

EUR 4869 e

COMMISSION OF THE EUROPEAN COMMUNITIES

**A PROGRAM FOR THE THEORETICAL
RECONSTRUCTION OF ESR SPECTRA**

by

L. MONGINI and C. THONET

1972



Joint Nuclear Research Centre
Ispra Establishment - Italy

Chemistry Division
and
Scientific Data Processing Centre - CETIS

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October 1972

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There are two versions of the program, ESR 2250 and ESRCALC. By the first version it is possible to obtain the display of the computed spectra on the IBM 2250 UNIT and, if required, on the CALCOMP Data Plotter; this version is fully interactive. By the second version the drawing of the spectra is obtained on the CALCOMP Data Plotter.

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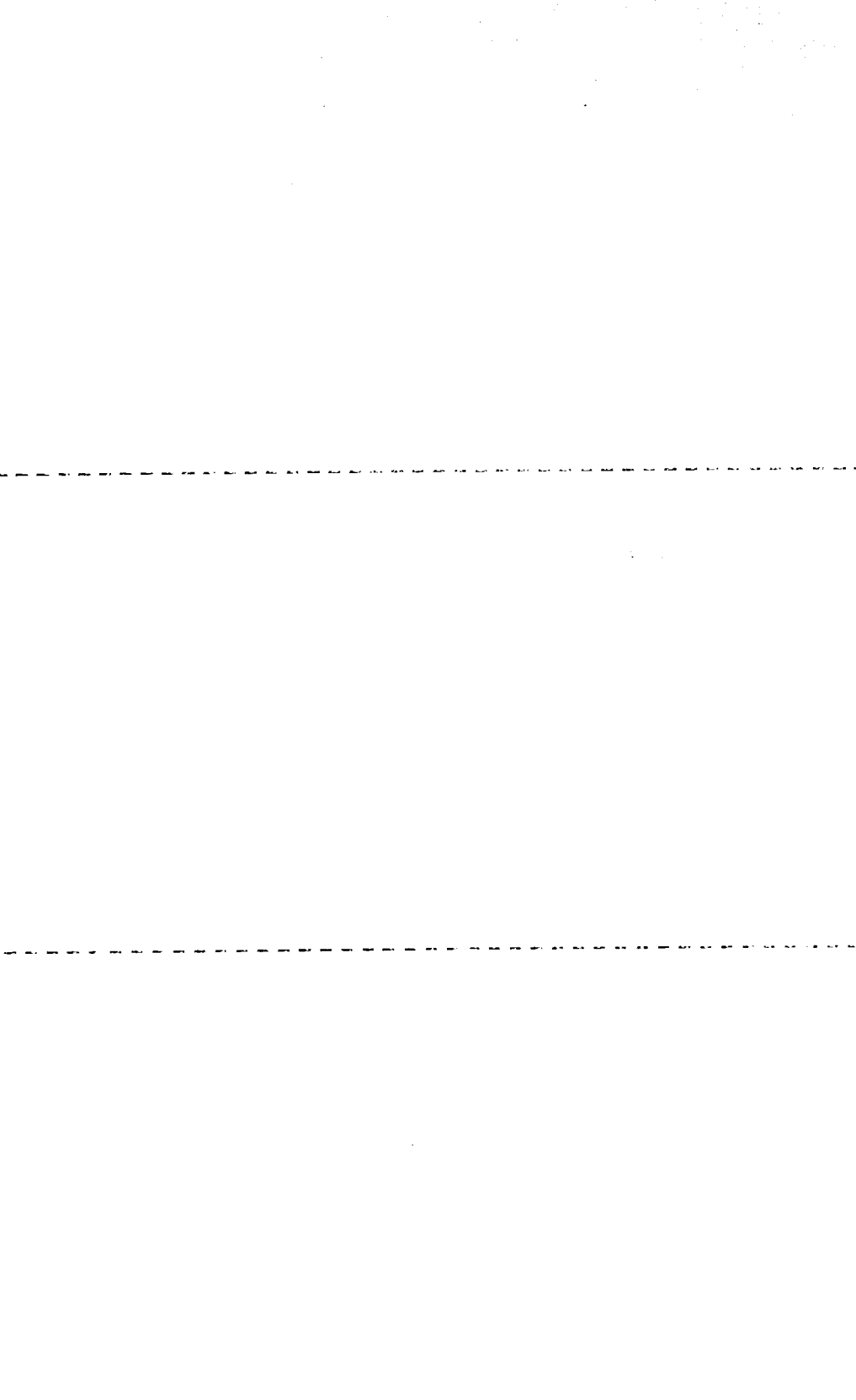
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ABSTRACT

The report describes an IBM 360/65 program for the computer simulation of Electron Spin Resonance Spectra. All the Hyperfine Interactions are considered in the program. The spectra can be obtained as stick spectrum, absorption spectrum, first or second derivative, with Lorentzian or Gaussian Line Shape. The calculation of the Spectra resulting from more than one radical is possible.

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KEYWORDS

ELECTRON SPIN RESONANCE
SPECTRA
PROGRAMMING
FORTRAN
IBM 360
PLOTTER
HYPERFINE STRUCTURE

MAGNETIC RESONANCE
LORENTZ LINE SHAPE
GAUSS FUNCTION
ETHYL RADICALS
METHYL RADICALS
SPIN

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1. INTRODUCTION

The program described in this report is the deeply modified new version of a program written in 1968 for the computer simulation of Electron Spin Resonance Spectra (1).

The program has now been completely rewritten (always for IBM 360/65, FORTRAN language) in order to take into account some exigences that were appearing during the use of the program in the ISPRA Joint Research Center and outside.

The program appears now in two versions, ESR 2250 and ESRCALC.

The first version is now structured in a main and 8 subroutines. By this version it is possible to obtain the display of the computed spectra on the IBM 2250 UNIT and, if required, on the CALCOMP Data Plotter.

The second version is structured in a main and 6 subroutines. By this version the drawing of the spectra is obtained on the CALCOMP Data Plotter.

We will now describe in some detail the most important features of the program.

2. MAIN FEATURES OF THE PROGRAM

2.1 Possibility of Taking into Account the Hyperfine Interaction with all nuclei

In the preceding version only the nuclear spins $1/2$, 1 and $3/2$ were considered. In the present version one can obtain the theoretical reconstruction of ESR spectra, without any restriction on the nuclei originating the Hyperfine interaction.

In order to do this for every set of equivalent nuclei (with spins different from $1/2$, 1 and $3/2$), the relative intensities of lines can be given directly in input.

