KFKI-72-74

J. Szőke

COMPUTERIZED MEASUREMENTS AND DATA PROCESSING

N° 6. Program for the elimination of instrument distortions and improvement of resolution

Hungarian Academy of Sciences

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BUDAPEST

COMPUTERIZED MEASUREMENTS AND DATA PROCESSING

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KFKI-72-74

COMPUTERIZED MEASUREMENTS AND DATA PROCESSING

PROGRAM FOR THE ELIMINATION OF INSTRUMENT DISTORTIONS AND IMPROVEMENT OF RESOLUTION

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ABSTRACT

A computer program using an iterative deconvolution algorithm for the generation of genuine /instrument-independent/ spectra and for the improvement of resolution is described.

РЕЗЮМЕ

В статье описывается программа ЭВМ, разработанная для получения истинных /независимых от прибора/ спектров, а также для улучшения разрешения при помощи итеративного алгоритма развертывания.

KIVONAT

Számitógépi programot ismertetünk, amely valódi /készüléktől független/ szinképek előállitására és a felbontás mesterséges javitására szolgál. A módszer iterativ dekonvoluciós algoritmussal dolgozik.

CONTENTS

1. INTRODUCTION

This program written in FORTRAN IV language using ICT 1900 machine representation eliminates instrumental distortions of convolute type from experimental data and/or improves the resolution by use of the deconvolution method described by J. Szőke in Chem. Phys. Letters, 1972. 5, 404.

The program is suitable also for solving other than spectral distortion deconvolution problems /e.g. chromatogram analysis/. A prerequisite is that the digital data be essentially free from experimental /systematic/ errors. Random errors usually do not interfere with the calculation, nevertheless, it is advisable to smooth the experimental data by methods which are insensitive to formal distortions of the processed data, such as e.g. the least squares method of A. Savitzky and M.J.E. Golay, Anal. Chem. 1964. 36, 1627. In the present program this method is applied after each deconvoluting cycle.

The deconvolution method can be applied also to calculate the convolute of an experimental data block.

2. INPUT, OUTPUT AND INSTRUCTIONS

a/ INPUT

The first set of the input data on the card or tape contains the basic entries which are

NT — Number of tasks to be solved /I6/

NA — Number of characters naming the task /spacings included/ in less than 72 characters /I6/

NAME/I/ — Name of the task in any number of characters below 72

NY — Number of elements in the data block /maximum number 512/ /9F8.1/ or /9F8.3/

IT — Number of iterations in subroutine DECONV /proposed number 10//I6/

KM — KEY to mode of operation /I6/

- EQ 1: Calculation of the genuine spectrum
- EQ 2: Improvement of resolution
- EQ 3: Calculation of genuine spectrum with subsequent improvement of resolution

KQ Key to prepare punch tape for least squares computation /I6/
NS Maximum allowed number of smoothing cycles /I6/
KY Key to read-in of data block /I6/
EQ 1: Read-in by 9F8.1
EQ 2: Read-in by 9F8.3
EQ 3: Read-in by subroutine ANAL in character form, each word terminates with ":"
DX Abscissal scale factor /9F8.3/
CS Limit of smoothing given by the ratio of two successive standard deviations /proposed value 1.2 /1.05-1.50/ /F8.3/
CJ Limit of deconvolution given by the ratio of two successive standard deviations /proposed value 1.2 /1.05-1.50/ /F8.3/
Y/I/ Data array of points equidistant on the X coordinate scale given in F8.1, F8.3 or an integer with arbitrary number of numerical characters
YK/I/ Data array of deconvoluting function containing maximum 100 data points with a scale factor DX, the same as that of Y/I/ /9F8.1/
NK Number of data points in the deconvoluting function /I6/
IM Serial number of the maximum point in the deconvoluting function /I6/
GS Variance of the calculated gaussian deconvoluting function /F8.3/
KJ Number of deconvoluting cycles, maximum 9 /I6/
KP Punched tape for analyzer /System KFKI/ /I6/
EQ 0: Don't punch
NE 0: Punch

b/ OUTPUT

1/ The program writes out its name before starting with the calculation: PROGRAM FOR CONVOLUTION AND DECONVOLUTION and specifies the name of the task /maximum 72 characters/.

2/ It writes out the type of the method used: GENUINE SPECTRUM or IMPROVEMENT OF RESOLUTION.
In a new line it specifies the input parameters in the arrangement employed in the input protocol by use of MASTER C4.

3/ Values of integral, maximum, its position, minimum, its position are written out by use of MASTER C5/e.

4/ The convoluting array YK/I/ is printed out as plotted by the line printer controlled by MASTER C6/i.

5/ The program writes out cyclically

a/ CALCULATION OF THE ith DECONVOLUTE by use of MASTER C7/a

b/ CONVOLUTE and convolute array C/I/ only in the first cycle of DECONV iteration by use of DECONV c2/e.

c/ INFORMATION ABOUT DECONVOLUTION, NUMBER OF ITERATIONS, STANDARD DEVIATIONS by use of DECONV C4

d/ DECONVOLUTE the non-smoothed value is punched by use of DECONV C5

e/ STANDARD DEVIATION OF SMOOTHING by use of SR. SMOOTH C2

f/ THE NUMBER OF ITERATIONS IS EXHAUSTED if this is the case

6/ The results of the calculation /genuine spectrum, spectrum with improved resolution/ are printed out as plotted by line printer.

c/ INSTRUCTIONS

Loading and running of the object program

The program PSCD is loaded into the memory from AF tape. The run starts from #GO # 20. The program requires a memory capacity of 23011 words.

Hardware requirements

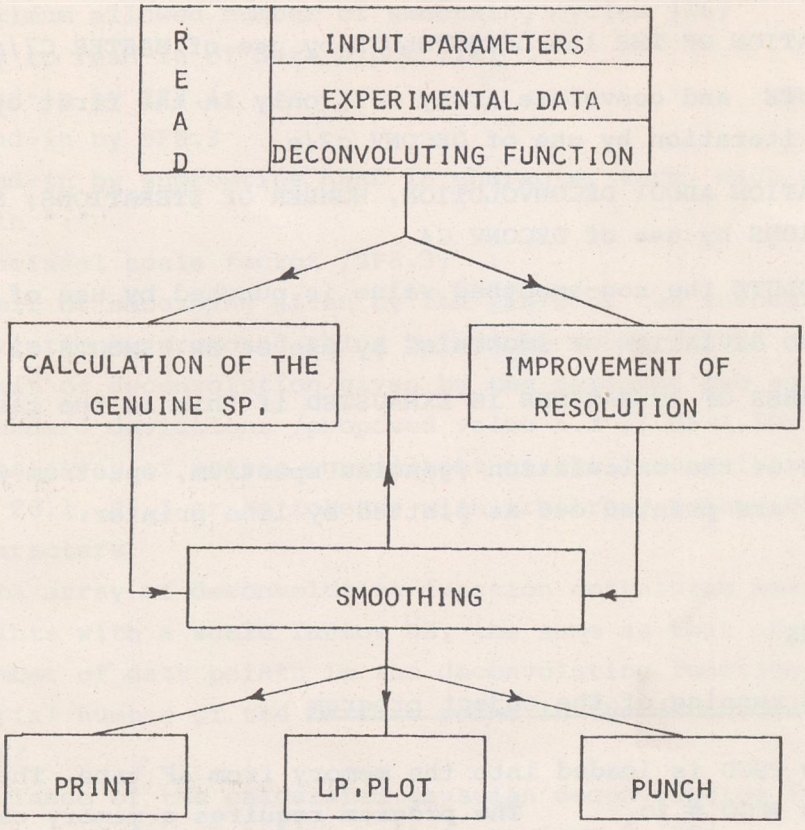
INPUT 1: Tape reader
OUTPUT 2: Line Printer
OUTPUT 3: Punch

Consol messages

The program does not provide for error protection and therefore comes to a halt in every case of "ERROR". The output message at the end of the run with error reads HALTED : EE
without error HALTED : FH

3. SCHEME OF PROGRAM OPERATIONS

The program operations are performed by the MASTER and 17 SUBROUTINES in the sequence as follows.

