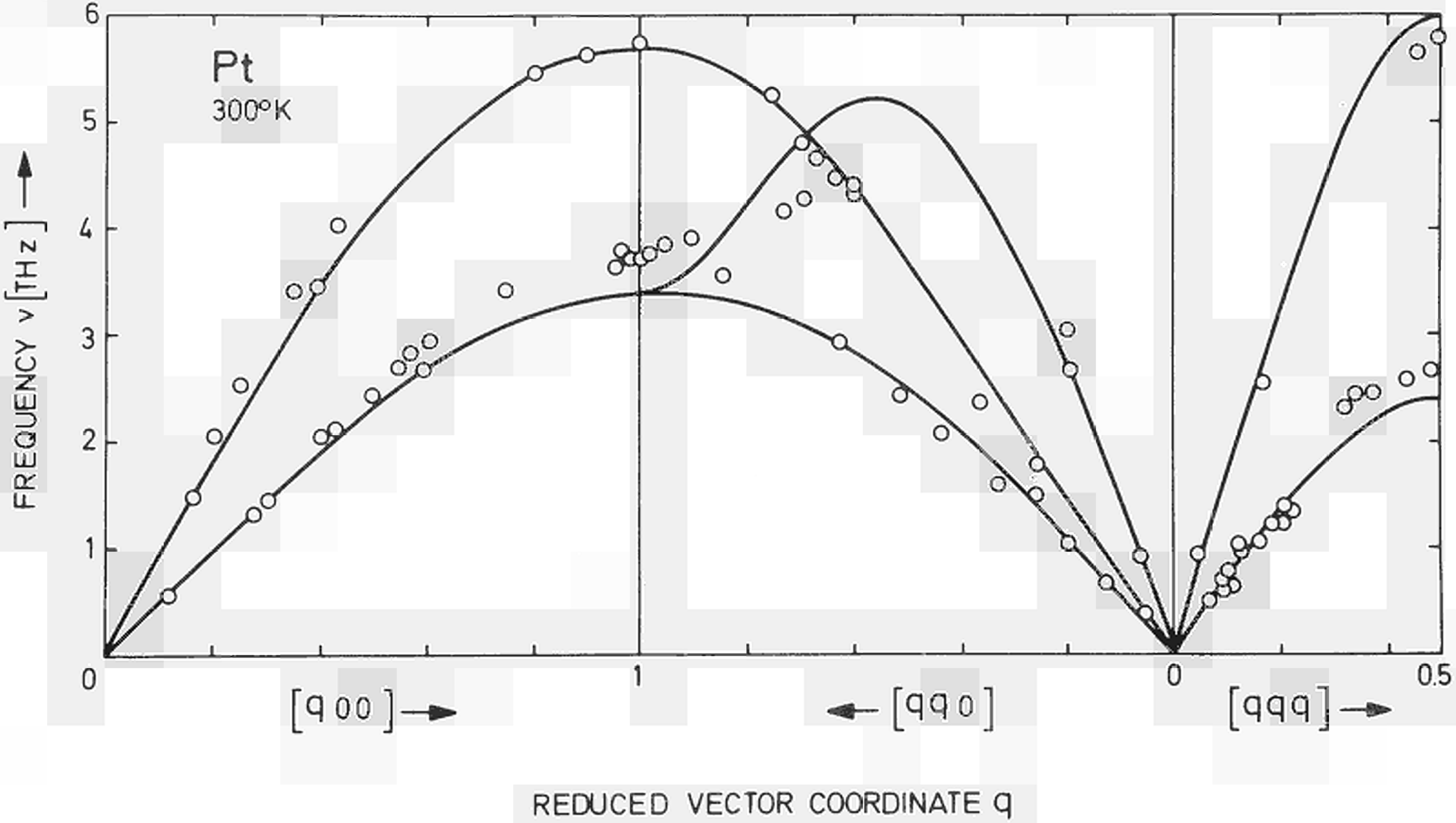

Pt
300°K
FREQUENCY ν [THz] →
6
5
4
3
2
1
0
1
0
0.5
[q00] →
← [qq0]
[qqq] →
REDUCED VECTOR COORDINATE q

