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
and
Chemistry Department - Organic Chemistry
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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 the Electron Spin Resonance Spectra of aromatic ions and radicals by A. Inzaghi and L. Mongini.
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.
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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.

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PROGRAMMING
IBM 360
SPIN
HYPERFINE STRUCTURE

ELECTRON SPIN RESONANCE
SPECTRA
SIMULATORS
AROMATICS
IONS
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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
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-
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

$^*)$ 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 $^1N$) 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)

\begin{verbatim}
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
\end{verbatim}
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: \( NL(I) = NMEK(I) \cdot INDGR(I) + 1 \)) it follows that the total memory occupied by the 2 above introduced vectors is equal, in the case of NMKD groups to:

\[
2 \cdot NL(1) \cdot NL(2) \cdots NL(NMKD)
\]

In the present version of the program we have reserved \( 2 \times 4096 \) 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:

<table>
<thead>
<tr>
<th>NL</th>
<th>NMKD maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>12</td>
</tr>
<tr>
<td>3</td>
<td>7</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
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<td>6</td>
<td>4</td>
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<td>3</td>
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<tr>
<td>9</td>
<td>3</td>
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<tr>
<td>10</td>
<td>3</td>
</tr>
<tr>
<td>11</td>
<td>3</td>
</tr>
<tr>
<td>12</td>
<td>3</td>
</tr>
<tr>
<td>13</td>
<td>3</td>
</tr>
</tbody>
</table>

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

36192

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


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 = 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 (l= 1, NMKD)
NMEK(I) = number of nuclei (l= 1, NMKD)
DHEK(I) = hyperfine splitting constant (l= 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

\[ \text{[NMEK(1) \times INDGR(1)+1] \times \cdots \times [NMEK(NMKD) \times INDGR(NMKD)+1]} \]

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:

A function being the absorption spectrum, sampled at intervals ANINT, having maximum height XXXX

IF IDEC = 07

YES

A function being the derivative spectrum, sampled at intervals ANINT, having maximum height XXXX

IF RIB > 07

YES

NO

Multiply ordinates by RIB

IF IWRT = 07

YES

Write ordinates and abscissae

NO

WRITE ORDINATES AND ABCISSAE

NUMBER OF PROBLEMS TREATED < NN?

YES

CALL CALCOMP - STOP
Call Calcomp and plot NN curves
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 4 | 5 | 6 | 7 | 8 | 9 | 10| 11| 12| 13| 14| 15| 16| 17| 18| 19| 20| 21| 22| 23| 24| 25| 26| 27| 28| 29| 30| 31| 32|
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| **Title Case 1** |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| **Title Case 2** |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| **Title Case 3** |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| **Title Case 4** |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| **END** |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |

**Input Instructions**
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<tbody>
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<td>4</td>
<td>9</td>
<td>10</td>
</tr>
</tbody>
</table>

**EURATOM - CETIS**

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

**TANNIN ABSORPTION**

<p>| | | |</p>
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<td>1</td>
<td>1.3</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>3.0</td>
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</table>

**TANNIN DERIVATIVE**

<p>| | | |</p>
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<td>5</td>
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**BIPHENYL NEGATIVE ION**

<p>| | | |</p>
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<tbody>
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<tr>
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<td>1</td>
<td>1.3</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>3.0</td>
</tr>
</tbody>
</table>

**END**

**INPUT DATA FOR CASES OF FIG. 3, 4, 6**
DIMENSION NMEK(12), NSHEK(12), H(13,12), 0(13,12), HS(4096), OS(4096)
DIMENSION X(6000), Y(6000), Z(6000), X(6000), Y(6000), Z(6000)
DIMENSION AA(18)
DIMENSION AP(90), AU(4,4), APX(12,13), AUX(6,13)
DIMENSION A(34), AQX(4,11)

DATE TEST,TEST,TEST,AU(4)END,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND

DATA TEST,TEST,TEST,AU(4)END,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND,4HEND