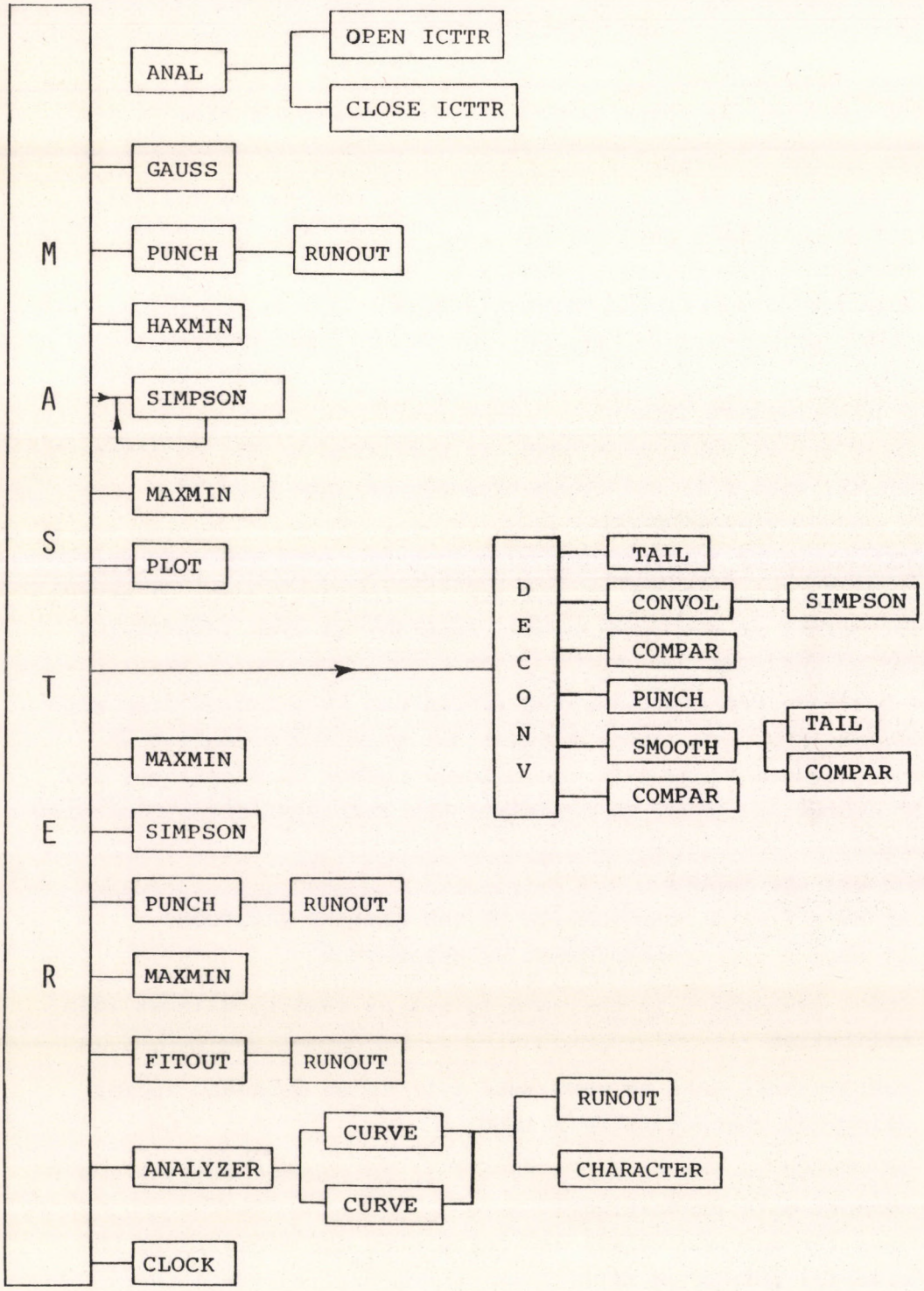


4. LIBRARY ROUTINES AND COMMON FIELDS

The program uses the following ICT Library routines: TIME, INONE, OPEN ICT TR, CLOSE TR, RUNOUT

IΘ /I/ array is in the COMMON FIELD /CHAR/, which is used in the MASTER and the subroutines: FITOUT, ANALYZER, CURVE and CHARACTER.

5. ORGANIZATION OF THE PROGRAM



6. DESCRIPTION OF THE PROGRAM

6.1 MASTER

The MASTER performs 12 steps of the program, specified from C1 to C12 in the listing

C1 The general information about the task is read-in as follows:

a/ Number of tasks into NT

b/ Number of characters in NAME into NA

c/ Characters specifying task into NAME

d/ Input parameters NY, IT, KM, KQ, NS, KY, KP, KPUNCH, DX, CS, CI

C2 Reads experimental data 9F8.1, 9F8.3 or subroutine ANAL, as specified by the position of switch KY, into Y/I/ and it is transferred into BASE/I/.

C3 Reads convoluting function as determined by the position of switch KM, into YK/I/ KM = 1 or 3 stands for calculation of the genuine spectrum, then NK experimental points of the instrumental function YK with identifying number IM are read

KM = 2 stands for improving the resolution by deconvolution with a Gaussian function, then it reads the standard deviation GS of the Gaussian along with the allowed number of iterations and calls subroutine GAUSS to calculate the points of the convoluting function.

C4 Writes out the inputs

a/ if KM = 1 or 3 CALCULATION OF THE GENUINE SPECTRUM
if KM = 2 IMPROVEMENT OF RESOLUTION

b/ INPUT PARAMETERS in the same format as read-in without identification

c/ EXPERIMENTAL DATA as read into Y/I/ in an extended format using 120 characters in a line

d/ If KPUNCH is not equal to zero Y/I/ is punched out for a subsequent data processing.

C5 Searches for max-min values and calculates the integral of the experimental points in Y/I/

a/ Checks whether the number of the experimental points is odd: NY1 = NY or even: NY1 = NY - 1

b/ Uses DO 7 to transfer the points from array Y/I/
- into array D/I/ to calculate the deconvolute, and
- into the integer array IA/I,1/ to plot the function NINT/Y/I//

c/ Calls MAXMIN to search for the maximum and minimum values and their serial numbers in the array D/I/

d/ Calls SIMPSON to integrate the array D/I/

e/ Writes out the results as INTEGRAL.... MAXIMUM .... AT .... MINIMUM .... AT ....

C6 Normalizes and plots the convoluting function

a/ Calls SIMPSON to calculate the integral of the convoluting function YK/I/

b/ Normalizes the integral of YK/I/ to 1.0

c/ Calls MAXMIN to search for the maxima and minima and their serial numbers in YK/I/

d/ Writes out the type of the convoluting function
for KM = 1 or 3 NORMALIZED EXPERIMENTAL INSTRUMENTAL FUNCTION
for KM = 2 NORMALIZED GAUSSIAN DECONVOLUTING FUNCTION

e/ Writes out the elements of the array YK/I/ in extended format using 120 characters

f/ Writes out the results of the operations on YK/I/ as INTEGRAL=... MAXIMUM ... AT ... MINIMUM ... AT .,..

g/ Normalizes YK/I/ setting minimum = 0, maximum = 100 for the plot by line printer

h/ Transfers the normalized function YK/I/ into JA/I,1/

i/ Plots YK/I/ by use of line printer.

C7 Calculates the deconvolute by use of DO 15 and plots the values by use of line printer.

a/ Writes out: CALCULATION OF THE ITH DECONVOLUTE

b/ Calls DECONV to calculate the deconvolute

c/ Uses DO 12 to transfer the points from arry E/I/ into Y/I/ and D/I/

d/ Calls MAXMIN to research for the maxima and minima and their serial numbers in D/I/

e/ Calls SIMPSON to calculate the integral of D/I/ and to re-normalize it to the original Y/I/ values

f/ Transfers D/I/ without normalization into IA

g/ Writes out D/I/ in normalized form with caption "NORMALIZED DECONVOLUTE"

h/ If KPUNCH is not equal to zero array D/I/ is punched out for a subsequent data processing by using subroutine PUNCH

i/ Writes out the results of the operations on D/I/ as INTEGRAL... MAXIMUM.... AT.... MINIMUM.... AT .....

j/ Calculates the normalizing factor for the plot of D/I/

C8 Punches by FITOUT subroutine the paper tape if a Gauss fit is required for, if KQ is not zero.

C9 Plots the results of the calculation by use of line printer. The details are listed under C7

a/ Writes out the title of the plot with captions chosen by
KM = 1 or 3 THE EXPERIMENTAL /1/ AND GENUINE /2/ SPECTRUM
KM = 2 IMPROVEMENT OF RESOLUTION
NUMBER 1 IN THE PLOT IS THE GENUINE SPECTRUM THE OTHERS ARE THE SUCCESSIVE DECONVOLUTES

b/ Normalizes and transfer the array IA/I,J/ into JA/I,J/
Uses DO 33 which normalizes IA/I,J/ by the last normalizing factor obtained in C7-i and transfers it into JA/I,J/

c/ Calls PLOT to plot the results of the calculation.

C10 Punches tape for processing by subroutine ANALYZER, if KP is nonzero.

C11 Calls new operation
D/I/ is fed into Y/I/ with the aid of DO 24.
If KM = 3, the next operation is to improve the resolution, therefore it sets KM = 2 and the program continues from statement 4

C12 Calls new task
Adds 1 to the task counter and if it is less than the input number NT the program continues at the statement 1, if not, it calls CLOCK to terminate the program.

