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EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM

An IBM 360/65 modified version of the L.C. Snyder's program for the computer simulation of the Electron Spin Resonance Spectra of aromatic ions and radicals. (Bell Telephone Lab.)

by

A. INZAGHI and L. MONGINI

1968

Joint Nuclear Research Center
Ispra Establishment - Italy

Scientific Data Processing Center - CETIS
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Chemistry Department - Organic Chemistry

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SUMMARY

The report describes an IBM 360/65 modified version of the "Electron Spin Resonance Spectrum Simulation Program" written by Lawrence C. Snyder (Bell Telephone Laboratories) for computer simulation of E.S.R. spectra of aromatic ions and radicals. CALCOMP spectrum plotting has been added to directly compare theoretical and experimental spectra. The possibility of hyperfine structure due to nuclei with spin 1 and 3/2 has been included.

KEYWORDS

COMPUTERS
PROGRAMMING
IBM 360
SPIN
HYPERFINE STRUCTURE
ELECTRON SPIN RESONANCE
SPECTRA
SIMULATORS
AROMATICS
IONS

CONTENTS

1. INTRODUCTION (*)

In order to arrive at the interpretation of E.S.R. spectra, a theoretical reconstruction and a comparison with the experimental spectra is necessary.

The hand made theoretical reconstruction is very time consuming; this is specially true for aromatic radicals and ions, with which we are mostly concerned, where the number of lines can be very high. Furthermore, with a hand made reconstruction it is not always easy to visualize the effect of overlapping between adjacent lines and the effect of line widths. Owing to these facts, several programs have been written to determine line positions and intensities from assumed hyperfine splitting constants. These programs can calculate absorption and derivative spectra using Gaussian or Lorentzian line shape.

This report describes an IBM 360/65 version of the "Electron Spin Resonance Spectrum Simulation Program" written by Lawrence C. Snyder [1] (Bell Telephone Laboratories) for computer simulation of E.S.R. spectra of aromatic ions and radicals.

The program has been written to compute and plot a theoretical reconstruction of the E.S.R. spectrum of an electron having isotropic interaction with several groups of protons; the protons belonging to the same group having the same value of hyperfine splitting constant. Lorentzian line shape is assumed.

We will now describe the modifications introduced in order to make the program suitable for our requirements and the machine.

2. MODIFICATIONS INTRODUCED IN THE PROGRAM

2.1 In the original version of the program, only the presence of hyperfine splittings due to protons or some other nucleus with spin 1/2 was con-

---

L. Mongini was concerned with the methodological and physical aspects of the problem, A. Inzaghi in writing the program for the IBM 360/65

(*) Manuscript received on June 10; 1968.

sidered. The program is now extended to the cases where the hyperfine splittings are due to nuclei with spin 1 and 3/2 *). The number of lines for n equivalent nuclei with spin I is given by the expression 2nI + 1; the relative intensities have been memorized by a data statement. For the sake of homogeneity, also for nuclear spin 1/2, the intensities are now introduced under the data statement; the part of the program calculating the intensities by a recursive formula is now suppressed.

2.2 The plotting by points is not suitable for spectra with a big number of lines. In fact in this case some lines are lost, or the output becomes very extended. In order to use the CALCOMP data plotter [2], and to obtain a continuous plotting of the spectra, the subroutine Plot has been suppressed from the program.

2.3 The height (cm) of the biggest line of the experimental spectrum is now given in input. This in order to obtain the superposition of theoretical and experimental spectrum along the Y axis. As concerns the X axis, the superposition is obtained by expressing in cm the line width at half height, the interval at which the spectrum is sampled and the hyperfine splitting constants.

2.4 The memory capacity of our machine, in comparison with the memory available for the original program in 1960, is much bigger. Owing to the fact that the cases to be treated until now do not need an enlargement in the memory capacity as concerned before, the excess of memory is now utilized in the present version, for memorizing 4 cases and plotting them together. With this method we can define only one file for CALCOMP; this means a great sparing in the number of control cards.

It is necessary to emphasize that this utilization of the memory capacity seems to be, at the moment, the more practical for our machine installation. It is obviously easy to modify the program in order to use

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*) A further extension to the cases of other nuclear spins, by the method outlined in 3.2, would be very easy.

the excess of memory also for a single case if the number of lines became very big. This point will be reconsidered later on.

3. DESCRIPTION OF THE MODIFIED PROGRAM

3.1 The program in its present version, apt to an IBM 360/65 computer, is able to calculate and plot by a CALCOMP data plotter, a theoretical expression for the E.S.R. spectrum (or its derivative) of an electron having isotropic hyperfine interaction with several groups of nuclei, with spin 1/2, 1, or 3/2. The spectrum is assumed to have a Lorentzian line shape.

In the program, the input data to be supplied for a given problem to be studied are in the first card:

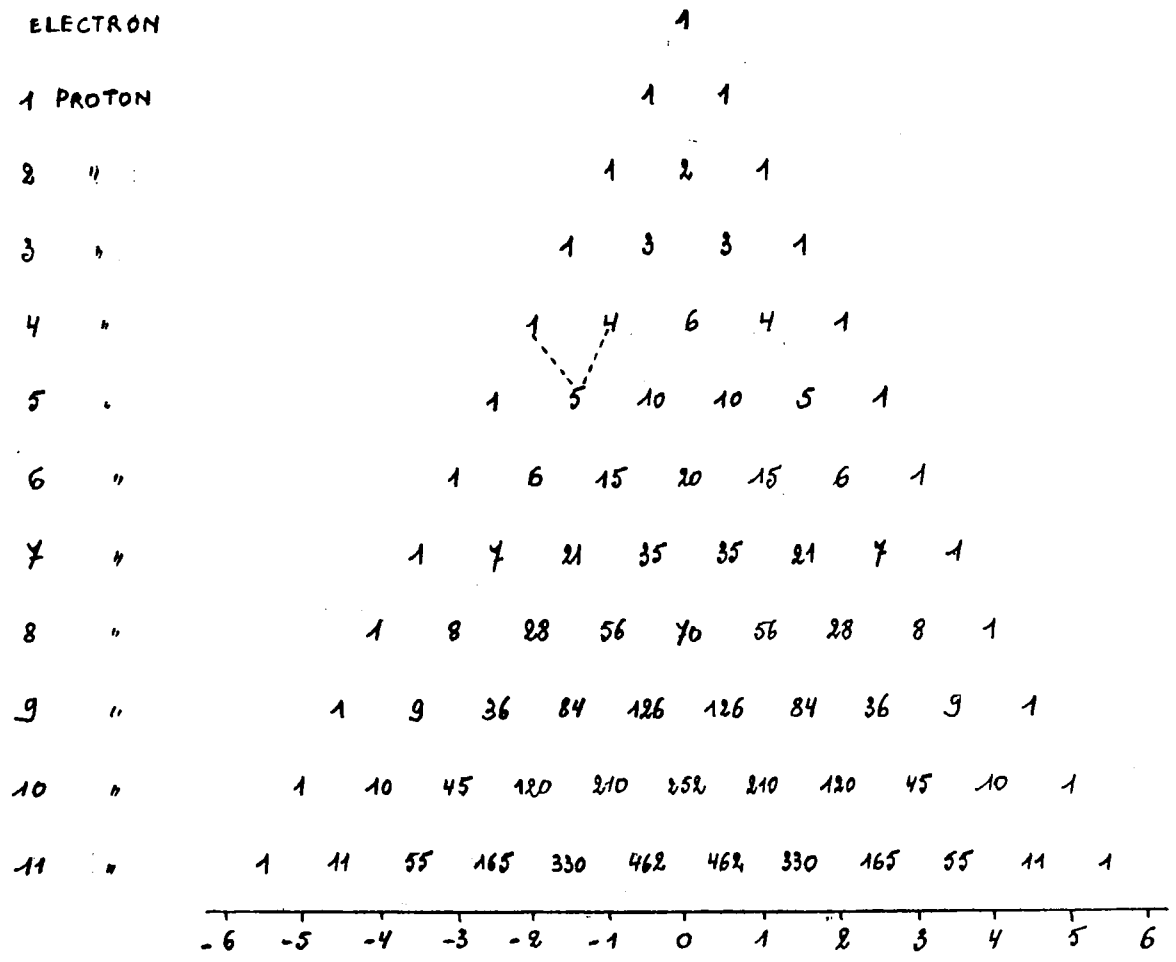
NMKD	- the total number of groups of equivalent nuclei, generating hyperfine patterns
IDEC	- an indicator specifying if the absorption spectrum or its derivative has to be calculated
W(cm)	- the half line width at half height (fig. 1)
ANINT (cm)	- the interval at which the spectrum has to be sampled
XXXX(cm)	- the height of the spectrum
RIB	- an indicator which states if the sign of ordinate of the plot is to be changed

Besides, for each of the groups, the following data have to be specified:

INDGR	- the nuclear spin multiplied by two
NMEK	- the number of nuclei belonging to the group
DHEK(cm)	- the hyperfine splitting constant

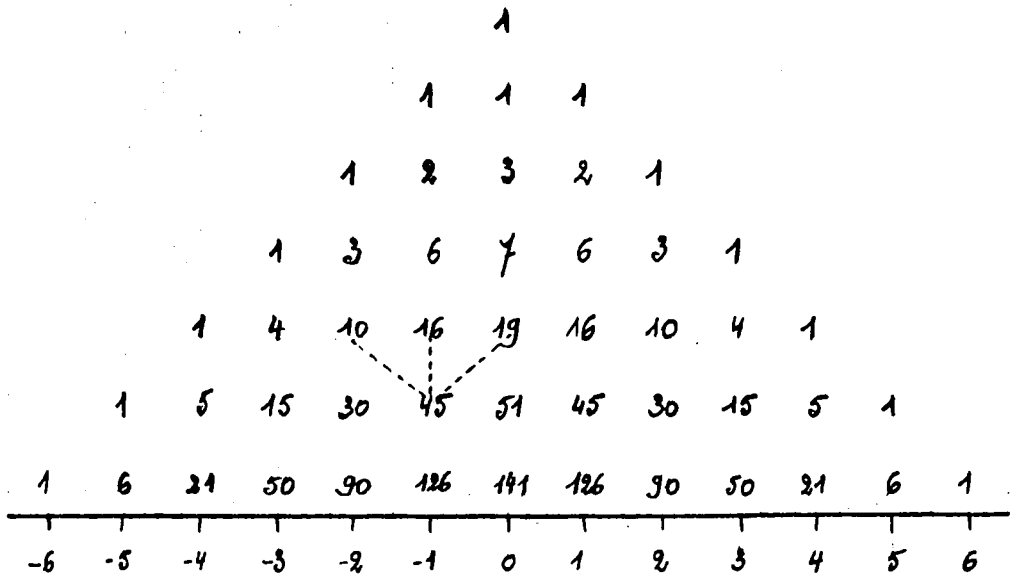
3.2 Now for the description of the work of the program after the reading of the input data, it is necessary to look into some detail at what happens in a single group. Let us consider first the case of protons or any nucleus of spin 1/2.

