DEUTSCHES ELEKTRONEN-SYNCHROTRON DESY

DESY SR-73/5
~~March~~ 1973

Kramers-Kronig Analysis of Reflection Data

by

R. Klucker and U. Nielsen

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KRAMERS - KRONIG - ANALYSIS OF REFLECTION DATA

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PROGRAM SUMMARY

Title of program: KRKRAN

Catalogue number:

Computer for which the program is designed and upon which it is operable

Computer: IBM 360/75 or IBM 360/65 Installation: Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Operating system or monitor under which the program is executed: OSMVT/Release 20.6

Programming languages used: FORTRAN IV

High speed store required 64 k bytes. No of bits in a byte: 8

Is the program overlaid? No

No of magnetic tapes required: None

What other peripherals are used: Card reader; Line printer

No of cards in combined program and test deck: 531

Card punching code: EBCDIC IBM 029

CPC library subprograms used: none

Reference to other published version of this program: none

Keywords descriptive of problem and method of solution:

Solid state physics, Dispersion-relation, Kramers-Kronig-Integral, Reflectance, Optical constants, Dielectric constants

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Nature of physical problem

Optical and dielectric constants of insulators and semiconductors are calculated from reflectance spectra using the Kramers-Kronig-Dispersion-relation[1]:

$$\mathrm{Im}(f(\omega_k)) = -\frac{2\omega_k}{\pi}\int_0^\infty \frac{\mathrm{Re}(f(\omega))}{\omega^2-\omega_k^2}\,d\omega \qquad (1)$$

$\mathrm{Im}(f(\omega))$, $\mathrm{Re}(f(\omega))$ are the imaginary and the real part of the complex function $f(\omega)$, respectively (e.g. $f(\omega) = \hat{\varepsilon}(\omega) = \varepsilon_1(\omega)+i\varepsilon_2(\omega)$).

Method of solution

Since reflectance spectra are only available in a restricted frequency range, say between ω_ℓ and ω_u, the integral of eq (1) is split into 3 parts:

$$\int_0^\infty = \int_0^{\omega_\ell} + \int_{\omega_\ell}^{\omega_u} + \int_{\omega_u}^\infty = I_{o\ell} + I_{\ell u} + I_{u\infty}$$

$I_{o\ell}$ and $I_{u\infty}$ are evaluated by assuming physical reasonable extrapolation functions:

1. For $0 \leq \omega \leq \omega_\ell$ $\mathrm{Re}(f(\omega)) = \mathrm{Re}(f(\omega_\ell))$ is assumed.
2. For $\omega > \omega_u$ the electrons of the material are treated as to behave like a free electron gas.

For $\omega_\ell \leq \omega \leq \omega_u$ $\mathrm{Re}(f(\omega))$ is expanded within small intervalls to powers of ω (up to some degree m). Then $I_{\ell u}$ is evaluated by using these approximations and by summation over all intervalls.

Restriction on the complexity of the problem

1. This program computes optical and dielectric constants only from reflectance spectra which are obtained with polarized light, the electrical field vector of which is lying either perpendicular or parallel to the plane of incidence.

2. For the integration only the linear term of the expansion of $Re(f(\omega))$ is used. But according to the long write-up this program may easily be modified if higher approximations are desired.

Typical running time

Typical running time is about 50 sec on the IBM 360/75 for one set of data and an output of 6000 lines printed.

Unusual features of the program

1. This program is especially suited to accept data in form of punched cards from a card punching machine (IBM 024). The original curves are converted by means of a X-Y-recorder with retransmitting slidewire potentiometers and an analog-digital converter connected to this punching machine[2].

2. This program provides a test on the accuracy of the results and the used extrapolation functions. Consistency of the results are tested by calculating $\varepsilon_2^{Test}(\omega)$ by means of eq (1) from the generated $\varepsilon_1(\omega)$-curve and comparing it with $\varepsilon_2(\omega)$.

References

1. D.M. Roessler, Brit.J.Appl.Phys. 16, 1359 (1965)

2. B. Sonntag, Thesis, University of Hamburg, Hamburg, Germany (1969)

LONG WRITE-UP

1. INTRODUCTION

1.1 Relation between $\hat{\varepsilon}(\omega)$ and $R(\omega)$

As Kramers[1] and Kronig[2] have shown, dispersion relations can be formulated for a large number of physical systems, for which complex functions describe the response of a system. Examples of such complex functions which are of relevance for solid state and optical physics are[3]:

a) complex dielectric constant $\hat{\varepsilon}(\omega) = \varepsilon_1(\omega) + i\cdot\varepsilon_2(\omega)$

b) complex refraction index $\hat{n}(\omega) = n(\omega) + i\cdot k(\omega)$

c) complex reflection ratio $\ln\hat{r}(\omega) = \ln(\sqrt{R}\cdot e^{i\cdot\Theta})$ (1)

where ω is the frequency, R the reflectance, and Θ the phaseshift between incident and reflected wave.

Real part $f_1(\omega)$ and imaginary part $f_2(\omega)$ of such functions are connected by:

$$f_2(\omega_k) = -\frac{2\omega_k}{\pi}\int_0^\infty \frac{f_1(\omega)}{\omega^2-\omega_k^2}\,d\omega \qquad (2)$$

To calculate $\hat{\varepsilon}(\omega)$ from $\hat{r}(\omega)$ we use Fresnel's equation for the reflectance of light with the electrical vector perpendicular to the plane of incidence (s-polarization, ϕ: angle of incidence; now we omit ω):

$$\hat{r} = \frac{(\hat{\varepsilon}-\sin^2\phi)^{1/2}-\cos\phi}{(\hat{\varepsilon}-\sin^2\phi)^{1/2}-\cos\phi} \qquad (3)$$

and a similar expression for p-polarization

Writing $(\hat{\varepsilon}-\sin^2\phi)^{1/2} = a+i\cdot b$ we obtain from eqs. (1) and (3) for ε_1 and ε_2 the following expressions:

$$\varepsilon_1 = a^2-b^2+\sin^2\phi$$

$$\varepsilon_2 = 2ab \qquad \text{with} \qquad a = (1-R)\cos\phi/c$$

$$b = 2\sqrt{R}\cdot\sin\Theta\cdot\cos\phi/c \qquad (4)$$

$$c = 1-2\sqrt{R}\cdot\cos\Theta+R$$

and by straight forward calculations the equations for the other optical constants, n, k etc.[4]

1.2 Extrapolation

Reflectance spectra are only given in the interval $\omega_\ell = \omega_1 \leq \omega \leq \omega_n = \omega_u$ for not necessary equally spaced discret frequency values (ω_i). Therefore we have to take physical reasonable values resulting for those parts of the integral spanning the intervals $0 \leq \omega \leq \omega_1$ and $\omega_n \leq \omega \leq \infty$.

These values here are obtained by extrapolating the reflectance spectra:

a) In the frequency region $0 \leq \omega \leq \omega_1$ $R(\omega) = R(\omega_1)$ is taken.

b) For $\omega > \omega_n$ the electrons of the material are treated to behave like a free electron gas. The high frequency dielectric constant then is given by eq. (5):[5]

$$\hat{\varepsilon}(\omega) = 1 + \frac{\omega_p^2}{\omega^2} \tag{5}$$

with ω_p = plasma frequency. From this equation we obtain the asymptotic high frequency behaviour of ε_1, ε_2 and R as follows

$$\begin{aligned} (\varepsilon_1 - 1) &\propto \omega^{-2} \\ \varepsilon_2 &\propto \omega^{-3} \\ R &\propto \omega^{-4} \end{aligned} \tag{6}$$

2. INTEGRATION OF DISPERSION INTEGRAL

2.1 Integration of eq. (2) between $\omega = 0$ and $\omega = \omega_n$

In the interval $\omega_i \leq \omega \leq \omega_{i+1}$ $(i=1,\ldots,n)$ function $f_1(\omega)$ is expanded to powers of ω:

$$f_1(\omega) = \sum_{j=0}^{\infty} a_{ji} \cdot \omega^j \tag{7}$$

Using $\int_0^\infty \frac{d\omega}{\omega^2-\omega_k^2} = 0$, one gets by simple straightforward evaluation

$$\frac{f_i(\omega) - f_i(\omega_k)}{\omega^2-\omega_k^2} = \frac{s_{1i}}{\omega+\omega_k} + \sum_{j=2}^{\infty} s_{ji}\omega^{j-2} \tag{8}$$

with $$s_{ji} = \sum_{\ell=0}^{\infty} a_{2\ell+j,i}\,\omega_k^{2\ell} \tag{9}$$

The contribution of the above interval to integral (2) then is given by

$$I_{i,i+1} = \begin{cases} s_{1i}\ln\dfrac{\omega_{i+1}+\omega_k}{\omega_i+\omega_k} + \displaystyle\sum_{j=2}^{\infty}\frac{s_{ji}}{j-1}\left(\omega_{i+1}^{j-1} - \omega_i^{j-1}\right) \\ + (s_o+\omega_k s_1)\cdot\dfrac{1}{2\omega_k}\left(\ln\left|\dfrac{\omega_{i+1}-\omega_k}{\omega_i-\omega_k}\right| - \ln\dfrac{\omega_{i+1}+\omega_k}{\omega_i+\omega_k}\right) \end{cases} \tag{10}$$

with $\omega_k \neq \omega_i,\ \omega_{i+1}$

Now only a linear approximation of $f_i(\omega)$ is used, leading to

$$s_{oi} = a_{o1},\ s_{1i} = a_{1i},\ \text{and } s_{j1} = 0 \text{ for } j \geq 2. \tag{11}$$

This gives

$$I_{i,i+1} = \frac{1}{2\omega_k}\left[(a_{oi}+\omega_k a_{1i})\ln\left|\frac{\omega_{i+1}-\omega_k}{\omega_i-\omega_k}\right| - (a_{oi}-\omega_k a_{1i})\ln\left(\frac{\omega_{i+1}+\omega_k}{\omega_i+\omega_k}\right)\right] \tag{12}$$

Extrapolation to $\omega=0$ is done by including the point $(\omega_o,R(\omega_o))=(0,R(\omega_1))$.

2.2 Integration of the high frequency extrapolation function

1. Case $\qquad f_i(\omega) = \ln\sqrt{R(\omega)}$

Consider $R(\omega) = R(\omega_n)\cdot(\omega_n/\omega)^\alpha$ as extrapolation function for high frequencies with exponent α which should be set equal to 4 according to eqs. (6). Then the extrapolation term is given by the integral

$$I_u = \frac{1}{2}\int_{\omega_u}^{\infty} \frac{\ln R(\omega_n)+\alpha\ \ln\ (\omega_n/\omega)}{\omega^2-\omega_k^2}\ d\omega \tag{13}$$

Evaluation of this integral results:

$$I_{u\infty} = -\frac{1}{4\omega_k}\left\{\ln R(\omega_n)\cdot\ln\frac{1-p}{1+p} + \alpha\cdot F(p)\right\} \tag{14}$$

with $p = \omega_k/\omega_n$

and

$$F(p) = \begin{cases} s(p) & \text{(a)} \\ -\pi^2/4 - \ln p\cdot\ln\frac{1-p}{1+p} - s\left(\frac{1-p}{1+p}\right) & \text{(b)} \end{cases} \tag{15}$$

$$s(x) = 2\cdot\sum_{j=1}^{\infty} x^{2j-1}/(2j-1)^2$$

For p-values $\sqrt{2}-1<p<1$ (b) gives better convergence of series s than (a).

2. Case $\quad (f_1(\omega)-1)\propto\omega^{-2}$

In analogy to 1. consider $f_1(\omega) = 1+(f_1(\omega_n)-1)\cdot(\omega_n/\omega)^2$. Then $I_{u\infty}$ is given by

$$I_{u\infty} = \int_{\omega_u=\omega_n}^{\infty} \frac{1+(f_1(\omega_n)-1)\cdot(\omega_n/\omega)^2}{\omega^2-\omega_k^2}\, d\omega \tag{16}$$

Evaluation of integral (16) gives:

$$I_{u\infty} = \frac{1}{2\omega_k}\left\{1+\left(\frac{\omega_n}{\omega_k}\right)^2\cdot(f_1(\omega_n)-1\right\}\cdot\ln\frac{\omega_n+\omega_k}{\omega_n-\omega_k} - \frac{\omega_n}{\omega_k^2}(f_1(\omega_n)-1) \tag{17}$$

2.3 Results

From eqs. (2) and (12), (14) and (17) follows the general equation:

$$f_2(\omega_k) = \{T - d\cdot F\}/(2\pi) \tag{18}$$

with

$$T = \begin{cases} \sum_{i=1}^{n}(a_{1i}-a_{1,i-1})\cdot(\omega_i+\omega_k)\cdot\ln(\omega_i+\omega_k) \\ +\sum_{\substack{i=1 \\ i\neq k}}^{n}(a_{1i}-1_{1,i-1})\cdot(\omega_k-\omega_i)\cdot\ln|\omega_k-\omega_i| \end{cases}$$

$$a_{1i} = \frac{f_1(\omega_{i+1})-f_1(\omega_i)}{\omega_{i+1}-\omega_i}\quad,\qquad a_{1o}=a_{1n}=0 \tag{19}$$

In the special case when $f_2(\omega_k) = \Theta(\omega_k)$ one has to take

$$f(\omega_i) = \ln R(\omega_i)$$

$$d = \alpha$$

the F as def. by eqs. (15a,b)

In case $f_2(\omega_k) = \varepsilon_2(\omega_k)$ one has to take

$$f_1(\omega_i) = 2\cdot\varepsilon_1(\omega_i)$$

$$d = 2\cdot(\varepsilon_1(\omega_n)-1)$$

$$F = \begin{cases} \dfrac{2}{p} + (1-\dfrac{1}{p^2})\cdot\ln\dfrac{1+p}{1-p} & \text{(20a)} \\ 4p\cdot\sum\limits_{j=1}^{\infty} p^{2j-2}/(4j^2-1) & \text{(20b)} \end{cases}$$

with $p = \omega_k/\omega_n$

(20b) avoids rounding errors for small p-values.