6.2 SUBROUTINE FITOUT

makes an input paper tape for the least squares program from the data array.
Setting the minimum equal to zero, the maximum equal to 1000. The elements of array D/I/ are transferred into the integer array IO being punched by the aid of the output FORMAT:
/6/I8, 4H ΔΔΔ 1//, where "1" is the weighting factor for Gauss-fit.
The subroutine produces a fit hole tape about 10 cm long before and after the output of the data block using subroutine RUNOUT. Array IΘ/I/ is in COMMON field.

Parameter list:

D/I/	Real array to be punched
N	Number of elements used in arrays D/I/ and IO/I/ /maximum:512/
DM	The highest value in array D/I/
DL	The lowest value in array D/I/

6.3 SUBROUTINE ANALYZER

prepares the experimental data array Y/I/, the last deconvolute D/I/ and the convoluting function YK/I/ applied in the calculation to punch on paper tape by using subroutine CURVE for processing by a KFKI 1024 channel analyzer. In the first step the procedure normalizes the highest value of Y/I/ and D/I/ to 60000 and their lowest value to zero.

After punch Y/I/ and D/I/ the same normalizing procedure is applied to the convoluting array JK/I/.

Parameter list:

Y/I/, D/I/	Real arrays to be punched
N	Number of elements of arrays Y/I/ and D/I/
DM	The highest value in arrays Y/I/ and D/I/
DL	The lowest value in arrays Y/I/ and D/I/
IK/I/	Convoluting function to be punched
NK	Number of elements of array YK/I/
FM	The highest value of array YK/I/
FL	The lowest value in array YK/I/

6.4 SUBROUTINE PUNCH

produces a punched tape from a real array A/I/ having N elements in the following FORMAT:/9F8.1/. Before punch subroutine RUNOUT is called for preparing about 10 cm long fit hole tape.

Parameter list:

A/I/	Real array to be punched
N	Number of elements in array A/I/

6.5 SUBROUTINE MAXMIN

This subroutine searches for the maximum and minimum values of the points in array Y/I/ and identifies their serial number.

Parameter list:

DM	Maximum point in the array Y/I/
DL	Minimum point in the array Y/I/
MD	Serial number of the maximum point
LD	Serial number of the minimum point
Y/I/	Real array to be investigated
N	Number of elements in the array I/I/

6.6 SUBROUTINE ANAL

reads the experimental data in characters of integer form by use of the INONE ICT library routine made in KFKI which converts the characters into real numbers of array Y/I/

Parameter list:

Y/I/	Real array
N	Number of data points in the array

6.7 SUBROUTINE CURVE

This subroutine normalizes the points of the array A/I/ to its lowest point, multiplying them by a normalizing constant C before transfer to the array of integers IΘ/I/ and calls subroutine CHARACTER to punch the points of IΘ/I/ in character form using the 20 cm long tapes supplied by the RUNOUT library routine. The array IO is in common field /CHAR/.

Parameter list:

A/I/	Real array to be punched
N	Number of points in array A/I/
C	Normalizing constant
D	The lowest point in array A/I/

6.8 SUBROUTINE CLOCK

This subroutine writes out the exact time by use of the TIME library routine, as

THE TIME IS NOW ... HOURS/MINUTES/SECONDS

6.9 SUBROUTINE SIMPSON

This subroutine calculates the integral S of the array Y in which the number of points N is odd and the points are equally spaced on the abscissal scale DX.

Parameters list:

Y/I/	Real array to be integrated
N	Number of points in array A/I/
S	Integral as calculated
DX	Abscissal scale

6.10 SUBROUTINE CONVOL

This subroutine calculates the convolute C/I/ of the one dimensional array Y/I/ of NY points with a numerical convoluting function YD/I/ of NK points by using SIMPSON quadrature. The two functions have identical abscissal scales. The identifying number of the YK/I/ points is IM. The algorithm of the calculation is

$$C/I/ = \frac{Dx}{3} \sum_{J=1}^{NK} w_J \cdot F/J/ =$$

$$= \frac{Dx}{3} \left| F/1/+4\cdot F/2/+2\cdot F/3/+\ldots+2\cdot F/NK-2/+4\cdot F/NK-1/+ \right.$$

$$\left. +F/NK/ \right|$$

F/I/ contains the products obtained by multiplying all the corresponding overlapping points of Y/I/ and YK/I/

a/ F/J/ = Y/K/ * YK/J/
   where
   J = 1 ... NK
   K = I - IM + J

b/ F/J/ is integrated by use of subroutine SIMPSON.

Parameter list:

Y/I/	Real array of the convoluted function
NY	Number of points in Y/I/ and C/I/
YK/I/	Real array of convoluting function
NK	Number of points in YK/I/
C/I/	Real array for the convolute
IM	Identifying element of YK/I/
DX	Spacing of abscissal scale
LP	Last point in the convoluting calculation

6.11 SUBROUTINE PLOT

This subroutine displays the points of the array IA of M dimensions in a plot made by line printer. The maximum number of curves to be plotted in a figure is 10.

The normalized positive integers constituting the points stored in IA/I,J/ are used by the subroutine to print the plots taking 100 points per line represented from by the 10th to 110th characters of the line printer, thus the values in IA/I,J/ must be kept between 0 and 100.

C1:	Calculation and print of the ordinate
C2:	Calculation of the plotting characters belonging to the subsequent abscissa
C2A:	Calculation of abscissal markers
C2B:	Calculation of adequat points of the curves
C2C:	Write out the plotting line
C2D:	Replacing of the calculated characters by "blank"

Parameter list:

IA/I,J/	M-dimensional integer block containing the curves to be plotted
N	Number of points in a column of IA/I,J/
M	Number of columns in IA/I,J/

6.12 SUBROUTINE DECONV

This subroutine calculates the deconvolute of the input curve A/I/ with the convoluting function B/I/. It continues the iteration up to an input number of cycles IT, or up to a deconvolute D/I/, deviat-

ing from the points of the input curve A/I/ by a factor less than CJ. The algorithm is

$$D/I/ = D/I/ * A/I/ \ / \ C/I/$$

C1: The length of the front and back tail is calculated and the array elements are transferred into a new, long array.

C2: The deconvolute is calculated cyclically. Cycle counter: IT.

a/ The front and back tail elements are computed in all cycles except of the second cycle.

b/ The deconvolute is improved by using of the following algorithm:

$$D_i^j = D_i^{j-1} * A_i \ / \ C_i^{j-1}$$

If D_i^j is negative NR = 1.
In the first cycle step b/ is omitted.

c/ The convolute is calculated by using subroutine CONVOL.

d/ Subroutine COMPAR computes the standard deviation between the original array and the convolute of the deconvolute array.

e/ After the first cycle the CONVOLUTE is written out.

f/ If the quotient of the last two standard deviation less than CJ or the last standard deviation higher then the previous one the deconvolution comes to an end.

C3: The deconvolute is prepared for smoothing. The front and back tail elements of the arrays A/I/ and E/I/ are reduced to 4.

C4: Informations and results of the deconvolution is printed and punched out before smoothing.

C5: Writes and punches out the deconvolute before smoothing.

C6: The original and the convolute of the deconvolute is compared by subroutine COMPAR and standard deviation is calculated.

C7: The array length of deconvolute is reduced to original dimension.

C8: If the iteration number of deconvolution is exhausted THE ITERATION NUMBER IS EXHAUSTED is written out.

Parameter list:

A/I/	Real array of the function to be deconvoluted
B/I/	Real array of the convoluting function
M	Number of points in B
C/I/	Array of the convolute
D/I/	Array of the deconvolute
E/I/	Auxiliary array to save the last deconvolute
IT	Number of iterations
IM	Identifying number of array B
DX	Abscissal scale unit
NR	Flag signalling the presence of a negative value in A
NS	Number of smoothing cycles
N1	Number of points in arrays A/I/, C/I/, D/I/ and E/I/ original number of data points + NK-1
CJ	Factor of improvement by deconvolution

6.13 SUBROUTINE COMPAR

This subroutine compares the arrays A/I/ and B/I/ from the element L to the element M and calculates the sum of square deviations S, as

$$S = \sum_{I=L}^{M} (A/I/ - B/I/)^2$$

and the standard deviation R, as

$$R = \sqrt{(S/(M-L))}$$

Parameter list:

A/I/, B/I/	Real arrays to be comparized
L	Serial number of the first calculated element
M	Serial number of the last calculated element
N	Number of elements of arrays A/I/ and B/I/
R	Standard deviation of the calculation.

6.14 SUBROUTINE SMOOTH

This subroutine uses the Savitzky-Golay /Anal. Chem. 1964, 36, 1627/

nine point quartic least squares method to smooth the one-dimensional data array Y/I/

C1A: Calculates front and back tails /both consisting of 4 points/

C2B: The algorithm of the smoothing is

$$C_i = 2.331.10^{-3} \left| 15(Y_{i-4} + Y_{i+4}) - 55(Y_{i-3} + Y_{i+3}) + 30(Y_{i-2} + Y_{i+2}) + 135(Y_{i-1} + Y_{i+1}) + 179\ Y_i \right|$$

The calculations are performed in double precision and the results are transferred into array C/I/.