DATA RR,RR,RR,AP/4H,4H

DATA FF,FF,FF,AQ/4H,4H

DO 24 JK=1,44540

24 XMEK(JK)=0

DO 997 K=1,12

997 CONTINUE

DO 998 J=1,10

998 CONTINUE
998 CONTINUE
   JX=0
   DO 996 K=1,W
      JY=JX+1
      J1=3*K
      JX=JY+K1
   J1=0
   DO 996 J=JY,JX
      J1=J1-1
      A3X(K,J1)=AQ(J)
   CONTINUE
   BLOCK 2-READ GENERAL INPUT-
READ(5,12) NN,IWRT
WRITE(6,12) NN,IWRT
1M=1
1111 CONTINUE
   DO321=1,12000
   32 X11(I)=0.
   BLOCK 3-READ INPUT FOR A PARTICULAR CASE-
READ(5,4) (AAA(I),I=1,18)
WRITE(6,10) (AAA(I),I=1,18)
IF(AAA(I),I=2,TEST) GJ TJ 2222
WRITE(5,8001)
READ(5,1) NMK,DHEK(1),1=1,NMK
WRITE(6,10) (NMK(I),I=1,NMK)
WRITE(5,11) NMK,DHEK,1=1,NMK
WRITE(6,18) (NMK(I),I=1,12)
WRITE(6,13) (DHEK(I),I=1,12)
WRITE(6,14) (DHEK(I),I=1,12)
WRITE(5,18) (DHEK(I),I=1,12)
WRITE(6,3)
   BLOCK 4-CALCULATION OF THE 2 VECTORS SPECIFYING INTENSITY AND POSITIONS OF EACH LINE-
   DO 150 1=1,NMK
      K = N1PR(1)
      L = N1GR(1)*K+1
JQ=INDGR(I)
GO TO (5000,5001,5006),JQ

AAIND=AAK*0.5
GO TO 5002

AAIND=AAK
GO TO 5002

AAIND=AAK*1.5
GO TO 150

JQ=INDGR(I)
GO TO (5000,5001,5006),JQ

AAIND=AAK*0.5
GO TO 5002

AAIND=AAK
GO TO 5002

AAIND=AAK*1.5
GO TO 150

LIST=0
IA=INDGR(1)*NMEK(1)+1
JQ=INDGR(1)*NMEK(1)+1
IA=INDGR(1)*NMEK(1)+1
IA=INDGR(1)*NMEK(1)+1

DO 201 J=1,IA
SH015=H(IY,1)
SHS=SH015
PD01S=D(IY,1)
PDS=PD01S
GO TO 150
IF (NMEK-2) 161,162,162
GO TO 201

DO 202 J=1,IA
SH02S=H(I2,2)+SH015
SHS=SH02S
PD02S=D(I2,2)*PD01S
PDS=PD02S
GO TO 150
IF (NMEK-3) 161,163,163
GO TO 202

DO 203 J=1,IC
SH03S=H(I3,3)+SH02S
SHS=SH03S
PD03S=D(I3,3)*PD02S
PDS=PD03S
GO TO 150
IF (NMEK-4) 161,164,164
GO TO 203

DO 204 J=1,ID
SH04S=H(I4,4)+SH03S
SHI = SH04S

PD04S = D([4,4] * PD03S)

IF (NMKD = 5) 161, 165, 165

404 GO TO 204

165 IE = INDGR(5) * NMEK(5) + 1

J0 205 IE = 1, IE

SH05S = H([5, 5]) * SH04S

SHS = SH05S

PD05S = D([5, 5] * PD04S)

PD5 = PD05S

IF (NMKD = 6) 161, 166, 166

405 GO TO 205

166 IG = INDGR(6) * NMEK(6) + 1

J0 206 IG = 1, IG

SH06S = H([6, 6]) * SH05S

SHS = SH06S

PD06S = D([6, 6] * PD05S)

PD6 = PD06S

IF (NMKD = 7) 161, 167, 167

406 GO TO 206

167 IH = INDGR(7) * NMEK(7) + 1

J0 207 IH = 1, IH

SH07S = H([7, 7]) * SH06S

SHS = SH07S

PD07S = D([7, 7] * PD06S)

PD7 = PD07S

IF (NMKD = 8) 161, 168, 168

407 GO TO 207

168 IJ = INDGR(8) * NMEK(8) + 1

J0 208 IJ = 1, IJ

SH08S = H([8, 8]) * SH07S

SHS = SH08S

PD08S = D([8, 8] * PD07S)

PD8 = PD08S

IF (NMKD = 9) 161, 169, 169

408 GO TO 208

169 IJ = INDGR(9) * NMEK(9) + 1

J0 209 IJ = 1, IJ

SH09S = H([9, 9]) * SH08S

SHS = SH09S

PD09S = D([9, 9] * PD08S)