2.2 The Resonance Line Shape

The first step in the reconstruction of the ESR spectra, as executed by the program is the generation of a spectrum (stick spectrum) where we have in abscissa the field in gauss and the ordinates are the relative intensities

of the peaks.

In order to obtain an acceptable representation of the resonance absorption line, which certainly cannot be given by a delta function, the program can calculate, starting from the stick spectrum, a shape function reproducing in the best way the true form of the broadened lines.

Magnetic resonance lines in solution very often show the so-called Lorentz line shape (2). For this reason only a Lorentzian shape function was used in the first version of the program.

However, due to the variety of processes influencing the line broadening, seems useful to have the possibility of using also the next most common shape function, that is the Gauss function.

This possibility has been introduced in the new version and the operator can now choose between two line shapes, Lorentzian or Gaussian. Fig. 1 shows the two lines, together with the absorption spectrum, as obtained by the CALCOMP data plotter.

2.3 The Second Derivative Curve

In most ESR spectrometers, a second modulative frequency, besides the first, can be applied to the sample, in order to obtain a second derivative curve of the absorption line. The second derivative curve is generally more sensitive than the first derivative to partly resolved hyperfine structure.

For this reason we have now included in the program the calculation of the second derivative of the absorption line. Hence, the spectra that can finally be plotted are the following:

- 1 - Absorption line:
 - a) Stick spectrum
 - b) Lorentz function
 - c) Gauss function

- 2 - First derivative:
 - a) of Lorentz function
 - b) of Gauss function

3 - Second derivative:

- a) of Lorentz function
- b) of Gauss function

2.4 Calculation of Spectra Resulting from more than one Radical

If the experimental spectrum results from more than one radical, the new version of the program (subroutine SPECAD and ADDT) can perform the addition of the component spectra.

In order to do this, the computed spectra are stored on a temporary Direct Data Set, with absolute address (3).

Three Data Sets are defined in the Define File statement. Two data sets (120 records, 7200 bytes per record, associated variable IPOINT) contain respectively the abscissa and the ordinates of the peaks. The other data set contains the dimension of the above vectors (1 record, 400 bytes, associated variable KPOINT).

The variable CORR in input allows for the different weights to be given to different spectra.

2.5 Display of the Spectra on the IBM 2250 UNIT (for the program ESR 2250)

For the interpretation of ESR spectra the input data have to be modified until the theoretical spectrum is not equal to the experimental one. The process requires very often a lot of iterations with different sets of parameters.

For this reason the utilization of an interactive system on a display unit is very useful for this work. We have hence added to the program the subroutine PL 2250 for the display of the spectra on the video of IBM 2250 UNIT, and for introducing the input data from the Alphanumeric Keyboard.

Once the display of the spectrum (single or resulting from a sum) is obtained, the operator can choose between three possibilities:

- a) to modify some parameters in order to obtain a better reconstruction of the spectrum of the radical,
- b) to introduce an entirely new set of data for a new radical,
- c) to obtain the CALCOMP plot of the spectrum.

In fact in order to obtain a permanent image of the spectrum, the operator can choose to store some computed spectra on a temporary storage. In a second step of the job the spectra are read from the temporary storage and sent to CALCOMP Data Plotter. The separate step is necessary because some routines utilized by Graphical Libraries (4, 5) and CALCOMP Library (6), have the same name.

Three remarks are necessary at this point:

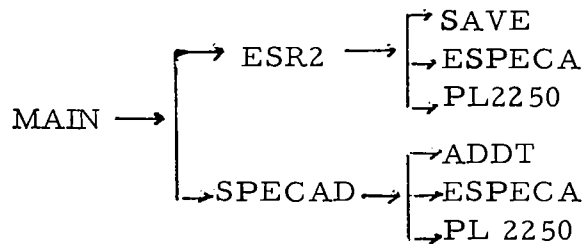
- 1) The buffer of 2250 UNIT cannot contain vectors longer than about 1000 points. For this reason longer spectra are displayed on the video in different fractions.
- 2) The maximum length of the spectrum on the screen can be 24 cm. If the calculated length is larger than 24 cm, the spectrum is reduced by a factor which appears on the screen.
- 3) At the end of a calculation the operator may type on the Keyboard either the title of the new case to executed, or the word END.

3. DESCRIPTION OF THE ROUTINES

3.1 General Structure of the Programs

3.1.1 Program ESR 2250

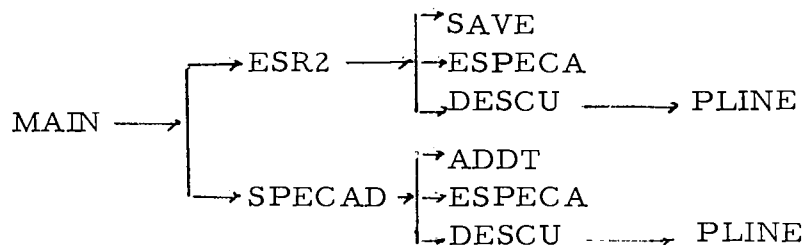
- The sequences of the first step are:



- For the second step we have:



3.1.2 Program ESRCALC



3.2 Description of the Main Sequences

3.2.1 Program ESR 2250

MAIN (1st step)

- initialization areas
- definition of the input type; two cases are possible:
 - 1) to introduce the data by the keyboard
 - 2) the data are read from cards, with the possibility to control and modify them by the keyboard
- introduction of the general data of the problem:
 - NN = number of single spectra
 - NSUM= number of sum of precalculated spectra
 - K1 = dimension of the vectors HS, DS (single spectra)
 - K2 = " " " " X1, Y1, DR2 (single spectra)
 - K3 = " " " " SUMX, SUMY (sum of spectra)
 - K4 = " " " " X1, Y1, DR2 " " "
- call of the subroutines ESR2 and SPECAD
- stop the 1st step.

Notes

- The variables of the subroutines ESR2 and SPECAD for which the dimensions are K1, K2, K3 and K4, are parts of an area (dimensioned 10,000) so that it will always be possible, according to the case, to select the dimensions of the vectors used to build the spectra.

When introducing the values of K1, K2, K3, K4, we must respect the next conditions:

1. for single spectra (ESR2 alone):

$$2K1 + 3K2 = 10000$$

2. if the spectrum results from a sum of single spectra (ESR2 and SPECAD):

$$2K1 + 2K3 + 3K4 = 10000$$

- If in the course of the execution, the effective dimension of the vectors abscissa and ordinates of the spectrum (HS, DS, X1, Y1) are greater than the value given in input for these vectors, it is possible to return to the main

and modify the failed value.