C1C: It calculates the sum of the standard deviations in arrays Y/I/ and C/I/ by using subroutine COMPAR.

C1D: It transfers C/I/ into Y/I/ and a new smoothing cycle begins

C1E: If the divergence between the two last standard deviations is less than a given value CS, the smoothing comes to an end, if not.

C2: Writes out the STANDARD DEVIATIONS of the smoothing cycles /not more than 20!/

Parameter list:

Y/I/	Real array to be smoothed the first and last 4 points are zero
C/I/	Empty auxiliary real array for the convolution
NS	Number of smoothing cycles
CS	Limiting factor of smoothing
N1	Number of points in Y/I/ and C/I/

6.15 SUBROUTINE TAIL

calculates the "tails" of the one-dimensional data array A/I/ if its extension is required.

The algorithm first determines the differences between the two first AL and between the two last AU points of A/I/. The additional points to form the tail are calculated as follows:

if the first or last points of A/I/ have values:

a/ Higher than the number of points J x AL of the front or J x AU of the back tail, the points of the front tail are evaluated as

|first A point| - I * AL and those of the back tail as
|last A point| - I * AU.

b/ Lower than or equal to J * AL and JL * AU, the sum S and the reciprocal R of the integers 1....J and 1....J1 are calculated and the points of the front and back tails evaluated as

[first A point] - A(1)/S(I), where I = 1,J

and

[last A point] - A last R(I) where I = 1,J1,

respectively.

Parameter list:

A/I/	Real array to be tailed
N1	Size of the extended array
IM	Identifying number of the convoluting function
NK	Number of points in the convoluting function.

6.16 SUBROUTINE GAUSS

This subroutine calculates the distribution function of the convolution /e.g. approximation to an experimental instrumental function or a deconvoluting function for improving the resolution/ using the algorithm

$$k_x = \exp\left[(x-x_o)^2/2\sigma^2\right]$$

where x_o and σ^2 are the maximum abscissal point and the variance of the distribution function, respectively.

Parameter list:

A/I/	Real array for distribution function
N	Number of data points in array A/I/
GS	Sigma parameter
DX	Abscissal scale factor

6.17 SUBROUTINE CHARACTER

This subroutine converts the integer form points of the normalized integer array IΘ/I/, the maximum value of which must be less than 65000, into characters so that every word has 5 characters. The thus obtained work array IY/J,L/ where L = 1,5 is then punched on tape, each word being terminated with /:/ and can be read by KFKI type analyser. In the first step the subroutine compares the number of points up to J in the array of integers IO with 10000, then uses DO 3 to convert the binary words of IO into characters of maximum 5 points each, and transfers the characters successively into the work array IY/I,J/ as follows.

1/ If the comparison of the J-th point in IΘ with 1000 gives

   a/ a negative value or zero, the character is zero and is transferred as such to the corresponding point of the IY/J,L/ integer array

   b/ a positive value, the transferred point must be greater than zero and its value is given by the value of J/10000. The numerical value of the character will be substracted from that of J in the calculation of the following character.

2/ The character at the place of the next digit is calculated by comparison of the J-th point of IΘ/I/ with 1000, 100, 10 and finally 1.

3/ On termination of the calculation, IY/I,L/ is punched out in the form

n(5A1, 1H:)

The program uses two given arrays IY/512,5 and IDIG/IO/ the latter being contained in the DATA block which accepts the characters to be used. The integer array IΘ/I/ is called from the COMMON field.

Parameter list:

N Number of points in IΘ/I/

7. LIST

FORTRAN COMPILATION BY #XFAM MK 4E DATE 20/03/73 TIME 12/27/14

```
LIST (LP)
SEND TO (MT,PROGRAM YSCA.PSCD)
PROGRAM (PSCD)
COMPRESS INTEGER AND LOGICAL
INPUT 1=TP0
OUTPUT 2=LP0
OUTPUT 3=TP0
END
```

```
      READ FROM (IT,PROGRAMOK AF.PS(D)
SUBFILE PSCD
      MASTER PSD2
      DIMENSION Y(512),BASE(512),C(512),D(512),E(512),VK(100),
     1IA(512,10),JA(512,1),NAME(70)
      COMMON/CHAR/IO(512)
C     PROGRAM FOR ITERATIVE DECONVOLUTION OF SPECTRA
C     WRITTEN BY DR.J.SZOKE CENTRAL RESEARCH INSTITUTE FOR PHYSICS
C     BUDAPEST, 1971-1972, FIRST VERSION
C1
      WRITE(2,200)
      MK=0
      NT1=0
      NDIM=512
      NC=10
      READ(1,202)NT
    1 MK=MK+1
      KK=0
      READ(1,202)NA
      READ(1,201)(NAME(I),I=1,NA)
      WRITE(2,201)(NAME(I),I=1,NA)
      READ(1,202)NY,IT,KM,KO,NS,KY,KP,KPUNCH
      READ(1,203)DX,CS,CJ
C2
      GO TO(0,2,3,19),KY
      READ(1,204)(Y(I),I=1,NY)
      GO TO 4
    2 READ(1,203)(Y(I),I=1,NY)
      GO TO 4
    3 CALL ANAL(Y,NY)
      GO TO 4
   19 READ(1,222)(Y(I),I=1,NY)
    4 DO 17 I=1,NY
   17 BASE(I)=Y(I)
   25 NST=1
      IF(NY.GT.256)NST=2
C3
      GO TO(0,5,0)KM
      KJ=1
      READ(1,202)NK,IM
      READ(1,204)(VK(I),I=1,NK)
      GO TO 6
    5 READ(1,203)GS
      READ(1,202)KJ
      NK=100
      CALL GAUSS(VK,NK,IM,GS,DX)
C4
    6 GO TO(0,23,0)KM
      WRITE(2,218)
      GO TO 27
   23 WRITE(2,215)
   27 WRITE(2,213)
      WRITE(2,202)NY,NK,IT,KM,KO,NS,KY,IM,KP,KJ,KPUNCH
      WRITE(2,203)DX,GS,CS,CJ
      WRITE(2,207)
      WRITE(2,205)(Y(I),I=1,NY)
      IF(KPUNCH.NE.0)CALL PUNCH (Y,NY)
C5
      NY1=NY
      NY2=NY/2+2
      IF(NY2.EQ.NY)NY1=NY-1
      DO 7 I=1,NY
      D(I)=Y(I)
```

```
      7 IA(I,1)=NINT(Y(I))
        CALL MAXMIN(DM,DL,MD,LD,Y,NY)
        SY=0.
        CALL SIMPSON(Y,NY1,SY,DX)
        WRITE(2,220)SY,DM,MD,DL,LD
C6
        S=0.
      8 CALL SIMPSON(YK,NK,S,DX)
        DO 9 I=1,NK
        YK(I)=YK(I)/S
      9 CONTINUE
        IF(S-1.)8,8,8
        CALL MAXMIN(FM,FL,MF,LF,YK,NK)
        IF(KM.EQ.2)GO TO 10
        WRITE(2,209)
        GO TO 11
     10 WRITE(2,208)
     11 WRITE(2,210)(YK(I),I=1,NK)
        WRITE(2,220)S,FM,MF,FL,LF
        YY=100./(FM-FL)
        DO 22 I=1,NK
        CY=(YK(I)-FL)*YY
     22 IA(I,1)=NINT(CY)
        WRITE(2,206)
        WRITE(2,214)
        CALL PLOT(IA,NK,1,NDIM)
        WRITE(2,206)
C7
        N1=NY+NK-1
        DO 15 II=1,KJ
        WRITE(2,221)IL
        IB=IL+1
     29 CALL DECONV(Y,YK,NK,C,D,E,IT,IM,DX,NS,CS,CJ,N1,KPUNCH)
        DO 12 JP=1,NY
        Y(JP)=E(JP)
     12 D(JP)=E(JP)
        CALL MAXMIN(DM,DL,MD,LD,D,NY)
        CALL SIMPSON(D,NY1,SD,DX)
        IF(SY-SD)0,14,0
        DY=SD/SY
        DL=DL/DY
        DO 13 II=1,NY
        D(II)=D(II)/DY
     13 IA(II,IB)=NINT(D(II)-DL)
     14 WRITE(2,211)
        WRITE(2,205)(D(K),K=1,NY)
        IF(KPUNCH.NE.0) CALL PUNCH(D,NY)
        CALL MAXMIN(DM,DL,MD,LD,D,NY)
        WRITE(2,220)SD,DM,MD,DL,LD
        Q=100./(DM-DL)
     15 CONTINUE
C8
        IF(KQ.NE.0)CALL FITOUT(D,NY,DM,DL)
C9
     18 WRITE(2,206)
        GO TO(0,20,0)KM
        WRITE(2,212)
        GO TO 21
     20 WRITE(2,216)
     21 DO 33 J=1,IB
        IG=0
        DO 33 I=1,NY,NST
        IG=IG+1
```

```
   33 IA(IG,J)=IA(I,I)*3
      CALL PLOT(IA,NY,IP,NDIM)
C10
      IF(KP.NE.0)CALL ANALYZER(BASE,D,NY,DM,DL,YK,NK,FM,FL)
C11
   35 IF(KM.NE.3)GO TO 26
      WRITE(2,206)
      DO 24 I=1,NY
   24 Y(I)=D(I)
      KM=2
      GO TO 25
C12
   26 NT1=NT1+1
      IF(NT-NT1)16,16,0
      WRITE(2,206)
      GO TO 1
   16 CALL CLOCK
      CALL EXIT
C FORMATS
  200 FORMAT(1H1,/,42H PROGRAM FOR CONVOLUTION AND DECONVOLUTION,//)
  201 FORMAT(1H0,20A1)
  202 FORMAT(12I6)
  203 FORMAT(9E8.3)
  204 FORMAT(9E8.1)
  205 FORMAT(12F10.2)
  206 FORMAT(1H1)
  207 FORMAT(1H0,10HINPUT DATA)
  208 FORMAT(1H0,42HNORMALISED GAUSSIAN DECONVOLUTING FUNCTION)
  209 FORMAT(1H0,43HNORMALISED EXPERIMENTAL INSTRUMENT FUNCTION)
  210 FORMAT(8F14.5)
  211 FORMAT(/,2X,23HNORMALISED DECONVOLUTE:)
  212 FORMAT(1H0,45HTHE EXPERIMENTAL (1) AND GENUINE (2) SPECTRUM)
  213 FORMAT(1H0,16HINPUT PARAMETERS)
  214 FORMAT(/)
  215 FORMAT(//,1H0,25HIMPROVEMENT OF RESOLUTION,/,1X,10H----------,
     115H----------)
  216 FORMAT(1H0,25HIMPROVEMENT OF RESOLUTION,/,1X,
     149HTHE NUMBER 1 IN THE PLOT IS THE GENUINE SPECTRUM,,
     146H THE OTHERS DENOTE THE SEQUENTIAL DECONVOLUTES)
  218 FORMAT(//,1X,35HCALCULATION OF THE GENUINE SPECTRUM,/,1X,
     135H-----------------------------------,/)
  219 FORMAT(5X,45HRESULTS OF THE IMPROVEMENT OF RESOLUTION AFTER,
     113,6HCYCLES)
  220 FORMAT(5X,10HINTEGRAL =,E12.4,5X,9HMAXIMUM =,E12.4,5X,4HAT =,I4,
     15X,9HMINIMUM =,E12.4,5X,4HAT =,I4)
  221 FORMAT(/,1H0,18HCALCULATION OF THE,I2,13H. DECONVOLUTE)
  222 FORMAT(6E12.5)
      END


END OF SEGMENT, LENGTH   890, NAME  PSD2
```

```
      SUBROUTINE FITOUT(D,N,DM,DL)
      DIMENSION D(N)
      COMMON/CHAR/IO(512)
      CALL RUNOUT(3)
      DS=1000./(DM-DL)
      DO 1 I=1,N
    1 IO(I)=NINT((D(I)-DL)*DS)
      WRITE(3,2)(IO(I),I=1,N)
      CALL RUNOUT(3)
    2 FORMAT(6(I8,4H    1))
      RETURN
      END

END OF SEGMENT, LENGTH     78, NAME  FITOUT
```

```
      SUBROUTINE ANALYZER(Y,D,N,DM,DL,YK,NK,FM,FL)
      DIMENSION Y(N),D(N),YK(NK)
      COMMON/CHAR/IO(512)
      DC=60000./(DM-DL)
      CALL CURVE(Y,N,DC,DL)
      CALL CURVE(D,N,DC,DL)
      DD=60000./(FM-FL)
      CALL CURVE(YK,NK,DD,FL)
      RETURN
      END
```