It is known that hyperfine interaction of the unpaired electron with n equivalent protons produces n + 1 lines having relative intensities and spacings as specified in the following diagram (the separation between any two lines being the value of the hyperfine splitting constant).

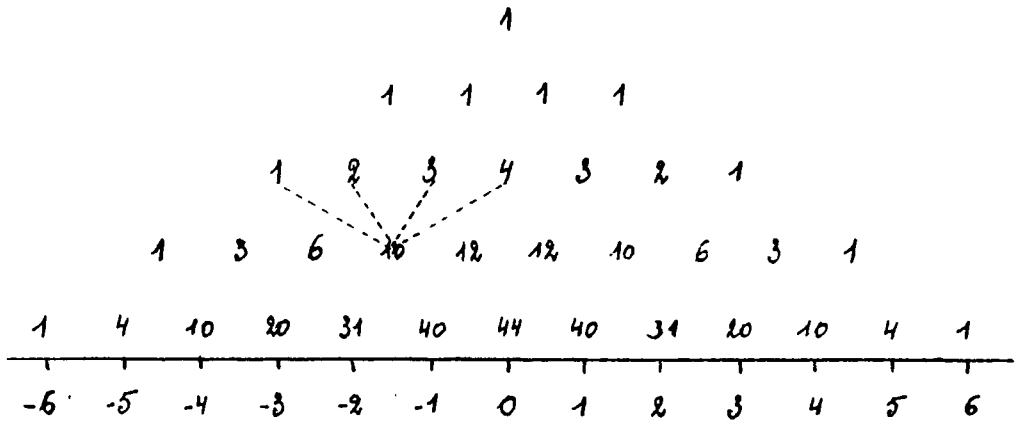


In this triangle the relative intensities of a line can be obtained by summing up the 2 immediate top elements of the upper row.

In the case of nuclei with spin 1 (for instance Deuterium and N^{14}) the hyperfine splitting produces 2n + 1 lines, if n is again the number of equivalent nuclei. The relative intensities and spacings are specified in the following diagram.



In this triangle the relative intensities of a line can be obtained by summing up the 3 immediate top elements of the upper row.
In the case of nuclei with spin 3/2 (for instance Na^{23}) the hyperfine splitting produces 3n + 1 lines. The relative intensities and spacings are



In this triangle the relative intensities of a line can be obtained by summing up the 4 immediate top elements of the upper row.

To shorten the execution time of the program, the values of the relative intensities in the above described triangular diagrams, have been stored in memory once for ever through a DATA statement. Relative intensities

for a given number of equivalent nuclei with spin 1/2, 1 and 3/2, can be asked for in the program till 12, 6 or 4 nuclei, respectively. That is up to 13 lines.

3.3 As soon as the input data are read the program starts to compute for each line both the distances from the origin and the relative intensities. To do so the following procedure is adopted, which, for the sake of clearness we will describe in a particular simple case rather than in general.

Suppose three groups are present having respectively 1 nucleus with spin 1/2, 2 nuclei with spin 1, and 1 nucleus with spin 3/2. In such a case we will have for the first group a splitting in 2 lines, for the second group in 5 lines and for the third group in 4 lines. Let us suppose then that the splitting constants are respectively 13, 2.5, 0.5. In such a case the diagram showing the computation of the relative intensities and of the distances from the origin is given in fig. 2.

The program follows each branch which appears in the diagram of fig. 2, from top to bottom, ordering the branches from the right-most side to the left-most side, and stores for the final points of each branch both the intensity and the distance from origin. That is, in the present case, 2 vectors of length 40 will be stored. These vectors named in the program DS(LIST) and HS(LIST) are respectively (positive part)

1	12.75
1	11.75
1	11.25
1	10.75
2	9.75
2	9.25
2	8.75
2	8.25
3	7.25
3	6.75
3	6.25
3	5.75
2	4.75
2	4.25
2	3.75
2	3.25
1	2.25
1	1.75
1	1.25
1	0.75

The ordering number of the considered branch (and of the corresponding position in the vectors) is named, in the program, LIST.
A CALCOMP plot for the above case is shown in fig. 3 and 4. It is important to note that the ordering numbers in the vectors are still the ordering numbers of the branches also in the cases in which the branches overlap.

3.4 In the program herein described, for the memorization of the above vectors, fast memory use is chosen with respect to tapes or disks, in order to shorten execution time. Consequently, some limitations must exist in the total number of groups to be considered and in the number of nuclei of each group.

If NL(I) is the number of lines of group I (being: NL(I) = NMEK(I) . INDGR(I) + 1) it follows that the total memory occupied by the 2 above introduced vectors is equal, in the case of NMKD groups to:

$$2\ NL(I)\ .\ NL(2)\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\ .\ NL(NMKD)$$

In the present version of the program we have reserved 2 x 4096 word-positions to the above product (see 3.6).

In order to give an idea of what such limitation really means, let us suppose the NL equal for all groups. In such a case the table given below holds

NL	NMKD maximum
2	12
3	7
4	6
5	5
6	4
7	4
8	4
9	3
10	3
11	3
12	3
13	3

3.5 The program assumes in each of the peaks which have been found, the presence of a Lorentzian curve having as half width at half height the input value W(cm). All such Lorentzian curves are summed up together

giving rise to a unique curve Y(X) of which, if so required, the derivative curve Y'(X) is calculated.

Such a curve is calculated and printed at a finite number of points on the abscissa scale, as specified by the input quantity ANINT. The choice of these 2 input parameters W and ANINT requires some skill and care. A too great value of W can give rise to spectra which, still being symmetric with respect to zero of abscissa, lose however some of their peaks; a too great ANINT can produce spectra which besides can also appear completely asymmetric. Generally it is advisable to have W/ANINT $\geq$ 5.

3.6 The program can deal with many cases, and the possibility of storing the points of Y(X) for each consecutive 4 cases is provided for. Two stops are provided in the program, one for number points to be plotted larger than 6000 and the other one for LIST indicator larger than 4096. These 2 stops are related to the memory utilization mode.

In fact, at our computer (IBM 360/65) the total memory capacity is of 128 K-words (K = 1024), of which about 60 K available for users. In the present version of the program, 56192 words are used for the storage of 4 cases. These 56192 words are distributed as follows:

Vector specifying intensities DS(LIST)	4096
Vector specifying distances HS(LIST)	4096
Abscissas of 4 curves Y(X) 6000 x 4	24000
Ordinates of 4 curves Y(X) 6000 x 4	24000
	56192

3.7 As already stated, the choice of the above described dimensions is mostly a matter of convenience. It is very easy, the case being, to change them, for instance in order to deal with larger vectors, that is with a greater number of allowed groups, or atoms in a group.

4. ACKNOWLEDGEMENT

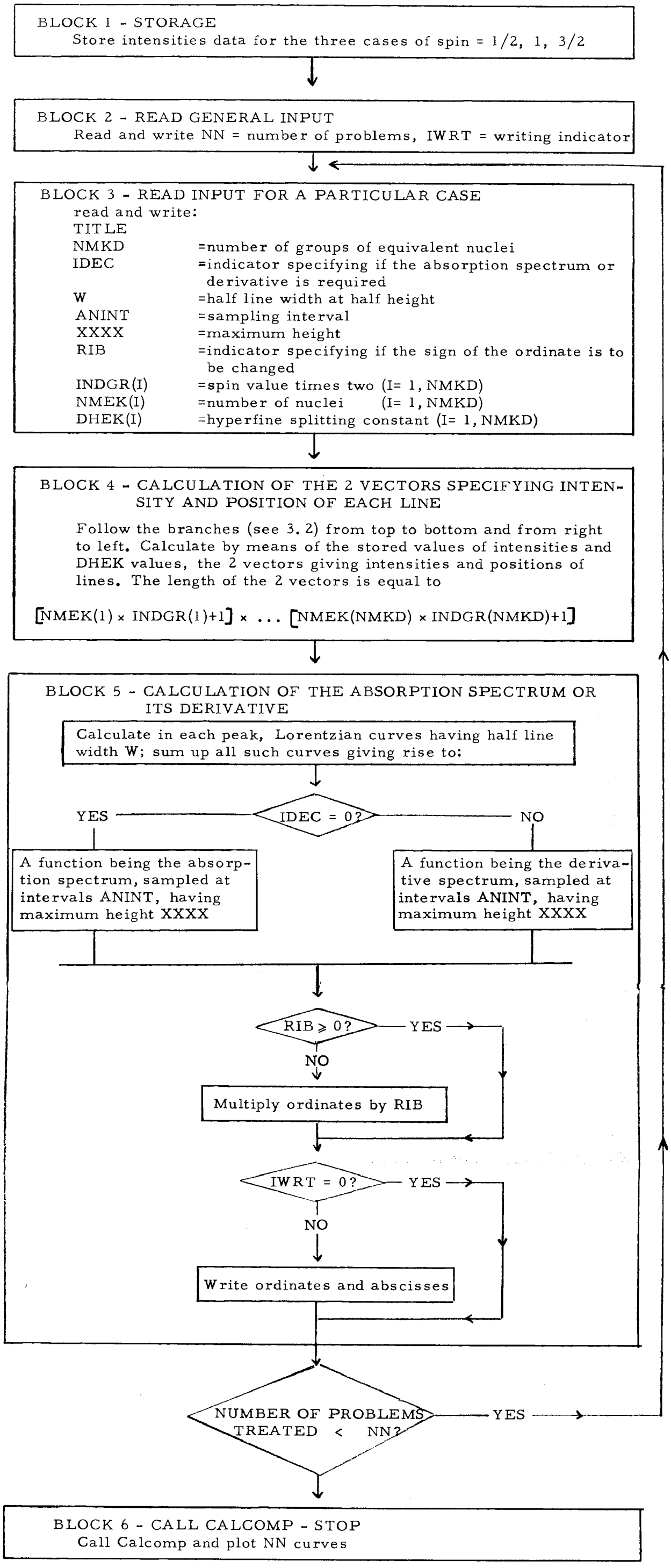
It is a pleasure to thank Dr. H. Hannaert for supporting this work and useful discussions. Thanks are due also to Dr. R. Van Steenwinkel (Magnetic Resonance) for the beautiful Diphenyl spectrum and valuable discussions.