ESR2

- Storage of the relative intensities for the 3 cases of spin equal to: $1/2$, 1, $3/2$. For other cases of spin we directly introduce the relative intensities.
- Introduction of the input data for a single spectrum:
 - NMKD = number of groups of equivalent nuclei
 - IDEC = indicator for the type of curve
 - IWRT = indicator to print output
 - ILINE = indicator to fix the type of line shape
 - W = half linewidth at half height
 - ANINT = sampling interval
 - XXXX = maximum height
 - RIB = indicator for the sign of the ordinates
 - CORR = correction factor for the height of the spectrum
 - SPIN(I) = spin value (I = 1, NMKD)
 - NMEK(I) = number of nuclei (I = 1, NMKD)
 - DHEK(I) = hyperfine splitting constant (I = 1, NMKD)

If SPIN(I) is different as $1/2$, 1, $3/2$ one must introduce:

 - D(J,I) = relative intensity of a line (J = 1, number of lines),
(I = 1, NMKD)
- Calculation of the 2 vectors of abscissa and ordinates (HS, DS) of the stick spectrum, and their dimension (LIST)
- Test on LIST with regard to K1
- Normalization of the biggest line to the height of the spectrum
- Recording of HS, DS and their dimension LIST, on data sets 1, 2, 3
- With the values of ANINT, W, calculation of the number of points I1 of the spectrum
- Test on I1 with regard to K2
- Calculation, according to the case of the:
 - absorption spectrum (IDEC = 0)
 - 1st derivative (IDEC = 1)

- 2nd derivative (IDEC = 2)

SAVE

Three data sets are used to record the elements of the stick spectrum. The routine SAVE performs the storage of the two vectors HS and DS and their relative dimensions on the three data sets.

ESPECA

From the stick spectrum, the program computes for every peak a Gaussian or a Lorentzian line shape, in order to obtain an:

- absorption spectrum (IDEC = 0)
- 1st derivative (IDEC = 1)
- 2nd derivative (IDEC = 2)

The 2 vectors resulting from this calculation and containing the abscissa and ordinates for the curve are called X1, Y1 (dimension I1).

PL 2250

This routine performs the display of the spectra on the screen of the 2250 UNIT. This is obtained by the subroutine "DESSIN" (5) for the:

- absorption spectrum
- 1st derivative
- 2nd derivative

and by the routines "STPOS" and "PLINE" (5) for the stick spectrum.

At this moment 3 options are presented to the operator:

1) to record the elements of the figure by using the "CALCOMP" plotter in the next step. To do this the function key 1 must be used; two temporary data sets are created:

- Data set 9: a record contains the type of curve (IDEC), the length (ZZX), the height (ZZY) of the spectrum and the dimension I1.
- Data set 11: a record contains the vectors X1 and Y1 (dimension I1)

2) In order to go on to the next case, the function key 2 must be used.

3) In order to correct the data of the present case, the function key 3 must

- if SPIN(I) is different as 1/2, 1, 3/2, NMKD groups of cards, each one with:

D(J,I) (format 6E12.6)

5.1.3 Input to Sum Single Spectra

- NSUM groups of cards, each one of them with:

- one card with:

AAAA Title of the case (format 18A4)

- one card with:

NADD, IDEC, IWRT, ILINE (format 4I12)

- one card with:

W, ANINT, XXXX, RIB (format 4E12.6)

- one card with:

NSPEC(I) (I = 1, NADD) (format 12I6)

Note

After the name of the job appears on the screen the variable INCA, which is to be set equal to 1 from the keyboard if the following data are introduced by cards (see fig. 2).

5.2 Sample of Input and Output for ESR2250 using the Keyboard

Figs. 3 to 14 correspond to the input and output of the ethyl and methyl radicals, for:

- absorption curve,
- first derivative,
- second derivative,
- stick spectrum.

The input and the output for the sum of these two radicals for the four types of representative curves is shown in figs. 15 to 21.

5.3 Sample of Input and Output for ESRCALC

The input is the same as given under 5.1.

The output for the ethyl radical is given in Figs. 22 to 25.