END OF SEGMENT, LENGTH 57, NAME ANALYZER

```
      SUBROUTINE PUNCH(A,N)
      DIMENSION A(N)
      CALL RUNOUT(3)
      WRITE(3,1)N
      WRITE(3,2)(A(I),I=1,N)
    1 FORMAT(I6)
    2 FORMAT(9F8.1)
      RETURN
      END

END OF SEGMENT, LENGTH     48, NAME   PUNCH
```

```
      SUBROUTINE MAXMIN(DH,DL,MD,LD,Y,N)
      DIMENSION Y(N)
      DM=Y(1)
      DL=Y(1)
      MD=1
      LD=1
      DO 2 I=1,N
      IF(DM.GT.Y(I))GO TO 1
      DM=Y(I)
      MD=I
      GO TO 2
    1 IF(DL.LT.Y(I))GO TO 2
      DL=Y(I)
      LD=I
    2 CONTINUE
      RETURN
      END
```

END OF SEGMENT, LENGTH 101, NAME MAXMIN

```
      SUBROUTINE ANAL(Y,N)
      REAL INONE
      DIMENSION Y(N)
      CALL OPENICTTR(0)
      DO 1 I=1,N
    1 Y(I)=INONE(J)
      CALL CLOSETR(0)
      RETURN
      END

END OF SEGMENT, LENGTH     44, NAME   ANAL
```

```
      SUBROUTINE CURVE(A,N,C,D)
      DIMENSION A(N)
      COMMON/CHAR/IO(512)
      DO 2 I=1,N
    2 IO(I)=0
      DO 1 I=1,N
      E=(A(I)-D)*C
    1 IO(I)=NINT(E)
      CALL RUNOUT(3)
      CALL RUNOUT(3)
      CALL CHARACTER(N)
      RETURN
      END
```

END OF SEGMENT, LENGTH 72, NAME CURVE

```
      SUBROUTINE CLOCK
      CALL TIME(TIM)
      WRITE(2,4)TIM
    4 FORMAT(18H (THE TIME IS NOW ,A8,1H))
      RETURN
      END

END OF SEGMENT, LENGTH     16, NAME   CLOCK
```

```
      SUBROUTINE SIMPSON(Y,N,S,DX)
      DIMENSION Y(N)
      A=Y(1)+Y(N)
      B=0.
      DO 1 L=2,N-1,2
    1 B=B+Y(L)
      B=4*B
      C=0.
      DO 2 M=3,N-2,2
    2 C=C+Y(M)
      S=C+C+A+B
      S=S*DX/3
      RETURN
      END
```

END OF SEGMENT, LENGTH 100, NAME SIMPSON

```
      SUBROUTINE CONVOL(Y,NY,YK,NK,C,IM,DX,LP)
      DIMENSION Y(NY),YK(NK),C(NY),E(100)
      DO 2 I=IM,LP
      I1=I-IM
      DO 1 J=1,NK
      K=I1+J
      E(J)=Y(K)*YK(J)
    1 CONTINUE
      CALL SIMPSON(E,NK,W,DX)
      C(I)=W
    2 CONTINUE
    3 RETURN
      END
```