FIG. 20

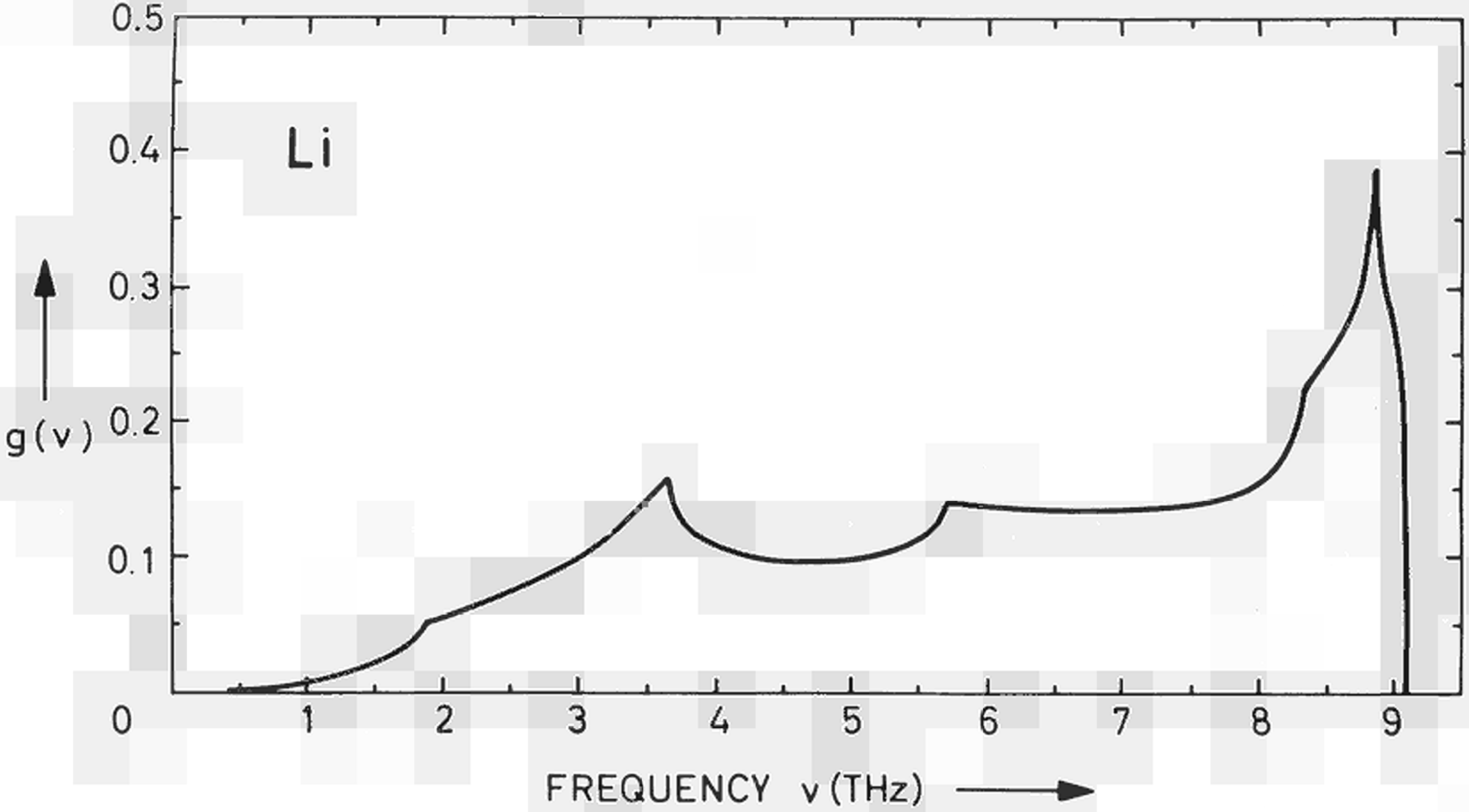


FIG. 21

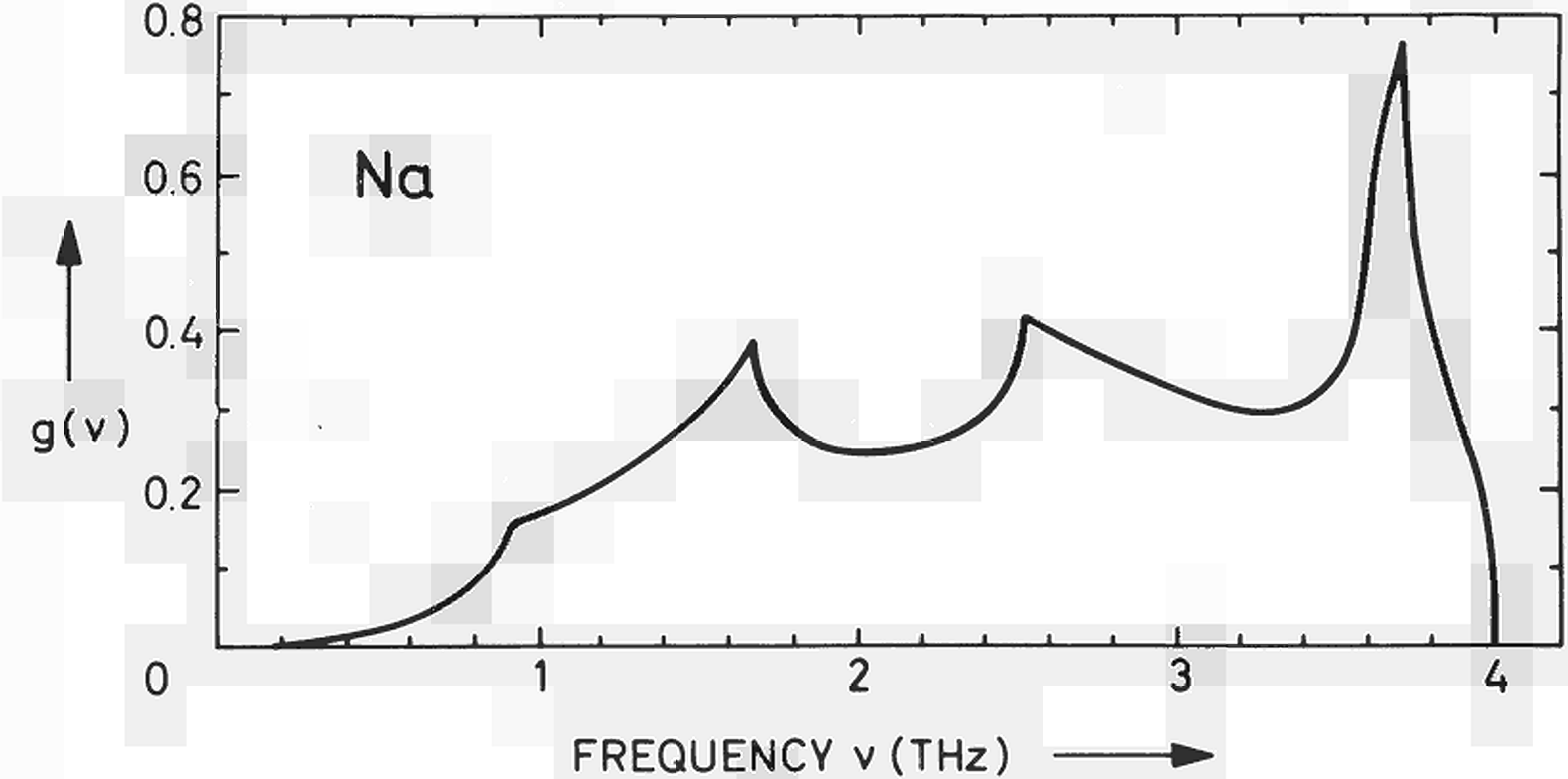


FIG. 22

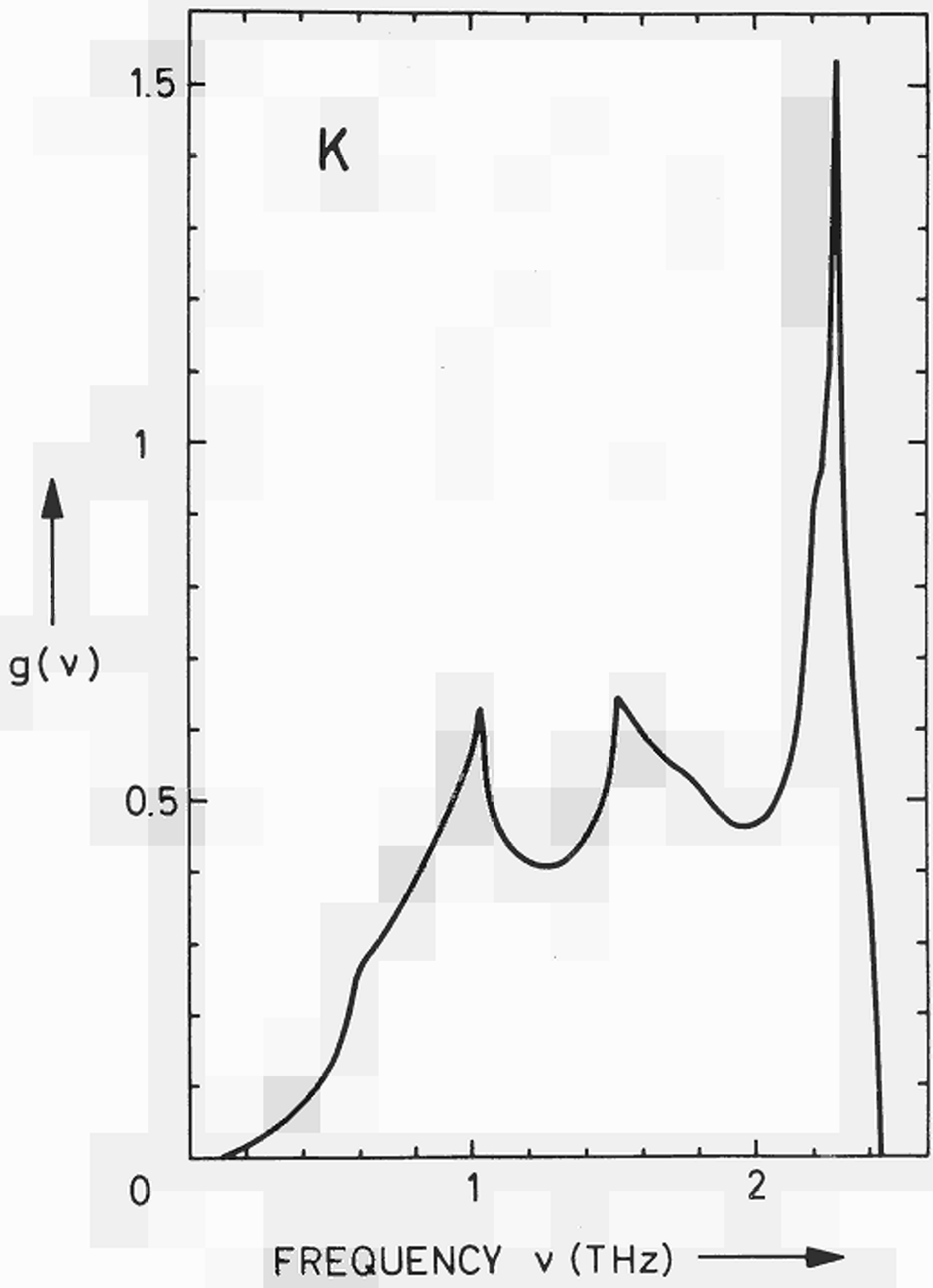


FIG. 23

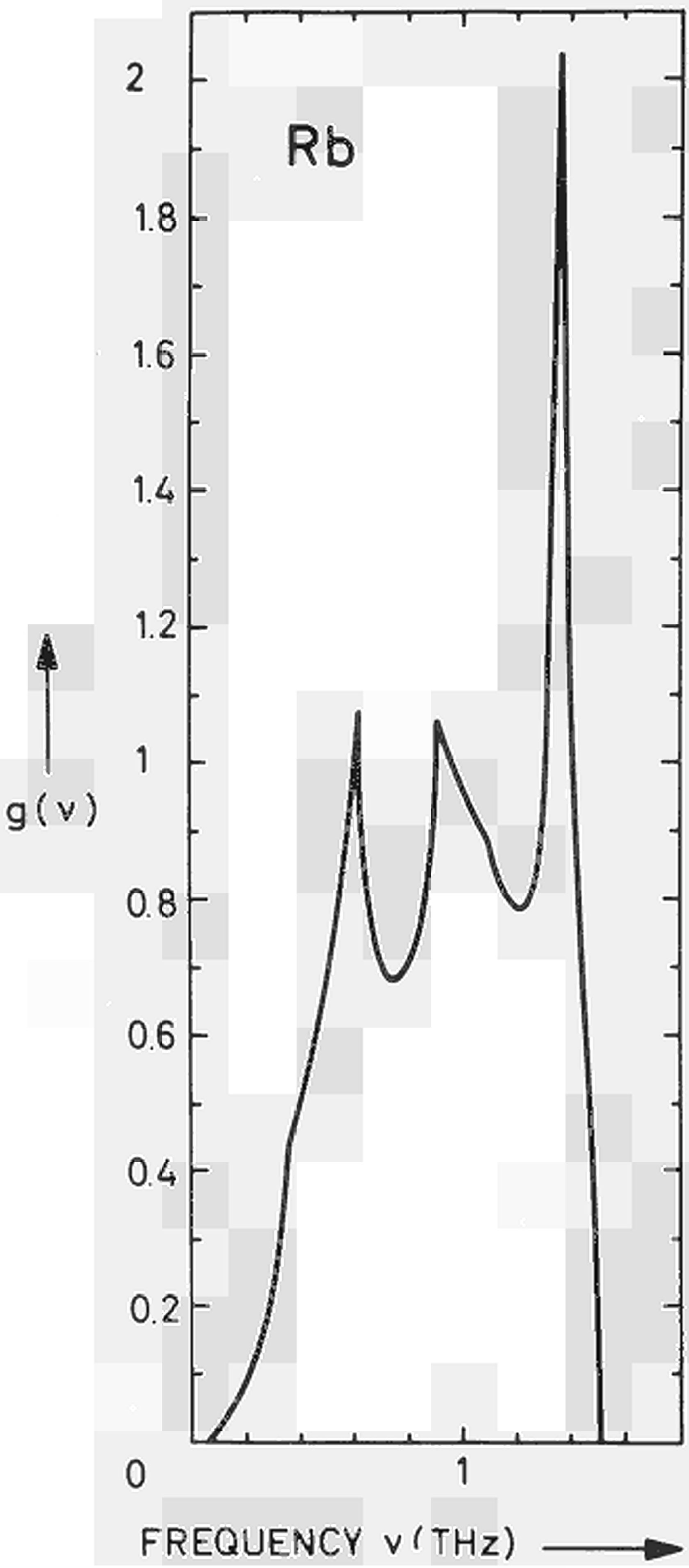


FIG. 24

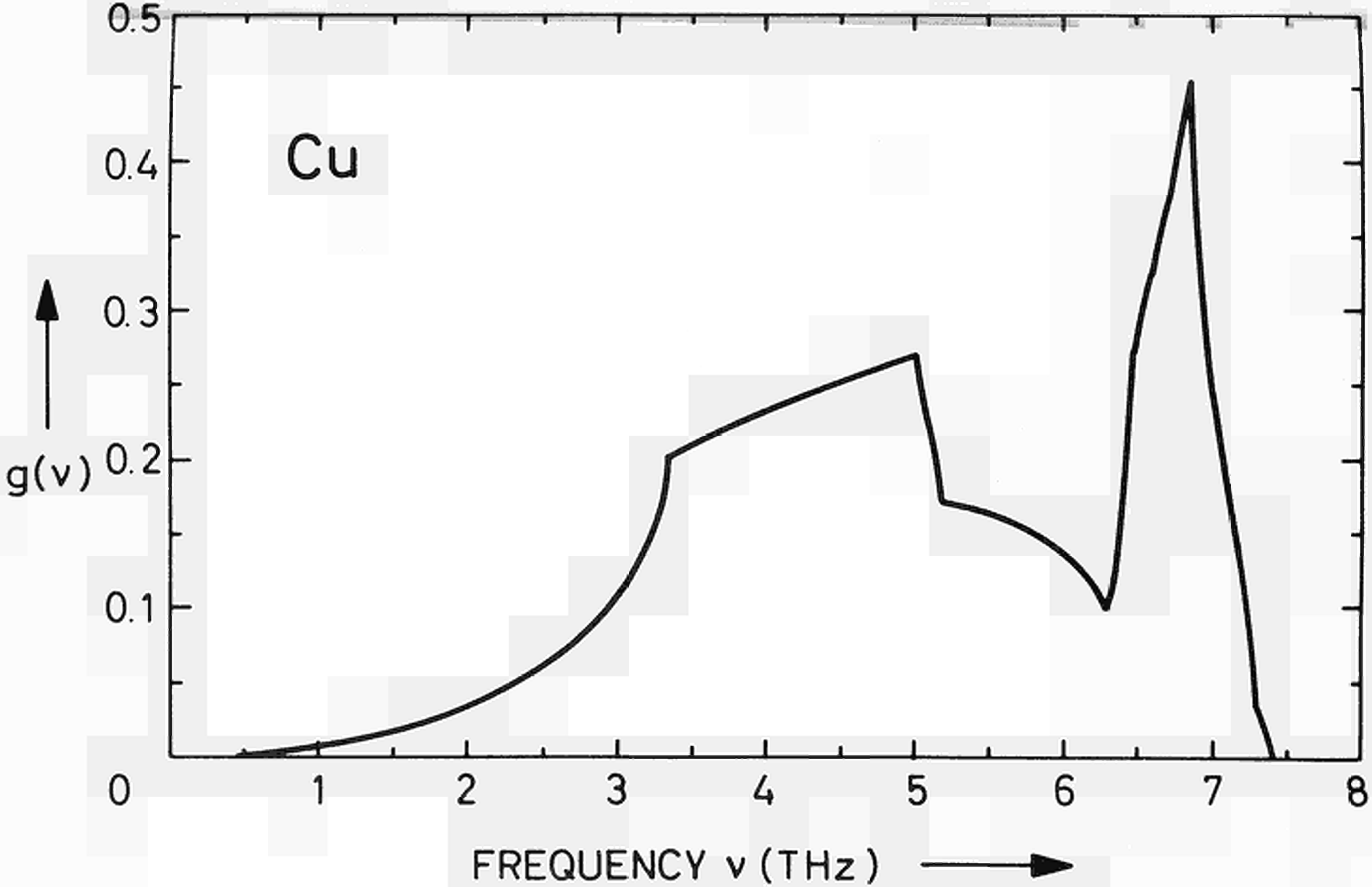


FIG. 25

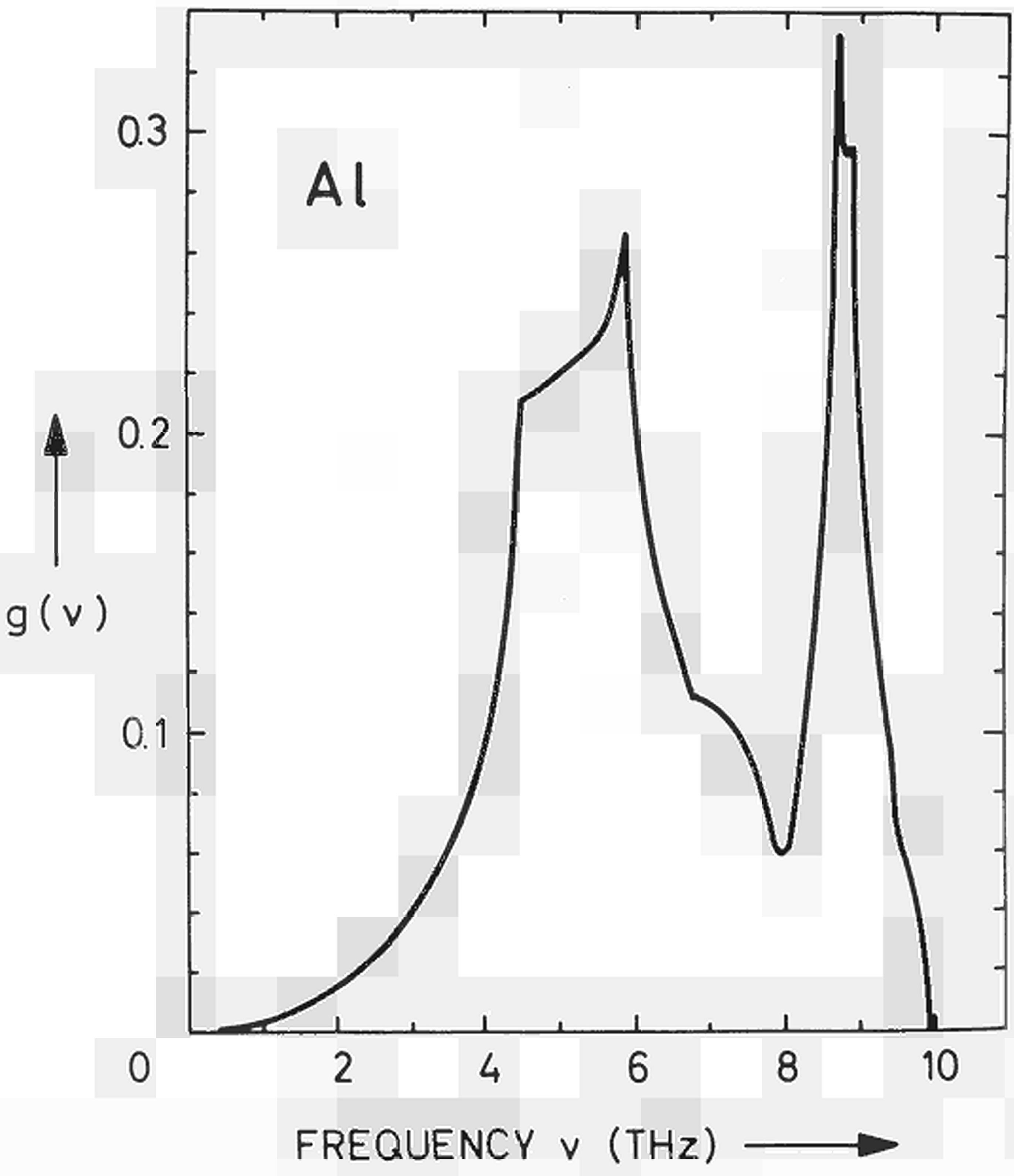


FIG. 26

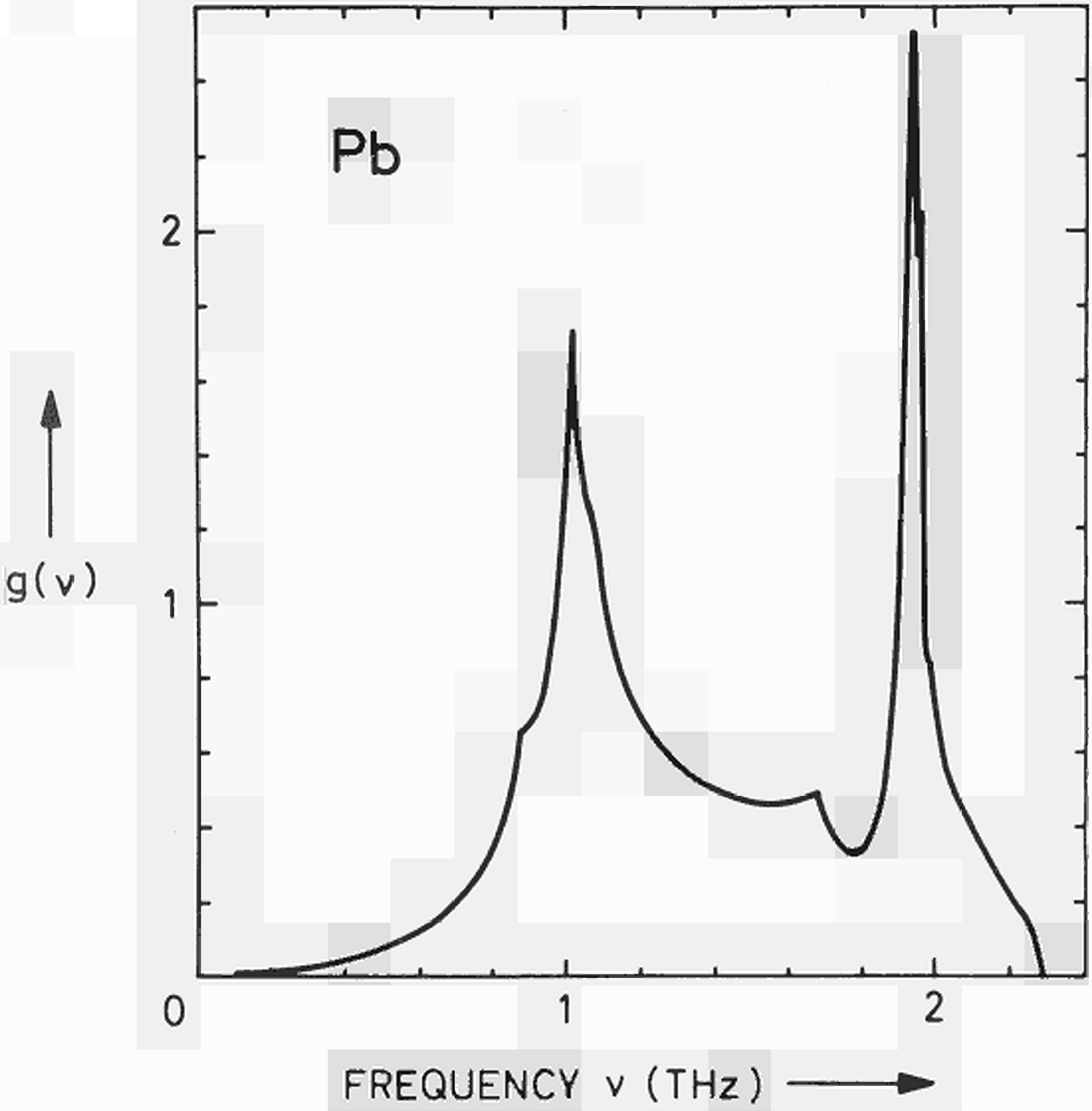


FIG. 27

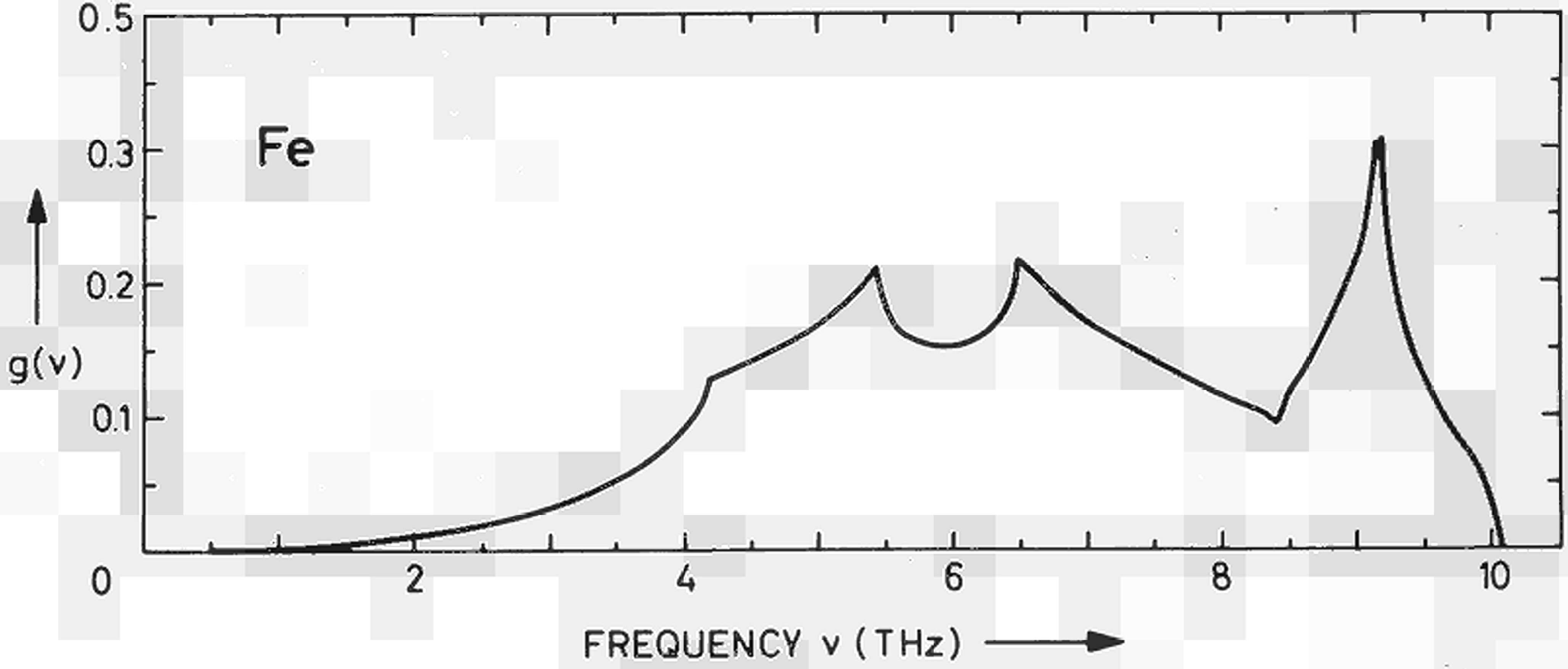


FIG. 28

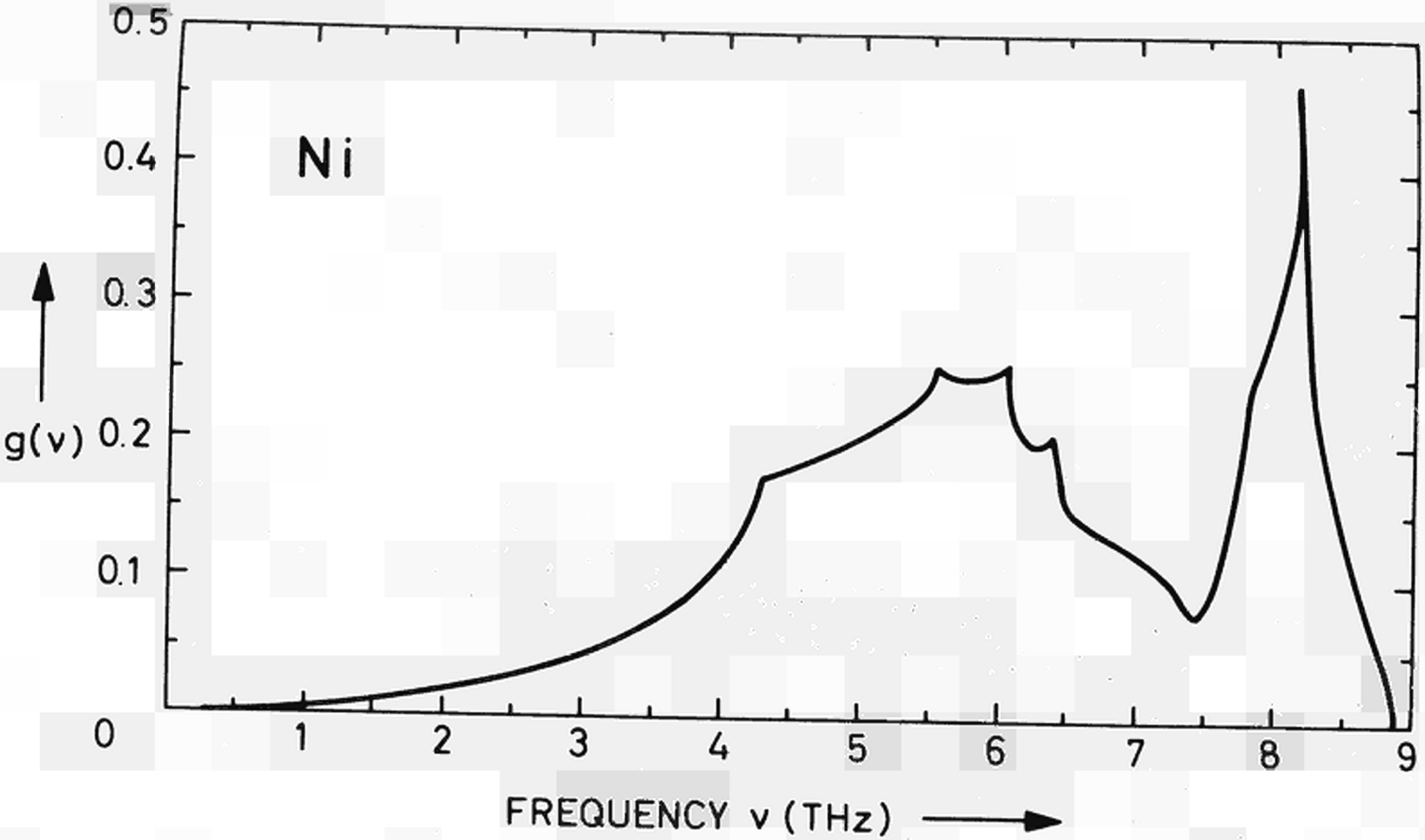


FIG. 29

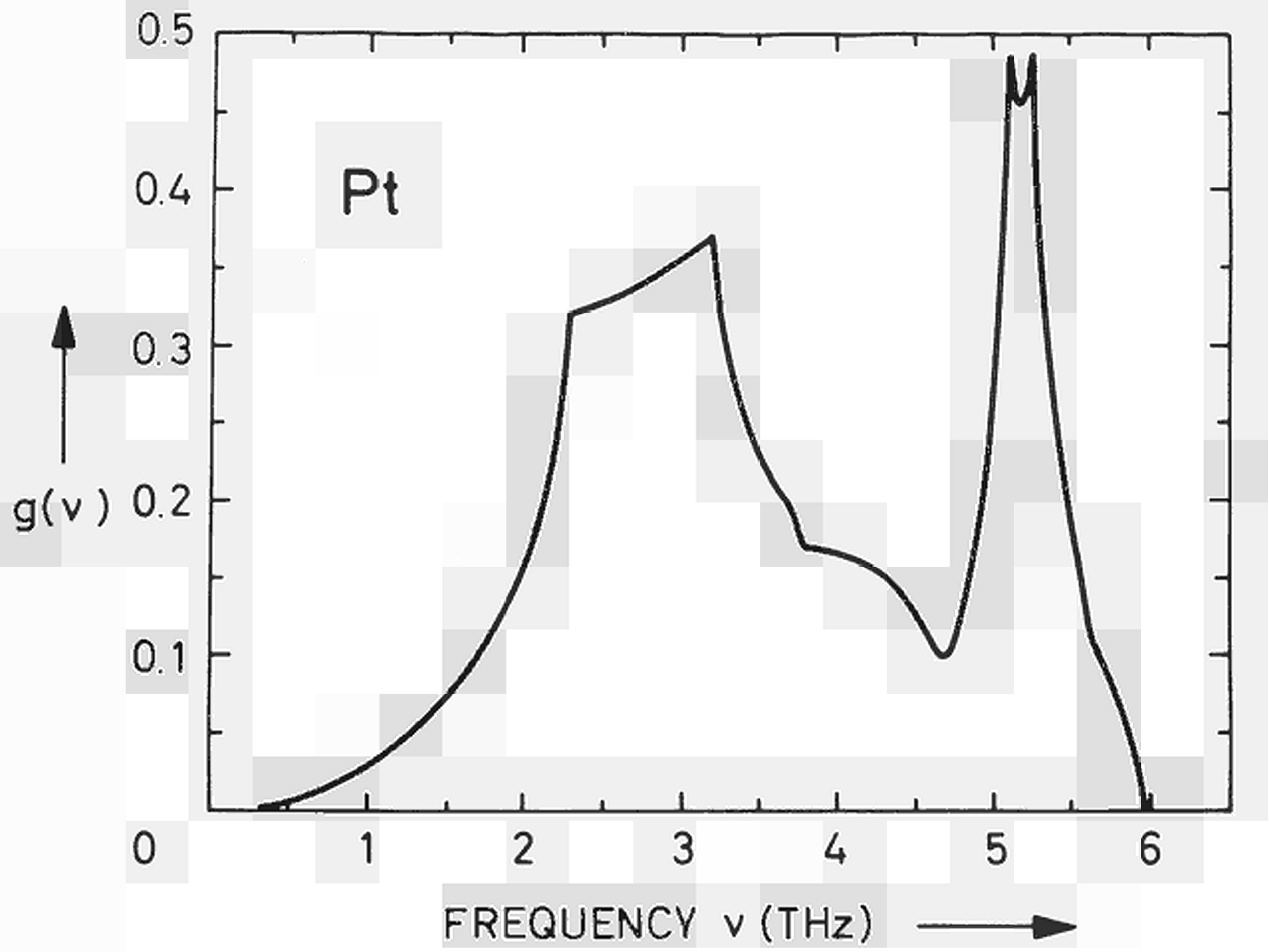
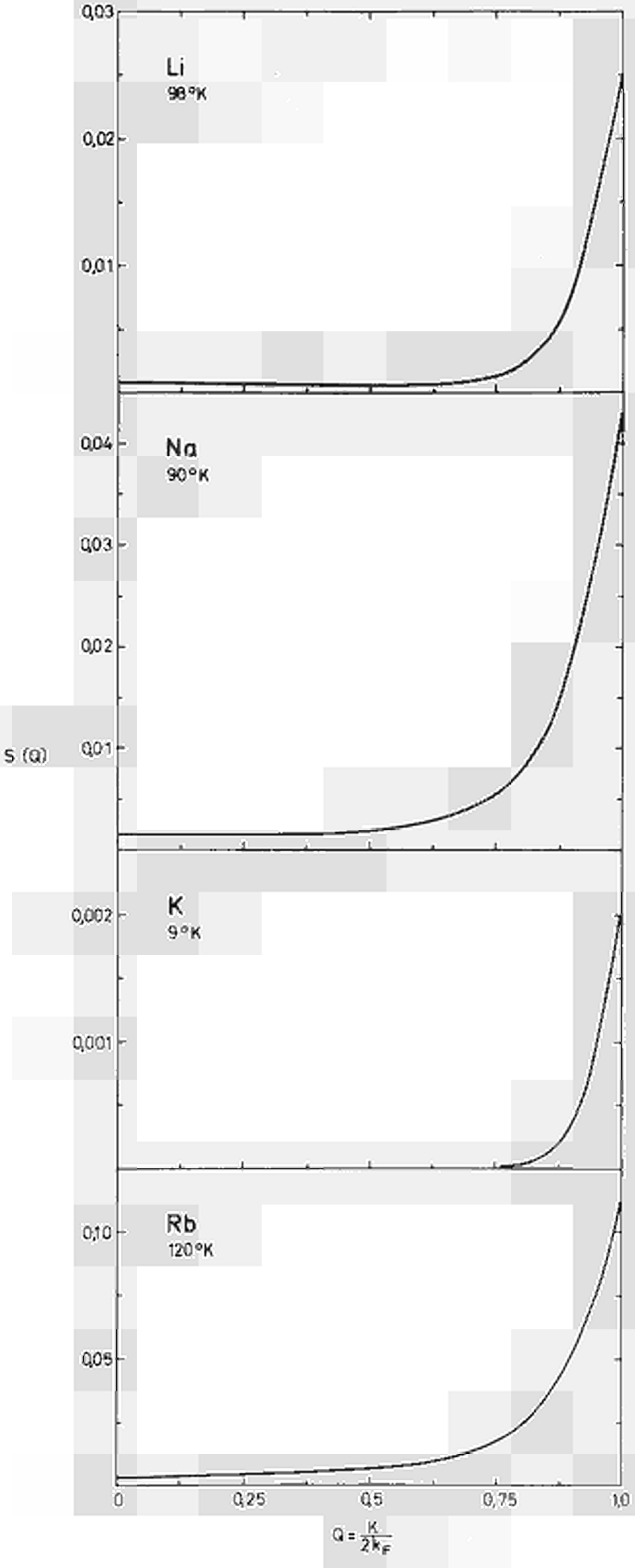
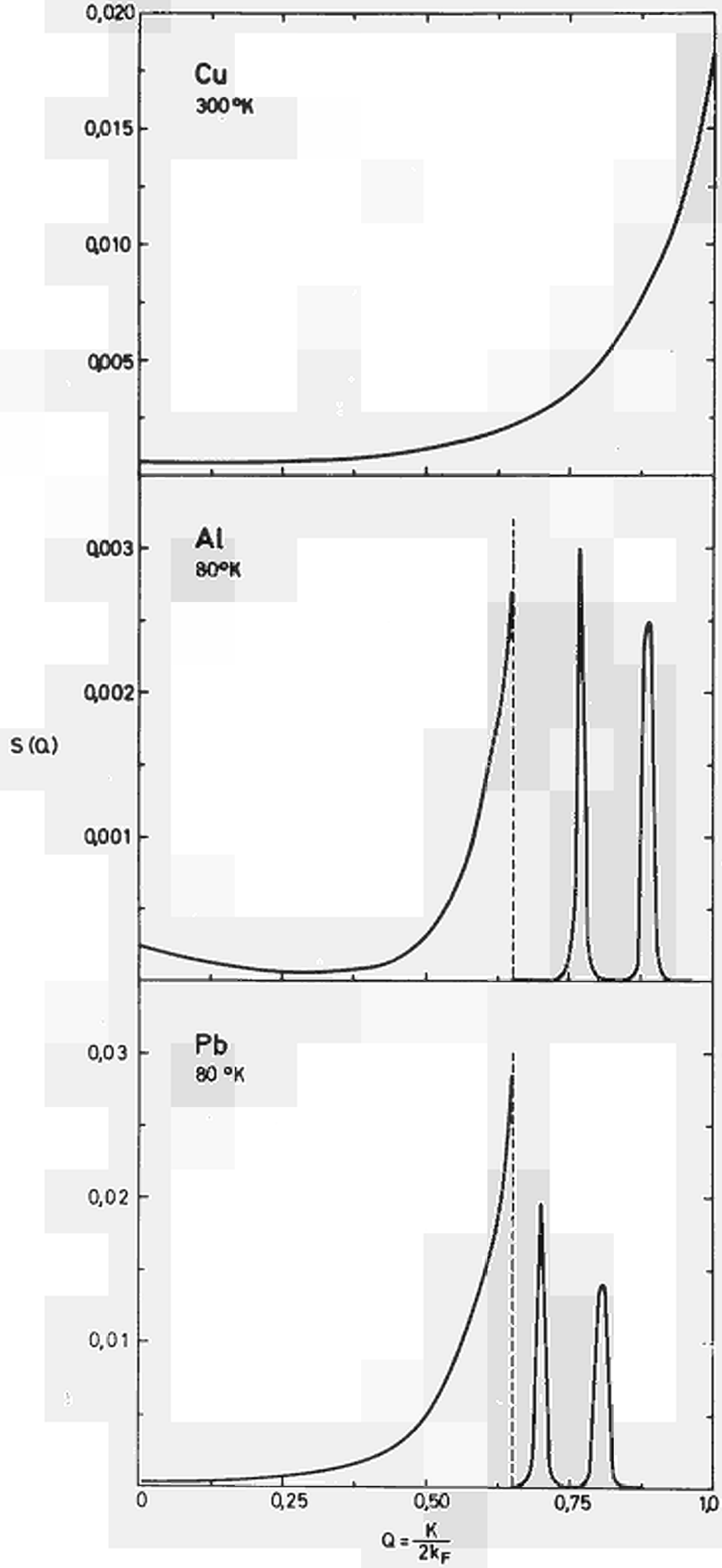


FIG. 30



Li
98 °K
Na
90 °K
K
9 °K
Rb
120 °K
S (Q)
0,03
0,02
0,01
0,04
0,03
0,02
0,01
0,002
0,001
0,10
0,05
0
0,25
0,5
0,75
1,0
$Q = \frac{K}{2k_F}$

FIG. 31



0,020
0,015
0,010
0,005
Cu
300 °K
0,003
0,002
0,001
Al
80°K
S (Q)
0,03
0,02
0,01
Pb
80 °K
0
0,25
0,50
0,75
1,0
Q = K / 2k_F

FIG. 32

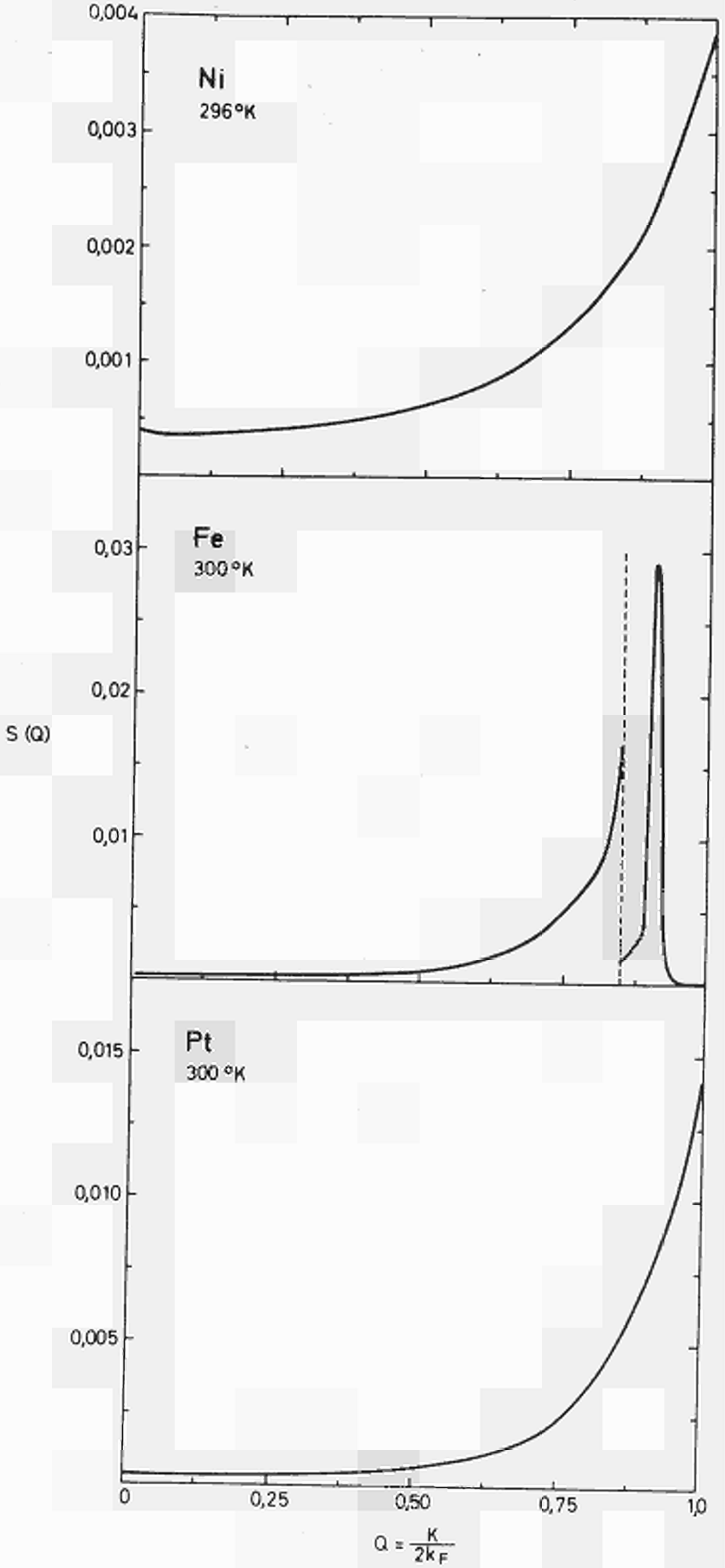

Ni
296 °K
0,004
0,003
0,002
0,001
Fe
300 °K
0,03
0,02
0,01
S (Q)
Pt
300 °K
0,015
0,010
0,005
0
0,25
0,50
0,75
1,0
Q = K / 2k_F

FIG. 33

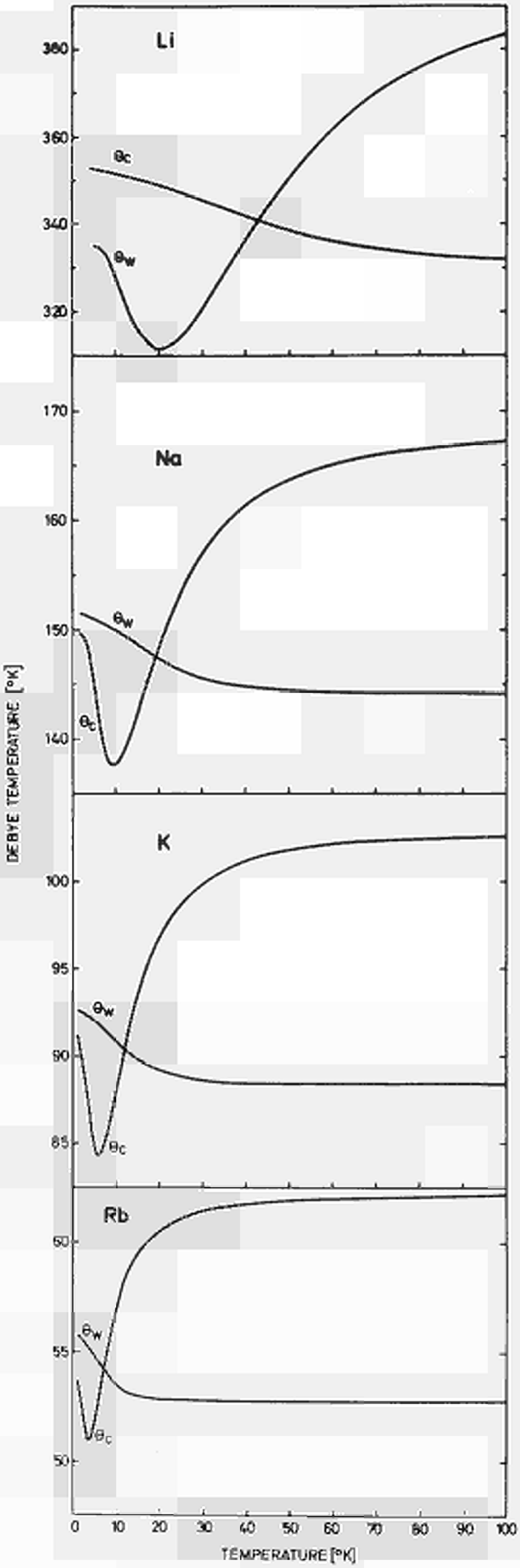
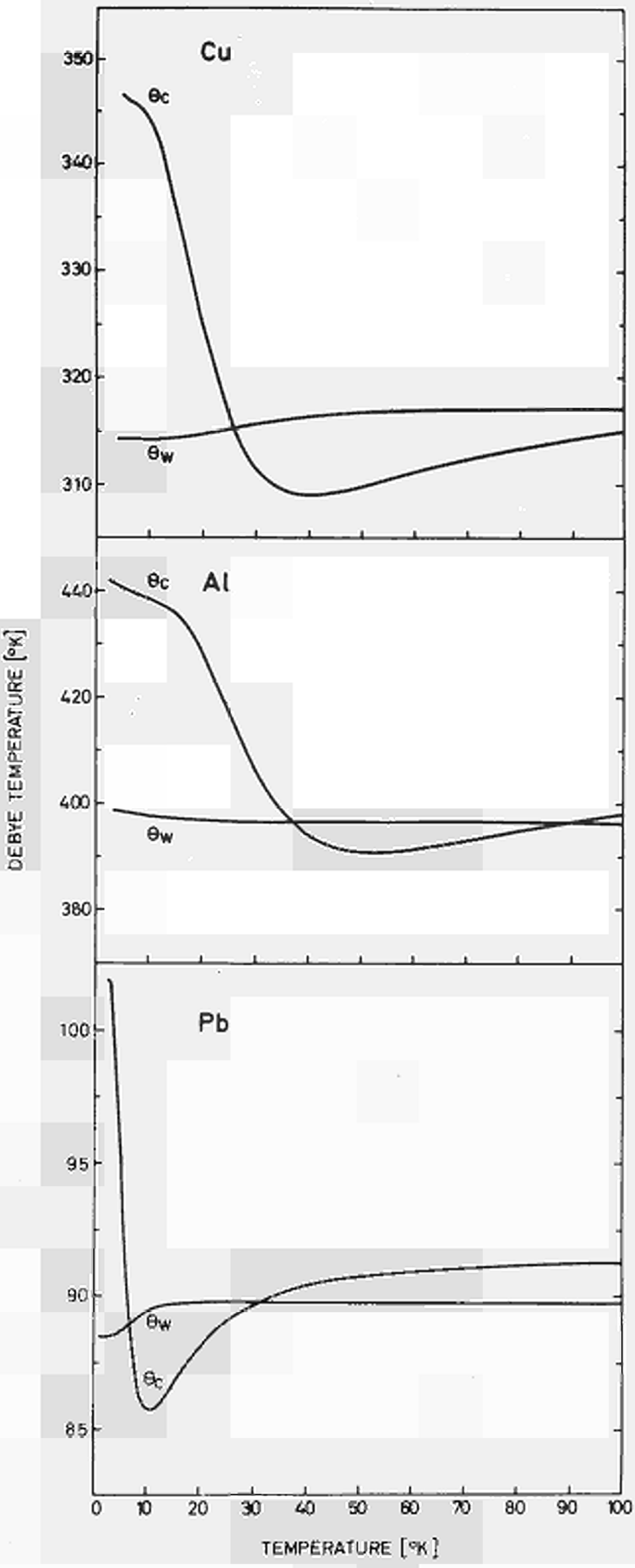
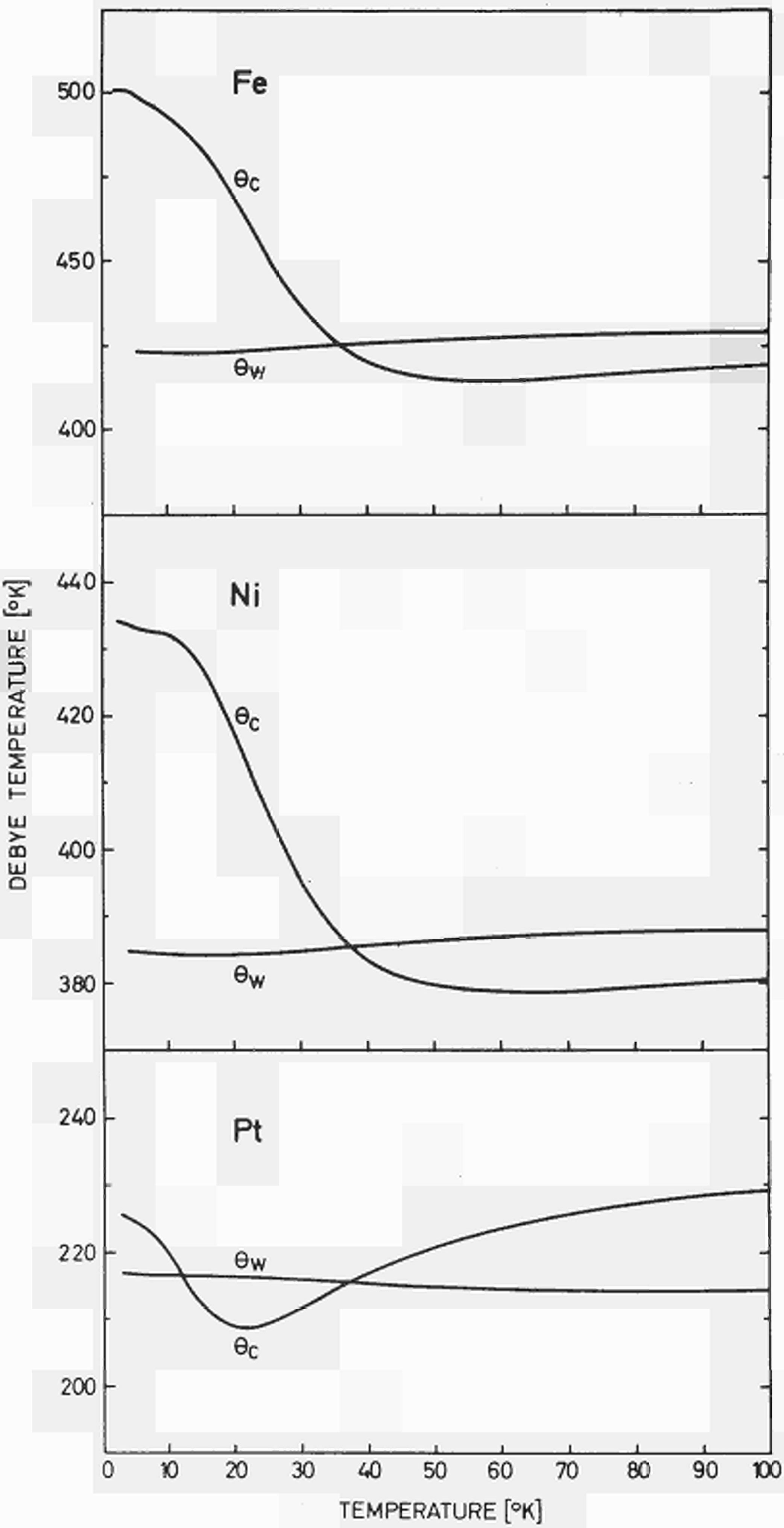

Li
θc
θw
380
360
340
320
Na
θw
θc
170
160
150
140
K
θw
θc
100
95
90
85
Rb
θw
θc
60
55
50
DEBYE TEMPERATURE [°K]
0
10
20
30
40
50
60
70
80
90
100
TEMPERATURE [°K]

FIG. 34



Cu
θc
θw
350
340
330
320
310
Al
θc
θw
440
420
400
380
Pb
θw
θc
100
95
90
85
DEBYE TEMPERATURE [°K]
0
10
20
30
40
50
60
70
80
90
100
TEMPERATURE [°K]

FIG. 35



Fe
θc
θw
500
450
400
Ni
θc
θw
440
420
400
380
Pt
θw
θc
240
220
200
DEBYE TEMPERATURE [°K]
0
10
20
30
40
50
60
70
80
90
100
TEMPERATURE [°K]