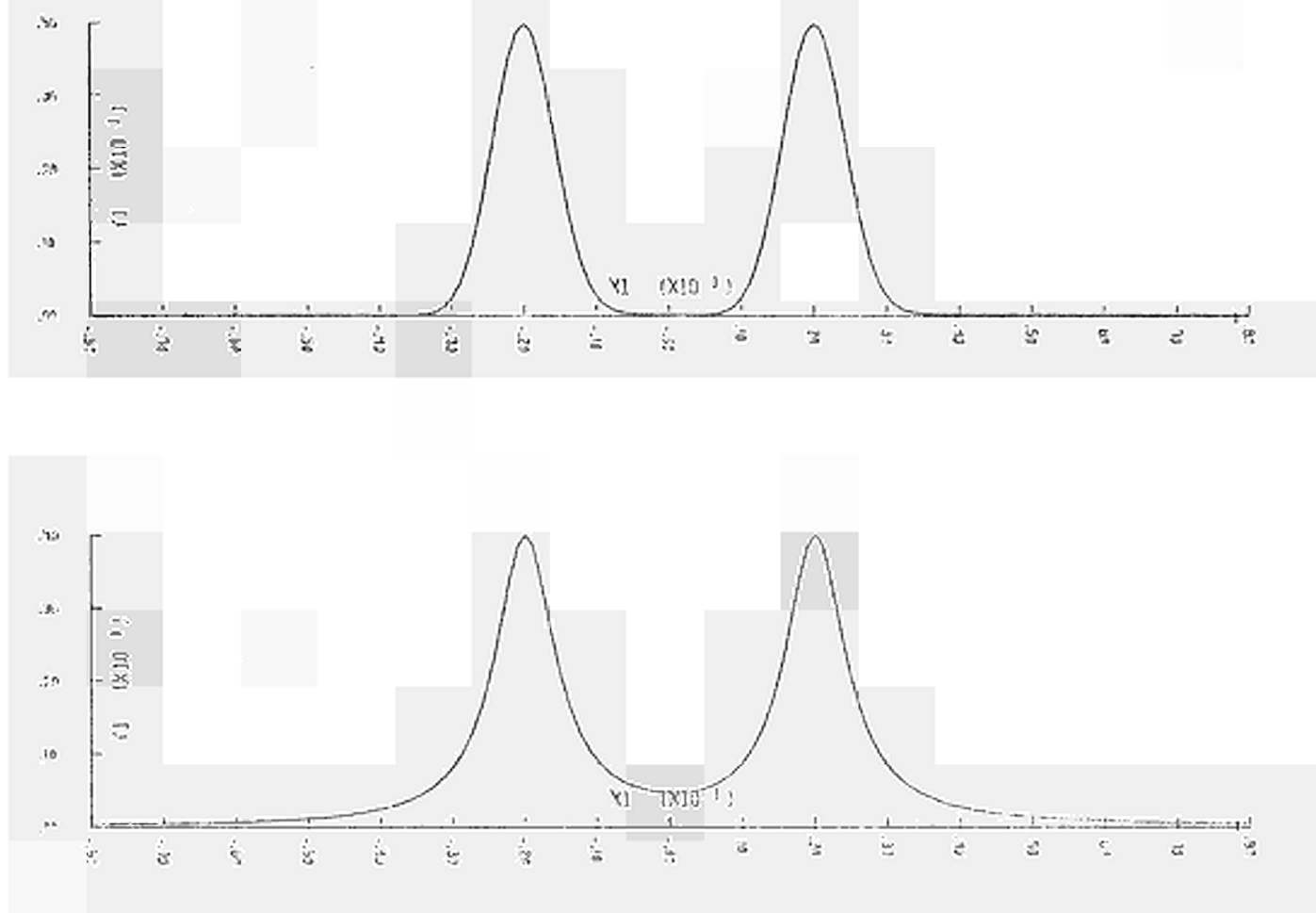


Fig. 1

INPUT DATA SPECIFICATION

INCA = 0 INPUT DATA BY THE KEYBOARD

INCA = 1 INPUT DATA BY CARDS

INCA (FORMAT 12) = 1

Fig. 2 - First picture appearing on the screen at the beginning of the job

GENERAL INPUT DATA

```
*****
TO FIX THE VALUES OF K1,K2,K3,K4 YOU MUST RESPECT THE 2 CONDITIONS
      2*K1 + 3*K2 = 10000 FOR SINGLE SPECTRA
      2*K1 + 2*K3 + 3*K4 = 10000 TO SUM SPECTRA
*****

NN    TOTAL NUMBER OF SINGLE SPECTRA (FORMAT I2)           8
NSUM  NUMBER OF SUM OF PRECALCULATED SPECTRA(FORMAT I2)    4
K1    MAX.DIMENSION OF HS,DS -SINGLE SPECTRA-(FORMAT I5)    800
K2    MAX.DIMENSION OF X1,Y1,DR2-SINGLE SPECTRA-(FORMAT I5) 1600
K3    MAX.DIMENSION OF SUMX,SUMY-SUM OF SPECTRA-(FORMAT I5) 800
K4    MAX.DIMENSION OF X1,Y1,DR2-SUM OF SPECTRA-(FORMAT I5) 1600

*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****
```

Fig. 3

```
CASE NUMBER      1                INPUT DATA FOR A SINGLE SPECTRUM
WRITE TITLE ON THE FOLLOWING LINE
ETHYL 1
NMKD NUMBER OF GROUPS OF EQUIVALENT NUCLEI (FORMAT I2)    2
IDEC=0 CALCULATION ABSORPTION SPECTRUM
IDEC=1 CALCULATION OF THE FIRST DERIVATIVE
IDEC=2 CALCULATION OF THE SECOND DERIVATIVE
IDEC=10 CALCULATION FIELD AND INTENSITY OF EACH TRANSITION
      IDEC (FORMAT I2) =                0
IWRT=1 IF YOU WANT TO WRITE OUTPUT
IWRT=0 IF NO OUTPUT IS REQUIRED
      IWRT (FORMAT I2) =                1
W  =HALF LINEWIDTH AT HALF HEIGHT (FORMAT E13.6)          0.100000E 00
ANINT =SAMPLING INTERVAL(FORMAT E13.6)                    0.500000E-01
RIB =INDICATOR SPECIFYING IF SIGN ORDINATES
      RIB (FORMAT E13.6) =              0.100000E 01
CORR =CORRECTION FACTOR FOR HEIGHT OF THE SPECTRUM (
      CORR (FORMAT E13.6) =              0.100000E 01
ILINE=0 LORENTZIAN LINE SHAPE FOR ABS.AND DERIVATIVE CURVES
ILINE=1 GAUSSIAN LINE SHAPE FOR ABS.AND DERIVATIVE CURVES
      ILINE (FORMAT I2) =                0
XXXX MAXIMUM HEIGHT(FORMAT E13.6) =                        0.100000E 02
*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****
```