END OF SEGMENT, LENGTH 93, NAME CONVOL

```
      SUBROUTINE PLOT(IA,N,M,NDIM)
      DIMENSION IA(NDIM,M),A(120),IB(20),DIG(10)
      DATA P,S,B,D/1H+,1H*,1H ,1H./
      DATA DIG(1),DIG(2),DIG(3),DIG(4),DIG(5),DIG(6),DIG(7),DIG(8),
     1DIG(9),DIG(10)/1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,1H0/
      K1=0
C1
      DO 1 I=1,9
      A(I)=B
    1 A(110+I)=B
      DO 2 I=10,110
    2 A(I)=D
      DO 3 I=1,9
      II=10*I+10
    3 A(II)=DIG(I)
      A(120)=B
      WRITE(2,21)(A(I),I=1,120)
      IC=0
      ID=0
      IE=0
      IG=0
      DO 4 I=10,110
    4 A(I)=B
C2
      DO 13 I=1,N
C2A
      IC=IC+1
      IF(IC.NE.10)GO TO 6
      IC=0
      ID=ID+1
      IF(ID.EQ.5)GO TO 8
      IF(ID.NE.10)GO TO 7
      IG=IG+1
      GO TO 9
    6 A(9)=P
      A(111)=P
      IB(1)=9
      IB(2)=111
      J1=2
      GO TO 10
    7 A(8)=S
      A(9)=S
      A(111)=S
      A(112)=S
      IB(1)=8
      IB(2)=9
      IB(3)=111
      IB(4)=112
      J1=4
      GO TO 10
    8 A(8)=DIG(5)
      A(9)=DIG(10)
      A(111)=S
      A(112)=S
      IB(1)=8
      IB(2)=9
      IB(3)=111
      IB(4)=112
      J1=4
      GO TO 10
    9 A(7)=DIG(IG)
      A(8)=DIG(10)
      A(9)=DIG(10)
```

```
      A(111)=S
      A(112)=S
      A(113)=S
      IB(1)=7
      IB(2)=8
      IB(3)=9
      IB(4)=111
      IB(5)=112
      IB(6)=113
      J1=6
C2B
   10 DO 11 J=1,M
      L1=IA(I,J)
      I=L1+10
      IB(J1+J)=L
      IF(IA(I,J).EQ.0) GO TO 11
      A(L)=DIG(J)
   11 CONTINUE
C2C
      WRITE(2,21)(A(I1),I1=1,120)
C2D
      DO 12 K=1,J1+M
      I1=IB(K)
      A(I1)=B
      IB(K)=0
   12 CONTINUE
   13 CONTINUE
   20 FORMAT(/)
   21 FORMAT(120A1)
      RETURN
      END

END OF SEGMENT, LENGTH   535, NAME  PLOT
```

```
      SUBROUTINE DECONV(A,B,M,C,D,E,IT,IM,DX,NS,CS,CJ,N1,KP)
      DIMENSION A(N1),D(N1),C(N1),B(M),Q(20),E(N1)
C1
      N=N1-M+1
      LP=N1-M+IM
      II=N-1
      NR=1
      M1=IM-1
      DO 1 I=1,N
      I4=N+1-I
      I3=N+IM-I
      A(I3)=A(I4)
      IF(I.GT.M1)GO TO 1
      D(I)=0.
    1 D(I3)=A(I4)
      DO 9 I1=1,IT
      DC=0.
      IF(I1.EQ.2)GO TO 3
    2 CALL TAIL(D,N1,IM,M)
      IF(I1.EQ.1)GO TO 5
C2
    3 DO 4 I=IM,LP
      D(I)=D(I)*A(1)/C(I)
      IF(D(I).LT.0)NR=-1
    4 CONTINUE
    5 CALL CONVOL(D,N1,B,M,C,IM,DX,LP)
      CALL COMPAR(A,C,IM,LP,N1,R)
      Q(I1)=R
      IF(I1.GT.1)GO TO 7
      WRITE(2,50)
      WRITE(2,51)(C(I),I=IM,LP)
    7 I2=I1-1
      DO 8 K=1,N1
    8 E(K)=D(K)
      IF(I1.EQ.1)GO TO 9
      IF(Q(I1).GT.Q(I2).OR.Q(I2)/Q(I1).LT.CJ)GO TO 10
    9 CONTINUE
C3
   10 DO 12 K=1,N
      A(K+4)=A(K+M1)
   12 E(K+4)=E(K+M1)
      N2=N+8
C4
      WRITE(2,54)
      WRITE(2,53)I2,NR
      WRITE(2,52)(Q(I),I=1,I2)
C5
      WRITE(2,56)
      WRITE(2,51)(E(I),I=5,N+4)
      IF(KP.NE.0)CALL PUNCH(E(5),LP-M1)
C6
      IF(NS.EQ.0)GO TO 6
      CALL SMOOTH(E,D,NS,CS,N2)
      CALL COMPAR(A,E,5,N+4,N2,R)
      WRITE(2,57)R
C7
    6 DO 11 I=5,N+4
   11 E(I-4)=E(I)
C8
      IF(I2.EQ.IT)WRITE(2,55)
   50 FORMAT(2X,10HCONVOLUTE:)
   51 FORMAT(12F10.2)
   52 FORMAT(10X,9F12.4)
```

```
   53 FORMAT(5X,28HNUMBER OF DECONV ITERATIONS=,I3,5X,3HNR.,I3,/,5X,
     136HSTANDARD DEVIATIONS OF DECONVOLUTION)
   54 FORMAT(/,4X,36HINFORMATIONS ABOUT THE DECONVOLUTION)
   55 FORMAT(1H0,33HTHE ITERATION NUMBER IS EXHAUSTED)
   56 FORMAT(5X,28HDECONVOLUTE BEFORE SMOOTHING)
   57 FORMAT(5X,36HSTANDARD DEVIATION AFTER SMOOTHING =,E12.5)
      RETURN
      END

END OF SEGMENT, LENGTH   537, NAME  DECONV
```

```
      SUBROUTINE COMPAR(A,B,L,M,N,R)
      DIMENSION A(N),B(N)
      S=0.
      DO 1 I=L,M
      H=A(I)-B(I)
      HH=H*H
    1 S=S+HH
      K=M-L
      R=SQRT(S/K)
      RETURN
      END

END OF SEGMENT, LENGTH    73, NAME  COMPAR
```

```
      SUBROUTINE SMOOTH(Y,C,NS,CS,N1)
      DOUBLE PRECISION CB
      DIMENSION Y(N1),C(N1),Q(20)
      N=N1-8
      LP=N+4
      NI=0
C1
      DO 3 IT=1,NS
      S2=0.
C1A
      CALL TAIL(Y,N1,5,8)
C1B
      DO 1 I=5,LP
      CB=15.D0*(Y(I-4)+Y(I+4))-55.D0*(Y(I-3)+Y(I+3))+30.D0*
     1(Y(I-2)+Y(I+2))+135.D0*(Y(I-1)+Y(I+1))+179.D0*Y(I)
      CB=CB*0.2331002331D-2
    1 C(I)=CB
C1C
      CALL COMPAR(Y,C,5,LP,N1,SD)
      NI=NI+1
      Q(NI)=SD
C1D
      DO 2 I=5,LP
    2 Y(I)=C(I)
      IF(NI.EQ.1)GO TO 3
C1E
      IF(Q(NI-1)/Q(NI).LT.CS)GO TO 4
    3 CONTINUE
C2
    4 WRITE(2,11)
      WRITE(2,12)(Q(I),I=1,NI)
   11 FORMAT(5X,32HSTANDARD DEVIATIONS OF SMOOTHING)
   12 FORMAT(10X,9E12.4)
      RETURN
      END

END OF SEGMENT, LENGTH   306, NAME  SMOOTH
```

```
      SUBROUTINE TAIL(A,N1,IM,NK)
      DIMENSION A(N1)
      J=IM-1
      J1=NK-IM
      K=N1-NK+IM
      KL=0
      KU=0
      AL=A(IM+1)-A(IM)
      IF(AL.LT.0.)GO TO 7
      IF(A(IM)-J*AL)0,0,2
    7 KL=1
      S=0.
      DO 3 I1=1,J
    3 S=S+1./I1
      AL=A(IM)/S
    2 AU=A(K-1)-A(K)
      IF(AU.LT.0.)GO TO 8
      IF(A(K)-J1*AU)0,0,4
    8 KU=1
      R=0.
      DO 5 J3=1,J1
    5 R=R+1./J3
      AU=A(K)/R
    4 I2=1
      DO 1 I=1,J
      M=IM-I
      IF(KL.EQ.1)I2=I
    1 A(M)=A(M+1)-AL/I2
      J2=1
      DO 6 I=1,J1
      L=K+I
      IF(KU.EQ.1)J2=I
    6 A(L)=A(L-1)-AU/J2
      RETURN
      END
```

END OF SEGMENT, LENGTH 271, NAME TAIL

```
      SUBROUTINE GAUSS(A,N,IM,GS,DX)
      DIMENSION A(N),B(49)
      P=0.
      J=0
    1 P=P+DX
      PP=P*P
      GG=GS*GS*2
      PG=PP/GG
      IF(J.EQ.49)GO TO 2
      J=J+1
      B(J)=EXP(-PG)
      IF(B(J)-0.001)0,1,1
    2 IM=J+1
      DO 3 I=1,J
      A(IM+I)=B(I)
    3 A(IM-I)=B(I)
      A(IM)=1.
      N=IM+J
      RETURN
      END
```