5. REFERENCES

[1] SNYDER, L. C., Proc. Symposium on Molecular Structure and Spectroscopy, Ohio State University, Columbus, June 13-17 (1960)

[2] MOINIL, P., PIRE, J., "Programmation relative au CALCOMP" EUR 2280-f

FLOWCHART


BLOCK 1 - STORAGE
Store intensities data for the three cases of spin = 1/2, 1, 3/2
BLOCK 2 - READ GENERAL INPUT
Read and write NN = number of problems, IWRT = writing indicator
BLOCK 3 - READ INPUT FOR A PARTICULAR CASE
read and write:
TITLE
NMKD =number of groups of equivalent nuclei
IDEC =indicator specifying if the absorption spectrum or derivative is required
W =half line width at half height
ANINT =sampling interval
XXXX =maximum height
RIB =indicator specifying if the sign of the ordinate is to be changed
INDGR(I) =spin value times two (I= 1, NMKD)
NMEK(I) =number of nuclei (I= 1, NMKD)
DHEK(I) =hyperfine splitting constant (I= 1, NMKD)
BLOCK 4 - CALCULATION OF THE 2 VECTORS SPECIFYING INTENSITY AND POSITION OF EACH LINE
Follow the branches (see 3.2) from top to bottom and from right to left. Calculate by means of the stored values of intensities and DHEK values, the 2 vectors giving intensities and positions of lines. The length of the 2 vectors is equal to
[NMEK(1) × INDGR(1)+1] × ... [NMEK(NMKD) × INDGR(NMKD)+1]
BLOCK 5 - CALCULATION OF THE ABSORPTION SPECTRUM OR ITS DERIVATIVE
Calculate in each peak, Lorentzian curves having half line width W; sum up all such curves giving rise to:
IDEC = 0?
YES
NO
A function being the absorption spectrum, sampled at intervals ANINT, having maximum height XXXX
A function being the derivative spectrum, sampled at intervals ANINT, having maximum height XXXX
RIB ≥ 0?
YES
NO
Multiply ordinates by RIB
IWRT = 0?
YES
NO
Write ordinates and abscisses
NUMBER OF PROBLEMS TREATED < NN?
YES
BLOCK 6 - CALL CALCOMP - STOP
Call Calcomp and plot NN curves

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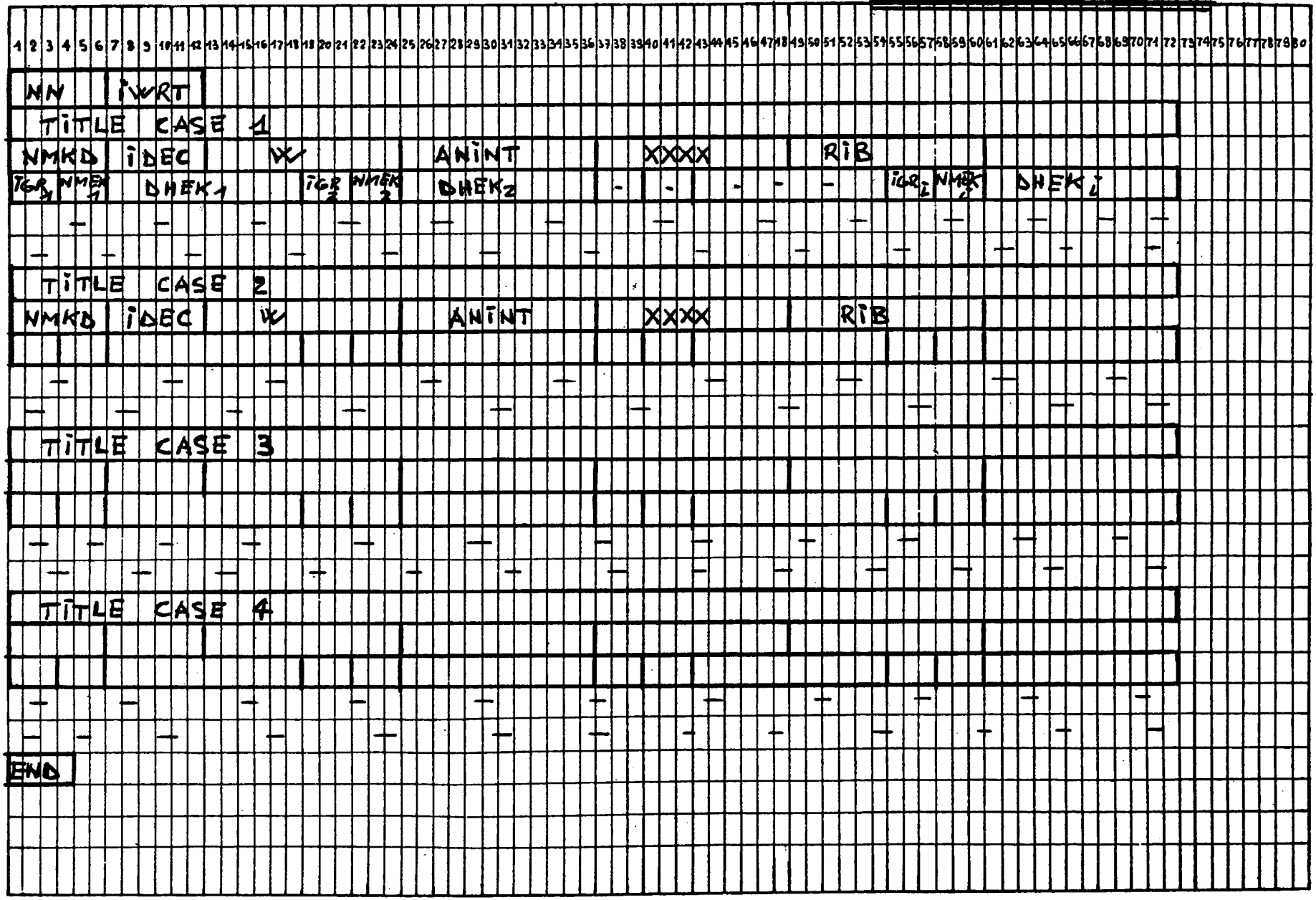
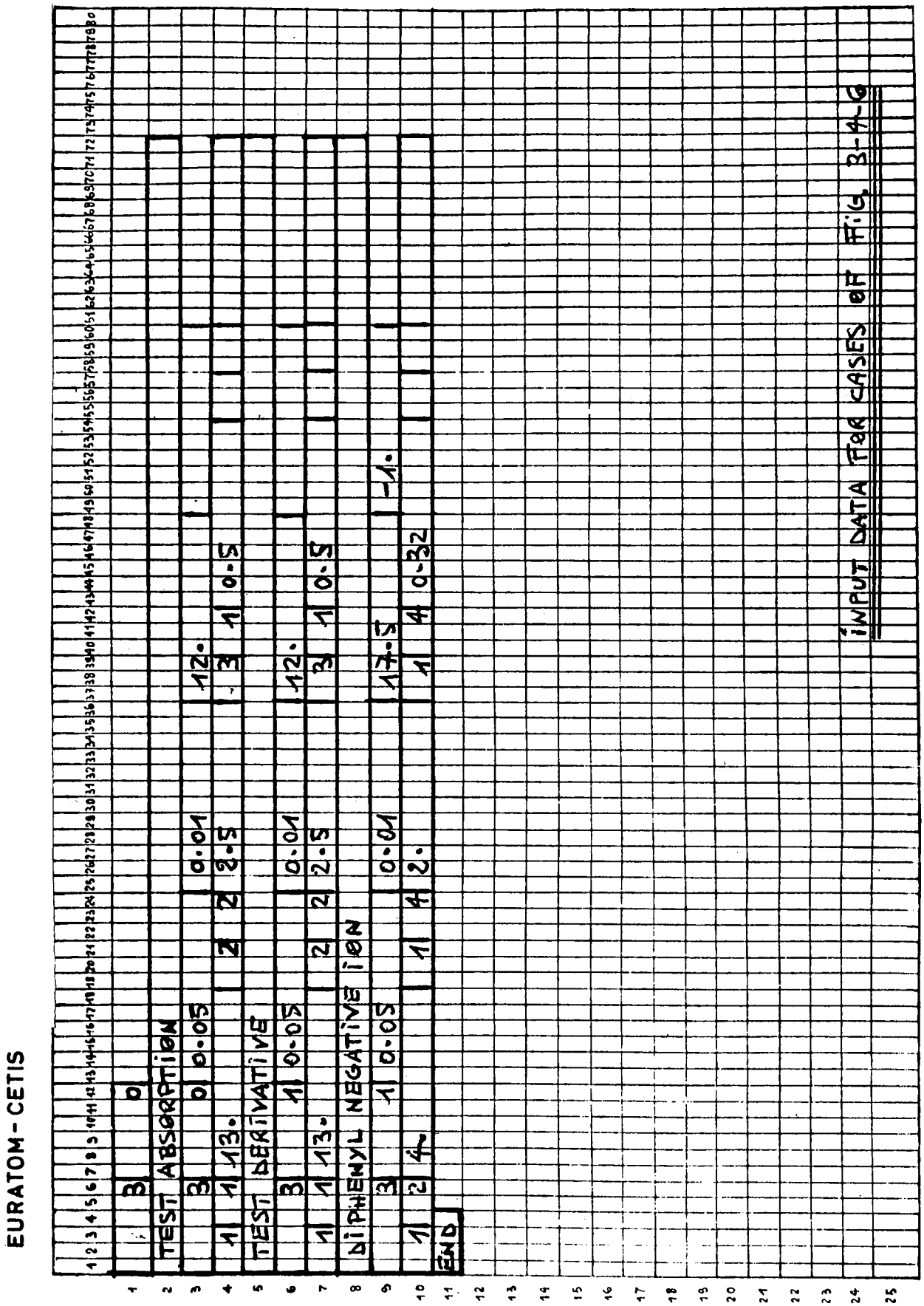
INPUT INSTRUCTIONS