PD9 = PD09S

IF (NMKD = 10) 161, 170, 170

409 GO TO 209

170 IK = INDGR(10) * NMEK(10) + 1

J0 210 IK = 1, IK

SH10S = H([10, 10]) * SH09S

SHS = SH10S

PD10S = D([10, 10] * PD09S)
BLOCK 5-CALCULATION OF THE ABSORPTION SPECTRUM OR ITS DERIVATIVE.
DO 740 IZ=2, LIST
  IF (A1-HS(I2)) 741,740,740 741 A1=HS(I2) 740 CONTINUE
  B1=-A1-W*10.0
  A1 = A14-W*10.0
  ART=(A1-B1)/(ANINT*20.0)
  JART = JART*10+1
  DO 450 K=1,II
    AJ=K-1
  450 X1(K)=A2+AJ*ANINT
  ANORM=3.0
  DO 455 K=1, LIST
    ANORM=ANORM+D(S(K))
  460 DS(K)=D(S(K))/ANORM
  DO 470 K=1, LIST
    Y1(K)=0.0
  470 Z=1.0/W
  S=Z/2.1416
  IF (IDEC) 500, 600, 500
  500 Y1(J)=Y1(J)+D(S(J))*(S/(1.0+W*(X(J)-HS(I))*X(J)-HS(I)))
  600 I=I+1
  630 CONTINUE
  620 J=J+1
  610 I=I-J+1
  599 Y1(J)=Y1(J)
  589 Y1(J)=Y1(J+1)
  579 DO 800 J=2, LIST
  569 Y1(J)=Y1(J)*Z
  559 CONTINUE
  549 ZZY=0.0
  539 DO 555 I=2, II
  529 IF (I+1)=558, 559, 559

FORTRAN IV & LEVEL 1, MOD 0  

MAIN  

DATE = 6/299  
20/24/50  

PAGE 0006
0249 DD1=0.
0250 GO TO 553
0251 DD1=Y1(I-1)
0252 IF(Y1(I))556,557,557
0253 DD2=0.
0254 GO TO 554
0255 DD2=Y1(I)
0256 IF(Y1-DO1)551,552,552
0257 IF(ZZY.LT.DD1) ZZY=DD1
0258 GO TO 556
0259 IF(ZZY.LT.DD2) ZZY=DD2
0260 CONTINUE
0261 IF(ZZY.LE.0.) GO TO 8222
0262 WRITE [6,17] ZZY
0263 RAPP=XXX/ZZY
0264 ZZY=XXX
0265 DD 515 I=1,II
0266 Y1(I)=Y1(I)*RAPP
0267 IF(RIB) 9000,9001,9001
0268 9000 DO 9002 I=1,II
0269 9002 Y1(I)=Y1(I)*RIB
0270 9001 CONTINUE
0271 WRITE(6,6) (X1(I),Y1(I),I=1,II)
0272 IF(IWRT.EQ.0) GO TO 23
0273 WRITE(6,7)
0274 WRITE(6,8) (X1(I),Y1(I),I=1,II)
0275 23 CONTINUE