FIG. 36

APPENDIX I - P R O G R A M PSAF

```
                 C
                 C
                 C
                 C     PROGRAM PSAF (PSEUDO-ATOM FIT)
                 C
                 C     THE MODEL PARAMETERS OF A PSEUDO-ATOM FORM FACTOR ARE FITTED TO
                 C     OBSERVED DISPERSION CURVES WHICH ARE FIRST REDUCED BY THE CLOSED
                 C     SHELL REPULSIVE INTERACTION. THE PARAMETERS ARE DETERMINED USING
                 C     A NONLINEAR LEAST SQUARES METHOD BASED ON SHARE-PROGRAM G2-DPE-
                 C     NLIN BY D.W.MARQUARDT.
                 C     THE PROGRAM IS RESTRICTED TO BCC-AND FCC-STRUCTURES. IT IS WRITTEN
                 C     IN FORTRAN 4 (360 G)
                 C
                 C     MODEL FORM FACTOR G(X)=EXP(-(B1*X/2)**2)*(1+B2*T+....+BK*T**(K-1))
                 C     REPULSIVE POTENTIAL=RAMP*EXP(-R/MY)
                 C
                 C          NWAY=1    T=B1*X/2
                 C          NWAY=2    T=(B1*X/2)**2
                 C          NWAY=3    T=X/2
                 C          NWAY=4    T=(X/2)**2
                 C
                 C     X IS THE PHONON WAVE VECTOR, BI=B(I) ARE THE PARAMETERS
                 C
                 C     MAX NO OF PARAMETERS IS K=25
                 C     MAX NO OF OBSERVATIONS IS N=150
                 C
                 C     EXTENSION OF THIS PROGRAM TO MORE THAN 25 PARAMETERS REQUIRES
                 C               CHANGE OF THE FOLLOWING STATEMENTS
                 C               FIRST DIMENSION IN MAIN AND FPCODE, DIMENSION IN GJR,
                 C               IN SUBZ (EXCEPT W ), IN MODEL AND LINGLS,
                 C               LABELED COMMONS /ALL/ AND /SULIN/.
                 C               THE EXTENDED PROGRAM USES TAPE 3 INSTEAD OF ASP ( SEE
                 C               DEF. OF IBKT) FOR INTERMEDIATE STORAGE OF THE MATRIX
                 C               A=PTP. TO SAVE STORAGE SPACE ASP OF MAIN MAY THEREFORE
                 C               BE DIMENSIONED AS ASP(1,1) IN THAT CASE.
                 C
                 C                  IBKT=1 MEANS USE UPPER A MATRIX
                 C                  IBKT=2 MEANS USE TAPE 3
                 C
                 C                  IWHER =-1 MEANS DO ANY SPECIAL INITIALIZING FOR CASE
                 C                  IWHER = 0 MEANS START NEW CASE OR END RUN
                 C                  IWHER = 1 MEANS GET P S AND F
                 C                  IWHER GREATER THAN 1 MEANS GET F ONLY
                 C
                 C     MODEL DEPENDANT PARTS OF THIS PROGRAM ARE MARKED BY MA
                 C     MODEL INDEPENDANT PARTS BY MU.
                 C
 0001                  DIMENSION BS(25),DR(25),BA(25),G(25),W(26),IB(24),SA(25),A(25,26),
```

```
                      1ASP(25,25)
0002                   DIMENSION FWS(150),EF(150),ITEXT(5)
0003                   COMMON PI,QP,K,CON4,CLB,PIA,CON1,NHSCON,F(150)
0004                   COMMON/ALL/P(150,25),B(25),BN(25)
0005                   COMMON/MASUFP/IFSS1,IFSS2,NWAY,NEX,CON2,IWHER,N,KZ(150),X(150),IEX
                      1IT
0006                   COMMON/MASU/CON3,FQ(150),FQZ(150),RT(150),Y(150),NGVE,CKF,ZEFF,CKC
                      1,WEIGHT(7),NWEIT
                C
0007                   DATA ITEXT(1),ITEXT(2),ITEXT(3),ITEXT(4),ITEXT(5)/1H ,1HQ,1HP,1HY,
                      11HX/
0008                   DATA ITEXT(1),ITEXT(2),ITEXT(3),ITEXT(4),ITEXT(5)/1H ,1HQ,1HP,1HY,
                      11HX/
                C
0009                   NPRNT=0
0010               650 IWHER = 0
0011               652 GO TO 4
0012               653 IWHER = IWHER
0013                   IF (IWHER.GT.0)GO TO 654
0014                   IF (IWHER.EQ.0)GO TO 660
0015               651 CONTINUE
                C                        CASE INITIALIZING
0016                   CALL SUBZ
0017                   IF(IBOUT.EQ.1.OR.IEXIT.EQ.1) GO TO 650
0018                   GO TO 652
0019               654 CONTINUE
                C
                C           GET FUNCTIONS F(I). F(I) IS Y HAT (I).
                C           GET DERIVATIVES P(I,J)=DF(I)/DB(J) ONLY IF IWHER=1 OR IFSS2=?
                C           IFSS2=1 MEANS GET ESTIMATED DERIVATIVES P(I,J).
                C
0020                   CALL FPCODE
0021                   IF(IEXIT.EQ.1) GO TO 650
0022                   GO TO 652
0023               660 CALL EXIT
                C                        THIS IS THE END OF THE MAIN ROUTINE
                C      ------------------------------------------------------------
0024                 4 IWHER = IWHER
                C                  -  0  +
0025                   IF (IWHER.LT.0)GO TO 50
0026                   IF (IWHER.EQ.0)GO TO 10
                C                     1   2    3    4
0027                 8 GO TO (75,304,606,620), IWHER
                C                        READ FIRST CARD OF NEXT CASE
0028                10 ITCT=0
0029                   IBOUT=0
0030                   IEXIT=0
0031                   READ (5,900)N,K,IP,M,IFP
```

```
0032                IF (N.GT.150.OR.K.GT.25) WRITE (6,944)
0033                IF (N.GT.150.OR.K.GT.25) GO TO 650
          C
          C         IP              NO OF OMITTED PARAMETERS, MAX. 24
          C         M               NO OF INDEPENDANT VARIABLES, HAS TO BE 1 IN THIS
          C                         APPLICATION
          C         IFP             =1 PLOT OF Y-OBS. AND Y-PRED.
          C                         =0 NO PLOT, TABULATION OF RESULTS
          C
0034                IF (N.LE.0)GO TO 20                                              0660
0035                READ (5,900)IWS1,IWS2,IWS3,IWS4,IWS5,IWS6                         0670
          C
          C         IWS1            DOESNOT APPLY
          C         IWS2            =0 ANAL., =1 ESTIM. DERIVATIVES
          C         IWS3            =0 ABBREV., =1 DETAIL PRINTOUT
          C         IWS4            =0 NO FORCE OFF, =I FORCED BRANCH TO CONF.
          C                         REGION CALCULATION AFTER I ITERATIONS
          C         IWS5            =0 SENSE SWITCHES NOT INTERROGATED,
          C                         =1 SENSE SWITCHES INTERROGATED
          C         IWS6            =0 NONLINEAR CONFIDENCE LIMITS DESIRED,
          C                         =1 OMITTED
          C
0036                IFSS1=2                                                          0680
0037                IF (IWS5.EQ.0)GO TO 210                                          0690
0038                PAUSE 5                                                          0700
0039                CALL SSWTCH(1,IFSS1)                                             0710
0040           210  CONTINUE                                                         0720
0041                WRITE (6,932)                                                    0730
0042                IF(IFSS1.NE.1)GO TO 211                                          0740
0043                WRITE (12,932)                                                   0750
0044           211  GO TO 21                                                         0760
          C                         END OF LAST PROBLEM                              0770
0045            20  CONTINUE
0046                IF(K.LE.25) IBKT=1
0047                IF(K.GT.25) IBKT=2
0048                IF(IBKT.EQ.2) REWIND 3
0049                IWHER=0
0050                GO TO 653                                                        0810
0051           21   IF (IFP.LE.0)GO TO 22                                            0820
0052            23  CONTINUE                                                         0830
0053                IBCH=ITEXT(1)
0054                IOCH=ITEXT(2)
0055                IPCH=ITEXT(3)
0056                IYCH=ITEXT(4)
0057                IXCH=ITEXT(5)
0058                READ (5,930)YMN,SPRD                                             0890
          C
          C         YMN             Y-VALUE AT LEFT END OF PLOTTING AREA. NOTE THAT THE
```

```
                  C                 Y-AXIS OF THE PLOT IS PARALLEL TO THE LINES OF THE
                  C                 PAGE.
                  C       SPRD      RANGE OF Y-VALUES OF PLOT
                  C
0059                 22 IF(IP.LE.0) GOTO 30
0060                 24 READ(5,900)(IB(I), I = 1,IP)
                  C
                  C       IB(I)     SUBSCRIPTS OF OMITTED PARAMETERS
                  C
0061                    DO 26 I=1,IP
0062                    IF (IB(I).GT.0)GO TO 26
0063               25   WRITE (6,926)
0064                    IF(IFSS1.NE.1)GO TO 212
0065                    WRITE (12,926)
0066              212   CONTINUE
0067                    IBOUT=1
0068                 26 CONTINUE
0069                 30 READ (5,931) FF,T,E,TAU,XL,GAMCR,DEL,ZETA
                  C                 DUB IN INPUT CONSTANTS IF NOT SUPPLIED
                  C                 ( XL IS CHECKED IN FIRST ITERATION )
0070                    IF(FF.GT.0.) GOTO 34
0071                 32 FF=4.
0072                 34 IF(E.GT.0.) GOTO 37
0073                 36 E=.00005
0074                 37 IF(TAU.GT.0.) GOTO 39
0075                 38 TAU=.001
0076                 39 IF(T.GT.0.) GOTO 42
0077                 40 T=2.
0078              42    IF (K .GT.25)GO TO 46
0079                 44 IBKT=1
0080                    GO TO 50
0081                 46 IBKT=2
0082                    REWIND 3
0083                 50 IF(GAMCR.GT. 0.) GOTO 52
0084                 51 GAMCR = 45.
0085                 52 IF (DEL.GT. 0.) GO TO 55
0086                    DEL=.00001
0087                 55 IF (ZETA.GT. 0.) GO TO 53
0088                    ZETA=.1E-30
0089                 53 XKOB = 1.
0090                 54 CONTINUE
0091                    READ (5,901)(B(I),I=1,K)
0092                    READ (5,902) (KZ(I),X(I),FQZ(I),EF(I),I=1,N)
0093                    READ (5,938) NUFIT,(WEIGHT(L),L=1,7)
                  C
                  C       B(I)      INITIAL GUESSES FOR PARAMETERS
                  C       KZ(I)     KENNZEICHEN, IN SUBR. FPCO DE DEF.
                  C       X(I)      PHONON-WAVE-VECTORS K/(2PI/A) (E+8/CM)
```

```
C       FQZ(I)          OBSERVED PHONON-FREQUENCIES (E+12/SEC)
C       EF(I)           EXPERIMENTAL ERRORS (E+12/SEC)
C       NWEIT           =0 MEANS NO WEIGHT
C                       =1 MEANS TAKE WEIGHT(L) AS WEIGHT OF L-TH BRANCH,
C                       =2 MEANS TAKE 1/FQZ(I)**2 AS WEIGHT OF I-TH POINT
C                       OF DC.
C                       =3 MEANS TAKE 1/(FQZ(I)*EF(I))**2 AS WEIGHT OF
C                       I-TH POINT OF DC.
C                       NOTE THAT THE SQARES OF THE FREQUENCIES ARE TO BE
C                       FITTED.
C       WEIGHT(L)       WEIGHT OF L-TH BRANCH OF DISPERSION RELATION (L=1 TO
C                       7) IN FORMAT (7E10.3). ARBITRARY FOR NWEIT=0,2 AND 3
C
        NWEIT1=NWEIT+1
        IF(NWEIT.EQ.0) WEIT2=1.
        IWHER=-1
        GO TO 653
     59 IBKA=1
C
C       ................................................................
C                       START THE CALCULATION OF THE PTP MATRIX
C    58 WRITE (6,907)N,K,IP,M,IFP,GAMCR,DEL,FF,T,E,TAU,XL,ZETA
        IF(IFSS1.NE.1)GO TO 213
        WRITE (12,907)N,K,IP,M,IFP,GAMCR,DEL,FF,T,E,TAU,XL,ZETA
    213 CONTINUE
     60 CONTINUE
        DO 62 I=1,K
        G (I) =0.
        DO 62 J=1,K
     62 A (I,J)=0.
        GO TO (63,69,69),IBKA
     63 IF (IWS5.EQ.0)GO TO 630
        CALL SSWTCH (3,IFSS3)
        CALL SSWTCH(2,IFSS2)
        CALL SSWTCH (1,IFSS1)
        GO TO (66,64),IFSS3
    630 IFSS3=IWS3
        IFSS2=IWS2
        GO TO 70
     64 IFSS3=0
     66 GO TO (70,65), IFSS2
     65 IFSS2=0
        GO TO 70
     69 IFSS3=1
        NGVE=1
     70 WRITE (6,908)(B(J),J=1,K)
        IF(IFSS1.NE.1)GO TO 214
        WRITE (12,908)(B(J),J=1,K)
```

```
0126          214  CONTINUE
0127               IF (IFSS3.EQ.0)GO TO 73
0128          71   IF (IFP.LE.0)GO TO 68
0129            67 WS = YMN+SPRD
0130               WRITE( 6,906)YMN,WS
0131               IF(IFSS1.NE.1) GOTO 258
0132               WRITE(12,906)YMN,WS
0133           258 CONTINUE
0134               GO TO 73
0135            68 CONTINUE
0136            73 IF (IFSS2.EQ.0) GO TO 57
0137               GO TO 600
0138         72    IF (IFSS2.EQ.1)GO TO 602
           C
           C             THIS IS THE FP-ROUTINE WITH ANALYTICAL P S
           C
0139            57 IWHER=1
           C             GET F AND ANALYTICAL P S
0140               GO TO 653
0141         75    IF (IP.LE.0)GO TO 80
0142            76 DO 77 II=1,IP
0143               IWS=IB(II)
0144               DO 77 I=1,N
0145            77 P(I,IWS)=0.0
0146               GO TO 80
           C       ..............................................................
           C
           C                           THIS IS THE ESTIMATED P S ROUTINE
           C
0147           600 CONTINUE
0148           602 IWHER=3
0149               GO TO 653
0150           606 DO 607 I=1,N
0151           607 TWS(I)=F(I)
0152               J=1
0153         608   IF (IP.LE.0)GO TO 618
0154           610 DO 612 II=1,IP
0155               IF ((J-IB(II)).EQ.0)GO TO 621
0156           612 CONTINUE
0157           618 DBW=B(J)*DEL
0158               TWS=B(J)
0159               B(J)=B(J)+DBW
0160               IWHER=4
0161               GO TO 653
0162           620 B(J)=TWS
0163               DO 361 I=1,N
0164           361 P(I,J)=(F(I)-FWS(I))/DBW
0165               GO TO 622
```

```
  621 DO 362 I=1,N
  362 P(I,J)=0.0
  622 J=J+1
      IF ((J-K).LE.0)GO TO 608
  624 DO 625 I=1,N
  625 F(I)=FWS(I)
C                    END OF ESTIMATED P S ROUTINE
C     .................................................................
C
C                    NOW, USE THE P S TO MAKE MATRIX A=PTP
C
   80 CONTINUE
      DO 82 I=1,N
      DYFW=Y(I)-F(I)
      GO TO (89,81,83,990),NWEIT1
   81 IKZ=KZ(I)
      WEIT=WEIGHT(IKZ)
      WEIT2=WEIT*WEIT
      GO TO 89
   83 YI=Y(I)
      WEIT2=1./(YI*YI)
      GO TO 89
  990 YI=Y(I)
      EFI=EF(I)
      YE=YI*EFI*EFI
      WEIT2=1./(YE*YE)
   89 DYFW=DYFW*WEIT2
      DO 82 J=1,K
      G(J)=G(J)+DYFW*P(I,J)
      DO 82 L=J,K
      A(L,J)=A(L,J)+P(I,L)*P(I,J)*WEIT2
   82 A(J,L)=A(L,J)
      IF (IFP.LE.0)GO TO 318
  800 IF (IFSS3.EQ.0)GO TO 314
C                    PLOTTING Y(I),F(I)
  802 DO 844 I=1,N
      IO = (Y(I)-YMN)*100./SPRD
      IPP = (F(I)-YMN)*100./SPRD
      IF (IO.EQ.IPP)GO TO 808
      IF (IO.GT. IPP)GO TO 812
C                    Y(I) OUT FIRST
  804 IP1=IOCH
      IP2=IPCH
      I1=IO
      I2=IPP
      GO TO 816
C                    ONLY ONE CHARACTER
  808 IP1=IYCH
```

```
0206              IP2=IBCH
0207              I1=IO
0208              I2=IPP
0209              GO TO 816
            C                          F OUT FIRST
0210          812 IP1=IPCH
0211              IP2=IOCH
0212              I1=IPP
0213              I2=IO
            C                          ZERO PLOTS IN THE LEFT HAND COLUMN, SO I1 IS ITS
            C                          OWN BLANK COUNTER
            C                          OVERFLOWS PLOT X IN COLUMN 102
            C                          UNDERFLOWS ALSO PLOT X IN COLUMN ZERO
0214         816  IF (I2.LE.101)GO TO 819
0215          817 I2=101
0216              IP2=IXCH
0217              IF (I1.LT.101)GO TO 819
0218          818 I1=101
0219              IP1=IXCH
0220              IP2=IBCH
0221              GO TO 825
0222         819  IF (I1.GE.0)GO TO 825
0223          822 I1=0
0224              IP1=IXCH
0225              IF (I2.GT.0)GO TO 825
0226          823 I2=1
0227              IP2=IBCH
0228          825 I1M1=I1
0229              I1M2=I2-I1-1
0230              IF (I1M1.GT.0)GO TO 832
0231         820  IF (I1M2.GT.0)GO TO 828
0232         824  WRITE (6,928)IP1,IP2
0233              IF(IFSS1.NE.1)GO TO 215
0234              WRITE (12,928)IP1,IP2
0235         215  CONTINUE
0236              GO TO 844
0237         828  WRITE (6,928)IP1,(IBCH,II=1,I1M2),IP2
0238              IF(IFSS1.NE.1)GO TO 216
0239              WRITE (12,928)IP1,(IBCH,II=1,I1M2),IP2
0240         216  CONTINUE
0241              GO TO 844
0242         832  IF (I1M2.GT.0)GO TO 840
0243         836  WRITE (6,928)(IBCH,II=1,I1M1),IP1,IP2
0244              IF(IFSS1.NE.1)GO TO 217
0245              WRITE (12,928)(IBCH,II=1,I1M1),IP1,IP2
0246         217  CONTINUE
0247              GO TO 844
0248          840 WRITE (6,928)(IBCH,II=1,I1M1),IP1,(IBCH,II=1,I1M2),IP2
```

```
      IF(IFSS1.NE.1)GO TO 218
      WRITE (12,923)(IBCH,II=1,I1M1),IP1,(IBCH,II=1,I1M2),IP2
  218 CONTINUE
  844 CONTINUE
      GO TO 314
  318 IF(IFSS3.EQ.0) GO TO 314
  308 CONTINUE
  310 CONTINUE
      WRITE (6,943)
      IF(IFSS1.NE.1) GO TO 376
      WRITE (12,943)
  376 PHI=0.0
      ICOUNT=0
      NDATA=N
      S1=0.0
      S2=0.0
      SL1=0.0
      SL2=0.0
      DO 350 L=1,N
      YL=Y(L)
      FL=F(L)
      FQZL=FQZ(L)
      RTL=RT(L)
      EFL=EF(L)
      EFL2=EFL**2
      FQL=FQ(L)
      FQTHL=FL+RTL
      IF(FQTHL.GE.0.0) GO TO 2000
      FQZTHL=-SQRT(ABS(FQTHL))
      GO TO 2001
 2000 FQZTHL=SQRT(FQTHL)
 2001 IF(FQZTHL.LT.1.0E-10.AND.FQZL.LT.1.0E-10) GO TO 2002
      IF(FQZL.LT.1.0E-10.AND.FQZTHL.GT.1.0E-10) GO TO 2003
      RFTHL=(FQZTHL-FQZL)/FQZL
      GO TO 2004
 2002 RFTHL=0.0
      GO TO 2004
 2003 RFTHL=1.0E+10
 2004 IF(FQZL.GT.1.0E-10) GO TO 2005
      IF(FQZL.LE.1.0E-10.AND.EFL.LE.1.0E-10) GO TO 2006
      IF(FQZL.LE.1.0E-10.AND.EFL.GT.1.0E-10) GO TO 2007
 2005 RFEXL=EFL/FQZL
      GO TO 2008
 2006 RFEXL=0.0
      GO TO 2008
 2007 RFEXL=1.0E+10
 2008 WS=FL-YL
      WSR=WS/YL
```

```
      GO TO (355,353,354,991),NWEIT1
  353 IKZ=KZ(L)
      WS=WS*WEIGHT(IKZ)
      GO TO 355
  354 WS=WSR
      GO TO 355
  991 WS=WSR/EFL2
  355 PHI=PHI+WS*WS
      WRITE (6,925) KZ(L),X(L),FQZTHL,FQZL,RTL,FL,YL,WSR,EFL,REEXL,RETHL
      IF(IFSS1.NE.1) GO TO 220
      WRITE (12,925) KZ(L),X(L),FQZTHL,FQZL,RTL,FL,YL,WSR,EFL,REEXL,RETH
     1L
  220 CONTINUE
      IF(KZ(L).NE.KZ(L+1))WRITE (6,937)
      IF(KZ(L).NE.KZ(L+1).AND.IFSS1.EQ.1)WRITE (12,937)
      IF(EFL.EQ.0.0)NCOUNT=NCOUNT+1
      IF(EFL.EQ.0.0) GO TO 350
      S1=S1+((FQTHL-FQL)/EFL2)**2
      S2=S2+(FQL/EFL2)**2
      SL1=SL1+(FQZTHL-FQZL)**2/EFL2
      SL2=SL2+FQL/EFL2
  350 CONTINUE
      CNDATA=NDATA-NCOUNT
      S1=S1-CNDATA
      SL1=SL1-CNDATA
      IF(SL1.GE.0.0)GO TO 4000
      RMSDL=-SQRT(ABS(SL1)/SL2)
      GO TO 4001
 4000 RMSDL=SQRT(SL1/SL2)
 4001 IF(S1.GE.0.0)GO TO 4002
      RMSD=-SQRT(ABS(S1)/S2)
      GO TO 4003
 4002 RMSD=SQRT(S1/S2)
 4003 CIR=S1/CNDATA
      WRITE (6,940) RMSD,RMSDL,CIR
      IF(IFSS1.EQ.1)WRITE (12,940) RMSD,RMSDL,CIR
      IF(NOVE.EQ.0) GO TO 352
C
C COMPUTE MODEL-FUNCTION G(K) AND V(K) AND E(K) / MA
C
      WRITE (6,942)
      IF(IFSS1.NE.1) GO TO 375
      WRITE (12,942)
  375 CL=B(1)
      CKF2=2.0*CKF
      CKC2=CKC**2
      AEX=CKF*CL
      IF(NWAY.GT.2)AE=CKF
```

```
      IF(NWAY.LE.2)AF=AEX
      DELA=0.1
      ARK=0.0
      DO 360 L=1,51
      ARGEX2=(AEX*ARK)**2
      ARGR=(AF*ARK)**NEX
      SS=0.0
      IF(K.LT.2) GO TO 365
      K2=K+2
      DO 369 I=2,K
      J=K2-I
  369 SS=(SS+B(J))*ARGR
  365 GK=EXP(-ARGEX2)*(1.0+SS)
      DEN=(ARK*CKF2)**2+FDC(ARK)*CKC2
      VK=CON3*GK/DEN
      EK=ZEFF*VK*GK
      VK=-VK
      ARKA=ARK/CON2
      WRITE (6,941) ARK,ARKA,GK,VK,EK
      IF(IFSS1.NE.1) GO TO 360
      WRITE (12,941) ARK,ARKA,GK,VK,EK
  360 ARK=ARK+DELA
      GO TO 352
  314 PHI=0.0
      DO 351 L=1,N
      WS=F(L)-Y(L)
      GO TO (351,356,357,992),NWEIT1
  356 IKZ=KZ(L)
      WS=WS*WEIGHT(IKZ)
      GO TO 351
  357 WS=WS/Y(L)
      GO TO 351
  992 EFL=EF(L)
      WS=WS/(Y(L)*EFL*EFL)
  351 PHI=PHI+WS*WS
  352 CONTINUE
   34 IF (IP.LE.0)GO TO 88
   85 DO 87 JJ=1,IP
      IWS=IB(JJ)
      DO 86 II=1,K
      A(IWS,II)=0.
   86 A(II,IWS)=0.
   87 A(IWS,IWS)=1.
   88 GO TO (90,704,706),IBKA
C                   SAVE SQUARE ROOTS OF DIAGONAL ELEMENTS
   90 DO 92 I=1,K
   92 SA(I)=SQRT (A(I,I))
      DO 106 I=1,K
```

```
                DO 100 J=1,K
                WS = SA(I)*SA(J)
                IF(WS.GT.0.) GOTO 98
          96    A(I,J) =0.
                GO TO 100
          98    A(I,J)=A(I,J)/WS
         100    CONTINUE
                IF(SA(I).GT.0.) GOTO 104
         102    G(I)=0.
                GO TO 106
         104    G(I)=G(I)/SA(I)
         106    CONTINUE
                DO 110 I=1,K
         110    A(I,I)=1.
                PHIZ=PHI
      C                        WE NOW HAVE PHI ZERO
                GO TO (1132,1130),IBKT
        1130    WRITE (3)A
                REWIND 3
                GO TO 1134
        1132    DO 1133 LZ=1,K
                DO 1133 JZ=1,K
        1133    ASP(LZ,JZ)=A(LZ,JZ)
      C         .............................................................
        1134    CONTINUE
                IF (ITCT.GT.0)GO TO 163
      C                        FIRST ITERATION
         150    IF(XL.GT.0.) GOTO 154
         152    XL=0.01
         154    ITCT=1
                DO 161 J=1,K
         161    BS(J)=B(J)
      C                        BS(J) CORRESPONDS TO PHIZ
         163    IBK1=1
                WS=N-K+IP
                SE=SQRT(PHIZ/WS)
                IF (IFSS3.GT.0)GO TO 165
         162    IF (IFSS2.EQ.0) GO TO 168
         167    WRITE (6,911)PHIZ,SE,XLL,GAMMA,XL,NHSCON
                IF(IFSS1.NE.1)GO TO 221
                WRITE (12,911)PHIZ,SE,XLL,GAMMA,XL,NHSCON
         221    CONTINUE
                GO TO 169
         168    WRITE (6,912)PHIZ,SE,XLL,GAMMA,XL,NHSCON
                IF(IFSS1.NE.1)GO TO 222
                WRITE (12,912)PHIZ,SE,XLL,GAMMA,XL,NHSCON
         222    CONTINUE
                GO TO 169
```

```
0432        165  IF (IFSS2.EQ.0)GO TO 1661                                        3670
0433        166  WRITE (6,903)PHIZ,SE,XL,NHSCON                                   3680
0434             IF(IFSS1.NE.1)GO TO 223                                          3690
0435             WRITE (12,903)PHIZ,SE,XL,NHSCON                                  3700
0436        223  CONTINUE                                                         3710
0437             GO TO 169                                                        3720
0438       1661  WRITE (6,909)PHIZ,SE,XL,NHSCON                                   3730
0439             IF(IFSS1.NE.1)GO TO 224                                          3740
0440             WRITE (12,909)PHIZ,SE,XL,NHSCON                                  3750
0441        224  CONTINUE                                                         3760
0442        169  GO TO 200                                                        3770
0443        164  PHIL=PHI                                                         3780
          C                  WE NOW HAVE PHI LAMBDA                               3790
0444             DO 170 J=1,K                                                     3800
0445             IF (ABS(DB(J)/(ABS(B(J)) + TAU)).GE.E) GOTO 172                  3810
0446        170  CONTINUE                                                         3820
0447             WRITE (6,923)                                                    3830
0448             IF(IFSS1.NE.1)GO TO 225                                          3840
0449             WRITE (12,923)                                                   3850
0450        225  CONTINUE                                                         3860
0451             GO TO 700                                                        3870
0452        172  IF (IWS5.EQ.0)GO TO 1720                                         3880
0453             CALL SSWTCH(4,IFSS4)                                             3890
0454             GO TO (171,173),IFSS4                                            3900
0455       1720  IF (IWS4.EQ.0)GO TO 173                                          3910
0456             IF (IWS4.EQ.1)GO TO 171                                          3920
0457             IWS4=IWS4-1                                                      3930
0458             GO TO 173                                                        3940
0459        171  WRITE (6,924)                                                    3950
0460             IF(IFSS1.NE.1)GO TO 226                                          3960
0461             WRITE (12,924)                                                   3970
0462        226  CONTINUE                                                         3980
0463             GO TO 700                                                        3990
0464        173  XKDB = 1.                                                        4000
0465             IF (PHIL.GT.PHIZ)GO TO 190                                       4010
0466        174  XLS=XL                                                           4020
0467             DO 176 J=1,K                                                     4030
0468             BA(J)=B(J)                                                       4040
0469        176  B(J)=BS(J)                                                       4050
0470             IF (XL.GT..00000001)GO TO 175                                    4060
0471       1175  DO 1176 J=1,K                                                    4070
0472             B(J)=BA(J)                                                       4080
0473       1176  BS(J)=B(J)                                                       4081
0474             GO TO 60                                                         4090
0475        175  XL=XL/10.                                                        4100