8. INPUT DATA FOR CASES OF FIG. 3, 4, 6



```
C      MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM
C
C
0001        DIMENSION NMEK(12),DMEK(12),H(13,12),D(13,12),HS(4096),DS(4096)
0002        DIMENSION INDGR(12)
0003        DIMENSION X2(6000),Y2(6000),X3(6000),Y3(6000),X4(6000),Y4(6000)
0004        DIMENSION X1(6000),Y1(6000)
0005        DIMENSION AAAA(18)
0006        DIMENSION AP(90),AU(48),APX(12,13),AUX(6,13)
0007        DIMENSION AQ(34),AQX(4,13)
C
C
C      BLOCK 1-STORAGE-
C
C
0008        DATA TEST,TEST,TEST,AU/4HEND ,4HEND ,4HEND ,1.,1.,1.,1.,2.,3.,2.,1
           A.,1.,3.,6.,7.,6.,3.,1.,1.,4.,10.,16.,19.,16.,10.,4.,1.,1.,5.,15.,3
           80.,45.,51.,45.,30.,15.,5.,1.,1.,6.,21.,50.,90.,126.,141.,126.,90.,
           C50.,21.,6.,1./
0009        DATA RR,RR,RR,AP/4H    ,4H    ,4H    ,1.,1.,1.,2.,1.,1.,3.,3.,1.,1
           A.,4.,6.,4.,1.,1.,5.,10.,10.,5.,1.,1.,6.,15.,20.,15.,6.,1.,1.,7.,21
           B.,35.,35.,21.,7.,1.,1.,8.,28.,56.,70.,56.,28.,8.,1.,1.,9.,36.,84.,
           C126.,126.,84.,36.,9.,1.,1.,10.,45.,120.,210.,252.,210.,120.,45.,10
           D.,1.,1.,11.,55.,165.,330.,462.,462.,330.,165.,55.,11.,1.,1.,12.,66
           E.,220.,495.,792.,924.,792.,495.,220.,66.,12.,1./
0010        DATA FF,FF,FF,AQ/4H    ,4H    ,4H    ,1.,1.,1.,1.,1.,2.,3.,4.,3.,2
           1.,1.,1.,3.,6.,10.,12.,12.,10.,6.,3.,1.,1.,4.,10.,20.,31.,40.,44.,4
           20.,31.,20.,10.,4.,1./
0011        DO 24 JK=1,44540
0012     24 NMEK(JK)=0
0013        JX=0
0014        DO 997 K=1,12
0015        JY=JX+1
0016        JX=JY+K
0017        J1=0
0018        DO 997 J=JY,JX
0019        J1=J1+1
0020        APX(K,J1)=AP(J)
0021     997 CONTINUE
0022        JX=0
0023        DO 998 K=1,6
0024        JY=JX+1
0025        K1=2*K
0026        JX=JY+K1
0027        J1=0
0028        DO 998 J=JY,JX
0029        J1=J1+1
0030        AUX(K,J1)=AU(J)
```

```
0031            998 CONTINUE
0032                JX=0
0033                DO 996 K=1,4
0034                JY=JX+1
0035                K1=3*K
0036                JX=JY+K1
0037                J1=0
0038                DO 996 J=JY,JX
0039                J1=J1+1
0040                AQX(K,J1)=AQ(J)
0041            996 CONTINUE
                C
                CC
                C       BLOCK 2-READ GENERAL INPUT-
                CC
                C
0042                READ (5,15) NN,IWRT
0043                WRITE (6,12) NN,IWRT
0044                MM=1
0045           1111 CONTINUE
0046                DO32I=1,12000
0047             32 X1(I)=0.
                C
                CC
                C       BLOCK 3-READ INPUT FOR A PARTICULAR CASE-
                CC
                C
0048                READ(5,4)(AAAA(I),I=1,18)
0049                WRITE (6,10) (AAAA(I),I=1,18)
0050                IF(AAAA(1).EQ.TEST) GO TO 2222
0051                WRITE (6,8001)
0052                READ(5,1) NMKD,IDEC,W,ANINT,XXXX,RIB
0053                READ (5,2) (INDGR(I),NMEK(I),DHEK(I),I=1,NMKD)
0054                WRITE (6,11) NMKD,IDEC,W,ANINT,XXXX
0055                WRITE (6,18) (INDGR(I),I=1,12)
0056                WRITE (6,13) (NMEK(I),I=1,12)
0057                WRITE (6,14) (DHEK(I),I=1,12)
0058                WRITE(6,3)
                C
                CC
                C       BLOCK 4-CALCULATION OF THE 2 VECTORS SPECIFYING
                C       INTENSITY AND POSITIONS OF EACH LINE-
                CC
                C
0059                DO 150 I=1,NMKD
0060                K=NMEK(I)
0061                AAK=K
0062                L=INDGR(I)*K+1
```

```
0063                JQ=INDGR(I)
0064                GO TO (5000,5001,5006),JQ
0065           5000 AAIND=AAK*0.5
0066                GO TO 5002
0067           5001 AAIND=AAK
0068                GO TO 5002
0069           5006 AAIND=AAK*1.5
0070           5002 DO 140 J=1,L
0071                AAJ=J
0072            140 H(J,I)=(AAIND-AAJ+1.)*DHEK(I)
0073                GO TO(5003,5004,5005),JQ
0074           5003 DO 130 J=1,L
0075            130 D(J,I)=APX(K,J)
0076                GO TO 150
0077           5004 DO 131 J=1,L
0078            131 D(J,I)=AUX(K,J)
0079                GO TO 150
0080           5005 DO 132 J=1,L
0081            132 D(J,I)=AQX(K,J)
0082            150 CONTINUE
0083                LIST=0
0084                IA=INDGR(1)*NMEK(1)+1
0085                DO 201 IY=1,IA
0086                SHO1S=H(IY,1)
0087                SHS=SHO1S
0088                PDO1S=D(IY,1)
0089                PDS=PDO1S
0090                IF (NMKD-2) 161,162,162
0091            401 GO TO 201
0092            162 IB=INDGR(2)*NMEK(2)+1
0093                DO 202 I2=1,IB
0094                SHO2S=H(I2,2)+SHO1S
0095                SHS=SHO2S
0096                PDO2S=D(I2,2)*PDO1S
0097                PDS=PDO2S
0098                IF (NMKD-3) 161,163,163
0099            402 GO TO 202
0100            163 IC=INDGR(3)*NMEK(3)+1
0101                DO 203 I3=1,IC
0102                SHO3S=H(I3,3)+SHO2S
0103                SHS=SHO3S
0104                PDO3S=D(I3,3)*PDO2S
0105                PDS=PDO3S
0106                IF (NMKD-4) 161,164,164
0107            403 GO TO 203
0108            164 ID=INDGR(4)*NMEK(4)+1
0109                DO 204 I4=1,ID
0110                SHO4S=H(I4,4)+SHO3S
```

```
0111                SHS=SH04S
0112                PD04S=D(I4,4)*PD03S
0113                PDS=PD04S
0114                IF (NMKD-5) 161,165,165
0115           404  GO TO 204
0116           165  IE=INDGR(5)*NMEK(5)+1
0117                DO 205 I5=1,IE
0118                SH05S=H(I5,5)+SH04S
0119                SHS=SH05S
0120                PD05S=D(I5,5)*PD04S
0121                PDS=PD05S
0122                IF (NMKD-6) 161,166,166
0123           405  GO TO 205
0124           166  IG=INDGR(6)*NMEK(6)+1
0125                DO 206 I6=1,IG
0126                SH06S=H(I6,6)+SH05S
0127                SHS=SH06S
0128                PD06S=D(I6,6)*PD05S
0129                PDS=PD06S
0130                IF (NMKD-7) 161,167,167
0131           406  GO TO 206
0132           167  IH=INDGR(7)*NMEK(7)+1
0133                DO 207 I7=1,IH
0134                SH07S=H(I7,7)+SH06S
0135                SHS=SH07S
0136                PD07S=D(I7,7)*PD06S
0137                PDS=PD07S
0138                IF (NMKD-8) 161,168,168
0139           407  GO TO 207
0140           168  II=INDGR(8)*NMEK(8)+1
0141                DO 208 I8=1,II
0142                SH08S=H(I8,8)+SH07S
0143                SHS=SH08S
0144                PD08S=D(I8,8)*PD07S
0145                PDS=PD08S
0146                IF (NMKD-9) 161,169,169
0147           408  GO TO 208
0148           169  IJ=INDGR(9)*NMEK(9)+1
0149                DO 209 I9=1,IJ
0150                SH09S=H(I9,9)+SH08S
0151                SHS=SH09S
0152                PD09S=D(I9,9)*PD08S
0153                PDS=PD09S
0154                IF (NMKD-10) 161,170,170
0155           409  GO TO 209
0156           170  IK=INDGR(10)*NMEK(10)+1
0157                DO 210 I10=1,IK
0158                SH10S=H(I10,10)+SH09S
```

```
0159                SHS=SH10S
0160                PD10S=D(I10,10)*PD09S
0161                PDS=PD10S
0162                IF (NMKD-11) 161,171,171
0163           410  GO TO 210
0164           171  IL=INDGR(11)*NMEK(11)+1
0165                DO 211 I11=1,IL
0166                SH11S=H(I11,11)+SH10S
0167                SHS=SH11S
0168                PD11S=D(I11,11)*PD10S
0169                PDS=PD11S
0170                IF (NMKD-12) 161,172,172
0171           411  GO TO 211
0172           172  IM=INDGR(12)*NMEK(12)+1
0173                DO 212 I12=1,IM
0174                SH12S=H(I12,12)+SH11S
0175                SHS=SH12S
0176                PD12S=D(I12,12)*PD11S
0177                PDS=PD12S
0178                GO TO 161
0179           212  CONTINUE
0180           211  CONTINUE
0181           210  CONTINUE
0182           209  CONTINUE
0183           208  CONTINUE
0184           207  CONTINUE
0185           206  CONTINUE
0186           205  CONTINUE
0187           204  CONTINUE
0188           203  CONTINUE
0189           202  CONTINUE
0190           201  CONTINUE
0191                GO TO 6005
0192           161  LIST=LIST+1
0193                IF(LIST-4096)6000,6000,6001
0194          6001  WRITE (6,6002) LIST
0195                GO TO 2222
0196          6000  CONTINUE
0197                HS(LIST)=SHS
0198                DS(LIST)=PDS
0199                NOWOT=NMK)
0200                GO TO(401,402,403,404,405,406,407,408,409,410,411,212),NOWOT
                C
                C
                C     BLOCK 5-CALCULATION OF THE ABSORPTION SPECTRUM OR ITS DERIVATIVE-
                C
                C
0201          6005  A1=HS(1)
```

```
0202                DO 740 IZ=2,LIST
0203                IF (A1-HS(IZ)) 741,740,740
0204           741  A1=HS(IZ)
0205           740  CONTINUE
0206                B1=-A1-W*10.0
0207                A1=A1+W*10.0
0208                ART=(A1-B1)/(ANINT*20.0)
0209                JART=ART+1.0
0210                BART=JART
0211                DELT=(BART-ART)*20.0*ANINT/2.0
0212                A1=A1+DELT
0213                A2=A1-BART*20.0*ANINT
0214                I1=JART*20+1
0215                IZ1=JART*10+1
0216                DO 450 K=1,I1
0217                AJ=K-1
0218           450  X1(K)=A2+AJ*ANINT
0219                ANORM=0.0
0220                DO 455 K=1,LIST
0221           455  ANORM=ANORM+DS(K)
0222                DO 460 K=1,LIST
0223           460  DS(K)=DS(K)/ANORM
0224                DO 470 K=1,I1
0225           470  Y1(K)=0.0
0226                Z=+1.0/W
0227                S=Z/3.1416
0228                IF(IDEC)500,600,500
0229           600  DO630I=1,LIST
0230                DO630J=1,IZ1
0231                Y1(J)=Y1(J)+DS(I)*(S/(1.0+Z*Z*(X1(J)-HS(I))*(X1(J)-HS(I))))
0232           630  CONTINUE
0233                DO999J=1,IZ1
0234                I=I1-J+1
0235           999  Y1(I)=Y1(J)
0236                GO TO 800
0237           500  DO 650 I=1,LIST
0238                DO 650 J=1,IZ1
0239                Y1(J)=Y1(J)+DS(I)*(-S*Z*Z*2.0*(X1(J)-HS(I))/((1.0+(X1(J)-HS(I))*(X
                   11(J)-HS(I))*Z*Z)*(1.0+(X1(J)-HS(I))*(X1(J)-HS(I))*Z*Z)))
0240           650  CONTINUE
0241                DO 899 J=1,IZ1
0242                I=I1-J+1
0243                Y1(I)=-Y1(J)
0244           899  Y1S=Y1(I)
0245           800  CONTINUE
0246                ZZY=0.
0247                DO 555 I=2,I1
0248                IF(Y1(I-1))558,559,559
```

```
0249           558 DD1=0.
0250               GO TO 553
0251           559 DD1=Y1(I-1)
0252           553 IF(Y1(I))556,557,557
0253           556 DD2=0.
0254               GO TO 554
0255           557 DD2=Y1(I)
0256           554 IF(DD2-DD1)551,552,552
0257           551 IF(ZZY.LT.DD1) ZZY=DD1
0258               GO TO 555
0259           552 IF(ZZY.LT.DD2) ZZY=DD2
0260           555 CONTINUE
0261               IF(ZZY.LE.0.) GO TO 8222
0262               WRITE (6,17) ZZY
0263               RAPP=XXXX/ZZY
0264               ZZY=XXXX
0265               DO 515 I=1,I1
0266           515 Y1(I)=Y1(I)*RAPP
0267               IF(RIB) 9000,9001,9001
0268          9000 DO 9002 I=1,I1
0269          9002 Y1(I)=Y1(I)*RIB
0270          9001 CONTINUE
0271               WRITE(6,5) JART,A1,A2,I1
0272               IF(IWRT.EQ.0) GO TO 23
0273               WRITE(6,7)
0274               WRITE (6,6) (X1(I),Y1(I),I=1,I1)
0275            23 CONTINUE
                C
                C
                C      BLOCK 6-CALL CALCONP-
                C
                C
0276               IF(I1.GT.6000) GO TO 4000
0277               GO TO (20,21,27,22),MM
0278            20 DO 25 I=1,I1
0279               X2(I)=X1(I)
0280            25 Y2(I)=Y1(I)
0281               MA=I1
0282               Z1X=A1-A2
0283               Z1Y=ZZY
0284               GO TO 22
0285            21 DO 26 I=1,I1
0286               X3(I)=X1(I)
0287            26 Y3(I)=Y1(I)
0288               MB=I1
0289               Z2X=A1-A2
0290               Z2Y=ZZY
0291               GO TO 22
```

```
0292            27 DO 29 I=1,I1
0293               X4(I)=X1(I)
0294            29 Y4(I)=Y1(I)
0295               MC=I1
0296               Z3X=A1-A2
0297               Z3Y=ZZY
0298            22 MM=MM+1
0299               IF(MM.GT.NN) GO TO 33
0300               GO TO 1111
0301            33 CONTINUE
0302               CALL FINIM (0.,0.)
0303               CALL DESSIN(X2,Y2,MA,1,1,1,0,0,Z1X,Z1Y,0,0,4H X1 ,-4,4H Y1 ,+4,0)
0304               IF(MM-2)3332,3334,3332
0305          3334 ZZB=Z1X+5.
0306               GO TO 3333
0307          3332 ZZA=Z1Y+3.
0308               CALL FINIM(0.,ZZA)
0309               CALL DESSIN(X3,Y3,MB,1,1,1,0,0,Z2X,Z2Y,0,0,4H X2 ,-4,4H Y2 ,+4,0)
0310               IF(MM-3)3335,3336,3335
0311          3336 ZZB=Z2X+5.
0312               GO TO 3333
0313          3335 ZZA=Z2Y+3.
0314               CALL FINIM(0.,ZZA)
0315               CALL DESSIN(X4,Y4,MC,1,1,1,0,0,Z3X,Z3Y,0,0,4H X3 ,-4,4H Y3 ,+4,0)
0316               IF(MM-4)3337,3338,3337
0317          3338 ZZB=Z3X+5.
0318               GO TO 3333
0319          3337 ZZA=Z3Y+3.
0320               CALL FINIM(0.,ZZA)
0321               ZZX=A1-A2
0322               CALL DESSIN(X1,Y1,I1,1,1,1,0,0,ZZX,ZZY,0,0,4H X4 ,-4,4H Y4 ,+4,0)
0323               ZZB=ZZX+5.
0324               ZZC=NN-1
0325               ZZC=-ZZC*ZZA
0326               CALL FINIM(ZZB,ZZC)
0327               CALL FINTRA
0328               GO TO 1111
0329          3333 CONTINUE
0330               ZZC=NN-1
0331               ZZC=-ZZC*ZZA
0332               CALL FINIM(ZZB,ZZC)
0333               CALL FINTRA
0334               GO TO 1111
                C
                C
                C      FORMAT STATEMENTS
                C
                C
```

```
0335              1 FORMAT(2I6,4E12.6)
0336              2 FORMAT (4(I3,I3,E12.6))
0337              3 FORMAT(1H1,30X,'MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATI
                   1ON PROGRAM'///)
0338              4 FORMAT (13A4)
0339              5 FORMAT (1H0,4HJART,I6,10X,2HA1,F6.2,10X,2HA2,F6.2,10X,2HI1,I6//)
0340              6 FORMAT(1H ,5X,6E16.6)
0341              7 FORMAT (1H ,45X,13HX1(I) , Y1(I)///)
0342              9 FORMAT (///1H ,'PROGRAM STOP FOR NUMBER POINTS TO PLOT LARGER THAN
                   1 6000'///)
0343             10 FORMAT (1H1,5X,18A4//)
0344             11 FORMAT (//1H ,10X,5HNMKD=I3,5X,5HIDEC=I3,5X,2HW=E12.4,5X,6HANINT=E
                   112.4,5X,16HLENG OF Y (CM) =E12.4)
0345             12 FORMAT (///1H ,20X,'NUMBER OF CASES  ',I2,10X,'IWRT = ',I2///)
0346             13 FORMAT (//1H ,10X,7HNMEK(I)/1H ,12I10)
0347             14 FORMAT (//1H ,10X,7HDHEK(I)/1H ,12E11.4//)
0348             16 FORMAT (2I6)
0349             17 FORMAT (///1H ,'MAX VALUE  OF Y1(I)  = ',E16.6///)
0350             18 FORMAT (//1H ,10X,8HINDGR(I)/1H ,12I10)
0351           6002 FORMAT (///1H ,'PROGRAM STOP FOR LIST INDICATOR LARGER THAN 4096'/
                   1//)
0352           8000 FORMAT (///1H ,'PROGRAM STOP FOR Y1(MAX) = ',E16.6///'
0353           8001 FORMAT (///1H ,50X,'INPUT DATA'///)
                C
                C
                C     CONTROL STATEMENTS FOR PROGRAM LIMITES
                C
                C
0354           4000 WRITE(6,9) I1
0355                GO TO 2222
0356           8222 WRITE (6,8000) ZZY
0357                GO TO 2222
0358           2222 STOP
0359                END
```