3. PROGRAM DESCRIPTION

The detailed working of the program is set out on Comment cards incorporated into the program. The program is directed by means of the MAIN segment. The input data are read in with the subroutine EINLES (IEND, K, NA, PHI, EXPO, A, RHO, NX, N, X, Y, TX), the phase Θ of the complex reflectivity is then computed in the subroutine KKAREF(N, 3·N, EXPO, X,Y). With the resulting $\Theta(\omega)$ the following optical constants as functions of ω are computed in subroutine OPTKON(N, 10·N, PHI, POL, EXPO, A, RHO, X, Y), using the Fresnel equations:

the complex dielectric constants	ε_1, ε_2
the complex refractive index	n, k
the energy loss function	$\mathrm{Im}(1/\hat{\varepsilon})$
the absorption coefficient	$\mu = 2\cdot k\cdot E/1.973$ (E(eV))

$\varepsilon_{o\ eff}$

N_{eff} = electrons/molecule

The resulting curves are then plotted together with the input data and $\Theta(\omega)$ on the lineprinter by the Subroutine PLOTLX(K, NA, NX, NY, X, Y, ITX, TY, TY). The results are then checked for their accuracy and extrapolation, by computing ε_2^{Test} (ω) by means of a Kramers-Kronig analysis using the calculated ε_1. This is done by the Subroutine KKAEPS (N, 6·N, X, Y) and a subsequent plotting of this result.

4. TEST RUN

One test example is included to illustrate the main features of the program. For solidified Xenon the optical constants are computed from 7.8 to 14.5 eV using near normal reflectance data.

4.1 Test run output

The output is to a wide extent self-explanatory, it contains in the first part all input data (for the special DESY-system) including those which are omitted for two possible reasons:

a) the energy-value of a point is less or equal the energy of the preceeding point

b) the reflectance value is less than 10^{-4}.

Next a record is given of the computed optical constants together with the energy of the incident light, the reflectance data and the phase shift. Then the single parameters are plotted as curves on the lineprinter.

References

1. H.A. Kramers, Atti Congr. Intern. Fis. Como 2, 545 (1927)

2. R. Kronig, J.Opt.Soc.Am. 12, 547 (1926)

3. F. Stern, in Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1963) Sec. III

4. R. Klucker and U. Nielsen, Interner Bericht DESY F 41 (to be published)

5. R.P. Godwin, in Springer Tracts in Modern Physics, edited by G. Höhler (Springer-Verlag Berlin, 1969), Vol. 51, sec. 5.1