Fig. 4

CASE NUMBER 1 INPUT DATA FOR A SINGLE SPECTRUM
ETHYL 1

FOR THE INDEX I VARYING FROM 1 TO NMKD = 2

INTRODUCE THE VALUES OF

I= 1

SPIN(I)=SPIN VALUE(FORMAT E13.6) 0.500000E 00

NMEK(I)=NUMBER OF NUCLEI(FORMAT I2) 3

DHEK(I)=HYPERFINE SPLITTING CONSTANT(FORMAT E13.6) 0.345000E 01

*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****

Fig. 5

CASE NUMBER 1 INPUT DATA FOR A SINGLE SPECTRUM
ETHYL 1

FOR THE INDEX I VARYING FROM 1 TO NMKD = 2

INTRODUCE THE VALUES OF

I= 2

SPIN(I)=SPIN VALUE(FORMAT E13.6) 0.500000E 00

NMEK(I)=NUMBER OF NUCLEI(FORMAT I2) 2

DHEK(I)=HYPERFINE SPLITTING CONSTANT(FORMAT E13.6) 0.255000E 01

*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****

Fig. 6

ETHYL 1

CASE NUMBER 1

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

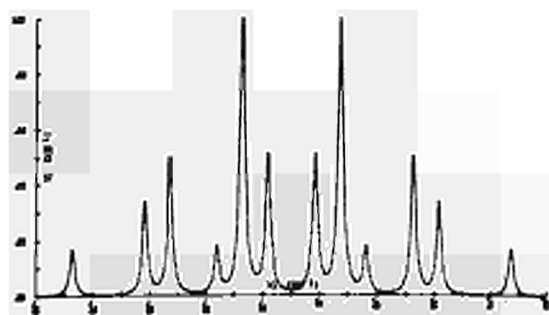


Fig. 7 - Ethyl absorption spectrum

ETHYL 2

CASE NUMBER 2

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

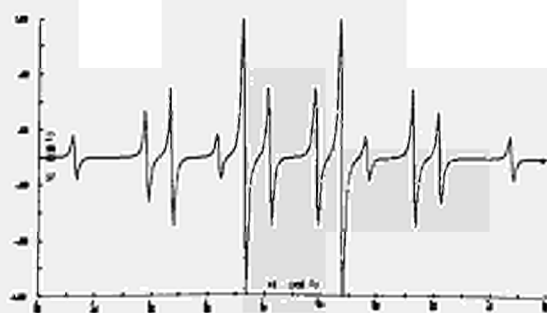


Fig. 8 - Ethyl first derivative

ETHYL 3

CASE NUMBER 3

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

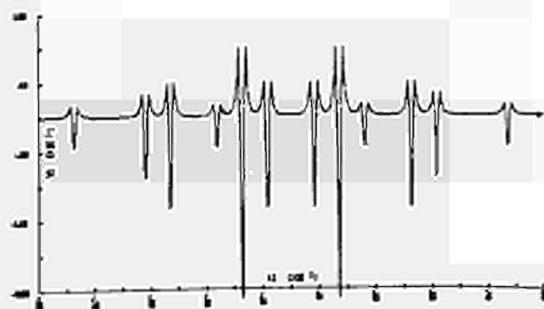


Fig. 9 - Ethyl second derivative

CASE NUMBER 4

ETHYL 4

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

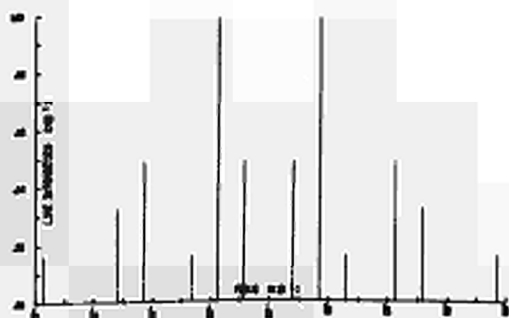


Fig. 10 - Ethyl stick spectrum

METHYL 1

CASE NUMBER 5

SCALE FACTOR FOR SPECTRUM LENGTH : 0.100000E 00

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

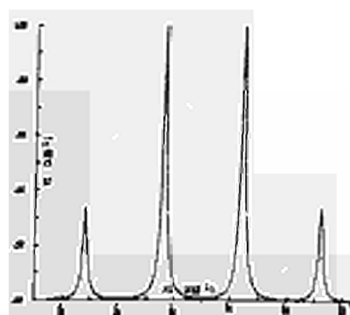


Fig. 11 - Methyl absorption spectrum

METHYL 2

CASE NUMBER 6

SCALE FACTOR FOR SPECTRUM LENGTH : 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

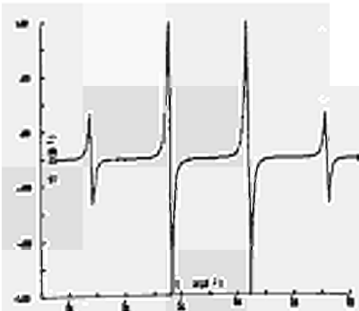


Fig. 12 - Methyl first derivative

METHYL 3

CASE NUMBER 7

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

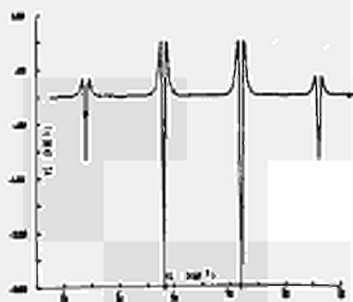


Fig. 13 - Methyl second derivative

CASE NUMBER 8

METHYL 4

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE

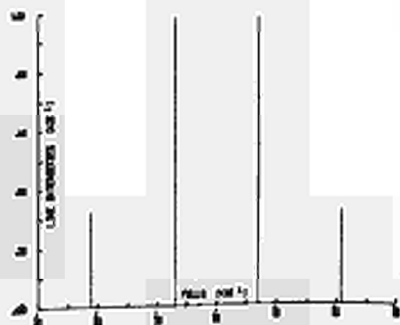


Fig. 14 - Methyl stick spectrum

```
CASE NUMBER      1                INPUT DATA FOR SUM OF SPECTRA
WRITE TITLE ON THE FOLLOWING LINE
SUM ETHYL 1 + METHYL 1

NADD NUMBER OF SPECTRA TO BE SUMMED(FORMAT I2)      2

IDEC=0 CALCULATION ABSORPTION SPECTRUM IDEC
IDEC=1 CALCULATION OF THE FIRST DERIVATIVE IDEC
IDEC=2 CALCULATION OF THE SECOND DERIVATIVE
IDEC=10 CALCULATION FIELD AND INTENSITY OF EACH TRANSITION

          IDEC (FORMAT I2) =                0

IWRT=1 IF YOU WANT TO WRITE OUTPUT
IWRT=0 IF NO OUTPUT IS REQUIRED

          IWRT (FORMAT I2) =                1

W  =HALF LINEWIDTH AT HALF HEIGHT (FORMAT E13.6)  0.100000E 00
ANINT =SAMPLING INTERVAL(FORMAT E13.6)           0.500000E-01
RIB  =INDICATOR SPECIFYING IF SIGN ORDINATES

          RIB (FORMAT E13.6) =              0.100000E 01

XXXX MAXIMUM HEIGHT(FORMAT E13.6) =              0.100000E 02

ILINE=0 LORENZTIAN LINE SHAPE FOR ABS.AND DERIVATIVE CURVES
ILINE=1 GAUSSIAN LINE SHAPE FOR ABS.AND DERIVATIVE CURVES

ILINE (FORMAT I2) =                0

*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****
```

Fig. 15

```
CASE NUMBER      1                INPUT DATA FOR SUM OF SPECTRA
SUM ETHYL 1 + METHYL 1

          THE INDEX I VARYING FROM 1 TO NADD =      2
          I =                1
NSPEC(I) = INDEX OF SPECTRA TO BE SUMMED (FORMAT I2)  1

*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****
```

Fig. 16


```
CASE NUMBER      1
SUM ETHYL 1 + METHYL 1
INPUT DATA FOR SUM OF SPECTRA
```

```
THE INDEX I VARYING FROM 1 TO NADD = 2
I = 2
NSPEC(I) = INDEX OF SPECTRA TO BE SUMMED (FORMAT I2) 5
```

*****TO CORRECT THESE DATA USE FK 1 TO GO ON USE FK 2 *****

Fig. 17

```
SUM ETHYL 1 + METHYL 1
CASE NUMBER      1
SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01
FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
FUNCTION KEY 2 = TO CONTINUE WITHOUT PLOTTING OF THIS FIGURE
FUNCTION KEY 3 = TO CORRECT THE INPUT DATA OF THIS CASE
```