0476             IBK1=2                                                           4110
0477             GO TO 200                                                        4120
0478        177  PHL4=PHI                                                         4130
```

```
              C                WE NOW HAVE PHI(LAMBDA/10)
0479                IF(PHL4.GT.PHIZ) GOTO 184
0480            182 DO 183 J=1,K
0481            183 BS(J)=B(J)
0482                GO TO 60
0483            184 XL=XLS
0484                DO 186 J=1,K
0485                BS(J)=BA(J)
0486            186 B(J)=BA(J)
0487                GO TO 60
0488            190 IBK1=4
0489                XLS=XL
0490                XL=XL/10.
0491                DO 185 J=1,K
0492            185 B(J)=BS(J)
0493                GO TO 200
0494           187  IF (PHI.LE.PHIZ)GO TO 196
0495            191 XL=XLS
0496                IBK1=3
0497            192 XL=XL*10.
0498            195 DO 193 J=1,K
0499            193 B(J)=BS(J)
0500                GO TO 200
0501            194 PHIT4=PHI
              C                WE NOW HAVE PHI(10*LAMBDA)
0502           180  IF (PHIT4.GT.PHIZ)GO TO 198
0503            196 DO 197 J=1,K
0504            197 BS(J)=B(J)
0505                GO TO 60
0506           198  IF (GAMMA.GE.GAMCR)GO TO 192
0507            199 XKDB = XKDB/2.
0508                DO 1199 J=1,K
0509                IF (ABS(DB(J)/(ABS(B(J))+TAU)).GE.E)GO TO 195
0510           1199 CONTINUE
0511                DO 1200 J=1,K
0512           1200 B(J)=BS(J)
0513                WRITE (6,934)
0514                IF(IFSS1.NE.1)GO TO 227
0515                WRITE (12,934)
0516           227  CONTINUE
0517                GO TO 700
              C
              C     ..............................................................
              C                SET UP FOR MATRIX INVERSION
0518            200 GO TO (1102,1100),IBKT
0519           1100 READ (3)A
0520                REWIND 3
0521                GO TO 1104
```

```
0522      1102 DO 1103 LZ=1,K
0523           DO 1103 JZ=1,K
0524      1103 A(LZ,JZ)=ASP(LZ,JZ)
0525      1104 DO 202 I=1,K
0526       202 A(I,I)=A(I,I)+XL
          C                 GET INVERSE OF A AND SOLVE FOR DB (J)S
0527           IBKM=1
          C    ...........................................................
          C                 THIS IS THE MATRIX INVERSION ROUTINE
          C                 K IS THE SIZE OF THE MATRIX
0528       404 CALL GJR(A,K,ZETA,MSING)
0529           GO TO (415,650), MSING
0530       415 GO TO (416,710), IBKM
          C                 END OF MATRIX INVERSION, SOLVE FOR DB(J)
0531       416 DO 420 I=1,K
0532           DB(I)=0.
0533           DO 421 J=1,K
0534       421 DB(I)=A(I,J)*G(J)+DB(I)
0535       420 DB(I)=XKDB*DB(I)
0536           XLL=0.
0537           DTG = 0.
0538           GTG = 0.
0539           DO 250 J=1,K
0540           DB(J)=DB(J)/SA(J)
0541           DTG = DTG + DB(J)*G(J)
0542           GTG = GTG + G(J)**2
0543           B(J)=B(J)+DB(J)
0544       250 XLL=XLL+DB(J)*DB(J)
0545           KIP=K-IP
0546           IF (KIP.EQ.1) GO TO 1257
0547           CGAM=DTG/SQRT(XLL*GTG)
0548           JGAM = 1
0549           IF(CGAM.GT..0) GOTO 253
0550       251 CGAM = ABS(CGAM)
0551           JGAM = 2
0552       253 GAMMA = 57.2957795*(1.5707288+CGAM*(-0.2121144+CGAM*(0.074261
              1-CGAM*.0187293)))*SQRT(1.-CGAM)
0553           GO TO (257,255), JGAM
0554       255 GAMMA = 180.-GAMMA
0555           IF (XL.LT.1.0)GO TO 257
0556      1255 WRITE(6,922)XL,GAMMA
0557           IF(IFSS1.NE.1)GO TO 228
0558           WRITE(12,922)XL,GAMMA
0559       228 CONTINUE
0560           GO TO 700
0561      1257 GAMMA=0.
0562       257 XLL=SQRT(XLL)
0563           IBK2=1
```

```
0564           GO TO 300
0565      252  IF (IFSS3.EQ.0)GO TO 256
0566      254  WRITE (6,904)(DB(J),J=1,K)
0567           IF(IFSS1.NE.1)GO TO 229
0568           WRITE (12,904)(DB(J),J=1,K)
0569      229  CONTINUE
0570           WRITE (6,905)PHI,XL,GAMMA,XLL,NHSCON
0571           IF(IFSS1.NE.1)GO TO 230
0572           WRITE (12,905)PHI,XL,GAMMA,XLL,NHSCON
0573      230  CONTINUE
0574       256 GO TO (164,177,194,187),IBK1
         C
         C     .....................................................
         C                     CALCULATE PHI
0575       300 PHI=0.
0576           IWHER=2
0577           IF (IWS5.EQ.0) GO TO 653
0578           CALL SSWTCH(5,NONSK)
0579           IF(NONSK.EQ.1) GOTO 650
0580       302 GO TO 653
0581       304 DO 370 I=1,N
0582           WS=Y(I)-F(I)
0583           GO TO (370,358,359,993),NWEIT1
0584       358 IKZ=KZ(I)
0585           WS=WS*WEIGHT(IKZ)
0586           GO TO 370
0587       359 WS=WS/Y(I)
0588           GO TO 370
0589       993 EFI=EF(I)
0590           WS=WS/(Y(I)*EFI*EFI)
0591       370 PHI=PHI+WS*WS
0592       316 GO TO (252,780,704,762,766,772),IBK2
         C
         C
         C     .....................................................
         C                     THIS IS THE CONFIDENCE LIMIT CALCULATION
0593       700 DO 702 J=1,K
0594       702 B(J)=BS(J)
0595           WRITE (6,933)N,K,IP,M,FF,T,E,TAU
0596           IF(IFSS1.NE.1)GO TO 231
0597           WRITE (12,933)N,K,IP,M,FF,T,E,TAU
0598      231  CONTINUE
0599           IBKA=2
         C                     THIS WILL PRINT THE Y,YHAT,DELTA Y
0600           GO TO 60
0601      704  IF (IFP.LE.0)GO TO 706
0602       705 IBKA=3
0603           IFP=0
```

```
      GO TO 60
  706 NS=N-K+IP
      SE=SQRT(PHI/NS)
      PHIZ=PHI
      IF (IFSS2.EQ.0)GO TO 709
  707 WRITE (6,903)PHIZ,SE,XL,NHSCON
      IF(IFSS1.NE.1)GO TO 232
      WRITE (12,903)PHIZ,SE,XL,NHSCON
  232 CONTINUE
      GO TO 708
  709 WRITE(6,909) PHIZ,SE,XL,NHSCON
      IF(IFSS1.NE.1)GO TO 233
      WRITE (12,909)PHIZ,SE,XL,NHSCON
  233 CONTINUE
C                      NOW WE HAVE MATRIX A
  708 GO TO (1122,1120),IBKT
 1120 WRITE (3)A
      REWIND 3
      GO TO 1124
 1122 DO 1123 LZ=1,K
      DO 1123 JZ=1,K
 1123 ASP(LZ,JZ)=A(LZ,JZ)
 1124 IBKM=2
      GO TO 404
C
C                      NOW WE HAVE C = A INVERSE
  710 DO 711 J=1,K
      IF(A(J,J).LT..0) GO TO 713
  711 SA(J)=SQRT(A(J,J))
      GO TO 715
  713 IBOUT=1
  715 KST=-4
      WRITE (6,916)
      IF(IFSS1.NE.1)GO TO 234
      WRITE (12,916)
  234 KST=KST+5
      KEND=KST+4
      IF (KEND.LT.K) GO TO 719
      KEND=K
  719 DO 712 I=1,K
      IF(IFSS1.NE.1)GO TO 235
      WRITE (12,918)I,(A(I,J),J=KST,KEND)
  235 CONTINUE
  712 WRITE (6,918)I,(A(I,J),J=KST,KEND)
      IF (KEND.LT.K) GO TO 234
      IF (IBOUT.EQ.0) GO TO 717
      WRITE (6,936)
      IF (IFSS1.NE.1) GO TO 650
```

```
0649          WRITE (12,936)
0650          GO TO 650
0651      717 DO 718 I=1,K
0652          DO 718 J=1,K
0653          WS=SA(I)*SA(J)
0654          IF(WS.GT. 0.) GOTO 716
0655      714 A(I,J)=0.
0656          GO TO 718
0657      716 A(I,J)=A(I,J)/WS
0658      718 CONTINUE
0659          DO 720 J=1,K
0660      720 A(J,J)=1.
0661          WRITE (6,917)
0662          IF(IFSS1.NE.1)GO TO 236
0663          WRITE (12,917)
0664     236  CONTINUE
0665          KST=-9
0666      721 KST=KST+10
0667          KEND=KST+9
0668          IF (KEND.LT.K) GO TO 722
0669          KEND=K
0670      722 DO 724 I=1,K
0671          IF(IFSS1.NE.1)GO TO 237
0672          WRITE (12,935)I,(A(I,J),J=KST,KEND)
0673     237  CONTINUE
0674     724  WRITE (6,935)I,(A(I,J),J=KST,KEND)
0675          IF (KEND.LT.K) GO TO 721
        C                       GET T*SE*SQRT(C(I,I))
0676          DO 726 J=1,K
0677      726 SA(J)=   SE*SA(J)
0678          GO TO (1112,1110),IBKT
0679     1110 READ (3)A
0680          REWIND 3
0681          GO TO 1114
0682     1112 DO 1113 LZ=1,K
0683          DO 1113 JZ=1,K
0684     1113 A(LZ,JZ)=ASP(LZ,JZ)
0685     1114 CONTINUE
0686     740  WRITE (6,919)
0687          IF(IFSS1.NE.1)GO TO 238
0688          WRITE (12,919)
0689     238  CONTINUE
0690          WS=K-IP
0691          DO 750 J=1,K
0692          IF (IP.LE.0)GO TO 743
0693      741 DO 742 I=1,IP
0694          IF (J.EQ.IB(I))GO TO 746
0695      742 CONTINUE
```

```
  743 HJTD=SQRT(WS*FF)*SA(J)
      STE=SA(J)
      OPL=BS(J)-SA(J)*T
      OPU=BS(J)+SA(J)*T
      SPL=BS(J)-HJTD
      SPU=BS(J)+HJTD
      WRITE ( 6,927)J,STE,OPL,OPU,SPL,SPU
      IF(IFSS1.NE.1)GO TO 239
      WRITE (12,927)J,STE,OPL,OPU,SPL,SPU
  239 CONTINUE
      GO TO 750
  746 WRITE (6,913)J
      IF(IFSS1.NE.1)GO TO 240
      WRITE (12,913)J
  240 CONTINUE
  750 CONTINUE
C                      NONLINEAR CONFIDENCE LIMIT
      IF (IWS6.EQ.1) GO TO 650
      WS=K-IP
      WS1=N-K+IP
      PKN=WS/WS1
      PC=PHIZ*(1.+FF*PKN)
      WRITE (6,920)PC
      IF(IFSS1.NE.1)GO TO 241
      WRITE (12,920)PC
  241 CONTINUE
      WRITE (6,921)
      IF(IFSS1.NE.1)GO TO 242
      WRITE (12,921)
  242 CONTINUE
      IFSS3=1
      J=1
 9790 IBKP=1
      DO 752 JJ=1,K
  752 B(JJ)=BS(JJ)
      IF (IP.LE.0)GO TO 758
  754 DO 756 JJ=1,IP
      IF (J.EQ.IB(JJ))GO TO 787
  756 CONTINUE
  758 DD=-1.
      IBKN=1
  760 D=DD
      B(J)=BS(J)+D*SA(J)
      IBK2=4
      GO TO 300
  762 PHI1=PHI
      IF (PHI1.GE.PC)GO TO 770
  764 D=D+DD
```

```
      IF (D/DD.GE.5.)GO TO 788
  765 B(J)=BS(J)+D*SA(J)
      IBK2=5
      GO TO 300
  766 PHID=PHI
      IF (PHID.LT.PC)GO TO 764
      IF (PHID.GE.PC) GO TO 778
  770 D=D/2.
      IF (D/DD.LE..001)GO TO 788
  771 B(J)=BS(J)+D*SA(J)
      IBK2=6
      GO TO 300
  772 PHID=PHI
      IF (PHID.GT.PC)GO TO 770
  778 XK1=PHIZ/D+PHI1/(1.-D)+PHID/(D*(D-1.))
      XK2=-(PHIZ*(1.+D)/D+D/(1.-D)*PHI1+PHID/(D*(D-1.)))
      XK3=PHIZ-PC
      BC = (SQRT(XK2*XK2-4.*XK1*XK3)-XK2)/(2.*XK1)
      GO TO (779,784),IBKN
  779 B(J)=BS(J)-SA(J)*BC
      GO TO 781
  784 B(J)=BS(J)+SA(J)*BC
  781 IBK2=2
      GO TO 300
  780 GO TO (782,786),IBKN
  782 IBKN=2
      DD=1.
      BL=B(J)
      PL=PHI
      GO TO 760
  786 BU=B(J)
      PU=PHI
      GO TO (783,795,785,789),IBKP
  783 WRITE (6,918) J, BL, PL, BU, PU
      IF(IFSS1.NE.1)GO TO 243
      WRITE (12,918)J,BL,PL,BU,PU
  243 CONTINUE
      GO TO 790
  795 WRITE (6,915) J, BU, PU
      IF(IFSS1.NE.1)GO TO 244
      WRITE (12,915)J,BU,PU
  244 CONTINUE
      GO TO 790
  785 WRITE (6,918)J,BL, PL
      IF(IFSS1.NE.1)GO TO 245
      WRITE (12,918)J,BL,PL
  245 CONTINUE
      GO TO 790
```

```
0791      787  WRITE (6,913)J
0792           IF(IFSS1.NE.1)GO TO 246
0793           WRITE (12,913)J
0794      246  CONTINUE
0795           GO TO 790
0796      789  WRITE (6,914)J
0797           IF(IFSS1.NE.1)GO TO 247
0798           WRITE (12,914)J
0799      247  CONTINUE
0800           GO TO 790
0801       788 GO TO (791,792),IBKN
         C                      DELETE LOWER PRINT
0802       791 IBKP=2
0803           GO TO 780
0804       792 GO TO (793,794),IBKP
         C                      DELETE UPPER PRINT
0805       793 IBKP=3
0806           GO TO 780
         C                      LOWER IS ALREADY DELETED, SO DELETE BOTH
0807       794 IBKP=4
0808           GO TO 780
0809       790 J=J+1
0810           IF(J.LE.K)GO TO 9790
0811           GO TO 10
         C     ..........................................................................
0812       900 FORMAT (25I3)
0813       901 FORMAT (6E12.5)
0814       902 FORMAT (I6,3E12.5)
0815       903 FORMAT (/13X,4H PHI 14X,4H S E                  9X,7H LAMBDA   6X,
          9031 25H ESTIMATED PARTIALS USED  //5X,2E18.8,  E13.3,4X,16HCONVERGENT
             2 WITH I2,9H H-SHELLS)
0816       904 FORMAT(/12H INCREMENTS 5E18.8/(12X,5E18.8) )
0817       905 FORMAT (13X,4H PHI 10X,7H LAMBDA 6X,7H GAMMA  6X, 7H LENGTH  /
          9051 5X, E18.8, 3E13.3,4X,16HCONVERGENT WITH I2,9H H-SHELLS)
0818       906 FORMAT(1X,1E9.2,86X,1E9.2 /1X,1H+ 99X,1H+ )
0819       907 FORMAT( 5HIN = I3,5X,5H K = I3,5X,5H P = I3,5X,5H M = I3,5X,
          9071 7H IFP = I3,5X,13HGAMMA CRIT = E10.3,5X,6HDEL = E10.3/6H FF =
          9072E10.3,5X,5H T = E10.3,5X,5H E = E10.3,5X,7H TAU = E10.3,5X,6H XL =
          9073  E10.3 , 4X, 7HZETA = E10.3 /)
0820       908 FORMAT(/12H PARAMETERS 5E18.8/(12X,5E18.8) )
0821       909 FORMAT (/13X,4H PHI 14X,4H S E                  9X,7H LAMBDA 6X,
          9091 25H ANALYTIC PARTIALS USED   /5X, 2E18.8,  E13.3,4X,16HCONVERGENT
             2 WITH I2,9H H-SHELLS)
0822       910 FORMAT(1H /5X,9X,4H OBS 13X,5H PRED 13X,5H DIFF  )
0823       911 FORMAT (/13X,4H PHI 14X,4H S E 11X,7H LENGTH 6X, 7H GAMMA 6X,
          9111 7H LAMBDA 6X, 25HESTIMATED PARTIALS USED  /5X, 2E18.8, 3E13.3,4X,
            216HCONVERGENT WITH I2,9H H-SHELLS)
0824       912 FORMAT (/13X,4H PHI 14X,4H S E 11X,7H LENGTH 6X, 7H GAMMA 6X,
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            9121 7H LAMBDA 6X, 24HANALYTIC PARTIALS USED  /5X, 2E18.8, 3E13.3,4X,1
                26HCONVERGENT WITH I2,9H H-SHELLS)
0825         913 FORMAT(2X,I3,20H PARAMETER NOT USED    )
0826         914 FORMAT(2X,I3,12H NONE FOUND    )
0827         915 FORMAT(2X,I3,36X,2E18.8  )
0828         916 FORMAT(1H /13H PTP INVERSE )
0829         917 FORMAT(1H /30H PARAMETER CORRELATION MATRIX   )
0830         918 FORMAT( 2X,I3,5E18.8)
0831         919 FORMAT( 1H /1H / 13X,4H STD 17X, 16H ONE - PARAMETER 21X,
            9191 14H SUPPORT PLANE / 3X, 2H B 7X,6H ERROR 12X, 6H LOWER 12X,
            9192 6H UPPER 12X, 6H LOWER 12X, 6H UPPER    )
0832         920 FORMAT( 1H /1H /30H  NONLINEAR CONFIDENCE LIMITS  / /
            9201 16H PHI CRITICAL = E15.8          )
0833         921 FORMAT(1H / 6H  PARA 6X,8H LOWER B 8X,10H LOWER PHI 10X,8H UPPER B
            9211 8X,10H UPPER PHI   )
0834         922 FORMAT(18H GAMMA LAMBDA TEST,5X,2E13.3)
0835         923 FORMAT(14H EPSILON TEST   )
0836         924 FORMAT(11H FORCE OFF   )
0837         925 FORMAT (I3,E12.3,5E13.4,4E12.3)
0838         926 FORMAT ( 40H BAD DATA, SUBSCRIPTS FOR UNUSED BS = 0    / / / )
0839         927 FORMAT(2X,I3,5E18.8 )
0840         928 FORMAT(1H , 110A1   )
0841         929 FORMAT(10A1)
0842         930 FORMAT (7F10.0)
0843         931 FORMAT (8F10.0)
0844         932 FORMAT(1H1)
0845         933 FORMAT( 5H1N = I3,5X,5H K = I3,5X,5H P = I3,5X,5H M = I3,5X,
            9331                                 /   6H FF = E10.3,5X,5H T = E10.3,
            9332 5X,5H E = E10.3,5X,7H TAU = E10.3   /     )
0846         934 FORMAT (19H GAMMA EPSILON TEST     )
0847         935 FORMAT (3X,I5,2X,10E10.4)
0848         936 FORMAT (27H0 NEGATIVE DIAGONAL ELEMENT    )
0849         937 FORMAT (/)
0850         938 FORMAT (I2,7E10.3)
0851         940 FORMAT (6H0RMSD=E12.5,6X,6HRMSDL=E12.5,6X,5HI.R.=E12.5)
0852         941 FORMAT (5E16.5)
0853         942 FORMAT (/19H0ADJUSTED FUNCTIONS//5X,10HX=K/(2*KF),5X,12HX=K/(2*PI/
                1A),8X,4HG(X),9X,10HV(X) IN EV,6X,10HE(X) IN EV//)
0854         943 FORMAT ( /15H0K2. K/(2*PI/A),4X,7HTH.EQZ.,6X,8HEXP.EQZ.,6X,6HR-TER
                1M,4X,36HE-TERM/PRED. E-TERM/OBS.    REL.DIFF.,4X,32HEXP.F.     REL.E
                2XP.F.    REL.TH.F.//)
0855         944 FORMAT (//79H0MORE THAN 152 DATA POINTS OR MORE THAN 25 PARAMETERS
                1. COMPUTATION INTERRUPTED.)
0856             END
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0001           SUBROUTINE SUBZ
          C
          C    EINMALIGE VORBEREITUNGEN. BERECHNUNG VON NAEH.WERTEN FUER DIE
          C    PARAMETER B(J),WENN NAPROX=1. REDUZIERUNG DER DISP.KURVEN DURCH
          C    DIE R-TERME.
          C
0002           DIMENSION XA(25),YA(25),W(18)
0003           COMMON PI,QP,KP,CON4,CLB,PIA,CON1,NHSCON,F(150)
0004           COMMON/ALL/P(150,25),B(25),BN(25)
0005           COMMON/SUFP/NBF,KNS(2,61),MAXM(2,61),IK1,IK2,KV1(4),KV2(4),PROZ,NH
              1EAUS,NSH
0006           COMMON/MASUFP/IFSS1,IFSS2,NWAY,NEX,CON2,IWHER,N,KZ(150),XI(150),IE
              1XIT
0007           COMMON/MASU/CON3,FQ(150),FQZ(150),RT(150),YI(150),NGVE,CKF,ZEFF,CK
              1C,WEIGHT(7),NWEIT
0008           COMMON/SUF/IFT,CORREX,QKCKF2
0009           COMMON/SULIN/CM(25,25),CS(25)
          C
0010           NSTEP=0
0011           KNS(1,1)=0
0012           DO 150 L=1,60
0013           IF(L.EQ.14.OR.L.EQ.29.OR.L.EQ.44.OR.L.EQ.53.OR.L.EQ.58)NSTEP=NSTEP
              1+2
0014       150 KNS(1,L+1)=2*L+NSTEP
0015           KP1=KP-1
          C
          C EINLESEN DER DATEN ( MA )
          C
0016           READ (5,3001) (W(I),I=1,18)
0017           READ (5,1000) CMASS,CLATT,CORRF,SCREEN,ZEFF,ETHA
0018           READ (5,1001) NBF,IFT,NWAY,NAPROX,NSR,NHRAUS,NHEAUS,NGVE,NSH
0019           READ (5,1000) CMY,RAMP,PROZ
0020           IF(NAPROX.EQ.0)GO TO 797
0021           READ (5,1000) (XA(L),YA(L),L=1,KP1)
0022       797 CONTINUE
          C
          C    W(I)            UEBERSCHRIFT
          C    CMASS           IONEN-MASSE IN E-24G
          C    CLATT           GITTER-KONSTANTE IN E-8CM
          C    CORRF           =1.0 FREE ELECTRON APPROXIMATION
          C    SCREEN          =1.0 THOMAS-FERMI-SCREENING
          C                    =0.18806 PINES-SCREENING
          C    SCREEN.PARAM.  CKC**2=CKF*(4/PI*A0)*SCREEN    A0=.529172E-8CM
          C    CLATT*CKF=CORRF*(6*ZEFF*PI**2)**0.333333
          C    ZEFF            EFFEKTIVE IONENLADUNG
          C    ETHA            DEF. IN UP. FCD
          C    NBF             =1 FUER BCC, =2 FUER FCC
          C    IFT             DEF. IN UP. FDC
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      C       NWAY           DEF. IM PROGR. PSAF/MAIN
      C       NAPROX         =1 AUS DATENPUNKTEN VON NAEH.KURVEN FUER V(K) WERDEN
      C                      NAEH.WERTE FUER DIE PARAMETER DES MODELLS BERECHNET
      C                      BEI VORGEGEBENEM PARAMETER B(1) ( EXP. DER E-WW ).
      C       NSR,NHRAUS     BERECHNUNG DER R-TERME BIS ZUR NSR-TEN SCHALE UND
      C                      AUSDRUCKEN AB DER NHRAUS-TEN SCHALE
      C                      NSR=0 HEISST RECHNUNG OHNE R-TERME
      C       NSH            BER. DER H-TERME BIS ZUR NSH-TEN SCHALE,
      C                      WENN KEINE SYMM.PUNKTE EINGEGEBEN SIND.
      C                      =0 HEISST, KONV. IST DURCH SYMM.PUNKTE ZU BESTIMMEN
      C       NHEAUS         AUSDRUCKEN DER E-TERME AB DER NHEAUS-TEN H-SCHALE
      C       NGVE           =1 G(K),V(K) UND E(K) WERDEN MIT DEN GEFUNDENEN
      C                      PARAMETERN BERECHNET UND AUSGEDRUCKT.
      C       CMY            EXPONENT DER REPULSIVE WW
      C       RAMP           AMPLITUDE DER REPULSIVE WW
      C       PROZ           WENN DER REL.FEHLER DER E-TERME VON SYMM.PUNKTEN
      C                      ZUEINANDER KLEINER ALS PROZ IST, WIRD DIE H-SUMM.
      C                      DER E-TERME ALS KONVERGENT ABGEBROCHEN.
      C       PRZPRZ         PROGRESSIVE VERGROESSERUNG DER KONVERGENZSCHRANKE
      C                      PROZ AB DER 60. H-SCHALE DURCH ERSETZEN VON PROZ
      C                      DURCH PROZ*(1+PRZPRZ) BEI JEDER NEUEN SCHALE.
      C       XA,YA          DATENPUNKTE EINER NAEH.KURVE FUER V(X) ZUR BERECHN.
      C                      VON NAEH.WERTEN FUER DIE PARAMETER DER POTENZ-REIHE.
      C                      LAMBDA IST IN CL VORZUGEBEN. XA IN K/(2PI/CLATT),
      C                      YA IN EV.
      C
      C BER. VON KONSTANTEN ( MU )
      C
0023          CL=B(1)
0024          CBF=NBF
0025          PI=3.14159
0026          QP=4.*PI
0027          CKF=CORRF/CLATT*(6.*PI**2*ZEFF*CBF)**0.333333
0028          SCRR=0.5*SQRT(PI*0.529172/(CKF*SCREEN))
0029          CKC=1./SCRR
0030          RATIOK=(CKC/CKF)**2
0031          QKCKF2=(CKC/CKF)**2
0032          RZERO=CLATT*(1.5/(QP*ZEFF*CBF))**0.333333
0033          CON1=CLATT**2/(QP*PI*SCRR**2)
0034          CON2=PI/(CLATT*CKF)
0035          CON3=(QP*ZEFF*46.124*CBF)/(1.60206*CLATT**3)
0036          CON4=20000.0*CBF*23.067*ZEFF**2/(PI*CMASS*CLATT**3)
0037          CON5=CON3*SCRR**2
0038          CON6=32041200.0*RAMP/(CMASS*CMY*QP*PI)
0039          EFERMI=1.5*CON5
0040          PIA=2.0*PI/CLATT
0041          IF(NWAY.LE.2)NEX=NWAY
0042          IF(NWAY.GT.2)NEX=NWAY-2
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```
0043           IF(IFT.EQ.3) CORREX=1.0+ETHA*RATIOK
0044           IF(IFT.EQ.4) CORREX=1.0+0.5*RATIOK
      C
      C AUSDRUCKEN
      C
0045           WRITE (6,3002) (W(I),I=1,18)
0046           WRITE (6,2000) CMASS,CLATT,CORRF,SCREEN,ZEFF,CKC,RZERO,SCRR
0047           WRITE (6,2001) NBF,IFT,NWAY,N,KP,NAPROX,NSR,NHRAUS,NHEAUS,NWEIT,NS
              1H
0048           WRITE (6,2002) CMY,RAMP,CKF,EFERMI,ETHA,PROZ
0049           IF(NWEIT.EQ.1) WRITE (6,2004) (WEIGHT(L),L=1,7)
0050           IF(NAPROX.EQ.0) GO TO 130
0051           WRITE (6,2003) (XA(L),YA(L),L=1,KP1)
0052       130 CONTINUE
      C
      C SYMMETRIE-PUNKTE DER X(I) SUCHEN ( MU )
      C
0053           IF(NSH.GT.0) GO TO 807
0054           IK1=0
0055           IK2=0
0056           DO 796 L=1,4
0057           KV1(L)=0
0058       796 KV2(L)=0
0059           GO TO(798,799),NBF
      C
      C FUER BCC-GITTER ( NBF=1)
      C
0060       798 DO 800 L=1,N
0061           X=XI(L)
0062           TV=ABS(X-1.0)
0063           IF(TV.GT.0.001)GO TO 802
0064           K=KZ(L)
0065           IF(K.EQ.1.OR.K.EQ.2.OR.K.EQ.6.OR.K.EQ.7)GO TO 801
0066           GO TO 800
0067       801 IK1=IK1+1
0068           KV1(IK1)=L
0069           GO TO 800
0070       802 TV=ABS(X-0.5)
0071           IF(TV.GT.0.0005)GO TO 800
0072           K=KZ(L)
0073           IF(K.EQ.6.OR.K.EQ.7)GO TO 803
0074           GO TO 800
0075       803 IK2=IK2+1
0076           KV2(IK2)=L
0077       800 CONTINUE
0078           GO TO 805
      C
      C FUER FCC-GITTER ( NBF=2)
```

```
                C
0079              799 DO 810 L=1,N
0080                  TV=ABS(XI(L)-1.0)
0081                  IF(TV.GT.0.001)GO TO 810
0082                  K=KZ(L)
0083                  IF(K.EQ.1.OR.K.EQ.5)GO TO 811
0084                  IF(K.EQ.2.OR.K.EQ.3.OR.K.EQ.4)GO TO 812
0085                  GO TO 810
0086              811 IK1=IK1+1
0087                  KV1(IK1)=L
0088                  GO TO 810
0089              812 IK2=IK2+1
0090                  KV2(IK2)=L
0091              810 CONTINUE
0092              805 IF(IK1.GT.1.OR.IK2.GT.1)GO TO 807
0093                  WRITE (6,1010)
0094                  IF(IESS1.NE.1)GO TO 806
0095                  WRITE (12,1010)
0096              806 IEXIT=1
0097                  RETURN
0098              807 IEXIT=0
                C
                C BER. VON NAEH.WERTEN FUER B(I), WENN NAPROX=1, AUS
                C NAEH.KURVEN FUER V(K) / MA
                C
0099                  IF(NAPROX.EQ.0)GO TO 520
0100                  CKC2=CKC**2
0101                  IF(NWAY.GT.2)AF=PIA/2.0
0102                  IF(NWAY.LE.2)AF=CL*PIA/2.0
0103                  AEX=CL*PIA/2.0
0104                  DO 500 L=1,KP1
0105                  ARG=XA(L)
0106                  ZFG=CON2*ABS(ARG)
0107                  DEN=(PIA*ARG)**2+FDC(ZFG)*CKC2
0108                  EXPO=EXP(-(AEX*ARG)**2)*CON3/DEN
0109                  CS(L)=-YA(L)-EXPO
0110                  CF=(AF*ARG)**NEX
0111                  PF=CF
0112                  DO 510 K=1,KP1
0113                  CM(L,K)=PF*EXPO
0114              510 PF=PF*CF
0115              500 CONTINUE
0116                  RELF=0.01
0117                  CALL LINGLS(KP1,RELF,B)
0118                  DO 505 L=1,KP1
0119                  LK=KP-L
0120              505 B(LK+1)=B(LK)
0121                  B(1)=CL
```

```
      520 CONTINUE
C
C     REDUZIERUNG DER EXP. DISP.KURVEN DURCH DIE R-TERME ( MU )
C
          DO 710 L=1,N
          FQ(L)=FQZ(L)**2
      710 RT(L)=0.0
C
C     BER. DER R-TERME ( MU )
C         NBF=1       BCC-GITTER
C         NBF=2       FCC-GITTER
C
          LF=NBF
          IF(NSR.EQ.0)GO TO 23
          IF(NHRAUS.GT.NSR)GO TO 711
          WRITE (6,9214)
          IF(IFSS1.NE.1)GO TO 711
          WRITE (12,9214)
      711 IF(NSR.GT.60)NSR=60
          IF(LF.EQ.1) LFR=2
          IF(LF.EQ.2) LFR=1
          NSR1=NSR+1
          DO 920 M=2,NSR1
          MR=M-1
          NPT=0
          LIM=MAXM(LFR,M)
          LIM1=LIM+1
          IRAD=KNS(LFR,M)
          LIM2=2*LIM+1
          DO 92 I=1,LIM2,LFR
          IX=I-LIM1
          DO 93 J=1,LIM2,LFR
          IY=J-LIM1
          DO 94 K=1,LIM2,LFR
          IZ=K-LIM1
          I2=IX*IX+IY*IY+IZ*IZ
          IF(I2.NE.IRAD) GO TO 94
          NPT=NPT+1
C
C     EIN R/L DER L-SUMME IST DAMIT BERECHNET
C     ES FOLGT DIE BERECHNUNG DER REPULSIVE-TERME FUER DIESES R/L
C
          R2=I2
          R1=SQRT(R2)
          RX=IX
          RY=IY
          RZ=IZ
          RXX=RX*RX
```

```
      RZZ=RZ*RZ
      RXY=RX*RY
      A2=CLATT/2.0
      P2=PI/2.0
      CR1=1.0/(A2*R1)
      CR2=(1.0/CMY+CR1)/R2
      EX=EXP(-A2*R1/CMY)
      CO1=CR2*RXX-CR1
      CO2=CR2*RZZ-CR1
      CO3=CR2*(RXX+RXY)-CR1
      CO4=CR2*(RXX-RXY)-CR1
      CO5=CR2*(RXX+2.0*RXY)-CR1
      DO 102 L=1,N
      KZZ=KZ(L)
C
C     DIE KENNZEICHEN KZ(L) SIND IM UP. EPCODE DEFINIERT.
C
      X=XI(L)
      IF(KZZ.LE.2) Y=0.0
      IF(KZZ.GT.2) Y=X
      IF(KZZ.LE.5) Z=0.0
      IF(KZZ.GT.5) Z=X
      ES=EX*(SIN(P2*(RX*X+RY*Y+RZ*Z)))**2
      IF(KZZ.EQ.1) RT(L)=RT(L)+ES*CO1*CON6
      IF(KZZ.EQ.2.OR.KZZ.EQ.5) RT(L)=RT(L)+ES*CO2*CON6
      IF(KZZ.EQ.3) RT(L)=RT(L)+ES*CO3*CON6
      IF(KZZ.EQ.4.OR.KZZ.EQ.7) RT(L)=RT(L)+ES*CO4*CON6
      IF(KZZ.EQ.6) RT(L)=RT(L)+ES*CO5*CON6
  102 CONTINUE
   94 CONTINUE
   93 CONTINUE
   92 CONTINUE
      IF(NR.LT.NHRAUS) GO TO 920
      WRITE (6,9212) NR,NPT,(RT(LR),LR=1,N)
      IF(IFSS1.NE.1)GO TO 920
      WRITE (12,9212) NR,NPT,(RT(LR),LR=1,N)
  920 CONTINUE
   23 CONTINUE
C
      DO 120 L=1,N
  120 YI(L)=EQ(L)-RT(L)
C
      RETURN
C
 1000 FORMAT (6E12.5)
 1001 FORMAT (9I6)
 1010 FORMAT (///85H1NO SYM.POINTS IN DATA, H-CONVERGENCY-TEST NOT POSSI
     1BLE, COMPUTATION INTERRUPTED.      )
```