Appendix A: Listing of the program

```
            COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                               SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
ISN 0002                  SUBROUTINE EINLES(IEND,K,NA,PHI,POL,EXPO,A,RHO,NX,N,X,Y,TX)
                 C=====================================================================
                 C
                 C    ORDER OF INPUTDATA FOR A SINGLE BLOCK
                 C           (THE NUMBER OF BLOCKS IS UNLIMITED)
                 C
                 C         1.CARD:
                 C           TX: TITLE (UP TO 80 CHAR.)
                 C         2.CARD:
                 C           PHI: ANGLE OF INCIDENCE IN DEGREE (F5.1)
                 C           EXPO: EXPONENT FOR EXTRAPOLATION (F5.1)
                 C           K: SEE SUBROUTINE PLOTLX (I5)
                 C           NA: CURVES ARE PLOTTED BETWEEN THE ENERGYVALUES
                 C               E(NA) AND E(N)      (I5)
                 C           A: ATOMIC OR MOLECULAR WEIGHT OF THE MATERIAL   (F5.2)
                 C           RHO: SPECIFIC MASS OF THE MATERIAL (G/CM**3)   (F5.2)
                 C           POL: POLARISATION (P OR S)   (A1)
                 C         3.CARD:
                 C           SCALING VALUES (SPECIAL FOR THE DESY-F41-SYSTEM TO PUNCH
                 C           CURVEPOINTS ON CARDS)
                 C         4. AND FOLLOWING CARDS CONTAIN THE DATAPOINTS (CURVES)
                 C
                 C
                 C---------------------------------------------------------------------
                 C
                 C    N IS THE NUMBER OF POINTS STORED IN THE ARRAYS
                 C    X (ENERGY IN ELECTRON-VOLTS) AND
                 C    Y (ABSOLUTE REFLECTIVITIES)
                 C
                 C---------------------------------------------------------------------
                 C
                 C    IEND=1 SENSES THE END OF THE INPUTDATA
                 C
                 C
                 C
                 C=====================================================================
ISN 0003                  REAL*4 X(NX)   ,Y(NX)   ,TX(20)
ISN 0004                  N=6
ISN 0005                  IEND=0
ISN 0006                  READ(5,5001,END=190) TX,PHI,EXPO,K,NA,A,RHO,POL,X1,Y1,X2,Y2,X01,
                        1      Y01,X02,Y02
ISN 0007                  WRITE(6,6001) TX,PHI,EXPO,K,NA,A,RHO,POL,X1,Y1,X2,Y2,X01,Y01,X02,
                        1      Y02
ISN 0008                  X02=(X02-X01)/(X2-X1)
ISN 0009                  Y02=(Y02-Y01)/(Y2-Y1)
ISN 0010              100 NN=N-5
ISN 0011                  READ (5,5002,END=190) (X(I),Y(I),I=NN,N),Y2
ISN 0012                  IF(Y2.LE.0.) GOTO 200
ISN 0014                  WRITE(6,6002) (X(I),Y(I),I=NN,N),Y2
ISN 0015                  DO 150 I=NN,N
ISN 0016                  X(I)=X01+X02*(X(I)-X1)
ISN 0017              150 Y(I)=(Y01+Y02*(Y(I)-Y1))*Y2
ISN 0018                  N=N+6
ISN 0019                  IF(N.GT.NX) N=N-6
ISN 0021                  GOTO 100
ISN 0022              190 IEND=1
```



```
ISN 0023              200 N=N-6
ISN 0024                  IF(N.LE.0) STOP
                 C
ISN 0026                  WRITE(6,6006)
ISN 0027                  I=0
ISN 0028              210 IF( Y(I+1).LT..0001 ) GOTO 250
ISN 0030                  I=I+1
ISN 0031                  WRITE(6,6003) X(I ),Y(I ),I
ISN 0032                  IF(I.GE.N) RETURN
ISN 0034              230 IF( X(I+1).GT.X(I) ) GOTO 210
ISN 0036              250 N=N-1
ISN 0037                  NN=I+1
ISN 0038                  WRITE(6,6003) X(NN),Y(NN)
ISN 0039                  IF(I.GE.N) RETURN
ISN 0041                  DO 260 M=NN,N
ISN 0042                  X(M)=X(M+1)
ISN 0043              260 Y(M)=Y(M+1)
ISN 0044                  GOTO 230
                 C
ISN 0045             5001 FORMAT(20A4/2F 5.1,2I5,2F5.2,4X,A1/2(F4.2,F5.3),2X,4F 5.2)
ISN 0046             5002 FORMAT(6(F4.2,F5.3),12X,F6.0)
ISN 0047             6001 FORMAT('1',20X,80('=')//40X,'KRAMERS-KRONIG-ANALYSIS OF REFLECTI',
                        1           'ONDATA'//21X,80(1H=)//////
                        2                                   //1X,20A4//' PHI =',F10.3/' EXPO=',
                        3      F10.3/' K    =',I6/' NA   =',I6/' MWHT=',F10.3/' RHO =',F10.3//
                        4      1X,A1,'-POLARISATION'//
                        5 ' SCALING-DATA     '/10X,2(F8.2,F7.3),4F10.4////' INPUT-CARDS:  ')
ISN 0048             6002 FORMAT(6(F9.2,F7.3),F20.5)
ISN 0049             6003 FORMAT(10X,'X=   ',F8.4,3X,'Y=   ',F9.6,I7)
ISN 0050             6006 FORMAT(   '1INPUT-VALUES'/1X,12('=')/10X,'FOR INTEGRATION USED VALU
                        1ES ARE NUMBERED'////)
ISN 0051                  END
*OPTIONS IN EFFECT*       NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,

*OPTIONS IN EFFECT*       SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =      50 ,PROGRAM SIZE =      2390

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                              141K BYTES OF CORE NOT USED
```

```
         COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                            SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
             C===================================================================      4
             C              KRAMERS-KRONIG-ANALYSIS       MAIN SEGMENT                    5
             C-------------------------------------------------------------------      6
             C                                                                          7
             C                                                                          8
             C       THE OPTICAL AND DIELECTRIC PROPERTIES OF SOLIDS ARE COMPUTED       9
             C       FROM THE ABSOLUTE REFLECTIVITIES USING KRAMERS-KRONIG-ANALYSIS    10
             C                                                                         11
             C       (S-REFLECTIVITY AT ANY ANGLE PHI )                                12
             C       (P-REFLECTIVITY AT ANGLES PHI LESS 45 DEGREE )                    13
             C                                                                         14
             C                                                                         15
             C-------------------------------------------------------------------     16
             C                                                                         17
             C                                                                         18
             C   DIMENSIONS:                                                           19
             C        X(NX),Y(10*NX)       MAXIMAL NX VALUES ARE READ IN               20
             C         (SEE CARD 52 AND CARD 63, IN THIS VERSION: NX=600)              21
             C       COMPUTATION IS DONE WITH N (LESS OR EQUAL NX) VALUES              22
             C                                                                         23
             C      STORAGE ORGANISATION                                               24
             C                                                                         25
             C       A) MAINRUN (CALCULATION OF THE OPTICAL CONSTANTS AND RELATED      26
             C                 VALUES FROM ABSOLUTE REFLECTIVITIES )                   27
             C                                                                         28
             C         X(L)    ENERGY                                                  29
             C         Y(    1),...,Y(  N) : ABSOLUTE REFLECTIVITIES                   30
             C         Y(  N+1),...,Y(2*N) : PHASE THETA OUT (DISPERSION INTEGRAL)     31
             C         Y(2*N+1),...,Y(3*N) : EPSILON 1                                 32
             C         Y(3*N+1),...,Y(4*N) : EPSILON 2                                 33
             C         Y(4*N+1),...,Y(5*N) : IMAGINARY PART (1/EPSILON)                34
             C         Y(5*N+1),...,Y(6*N) : REFRACTIONINDEX N                         35
             C         Y(6*N+1),...,Y(7*N) : ABSORPTIONINDEX K                         36
             C         Y(7*N+1),...,Y(8*N) : ABSORPTIONCOEFFICIENT  MY=2*K*E/1.973     37
             C         Y(8*N+1),...,Y(9*N) : EPSILON-0-EFFECTIV                        38
             C         Y(9*N+1),...,Y(10*N): N-EFFECTIV (ELECTRONS/MOLECULE)           39
             C                                                                         40
             C       B) TESTRUN (CALCULATION OF EPSILON2(TEST) FROM EPSILON1)          41
             C                                                                         42
             C         X(L)    ENERGY                                                  43
             C         Y(    1),...,Y(  N) : ABSOLUTE REFLECTIVITIES                   44
             C         Y(  N+1),...,Y(2*N) : PHASE THETA (OLD VALUES)                  45
             C         Y(2*N+1),...,Y(3*N) : EPSILON 1    (OLD VALUES)                 46
             C         Y(3*N+1),...,Y(4*N) : EPSILON 2    (OLD VALUES)                 47
             C         Y(4*N+1),...,Y(5*N) : EPSILON2(TEST)                            48
             C         Y(5*N+1),...,Y(6*N) : EPSILON2(TEST)-EPSILON2                   49
             C                                                                         50
             C===================================================================     51
   ISN 0002         REAL*4 TX(20),X( 600),Y( 6000)                                     52
   ISN 0003         REAL*4 TY(80)/'REFL','ECTI','VITY',' R  ',4*'  ','PHAS','E TH',    53
                   1 'ETA ',5*'  ','EPSI','LON ','1   ',5*'  ','EPSI','LON ','2   ',   54
                   25*'  ','IMAG','(1/E','PSIL','ON) ',4*'  ','REFR','ACTI','VE I','NDEX 55
                   3',' N ',3*'  ','ABSO','RPTI','ONIN','DEX ','K   ',3*'  ','ABSO',   56
                   4 'RPTI','ONCO','EFFI','CIEN','T MY','    ',' ','EPSI','LON-',      57
                   5 '0-EF','FECT','IV  ',3*'  ','N-EF','FECT','IV (','ELEC','TRON',   58
                   6 'S/MO','LECU','LE) '/                                             59
```



```
             C                                                                         60
             C-------------------------------------------------------------------     61
             C                                                                         62
   ISN 0004         NX=600                                                             63
             C                                                                         64
   ISN 0005       1 CALL EINLES(IEND,K,NA,PHI,POL,EXPO,A,RHO, 600,N,X,Y,TX)            65
   ISN 0006         IF(N.LE.5) GOTO 3                                                  66
   ISN 0008         IF(K.EQ.1 .OR. K.EQ.0) K=N                                         67
             C                                                                         68
             C-------------------------------------------------------------------     69
             C                      M A I N R U N                                      70
             C-------------------------------------------------------------------     71
             C                                                                         72
   ISN 0010         CALL KKAREF(N,3*N,EXPO,X,Y)                                        73
             C                                                                         74
             C-------------------------------------------------------------------     75
   ISN 0011         CALL OPTKON(N,10*N,PHI,POL,A,RHO,X,Y)                              76
   ISN 0012         WRITE(6,6001) (I,X(I),(Y(I+N*L-N),L=1,10),I=1,N)                   77
             C-------------------------------------------------------------------     78
   ISN 0013         DO 2 I=1,10                                                        79
   ISN 0014       2 CALL PLOTLX(K,NA,N,N*I,X,Y,20,TX,I*8,8,TY)                         80
             C                                                                         81
             C-------------------------------------------------------------------     82
             C                      T E S T R U N                                      83
             C-------------------------------------------------------------------     84
             C                                                                         85
   ISN 0015         CALL KKAEPS(N, 5*N,X,Y)                                            86
   ISN 0016         CALL PLOTLX(   K,NA,N,N*5 ,X,Y,20,TX,6,6,'EPSILON2 FR. EPSILON1')  87
             C                                                                         88
   ISN 0017         DO    4    I=1,N                                                   89
   ISN 0018       4 Y(5*N+I)=Y(4*N+I)-Y(3*N+I)                                         90
   ISN 0019         CALL PLOTLX(K,NA,N,N*6,X,Y,20,TX,6,6,'EPSILON2(TEST)-EPSILON2')    91
             C                                                                         92
             C-------------------------------------------------------------------     93
             C                                                                         94
   ISN 0020       3 IF(IEND.EQ.0) GOTO 1                                               95
   ISN 0022         STOP                                                               96
   ISN 0023    6001 FORMAT('1        I     ENERGY      REFLECT PHAS.THETA  EPSILON.1  E',  97
                  1    'PSILON.2  IM(1/EPS)  RF.INDX N  ABSINDX K ABSCOEF MY  EPS.0',     98
                  2    '.EFF    N.EFF'   /4X,'----',11(' ----------')/5(I8,11F11.5/))    99
   ISN 0024         END                                                               100
*OPTIONS IN EFFECT*      NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,

*OPTIONS IN EFFECT*      SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =       23 ,PROGRAM SIZE =     28136

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                              145K BYTES OF CORE NOT USED
```

```
          COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                             SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
 ISN 0002             SUBROUTINE KKAREF(NX,NY,EXPO,X,Y)
                C=====================================================================
                C
                C    DISPERSION-INTEGRAL  WITH EXTRAPOLATION
                C                 COMPUTES FOR NX NON EQUIDISTANT POINTS (X,Y)
                C                 (0<X(L)<X(L+1) ) FROM REFLACTANCEVALUES THE
                C                 PHASE THETA OF THE COMPLEX REFLACTANCE
                C
                C                 X(L) = ENERGYVALUES
                C                 Y(L) = ABSOLUTE REFLECTIVITIES
                C                 IN Y(NX+1),...,Y(2*NX) THETA
                C                 Y(2*NX+1),...,Y(3*NX) SCRATCH STORAGE
                C
                C                 THE THETAVALUE OF THE FIRST POINT =0.0
                C                 THE THETAVALUE OF THE LAST POINT IS EXTRAPOLATED
                C
                C=====================================================================
 ISN 0003             REAL*4 X(NX)   ,Y(NY)
 ISN 0004             NX2=NX+NX
 ISN 0005             Y(NX2+1)=ALOG(Y(1))
 ISN 0006             DO 1 I=2,NX
 ISN 0007             K=NX2+I
 ISN 0008             Y(K)=ALOG(Y(I))
 ISN 0009           1 Y(K-1)=(Y(K)-Y(K-1))/(X(I)-X(I-1))
 ISN 0010             Y(K)=0.
 ISN 0011             DO 2 I=2,NX
 ISN 0012             K=K-1
 ISN 0013           2 Y(K+1)=Y(K+1)-Y(K)
                C
 ISN 0014             Y(NX+1)=0.
 ISN 0015             DO 9999 K=3,NX
 ISN 0016             XK=X(K-1)
 ISN 0017             XX=XK+XK
 ISN 0018             T=Y(NX2+K-1)*XX*ALOG(XX)
 ISN 0019             DO 3 I=3,K
 ISN 0020             XX=XK+X(I-2)
 ISN 0021             XY=XK-X(I-2)
 ISN 0022           3 T=T+Y(NX2+I-2)*(XX*ALOG(XX)+XY*ALOG(XY))
 ISN 0023             DO 4 I=K,NX
 ISN 0024             XX=X(I)+XK
 ISN 0025             XY=X(I)-XK
 ISN 0026           4 T=T+Y(NX2+I)   *(XX*ALOG(XX)-XY*ALOG(XY))
                C
 ISN 0027             F=0
 ISN 0028             XK=XK/X(NX)
 ISN 0029             IF(XK.LE..4142136) GOTO 6
 ISN 0031             XX=(1.-XK)/(1.+XK)
 ISN 0032             F=2.477401-ALOG(XK)*ALOG(XX)
 ISN 0033             XK=-XX
 ISN 0034           6 XX=XK*XK
 ISN 0035             F=F+XK*(2.+XX*(.2222222+XX*(.08+XX*(.040816+XX*(.02469+XX*(.0165
                     1       +XX*.012))))))
 ISN 0036        9999 Y(NX+K-1)=(T+F*EXPO)*.1591549
                C
 ISN 0037             Y(NX+1)=Y(NX+2)+(Y(NX+3)-Y(NX+2))*(X(1)-X(2))/(X(3)-X(2))
 ISN 0038             Y(NX2)=Y(NX2-1)+(Y(NX2-1)-Y(NX2-2))/(X(NX-1)-X(NX-2))
```



```
                     1         *(X(NX)-X(NX-1))
 ISN 0039             RETURN
 ISN 0040             END
*OPTIONS IN EFFECT*       NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,

*OPTIONS IN EFFECT*       SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =       39 ,PROGRAM SIZE =      2050

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                            141K BYTES OF CORE NOT USED
```

```
         COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                            SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
  ISN 0002            SUBROUTINE OPTKON(NX,NY,PHI,POL,A,RHO,X,Y)
                C=====================================================================
                C
                C     COMPUTATION OF THE OPTICAL CONSTANTS  (BY FRESNELS FORMULA)
                C     AND ASSOCIATED VALUES
                C
                C---------------------------------------------------------------------
                C
                C        X(L)      ENERGY
                C        Y(      1),...,Y(   NX) : ABSOLUT REFLECTIVITIES
                C        Y(   NX+1),...,Y(2*NX) : PHASE THETA
                C        Y(2*NX+1),...,Y(3*NX) : EPSILON 1
                C        Y(3*NX+1),...,Y(4*NX) : EPSILON 2
                C        Y(4*NX+1),...,Y(5*NX) : IMAGINARY PART (1/EPSILON)
                C        Y(5*NX+1),...,Y(6*NX) : REFRACTIONINDEX N
                C        Y(6*NX+1),...,Y(7*NX) : ABSORPTIONINDEX K
                C        Y(7*NX+1),...,Y(8*NX) : ABSORPTIONCOEFFICIENT  MY=2*K*E/1.973
                C        Y(8*NX+1),...,Y(9*NX) : EPSILON-O-EFFECTIV
                C        Y(9*NX+1),...,Y(10*NX): N-EFFECTIV (ELECTRONS/MOLECULE)
                C
                C=====================================================================
  ISN 0003            REAL*4 X(NX),Y(NY),P/'P'/
  ISN 0004            LOGICAL*4 L
  ISN 0005            L=POL.EQ.P
  ISN 0006            PHI=PHI*.01745329
  ISN 0007            CNEFF=7.66686E-4*A/RHO
  ISN 0008            CB=SIN(PHI)**2
  ISN 0009            CA=1.-CB
  ISN 0010            CG=1.5708
  ISN 0011            CH=0.
  ISN 0012            DO 1000 I=1,NX
  ISN 0013            CC=Y(NX+I)
  ISN 0014            CD=Y(I)
  ISN 0015            CE=SQRT(CD)
  ISN 0016            CE=CE+CE
  ISN 0017            CF=    1.+CD-CE*COS(CC)
  ISN 0018            CD=   (1.-CD)/CF
  ISN 0019            CE=CE/CF*SIN(CC)
  ISN 0020            CF=CD*CD-CE*CE
  ISN 0021            CD=CD+CD
  ISN 0022            CE=CD*CE
  ISN 0023            IF(L) GOTO 6
  ISN 0025            CF=CF*CA+CB
  ISN 0026            CE=CE*CA
  ISN 0027            GOTO 8
  ISN 0028          6 CF=CF/CA
  ISN 0029            CE=CE/CA
  ISN 0030            CF1=CF
  ISN 0031            CE1=CE
  ISN 0032            CC=CF*(CF-4.*CB)-CE*CE
  ISN 0033            CD=CE*(CF+CF-4.*CB)
  ISN 0034            CI=SQRT(CC*CC+CD*CD)
  ISN 0035            CJ=SQRT(.5*(CI-CC))
  ISN 0036            CK=SQRT(.5*(CI+CC))
  ISN 0037            IF(CD.LT.0.) CK=-CK
  ISN 0039            CF=.5*(CF+CK)
```



```
  ISN 0040            CE=.5*(CE+CJ)
  ISN 0041          8 Y(2*NX+I)  =CF
  ISN 0042            IF(I.EQ.1) GOTO 9
  ISN 0044            CC=CE*(X(I)  -X(I-1))
  ISN 0045            CG=CG+CC/X(I)
  ISN 0046            CH=CH+CC*X(I)
  ISN 0047          9 Y(3*NX+I)  =CE
  ISN 0048            CC=CF*CF+CE*CE
  ISN 0049            Y(4*NX+I)  =CE/CC
  ISN 0050            CC=SQRT(.5*(SQRT(CC)+CF))
  ISN 0051            Y(5*NX+I)  =CC
  ISN 0052            CE=CE/(CC+CC)
  ISN 0053            Y(6*NX+I)  =CE
  ISN 0054            Y(7*NX+I)  =X(I)  *CE/.9865
  ISN 0055            Y(8*NX+I)  =CG*.63662
  ISN 0056       1000 Y(9*NX+I)  =CH*CNEFF
  ISN 0057            RETURN
  ISN 0058            END
*OPTIONS IN EFFECT*       NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,

*OPTIONS IN EFFECT*       SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =       57 ,PROGRAM SIZE =      1718

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                              145K BYTES OF CORE NOT USED
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
ISN 0002           SUBROUTINE KKAEPS(NX,NY,X,Y)
             C=====================================================================
             C
             C        PROGRAM KKAEPS IS IDENTICAL WITH KKAREF EXCEPT FOR THE
             C        EXTRAPOLATION
             C
             C    DISPERSION-INTEGRAL  WITH EXTRAPOLATION
             C                  COMPUTES FOR NX NON EQUIDISTANT POINTS (X,Y)
             C                  (0<X(L)<X(L+1))     FROM THE REAL-PART THE IMAG.-PART
             C                  OF THE DIELECTRIC CONSTANT
             C
             C        X(L)        ENERGY
             C        Y(      1),...,Y(   NX) : ABSOLUT REFLECTIVITIES
             C        Y(   NX+1),...,Y(2*NX)  : SCRATCHBUFFER
             C        Y(2*NX+1),...,Y(3*NX)   : EPSILON 1
             C        Y(3*NX+1),...,Y(4*NX)   : EPSILON 2
             C        Y(4*NX+1),...,Y(5*NX)   : EPSILON2(TEST) FROM EPSILON1
             C
             C=====================================================================
ISN 0003           REAL*4 X(NX)   ,Y(NY)
ISN 0004           NX2=NX+NX
ISN 0005           NXX=NX
ISN 0006           NXY=NX*4
ISN 0007           YN1=Y(NX2+NX)-1.
ISN 0008           Y(NXX+1)=Y(NX2+2)
ISN 0009           DO 1 I=2,NX
ISN 0010           K=NXX+I
ISN 0011           Y(K)=Y(NX2+I)
ISN 0012         1 Y(K-1)=(Y(K)-Y(K-1))/(X(I)-X(I-1))
ISN 0013           Y(K)=0.
ISN 0014           DO 2 I=2,NX
ISN 0015           K=K-1
ISN 0016         2 Y(K+1)=Y(K+1)-Y(K)
             C
ISN 0017           Y(NXY+1)=0.
ISN 0018           DO 9999 K=3,NX
ISN 0019           XK=X(K-1)
ISN 0020           XX=XK+XK
ISN 0021           T=Y(NXX+K-1)*XX*ALOG(XX)
ISN 0022           DO 3 I=3,K
ISN 0023           XX=XK+X(I-2)
ISN 0024           XY=XK-X(I-2)
ISN 0025         3 T=T+Y(NXX+I-2)*(XX*ALOG(XX)+XY*ALOG(XY))
ISN 0026           DO 4 I=K,NX
ISN 0027           XX=X(I)+XK
ISN 0028           XY=X(I)-XK
ISN 0029         4 T=T+Y(NXX+I)   *(XX*ALOG(XX)-XY*ALOG(XY))
             C
ISN 0030           XK=XK/X(NX)
ISN 0031           XX=XK*XK
ISN 0032           IF(XK.LE..4142136) GOTO 6
ISN 0034           F=2./XK+(1.-1./XX)*ALOG((1.+XK)/(1.-XK))
ISN 0035           GOTO 9999
ISN 0036         6 F=XK*(1.333333+XX*(.2666667+XX*(.11429+XX*(.06349+XX*(.0404
                  1      +XX*(.028+XX*.021)))))
ISN 0037      9999 Y(NXY+K-1)=(T+F*YN1)*.3183099
```



```
             C
ISN 0038           Y(NXY+NX)=Y(NXY+NX-1)
ISN 0039           RETURN
ISN 0040           END

*OPTIONS IN EFFECT*      NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,

*OPTIONS IN EFFECT*      SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*     SOURCE STATEMENTS =      39 ,PROGRAM SIZE =      1692

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                          141K BYTES OF CORE NOT USED
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF
 ISN 0002            SUBROUTINE PLOTLX(K,NA,NX,NY,X,Y,ITX,TX,ITY,IY,TY)
               C======================================================================
               C
               C     PLOT
               C     PLOT TREATS ( X(L),Y(L+NY-NX) ) AS A POINT
               C               (NA-1<L<NX+1 , X(L)<X(L+1) NON AEQUIDISTANT )
               C          INTERPOLATION IS DONE BETWEEN THE INPUTVALUES
               C          INPUTVALUES ARE PLOTTED WITH '*',INTERPOLATED WITH 'O'
               C          ARE THERE MORE THAN ONE INPUTPOINT AT THE PRINTERPOINT
               C          THE PLOTSYMBOL IS 'X'
               C
               C       K>1: THE PLOT HAS K LINES,DX=(X(NX)-X(NA))/(K-1)
               C       K<0: THE PLOT HAS N=(N(NX)-X(NA))/DX LINES,DX=ABS(K/1000)
               C       K=0,K=1: PLOT PRINTS ONLY THE HEADING
               C       THE TEXTBUFFER TX IS PRINTED AHEAD THE CURVE
               C       THE LAST PLACES OF TY(ITY) ARE PRINTED (4*IY CHAR)
               C
               C======================================================================
 ISN 0003            REAL G*8(26)/'I',5*' ',' I',5*' ','    I','I-------','--+-----',
                   1              '----+---','------+-','--------','+-------','--I-----',
                   2              '----+---','------+-','--------','+-------','--+-----',
                   3              '-----I'/,Z*8(13),YM(11),X(NX),Y(NY),TX(ITX),TY(ITY)
 ISN 0004            LOGICAL*1 S(104),SL(6)/' ','O','*','O','X','O'/
 ISN 0005            INTEGER*2 SI(3)
 ISN 0006            EQUIVALENCE (Z(1),YM(1),S(1)),(SI(1),SL(1))
 ISN 0007            IF(K.LE.1) GOTO 100
 ISN 0009            DX=(X(NX)-X(NA))/(K-1)
 ISN 0010            GOTO 120
 ISN 0011        100 DX=-K*.001
 ISN 0012        120 NB=NY-NX+NA
 ISN 0013            YMIN=Y(NB)
 ISN 0014            YMAX=YMIN
 ISN 0015            DO 140 I=NB,NY
 ISN 0016            IF(Y(I).LT.YMIN) YMIN=Y(I)
 ISN 0018            IF(Y(I).GT.YMAX) YMAX=Y(I)
 ISN 0020        140 CONTINUE
 ISN 0021            NB=NY-NX
 ISN 0022            DY=(YMAX-YMIN)/10.
 ISN 0023            DO 160 I=1,11
 ISN 0024        160 YM(I)=YMIN+(I-1)*DY
 ISN 0025            J=ITY-IY+1
 ISN 0026            WRITE(6,6001) TX,(TY(I),I=J,ITY)
 ISN 0027            WRITE(6,6002) YMAX,X(NX),YMIN,X(NA),DY,DX,YM
 ISN 0028            IF(DY.LE.0. .OR. DX.LE.0.) RETURN
 ISN 0030            DY=10./DY
               C----------------------------------------------------------------------
 ISN 0031            I=NA+1
 ISN 0032            J=NA
 ISN 0033            L=0
 ISN 0034            XX=X(NA)
 ISN 0035            XO=XX+.5*DX
 ISN 0036        200 LL=0
 ISN 0037            IF(L/20*20.EQ.L) LL=13
 ISN 0039            DO 210 LM=1,13
 ISN 0040        210 Z(LM)=G(LM+LL)
 ISN 0041        220 IF(XX.LE.X(I)) GOTO 240
```



```
 ISN 0043            IF(I.GE.NX) GOTO 260
 ISN 0045            I=I+1
 ISN 0046            GOTO 220
 ISN 0047        240 LM=I+NB
 ISN 0048            LL=(Y(LM)-YMIN+(Y(LM)-Y(LM-1))*(XX-X(I))/(X(I)-X(I-1)))*DY+1.5
 ISN 0049            S(LL)=SL(4)
 ISN 0050        260 IF(X(J).GE.XO) GOTO 280
 ISN 0052            LL=(Y(J+NB)-YMIN)*DY+1.5
 ISN 0053            SL(1)=S(LL)
 ISN 0054            IF(SI(1).NE.SI(2)) GOTO 265
 ISN 0056            S(LL)=SL(5)
 ISN 0057            GOTO 270
 ISN 0058        265 IF(SI(1).NE.SI(3)) S(LL)=SL(3)
 ISN 0060        270 J=J+1
 ISN 0061            IF(J.LE.NX) GOTO 260
 ISN 0063        280 L=L+1
 ISN 0064            WRITE(6,6003) XX,Z
 ISN 0065            IF(XO.GT.X(NX)) RETURN
 ISN 0067            XX=XX+DX
 ISN 0068            XO=XO+DX
 ISN 0069            GOTO 200
               C----------------------------------------------------------------------
 ISN 0070       6001 FORMAT('1'/(1X,20A4))
 ISN 0071       6002 FORMAT(/'OYMAX=',1PE13.6,9X,'XMAX=',E13.6/' YMIN=',E13.6,9X,
                   1  'XMIN=',E13.6/' DY=',E15.6,9X,'DX=',E15.6//8X,11(1X,0PF9.4))
 ISN 0072       6003 FORMAT(1X,F10.3,2X,13A8)
 ISN 0073            END
*OPTIONS IN EFFECT*       NAME=  MAIN,OPT=00,LINECNT=60,SIZE=0000K,

*OPTIONS IN EFFECT*       SOURCE,EBCDIC,NOLIST,NODECK,LOAD,NOMAP,NOEDIT,NOID,NOXREF

*STATISTICS*    SOURCE STATEMENTS =      72 ,PROGRAM SIZE =      2610

*STATISTICS*  NO  DIAGNOSTICS GENERATED

****** END OF COMPILATION ******                                141K BYTES OF CORE NOT USED

*STATISTICS*  NO  DIAGNOSTICS THIS STEP
```