CBLUC 6-CALL CALCONP-

0276 IF(Ilt.6000) GO TO 4000
0277 GO TO (20,21,27,22),MM
0278 20 DO 25 I=1,II
0279 X2(I)=X1(I)
0280 25 Y2(I)=Y1(I)
0281 MA=II
0282 LA=AI-A2
0283 LY=ZZY
0284 GO TO 27
0285 21 DO 27 I=1,II
0287 X3(I)=X1(I)
0287 29 Y3(I)=Y1(I)
0288 MB=II
0289 LA=AI-A2
0290 Z2Y=ZZY
0291 GO TO 27
27 \text{ DO } 29 \text{ I}=1,11 \\
29 \text{ X4(I)}=\text{X1(I)} \\
29 \text{ Y4(I)}=\text{Y1(I)} \\
29 \text{ MC}=11 \\
29 \text{ Z3X}=\text{A1-A2} \\
29 \text{ Z3Y}=\text{Z2Y} \\
29 \text{ MM}=\text{MM}+1 \\
29 \text{ IF}(\text{MM">NN}) \text{ GO TO } 33 \\
30 \text{ GO TO } 1111 \\
33 \text{ CONTINUE} \\
30 \text{ CALL } \text{FINIM}(0.,0.) \\
30 \text{ CALL } \text{DESSIN}(X2,Y2,MA,1,1,1,0,0,Z1X,Z1Y,0,0,4H X1,-4,4H Y1,+4,0) \\
30 \text{ IF}(\text{MM}=2)3332,3334,3332 \\
30 \text{ ZZA}=Z1X+5. \\
30 \text{ GO TO } 3333 \\
3332 \text{ ZZA}=Z1Y+3. \\
30 \text{ CALL } \text{FINIM}(0.,ZZA) \\
30 \text{ CALL } \text{DESSIN}(X3,Y3,MB,1,1,1,0,0,Z2X,Z2Y,0,0,4H X2,-4,4H Y2,+4,0) \\
30 \text{ IF}(\text{MM}=3)3335,3336,3335 \\
30 \text{ ZZA}=Z2X+5. \\
30 \text{ GO TO } 3333 \\
3335 \text{ ZZA}=Z2Y+3. \\
30 \text{ CALL } \text{FINIM}(0.,ZZA) \\
30 \text{ CALL } \text{DESSIN}(X4,Y4,MC,1,1,1,0,0,Z3X,Z3Y,0,0,4H X3,-4,4H Y3,+4,0) \\
30 \text{ IF}(\text{MM}=4)3337,3338,3337 \\
30 \text{ ZZA}=Z3X+5. \\
30 \text{ GO TO } 3333 \\
3337 \text{ ZZA}=Z3Y+3. \\
30 \text{ CALL } \text{FINIM}(0.,ZZA) \\
30 \text{ CALL } \text{DESSIN}(X1,Y1,1,1,1,1,0,0,ZZX,ZZY,0,0,4H X4,-4,4H Y4,+4,0) \\
30 \text{ ZZA}=Z2X+5. \\
30 \text{ ZGC}=\text{NN}-1 \\
30 \text{ ZGC}=-\text{ZGC}+\text{ZZA} \\
30 \text{ CALL } \text{FINIM}(ZZB,ZGC) \\
30 \text{ CALL } \text{FINTRA} \\
30 \text{ GO TO } 1111 \\
30 \text{ CONTINUE} \\
30 \text{ ZGC}=\text{NN}-1 \\
30 \text{ ZGC}=-\text{ZGC}+\text{ZZA} \\
30 \text{ CALL } \text{FINIM}(ZZB,ZGC) \\
30 \text{ CALL } \text{FINTRA} \\
30 \text{ GO TO } 1111 \\
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1 FORMAT(2I6,4E12.6)
2 FORMAT(4(4(I3,13,E12.6))
3 FORMAT([H1:130X],"MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATI"
       1HN,PROGRAM////)
4 FORMAT(4H4)
5 FORMAT(1H1,4:8HART,16,10X,2HAI,F6.2,10X,7HA2,F6.2,10X,2H11,16////)
6 FORMAT(1H1,5X,6F6.6)
7 FORMAT(1H1,5X,13H1(1),Y1(1)////)
8 FORMAT(/1H ,"PROGRAM STOP FOR NUMBER POINTS TO PLOT LARGER THAN"
       1GOOD////)
9 FORMAT(1H1,5X,13H4 ////)
10 FORMAT(1H1,5X,13H4 ////)
11 FORMAT(/1H ,4:8HNM=I13,5X,5HDEC=I13,5X,2H1=W=E12.4,5X,6H1=N=I12,4,5X,15HLEG OF Y (CM) =E12,4)
12 FORMAT(/1H ,7HNMKE(1)/1H ,12110)
13 FORMAT(/1H ,10X,7HDEK(1)/1H ,1?E14.4 //)
14 FORMAT(2I6)
15 FORMAT(2I6)
16 FORMAT(2I6)
17 FORMAT(/1H ,"MAX VALUE OF Y1(1) = 'E16.6////)
18 FORMAT(/1H ,"PROGRAM STOP FOR LIST INDICATOR LARGER THAN 40964"
        1//)
19 FORMAT(/1H ,"PROGRAM STOP FOR Y1(MAX) = 'E16.6////)
20 FORMAT(/1H ,50X,"INPUT DATA\\\\"
21 CONTROL STATEMENTS FOR PROGRAM LIMITES
22 10 FORMAT(6,9) 11
23 GO TO 2222
24 8222 WRITE (6,8000) ZY
25 GO TO 2222
26 2222 STOP
27 END
### SCALAR MAP