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0199      2000 FORMAT (////16H0METAL CONSTANTS///9X,11HMASS(E-24G),3X,12HLATTC(E-
              18CM),4X,10HCORP-FERMI,4X,13HSCREEN.COEFF.,3X,11HZ-EFFECTIVE,2X,14H
              2K-SCR.(E+8/CM),2X,13HR-ZERO(E-8CM),1X,15HSCR.RAD.(E-8CM)//5X,8E15.
              35)
0200      2001 FORMAT (//33H0MODEL AND COMPUTATION PARAMETERS//7X,4HNBF=I2,3X,4HI
              1FT=I2,3X,5HNWAY=I2,3X,7HN-DATA=I4,3X,7HK-PAR.=I3,3X,8HN-APPR.=I2,3
              2X,4HNSR=I3,3X,7HNHRAUS=I3,3X,7HNHEAUS=I3,3X,6HNWEIT=I2,3X,4HNSH=I3
              3)
0201      2002 FORMAT (//9X,9HMY(E-8CM),6X,11HA-REP.(KEV),3X,15HK-FERMI(E+8/CM),3
              1X,11HE-FERMI(EV),8X,4HETHA,11X,7HPERCENT//3X,6E16.5)
0202      2003 FORMAT (///34H0DATA-POINTS OF APPROX. V(K)-CURVE  //7X,12HX=K/(2*P
              1I/A),5X,10HV(X) IN EV//(3X,2E16.5))
0203      2004 FORMAT (//53H0WEIGHTS OF THE 7 BRANCHES OF THE DISPERSION CURVES
              1  //5X,7E15.5)
0204      3001 FORMAT (18A4)
0205      3002 FORMAT (1H1,18A4)
0206      9212 FORMAT (//I5,I9,2X,8E14.5,/,(16X,8E14.5))
0207      9214 FORMAT (57H1L-SHELL  POINTS  R-TERMS INCLUSIVE CORRESPONDENT L-SHE
              1LL///)
0208           END
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```
0001                SUBROUTINE FPCODE
              C
              C     ZU VOR GEGEBENEN DATEN-PUNKTEN X(I),Y(I) UND PARAMETERN B(J)
              C     WERDEN ENTSPRECHEND DEM IN MAIN ANGEGEBENEN MODELL DIE
              C     FUNKTIONSWERTE F(I) (=E-TERME DER DISP.KURVEN) BERECHNET.DIE
              C     ABLEITUNGEN P(I,J)=DF(I)/DB(J) DAZU NUR, WENN IFSS2=0 ODER
              C     IWHER=1.
              C
0002                DIMENSION PRH(25),PRQH(25),PRQHSP(40,25)
0003                DIMENSION QHSP(40),FSPSP(40),HPX(300),HPY(300),HPZ(300)
0004                COMMON PI,QP,KP,CON4,CLB,PIA,CON1,NHSCON,F(150)
0005                COMMON/ALL/P(150,25),B(25),BN(25)
0006                COMMON/SUFP/NBF,KNS(2,61),MAXM(2,61),IK1,IK2,KV1(4),KV2(4),PROZ,NH
                   1EAUS,NSH
0007                COMMON/MASUFP/IFSS1,IFSS2,NWAY,NEX,CON2,IWHER,N,KZ(150),XI(150),IE
                   1XIT
              C
              C VORBEREITUNGEN ( MA )
              C
0008                IF(IFSS2.EQ.1.OR.IWHER.NE.1)NZW=1
0009                IF(IFSS2.EQ.0.AND.IWHER.EQ.1.AND.NWAY.LE.2)NZW=2
0010                IF(IFSS2.EQ.0.AND.IWHER.EQ.1.AND.NWAY.GT.2)NZW=3
              C
              C          NZW=1 NUR F(L)
              C          NZW=2 F(I) UND P(I,J),POT.REIHE LAMBDA-ABHAENGIG
              C          NZW=3 F(I) UND P(I,J),POT.REIHE NICHT VON LAMBDA ABH.
              C
0011                CNEX=NEX
0012                IF(KP.EQ.1) GO TO 217
0013                GO TO(215,216,217),NZW
0014            216 DO 214 KL=2,KP
0015                CKL=KL-1
0016            214 BN(KL)=CKL*B(KL)
0017                GO TO 217
0018            215 NEND=(KP-1)/2+1
0019                DO 218 KL=2,NEND
0020                I=KP+2-KL
0021                ZS1=B(I)
0022                B(I)=B(KL)
0023            218 B(KL)=ZS1
0024            217 CONTINUE
0025                DO 212 L=1,N
0026            212 F(L)=0.0
0027                IF(NZW.EQ.1)GO TO 213
0028                DO 211 L=1,N
0029                DO 211 K=1,KP
0030            211 P(L,K)=0.0
0031            213 CONTINUE
```

```
              CL=B(1)
              CLB=CL*PIA/2.C
C
C BERECHNUNG DER H-SUMMEN / L=H-SCHALEN-INDEX ( MU )
C
              KNP=0
              N1=3
              N2=1
              N3=4
              LF=NBF
              L=1
  220         CONTINUE
C
C SUCHEN DER H-PUNKTE ZUR L-TEN H-SCHALE ( MU )
C DIE H-PUNKTE WERDEN IN HPX(300), HPY(300), HPZ(300) GESPEICHERT.
C
              LIM=MAXM(LF,L)
              IRAD=KNS(LF,L)
  342         LIM1=LIM+1
              LIM2=2*LIM+1
              NPT=C
              DO 1 I=1,LIM2,LF
              IX=I-LIM1
              DO 1 J=1,LIM2,LF
              IY=J-LIM1
              DO 1 K=1,LIM2,LF
              IZ=K-LIM1
              I2=IX*IX+IY*IY+IZ*IZ
              IF(I2.NE.IRAD) GO TO 1
              NPT=NPT+1
              IF(NPT.GT.300) GO TO 350
              HPX(NPT)=IX
              HPY(NPT)=IY
              HPZ(NPT)=IZ
    1         CONTINUE
              IF(L.GT.1.AND.NPT.EQ.0) GO TO 341
C
C ALLE H-PUNKTE DER L-TEN H-SCHALE GEFUNDEN
C    BER. VON U(H) UND DU(H)/DB (NUR VOM BETRAGC VON H ABH.) FUER DIE
C L-TE H-SCHALE ( MA ). U(H) IST DIE FOURIER-TR. DES LOK. PSEUDO-ATOM
C -POTENTIALS.
C
              H2=IRAD
              H1=SQRT(H2)
              T2=CON2*H1
              CALL MODEL(H1,NWAY,NEX,NZW,PRH,FSP2,T2)
C
C U(H) IN FSP2, DU(H)/DB IN PRH.
```

```
                C BER. F UND P ZU DER L-TEN H-SCHALE
                C ZUERST MODELL-UNABH. FAKTOREN ( MU ).
                C LN=INDEX DER DATEN PUNKTE.
                C
0065                  DO 100 LN=1,N
0066                  KZZ=KZ(LN)
0067                  X=XI(LN)
0068                  IF(KZZ.LE.2)Y=0.0
0069                  IF(KZZ.GT.2)Y=X
0070                  IF(KZZ.LE.5)Z=0.0
0071                  IF(KZZ.GT.5)Z=X
0072                  NZZ=0
0073                  DO 2 LH=1,NPT
0074                  HX=HPX(LH)
0075                  HY=HPY(LH)
0076                  HZ=HPZ(LH)
0077                  QH2=(HX+X)**2+(HY+Y)**2+(HZ+Z)**2
0078                  QH=SQRT(QH2)
0079                  T1=CON2*QH
                C
                C DIE KENNZEICHEN KZ GEBEN AN,VON WELCHEM ZWEIG DER DISPERSIONSKURVE DIE
                C MESS DATEN XI,YI,ZI UND FQ KOMMEN.
                C R=RICHTUNG, L=LONGITUDINAL, T=TRANSVERSAL, (I,J)=ELEM. DER DYN. MATRIX
                C
                C     KZ=1   R(1,0,0)   L    FQ=FQZ**2=(X,X)
                C     KZ=2   R(1,0,0)   T    FQ=FQZ**2=(Y,Y)=(Z,Z)
                C     KZ=3   R(1,1,0)   L    FQ=FQZ**2=(X,X)+(X,Y)
                C     KZ=4   R(1,1,0)   T1   FQ=FQZ**2=(X,X)-(X,Y)
                C     KZ=5   R(1,1,0)   T2   FQ=FQZ**2=(Z,Z)
                C     KZ=6   R(1,1,1)   L    FQ=FQZ**2=(X,X)+2(X,Y)
                C     KZ=7   R(1,1,1)   T    FQ=FQZ**2=(X,X)-(X,Y)
                C
0080                  GO TO (201,202,203,204,202,205,204),KZZ
0081              201 Z1=(X+HX)*(X+HX)
0082                  Z2=HX*HX
0083                  GO TO 210
0084              202 Z1=(Z+HZ)*(Z+HZ)
0085                  Z2=HZ*HZ
0086                  GO TO 210
0087              203 Z1=(X+HX)*((X+HX)+Y+HY)
0088                  Z2=HX*(HX+HY)
0089                  GO TO 210
0090              204 Z1=(X+HX)*((X+HX)-Y-HY)
0091                  Z2=HX*(HX-HY)
0092                  GO TO 210
0093              205 Z1=(X+HX)*((X+HX)+2.*(Y+HY))
0094                  Z2=HX*(HX+2.*HY)
0095              210 CONTINUE
```

```
C
C  JETZT MODELL-UND NUR VOM BETRAG (Q+H)-ABH. FACTOREN ( MA )
C
          IF(NZZ.EQ.0) GO TO 150
          DO 152 LZ=1,NZZ
          IF(QH.EQ.QHSP(LZ)) GO TO 155
  152     CONTINUE
  150     CALL MODEL(QH,NWAY,NEX,NZW,PRQH,FSP1,T1)
          NZZ=NZZ+1
          IF(NZZ.GT.40) GO TO 351
          QHSP(NZZ)=QH
          FSPSP(NZZ)=FSP1
          IF(NZW.EQ.1) GO TO 270
          DO 153 LL=1,KP
  153     PRQHSP(NZZ,LL)=PRQH(LL)
          GO TO 157
  155     FSP1=FSPSP(LZ)
          IF(NZW.EQ.1) GO TO 270
          DO 156 LL=1,KP
  156     PRQH(LL)=PRQHSP(LZ,LL)
C
C  BER. DER F(I) UND P(I,J)
C
  157     CONTINUE
          DO 275 KL=1,KP
  275     P(LN,KL)=P(LN,KL)+CON4*(Z1*PRQH(KL)-Z2*PRH(KL))
  270     F(LN)=F(LN)+CON4*(Z1*FSP1-Z2*FSP2)
    2     CONTINUE
  100     CONTINUE
C
C  F UND P BIS EINSCHL. L-TE H-SCHALE GERECHNET.
C  AUSDRUCKEN DER F ( MU )
C
          L1=L-1
          IF(L1.LT.NHEAUS) GO TO 20
          IF(KNP.EQ.1)GO TO 21
          KNP=1
          WRITE (6,2213)
          IF(IFSS1.NE.1)GO TO 21
          WRITE (12,2213)
   21     WRITE (6,2212) L1,NPT,(F(IL),IL=1,N)
          IF(IFSS1.NE.1)GO TO 20
          WRITE (12,2212)L1,NPT,(F(IL),IL=1,N)
   20     CONTINUE
C
C  KONVERGENZ-ABFRAGE DER H-SUMMIERUNG ( MU )
C
          IF(NSH.GT.0) GO TO 304
```

```
      IF(IK1.LE.1)GO TO 310
      CIK1=IK1
      S=0.0
      DO 300 I=1,IK1
      M=KV1(I)
  300 S=S+F(M)
      S=S/CIK1
      DO 301 I=1,IK1
      M=KV1(I)
      RDF=ABS((F(M)-S)/S)
      IF(RDF.GT.PROZ)GO TO 320
  301 CONTINUE
      IF(IK2.LE.1)GO TO 330
  310 CIK2=IK2
      S=0.0
      DO 302 I=1,IK2
      M=KV2(I)
  302 S=S+F(M)
      S=S/CIK2
      DO 303 I=1,IK2
      M=KV2(I)
      RDF=ABS((F(M)-S)/S)
      IF(RDF.GT.PROZ)GO TO 320
  303 CONTINUE
      GO TO 330
  304 IF(L.GT.NSH) GO TO 330
C
C H-SUMME NOCH NICHT KONVERGENT. NEUE H-SCHALE ( MU ).
C
  320 L=L+1
      IF(L.GE.62)GO TO 341
      GO TO 220
  341 LF=1
      GO TO (343,344),NBF
  343 IRAD=IRAD+2
      CIRAD=IRAD
      CLIM=SQRT(CIRAD)
      LIM=CLIM
      GO TO 342
  344 IRAD=IRAD+N1
      CIRAD=IRAD
      CLIM=SQRT(CIRAD)
      LIM=CLIM
      NSPI=N1
      N1=N2
      N2=N3
      N3=NSPI
      GO TO 342
```

```
      C
      C H-SUMME KONVERGENT
      C
        330 NHSCON=L1
            IF(NZH.GT.1.OR.KP.LE.2) GO TO 340
            DO 335 KL=2,NEND
            I=KP+2-KL
            ZS1=B(I)
            B(I)=B(KL)
        335 B(KL)=ZS1
        340 CONTINUE
            RETURN
        350 L1=L-1
            IEXIT=1
            WRITE (6,2216) L1
            RETURN
        351 L1=L-1
            IEXIT=1
            WRITE (6,2217) L1
            RETURN
       2212 FORMAT (/I5,I9,2X,8E14.5,/,(16X,8E14.5))
       2213 FORMAT (59H1H-SHELL  POINTS  E+C-TERMS INCLUSIVE CORRESPONDENT H-S
           1HELL/)
       2215 FORMAT (55H1E-TERMS OF H-SUMMATION NOT CONVERGENT WITH 60 H-SHELLS
           1)
       2216 FORMAT (5H1THE I3,43H. H-SHELL CONTAINS MORE THAN 300 H-POINTS.   ,
           152H(DIMENSION OF HPX, HPY AND HPZ MUST BE INCREASED.    )
       2217 FORMAT (1H1,I3,80H. H-SHELL / DIMENSION OF WORKING STORAGES PRQHSP
           1, QHSP AND FSPSP TOO SMALL.             )
            END
```

```
0001           SUBROUTINE GJR(A,N,EPS,MSING)
      C
      C        GAUSS-JORDAN-RUTISHAUSER MATRIX INVERSION WITH DOUBLE PIVOTING.
      C
0002           DIMENSION A(25,26),B(25),C(25),P(25),Q(25)
0003           INTEGER P,Q
      C
0004           MSING=1
0005           DO 10 K=1,N
      C        DETERMINATION OF THE PIVOT ELEMENT
0006           PIVOT=0.
0007           DO 20 I=K,N
0008           DO 20 J=K,N
0009           IF(ABS(A(I,J))-ABS(PIVOT))20,20,30
0010        30 PIVOT=A(I,J)
0011           P(K)=I
0012           Q(K)=J
0013        20 CONTINUE
0014           IF(ABS(PIVOT)-EPS)40,40,50
      C        EXCHANGE OF THE PIVOTAL ROW WITH THE KTH ROW
0015        50 IF(P(K)-K)60,80,60
0016        60 DO 70 J=1,N
0017           L=P(K)
0018           Z=A(L,J)
0019           A(L,J)=A(K,J)
0020        70 A(K,J)=Z
      C        EXCHANGE OF THE PIVOTAL COLUMN WITH THE KTH COLUMN
0021        80 IF(Q(K)-K)85,90,85
0022        85 DO 100 I=1,N
0023           L=Q(K)
0024           Z=A(I,L)
0025           A(I,L)=A(I,K)
0026       100 A(I,K)=Z
0027       90  CONTINUE
      C        JORDAN STEP
0028           DO 110 J=1,N
0029           IF(J-K)130,120,130
0030       120 B(J)=1./PIVOT
0031           C(J)=1.
0032           GO TO 140
0033       130 B(J)=-A(K,J)/PIVOT
0034           C(J)=A(J,K)
0035       140 A(K,J)=0.
0036       110 A(J,K)=0.
0037           DO 10 I=1,N
0038           DO 10 J=1,N
0039        10 A(I,J)=A(I,J)+C(I)*B(J)
      C        REORDERING THE MATRIX
```

```
      DO 155 M=1,N
      K=N-M+1
      IF(P(K)-K)160,170,160
  160 DO 180  I=1,N
      L=P(K)
      Z=A(I,L)
      A(I,L)=A(I,K)
  180 A(I,K)=Z
  170 IF(Q(K)-K)190,155,190
  190 DO 150  J=1,N
      L=Q(K)
      Z=A(L,J)
      A(L,J)=A(K,J)
  150 A(K,J)=Z
 155  CONTINUE
  151 RETURN
   40 WRITE (6,45) P(K),Q(K),PIVOT
   45 FORMAT(16H0SINGULAR MATRIX3H I=I3,3H J=I3,7H PIVOT=E16.8/)
      NSING=2
      GO TO 151
      END
```

```
      SUBROUTINE MODEL(X,NWAY,NEX,NZW,PRX,FSP,T)
C
C    COMPUTES THE FOURIER TRANSFORM FSP OF THE MODEL POTENTIAL
C    AND, IF NZW=2 OR 3, ITS DERIVATIVES PRX WITH RESPECT
C    TO THE MODEL PARAMETERS.
C
      DIMENSION PRX(25)
      COMMON PI,QP,KP,CON4,CLB,PIA,CON1,NHSCON,F(150)
      COMMON/ALL/P(150,25),B(25),BN(25)
C
      CNEX=NEX
      X2=X*X
      DEN=X2+CON1*FDC(T)
      CLBX2=X2*CLB*CLB
      EXX2=EXP(-2.0*CLBX2)
      IF(KP.EQ.1) GO TO (100,200,200),NZW
      IF(NWAY.GT.2)AX=(PIA*X/2.0)**NEX
      IF(NWAY.LE.2)AX=(CLB*X)**NEX
      S1=0.0
      S2=0.0
      PRX(1)=0.0
      GO TO(1,2,3),NZW
    1 DO 10 KL=2,KP
   10 S1=(S1+B(KL))*AX
      S1=1.0+S1
      GO TO 50
    2 CX=AX
      DO 20 KL=2,KP
      PRX(KL)=CX
      S1=S1+B(KL)*CX
      S2=S2+BN(KL)*CX
   20 CX=CX*AX
      S1=1.0+S1
      PRX(1)=CNEX*S2
      GO TO 60
    3 CX=AX
      DO 30 KL=2,KP
      PRX(KL)=CX
      S1=S1+B(KL)*CX
   30 CX=CX*AX
      S1=1.0+S1
   60 PRX(1)=(PRX(1)-2.0*CLBX2*S1)*S1*EXX2*2.0/(B(1)*DEN)
      SEX=2.0*EXX2*S1/DEN
      DO 70 KL=2,KP
   70 PRX(KL)=PRX(KL)*SEX
   50 FSP=EXX2*S1*S1/DEN
      RETURN
  200 PRX(1)=-4.0*CLBX2*EXX2/(B(1)*DEN)
```

```
        100 FSP=EXX2/DEN
            RETURN
            END
```

```
0001                 FUNCTION FDC(T)
               C
               C     CALCULATION OF A SCREENING FUNCTION.
               C
               C        IFT=1  K-INDEP. SCREENING
               C        IFT=2  K-DEP.  SCREEN., HARTREE-APPR., NO EXCHANGE
               C        IFT=3  AS 2, BUT WITH EXCHANGE, GENERAL FORMULA
               C        IFT=4  AS 3, BUT SPECIAL EXCHANGE ACCORDING TO HUBBARD
               C        IFT=5  AS 3, BUT SPECIAL EXCHANGE ACCORDING TO HARRISON
               C        IFT=6  EFFECTIVE FDC WITH GENERAL EXCHANGE TERM
               C        IFT=7  EFFECTIVE FDC WITH EXCHANGE ACCORDING TO HARRISON
               C
               C     CORREX=1+ETHA*(KC/KF)**2 MUST BE COMPUTED IN THE CALLING PROGRAM
               C     FOR CASES 4 ( ETHA=0.5) AND 3 ( DESIRED VALUE OF ETHA), IT DOES
               C     NOT APPLY FOR IFT=1,2 AND 5. WHERE USED THE MEANING OF ETHA IS
               C
               C        ETHA=(KS/KC)**2, KC=SCREEN.PARAM. FOR THE HARTREE-APPROX.
               C                         KS=SCREEN.PARAM. FOR THE EXCHANGE CORRECTION.
               C
0002                 COMMON/SUF/IFT,CORREX,QKCKF2
               C
0003                 IF(IFT.EQ.1.OR.T.EQ.0.0) GO TO 1
0004                 IF(T.EQ.1.0) GO TO 2
0005                 AB=ABS((1.0+T)/(1.0-T))
0006                 TT=T**2
0007                 FDC=0.5+(1.0-TT)*ALOG(AB)/(4.0*T)                          IFT=2
0008               3 GO TO (4,4,5,5,6,7,8),IFT
0009               5 FDC=FDC*(1.0-2.0*TT/(4.0*TT+CORREX))                       IFT=3,4
0010                 RETURN
0011               6 FDC=FDC*(1.0-3.0*TT/(2.0+6.0*TT))                          IFT=5
0012                 RETURN
0013               7 FDC=FDC/(1.-(.5*QKCKF2*FDC)/(4.*TT+CORREX))                IFT=6
0014                 RETURN
0015               8 FDC=FDC/(1.-(3.0*QKCKF2*FDC/8.0)/(1.0+3.0*TT))             IFT=7
0016                 RETURN
0017               1 FDC=1.0                                                     IFT=1
0018                 IF(IFT.LE.5)RETURN
0019                 TT=0.0
0020                 GO TO 3
0021               4 RETURN
0022               2 FDC=0.5
0023                 TT=1.0
0024                 GO TO 3
0025                 END
```

```
            SUBROUTINE LINGLS(IG,RELF,B)
      C
      C     LOESUNG EINES INHOMOG. LIN. GLEICH.-SYSTEMS CM*B=C.
      C SCHRITTWEISE VERBESSERUNG DER LOESUNGEN B BIS DER PFL. RUNDUNGS-
      C FEHLER DER KONST.SPALTE C KLEINER ALS RELF IST.
      C IG=ZAHL DER GLEICHUNGEN BZW. UNBEKANNTEN (MAXIMAL 25).
      C
            DIMENSION SNR(25,26),ST(25,25),B(25),AN(25),RF(25),CP(25),KZU(25)
            COMMON/SULIN/CM(25,25),C(25)
      C
            IF(IG.GE.2) GO TO 700
            B(1)=C(1)/CM(1,1)
            RETURN
      C
        700 DO 800 K=1,IG
            B(K)=0.0
            KZU(K)=K
            DO 800 L=1,IG
        800 ST(K,L)=0.0
      C
      C UEBERTRAGUNG DER MATRIZEN CM UND C  IN SPEICHER SNR
      C
            IL=IG-1
            IG1=IG+1
            DO 400 I=1,IG
            DO 401 J=1,IG
        401 SNR(I,J)=CM(I,J)
        400 SNR(I,IG1)=C(I)
            WRITE (6,4999)                                                  TEST
       4999 FORMAT (1H1)                                                    TEST
            DO 6000 I=1,IG                                                  TEST
       6000 WRITE (6,5000) (SNR(I,K),K=1,IG1)                               TEST
       5000 FORMAT (10E12.5)                                                TEST
      C
      C GAUSS-SCHER ALGORITHMUS
      C
            DO 410 I=1,IL
      C
      C SUCHEN DES GROESSTEN ELEMENTES DER I-TEN SPALTE
      C
            NM=I
            DO 411 L=I,IL
            IF(ABS(SNR(L+1,I)).LE.ABS(SNR(NM,I)))GO TO 411
            NM=L+1
        411 CONTINUE
            IF(NM.EQ.I)GO TO 414
      C
      C UMSTELLUNG DER GLEICHUNGEN/DIE UMSTELLUNG WIRD IN KZU REGISTRIERT
```

```
                C
0030                  KZUSP=KZU(I)
0031                  KZU(I)=KZU(NM)
0032                  KZU(NM)=KZUSP
0033                  DO 412 L=I,IG1
0034                  SPEI=SNR(I,L)
0035                  SNR(I,L)=SNR(NM,L)
0036              412 SNR(NM,L)=SPEI
                C
                C REDUKTION DER NORMALGLEICHUNGEN NACH GAUSS
                C
0037              414 DO 415 J=I,IG
0038                  ST(J,I)=SNR(J,I)
0039              415 SNR(I,J)=SNR(I,J)/ST(I,I)
0040                  SNR(I,IG1)=SNR(I,IG1)/ST(I,I)
0041                  IGI=IG-I
0042                  I1=I+1
0043                  DO 410 K=1,IGI
0044                  IK=I+K
0045                  DO 410 J=I1,IG1
0046              410 SNR(IK,J)=SNR(IK,J)-SNR(I,J)*ST(IK,I)
0047                  DO 6001 I=1,IG                                       TEST
0048             6001 WRITE (6,5000) (SNR(I,K),K=1,IG1)                    TEST
0049                  DO 6002 I=1,IG                                       TEST
0050             6002 WRITE (6,5001) KZU(I),(ST(I,K),K=1,IG)               TEST
0051             5001 FORMAT (/I6,9E12.5/(6X,9E12.5))                      TEST
                C
                C BERECHNUNG DER LOESUNGEN
                C
0052              450 AN(IG)=SNR(IG,IG1)/SNR(IG,IG)
0053                  DO 500 L=1,IL
0054                  IGL=IG-L
0055                  AN(IGL)=SNR(IGL,IG1)
0056                  KL=IG1-L
0057                  DO 500 K=KL,IG
0058              500 AN(IGL)=AN(IGL)-SNR(IGL,K)*AN(K)
                C
                C BERECHNUNG DER KORRIGIERTEN LOESUNGEN
                C
0059                  DO 510 L=1,IG
0060              510 B(L)=B(L)+AN(L)
                C
                C BERECHNUNG DER RUNDUNGSFEHLER RF=C-CM*B
                C
0061                  NZ=0
0062                  DO 600 K=1,IG
0063                  RF(K)=C(K)
0064                  CP(K)=C(K)*RELF
```

```
0065            DO 601 L=1,IG
0066        601 RF(K)=RF(K)-CM(K,L)*B(L)
0067            IF(ABS(CP(K)).LT.ABS(RF(K)))NZ=NZ+1
0068        600 CONTINUE
0069            WRITE (6,5003) (SNR(L,IG1),AN(L),B(L),RF(L),CP(L),L=1,IG)        TEST
0070       5003 FORMAT (//,(5E12.5))                                               TEST
0071            IF(NZ.EQ.0)RETURN
          C
          C RUNDUNGSFEHLER ZU GROSS.BERECHNUNG VON KORREKTUREN.DAZU MUSS DIE
          C KONSTANTENSPALTE SNR(*,IG1) DER REDUZIERTEN NORMALGLEICHUNGEN
          C MITTELS DER RF NEU GEBILDET WERDEN.
          C UEBERTRAGEN DER RF ENTSPRECHEND KZU NACH SNR(*,IG1).
          C
0072            DO 605 L=1,IG
0073            MK=KZU(L)
0074        605 SNR(L,IG1)=RF(MK)
0075            WRITE (6,5004) (SNR(L,IG1),L=1,IG)                                TEST
0076       5004 FORMAT (//,(4E12.5))                                               TEST
          C
          C GAUSS-ALGORITHMUS FUR SNR(*,IG1)
          C
0077            DO 610 I=1,IL
0078            SNR(I,IG1)=SNR(I,IG1)/ST(I,I)
0079            IGI=IG-I
0080            DO 610 K=1,IGI
0081            IK=I+K
0082        610 SNR(IK,IG1)=SNR(IK,IG1)-SNR(I,IG1)*ST(IK,I)
0083            GO TO 450
0084            END
```