Appendix B: Testdeck output

(shortened, only the first page of each output segment is given)

==

KRAMERS-KRONIG-ANALYSIS OF REFLECTIONDATA

==

XENON (SOLID, 20 K)   NEARNORMALINCIDENCE (15 DEGREE)   467

PHI = 15.000
EXPO= 4.000
K = 400
NA = 5
MWHT= 131.300
RHO = 3.780

S-POLARISATION

SCALING-DATA

2.49 1.007 26.20 19.293 8.0000 0.0 14.0000 0.0370

INPUT-CARDS:

0.66	3.345	0.80	3.337	1.03	3.338	1.51	3.383	1.85	3.487	2.12	3.620			4.00000
2.42	3.858	2.65	4.124	2.84	4.299	3.00	4.609	3.12	4.932	3.28	5.277			4.00000
3.39	5.684	3.46	6.044	3.54	6.462	3.65	6.984	3.74	7.563	3.78	7.930			4.00000
3.88	8.684	3.97	9.155	4.00	9.729	4.02	10.399	4.08	11.074	4.10	11.630			4.00000
4.10	12.057	4.15	12.572	4.15	13.332	4.17	13.846	4.17	14.475	4.17	15.172			4.00000
4.20	15.582	4.22	16.296	4.26	16.889	4.29	17.309	4.31	17.759	4.31	18.043			4.00000
4.31	18.420	4.33	18.743	4.36	19.061	4.42	19.224	4.42	19.262	4.44	19.271			4.00000
4.45	19.311	4.52	19.205	4.52	18.999	4.55	18.766	4.55	18.639	4.55	18.562			4.00000
4.59	18.168	4.67	17.661	4.67	17.232	4.67	16.821	4.70	16.439	4.71	16.128			4.00000
4.76	15.549	4.80	14.932	4.84	14.509	4.86	13.996	4.87	13.461	4.89	12.961			4.00000
4.89	12.333	4.89	11.602	4.89	10.886	4.91	10.105	4.92	9.617	4.92	9.127			4.00000
4.94	8.371	4.94	7.801	4.94	7.082	4.94	6.672	4.94	5.990	4.94	5.476			4.00000
4.94	4.801	4.99	4.324	5.06	3.918	5.08	3.623	5.22	3.508	5.44	3.779			4.00000
5.62	4.447	5.81	4.847	5.98	5.322	6.09	5.853	6.16	6.197	6.28	6.851			4.00000
6.52	7.726	6.69	8.474	6.80	9.188	6.85	9.743	6.88	10.195	6.90	10.700			4.00000
6.96	11.620	6.96	12.210	6.98	12.651	6.99	13.182	6.99	13.640	6.99	14.047			4.00000
7.06	14.141	7.06	14.133	7.08	14.065	7.09	13.875	7.10	13.549	7.11	13.085			4.00000
7.10	12.465	7.14	11.991	7.15	11.414	7.15	10.944	7.15	10.291	7.15	9.834			4.00000
7.13	9.249	7.14	8.651	7.14	8.123	7.14	7.544	7.12	7.127	7.12	6.741			4.00000
7.15	6.468	7.16	5.979	7.15	5.547	7.16	5.238	7.19	5.182	7.22	5.198			4.00000
7.25	5.531	7.27	5.854	7.33	6.576	7.33	6.999	7.35	7.540	7.36	7.949			4.00000
7.36	8.276	7.40	8.646	7.44	9.016	7.49	9.263	7.52	9.282	7.54	9.230			4.00000
7.54	9.083	7.54	8.863	7.54	8.660	7.58	8.438	7.59	8.115	7.59	8.021			4.00000
7.62	7.927	7.65	7.817	7.70	7.773	7.72	7.809	7.76	8.132	7.77	8.437			4.00000
7.77	8.744	7.85	8.988	7.94	9.278	7.98	9.535	8.01	9.905	8.01	10.148			4.00000
8.02	10.331	8.10	10.794	8.25	11.358	8.32	11.843	8.38	12.314	8.42	12.717			4.00000
8.42	12.955	8.47	13.589	8.57	14.429	8.62	15.506	8.64	16.011	8.65	16.536			4.00000
8.65	16.812	8.69	17.461	8.70	18.197	8.69	18.432	8.74	18.578	8.81	18.559			4.00000
8.87	18.332	8.90	18.181	8.90	17.824	8.96	17.278	8.96	16.857	8.99	16.457			4.00000
9.00	16.363	9.03	15.883	9.03	15.208	9.05	14.538	9.10	14.037	9.16	13.579			4.00000
9.17	13.302	9.24	12.853	9.30	12.370	9.30	12.001	9.37	11.297	9.38	11.069			4.00000
9.46	10.895	9.64	10.655	9.77	10.524	9.91	10.504	10.02	10.467	10.12	10.368			4.00000
10.17	10.284	10.28	9.967	10.34	9.516	10.38	9.060	10.48	8.589	10.52	8.115			4.00000
10.53	7.979	10.59	7.611	10.61	7.145	10.66	6.721	10.66	6.236	10.69	5.823			4.00000
10.75	5.492	10.84	5.436	10.89	5.436	10.92	5.494	10.97	5.783	11.00	6.299			4.00000
11.01	6.265	11.08	7.057	11.11	7.645	11.15	8.338	11.21	9.183	11.26	9.544			4.00000
11.31	9.948	11.38	10.385	11.46	10.746	11.65	10.917	11.72	10.927	11.82	10.893			4.00000
11.86	10.704	11.97	10.404	12.06	9.995	12.07	9.558	12.12	9.254	12.14	8.909			4.00000
12.19	8.732	12.23	8.205	12.27	7.744	12.28	7.221	12.29	6.753	12.33	6.393			4.00000
12.33	6.206	12.33	5.652	12.38	5.189	12.40	4.562	12.41	4.165	12.43	3.866			4.00000