END OF SEGMENT, LENGTH 138, NAME GAUSS

```
      SUBROUTINE CHARACTER(N)
      DIMENSION IY(512,5),IDIG(10)
      COMMON/CHAR/IO(512)
      DATA IDIG(1),IDIG(2),IDIG(3),IDIG(4),IDIG(5),IDIG(6),IDIG(7),
     1IDIG(8),IDIG(9),IDIG(10)/1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,1H0/
      DO 3 J=1,N
      IA=IO(J)
      IQ=10000
      DO 3 L=1,5
      IF(IA-IQ)1,0,0
      IB=IA/IQ
      IA=IA-IB*IQ
      GO TO 2
    1 IB=10
    2 IY(J,L)=IDIG(IB)
      IQ=IQ/10
    3 CONTINUE
      WRITE(3,50)((IY(KJ,NI),NI=1,5),KJ=1,N)
   50 FORMAT(1024(5A1,1H:))
      RETURN
      END

END OF SEGMENT, LENGTH    96, NAME  CHARACTER
```

```
 END OF SUBFILE
      FINISH
= 55 250 1156 1217 2205 2257 16717 17717 20007 53743 4
> 533 6740003 60634344 54743 1172 4
? 41002330 %%%F 4
? 33002261 %FMARK   4
? 13017717 %FIOINF  4
? 33002262 %FIOLIST 4
? 41014172 %FIOPT   4
? 41014477 %FIOLP   4
? 41011705 %FERROR  4
? 41002330 PSD2 4
? 41011410 %FAP4    4
? 3053743 CHAR 4
? 41012241 %FINOUT  4
? 41004556 ANAL 4
? 41010555 GAUSS    4
? 41004331 PUNCH    4
? 41016516 NINT 4
? 41004411 MAXMIN   4
? 41004762 SIMPSON  4
? 41005263 PLOT 4
? 41006312 DECONV   4
? 41004122 FITOUT   4
? 41004240 ANALYZER 4
? 41004742 CLOCK    4
? 41015341 EXIT 4
? 2012064 %FERND   4
? 2011741 %FRL 4
? 41015352 %FARHD   4
? 41012140 RUNOUT   4
? 41004632 CURVE    4
? 41011127 OPENICTTR     4
? 41011205 INONE    4
? 41011401 CLOSETR  4
? 41010767 CHARACTER     4
? 41016511 TIME 4
? 41005126 CONVOL   4
? 41010136 TAIL 4
? 41007343 COMPAR   4
? 41007454 SMOOTH   4
? 41016551 SQRT 4
? 41015515 %FDP 4
? 41016623 EXP  4
? 23001156 TABLA    4
? 23001157 MIST 4
? 23001161 %LIB 4
? 23001204 %FMC 4
? 33002271 %F1  4
? 2012066 %FER 4
? 33002273 %FRMK    4
? 33002275 %FITER   4
? 2011705 FTRAP     4
? 2011710 FRESET    4
? 2011713 %FLOC     4
? 2012241 %FIOAUX   4
? 41012147 %FSTOP   4
```

```
? 33002276 %FER 4
? 33002311 %FDIS    4
? 33002313 %ACIOS   4
? 33002314 %FPNO    4
? 33002315 %FDMK    4
? 41014127 %FINF    4
? 23001207 %FIOLEN  4
? 13017736 %FIOBUF  4
? 23001211 %FMTP    4
? 23001212 %FLK 4
? 23001213 %FINCH   4
? 33002316 %FIOZ    4
? 2013004 %FIOF    4
? 2013151 %FIOF    4
? 2013260 %FIOB    4
? 2013322 %FIOA    4
? 2013530 %FIOC    4
? 2013577 %FIOG    4
? 2013721 %FIOD    4
? 23001214 %FIOPER  4
? 2014644 %FIOND   4
? 2014662 %FOTR    4
? 41014635 %FINIL   4
? 2014760 %CICA    4
? 41014717 %LPMT    4
? 2015161 EXT  4
? 2016260 %FDPNRM  4
? 23001215 %LIBA    4

PROGRAM NAME #PSCD, CORE  23011,LOWER AREA  1240,PROGRAM   7631

END OF COMPILATION -  NO ERRORS
```

8. TEST OF PROGRAM OPERATION

The test example illustrates the operation of the program which analyses the environment of the 0.0 transition in the fluorescence spectrum of ammonium-uranyl-tris-carbonate between 20000 and 19000 cm^{-1}. The experimental instrumental function was measured at 508 nm using the Cd line.

Applying the combined modes of operation the genuine spectrum was evaluated in the first and the resolution of the spectrum improved in the second step in three cycles.

The set of serial numbers at the start and end of the protocol of the input tape serves to the better understanding of the FORMAT structure.

NOTE

To protect the experimental data array from being too short or distorted, front and back tails are needed which must be of the appropriate length and low information content. If the values of the tails are high relative to those of the array, the spectrum is easily distorted. It is advisable to choose an interval of the experimental curve where both ends tend toward zero because the algorithm of the TAIL produces tails going to zero.

ACKNOWLEDGEMENTS

Many thanks are due to Mrs. J. Linder for valuable computational assistance and to Mr. G. Kötél for useful discussions.

```
   1
  20
TEST - 9 COMPONENTS
  151     10      3      0     20      1      1      0
 1.000   1.050   1.050
  87.5   108.9   133.8   163.1   196.6   234.7   277.4   324.7   376.3
 431.9   491.0   553.1   617.3   682.8   748.4   813.2   876.0   935.9
 991.8  1043.3  1089.7  1131.1  1167.7  1200.0  1229.1  1256.1  1282.3
1308.9  1337.0  1367.5  1400.6  1436.1  1473.4  1511.3  1548.2  1582.3
1611.7  1634.5  1649.4  1655.3  1651.6  1638.2  1615.7  1584.8  1546.7
1502.7  1454.4  1405.0  1350.0  1296.5  1243.7  1192.5  1143.9  1098.7
1057.8  1021.7   990.9   965.8   946.6   933.1   925.0   921.8   922.9
 927.6   935.3   945.5   958.2   973.4   991.4  1013.0  1038.8  1069.6
1106.2  1148.7  1197.1  1250.9  1308.8  1369.4  1430.6  1490.2  1546.1
1596.2  1638.9  1673.1  1696.4  1714.9  1723.5  1725.2  1721.5  1713.7
1705.0  1689.9  1674.9  1657.4  1636.8  1611.8  1581.2  1545.6  1498.2
1444.5  1382.8  1314.0  1239.7  1162.2  1084.1  1008.3   937.7   874.9
 822.0   780.4   751.1   733.8   728.0   732.1   744.2   761.8   782.4
 805.4   822.4   837.2   846.2   848.2   842.4   828.6   807.2   778.7
 744.1   704.4   660.9   614.7   566.9   518.6   470.5   425.5   378.1
 334.8   293.8   255.6   220.3   188.0   158.7   132.5   109.4    89.3
  71.9    57.2    45.0    34.9    26.8    20.3    15.3
  29     11
   3.2    16.8    59.8   159.8   286.8   452.5   595.4   743.1   896.4
1021.4  1086.5  1028.7   884.4   709.5   554.1   407.5   292.3   219.5
 104.1   119.5    85.8    64.1    47.8    35.9    26.1    19.6    13.0
   6.5     1.0
 2.500
   5
```