SCALAR MAP

SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION
TEST	410	PD	414	FF	418	JK	41C	JX	420
K	424	JY	428	J1	42C	J	430	K1	434
NN	438	IWRT	43C	MM	440	I	444	NMKD	448
IDEC	44C	N	450	ANINT	454	XXXX	458	RIB	45C
AAK	460	L	464	JQ	468	AAIND	46C	AAJ	470
LIST	474	IA	478	IY	47C	SH01S	480	SHS	484
PD01S	488	PDS	48C	I8	490	I2	494	SH02S	498
PD02S	49C	TC	4A0	I3	4A4	SH03S	4A8	PD03S	4AC
I9	4B0	I4	4B4	SH04S	4B8	PD04S	4BC	IE	4C0
I5	4C4	SH05S	4C8	PD05S	4CC	IG	4D0	I6	4D4
SH06S	4D8	PD06S	4DC	IH	4E0	I7	4E4	SH07S	4E8
PD07S	4EC	II	4F0	I8	4F4	SH08S	4F8	PD08S	4FC
IJ	500	I9	504	SH09S	508	PD09S	50C	IK	510
I10	514	SH10S	518	PD10S	51C	IL	520	I11	524
SH11S	528	PD11S	52C	IM	530	I12	534	SH12S	538
PD12S	53C	NUMOT	540	A1	544	IZ	548	B1	54C
ART	550	JART	554	BART	558	DELT	55C	A2	560
II	564	IZ1	568	AJ	56C	ANORM	570	Z	574
S	578	YIS	57C	ZZY	580	DD1	584	DD2	588
SAPP	58C	MA	590	Z1X	594	Z1Y	598	MB	59C
Z2X	5A0	Z2Y	5A4	MC	5A8	Z3X	5AC	Z3Y	5B0
ZZB	5B4	ZZ	5B8	ZZX	5BC	ZZC	5C0		

ARRAY MAP

SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION
NMEK	5C4	CHCK	5E4	H	624	D	894	HS	B04
DS	4B04	INDGR	8B04	X2	8B34	Y2	1E8E4	X3	146B4
Y3	1A474	X4	20234	Y4	25FE4	X1	28DB4	Y1	31B74
AAAA	37934	AP	3797C	AU	37AE4	APX	37BA4	AUX	37E14
AQ	37F4C	AQX	37F04						

SUBPROGRAMS CALLED

SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION
IBCOM=	380A4	FINIM	380A8	DESSIN	380AC	FINTRA	380B0		

FORMAT STATEMENT MAP

SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION	SYMBOL	LOCATION
1	38214	2	3821F	3	3822B	4	38273	5	38279
6	382A2	7	382AE	9	382C7	10	3830B	11	38318
12	38362	13	38391	14	383AB	16	383C8	17	383CE
18	383F5	8002	38410	8000	3844D	8001	38478		

TOTAL MEMORY REQUIREMENTS 03A064 BYTES

28

```
IEF285I   SYSOUT                                        SYSOUT
IEF285I   VOL SER NOS=                                  PASSED
IEF285I   PUNCH1                                        PASSED
IEF285I   VOL SER NOS= PUNCH1.
IEF285I   LOADSET.SPIN
IEF285I   VOL SER NOS= EURSY1.
     EURFT      DATE 68.04.08          13  DURATION 0.006 N.OPER= 504 INP=001
IEF236I ALLOC. FOR SPIN      EURL
IEF237I SYSLIB   ON 190
IEF237I SYSLMOD  ON 390
IEF237I SYSLIN   ON 00C
IEF237I SYSUT1   ON 391
IEF237I SOURCEFT ON 190
```