INPUT-VALUES
============

FOR INTEGRATION USED VALUES ARE NUMBERED

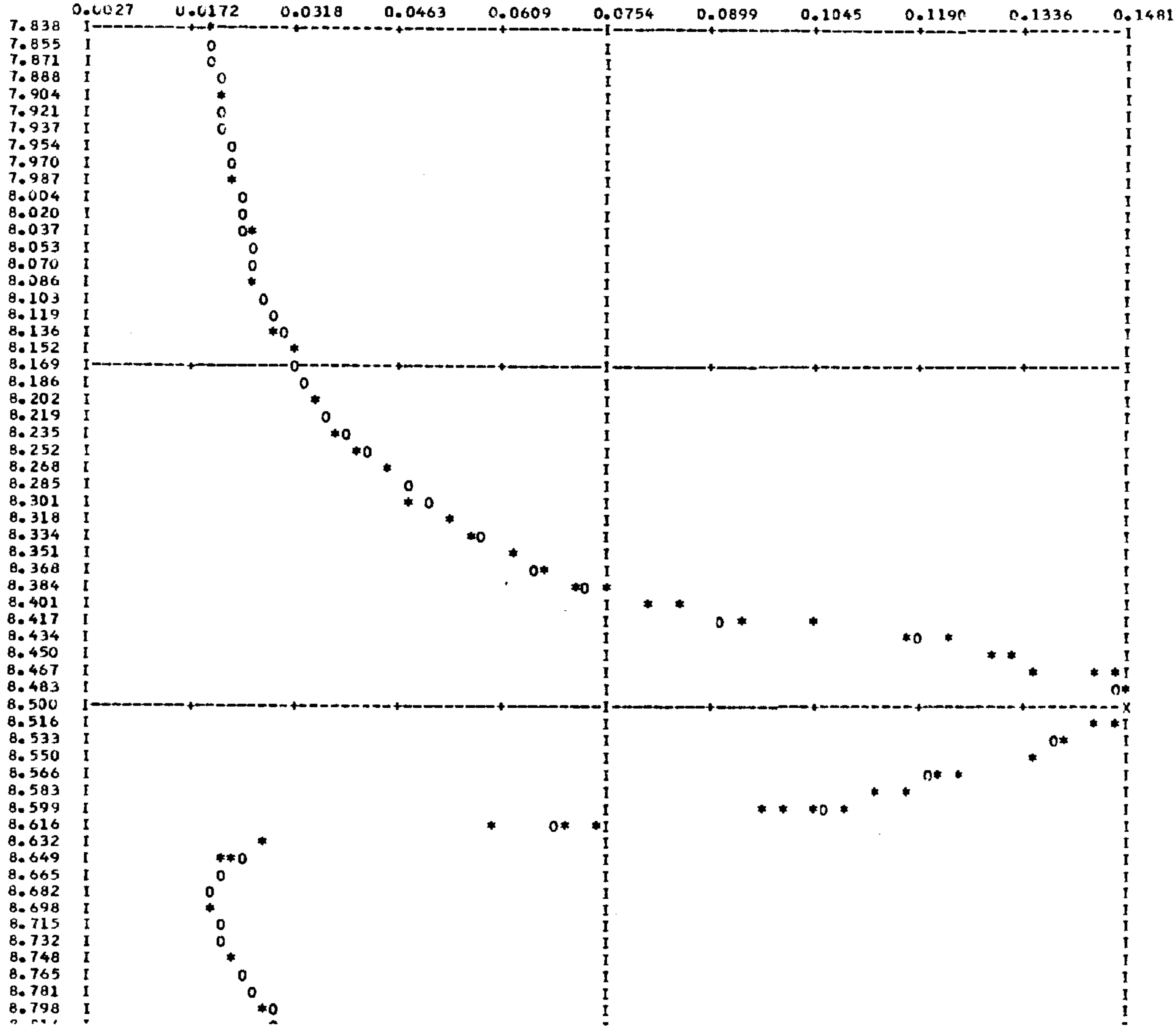
X=	7.5369	Y=	0.018923	1
X=	7.5723	Y=	0.018858	2
X=	7.6305	Y=	0.018866	3
X=	7.7520	Y=	0.019230	4
X=	7.8380	Y=	0.020072	5
X=	7.9064	Y=	0.021149	6
X=	7.9823	Y=	0.023075	7
X=	8.0405	Y=	0.025228	8
X=	8.0886	Y=	0.026644	9
X=	8.1291	Y=	0.029153	10
X=	8.1594	Y=	0.031767	11
X=	8.1999	Y=	0.034560	12
X=	8.2278	Y=	0.037854	13
X=	8.2455	Y=	0.040768	14
X=	8.2657	Y=	0.044151	15
X=	8.2935	Y=	0.048376	16
X=	8.3163	Y=	0.053062	17
X=	8.3264	Y=	0.056032	18
X=	8.3517	Y=	0.062135	19
X=	8.3745	Y=	0.065947	20
X=	8.3821	Y=	0.070593	21
X=	8.3872	Y=	0.076015	22
X=	8.4024	Y=	0.081478	23
X=	8.4074	Y=	0.085979	24
X=	8.4074	Y=	0.089435	
X=	8.4201	Y=	0.093603	25
X=	8.4201	Y=	0.099754	
X=	8.4251	Y=	0.103914	26
X=	8.4251	Y=	0.109005	
X=	8.4251	Y=	0.114646	
X=	8.4327	Y=	0.117965	27
X=	8.4378	Y=	0.123743	28
X=	8.4479	Y=	0.128543	29
X=	8.4555	Y=	0.131942	30
X=	8.4606	Y=	0.135584	31
X=	8.4606	Y=	0.137883	
X=	8.4606	Y=	0.140934	
X=	8.4656	Y=	0.143548	32
X=	8.4732	Y=	0.146122	33
X=	8.4884	Y=	0.147442	34
X=	8.4884	Y=	0.147749	
X=	8.4935	Y=	0.147822	35
X=	8.4960	Y=	0.148146	36
X=	8.5137	Y=	0.147288	37
X=	8.5137	Y=	0.145620	
X=	8.5213	Y=	0.143735	38
X=	8.5213	Y=	0.142707	
X=	8.5213	Y=	0.142083	
X=	8.5314	Y=	0.138895	39
X=	8.5517	Y=	0.134791	40
X=	8.5517	Y=	0.131319	
X=	8.5517	Y=	0.127993	
X=	8.5593	Y=	0.124901	41
X=	8.5618	Y=	0.122384	42
X=	8.5744	Y=	0.117697	43
X=	8.5846	Y=	0.112704	44
X=	8.5947	Y=	0.109280	45
X=	8.5997	Y=	0.105128	46
X=	8.6023	Y=	0.100798	47
X=	8.6073	Y=	0.096751	48
X=	8.6073	Y=	0.091668	
X=	8.6073	Y=	0.085752	
[illegible]	[illegible]	[illegible]	[illegible]	

I	ENERGY	REFLECT	PHAS.THETA	EPSILON.1	EPSILON.2	IM(1/EPS)	RF.INDX N	ABSINDX K	ABSCOEFF MY	EPS.0.EFF	N.EFF
1	7.53690	0.01892	0.81940	1.31250	0.53283	0.26555	1.16812	0.22807	1.74247	1.00000	0.0
2	7.57233	0.01886	0.81039	1.31842	0.52942	0.26228	1.17029	0.22619	1.73624	1.00158	0.00378
3	7.63054	0.01887	0.79559	1.32887	0.52576	0.25743	1.17430	0.22386	1.73155	1.00413	0.01009
4	7.75200	0.01923	0.76346	1.35426	0.52340	0.24830	1.18451	0.22094	1.73613	1.00935	0.02313
5	7.83804	0.02007	0.72851	1.38634	0.52752	0.23976	1.19784	0.22020	1.74953	1.01304	0.03260
6	7.90637	0.02115	0.69396	1.42160	0.53416	0.23161	1.21248	0.22028	1.76541	1.01598	0.04028
7	7.98229	0.02307	0.66601	1.46152	0.55644	0.22752	1.22992	0.22621	1.83039	1.01935	0.04926
8	8.04049	0.02523	0.64603	1.49880	0.58431	0.22579	1.24649	0.23438	1.91034	1.02204	0.05655
9	8.06857	0.02664	0.62555	1.53064	0.59795	0.22143	1.25975	0.23733	1.94593	1.02430	0.06274
10	8.12906	0.02915	0.60273	1.57690	0.62708	0.21775	1.27944	0.24506	2.01939	1.02629	0.06824
11	8.15943	0.03177	0.59387	1.61176	0.66470	0.21868	1.29522	0.25660	2.12234	1.02786	0.07262
12	8.19991	0.03456	0.58052	1.65349	0.70150	0.21744	1.31332	0.26707	2.21993	1.03007	0.07882
13	8.22775	0.03785	0.56853	1.69938	0.74627	0.21664	1.33331	0.27986	2.33412	1.03168	0.08338
14	8.24547	0.04077	0.56368	1.73312	0.78948	0.21767	1.34862	0.29270	2.44645	1.03276	0.08645
15	8.26571	0.04415	0.57122	1.75323	0.84966	0.22385	1.36042	0.31228	2.61652	1.03408	0.09023
16	8.29355	0.04838	0.58068	1.77378	0.92514	0.23116	1.37374	0.33672	2.83084	1.03606	0.09592
17	8.31632	0.05306	0.58268	1.80554	1.00273	0.23508	1.39119	0.36039	3.03809	1.03780	0.10098
18	8.32644	0.05603	0.58618	1.81994	1.05377	0.23827	1.40053	0.37620	3.17531	1.03862	0.10334
19	8.35175	0.06213	0.61059	1.80919	1.17070	0.25210	1.40786	0.41578	3.51997	1.04088	0.10993
20	8.37453	0.06595	0.60722	1.83565	1.23098	0.25200	1.42229	0.43275	3.67363	1.04301	0.11619
21	8.38212	0.07059	0.59493	1.88615	1.29925	0.24768	1.44507	0.44954	3.81969	1.04376	0.11839
22	8.38718	0.07602	0.60462	1.88687	1.39534	0.25336	1.45493	0.47952	4.07687	1.04429	0.11997
23	8.40236	0.08148	0.62483	1.85298	1.49649	0.26379	1.45513	0.51421	4.37972	1.04601	0.12505
24	8.40742	0.08598	0.62871	1.85372	1.57222	0.26611	1.46362	0.53710	4.57741	1.04662	0.12683
25	8.42008	0.09360	0.63135	1.86017	1.69871	0.26769	1.47974	0.57399	4.89916	1.04824	0.13165
26	8.42514	0.10391	0.63020	1.87466	1.86885	0.26671	1.50362	0.62145	5.30747	1.04896	0.13377
27	8.43273	0.11796	0.67510	1.70384	2.08804	0.28749	1.48304	0.70397	6.01764	1.05015	0.13733
28	8.43779	0.12374	0.71754	1.53307	2.14614	0.30852	1.44405	0.74310	6.35593	1.05097	0.13977
29	8.44791	0.12854	0.78095	1.29480	2.14054	0.34203	1.37777	0.77681	6.65226	1.05260	0.14465
30	8.45550	0.13194	0.81713	1.16190	2.12936	0.36188	1.33933	0.79493	6.81352	1.05382	0.14829
31	8.46056	0.13558	0.83539	1.08488	2.14044	0.37170	1.31995	0.81080	6.95372	1.05464	0.15073
32	8.46563	0.14355	0.86866	0.93658	2.16064	0.38962	1.28286	0.84212	7.22659	1.05546	0.15320
33	8.47322	0.14612	0.92198	0.78062	2.07361	0.42239	1.22399	0.84707	7.27563	1.05664	0.15675
34	8.48840	0.14744	1.01681	0.57395	1.87992	0.48658	1.12684	0.83416	7.17756	1.05878	0.16320
35	8.49346	0.14782	1.04421	0.52454	1.82367	0.50645	1.10049	0.82857	7.13377	1.05947	0.16529
36	8.49599	0.14815	1.06009	0.49710	1.79177	0.51822	1.08548	0.82533	7.10796	1.05981	0.16631
37	8.51371	0.14729	1.16553	0.36717	1.57317	0.60282	0.99564	0.79003	6.81809	1.06190	0.17263
38	8.52130	0.14373	1.20887	0.34751	1.47903	0.64075	0.96613	0.76544	6.61180	1.06273	0.17518
39	8.53142	0.13889	1.26371	0.33158	1.36787	0.69049	0.93249	0.73345	6.34303	1.06377	0.17833
40	8.55167	0.13479	1.38607	0.27939	1.16551	0.81137	0.85962	0.67792	5.87665	1.06552	0.18370
41	8.55926	0.12490	1.43338	0.31025	1.08174	0.85418	0.84723	0.63840	5.53899	1.06613	0.18557
42	8.56179	0.12238	1.44295	0.31927	1.06465	0.86178	0.84580	0.62937	5.46230	1.06633	0.18619
43	8.57444	0.11770	1.50599	0.31779	0.97864	0.92435	0.82059	0.59630	5.18294	1.06725	0.18901
44	8.58456	0.11270	1.57409	0.31955	0.89434	0.99156	0.79664	0.56132	4.88464	1.06792	0.19108
45	8.59469	0.10928	1.66271	0.31233	0.79942	1.08524	0.76505	0.52247	4.55187	1.06852	0.19293
46	8.59975	0.10513	1.72766	0.31734	0.73485	1.14693	0.74759	0.49148	4.28442	1.06880	0.19379
47	8.60228	0.10080	1.75792	0.33031	0.70458	1.16356	0.74447	0.47321	4.12639	1.06893	0.19419
48	8.60734	0.09675	1.85111	0.33268	0.62584	1.24582	0.72161	0.43364	3.78358	1.06916	0.19492
49	8.61240	0.07364	1.91629	0.41950	0.55828	1.14482	0.74760	0.37338	3.25969	1.06937	0.19557
50	8.61493	0.06969	1.92474	0.43576	0.54787	1.11799	0.75359	0.36351	3.17446	1.06947	0.19589
51	8.61999	0.05960	1.97993	0.47273	0.50002	1.05602	0.76185	0.32816	2.86747	1.06966	0.19647
52	8.63264	0.02685	1.90484	0.68424	0.43695	0.66294	0.86495	0.25260	2.21046	[illegible]	0.19774
53	8.65036	0.02356	1.67971	0.78552	0.49775	0.57557	0.92614	0.26872	2.35637	1.07072	0.19977
54	8.65542	0.02117	1.63001	0.82300	0.49210	0.53519	0.94395	0.26068	2.28713	1.07090	0.20034
55	8.69085	0.02024	1.36803	0.95471	0.54955	0.45288	1.01397	0.27099	2.38734	1.07233	0.20485
56	8.74652	0.02244	1.14470	1.08516	0.61622	0.39569	1.08026	0.28527	2.52924	1.07482	0.21284
57	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

XENON (SOLID,20 K)   NEARNORMAL INCIDENCE (15 DEGREE)