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### SUBPROGRAMS CALLED

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### FORMAT STATEMENT MAP

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### TOTAL MEMORY REQUIREMENTS 03AO64 BYTES
E-LEVEL LINKAGE EDIT OPTIONS SPECIFIED MAP

***RUN*** DOES NOT EXIST BUT HAS BEEN ADDED TO DATA SET

### MODULE MAP

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<td>IHCJTRCH *</td>
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| DESSIN= | 387A0  | 1350   |
| IHCFCVTH* | 3CAFC  | 107C   |
| IHCFIOSH* | 30370  | 07A    |

| IHCFAUATL* | 3B880  | 6322   |
| MXMN= | 3F110  | 1GC    |
| SCALE= | 3F260  | 95C    |
| DXLG= | 3FC70  | 32C    |
| AXIS= | 40298  | 030    |
| AXLOG= | 40A30  | 346    |
| AXCIR= | 41616  | 7AC    |
| LINESC= | 410C6  | 530    |
| LIPOSC= | 42378  | 580    |
| NUMB= | 42603  | 25A    |
| MAPOSC= | 42630  | 360    |
| SYMB= | 42C98  | 419    |
| MARKSC= | 43230  | 37B    |
| IHCSLUS* | 43528  | 17C    |
| IHCSOC* | 43730  | 174    |

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**ENTRY ADDRESS**

**TOTAL LENGTH** 4464

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**IEF235I**

SYSOUT                                SYSDUT
VOL SER NUS=                            KEPT
VOL SER NOS= EURSY1.                   PASSED
GOTEI,SPIN                              
VOL SCL NUS= EURSY3.                   DELETED
AAAAAAA.AAAAAAAA.AAAAAAAA.AAAAAAAA.00000425
VOL SER NUS= EURSY2.                   DELETED
LOADSET,SPIN                            
VOL SER NUS= EURSY1.                   
CPU=FT DATE 09.04.08 SEG.T. 20.419 DURATION 0.010 N.OPER= 504 INP=001
ALLOC. FOR SPIN                        FURX
PGM=*.*.DD UN 390
FT02F001 UN 190
FT03F001 UN 291
FT04F001 UN 390
FT05F001 UN 00C
FT07F001 UN 000
FT08F001 UN 390
FT16F001 UN 280

**NUMBER OF CASES** 3

**IWRT = 0**
## INPUT DATA

<table>
<thead>
<tr>
<th>NMKD</th>
<th>DEC</th>
<th>W</th>
<th>ANINT</th>
<th>LENG OF Y (CM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0</td>
<td>0.5000E-01</td>
<td>0.1000E-01</td>
<td>0.1200E 02</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>INDOGR(I)</th>
<th>NMEK(I)</th>
<th>DHEK(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2 3 0 0 0 0 0 0 0</td>
<td>1 2 1 0 0 0 0 0 0 0</td>
<td>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 0.0 0.0</td>
</tr>
</tbody>
</table>

**MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM**

**MAX VALUE OF Y1(I) = 0.271997E 00**

<table>
<thead>
<tr>
<th>JART</th>
<th>A1</th>
<th>A2</th>
<th>II</th>
<th>2561</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>12.30</td>
<td>-12.30</td>
<td>112</td>
<td>2561</td>
</tr>
</tbody>
</table>
TEST DERIVATIVE

INPUT DATA

NMKD = 3  IDEC = 1  \( \gamma = 0.5000 \times 10^{-1} \)  ANINT = 0.1000E-01  LENG OF Y (CM) = 0.1200E 02

INDOR(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  N1  2561
DIPHENYL NEGATIVE ION

INPUT DATA

NMKD = 3
IDEC = 1
W = 0.5000E-01
ANINT = 0.1000E-01
LEN5 OF Y (C4) = 0.1750E 02

INOGR(I)
  1  1  0  0  0  0  0  0  0  0  0

NMEK(I)
  2  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

MODIFIED ELECTRON SPIN RESONANCE SPECTRUM SIMULATION PROGRAM

MAX VALUE OF Y1(I) = 0.574749E 01

JART = 02
A1 = 0.20
A2 = 0.20
II = 1841
HASP JOB STATISTICS — 444 CARDS READ — 758 LINES PRINTED — 224 CARDS PUNCHED — 1.93 MINUTES EXECUTION TIME
Fig. 1. Lorentzian line and its derivative; $w = 0.5 \text{ cm}$
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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Alfred Nobel
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