E-LEVEL LINKAGE EDITOR OPTIONS SPECIFIED MAP
****RUN DOES NOT EXIST BUT HAS BEEN ADDED TO DATA SET

MODULE MAP

CONTROL SECTION

NAME		ORIGIN	LENGTH
MAIN=		00	3A064
IHCFCOMH*		3A063	1000
IHCUOPT	*	3B073	8
IHCTRCH	*	3B080	278
PLT	*	3B2F8	4A6
DESSIN=	*	3B7A0	1350
IHCFCVTH*		3CAF0	107C
IHCFIOSH*		3DB70	D0A
IHCUATBL*		3E880	638
MXMN=	*	3EE88	252
MXMNL=	*	3F110	1CC
SCALE=	*	3F2E0	98C
DXLG=	*	3FC70	625
AXIS=	*	40298	636
AXLOG=	*	40AD0	848
AXCIR=	*	41618	7AC
LINESC=	*	41DC8	580
LIPOSC=	*	42378	560
NUMB	*	428D8	25A
MAPOSC=	*	42B38	360
SYMB	*	42E98	418
MARKSC=	*	432B0	378
IHCSLOG	*	43628	10C
IHCSSCN	*	43738	104

ENTRY

NAME	LOCATION	NAME	LOCATION	NAME	LOCATION	NAME	LOCATION
MAIN	00						
IBCOM=	3A068	FDIOCS=	3A124				
PLOT	3B2FC	PLTIR	3B30A	FINIM	3B328	FINTRA	3B346
DESSIN	3B7A0						
ADCON=	3CAF0	FCVZO	3CC3C	FCVAO	3CCE2	FCVLO	3CD72
FCVIO	3D0A8	FCVEO	3D59A	FCVCO	3D79C	INT6SW	3DB51
FIOCS=	3DB70						
MXMN	3EEB8						
MXMNL	3F110						
SCALE	3F2E0	DXDY	3F310				
DXLG	3FC70						
AXIS	40298						
AXLOG	40AD0						
AXCIR	41618						
LINESC	41DC8	DASHSC	41DF8				
LIPOSC	42378	DAPOSC	423A8				
SNUM	42BDC	NUMBER	428E8				
MAPOSC	42B38						
CARSP	42E9C	SYMBL4	42EBA	SYMBOL	42EC6		
MARKSC	43280						
ALOG10	43628	ALOG	43644				

NAME	ORIGIN	LENGTH
GIST *	43840	74
IHCFOVER*	43888	50
CALERR= *	43908	3F6
IHCSEXP *	43D00	11E
IHCFRXPI*	43E20	D4
SYMT *	43EB8	60C

ENTRY ADDRESS 00
TOTAL LENGTH 444C4

NAME	LOCATION	NAME	LOCATION	NAME	LOCATION	NAME	LOCATION
COS	43738	SIN	43754				
GIVE	43846	STORE	43852				
OVERFL	43888						
CALERR	43908						
EXP	43D00						
FRXPI=	43E20						
SYMBTB	43EBE						


```
IEF285I    SYSOUT                                                SYSOUT
IEF285I    VOL SER NOS=
IEF285I    SYS1.FORTLIB                                          KEPT
IEF285I    VOL SER NOS= EURSY1.
IEF285I    GOSET.SPIN                                            PASSED
IEF285I    VOL SER NOS= EURSY3.
IEF285I    AAAAAAAA.AAAAAAAA.AAAAAAAA.AAAAAAAA.00000625 DELETED
IEF285I    VOL SER NOS= EURSY2.
IEF285I    LOADSET.SPIN                                          DELETED
IEF285I    VOL SER NOS= EURSY1.
    EURLFRT    DATE 68.04.08    BEG.T. 20.419  DURATION 0.010 N.OPER= 504 INP=001
IEF236I ALLOC. FOR SPIN      EURX
IEF237I PGM=*.DD ON 390
IEF237I FT02F001 ON 190
IEF237I FT03F001 ON 291
IEF237I FT04F001 ON 390
IEF237I FT05F001 ON 00C
IEF237I FT07F001 ON 00D
IEF237I FT08F001 ON 390
IEF237I FT16F001 ON 280
```

NUMBER OF CASES 3 IWRT = 0

TEST ABSORPTION

INPUT DATA

NMKD= 3 IDEC= 0 W= 0.5000E-01 ANINT= 0.1000E-01 LENG OF Y (CM) = 0.1200E 02

INDGR(I)

1 2 3 0 0 0 0 0 0 0 0 0

NMEK(I)

1 2 1 0 0 0 0 0 0 0 0 0

DHEK(I)

0.1300E 02 0.2500E 01 0.5000E 00 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM

MAX VALUE OF Y1(I) = 0.271997E 00

JART 128 A1 12.30 A2-12.80 I1 2561

TEST DERIVATIVE

INPUT DATA

NMKD= 3 IDEC= 1 W= 0.5000E-01 ANINT= 0.1000E-01 LENG OF Y (CM) = 0.1200E 02

INDGR(I)

1 2 3 0 0 0 0 0 0 0 0 0

NMEK(I)

1 2 1 0 0 0 0 0 0 0 0 0

DHEK(I)

0.1300E 02 0.2500E 01 0.5000E 00 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM

MAX VALUE OF Y1(I) = 0.345102E 01

JART 128 A1 12.80 A2-12.80 I1 2561

DIPHENYL NEGATIVE ION

INPUT DATA

NMKD= 3 IDEC= 1 W= 0.5000E-01 ANINT= 0.1000E-01 LENG OF Y (CM) = 0.1750E 02

INDGR(I)

1 1 1 0 0 0 0 0 0 0 0 0

NMEK(I)

2 4 4 0 0 0 0 0 0 0 0 0

DHEK(I)

0.4000E 01 0.2000E 01 0.3200E 00 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

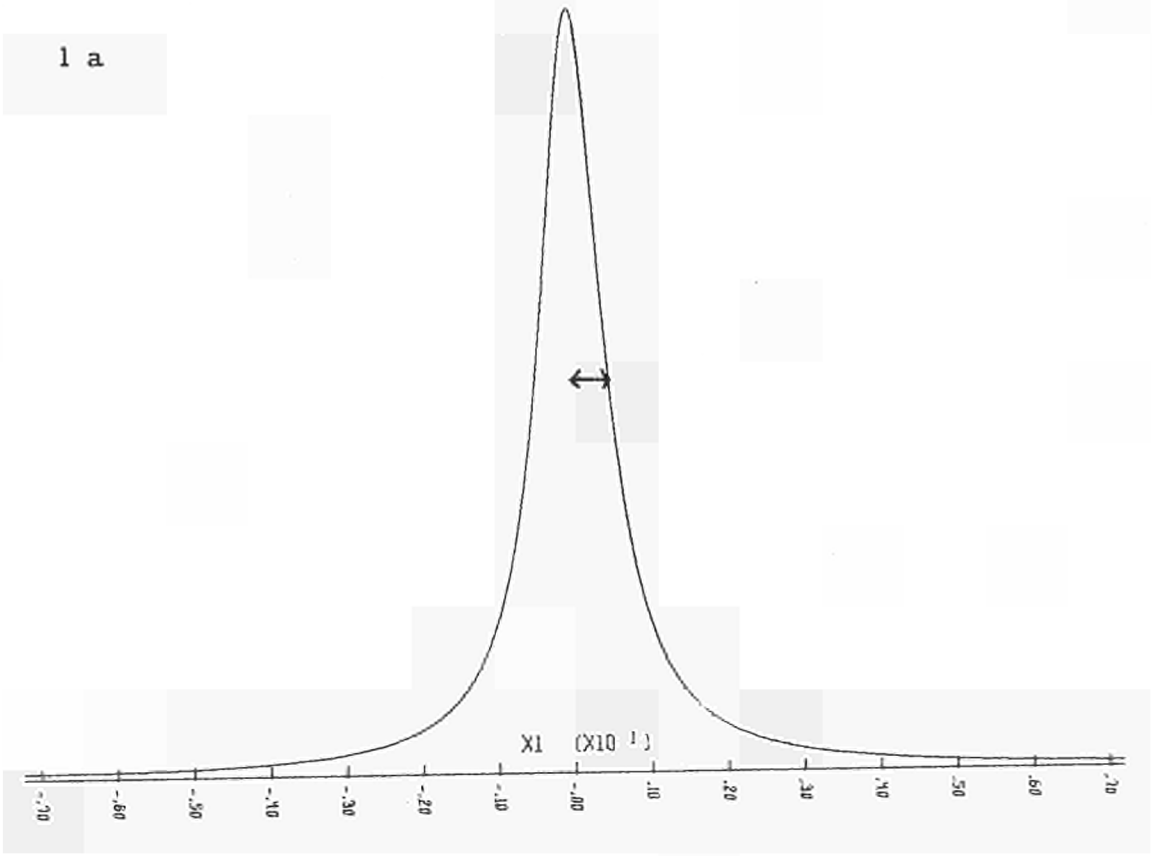
MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM

MAX VALUE OF YI(I) = 0.674749E 01

JART 02 A1 9.20 A2 -9.20 I1 1841

```
IEF285I    GOSET.SPIN                                       PASSED
IEF285I    VOL SER NOS= EURSY3.
IEF285I    EURSCR02.SPIN                                    PASSED
IEF285I    VOL SER NOS= EURSY1.
IEF285I    EURSCR03.SPIN                                    PASSED
IEF285I    VOL SER NOS= EURSY2.
IEF285I    EURSCR04.SPIN                                    PASSED
IEF285I    VOL SER NOS= EURSY3.
IEF285I    SYSOUT                                           SYSOUT
IEF285I    VOL SER NOS=      .
IEF285I    PUNCH1                                           PASSED
IEF285I    VOL SER NOS= PUNCH1.
IEF285I    EURSCR03.SPIN                                    PASSED
IEF285I    VOL SER NOS= EURSY3.
IEF285I    CALCP1                                           DELETED
IEF285I    VOL SER NOS= CALCP1.
IEF280I K 280,CALCP1,SPIN
    EURX        DATE 68.04.08    BEG.T. 20.429  DURATION 0.013 N.OPER= 504 INP=001
IEF285I    GOSET.SPIN                                       DELETED
IEF285I    VOL SER NOS= EURSY3.
IEF285I    EURSCR02.SPIN                                    DELETED
IEF285I    VOL SER NOS= EURSY1.
IEF285I    EURSCR03.SPIN                                    DELETED
IEF285I    VOL SER NOS= EURSY2.
IEF285I    EURSCR04.SPIN                                    DELETED
IEF285I    VOL SER NOS= EURSY3.
IEF285I    EURSCR03.SPIN                                    DELETED
IEF285I    VOL SER NOS= EURSY3.
    SPIN        DATE 68.04.08    BEG.T. 20.412  DURATION 0.031 N.OPER= 504 INP=001


H A S P  JOB STATISTICS --    444 CARDS READ --      758 LINES PRINTED --    224 CARDS PUNCHED --   1.93 MINUTES EXECUTION TIME
```