REFLECTIVITY R

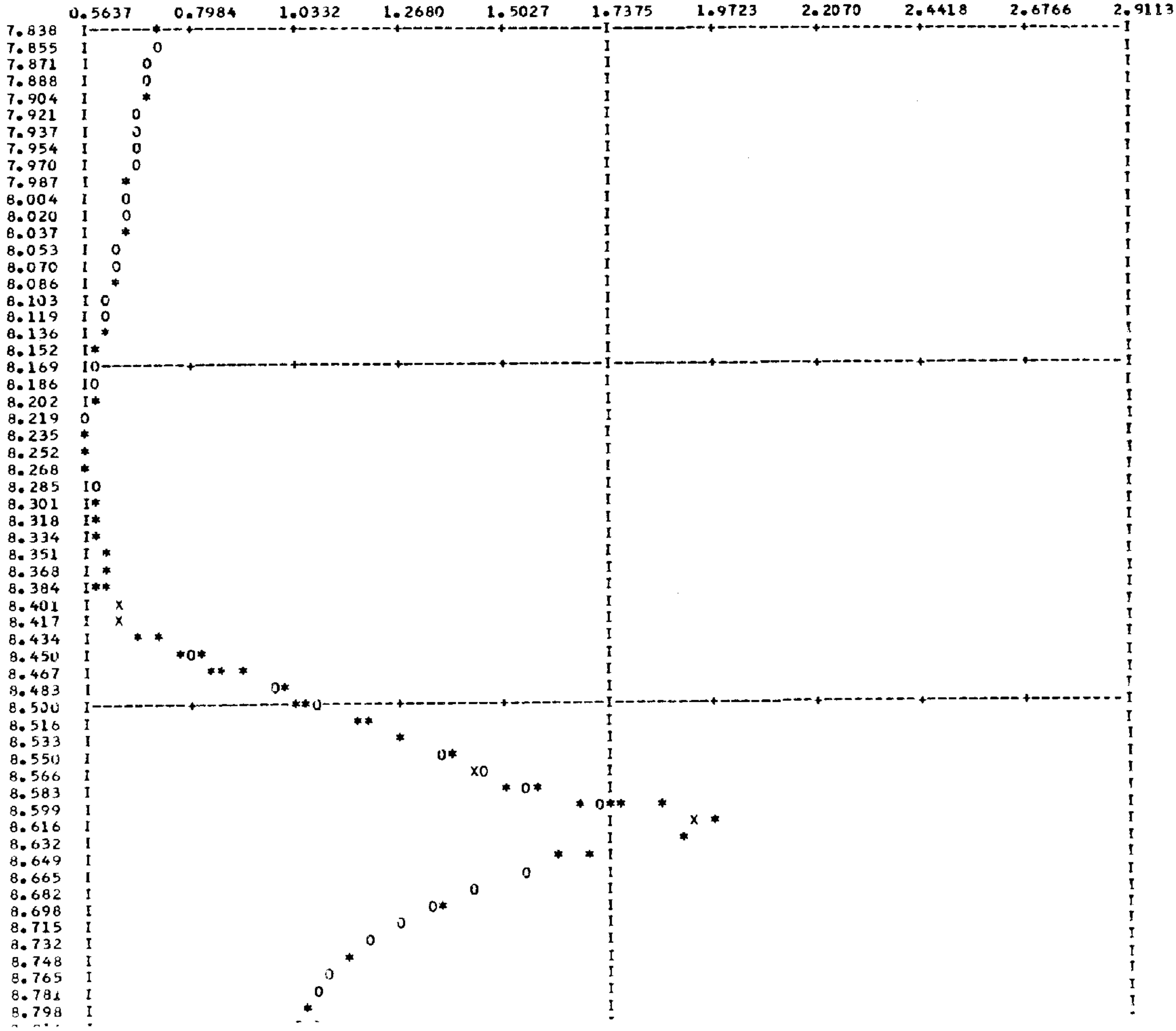
YMAX= 1.481456E-01   XMAX= 1.444032E 01
YMIN= 2.654707E-03   XMIN= 7.838042E 00
DY= 1.454908E-02   DX= 1.654705E-02



XENON (SOLID,20 K)   NEARNORMAL INCIDENCE (15 DEGREE)

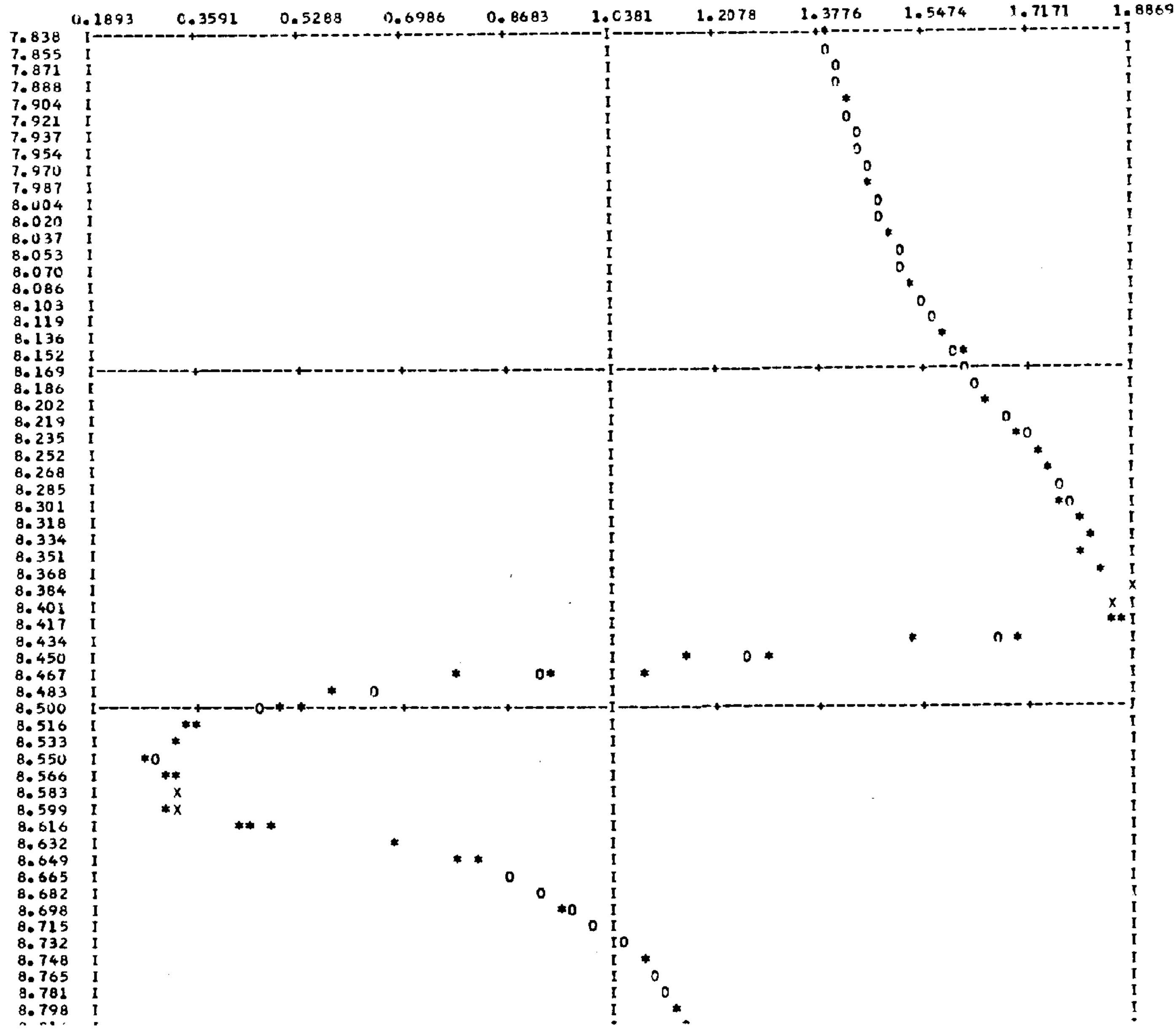
PHASE THETA

YMAX= 2.911342E 00   XMAX= 1.444032E 01
YMIN= 5.636840E-01   XMIN= 7.838042E 00
DY=   2.347657E-01   DX=   1.654705E-02



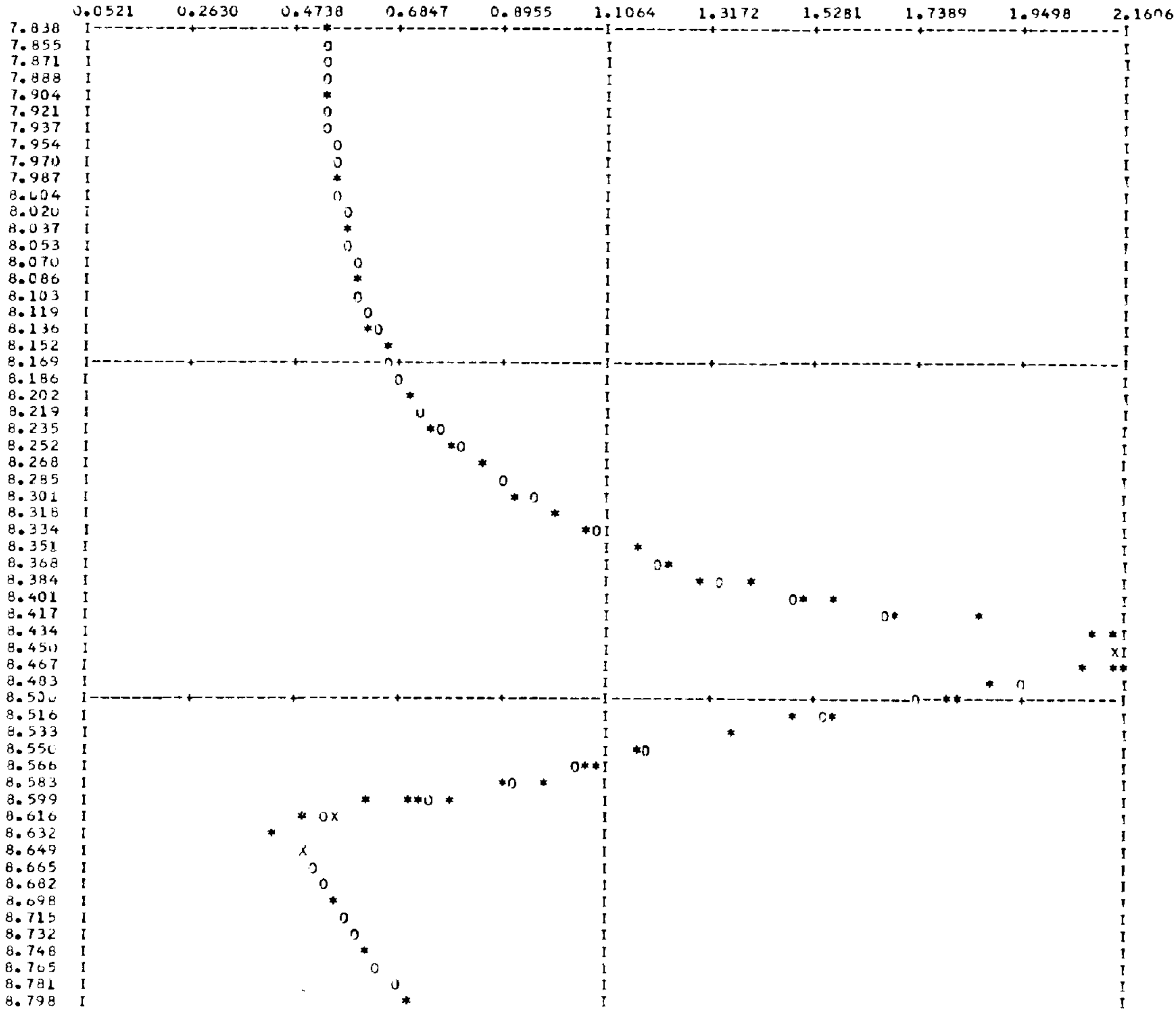
XENON (SOLID,20 K)   NEARNORMAL INCIDENCE (15 DEGREE)
EPSILON 1

YMAX= 1.886871E 00   XMAX= 1.444032E 01
YMIN= 1.893201E-01   XMIN= 7.838042E 00
DY= 1.697550E-01   DX= 1.654705E-02



XENON (SOLID,20 K) NEARNORMALINCIDENCE (15 DEGREE)
EPSILON 2

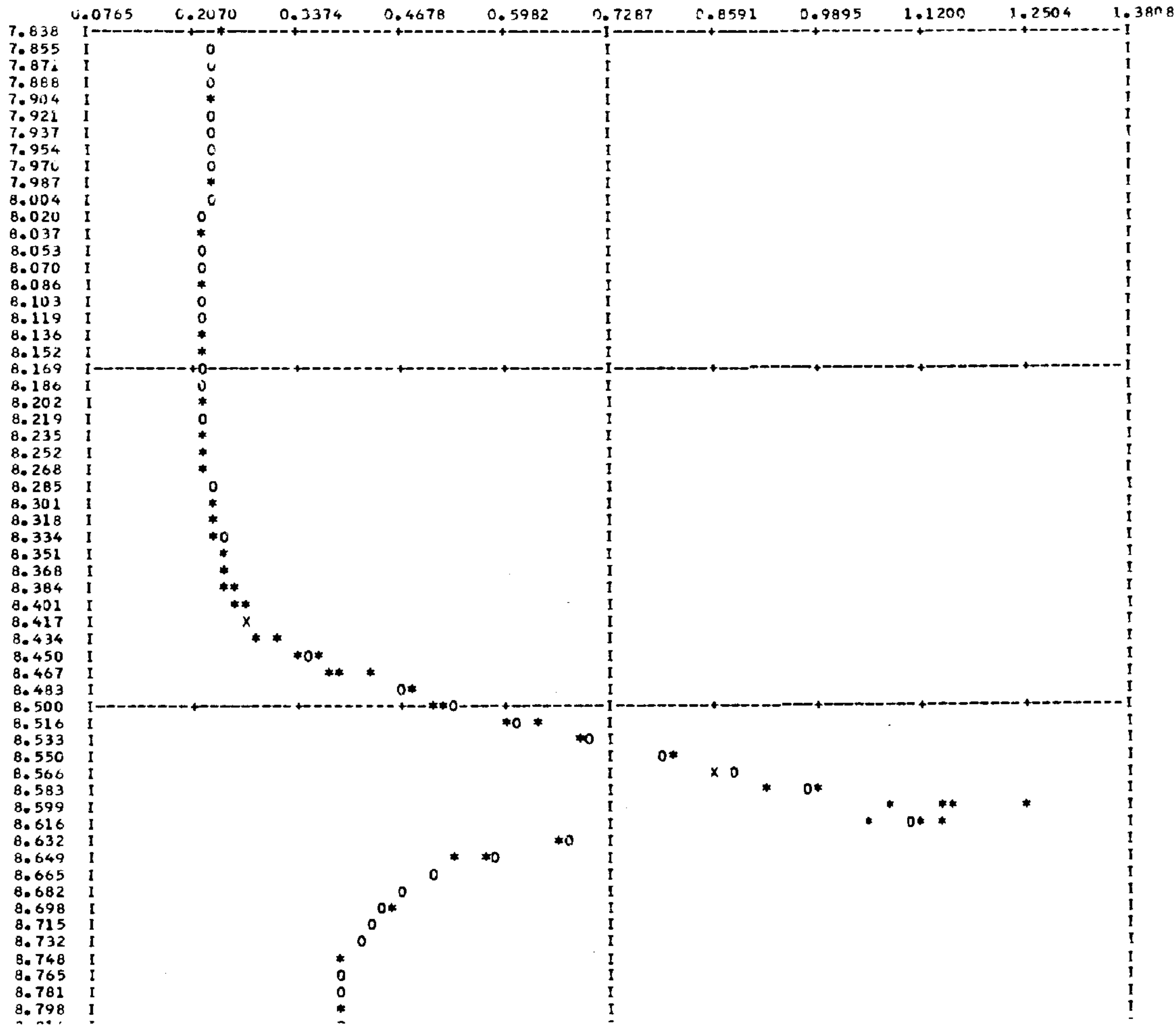
YMAX= 2.160636E 00 XMAX= 1.444032E 01
YMIN= 5.211153E-02 XMIN= 7.838042E 00
DY= 2.108524E-01 DX= 1.654705E-02