```
 0001            BLOCK DATA
          C
 0002            COMMON/SUFP/NBF,KNS(2,61),MAXM(2,61),IK1,IK2,KV1(4),KV2(4),PROZ,NH
                1EAUS
          C
 0003            DATA MAXM(1,1),MAXM(1,2),MAXM(1,3),MAXM(1,4),MAXM(1,5),MAXM(1,6),M
                1AXM(1,7),MAXM(1,8),MAXM(1,9),MAXM(1,10),MAXM(1,11),MAXM(1,12),MAXM
                2(1,13),MAXM(1,14),MAXM(1,15),MAXM(1,16),MAXM(1,17),MAXM(1,18),MAXM
                3(1,19),MAXM(1,20),MAXM(1,21),MAXM(1,22),MAXM(1,23),MAXM(1,24),MAXM
                4(1,25),MAXM(1,26),MAXM(1,27),MAXM(1,28),MAXM(1,29),MAXM(1,30),MAXM
                5(1,31),MAXM(1,32),MAXM(1,33),MAXM(1,34),MAXM(1,35),MAXM(1,36),MAXM
                6(1,37),MAXM(1,38),MAXM(1,39),MAXM(1,40),MAXM(1,41),MAXM(1,42),MAXM
                7(1,43),MAXM(1,44),MAXM(1,45),MAXM(1,46),MAXM(1,47),MAXM(1,48),MAXM
                8(1,49),MAXM(1,50),MAXM(1,51),MAXM(1,52),MAXM(1,53),MAXM(1,54),MAXM
                9(1,55),MAXM(1,56),MAXM(1,57),MAXM(1,58),MAXM(1,59),MAXM(1,60),MAXM
                A(1,61)/0,1,2,2,2,3,2,3,4,4,4,3,4,5,5,4,5,6,6,6,5,6,6,4,7,6,7,6,7,7
                B,8,8,8,6,8,8,6,7,8,9,8,9,6,9,9,8,9,10,10,10,9,10,10,8,10,10,10,11,
                C11,8,11/,MAXM(2,1),MAXM(2,2),MAXM(2,3),MAXM(2,4),MAXM(2,5),MAXM(2,
                D6),MAXM(2,7),MAXM(2,8),MAXM(2,9),MAXM(2,10),MAXM(2,11),MAXM(2,12),
                EMAXM(2,13),MAXM(2,14),MAXM(2,15),MAXM(2,16),MAXM(2,17),MAXM(2,18),
                FMAXM(2,19),MAXM(2,20),MAXM(2,21),MAXM(2,22),MAXM(2,23),MAXM(2,24),
                GMAXM(2,25),MAXM(2,26),MAXM(2,27),MAXM(2,28),MAXM(2,29),MAXM(2,30),
                HMAXM(2,31),MAXM(2,32),MAXM(2,33),MAXM(2,34),MAXM(2,35),MAXM(2,36),
                IMAXM(2,37),MAXM(2,38),MAXM(2,39),MAXM(2,40),MAXM(2,41),MAXM(2,42),
                JMAXM(2,43),MAXM(2,44),MAXM(2,45),MAXM(2,46),MAXM(2,47),MAXM(2,48),
                KMAXM(2,49),MAXM(2,50),MAXM(2,51),MAXM(2,52),MAXM(2,53),MAXM(2,54),
                LMAXM(2,55),MAXM(2,56),MAXM(2,57),MAXM(2,58),MAXM(2,59),MAXM(2,60),
                MMAXM(2,61)/0,1,2,2,3,2,4,3,4,4,5,4,5,6,6,5,6,4,7,6,6,7,8,7,8,8,7,6
                N,8,9,8,6,9,8,9,10,10,9,10,9,10,10,11,8,11,10,10,11,10,12,11,12,12,
                O11,12,9,12,10,13,10,12/,KNS(2,1),KNS(2,2),KNS(2,3),KNS(2,4),KNS(2,
                P5),KNS(2,6),KNS(2,7),KNS(2,8),KNS(2,9),KNS(2,10),KNS(2,11),KNS(2,1
                Q2),KNS(2,13),KNS(2,14),KNS(2,15),KNS(2,16),KNS(2,17),KNS(2,18),KNS
                R(2,19),KNS(2,20),KNS(2,21),KNS(2,22),KNS(2,23),KNS(2,24),KNS(2,25)
                S,KNS(2,26),KNS(2,27),KNS(2,28),KNS(2,29),KNS(2,30),KNS(2,31),KNS(2
                T,32),KNS(2,33),KNS(2,34),KNS(2,35),KNS(2,36),KNS(2,37),KNS(2,38),K
                UNS(2,39),KNS(2,40),KNS(2,41),KNS(2,42),KNS(2,43),KNS(2,44),KNS(2,4
                V5),KNS(2,46),KNS(2,47),KNS(2,48),KNS(2,49),KNS(2,50),KNS(2,51),KNS
                W(2,52),KNS(2,53),KNS(2,54),KNS(2,55),KNS(2,56),KNS(2,57),KNS(2,58)
                X,KNS(2,59),KNS(2,60),KNS(2,61)/0,3,4,8,11,12,16,19,20,24,27,32,35,
                Y36,40,43,44,48,51,52,56,59,64,67,68,72,75,76,80,83,84,88,91,96,99,
                Z100,104,107,108,115,116,120,123,128,131,132,136,139,140,144,147,14
                *8,152,155,160,163,164,168,171,172,176/
          C
 0004            END
```

```
0001              SUBROUTINE SSWTCH(N,IFSSN)
            C
0002              RETURN
            C
0003              END
```

```
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
ROOM 121   ***HASP***HASP***HASP**   ooEND  JOB   59   ROOM 121   -KREBS   5   **HASP***HASP***HASP***HASP***HASP*
```

APPENDIX II - P R O G R A M SKFD

```
            C
            C
            C      PROGRAM SKFD (STRUCTURE FACTOR AND FREQUENCY DISTRIBUTION)
            C
            C      SKFD IS AN EXTENSION OF A PROGRAM - GNU, ORNL-TM 1425 BY
            C      L.J.RAUBENHEIMER AND G.GILAT ( CALCULATION OF FREQUENCY-
            C      DISTRIBUTION FUNCTIONS OF CUBIC CRYSTALS ) - TO CALCULATE ALSO
            C      THE STRUCTURE-FACTOR S(K) AVERAGED OVER ALL DIRECTIONS FOR FIXED
            C      K AND THE ELECTRICAL RESISTIVITY.
            C      SKFD IS RESTRICTED TO BCC AND FCC CRYSTALS AND WRITTEN IN
            C      FORTRAN 4 LANGUAGE.
            C
            C      MODEL FORM FACTOR USED FOR THE DESCRIPTION OF THE CRYSTAL PHONONS
            C      G(X)=EXP(-(B1*X/2)**2)*(1+B2*T+.....BK*T**(K-1))
            C
            C          NWAY=1    T=B1*X/2
            C          NWAY=2    T=(B1*X/2)**2
            C          NWAY=3    T=X/2
            C          NWAY=4    T=(X/2)**2
            C
            C      X IS THE PHONON WAVE VECTOR, BI=B(I) ARE THE PARAMETERS (MAX. 25)
            C                                                                          2
 0001              DIMENSION CTC(3103)
 0002              DIMENSION AL(3),Q(3),V(3),GD1(3),GD2(3),GD3(3),PX(60)
 0003              DIMENSION AMAS(12)                                                  5
 0004              DIMENSION EV(3,3)
 0005              DIMENSION MAXM(2,61),KNS(2,61)
 0006              DIMENSION ITB(33),JTB(33),KTB(33),ITF(33),JTF(33),KTF(33)
            C
 0007              COMMON/C2/AMM
 0008              COMMON/C3/PI,CPT,PX,GU,SC,NSF3,AMAS,DQ
 0009              COMMON/C4/EV,V
 0010              COMMON/C5/CTA(3000),LA,DVA,AHALF,VOLUME,ASQ,NPRINT,XM
 0011              COMMON/C6/KM,KK,I,J,K
 0012              COMMON/C7/NNN
 0013              COMMON/MAELGN/NSH1,CLB2,CLB,KP,NWAY,PIA2,CON1,CON2,CON4,SUS,NEX,B(
                  125),NPPS(60),HPX(3103),HPY(3103),HPZ(3103),FSPH(60),FSIMP(3000)
 0014              COMMON/MAFD/IFT,CORREX,QKCKF2
 0015              COMMON/MAGN/N(18)
 0016              COMMON/MAFRE/RMAX,NT,DELK,NSK,CON10,XT(33),YT(33),ZT(33),CNR(502),
                  1SK(502)
 0017              COMMON/MASK/CON3,CON7,CON8,CON9,PIA,NRES,NSKPL,NPLOT,NCAN,DWF,TEMP
                  1,FQMAX
            C
            C COMMON/MAELGN/ REFERS ALSO TO SUBR.S SIMPC AND SKRES
            C COMMONS/MAGN/ AND /MAFRE/ REFER ALSO TO SUBR. SKRES
            C
 0018              EQUIVALENCE (HPX,CTC)
```

```
      C
0019        DATA MAXM(1,1),MAXM(1,2),MAXM(1,3),MAXM(1,4),MAXM(1,5),MAXM(1,6),M
           1AXM(1,7),MAXM(1,8),MAXM(1,9),MAXM(1,10),MAXM(1,11),MAXM(1,12),MAXM
           2(1,13),MAXM(1,14),MAXM(1,15),MAXM(1,16),MAXM(1,17),MAXM(1,18),MAXM
           3(1,19),MAXM(1,20),MAXM(1,21),MAXM(1,22),MAXM(1,23),MAXM(1,24),MAXM
           4(1,25),MAXM(1,26),MAXM(1,27),MAXM(1,28),MAXM(1,29),MAXM(1,30),MAXM
           5(1,31),MAXM(1,32),MAXM(1,33),MAXM(1,34),MAXM(1,35),MAXM(1,36),MAXM
           6(1,37),MAXM(1,38),MAXM(1,39),MAXM(1,40),MAXM(1,41),MAXM(1,42),MAXM
           7(1,43),MAXM(1,44),MAXM(1,45),MAXM(1,46),MAXM(1,47),MAXM(1,48),MAXM
           8(1,49),MAXM(1,50),MAXM(1,51),MAXM(1,52),MAXM(1,53),MAXM(1,54),MAXM
           9(1,55),MAXM(1,56),MAXM(1,57),MAXM(1,58),MAXM(1,59),MAXM(1,60),MAXM
           A(1,61)/0,1,2,2,2,3,2,3,4,4,4,3,4,5,5,4,5,6,6,6,5,6,6,4,7,6,7,6,7,7
           B,8,8,8,6,8,8,6,7,8,9,8,9,6,9,9,8,9,10,10,10,9,10,10,8,10,10,10,11,
           C11,8,11/,MAXM(2,1),MAXM(2,2),MAXM(2,3),MAXM(2,4),MAXM(2,5),MAXM(2,
           D6),MAXM(2,7),MAXM(2,8),MAXM(2,9),MAXM(2,10),MAXM(2,11),MAXM(2,12),
           EMAXM(2,13),MAXM(2,14),MAXM(2,15),MAXM(2,16),MAXM(2,17),MAXM(2,18),
           FMAXM(2,19),MAXM(2,20),MAXM(2,21),MAXM(2,22),MAXM(2,23),MAXM(2,24),
           GMAXM(2,25),MAXM(2,26),MAXM(2,27),MAXM(2,28),MAXM(2,29),MAXM(2,30),
           HMAXM(2,31),MAXM(2,32),MAXM(2,33),MAXM(2,34),MAXM(2,35),MAXM(2,36),
           IMAXM(2,37),MAXM(2,38),MAXM(2,39),MAXM(2,40),MAXM(2,41),MAXM(2,42),
           JMAXM(2,43),MAXM(2,44),MAXM(2,45),MAXM(2,46),MAXM(2,47),MAXM(2,48),
           KMAXM(2,49),MAXM(2,50),MAXM(2,51),MAXM(2,52),MAXM(2,53),MAXM(2,54),
           LMAXM(2,55),MAXM(2,56),MAXM(2,57),MAXM(2,58),MAXM(2,59),MAXM(2,60),
           MMAXM(2,61)/0,1,2,2,3,2,4,3,4,4,5,4,5,6,6,5,6,4,7,6,6,7,8,7,8,8,7,6
           N,8,9,8,6,9,8,9,10,10,9,10,9,10,10,11,8,11,10,10,11,10,12,11,12,12,
           O11,12,9,12,10,13,10,12/,KNS(2,1),KNS(2,2),KNS(2,3),KNS(2,4),KNS(2,
           P5),KNS(2,6),KNS(2,7),KNS(2,8),KNS(2,9),KNS(2,10),KNS(2,11),KNS(2,1
           Q2),KNS(2,13),KNS(2,14),KNS(2,15),KNS(2,16),KNS(2,17),KNS(2,18),KNS
           R(2,19),KNS(2,20),KNS(2,21),KNS(2,22),KNS(2,23),KNS(2,24),KNS(2,25)
           S,KNS(2,26),KNS(2,27),KNS(2,28),KNS(2,29),KNS(2,30),KNS(2,31),KNS(2
           T,32),KNS(2,33),KNS(2,34),KNS(2,35),KNS(2,36),KNS(2,37),KNS(2,38),K
           UNS(2,39),KNS(2,40),KNS(2,41),KNS(2,42),KNS(2,43),KNS(2,44),KNS(2,4
           V5),KNS(2,46),KNS(2,47),KNS(2,48),KNS(2,49),KNS(2,50),KNS(2,51),KNS
           W(2,52),KNS(2,53),KNS(2,54),KNS(2,55),KNS(2,56),KNS(2,57),KNS(2,58)
           X,KNS(2,59),KNS(2,60),KNS(2,61)/0,3,4,8,11,12,16,19,20,24,27,32,35,
           Y36,40,43,44,48,51,52,56,59,64,67,68,72,75,76,80,83,84,88,91,96,99,
           Z100,104,107,108,115,116,120,123,128,131,132,136,139,140,144,147,14
           *8,152,155,160,163,164,168,171,172,176/
0020        DATA ITF(1),JTF(1),KTF(1),ITF(2),JTF(2),KTF(2),ITF(3),JTF(3),KTF(3
           1),ITF(4),JTF(4),KTF(4),ITF(5),JTF(5),KTF(5),ITF(6),JTF(6),KTF(6),I
           2TF(7),JTF(7),KTF(7),ITF(8),JTF(8),KTF(8),ITF(9),JTF(9),KTF(9),ITF(
           310),JTF(10),KTF(10),ITF(11),JTF(11),KTF(11),ITF(12),JTF(12),KTF(12
           4),ITF(13),JTF(13),KTF(13),ITF(14),JTF(14),KTF(14),ITF(15),JTF(15),
           5KTF(15),ITF(16),JTF(16),KTF(16),ITF(17),JTF(17),KTF(17),ITF(18),JT
           6F(18),KTF(18),ITF(19),JTF(19),KTF(19),ITF(20),JTF(20),KTF(20),ITF(
           721),JTF(21),KTF(21),ITF(22),JTF(22),KTF(22),ITF(23),JTF(23),KTF(23
           8),ITF(24),JTF(24),KTF(24),ITF(25),JTF(25),KTF(25),ITF(26),JTF(26),
           9KTF(26),ITF(27),JTF(27),KTF(27),ITF(28),JTF(28),KTF(28),ITF(29),JT
```

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                    AF(29),KTF(29),ITF(30),JTF(30),KTF(30),ITF(31),JTF(31),KTF(31),ITF(
                    B32),JTF(32),KTF(32),ITF(33),JTF(33),KTF(33)/0,0,0,1,1,1,2,0,0,2,2,
                    C0,3,1,1,2,2,2,4,0,0,3,3,1,4,2,0,4,2,2,5,1,1,3,3,3,4,4,0,5,3,1,6,0,
                    D0,4,4,2,6,2,0,5,3,3,6,2,2,4,4,4,5,5,1,6,4,0,6,4,2,7,3,1,5,5,3,8,0,
                    E0,7,3,3,3,2,0,6,4,4,3,2,2,6,6,0,7,5,1,5,5,5/,ITB(1),JTB(1),KTB(1),
                    FITB(2),JTB(2),KTB(2),ITB(3),JTB(3),KTB(3),ITB(4),JTB(4),KTB(4),ITB
                    G(5),JTB(5),KTB(5),ITB(6),JTB(6),KTB(6),ITB(7),JTB(7),KTB(7),ITB(8)
                    H,JTB(8),KTB(8),ITB(9),JTB(9),KTB(9),ITB(10),JTB(10),KTB(10),ITB(11
                    I),JTB(11),KTB(11),ITB(12),JTB(12),KTB(12),ITB(13),JTB(13),KTB(13),
                    JITB(14),JTB(14),KTB(14),ITB(15),JTB(15),KTB(15),ITB(16),JTB(16),KT
                    KB(16),ITB(17),JTB(17),KTB(17),ITB(18),JTB(18),KTB(18),ITB(19),JTB(
                    L19),KTB(19),ITB(20),JTB(20),KTB(20),ITB(21),JTB(21),KTB(21),ITB(22
                    M),JTB(22),KTB(22),ITB(23),JTB(23),KTB(23),ITB(24),JTB(24),KTB(24),
                    NITB(25),JTB(25),KTB(25),ITB(26),JTB(26),KTB(26),ITB(27),JTB(27),KT
                    OB(27),ITB(28),JTB(28),KTB(28),ITB(29),JTB(29),KTB(29),ITB(30),JTB(
                    P30),KTB(30),ITB(31),JTB(31),KTB(31),ITB(32),JTB(32),KTB(32),ITB(33
                    Q),JTB(33),KTB(33)/0,0,0,1,1,0,2,0,0,2,1,1,2,2,0,3,1,0,2,2,2,3,2,1,
                    R4,0,0,3,3,0,4,1,1,4,2,0,3,3,2,4,2,2,5,1,0,4,3,1,5,2,1,4,4,0,5,3,0,
                    S4,2,3,6,0,0,4,4,2,6,1,1,5,3,2,6,2,0,5,4,1,6,2,2,6,3,1,4,4,4,7,1,0,
                    T5,5,0,5,4,3,6,4,0/
               C                                                                        13
               C  THE ONLY (DIMENSIONED) ARRAYS IN COMMON STATEMENTS ARE CTA(3000),     14
               C  EV( 3, 3) AND V( 3) ,  V IN GNU IS EQUIVALENT TO PH IN SUBR. FREQ     15
               C                                                                        16
0021             101 FORMAT(1H0)                                                        17
0022             104 FORMAT  (4H EV=9E12.5)
0023             105 FORMAT(1X,I4,3I3,2X,3HGU=,F4.1,5X,3HQ =,3F9.5,5X,3HV =,6F9.5)      19
0024             106 FORMAT(1H0,10X, 22HARRAY OF G(NU)/(NU)**2  ///)                    20
0025             107 FORMAT(1X,I5,3I3,F5.1,4X,6F9.5/8F9.5)                              21
0026             108 FORMAT(1H0,10X,18HATOMIC MASS(ES) =   ,4F10.4 )                    23
0027             119 FORMAT(8F10.0)                                                     27
0028             125 FORMAT(10F8.0)                                                     33
0029             447 FORMAT (9A4,I6,E12.5)
0030             547 FORMAT (I5,1P5E15.3)
0031            1000 FORMAT (6E12.5)
0032            1001 FORMAT (12I6)
0033            1002 FORMAT(1H1)                                                        35
0034            1003 FORMAT(1H1/35H       *NEGATIVE* FREQUENCY CHANNELS   /1H0)         36
0035            1111 FORMAT(33H    (NSFB, NNN, KK, IMIN, IMAX) =    ,10I4)              25
0036            1112 FORMAT(44H0       CYCLE NO., KK, NO. CUBES, IMIN, IMAX =   ,10I5)  26
0037            1120 FORMAT(20I5)                                                       28
0038            2000 FORMAT (////16HMETAL CONSTANTS///9X,11HMASS(E-24G),3X,12HLATTC(E-
                    18CM),4X,10HCORR-FERMI,4X,13HSCREEN.COEFF.,3X,11HZ-EFFECTIVE,2X,14H
                    2K-SCR.(E+8/CM),2X,13HR-ZERO(E-8CM),1X,15HSCR.RAD.(E-8CM)//5X,8E15.
                    35)
0039            2001 FORMAT (//33H0MODEL AND COMPUTATION PARAMETERS//9X,4HNBF=I2,5X,4HI
                    1FT=I2,5X,3HKP=I3,5X,5HNWAY=I2,5X,4HNSH=I3)
0040            2002 FORMAT (//9X,8HE-F(EV)=E12.5,5X,12HK-F(E+8/CM)=E12.5,5X,5HETHA=E12
```

```
                 1.5)
0041       2003 FORMAT (//15H0FIT-PARAMETERS//(5X,3E15.5))
0042       2004 FORMAT (50H1WORKING STORAGE HPX, HPY, HPZ OR NPPS EXCEEDED     /56H
               10MORE THAN 30 ( 35 ) H-SHELLS FOR BCC- ( FCC- ) CASE.      /30H0COM
               2PUTATION INTERRUPTED.           )
0043       2107 FORMAT(4F20.6)                                                    22
0044       2109 FORMAT (16H0FORCE CONSTANTS//)
0045       2120 FORMAT(1H0, 10E11.4)                                              29
0046       3001 FORMAT (18A4)
0047       3002 FORMAT (1H1,18A4)
0048       7102 FORMAT(5X,22HFREQ, CHANNEL WIDTH =  ,F6.4 )                        18
0049       8123 FORMAT(18H0FREQ(10**12 CPS). ,20X, 24HG(NU) HISTOGRAM CHANNELS //)  31
0050       9123 FORMAT (1H0,10X,18A4/1H0)
0051       9125 FORMAT(5E16.8)                                                    34
0052       9126 FORMAT (/38H0NOTE THAT INPUT RMAX WAS CHANGED FROM,E12.5,3H TO,E12
               1.5,35H TO AVOID OVERFLOW IN CNR AND SK.        )
0053       9127 FORMAT (/52H0NUMBER OF TRANSL.VECTORS TOO SMALL FOR INPUT RMAX.
               1/37H0RESULTS RELIABLE FOR K/(2*PI/A).LT. E12.5)
          C
          C                                                                        37
          C   ALL *LOGICAL IF* STATEMENTS HAVE BEEN REPLACED BY ARITHMETIC IF*S     38
          C   SOME LOGICAL IFS HAVE BEEN LEFT IN AS COMMENTS, INDICATED BY C*     39
          C                                                                        43
          C   NDIMA AND NDIMC ARE THE DIMENSIONS OF CTA AND CTC                    44
0054              NDIMA=3000                                                       45
0055              NDIMC=NDIMA                                                      46
          C                                                                        50
0056              NSTEP=0
0057              KNS(1,1)=0
0058              DO 160 L=1,60
0059              IF(L.EQ.14.OR.L.EQ.29.OR.L.EQ.44.OR.L.EQ.53.OR.L.EQ.58)NSTEP=NSTEP
                 1+2
0060        160 KNS(1,L+1)=2*L+NSTEP
0061              READ (5,3001) (W(I),I=1,18)
0062              READ (5,1000) CMASS,CLATT,CORRF,SCREEN,ZEFF,ETHA
0063              READ (5,1001) NBF,IFT,NWAY,KP,NSH
0064              READ (5,1000) (B(I),I=1,KP)
0065              READ (5,119) DVA,XM,DQ                                           58
0066              READ (5,1120) NCTA,NCTC,NTAPE,NPLOT,KK,KG,IMIN,IMAX,NDIV,NPRINT,NP
                 1UNCH,NSK,NSKPL,NRES
0067              IF(NPLOT)710,710,402                                             77
0068        402 READ (5,119) XFACT,YFACT
0069        710 CONTINUE
0070              IF(NSK.NE.0) READ (5,1000) RMAX,TEMP,DWF,FQMAX
0071              IF(NRES.EQ.1.AND.NSK.EQ.0)NSK=1
0072              IF(NRES.EQ.1.AND.RMAX.LE.1.0)RMAX=1.1
0073              IF(NSK.EQ.0) NSKPL=0
          C
```

```
      C     CMASS        IONEN-MASSE IN E-24G
      C     CLATT        GITTER-KONSTANTE IN E-8CM
      C     CORRF        =1.0 FREE ELECTRON APPROXIMATION
      C     SCREEN       =1.0 THOMAS-FERMI-SCREENING
      C                  =0.18336 PINES-SCREENING
      C     SCREEN.PARAM. CKC**2=CKF*(4/PI*A0)*SCREEN    A0=.529172E-8CM
      C     CLATT*CKF=CORRF*(6*ZEFF*PI**2)**0.333333
      C     ZEFF         EFFEKTIVE IONENLADUNG
      C     ETMA         DEF. IN UP. FCD
      C     IBF          =1 FUER BCC, =2 FUER FCC
      C     IFT          DEF. IN UP. FDC
      C     NWAY         DEF. IN PROGR. PSAF/MAIN
      C     KP           ANZAHL DER MODELL-PARAMETER, MAX. 25
      C     NSH          BER. DER H-TERME BIS ZUR NSH-TEN SCHALE,
      C     B(I)         FIT PARAMETER
      C  DVA = CHANNEL WIDTH OF HISTOGRAM (IN 10**12 C/S)
      C  XM = MAX FREQ  (UNITS OF 10**12 C/S)
      C  DQ = DELTA Q FOR COMPUTING GRAD(NU), USUALLY DQ = 0.0001
      C     XFACT, YFACT DETERMINES SIZE OF GNU-PLOT / LENGTH OF X-AXIS WILL
      C                  BE XFACT*VU-MAX., LENGTH OF Y-AXIS YFACT*GNU-MAX.
      C     IPLOT        =1, PLOT OF GNU. OTHERWISE=0
      C     IPUNCH       =1, PUNCH OF GNU ( FOR INTERMEDIATE STORAGE TAPE 11
      C                  IS USED ). OTHERWISE =0
      C     NSK          =0, COMPUTE ONLY GNU
      C                  =1, COMPUTE GNU AND S(K)
      C                  =2, COMPUTE ONLY S(K)
      C     NSKPL        =1, PLOT OF S(K). OTHERWISE =0
      C     NRES         =1, COMPUTE THE ELECTRICAL RESISTIVITY.
      C                  OTHERWISE=0
      C     RMAX         S(K) IS COMPUTED FOR K=DELTAK/2 UNTIL K=RMAX.
      C                  THE STEP SIZE DELTAK IS DETERMINED BY KK
      C                  DELTAK=1/(3*KK) FOR FCC AND =1/(4*KK) FOR BCC IN
      C                  UNITS OF (2*PI/A).
      C                  RMAX HAS TO BE INPUT IN UNITS OF (2*KFERMI).
      C     TEMP         TEMPERATURE AT WHICH THE FITTED DISP. CURVES ARE
      C                  MEASURED.
      C     DWF          DEBYE-WALLER FACTOR AT THAT TEMPERATURE. IF NOT
      C                  KNOWN =0.0. S(K) IS THEN COMPUTED WITHOUT THE D.W.F.
      C     FQMAX        MAX. FREQUENCY OF THE FREQU.DISTRIB. USED FOR
      C                  COMPUTING THE D.W.F.. IF DWF=0.0 ALSO FQMAX=0.0
      C
0074     310 LA=XM/DVA+51.0
      C
      C  WE START STORING G(NU) IN LOC. 51 OF CTA IN CASE OF *NEG* FREQS
      C
0075         MS=0
      C
      C  MS IS TO BE THE MESH POINT SEQUENCE NUMBER
```

```
C FIND SOME CONVENIENT CONSTANTS ETC.
C                                                                        93
      CL=B(1)
      KP1=KP-1
      CBF=NBF
      PI=3.14159
      QP=4.*PI
      CKF=CORRF/CLATT*(6.*PI**2*ZEFF*CBF)**0.333333
      SCRR=0.5*SQRT(PI*0.529172/(CKF*SCREEN))
      CKC=1./SCRR
      RATIOK=(CKC/CKF)**2
      QKCKF2=(CKC/CKF)**2
      RZERO=CLATT*(1.5/(QP*ZEFF*CBF))**0.333333
      CON1=CLATT**2/(QP*PI*SCRR**2)
      CON2=PI/(CLATT*CKF)
      CON3=(QP*ZEFF*45.124*CBF)/(1.60205*CLATT**3)
      CON6=20000.0*CBF*23.067*ZEFF**2*QP/CLATT**3
      CON5=CON3*SCRR**2
      EFERMI=1.5*CON5
      PIA=2.0*PI/CLATT
      CLB=CL*PIA/2.0
      CLB2=CLB*CLB
      IF( NWAY.LE.2) NEX=NWAY
      IF( NWAY.GT.2) NEX=NWAY-2
      CNEX=NEX
      IF(IFT.EQ.3) CORREX=1.0+ETHA*RATIOK
      IF(IFT.EQ.4) CORREX=1.0+0.5*RATIOK
      PIA2=PI/CLATT
      HH=1.66043
      AMAS(1)=CMASS/HH
      NNN=3
      IF(NBF.EQ.1) NSFB=3
      IF(NBF.EQ.2) NSFB=2
C                                                                        56
C  NSFB = 1 FOR SIMPLE CUBE,  =2 FOR FCC  AND =3 FOR BCC .               53
C  NNN = DIMENSION  ( =3 TIMES NO. OF ATOMS/UNIT CELL )                  54
C
      SC=QP*PI*HH
      ANN=0.5/(D0*SC*AMAS(1))
      SC=SC*AMAS(1)
      CON4=CON6
C
C AUSDRUCKEN
C
      WRITE (6,3002) (H(I),I=1,18)
      WRITE (6,2000) CMASS,CLATT,CORRF,SCREEN,ZEFF,CKC,RZERO,SCRR
      WRITE (6,2003) (B(I),I=1,KP)
      WRITE (6,2001) NBF,IFT,KP,NWAY,NSH
```

```
              WRITE (6,2002) EFERMI,CKF,ETHA
        C
              IF(NSK.EQ.0) GO TO 330
              CON7=(10.544*10.544)/(CMASS*TEMP*1.38044)
              CON8=(3.0*10.544*10.544*PIA*PIA)/(CMASS*66.2517)
              CON9=101.635*CLATT**3/(2.0*CBF*EFERMI)
              IF(TEMP.GT.0.0) CON10=47.993/TEMP
              RMAX=RMAX/CON2
              CKK=KK
              GO TO (841,842),NBF
          841 DELK=1.0/(4.0*CKK)
              COMP=1.25*1.25
              DO 843 L=1,33
              XT(L)=ITB(L)
              CJ=J
          863 DO 350 K=1,J
              YT(L)=JTB(L)
          843 ZT(L)=KTB(L)
              GO TO 845
          842 DELK=1.0/(8.0*CKK)
              COMP=1.0
              DO 844 L=1,33
              XT(L)=ITF(L)
              YT(L)=JTF(L)
          844 ZT(L)=KTF(L)
          845 CONTINUE
              RMAX2=RMAX*RMAX
              DO 846 L=1,33
              XTL=XT(L)
              YTL=YT(L)
              ZTL=ZT(L)
              SM=XTL*XTL+YTL*YTL+ZTL*ZTL-RMAX2
              IF(SM.GT.COMP) GO TO 847
          846 CONTINUE
              RMAXC=SQRT(SM+RMAX2-COMP)
              WRITE (6,9127) RMAXC
          847 NT=L
              NCAN=RMAX/DELK+1.0
              IF(2*(NCAN/2).EQ.NCAN)NCAN=NCAN+1
              CNCAN=NCAN
              RMAX=CNCAN*DELK
              IF(NCAN.LE.501)GO TO 849
              CRMAX=RMAX
              RMAX=501.*DELK
              NCAN=501
              WRITE (6,9126) CRMAX,RMAX
          849 CONTINUE
              DO 848 L=1,NCAN
```