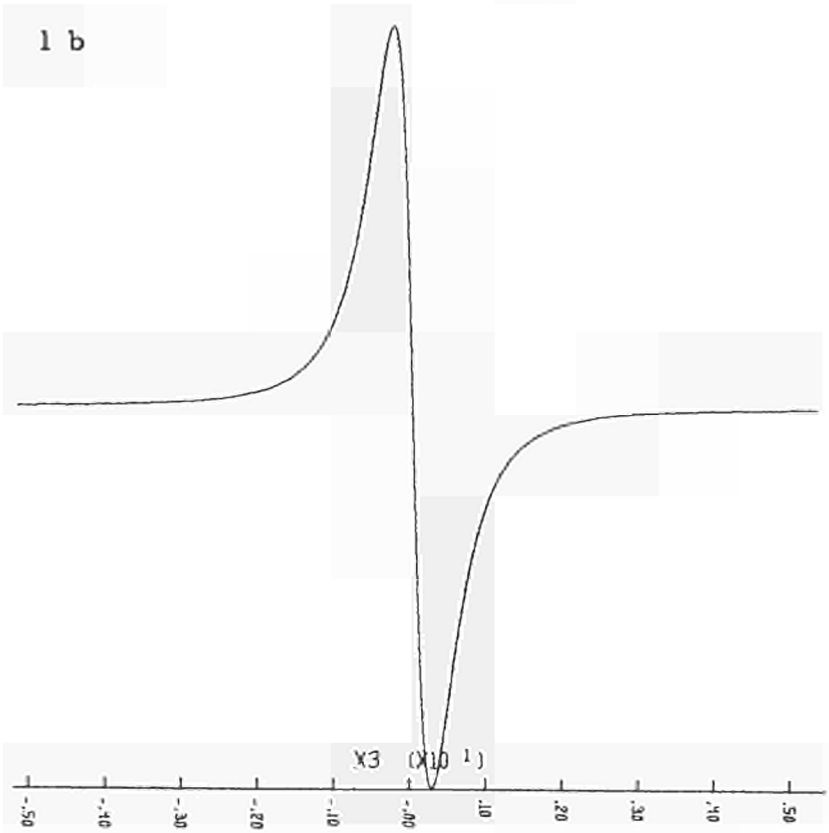


Fig. 1. Lorentzian line and its derivative; w = 0.5 cm

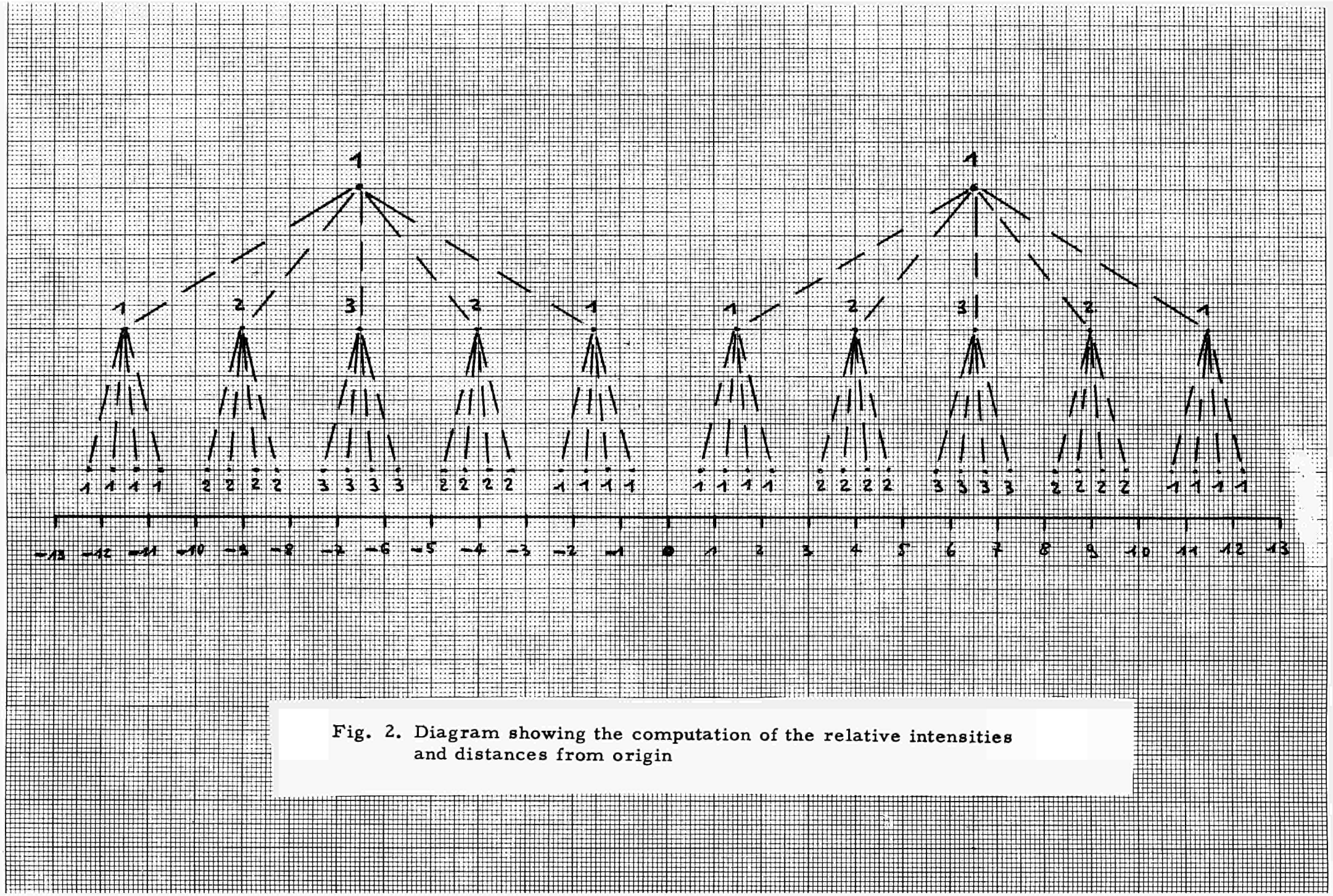


Fig. 2. Diagram showing the computation of the relative intensities and distances from origin