XENON (SOLID,20 K)   NEARNORMALINCIDENCE (15 DEGREE)

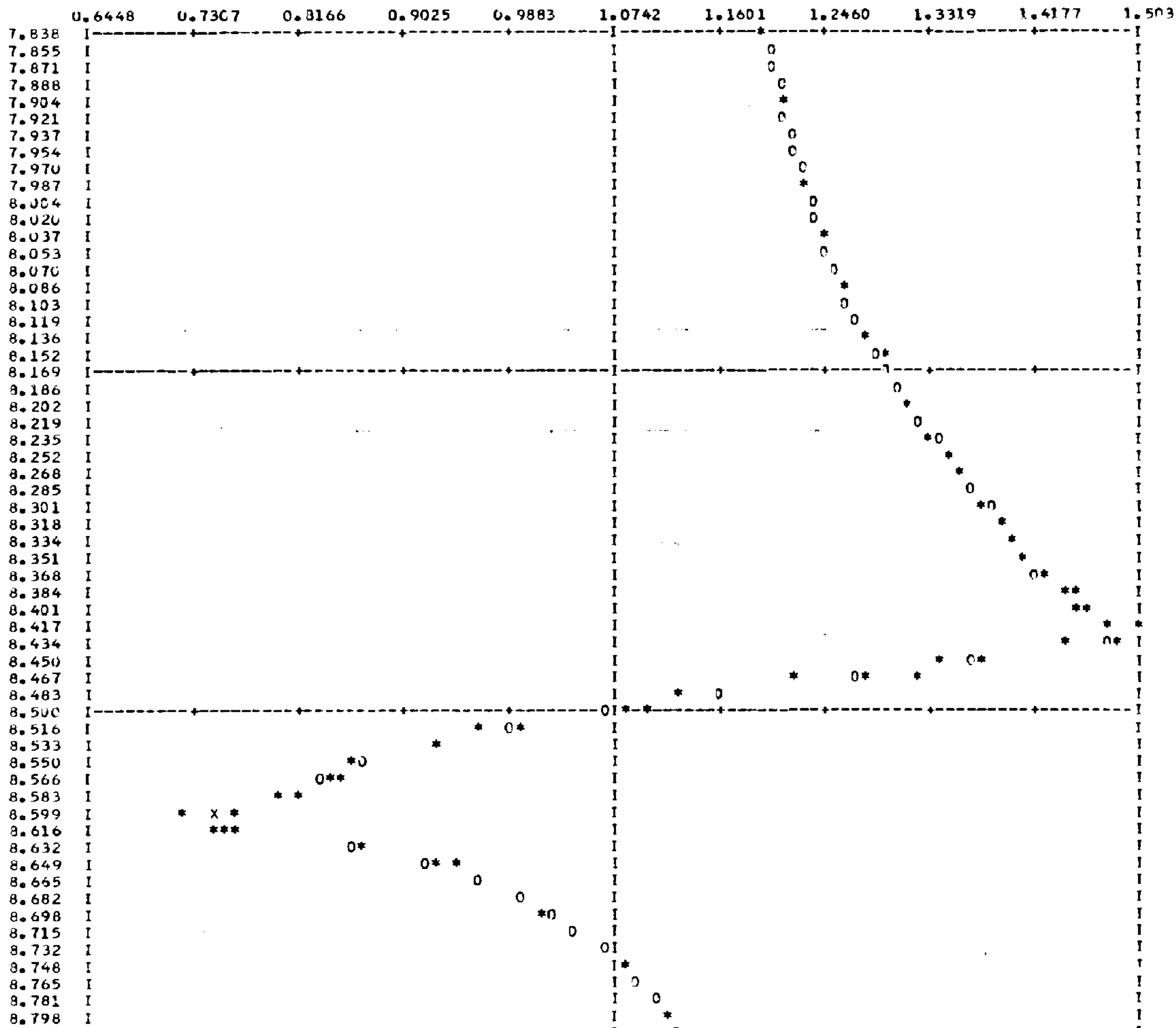
IMAG(1/EPSILON)

YMAX= 1.380826E 00 XMAX= 1.444032E 01
YMIN= 7.653117E-02 XMIN= 7.838042E 00
DY= 1.304294E-01 DX= 1.654705E-02



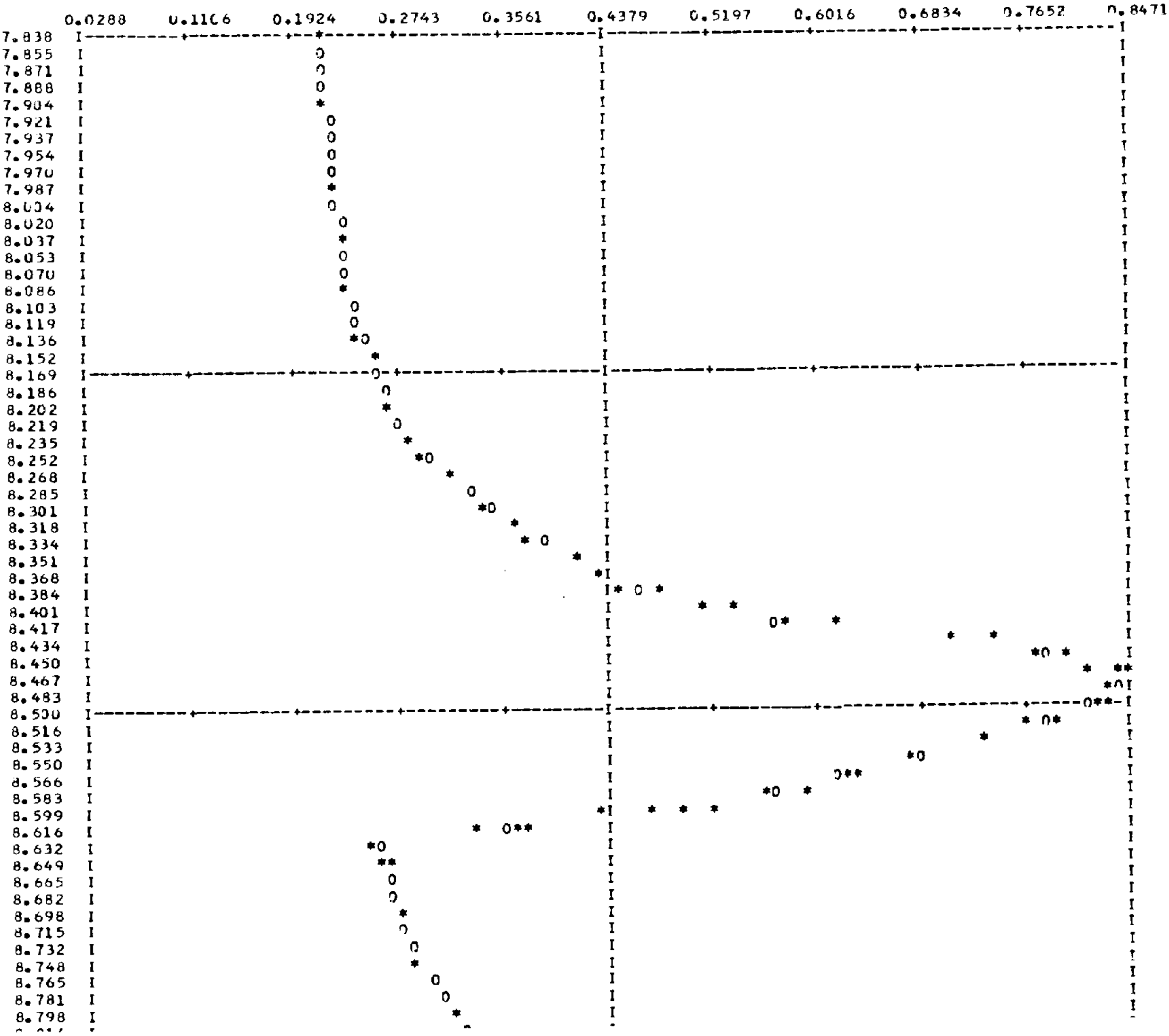
XENON (SOLID, 20 K)   NEARNORMALINCIDENCE (15 DEGREE)   467
REFRACTIVE INDEX N

YMAX= 1.503616E 00   XMAX= 1.444032E 01
YMIN= 6.448148E-01   XMIN= 7.838042E 00
DY= 8.588010E-02   DX= 1.654705E-02



XENON (SOLID, 20 K)   NEARNORMALINCIDENCE (15 DEGREE)
ABSORPTIONINDEX K

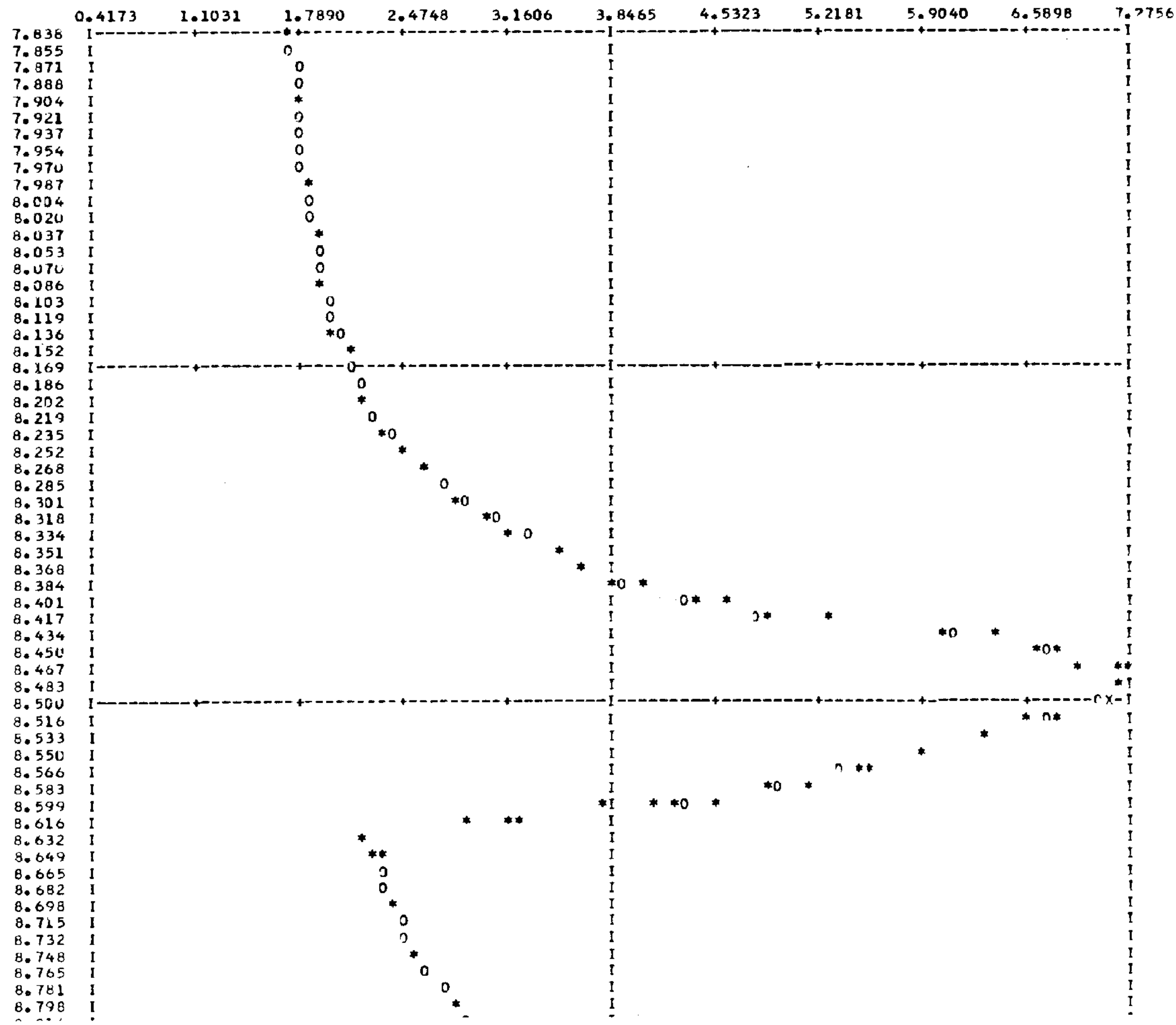
YMAX= 8.470705E-01   XMAX= 1.444032E 01
YMIN= 2.876575E-02   XMIN= 7.838042E 00
DY= 8.183044E-02   DX= 1.654735E-02