82

```
0162          CNR(L)=0.0
0163      348 SK(L)=0.0
0164      830 CONTINUE
0165          IF(KP.EQ.1) GO TO 217
0166      215 NEND=(KP-1)/2+1
0167          DO 218 KL=2,NEND
0168          I=KP+2-KL
0169          ZS1=B(I)
0170          B(I)=B(KL)
0171      218 B(KL)=ZS1
0172      217 CONTINUE
        C
        C PREPARATION OF H-SUMS
        C
0173          IF(NBF.EQ.1.AND.NSH.GE.31.OR.NBF.EQ.2.AND.NSH.GE.36) GO TO 91
0174          NSH1=NSH+1
0175          NPT=0
0176          SHS=0.0
0177          L=1
0178       99 LIM=MAXM(NBF,L)
0179          IRAD=KNS(NBF,L)
0180          H2=IRAD
0181          H1=SQRT(H2)
        C
        C CALCULATION OF U(H)*G(H)
        C
0182          CLBX2=H2*CLB2
0183          EXX2=EXP(-2.0*CLBX2)
0184          IF(KP.EQ.1) GO TO 98
0185          IF(NWAY.GT.2)AX=(PIA2*H1)**NEX
0186          IF(NWAY.LE.2) AX=(CLB*H1)**NEX
0187          S1=0.0
0188          DO 97 KL=2,KP
0189       97 S1=(S1+B(KL))*AX
0190          S1=1.+S1
0191          FSP=EXX2*S1*S1/(H2+CON1*FDC(CON2*H1))
0192          GO TO 96
0193       98 FSP=EXX2/(H2+CON1*FDC(CON2*H1))
        C
        C U(H)*G(H) ZU EINER H-SCHALE IN FSP GESPEICHERT.
        C SUCHEN DER H-PUNKTE ZU DER SCHALE.
        C
0194       96 FSPH(L)=FSP
0195          LIM1=LIM+1
0196          LIM2=LIM1+LIM
0197          NPTS=0
0198          DO 94 I=1,LIM2,NBF
0199          IX=I-LIM1
```

```
            DO 94 J=1,LIM2,NBF
            IY=J-LIM1
            DO 94 K=1,LIM2,NBF
            IZ=K-LIM1
            IXX=IX*IX
            IYY=IY*IY
            IZZ=IZ*IZ
            I2=IXX+IYY+IZZ
            IF(I2.NE.IRAD) GO TO 94
            NPTS=NPTS+1
            NPT=NPT+1
            IF(NPT.GT.3103) GO TO 91
            HPX(NPT)=IX
            HPY(NPT)=IY
            HPZ(NPT)=IZ
         94 CONTINUE
            NPPS(L)=NPTS
      C
      C EINE H-SCHALE FERTIG, H-PUNKTE IN HPX,HPY UND HPZ
      C
            IF(L.GE.NSH1) GO TO 90
            L=L+1
            GO TO 99
         91 WRITE (6,2004)
            CALL EXIT
         90 CONTINUE
      C                                                          95
            DO 10 I=1,NDIMA                                      96
         10 CTA(I)=0.0                                           97
      C                                                         100
        311 GO TO (312,313,314),NSFB                            101
        312 JIMAX=KK                                            102
            CJIMAX=JIMAX
            PP=0.5                                              103
            GO TO 320                                           104
        313 JIMAX=4*KK                                          105
            CJIMAX=JIMAX
            PP=1.0                                              106
            GO TO 320                                           107
        314 JIMAX=2*KK                                          108
            CJIMAX=JIMAX
            PP=1.0                                              109
        320 CUBE=PP/CJIMAX
            IF(IMAX)1320,1320,2320                              111
       1320 IMAX=JIMAX                                          112
       2320 IF(IMIN)321,321,401                                 113
        321 IMIN=3                                              114
      C
```

```
0242      401 WRITE (6,1111) NSFB,NNN,KK,IMIN,IMAX                              115
0243          WRITE (6,101)                                                     116
        C                                                                       117
        C  BRILLOUIN ZONE NOW BROKEN UP INTO THREE PARTS (KM = 1,3)             118
        C    AHALF IS HALF THE LENGTH OF A LITTLE CUBE EDGE .                   123
        C                                                                       119
0244          DO 69 KM=1,3                                                      120
0245       11 AHALF=CUBE/2.0                                                    121
0246          VOLUME=8.0*AHALF**3                                               122
0247          ASQ=AHALF**2                                                      124
0248          CKK=KK
        C                                                                       125
0249          DO 350 I=IMIN,IMAX                                                126
0250          CI=I
0251          GO TO (864,865,866),NSFB                                          127
0252      864 JMAX=I                                                            128
0253          GO TO 867                                                         129
0254      865 JMAX=3.0*CKK+0.5001-ABS(3.0*CKK+0.5-CI)                           130
0255          KFCC=6*KK+1                                                       131
0256          GO TO 367                                                         132
0257      866 JMAX=CKK+0.5001-ABS(CKK+0.5-CI)                                   133
0258      867 DO 350 J=1,JMAX                                                   134
0259          CK=K
0260          GO TO (345,870,345),NSFB                                          136
0261      870 IF(I+J+K-KFCC)345,345,350                                         137
0262      345 Q(1)=(CI-0.5)*CUBE                                                138
0263          Q(2)=(CJ-0.5)*CUBE                                                139
0264          Q(3)=(CK-0.5)*CUBE                                                140
        C
        C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S), IS        141
        C*        IF(JMAX.NE.J.AND.J.NE.K) 349,346                              142
        C
0265          IF((JMAX-J)*(J-K))349,346,349                                     143
0266      346 IF(K-JMAX)348,347,347                                             144
0267      347 GU=1.0                                                            145
0268          GO TO 19                                                          146
0269      348 GU=3.0                                                            147
0270          GO TO 19                                                          148
0271      349 GU=6.0                                                            149
0272       19 MS=MS+1                                                           150
0273          NEG=0
        C                                                                        65
0274          CALL FREQ(Q,GD1,GD2,GD3,NEG)
        C
0275          IF(NEG.EQ.1) GO TO 350
0276       31 IF(KG-1)34,34,29                                                  152
0277       34 WRITE (6,105) MS,I,J,K,GU,(Q(M),M=1,3),(V(M),M=1,NNN)             153
0278          WRITE (6,104) ((EV(II,JJ),II=1,3),JJ=1,3)
```

```
                C
                C  THE *LOGICAL IF* FORM OF THE STATEMENT(S) WHICH FOLLOW(S), IS        154
                C* 29 IF(KG.EQ.0.OR.KG.EQ.2) 35,370                                      155
                C
0279               29 IF(KG*(KG-2))370,35,370                                            156
0280               35 WRITE ( 7,107) MS,I,J,K,GU,(Q(M),M=1,3),(V(M),M=1,NNN)
0281                  IF(ISK.EQ.2) GO TO 350
                C                                                                        158
0282              370 CALL SWEEP(J,G01,G02,G03)                                          159
                C
0283              350 CONTINUE                                                           160
0284                  IF(ISK.EQ.2) GO TO 746
                C
0285                  WRITE (6,101)                                                      161
                C                                                                        162
0286                  IF(NCTA.GT.0.AND.IMIN.GT.1) GO TO 63
0287                  GO TO 746
                C
0288               63 SA=0.0
0289                  DO 502 I=1,LA
0290              502 SA = SA + CTA(I)
0291                  RA=SA*DVA
0292                  DO 503 J=1,LA
0293              503 CTA(J)=CTA(J)/RA
0294                  CALL WRITE(CTA,DIMA,DVA,51,LA,2)
                C
0295                  WRITE (6,101)
                C
0296                  DO 504 J=1,LA
0297              504 CTA(J)=CTA(J)*RA
                C
0298              746 WRITE (6,1112) KM,KK,MS,IMIN,IMAX                                  191
0299                  WRITE (6,101)                                                      192
                C
0300                  KK=3*KK                                                            193
0301                  CUBE=CUBE/3.0                                                      194
0302                  IF(IMIN-1)202,202,76                                              194A
0303               76 CONTINUE                                                          194B
0304                  IMAX=(IMIN-1)*3                                                    195
0305                  GO TO (71,70,69),KM                                                196
0306               70 IMIN=1                                                             197
0307                  GO TO 69                                                           198
0308               71 IMIN=4                                                             199
0309               69 CONTINUE                                                           200
0310                  IF(NSK.EQ.2) GO TO 331
                C                                                                        201
0311              202 SA=0.0                                                             163
0312               47 DO 56 I=1,LA                                                       169
```

```
   56 SA = SA + CTA(I)
      RA=SA*DVA
      DO 57 J=1,LA                                                    172
   57 CTA(J)=CTA(J)/RA
C
   68 WRITE (6,101)                                                   174
      IF(NPUNCH.EQ.0) GO TO 647
      LA1=LA-50
      WRITE ( 7,447) (W(I),I=1,9),LA1,DVA
      LA5=LA1/5
      LA55=5*LA5
      LDIFF=LA1-LA55
      K=46
      DO 500 I=1,LA5
      K=K+5
      K5=K+4
  500 WRITE ( 7,547) I,(CTA(L),L=K,K5)
      IF(LDIFF.EQ.0) GO TO 501
      I1=I+1
      K=LA55+51
      KE=LA55+LDIFF+50
      WRITE ( 7,547) I1,(CTA(L),L=K,KE)
  501 CONTINUE
      END FILE 7
  647 CONTINUE
      WRITE (6,1003)                                                  202
      WRITE (6,2120) (CTA(J),J=1,50)                                  203
C
  201 DO 298 I=51,LA                                                  204
  298 CTA(I-50)=CTA(I)                                                205
      NA=LA-50                                                        206
      NAA=NA+1                                                        207
      DO 4008 J=NAA,LA                                                208
 4008 CTA(J)=0.0                                                      209
      IF(NCTA)6298,3298,3298                                          210
C
 3298 WRITE (6,1002)                                                  211
      WRITE (6,9123) (W(II),II=1,9)
      WRITE (6,7102) DVA                                              213
      WRITE (6,8123)                                                  214
C
      CALL WRITE(CTA,NDIMA,DVA,1,NA,2)                                215
C
 6298 IF(NCTC)5298,5298,4298
 4298 WRITE (6,1002)                                                  217
C
      DO 406 I=1,NDIMC                                                 98
  406 CTC(I)=0.0                                                       99
```

```
0355                FAC=3./DVA**3.
0356                NFRAC=NA/NCTC                                                         219
0357                DO 61 J=1,NFRAC                                                       220
0358                R=J                                                                   221
0359             61 CTC(J)=FAC*CTA(J)/(3.0*(R**2.-R)+1.0)
           C
0360                WRITE (6,106)                                                         226
           C
0361                CALL WRITE(CTC,NDIMC,DVA,1,NFRAC,2)                                   227
           C
0362           5298 CONTINUE
0363                IF(NPLOT.GT.0) CALL GNPLOT(XFACT,YFACT)
           C
0364           2293 IF(NTAPE)306,306,199
0365            199 WRITE ( 7,3001) (W(II),II=1,6)
0366            299 WRITE ( 7,9125) (CTA(J),J=1,NA)
           C
0367                END FILE 7
           C                                                                              362
0368            306 IF(NSK.EQ.0) GO TO 200
0369            831 CALL SKRES
0370            200 IF(NPLOT.NE.0.OR.NSKPL.NE.0) CALL FINTRA
0371                STOP
0372                END
```

```
0001             SUBROUTINE GRAD(A,GG)                                          556
           C                                                                    557
0002             DIMENSION EV(3,3),A(3,3),GG(3),P(3,3),V(3)
           C
0003             COMMON/C2/ANN
0004             COMMON/C4/EV,V
0005             COMMON/C7/N
           C
0006             DO 10 I=1,N                                                    562
0007             Y=0.0                                                          563
0008             DO 11 J=1,N                                                    564
0009             X=0.0                                                          565
0010             DO 12 K=1,N                                                    566
0011          12 X=X+EV(K,I)*A(K,J)                                             567
0012          11 P(I,J)=X                                                       568
0013             DO 13 K=1,N                                                    569
0014          13 Y=Y+P(I,K)*EV(K,I)                                             570
0015          10 GG(I)=Y*ANN/V(I)                                               571
           C
0016             RETURN                                                         572
0017             END                                                            573
```

```
0001          FUNCTION SIMPC(DT,LIMIT)
        C
        C INTEGRATION EINER FUNCTION FUNC NACH SIMPSON
        C
        C     LIMIT IST DIE ANZAHL DER FUNKTIONSWERTE FUNC, DIE FUER
        C     AEQUIDISTANTE PUNKTE ( SCHRITTWEITE DT) IHRES ARGUMENTES GEGEBEN
        C     IST.
        C
0002          COMMON/JAELSN/NSH1,CLB2,CLB,KP,NWAY,PIA2,CON1,CON2,CON4,SHS,NEX,B(
             125),MPPS(60),MPX(3103),MPY(3103),MPZ(3103),FSPH(60),FUNC(3000)
        C
0003          LIMIT1=LIMIT-1
0004          SUM=0.0
0005          SUM1=0.0
0006          FUNC(1)=FUNC(1)*0.5
0007          FUNC(LIMIT)=FUNC(LIMIT)*0.5
0008          DO 1 I=1,LIMIT,2
0009        1 SUM=SUM+FUNC(I)
0010          DO 2 I=2,LIMIT1,2
0011        2 SUM1=SUM1+FUNC(I)
0012          SIMPC=((0.333333*DT)*(4.*SUM1+2.*SUM)
0013          RETURN
0014          END
```

```
0001          SUBROUTINE ELEM(Q,A)
        C
0002          DIMENSION Q(3),A(3,3),QISP(50),FSPSP(50)
0003          COMMON/MAELGN/NSH1,CLB2,CLB,KP,NWAY,PIA2,CON1,CON2,CON4,SHS,NEX,B(
             125),NPPS(50),HPX(3103),HPY(3103),HPZ(3103),FSPH(60),FSIMP(3000)
        C
0004          DO 3 L=1,3
0005          DO 3 K=1,3
0006        3 A(L,K)=0.0
0007          NZZ=0
0008          NSTART=1
0009          NEND=0
0010          DO 1 L=1,NSH1
0011          FSP2=FSPH(L)
0012          NEND=NPPS(L)+NEND
0013          DO 2 K=NSTART,NEND
0014          HX=HPX(K)
0015          HY=HPY(K)
0016          HZ=HPZ(K)
0017          XHX=Q(1)+HX
0018          YHY=Q(2)+HY
0019          ZHZ=Q(3)+HZ
0020          XHX2=XHX*XHX
0021          YHY2=YHY*YHY
0022          ZHZ2=ZHZ*ZHZ
0023          QH2=XHX2+YHY2+ZHZ2
0024          QH=SQRT(QH2)
0025        4 CLBX2=QH2*CLB2
0026          EXX2=EXP(-2.0*CLBX2)
0027          IF(KP.EQ.1) GO TO 8
0028          IF(NWAY.GT.2) AX=(PIA2*QH)**NEX
0029          IF(NWAY.LE.2) AX=(CLB*QH)**NEX
0030          S1=0.0
0031          DO 7 KL=2,KP
0032        7 S1=(S1+B(KL))*AX
0033          S1=1.+S1
0034          FSP=EXX2*S1*S1/(QH2+CON1*FDC(CON2*QH))
0035          GO TO 10
0036        8 FSP=EXX2/(QH2+CON1*FDC(CON2*QH))
0037       10 CONTINUE
0038          A(1,1)=A(1,1)+XHX2*FSP-HX*HX*FSP2
0039          A(1,2)=A(1,2)+XHX*YHY*FSP
0040          A(1,3)=A(1,3)+XHX*ZHZ*FSP
0041          A(2,2)=A(2,2)+YHY2*FSP-HY*HY*FSP2
0042          A(2,3)=A(2,3)+YHY*ZHZ*FSP
0043          A(3,3)=A(3,3)+ZHZ2*FSP-HZ*HZ*FSP2
0044        2 CONTINUE
0045          NSTART=NEND+1
```

```
0046           IZZ=0
0047         1 CONTINUE
0048           DO 11 L=1,3
0049           DO 11 K=L,3
0050        11 A(L,K)=A(L,K)*CON4
0051           A(2,1)=A(1,2)
0052           A(3,1)=A(1,3)
0053           A(3,2)=A(2,3)
0054           RETURN
0055        12 WRITE (6,13)
0056        13 FORMAT (7?H WORKING STORAGES QHSP AND FSPSP TO SMALL, COMPUTATION
             1INTERRUPTED.        )
0057           STOP
0058           END
```

```
0001          SUBROUTINE WRITE (ARRAY,NDIM,DELF,NA,NB,NFMT)
        C
0002          DIMENSION ARRAY(NDIM)
0003      101 FORMAT(1X,F10.5,7X,10F10.0)
0004      102 FORMAT(1X,F10.5,7X,10E10.3)
        C
0005          NLINES=(NB-NA+9)/10
0006          N2=NA-1
0007          FINCR=10.*DELF
0008          FRQ=-FINCR
0009          DO 5 J=1,NLINES
0010          N1=N2+1
0011          N2=N1+9
0012          FRQ=FRQ+FINCR
0013          GO TO (1,2), NFMT
0014        1 WRITE (6,101) FRQ,(ARRAY(K),K=N1,N2)
0015          GO TO 5
0016        2 WRITE (6,102) FRQ,(ARRAY(K),K=N1,N2)
0017        5 CONTINUE
        C
0018          RETURN
0019          END
```

```
      SUBROUTINE SWEEP(Q,GD1,GD2,GD3)
C
      COMMON/C3/PI,CPT,PX,GU,SC,NSFB,AMAS,DQ
      COMMON/C4/EV,V
      COMMON/C5/CTA(3000),LA,DVA,AHALF,VOLUME,ASQ,NPRINT,XM
      COMMON/C6/K1,KK,I,J,K
      COMMON/C7/NNN
C
      DIMENSION AL(3),V(3),GD1(3),GD2(3),GD3(3)
      DIMENSION PX(60),Q(3)
      DIMENSION AMAS(12)
      DIMENSION EV(3,3)
C
 1000 FORMAT(5X, 7F11.6, 2E15.5, I6)
 1002 FORMAT(26H0V(L).GT.MAX FREQ  V(L) =  ,E15.6/ 1H0)
C
      DO 20 L=1,NNN
      IF(V(L)-XM)21,21,19
   19 WRITE (6,1002) V(L)
      GO TO 20
   21 GRD=SQRT(GD1(L)**2+GD2(L)**2+GD3(L)**2)
      DELW=DVA/GRD
      AL(1)=ABS(GD1(L))/GRD
      AL(2)=ABS(GD2(L))/GRD
      AL(3)=ABS(GD3(L))/GRD
      ALMN=1.0/(AL(1)*AL(2)*AL(3))
      IF(AL(1)-AL(2))521,521,522
  521 AP=AL(1)
      AL(1)=AL(2)
      AL(2)=AP
  522 IF(AL(2)-AL(3))523,523,527
  523 IF(AL(3)-AL(1))524,524,525
C
  524 AP=AL(2)
      AL(2)=AL(3)
      AL(3)=AP
      GO TO 527
  525 AP=AL(3)
      AL(3)=AL(2)
      AL(2)=AL(1)
      AL(1)=AP
  527 CONTINUE
      W1=(-AL(1)+AL(2)+AL(3))*AHALF
      W2=(AL(1)-AL(2)+AL(3))*AHALF
      W3=(AL(1)+AL(2)-AL(3))*AHALF
      W4=(AL(1)+AL(2)+AL(3))*AHALF
C
C  CONSTANTS NEEDED
```

```
                 C
0042                   ULMN=GO*ALMN
0043                   COM=0.5*ULMN
0044                   WSQ=W1**2
0045                   AL23=4.0*AL(2)*AL(3)*ASQ
0046                   B3=COM*W4
0047                   A3=B3*W4
0048                   C3=ULMN/6.0
0049                   B42=ULMN*AHALF*AL(3)
0050                   A42=2.0*B42*AHALF*(AL(1)+AL(2))
0051                   A5=COM*(2.0*AL23-WSQ)
0052                   B5=COM*W1
0053                   C5=-C3
0054                   A6=ULMN*(AL23-WSQ)
0055                   A41=4.0*GO*ASQ/AL(1)
0056                   SUM=0.0
                 C
0057                   DO 900 JJJ=1,7
0058                   GO TO (751,752,753,754,755,756,757),JJJ
0059               751 A=A3
0060                   B=B3
0061                   C=C3
0062                   WN=-W4
0063                   WX=-W3
0064                   FMAX=V(L)+WN*GRD
0065                   NN2=FMAX/DVA+1.0
0066                   AN2=NN2-1
0067                   N2=NN2+50
0068                   NMIN=N2
0069                   BW=(FMAX-AN2*DVA)/GRD
0070                   GO TO 770
                 C
0071               752 A=A42
0072                   B=B42
0073                   C=0.0
0074                   WX=-W2
0075                   GO TO 770
                 C
0076               753 A=A5
0077                   B=B5
0078                   C=C5
0079                   WX=-ABS(W1)
0080                   GO TO 770
                 C
0081               754 IF(W1)4754,900,4754
0082              4754 A=A41
0083                   B=0.0
0084                   C=0.0
```

```
0085                 JX=-J1
0086                 GO TO 770
               C
0087             754 A=A6
0088                 B=[illegible]
0089                 C=-JL11/3.0)
0090                 JX=J1
0091                 GO TO 770
               C
0092             755 A=A5
0093                 B=-B5
0094                 C=C5
0095                 JX=J2
0096                 GO TO 770
               C
0097             756 A=A42
0098                 B=-B42
0099                 C=[illegible]
0100                 JX=J3
0101                 GO TO 770
               C
0102             757 A=A3
0103                 B=-B3
0104                 C=C3
0105                 JX=J4
               C
0106             770 FMIN=FMAX
0107                 FMAX=V(L)+JX*GRD
0108                 N1=N2
0109                 MN2=FMAX/DVA+1.0
0110                 AN2=MN2-1
0111                 N2=MN2+50
0112                 AW=DELW-BW
0113                 BW=(FMAX-AN2*DVA)/GRD
0114                 IF(N2-N1)350,350,780
0115             780 NFRST=N1+1
0116                 NLAST=N2-1
0117                 W=WN+AW
               C
0118                 DELN=AW*(A+B*(WN+W)+C*(WN**2+WN*W+W**2))
0119                 CTA(N1)=DELN+CTA(N1)
0120                 SUM=SUM+DELN
               C
0121                 IF(NLAST-NFRST)3001,3000,3000
               C
0122            3000 DO 300 KN=NFRST,NLAST
0123                 WW=W+DELW
0124                 DELN=DELW*(A+B*(W+WW)+C*(W**2+W*WW+WW**2))
```

```
0125              CTA(KN)=DELW+CTA(KN)
0126              SUM=SUM+DELW
0127          800 W=W+DELW
            C
0128         8001 WW=W+BW
0129              DELW=BW*(A+B*(W+WW)+C*(W**2+W*WW+WW**2))
0130              CTA(N2)=DELW+CTA(N2)
0131              SUM=SUM+DELW
0132              W=WW
0133              GO TO 900
            C
0134          850 CW=WX-WN
0135              DELW=CW*(A+B*(WN+WX)+C*(WN**2+WN*WX+WX**2))
0136              CTA(N1)=DELW+CTA(N1)
0137              SUM=SUM+DELW
0138          900 WN=WX
            C
0139              GO TO (20,30),NPRINT
0140           30 SUM=SUM/GU
0141              NDEL=N2-NMIN+1
0142         7654 DIFF=VOLUME-SUM
0143              WRITE (6,1000) V(L),GRD,AL(1),AL(2),AL(3),DELW,W1,VOLUME,DIFF,NDEL
            C
            C   THE VOLUME PRINTED HERE IS THE CORRECT VALUE , DIFF=CORRECT-SUMMED
            C
0144           20 CONTINUE
            C
0145              RETURN
0146              END
```

```
      SUBROUTINE JACOBI(A,B,E,N)
C
      DIMENSION A(3,3),B(3,3),E(3)
      DOUBLE PRECISION DENOM,YY,DD,YA
C
      EQUIVALENCE (Y,YA)
C
      S=0.0
      DO 10 I=1,N
   10 S=S+ABS(A(I,I))
      XN=N
      TEST=S/XN
      DO 12 I=1,N
      DO 11 J=1,N
   11 B(I,J)=0.0
   12 B(I,I)=1.0
      GO TO 15
   25 DO 13 I=2,N
      II=I-1
      DO 13 J=1,II
      P=A(I,J)
      IF(ABS(P)-AMAX)13,16,16
   16 Y=(A(J,J)-A(I,I))/2.
      D=Y**2+P*A(J,I)
      IF(D)18,18,80
   80 YSQ=Y+SQRT(D)
      IF(YSQ)31,31,17
   31 DD=YA**2+P*A(J,I)
      YY=DSQRT(DD)
      DENOM=Y+YY
      YSQ=DABS(DENOM)
      SIGNX=P*A(I,J)
      IF(SIGNX)32,75,75
   32 YSQ=-YSQ
   75 IF(YSQ)17,77,17
   77 C=0.
      S=1.
      GO TO 78
   17 X=P/YSQ
      GO TO 19
   18 X=P/Y
   19 U=SQRT(1.+X*X)
      C=1.0/U
      S=X*C
   78 DO 20 K=1,N
      Y=A(K,I)
      Z=A(K,J)
      A(K,I)=C*Y-S*Z
```

```
      A(K,J)=S*Y+C*Z
      Y=B(K,I)
      Z=B(K,J)
      B(K,I)=C*Y-S*Z
   20 B(K,J)=S*Y+C*Z
      DO 1 K=1,N
      Y=A(I,K)
      Z=A(J,K)
      A(I,K)=C*Y-S*Z
    1 A(J,K)=S*Y+C*Z
   13 CONTINUE
   15 S=0.0
      DO 21 I=2,N
      II=I-1
      DO 21 J=1,II
      IF(ABS(A(I,J))-S)21,21,22
   22 S=ABS(A(I,J))
   21 CONTINUE
   23 R=S/TEST
      AMAX=S/5.0
      IF(R-1.0E-5)24,24,25
   24 DO 26 I=1,N
   26 E(I)=A(I,I)
C
      RETURN
      END
```

```
      FUNCTION FDC(T)
C
C DIELECTRIC CONSTANT
C
C     CALCULATION OF A SCREENING FUNCTION.
C
C        IFT=1  K-INDEP. SCREENING
C        IFT=2  K-DEP.  SCREEN., HARTREE-APPR., NO EXCHANGE
C        IFT=3  AS 2, BUT WITH EXCHANGE, GENERAL FORMULA
C        IFT=4  AS 3, BUT SPECIAL EXCHANGE ACCORDING TO HUBBARD
C        IFT=5  AS 3, BUT SPECIAL EXCHANGE ACCORDING TO HARRISON
C        IFT=6  EFFECTIVE FDC WITH GENERAL EXCHANGE TERM
C        IFT=7  EFFECTIVE FDC WITH EXCHANGE ACCORDING TO HARRISON
C
C     CORREX=1+ETHA*(KC/KF)**2 MUST BE COMPUTED IN THE CALLING PROGRAM
C     FOR CASES 4 ( ETHA=0.5) AND 3 ( DESIRED VALUE OF ETHA), IT DOES
C     NOT APPLY FOR IFT=1,2 AND 5. WHERE USED THE MEANING OF ETHA IS
C
C        ETHA=(KS/KC)**2, KC=SCREEN.PARAM. FOR THE HARTREE-APPROX.
C                         KS=SCREEN.PARAM. FOR THE EXCHANGE CORRECTION.
C
      COMMON/NAFD/IFT,CORREX,QKCKF2
C
      IF(IFT.EQ.1.OR.T.EQ.0.0) GO TO 1
      IF(T.EQ.1.0) GO TO 2
      AB=ABS((1.0+T)/(1.0-T))
      TT=T**2
      FDC=0.5+(1.0-TT)*ALOG(AB)/(4.0*T)                              IFT=2
    3 GO TO (4,4,5,5,6,7,8),IFT
    5 FDC=FDC*(1.0-2.0*TT/(4.0*TT+CORREX))                           IFT=3,4
      RETURN
    6 FDC=FDC*(1.0-3.0*TT/(2.0+6.0*TT))                              IFT=5
      RETURN
    7 FDC=FDC/(1.-(.5*QKCKF2*FDC)/(4.*TT+CORREX))                    IFT=6
      RETURN
    8 FDC=FDC/(1.-(3.0*QKCKF2*FDC/8.0)/(1.0+3.0*TT))                 IFT=7
      RETURN
    1 FDC=1.0                                                        IFT=1
      IF(IFT.LE.5)RETURN
      TT=0.0
      GO TO 3
    4 RETURN
    2 FDC=0.5
      TT=1.0
      GO TO 3
      END
```

```
0001              SUBROUTINE FREQ(Q,GD1,GD2,GD3,NEG)
           C                                                                290
0002              DIMENSION Q(3),PH(3),A(3,3),B(3,3)
0003              DIMENSION EV(3,3),AA(3,3),DA(3,3),V(3),W(3),PX(60),QL(3)
0004              DIMENSION GD1(3),GD2(3),GD3(3)
0005              DIMENSION AMAS(12),DEN(3)                                 294
           C
0006              COMMON/C2/ANN
0007              COMMON/C3/PI,CPT,PX,GU,SC,NSFB,AMAS,GQ
0008              COMMON/C4/EV,PH
0009              COMMON/C7/N
0010              COMMON/FREPE/XP(4,48),YP(4,48),ZP(4,48)
0011              COMMON/MAFRE/RMAX,NT,DELK,NSK,CONIC,XT(33),YT(33),ZT(33),CNR(502),
                 1SK(502)
           C
0012              X=Q(1)
0013              Y=Q(2)
0014              Z=Q(3)
           C                                                                299
0015           90 FAC=0.0                                                   300
0016              IF(GQ-1.0)10,1004,10
0017         1004 D1Q=1.0E-4                                                302
0018              D2Q=-1.0E-4                                               303
0019              D3Q=1.0E-4                                                304
0020              Q(1)=Q(1)+D1Q                                             305
0021              Q(2)=Q(2)+D2Q                                             306
0022              Q(3)=Q(3)+D3Q                                             307
0023              FAC=1.0                                                   308
           C
0024           10 CALL ELEM(Q,A)                                            309
           C
0025              DO 12 I=1,N                                               310
0026              DO 12 J=1,N                                               311
0027           12 B(I,J)=A(I,J)                                             312
           C
0028              CALL JACOBI(B,EV,V,3)
           C
0029              DO 16 I=1,N
0030              IF(V(I))50,51,51
0031           51 PH(I)=SQRT(V(I)/SC)
0032           16 CONTINUE
           C
           C MIT * CALL EIGEN(B,V,3,1) * IST * 16 CONTINUE * ZU ERSETZEN DURCH
           C      DO 16 J=1,N
           C   16 EV(I,J)=B(I,J)
           C
0033              IF(NSK.EQ.0) GO TO 105
           C
```

```
C COMPUTE S(K)
C
C        APPLY ALL SYMMETRY OPERATIONS TO Q(I)=(X,Y,Z)
C        AND TO THE 3 POLARIZATION-VECTORS EV(I,2),EV(I,2),EV(I,3)
C        BELONGING TO Q(I)
C
      CALL PERM(X,Y,Z,1)
      CALL PERM(EV(1,1),EV(2,1),EV(3,1),2)
      CALL PERM(EV(1,2),EV(2,2),EV(3,2),3)
      CALL PERM(EV(1,3),EV(2,3),EV(3,3),4)
C
      DO 102 I=1,3
      ARG=CONIO*PH(I)
      IF(ARG.GT.33.0) GO TO 110
      EXPA=EXP(-ARG)
      EXPA1=1.0-EXPA
      DEN(I)=EXPA/(EXPA1*EXPA1)
      GO TO 102
  110 DEN(I)=0.0
  102 CONTINUE
C
C USE THE TRANSLATIONAL INVARIANCE OF THE LATTICE TO PASS TO THE
C REPEATED ZONE SCHEME.
C
      DO 101 J=1,48
      PQX=XP(1,J)
      PQY=YP(1,J)
      PQZ=ZP(1,J)
      PLX=XP(2,J)
      PLY=YP(2,J)
      PLZ=ZP(2,J)
      PT1X=XP(3,J)
      PT1Y=YP(3,J)
      PT1Z=ZP(3,J)
      PT2X=XP(4,J)
      PT2Y=YP(4,J)
      PT2Z=ZP(4,J)
      DO 101 L=1,NT
      XH=PQX+XT(L)
      YH=PQY+YT(L)
      ZH=PQZ+ZT(L)
      XYZ=SQRT(XH*XH+YH*YH+ZH*ZH)
C
C POINTS NOT LYING IN THE BRILLOUIN ZONE SECTOR ARE EXCLUDED
C BY THE FOLLOWING STATEMENTS. ALSO POINTS THAT ARE FARTHER AWAY
C FROM THE ORIGIN THAN RMAX ( SEE INPUT ).
C
      IF(ZH.LE.0.0.OR.XH.LT.YH.OR.YH.LT.ZH) GO TO 101
```

```
      IF(XH.GT.RMAX.OR.YH.GT.RMAX.OR.ZH.GT.RMAX.OR.XYZ.GT.RMAX)GO TO 101
      IF(XH.LE.0.0.OR.YH.LE.0.0) GO TO 101
C
C COMPUTE S(K) FOR THE ALLOWED POINTS
C
C DETERMINE THE STATISTICAL WEIGHT OF THE POINT
C
      XY=XH-YH
      YZ=YH-ZH
      ZX=ZH-XH
      GUT=6.0
      IF(XY.NE.0.0.AND.YZ.NE.0.0.AND.ZX.NE.0.0) GO TO 150
      GUT=1.0
      IF(XY.EQ.0.0.AND.YZ.EQ.0.0.AND.ZX.EQ.0.0) GO TO 150
      GUT=3.0
  150 CONTINUE
      PROD=XH*PLX+YH*PLY+ZH*PLZ
      SUM=PROD*PROD*DEN(1)
      PROD=XH*PT1X+YH*PT1Y+ZH*PT1Z
      SUM=SUM+PROD*PROD*DEN(2)
      PROD=XH*PT2X+YH*PT2Y+ZH*PT2Z
      SUM=SUM+PROD*PROD*DEN(3)
      SUM=SUM*GUT
      NK=XYZ/DELK+1.0
      CNR(NK)=CNR(NK)+GUT
      SK(NK)=SK(NK)+SUM
  101 CONTINUE
      IF(NSK.EQ.2) RETURN
  105 CONTINUE
C
   17 QL(1)=Q(1)+DQ
      QL(2)=Q(2)
      QL(3)=Q(3)
C
      CALL ELEM(QL,AA)
C
      DO 19 I=1,N
      DO 19 J=1,N
   19 DA(J,I)=        AA(I,J)-A(I,J)
      DA(I,J)=DA(J,I)
C
   22 CALL GRAD(DA,GD1)
C
      IF(Q(1)-Q(2))24,23,24
   24 QL(1)=Q(1)
      QL(2)=Q(2)+DQ
      QL(3)=Q(3)
C
```

```
0103          CALL ELEM(QL,AA)                                          328
        C
0104          DO 29 I=1,N                                               329
0105          DO 29 J=1,N                                               330
0106       29 DA(J,I)=          AA(I,J)-A(I,J)                          331
0107          DA(I,J)=DA(J,I)
        C
0108       32 CALL GRAD(DA,GD2)                                         332
        C
0109          IF(Q(2)-Q(3))23,25,26                                     333
0110       23 DO 33 J=1,N                                               334
0111       33 GD2(J)=GD1(J)                                             335
0112       26 QL(1)=Q(1)                                                336
0113          QL(2)=Q(2)                                                337
0114          QL(3)=Q(3)+DQ                                             338
        C
0115          CALL ELEM(QL,AA)                                          339
        C
0116          Q(1)=Q(1)-FAC*D1Q                                         340
0117          Q(2)=Q(2)-FAC*D2Q                                         341
0118          Q(3)=Q(3)-FAC*D3Q                                         342
0119          DO 34 I=1,N                                               343
0120          DO 34 J=1,N                                               344
0121       34 DA(J,I)=          AA(I,J)-A(I,J)                          345
0122          DA(I,J)=DA(J,I)
        C
0123       37 CALL GRAD(DA,GD3)                                         346
        C
0124          DO 370 J=1,N                                              347
0125      370 PH(J)=PH(J)-(GD1(J)*D1Q+GD2(J)*D2Q+GD3(J)*D3Q)*FAC        348
        C
0126          RETURN                                                    349
0127       25 DO 40 J=1,N                                               350
0128       40 GD3(J)=GD2(J)                                             351
        C
0129       38 RETURN                                                    352
        C
0130       50 WRITE (6,52) (Q(I),I=1,3),(V(I),I=1,3)
0131       52 FORMAT (////17HOMESH POINT Q(I)=E14.5,1H,E14.5,1H,E14.5,40H  NOT C
             1OUNTED IN FREQUENCY DISTRIBUTION    ,/35HOBECAUSE OF NEGATIVE EIGEN
             2 VALUES    3E14.5,20H    OF THE DYNAMICAL MATRIX.    )
0132          NEG=1
0133          RETURN
0134          END                                                       353
```

```
0001            SUBROUTINE PERM1(X,Y,Z,I)
          C     SYMMETRY OPERATIONS OF A CUBIC (SC,BCC,FCC) LATTICE
          C     ARE APPLIED TO A VECTOR X,Y,Z.
          C
          C     I=1    X,Y,Z=RED Q-VECTOR
          C     I=2    X,Y,Z=*LONGITUDINAL*-POLARIZATION-VECTOR
          C     I=3    X,Y,Z=*1.TRANSVERSAL*-POL.VECTOR
          C     I=4    X,Y,Z=*2.TRANSVERSAL*-POL.VECTOR
          C
          C     RESULT IN XP(I,N),YP(I,N),ZP(I,N)
          C     N=1,...48 IS THE NUMBER OF PERMUTATION
          C
0002            COMMON/FREPE/XP(4,48),YP(4,48),ZP(4,48)
0003            N=1
0004            K=0
0005         10 XP(I,N)=X
0006            XP(I,N+1)=X
0007            XP(I,N+2)=Y
0008            XP(I,N+3)=Y
0009            XP(I,N+4)=Z
0010            XP(I,N+5)=Z
0011            YP(I,N)=Y
0012            YP(I,N+1)=Z
0013            YP(I,N+2)=X
0014            YP(I,N+3)=Z
0015            YP(I,N+4)=Y
0016            YP(I,N+5)=X
0017            ZP(I,N)=Z
0018            ZP(I,N+1)=Y
0019            ZP(I,N+2)=Z
0020            ZP(I,N+3)=X
0021            ZP(I,N+4)=X
0022            ZP(I,N+5)=Y
0023            N=N+6
0024            K=K+1
0025            GO TO (1,2,3,4,5,6,7,8),K
0026          1 X=-X
0027            GO TO 10
0028          2 Y=-Y
0029            GO TO 10
0030          3 Z=-Z
0031            GO TO 10
0032          4 X=-X
0033            GO TO 10
0034          5 Y=-Y
0035            GO TO 10
0036          6 X=-X
0037            GO TO 10
```

```
0038      7 X=-X
0039        Y=-Y
0040        Z=-Z
0041        GO TO 10
0042      8 Y=-Y
0043        RETURN
0044        END
```

```
      SUBROUTINE GIPLOT(XFACT,YFACT)
C
      COMMON/MAGN/W(13)
      COMMON/C5/G(3000),LA,DF,AHALF,VOLUME,ASQ,NPRINT,XMAX
      COMMON/MAELGN/NSH1,CL32,CLB,KP,NWAY,PIA2,CON1,CON2,CON4,SHS,NEX,B(
     125),NPPS(60),HPX(3103),HPY(3103),HPZ(3103),FSPH(60),X(3000)
C
      NDIM=XMAX/DF
      NDIM1=NDIM+1
      DO 2 L=1,NDIM
      K=NDIM1-L
      IF(G(K).GT.0.0) GO TO 3
    2 CONTINUE
    3 CK=K
      XMAX=CK*DF
      GMAX=0.0
      DO 4 L=1,K
      IF(G(L).LE.GMAX) GO TO 4
      GMAX=G(L)
    4 CONTINUE
      X(1)=DF/2.0
      DO 1 L=2,K
    1 X(L)=X(L-1)+DF
      PLOTX=XMAX*XFACT
      PLOTX1=PLOTX+10.0
      PLOTY=GMAX*YFACT
      SYMBY=PLOTY+2.0
      CALL FINM(10.,10.)
      CALL SYMBL4(0.,SYMBY,.4,0.,W(1),30,0.)
      CALL DESSIN(X,G,K,1,1,1,0,0,PLOTX,PLOTY,0,0,1H ,1,1H ,1,0)
      CALL FINM(PLOTX1,0.0)
      RETURN
      END
```

```
0001          SUBROUTINE SKRES
        C
0002          DIMENSION SR(502),XKFF(502),DWFSP(502),EXPWSP(502)
0003          COMMON/ MAELGN/NSHI,CLB2,CLB,KP,NWAY,PIA2,CON1,CON2,CON4,SHS,NEX,B(
             125),NPPS(50),NPX(3103),NPY(3103),NPZ(3103),FSPH(60),FSIMP(3000)
0004          COMMON/C5/CTA(3000),LA,DVA,AHALF,VOLUME,ASQ,NPRINT,XM
0005          COMMON/ MAFRE/RMAX,NT,DELK,NSK,CON10,DUMMY(99),CNR(502),SK(502)
0006          COMMON/ MAGN/ N(13)
0007          COMMON/ MASK/CON3,CON7,CON8,CON9,PIA,NRES,NSKPL,NPLOT,NCAN,DWF,TEMP
             1,VUMAX
0008          EQUIVALENCE (FSIMP,SR),(FSIMP(503),XKFF),(FSIMP(1005),DWFSP),(FSIM
             1P(1507),EXPWSP)
        C
0009          IF(DWF.NE.0.0.OR.NSK.EQ.2)GO TO 801
        C
        C COMPUTE DEBYE-WALLER FACTOR DWF TO TEMPERATURE TEMP
        C
0010          MA=LA-50
0011          MA1=MA+1
0012          DO 802 L=1,MA
0013          KK=MA1-L
0014          IF(CTA(KK).GT.0.0)GO TO 803
0015      802 CONTINUE
0016      803 CK=KK
0017          VUMAX=(CK-0.5)*DVA
0018          IF(2*(KK/2).EQ.KK)KK=KK+1
0019          DO 804 KL=1,KK
0020          CKL=KL
0021          VU=(CKL-0.5)*DVA
0022          X=CON10*VU
0023          IF(X.GT.88.0) GO TO 805
0024          EX1=EXP(X)-1.0
        C NOTE THAT FSIMP IS EQUIVALENT TO CTC
0025          FSIMP(KL)=CTA(KL)*(0.5+1./EX1)/VU
0026          GO TO 804
0027      805 FSIMP(KL)=0.5*CTA(KL)/VU
0028      804 CONTINUE
0029          DWF=(VUMAX/3.0)*(SIMPC(DVA,KK)+(5.0*FSIMP(1)-FSIMP(2))*DVA/8.0)
0030      801 CONTINUE
        C
0031          WRITE (6,1002) (N(L),L=10,13)
0032          WRITE (6,9123) TEMP
0033          IF(DWF.NE.0.0) GO TO 833
0034          WRITE (6,9120)
0035          DO 832 L=1,NCAN
0036      832 SK(L)=CON7*(SK(L)/CNR(L))
0037          GO TO 834
0038      833 X=-DELK/2.0
```

```
            DO 835 L=1,NCAN
            X=X+DELK
            X2=X*X*CON8*DWF/VUMAX
            DWFSP(L)=X2
            EXPW=EXP(-X2)
            EXPWSP(L)=EXPW
        835 SK(L)=CON7*EXPW*(SK(L)/CNR(L))
            WRITE (6,9133) DWF
        834 X=-DELK/2.0
            WRITE (6,9132)
            FSP=0.0
            DO 836 L=1,NCAN
            X=X+DELK
            XKF=X*CON2
            XKFF(L)=XKF
            IF(NRES.EQ.0)GO TO 838
            X2=X*X
            EXX2=EXP(-X2*CLB2)
            IF(KP.EQ.1)GO TO 822
            IF(NWAY.GT.2)AX=(PIA2*X)**NEX
            IF(NWAY.LE.2)AX=(CLB*X)**NEX
            S1=0.0
            DO 823 KL=2,KP
        823 S1=(S1+B(KL))*AX
            S1=1.+S1
            FSP=EXX2*S1/(X2+CON1*FDC(CON2*X))
            GO TO 824
        822 FSP=EXX2/(X2+CON1*FDC(CON2*X))
        824 FSP=-FSP*CON3/(PIA*PIA)
            SR(L)=FSP*FSP*SK(L)*XKF*XKF*XKF
        838 NCNR=CNR(L)
        836 WRITE (6,9131) X,XKF,FSP,SK(L),DWFSP(L),EXPWSP(L),NCNR
            IF(ISKPL.EQ.0) GO TO 837
      C
      C PLOT S(K)
      C
            IF(IPLOT.EQ.0) CALL FINIM(10.,10.)
            PLOTX=XKFF(NCAN)*10.0
            CALL SYMBL4(0.,10.,.4,0.,W(10),36,0.)
            CALL DESSIN(XKFF,SK,NCAN,1,1,1,0,0,PLOTX,10.,0,0,1H , 1,1H ,1,0)
            PLOTX1=PLOTX+10.0
            CALL FINIM(PLOTX1,0.0)
        837 CONTINUE
            IF(NRES.EQ.0)GO TO 825
      C
      C COMPUTE THE ELECTRICAL RESISTIVITY.
      C
            IF(IFT.GT.5) IFT = IFT-2
```

```
              C
0081                DELKF=DELK*CON2
0082                CLIM=1.0
0083                N=CLIM/DELKF+1.0
0084                IF(2*(N/2).EQ.N) N=N+1
0085                IF(N.LE.NCAN) GO TO 825
0086                CNCAN=NCAN
0087                CLIMCR=(CNCAN-0.5)*DELKF
0088                WRITE (6,9133) CLIMCR
0089                N=NCAN
0090            825 SPRES=SIMPC(DELK,N)
              C
              C CORRECTIONS FOR THE INTEGRAL
              C
0091                CORR2=0.0
0092                DIFF=CLIM-XKFF(N)
0093                IF(DIFF)828,826,827
0094            827 FC=SR(N)+DIFF*(SR(N+1)-SR(N))/(2.0*DELKF)
0095                CORR2=FC*DIFF
0096                GO TO 826
0097            828 Y=DELKF+DIFF/2.0
0098                FC=SR(N-1)+Y*(SR(N)-SR(N-1))/DELKF
0099                CORR2=FC*DIFF
0100            826 CONTINUE
0101                CORR1=(5.0*SR(1)-SR(2))*DELKF/8.0
0102                WRITE (6,9134) SPRES,CORR1,CORR2
0103                SPRES=(SPRES+CORR1+CORR2)*CON9
0104                WRITE (6,9135) SPRES
0105                RETURN
              C
0106           1002 FORMAT (1H1,9A4)
0107           9128 FORMAT (//,95H STRUCTURE FACTOR S(Q) AVERAGED OVER ALL DIRECTIONS
                   1FOR FIXED Q / ONE PHONON APPROXIMATION / T=F7.2)
0108           9129 FORMAT (35H DEBYE-WALLER FACTOR NOT INCLUDED        )
0109           9130 FORMAT (34H DEBYE-WALLER FACTOR INCLUDED DWF=E12.5)
0110           9131 FORMAT (6E16.5,I9)
0111           9132 FORMAT (//,4X,12HQ=K/(2*PI/A),6X,10HQ=K/(2*KF),5X,10HV(Q) IN EV,9X
                   1,4HS(Q),13X,2H2Q,11X,8HEXP(-2W),3X,13HQ-PTS/CHANNEL,//)
0112           9133 FORMAT (//92H RESULT FOR THE ELECTRICAL RESISTIVITY MIGHT BE INCOR
                   1RECT, BECAUSE HIGHER INTEGRATION LIMIT=E12.5,15H INSTEAD OF 1.0)
0113           9134 FORMAT (/10H INTEGRAL=E12.5,10H     CORR1=E12.5,10H     CORR2=E12.5)
0114           9135 FORMAT (//24H ELECTRICAL RESISTIVITY=E12.5,15H MICRO-OHM*CM     )
              C
0115                END
```