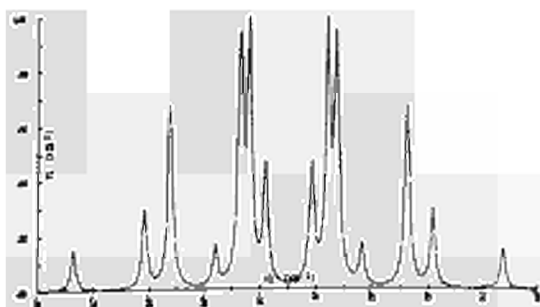


Fig. 18 - Sum Ethyl + Methyl radicals; absorption spectrum

SUM ETHYL 2 + METHYL 2

CASE NUMBER 2

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

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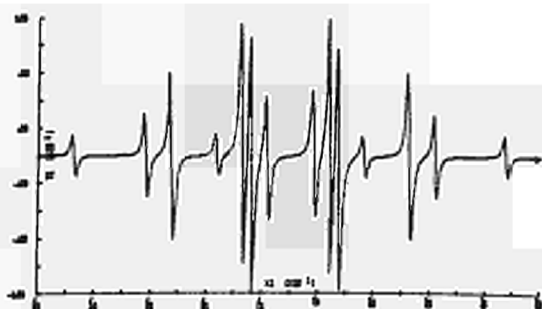


Fig. 19 - Sum Ethyl + Methyl first derivative

SUM ETHYL 3 + METHYL 3

CASE NUMBER 3

SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

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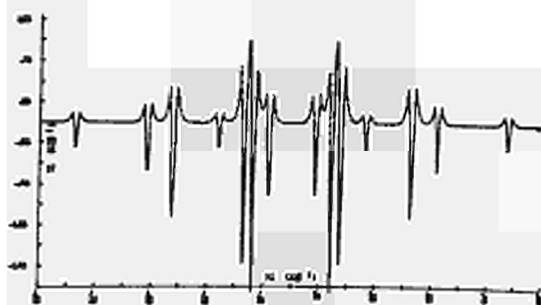


Fig. 20 - Sum Ethyl + Methyl second derivative

CASE NUMBER 4

SSUM ETHYL 4 + METHYL 4
SCALE FACTOR FOR SPECTRUM LENGTH = 0.100000E 01

FUNCTION KEY 1 = TO PLOT THIS FIGURE BY THE DATA-PLOTTER
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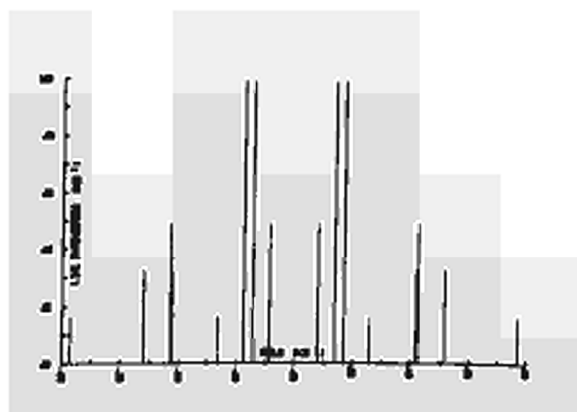