XENON (SOLID,20 K)   NEARNORMALINCIDENCE (15 DEGREE)

ABSORPTIONCOEFFICIENT MY

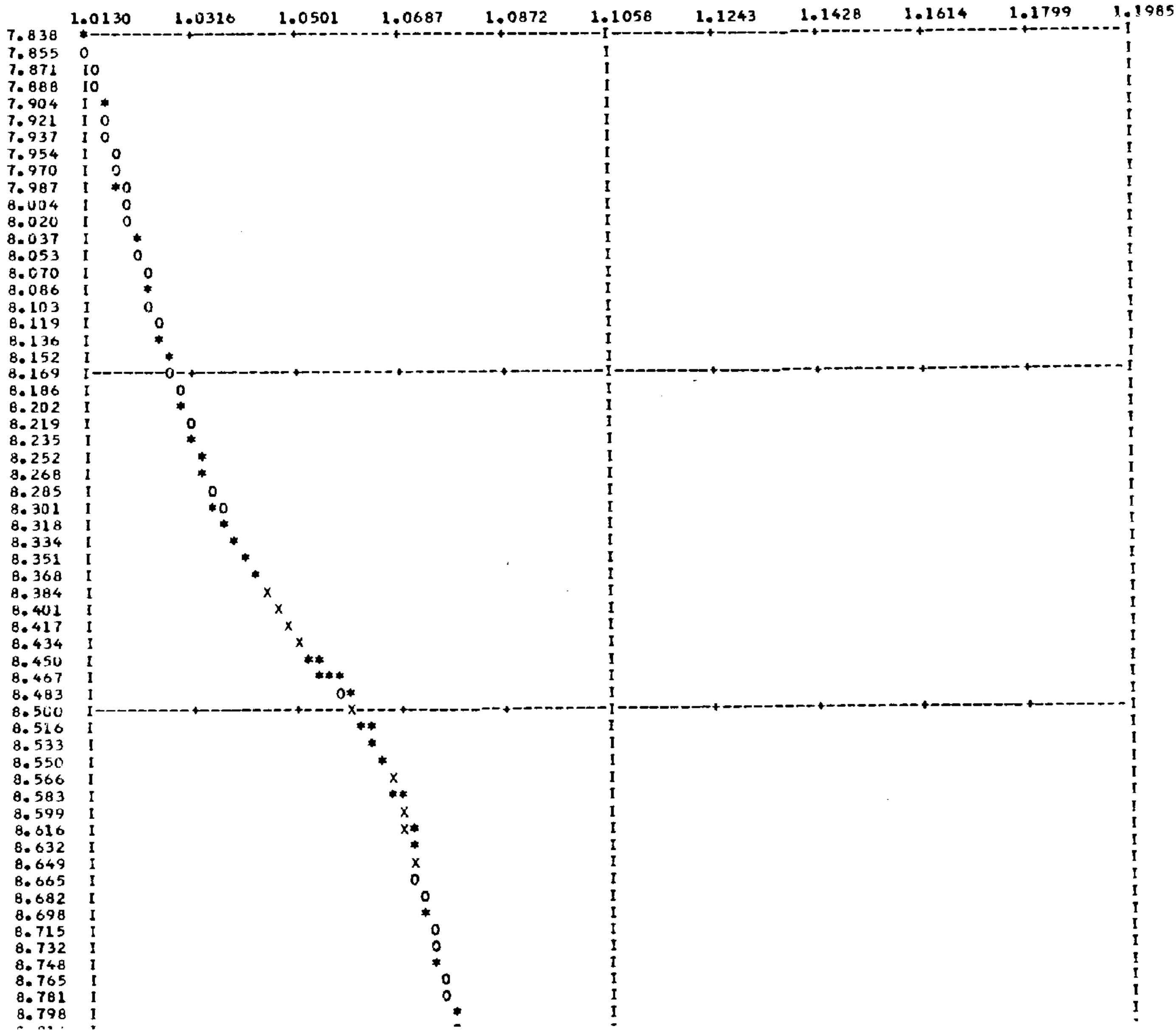
YMAX= 7.275633E 00   XMAX= 1.444032E 01
YMIN= 4.173077E-01   XMIN= 7.838042E 00
DY= 6.858325E-01   DX= 1.654705E-02



XENON (SOLID,20 K)   NEARNORMALINCIDENCE (15 DEGREE)

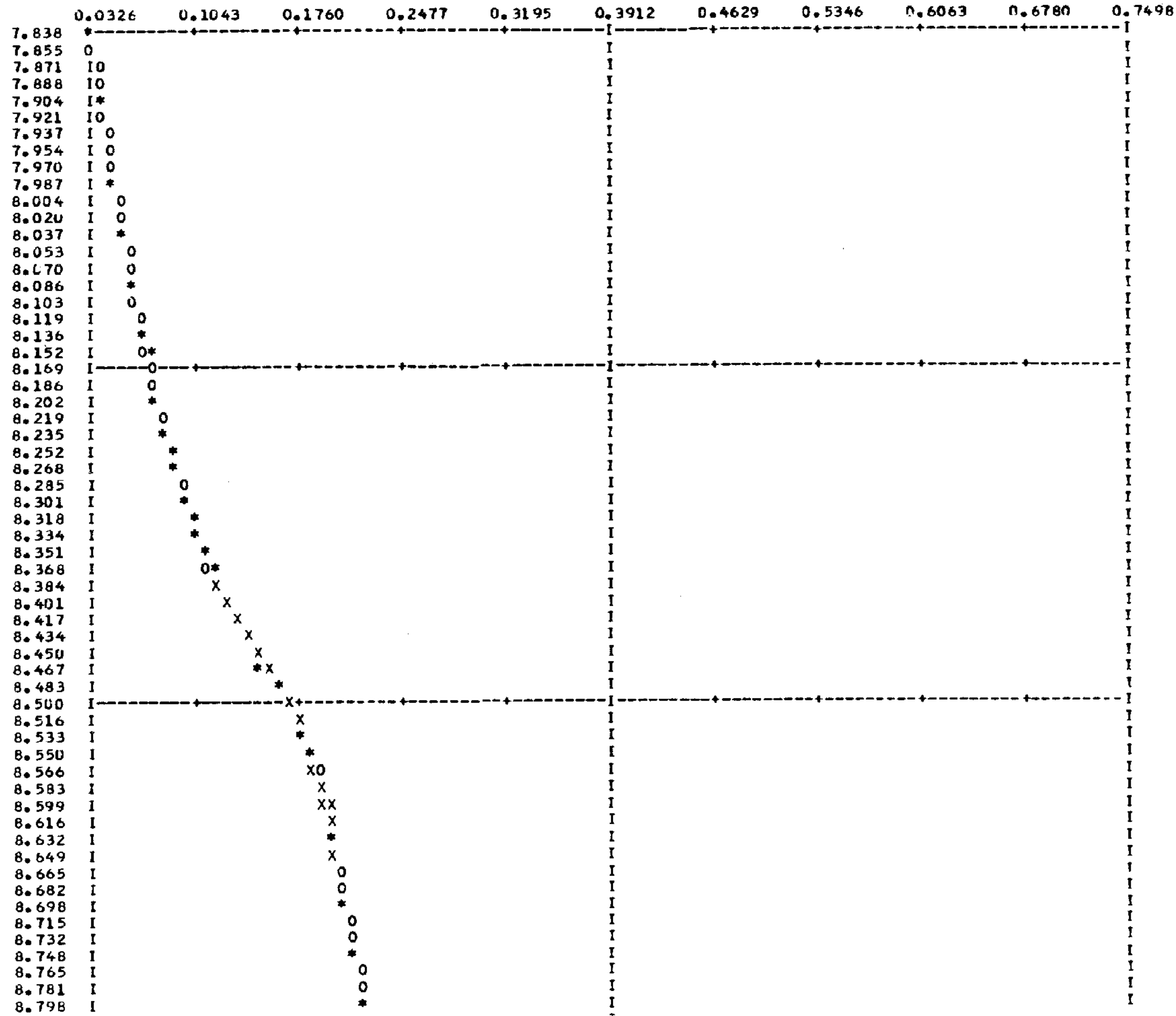
EPSILON-O-EFFECTIV

YMAX= 1.198469E 00   XMAX= 1.444032E 01
YMIN= 1.013039E 00   XMIN= 7.838042E 00
DY= 1.854305E-02   DX= 1.654705E-02



XENON (SOLID,20 K) NEARNORMALINCIDENCE (15 DEGREE)
N-EFFECTIV (ELECTRONS/MOLECULE)

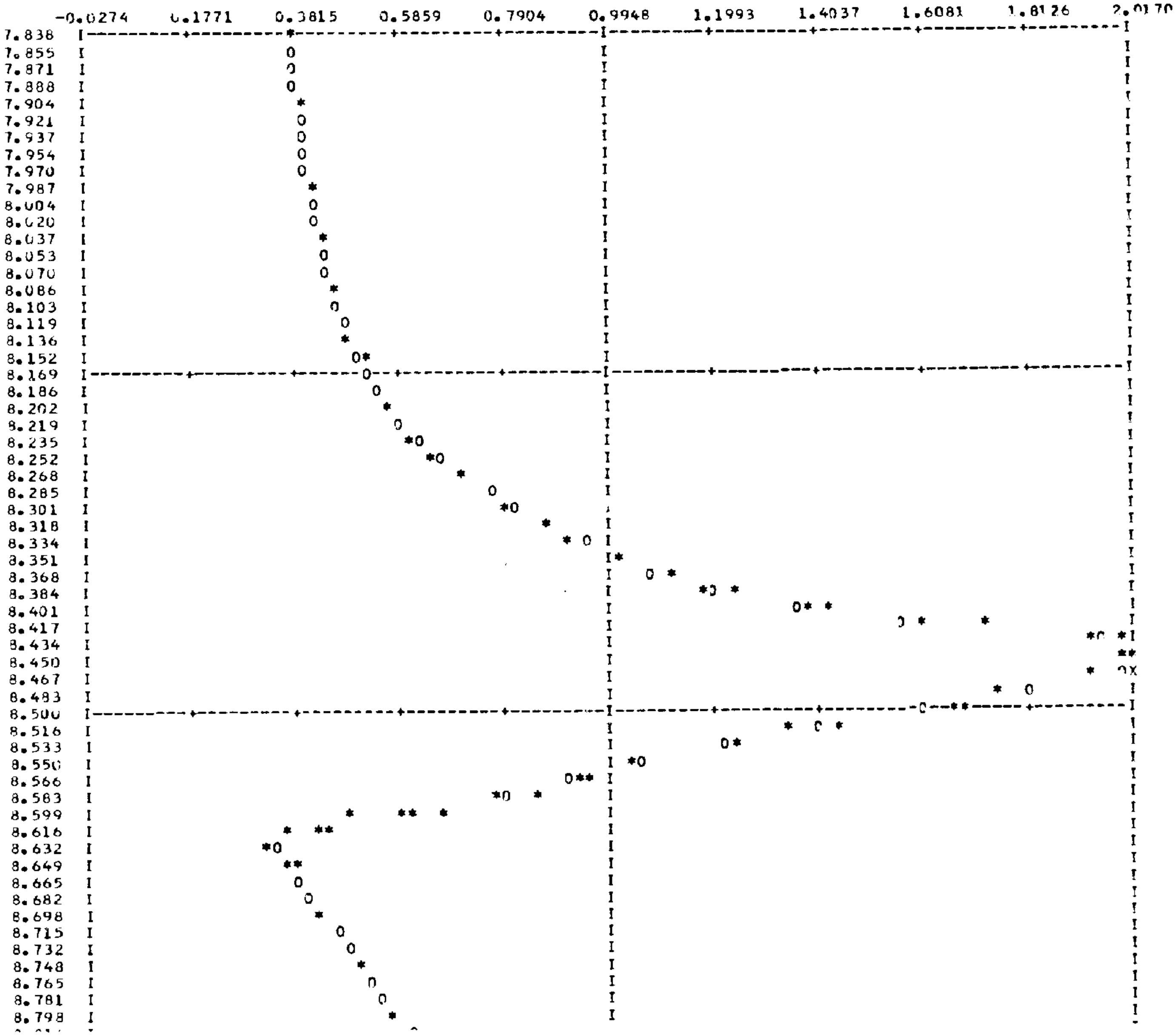
YMAX= 7.497626E-01 XMAX= 1.444032E 01
YMIN= 3.259977E-02 XMIN= 7.838042E 00
DY= 7.171625E-02 DX= 1.654705E-02



XENON (SOLID,20 K)   NEARNORMAL INCIDENCE (15 DEGREE)

EPSILON2 FR. EPSILON1

YMAX= 2.017005E 00   XMAX= 1.444032E 01
YMIN=-2.736678E-02   XMIN= 7.838042E 00
DY=   2.044371E-01   DX=   1.654705E-02



XENON (SOLID,20 K)   NEARNORMAL INCIDENCE (15 DEGREE)
EPSILON2(TEST)-EPSILON2

YMAX=-6.921440E-02   XMAX= 1.444032E 01
YMIN=-1.617523E-01   XMIN= 7.838042E 00
DY= 9.253792E-03   DX= 1.654705E-02