APPENDIX III - P R O G R A M CVDWF

```
      C
      C        PROGRAM CVDWF (SPECIFIC HEAT AND DEBYE-WALLER FACTOR)
      C
      C        CVDWF  CALCULATES THE SPECIFIC HEAT AT CONSTANT VOLUME CV AND THE
      C        DEBYE-WALLER FACTOR DWF OF BCC OR FCC CRYSTALS TO AN INPUT
      C        FREQUENCY-DISTRIBUTION FUNCTION. THE DEBYE-TEMPERATURE AS A
      C        FUNCTION OF THE ABSOLUTE TEMPERATURE IS AVAILABLE OF BOTH OF THEM
      C        WRITTEN IN FORTRAN 4 LANGUAGE
      C
      C
0001           DIMENSION W(9),CD(3001),DW(5001),ARG(300),CT(300),WT(300),WD(300),
              1T(300),F2(2051),GN(2051) ,TEXT(16),Z(5001)
      C
0002           COMMON F1(2051)
      C
0003           DATA   W/36HTEST / DEBYE FREQU.DISTRIB. FOR GN   /
0004           DATA   W/36HTEST / DEBYE FREQU.DISTRIB. FOR GN   /
      C
0005           NDIMGN=2051
0006           DO 200  I=1,NDIMGN
0007       200 GN(I)=0.0
      C
0008           NDIMCD=3001
0009           DO 201  I=1, NDIMCD
0010       201 CD(I)=0.0
      C
0011           NDIMDW=5001
0012           DO 202  I=1,NDIMDW
0013       202 DW(I)=0.0
      C
      C        NTEST=1    ES WIRD MIT EINER FREQUENZVERTEILUNG NACH DEBYE
      C                   GERECHNET MIT VUMAX=(NV-1/2)*DELTAV
      C        NTEST=0    NV, DELTAV WIRD BEIM EINLESEN DER ZU VERWENDENDEN
      C                   FREQU.VERTEILUNG GN UEBERLESEN
      C
0014           READ (5,11) N1,N2,NPLOT,NT,DELTAT,NTEST,NV,DELTAV
0015           WRITE (6,11) N1,N2,NPLOT,NT,DELTAT,NTEST,NV,DELTAV
      C
0016           IF(NV.GT.2051)  GO TO 101
0017           NDATA=0
0018           NDW=0
0019           IF(N1.NE.2)  GO TO 89
0020           READ (5,13)  NDATA,DELTAX
0021           WRITE (6,13)  NDATA,DELTAX
0022           READ (5,12)  (CD(L),L=1,NDATA)
      C
0023        89 IF(N2.NE.2)  GO TO 90
0024           READ (5,13)  NDW,DELXW
```

```
      WRITE (6,13) NDW,DELXW
      READ (5,8) (DW(L),L=1,NDW)
C
      DO 222 I=1,NDW
      Z(I)=I*DELXW
  222 DW(I)=DW(I)*3*47.993/Z(I)
C
   90 IF(NTEST.GT.0) GO TO 102
      READ (5,14) N,NV,DELTAV
      WRITE (6,14) N,NV,DELTAV
      NV5=NV/5
      NV55=5*NV5
      NVDIFF=NV-NV55
      K=-4
      DO 70 I=1,NV5
      K=K+5
      K5=K+4
      READ (5,15) NI,(GN(L),L=K,K5)
      WRITE (6,15) NI,(GN(L),L=K,K5)
      IF(NI.NE.I) GO TO 71
   70 CONTINUE
      IF(NVDIFF.EQ.0) GO TO 72
      K=NV55+1
      KE=NV55+NVDIFF
      READ (5,15) NI,(GN(L),L=K,KE)
      WRITE (6,15) NI,(GN(L),L=K,KE)
      I=I+1
      IF(NI.NE.I) GO TO 71
   72 CONTINUE
      IF(NT.GT.3001.OR.NDATA.GT.3001.OR.NDW.GT.5001.OR.NV.GT.2051) GO TO
     1101
C
      WRITE (6,19)
      WRITE (6,9) N
      WRITE (6,20) NV,DELTAV
      WRITE (6,17) (GN(L),L=1,NV)
      WRITE (6,1 )
C
      DO 54 L=1,NT
      ARG(L)=0.0
      CT(L)=0.
      WT(L)=0.
   54 WP(L)=0.
      T(1)=0.
      DO 53 L=2,NT
   53 T(L)=T(L-1)+DELTAT
      NV1=NV+1
      DO 95 L=1,NV
```

TEST

```
0068           KK=NV1-L
0069           IF(GN(KK).GT.0.0) GO TO 96
0070        95 CONTINUE
0071        96 CNV=KK
0072           CNV=CNV-0.5
0073           VMAX=CNV*DELTAV
0074           VMAX2=VMAX/2.
0075           KK=KK+1
0076           IF(2*(KK/2).EQ.KK) KK=KK+1
0077           IF(KK.GT.201) KK=KK-2
      C
      C BERECHNE CV UND DWF
      C
0078           DO 3 K=2,NT
0079           VU=-DELTAV/2.0
0080           TT=47.993/T(K)
0081           DO 4 KL=1,KK
0082           VU=VU+DELTAV
0083           X=TT*VU
0084           IF(X.GT.85.0) GO TO 100
0085           EX=EXP(X)
0086           EX1=EX-1.
      C
0087           IF(N1.GT.0)F1(KL)=GN(KL)*EX*(X/EX1)*(X/EX1)
0088           IF(N2.GT.0)F2(KL)=GN(KL)*(0.5+1./EX1)/VU
0089           GO TO 4
0090       100 IF(N1.GT.0) F1(KL)=0.0
0091           IF(N2.GT.0) F2(KL)=0.5*GN(KL)/VU
0092         4 CONTINUE
0093           IF(N1.GT.0)CT(K)=SIMPCR(DELTAV,KK,1)
0094           IF(N2.LE.0) GO TO 3
0095           DO 104 L=1,KK
0096       104 F1(L)=F2(L)
0097           WT(K)=SIMPCR(DELTAV,KK,1)*T(K)
0098         3 CONTINUE
      C
      C T-DEBYE ALS FUNKTION VON T-ABS. MIT CV
      C
0099           IF(N1.NE.2) GO TO 21
0100           NDATA1=NDATA-1
0101           CDMAX=CD(NDATA1)
0102           DO 55 L=2,NT
0103           CTL=CT(L)
0104           IF(CTL.GE.CDMAX) GO TO 57
0105           IF(CTL.GT.0.0) GO TO 58
0106           ARG(L)=0.0
0107           GO TO 55
0108        58 ARG(L)=T(L)*(77.92727/CTL)**0.3333333
```

```
   55 CONTINUE
      GO TO 21
   57 NN=L
      DO 51 K=1,NDATA1
      IF(CTL.GE.CD(K)) GO TO 52
   51 CONTINUE
      WRITE (6,5) CTL,T(L)
      STOP
   52 KEFF=K
      KEFF1=KEFF+1
      KIN=1
      DO 50 L=NN,NT
      IF(CT(L).GT.CT(L-1)) GO TO 106
      WRITE (6,105) T(L)
  106 DO 94 K=KIN,KEFF
      KK=KEFF1-K
      DIFF=CD(KK)-CT(L)
      IF(DIFF)94,60,60
   94 CONTINUE
   60 CKK=KK-1
      DF=CD(KK)-CD(KK+1)
      APC(L)=(CKK+DIFF/DF)*DELTAX*T(L)
      KIN=K
   50 CONTINUE
   21 CONTINUE
C
C T-DEBYE ALS FUNKTION VON T-ABS. MIT DWF
C
      IF(N2.NE.2) GO TO 23
      PI=3.141592
      NDW1=NDW-1
      DWMAX=DW(NDW1)
      DO 65 L=2,NT
      WTL=WT(L)
      IF(WTL.GE.DWMAX) GO TO 67
      WTL25=WTL-.25
      IF(WTL25.GT.1.0E-30) GO TO 63
      WD(L)=0.0
      GO TO 65
   63 WD(L)=T(L)*PI/SQRT(6.*WTL25)
   65 CONTINUE
      GO TO 23
   67 NN=L
      DO 61 K=1,NDW
      IF(WTL.GE.DW(K)) GO TO 62
   61 CONTINUE
      WRITE (6,7) WTL,T(L)
      STOP
```

```
0154         62 KEFF=K
0155            KEFF1=K+1
0156            KIN=1
0157            DO 69 L=NN,NT
0158            IF(WT(L).GT.WT(L-1)) GO TO 107
0159            WRITE (6,108) T(L)
0160        107 DO 93 K=KIN,KEFF
0161            KK=KEFF1-K
0162            DIFF=DW(KK)-WT(L)
0163            IF(DIFF)93,68,68
0164         93 CONTINUE
0165         68 CKK=KK
0166            DF=DW(KK)-DW(KK+1)
0167            WD(L)=(CKK+DIFF/DF)*DELXW*T(L)
0168            KIN=K
0169         69 CONTINUE
0170         23 CONTINUE
      C
      C         AUSGABE
      C
0171            WRITE (6,6) (T(L),CT(L),ARG(L),WT(L),WD(L),L=2,NT)
0172         22 CONTINUE
0173            STOP
0174         71 I=I-1
0175            WRITE (6,16) I
0176            STOP
0177        101 WRITE (6,18)
0178            STOP
      C
      C BERECHNE FREQU.VERTEILUNG NACH DEBYE
      C
0179        102 IF(2*(NV/2).EQ.NV) NV=NV+1
0180            CNV=NV
0181            VUMAX=(CNV-0.5)*DELTAV
0182            VUMAX3=VUMAX*VUMAX*VUMAX/3.0
0183            VU=-DELTAV/2.0
0184            DO 103 L=1,NV
0185            VU=VU+DELTAV
0186        103 CN(L)=VU*VU/VUMAX3
0187            GO TO 72
      C
0188          5 FORMAT (4H1CV=,E12.5,8H  FOR T=,E12.5,53H  NOT FOUND IN TAB. DEBYE
             1-SPECIFIC-HEAT FUNCTION.          )
0189          6 FORMAT (/,(F10.2,E16.5,E12.4,E16.5,F15.4))
0190          7 FORMAT (7H1DW-F.=,E12.5,8H  FOR T=,E12.7,45H  NOT FOUND IN TAB. DE
             1BYE-WALLER FUNCTION.         )
0191          8 FORMAT (5E14.9)
0192          9 FORMAT (//,1H0,9A4)
```

```
0193          10 FORMAT (//105H0SPECIFIC HEAT CV, DEBYE-TEMPERATURE AND DEBYE WALLE
                1R FACTOR AS FUNCTIONS OF THE ABSOLUTE TEMPERATURE.       //4X,6HT-
                2ABS.,7X,8HCV/MODEL,3X,10HT-DEBYE/CV,5X,11HDW-F./MODEL,5X,11HT-DEBY
                3E/DWF)
0194          11 FORMAT (4I3,E12.5,2I6,E12.5)
0195          12 FORMAT (6F12.9)
0196          13 FORMAT (I6,F12.8)
0197          14 FORMAT (9A4,I6,E12.5)
0198          15 FORMAT (I5,5D15.8)
0199          16 FORMAT (77H1SEQUENCE OF DATA DECK ON NOT CORRECT, LAST CORRECT CAR
                1D HAS SEQUENCE NUMBER ,I4,3H  .)
0200          17 FORMAT (//,(10E11.3))                                                TEST
0201          18 FORMAT (78H1TOO LARGE NT, NDATA, NDW OR NV. STORAGE OVER FLOW. COM
                1PUTATION INTERRUPTED.      )
0202          19 FORMAT (30H1THERMODYNAMICAL QUANTITIES      )
0203          20 FORMAT (4H0NV=,I4,3X,7H0DELTAV=E12.5)
0204         105 FORMAT (21H0CHECK CV/MODEL AT T=F6.2,34H,  T-DEBYE/CV COULD BE INC
                1ORRECT.      )
0205         108 FORMAT (24H0CHECK DW-F./MODEL AT T=F6.2,36H,  T-DEBYE/DWF COULD BE
                1 INCORRECT.      )
           C
0206             END
```

```
0001            FUNCTION SIMPCR(DT,LIMIT,NCORR)
          C
          C  INTEGRATION EINER FUNCTION FUNC NACH SIMPSON
          C
          C       LIMIT IST DIE (UNGERADE) ANZAHL DER FUNKTIONSWERTE FUNC, DIE FUER
          C       AEQUIDISTANTE PUNKTE ( SCHRITTWEITE DT) IHRES ARGUMENTES GEGEBEN
          C       SIND. FUNC(1) UND FUNC(LIMIT)=F-WERTE AN DEN INT.GRENZEN.
          C
0002            COMMON FUNC(2051)
          C
0003            LIMIT1=LIMIT-1
0004            SUM=0.0
0005            SUM1=0.0
0006            FUNC(1)=FUNC(1)*0.5
0007            FUNC(LIMIT)=FUNC(LIMIT)*0.5
0008            DO 1 I=1,LIMIT,2
0009          1 SUM=SUM+FUNC(I)
0010            DO 2 I=2,LIMIT1,2
0011          2 SUM1=SUM1+FUNC(I)
0012            SIMPCR=(0.333333*DT)*(4.*SUM1+2.*SUM)
          C
          C KORREKTUR, WENN FUNC(1)=F-WERT FUER DAS ARGUMENT X=DT/2 ( UND NICHT
          C FUER X=0 ).
          C
0013            IF(NCORR.EQ.0) RETURN
0014            Y=(FUNC(2)-FUNC(1))/4.0
0015            SIMPCR=SIMPCR+(FUNC(1)-Y)*DT/2.0
0016            RETURN
0017            END
```

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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