Fig. 21 - Sum Ethyl + Methyl stick spectrum

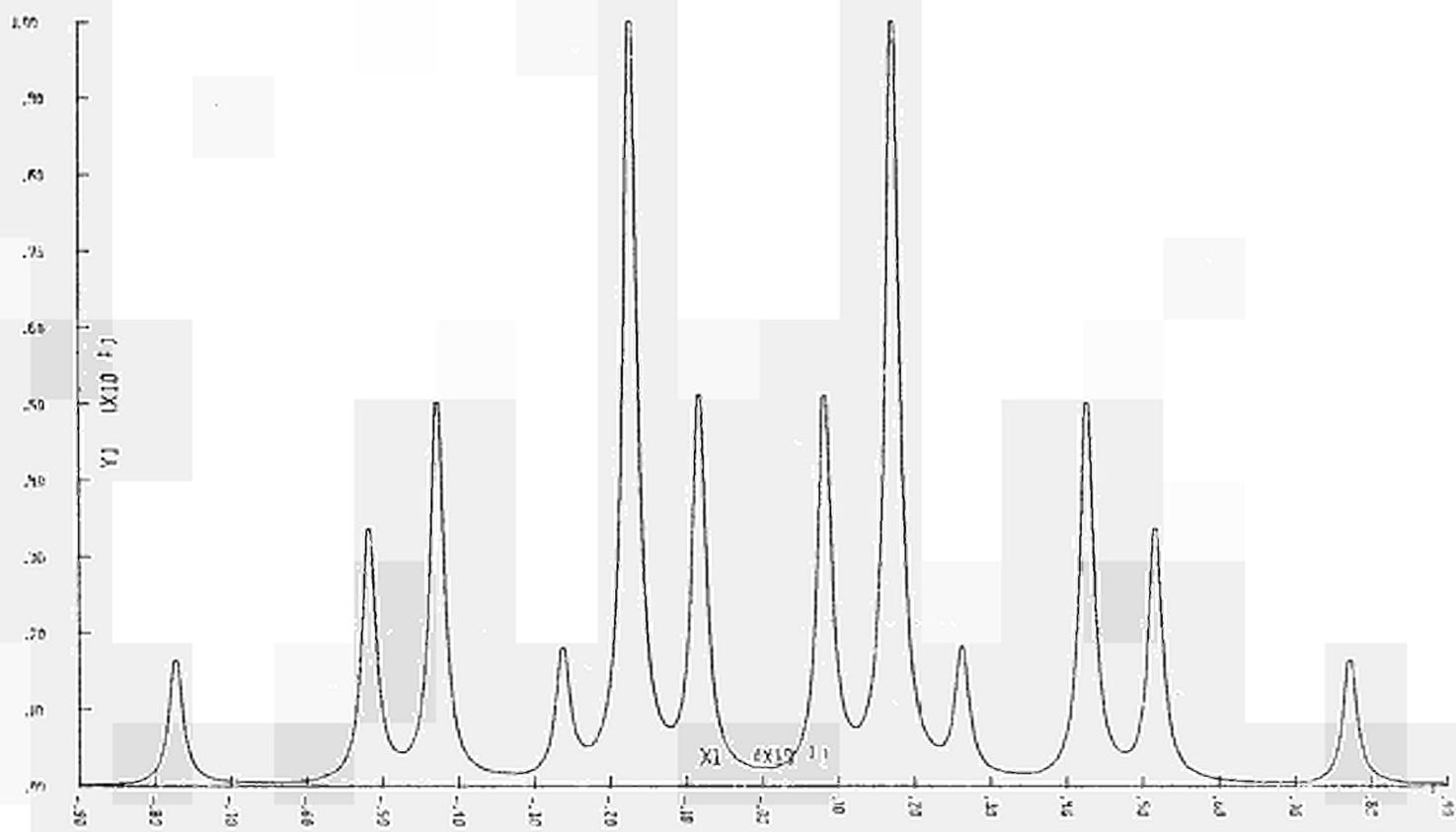


Fig. 22 - Ethyl absorption spectrum

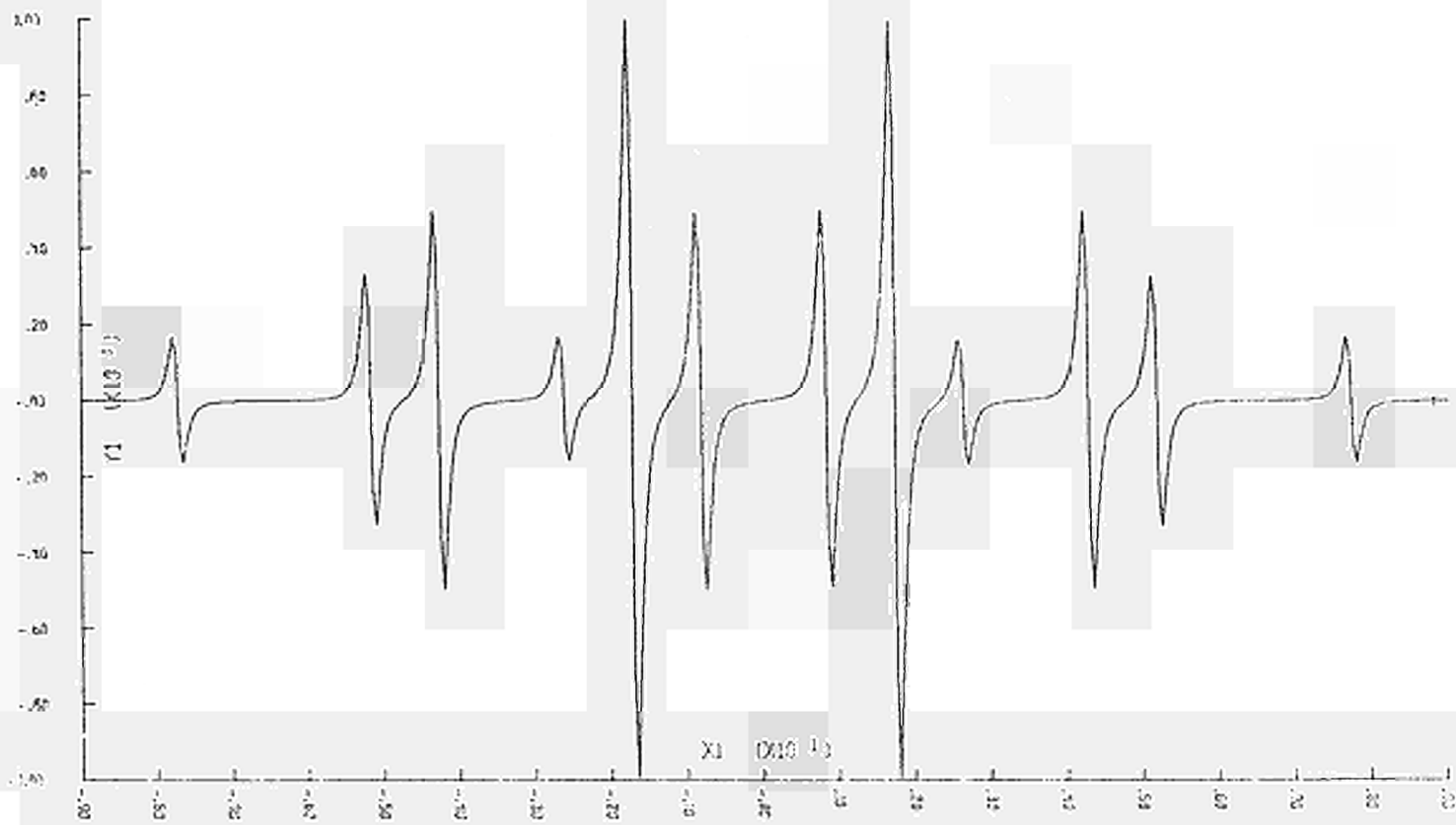


Fig. 23 - Ethyl first derivative

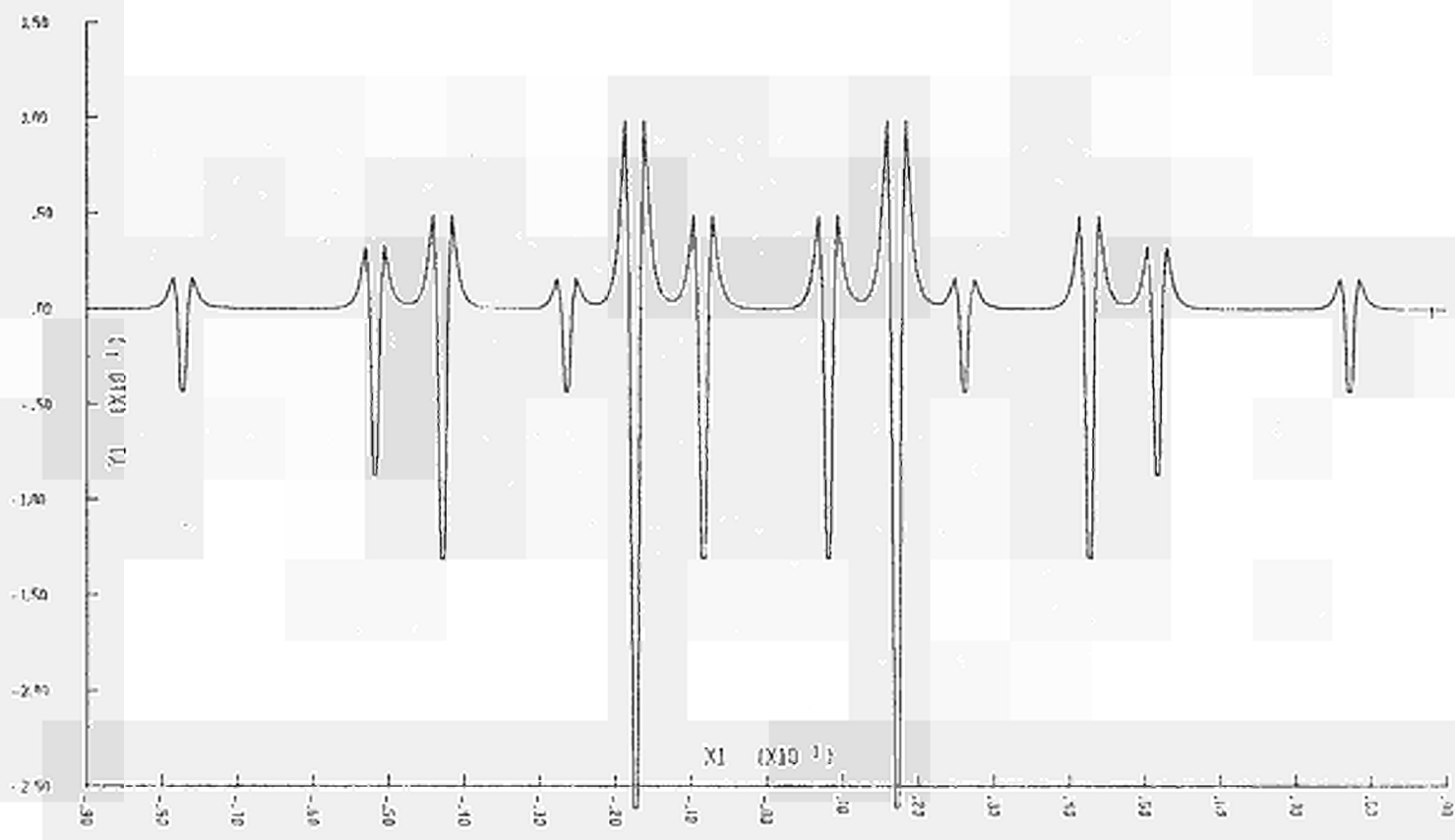