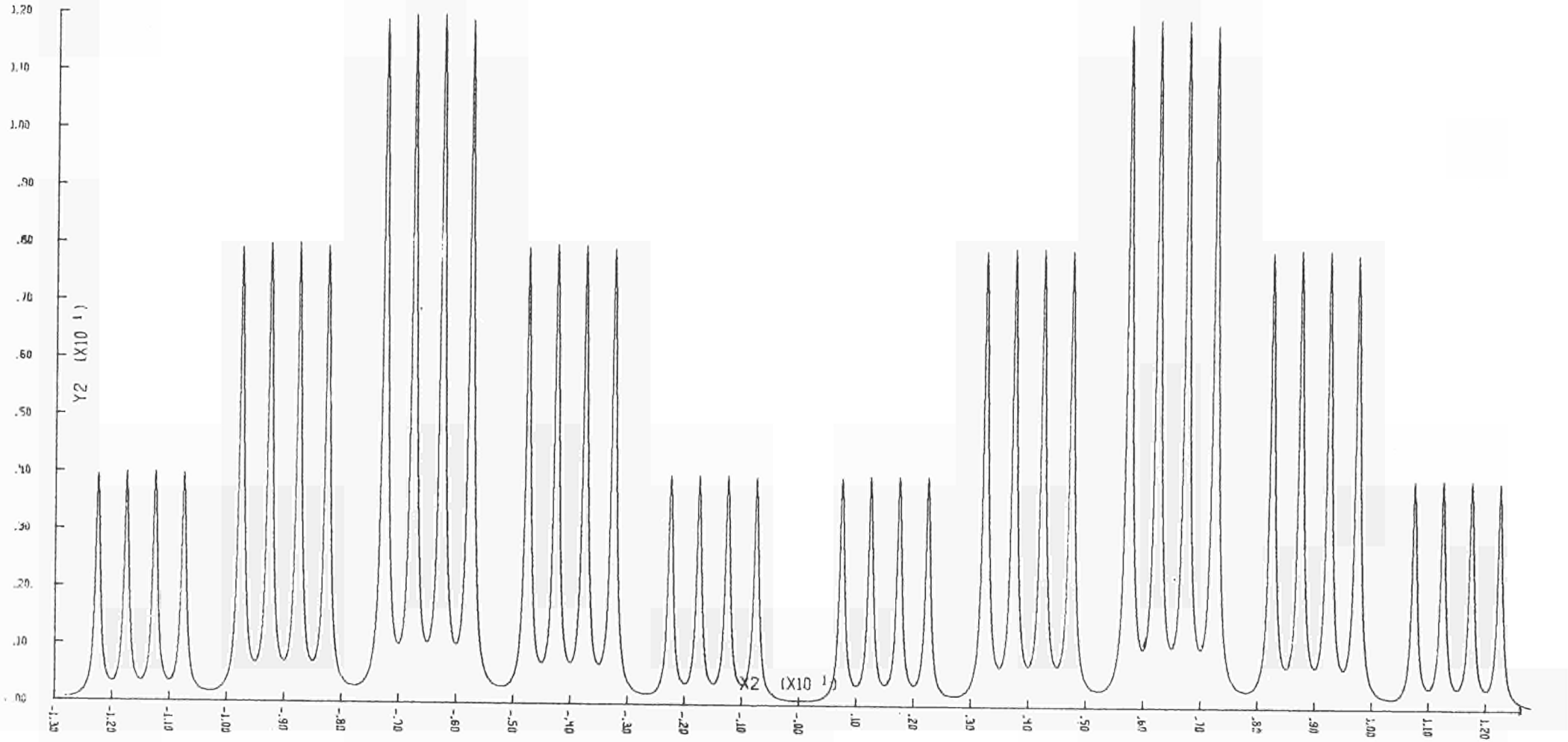


Fig. 3. CALCOMP plot of the case discussed in 3.3. Absorption curve

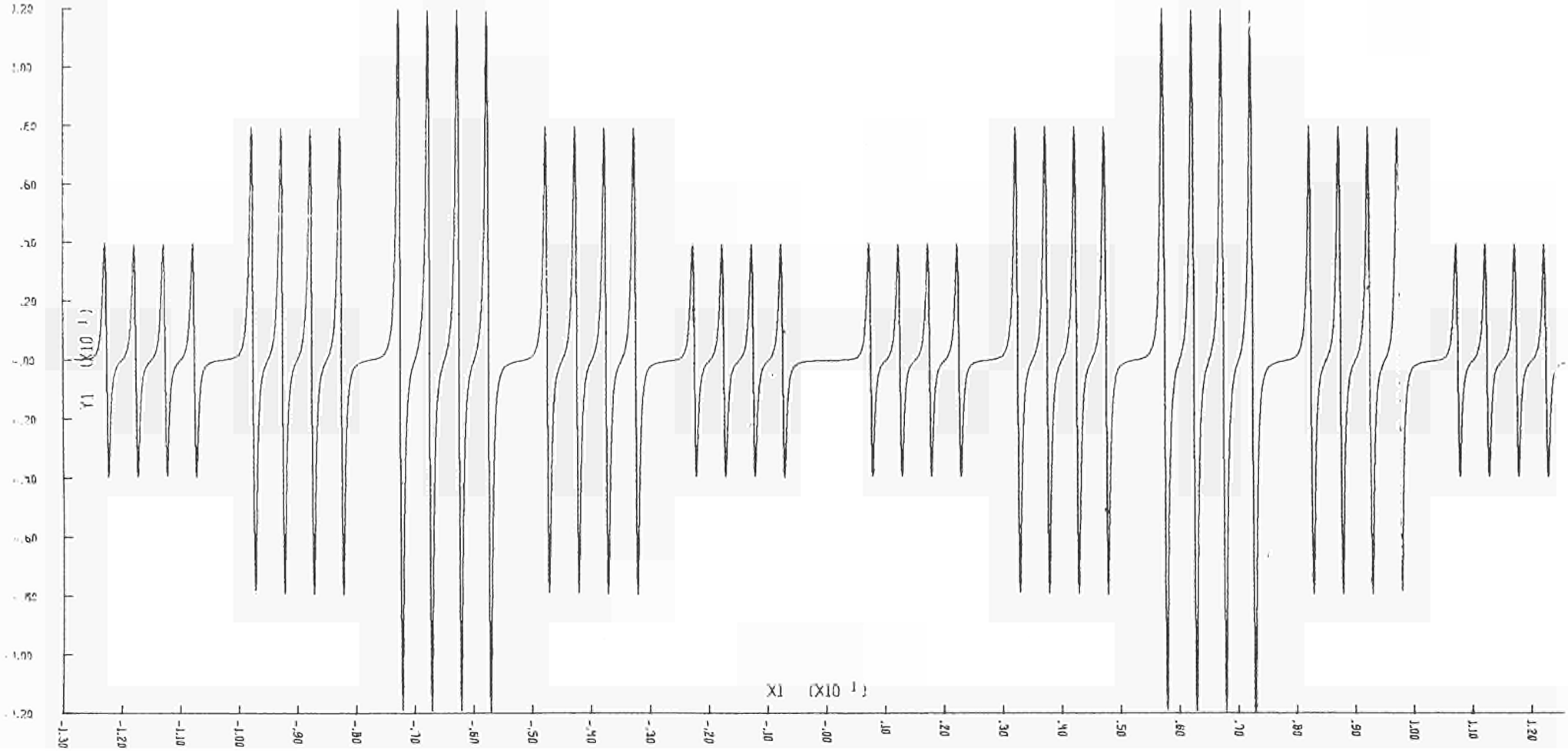


Fig. 4. CALCOMP plot of the case discussed in 3.3. Derivative curve

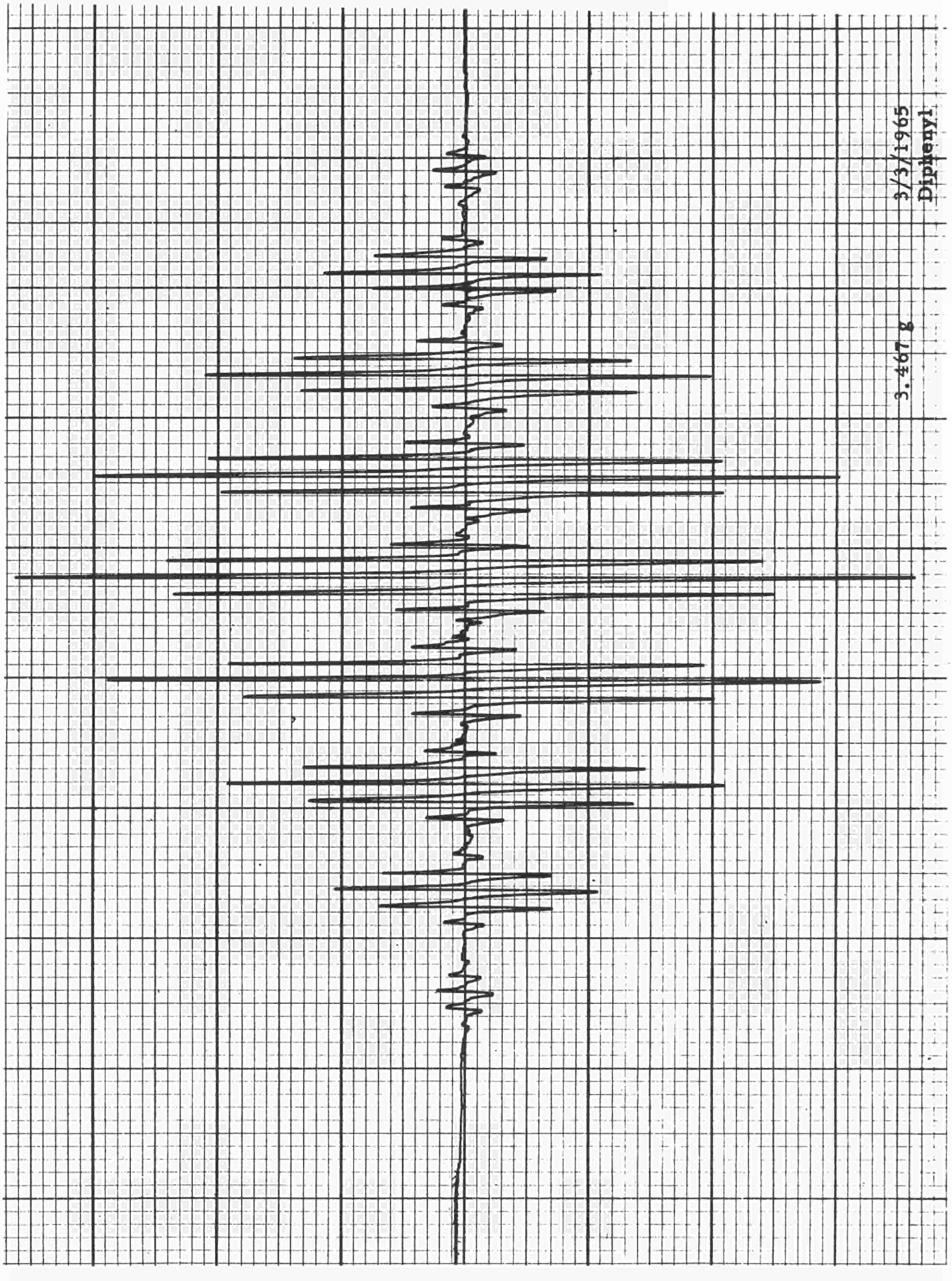


Fig. 5. Experimental spectrum of Diphenyl negative ion

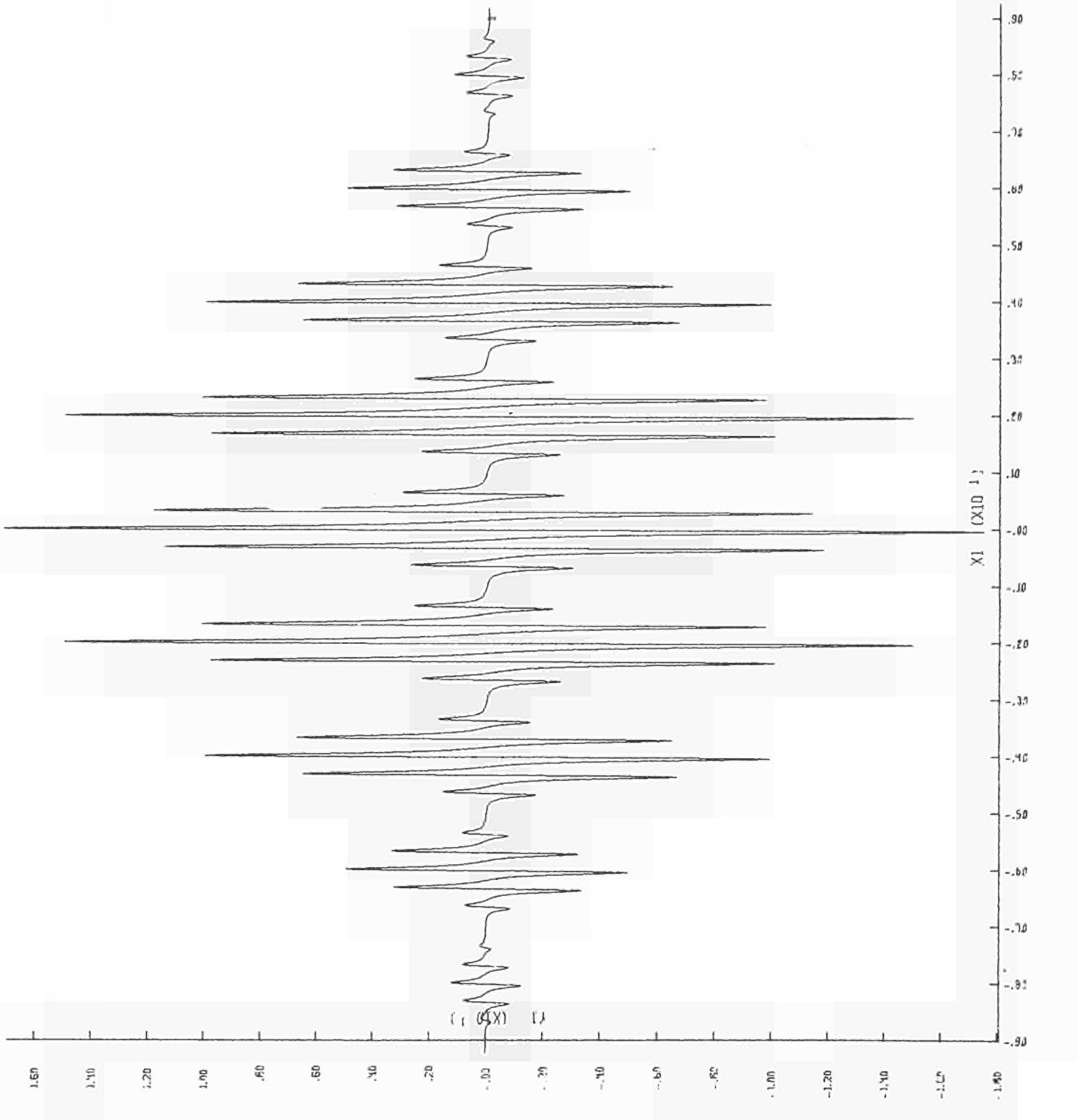


Fig. 6. Calculated spectrum of Diphenyl negative ion

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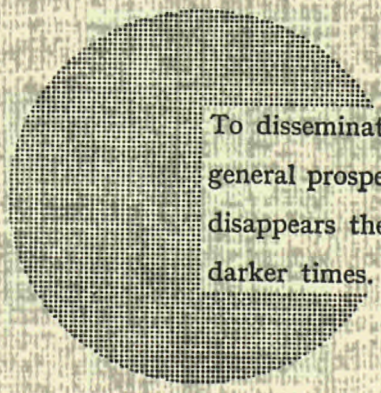

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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