Fig. 24 - Ethyl second derivative

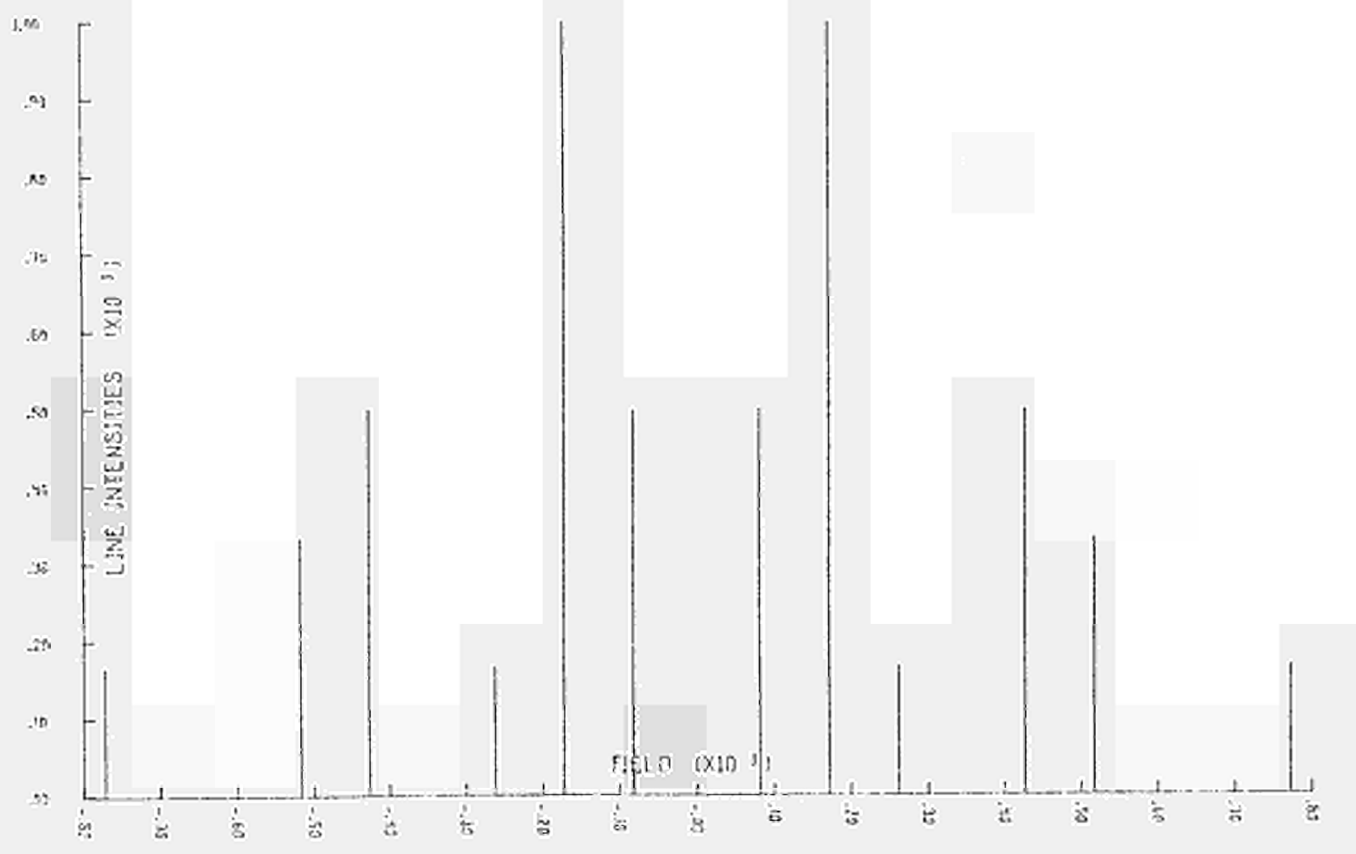


Fig. 25 - Ethyl stick spectrum

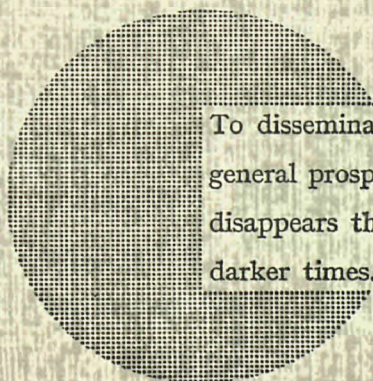
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Alfred Nobel

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