8.2 RESULTS OF CALCULATION IN LP REPRESENTATION

PROGRAM FOR CONVOLUTION AND DECONVOLUTION

TEST - 9 COMPONENTS

CALCULATION OF THE GENUINE SPECTRUM

INPUT PARAMETERS

151	29	10	3	0	20	4	11	1	1	0
1.000	0.000	1.050	1.050							

INPUT DATA

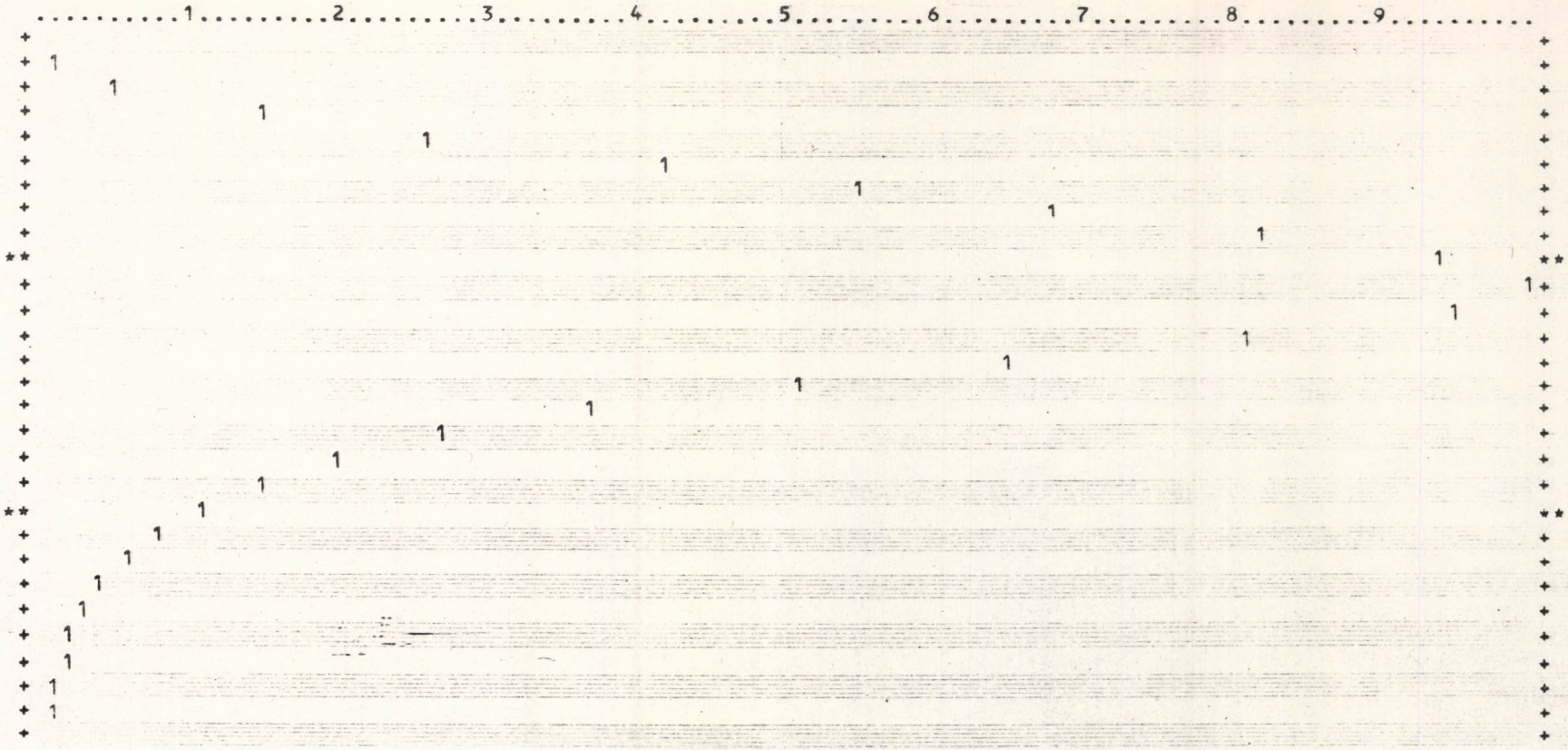
87.53	108.89	133.82	163.09	196.58	234.75	277.42	324.68	376.26	431.88	491.05	553.13
617.35	682.78	748.42	813.19	876.01	935.86	991.84	1043.27	1089.73	1131.11	1167.68	1200.05
1229.15	1256.14	1282.30	1308.91	1337.04	1367.48	1400.56	1436.12	1473.44	1511.35	1548.25	1582.32
1611.67	1634.55	1649.45	1655.32	1651.60	1638.23	1615.67	1584.76	1546.68	1502.75	1454.40	1403.04
1350.00	1296.50	1243.66	1192.48	1143.89	1098.74	1057.77	1021.66	990.90	965.85	946.62	933.12
925.03	921.33	922.90	927.58	935.27	945.54	958.21	973.38	991.43	1012.98	1038.80	1069.65
1106.16	1148.67	1197.10	1250.86	1308.83	1369.40	1430.61	1490.25	1546.11	1596.19	1636.87	1673.08
1698.36	1714.92	1723.49	1725.25	1721.54	1713.74	1702.97	1689.94	1674.88	1657.44	1636.80	1611.81
1581.15	1543.58	1498.17	1444.49	1382.78	1313.96	1239.68	1162.17	1084.09	1008.32	937.72	874.89
821.95	780.42	751.06	733.85	728.02	732.12	744.17	761.78	782.89	803.40	822.39	837.24
846.24	848.19	842.38	828.63	807.19	778.70	744.07	704.41	660.89	614.68	566.91	518.57
470.53	423.51	378.10	334.76	293.85	255.63	220.29	187.96	158.71	132.54	109.43	89.27
71.93	57.24	44.97	34.90	26.77	20.33	15.33					

INTEGRAL = 0.1487E 06 MAXIMUM = 0.1725E 04 AT = 88 MINIMUM = 0.1583E 02 AT = 151

NORMALISED EXPERIMENTAL INSTRUMENT FUNCTION

0.51993E-03	0.16796E-02	0.59786E-02	0.15976E-01	0.28674E-01	0.45240E-01	0.59527E-01	0.74293E-01
0.89620E-01	0.10212E 00	0.10863E 00	0.10285E 00	0.88420E-01	0.70934E-01	0.55397E-01	0.40741E-01
0.29223E-01	0.21965E-01	0.16406E-01	0.11947E-01	0.85781E-02	0.64085E-02	0.47789E-02	0.35892E-02
0.26094E-02	0.19596E-02	0.12997E-02	0.64985E-03	0.99977E-04			

INTEGRAL = 0.1000E 01 MAXIMUM = 0.1086E 00 AT = 11 MINIMUM = 0.9998E-04 AT = 29



CALCULATION OF THE 1. DECONVOLUTE

CONVOLUTE:

124.62	150.81	179.70	212.66	248.73	288.75	331.96	378.64	428.55	480.88	535.81	592.60
650.65	709.29	767.83	825.57	881.84	936.04	987.68	1036.40	1082.00	1124.43	1163.85	1200.53
1234.90	1267.46	1298.74	1329.23	1359.32	1389.22	1418.98	1448.39	1477.01	1504.19	1529.11	1550.85
1568.45	1581.01	1587.75	1588.08	1581.65	1568.38	1548.46	1522.33	1490.66	1454.27	1414.13	1371.27
1326.74	1281.58	1236.77	1193.23	1151.78	1113.17	1077.99	1046.76	1019.84	997.50	979.85	966.91
958.60	954.75	955.13	959.52	967.69	979.48	994.76	1013.52	1035.79	1061.65	1091.17	1124.42
1161.32	1201.70	1245.15	1291.10	1338.74	1387.07	1434.98	1481.26	1524.71	1564.23	1598.89	1627.96
1651.00	1667.81	1678.45	1683.19	1682.40	1676.53	1665.99	1651.10	1632.03	1608.84	1581.42	1549.58
1513.13	1471.91	1425.93	1375.39	1320.78	1262.90	1202.83	1141.88	1081.57	1023.48	969.19	920.10
877.41	841.94	814.15	794.06	781.26	774.94	773.96	776.94	782.33	788.54	794.00	797.30
797.23	792.86	783.53	768.90	748.93	723.84	694.06	660.21	623.01	583.25	541.75	499.30
456.63	414.41	373.21	333.51	295.70	260.10	226.93	196.33	168.39	143.15	120.58	100.61
83.14	68.04	55.13	44.26	35.18	27.78	21.76					

INFORMATIONS ABOUT THE DECONVOLUTION

NUMBER OF DECONV ITERATIONS= 9 NR: 1

STANDARD DEVIATIONS OF DECONVOLUTION

0.3856E 02 0.1095E 02 0.4896E 01 0.2564E 01 0.1457E 01 0.8755E 00 0.5494E 00 0.3571E 00 0.2391E 00

DECONVOLUTE BEFORE SMOOTHING

46.48	62.91	81.90	106.90	135.56	171.07	211.20	258.28	310.57	369.31	433.04	502.00
574.64	650.30	727.20	803.95	878.53	949.14	1013.81	1070.95	1119.32	1158.35	1188.26	1210.17
1226.00	1238.39	1250.37	1265.00	1285.04	1312.59	1348.78	1393.64	1445.97	1503.41	1562.61	1619.63
1670.37	1711.04	1738.72	1751.57	1749.07	1731.89	1701.67	1660.66	1611.37	1556.22	1497.31	1436.29
1374.39	1312.50	1251.35	1191.65	1134.26	1080.26	1030.89	987.48	951.25	923.12	903.54	892.36
888.82	891.55	898.77	908.45	918.69	928.03	935.80	942.24	948.62	956.99	969.90	990.05
1019.81	1060.98	1114.38	1179.71	1255.37	1338.49	1425.05	1510.32	1589.32	1657.54	1711.48	1749.20
1770.52	1777.00	1771.62	1758.24	1741.03	1723.79	1709.45	1699.65	1694.59	1692.94	1692.01	1688.11
1677.03	1654.63	1617.47	1563.43	1492.04	1404.70	1304.56	1196.24	1085.28	977.54	878.57	793.05
724.41	674.70	644.64	633.77	640.64	662.84	697.13	739.48	785.42	830.37	870.15	901.36
921.58	929.53	924.90	908.28	880.90	844.42	800.70	751.65	699.06	644.57	589.45	534.84
481.44	429.92	380.60	333.90	289.91	249.03	211.25	176.99	146.09	118.96	95.21	75.16
58.16	44.48	33.22	24.63	17.71	12.77	8.83					

STANDARD DEVIATIONS OF SMOOTHING

0.1114E 01 0.5337E 00 0.3765E 00 0.2978E 00 0.2493E 00 0.2161E 00 0.1917E 00 0.1729E 00 0.1580E 00

0.1458E 00 0.1357E 00 0.1270E 00 0.1196E 00 0.1132E 00 0.1075E 00 0.1025E 00

STANDARD DEVIATION AFTER SMOOTHING = 0.53616E 02

NORMALISED DECONVOLUTE:

55.94	57.27	81.75	107.90	137.15	170.96	210.84	257.22	309.97	368.58	432.50	501.16
573.75	649.19	726.05	802.65	877.13	947.55	1012.05	1068.99	1117.19	1156.09	1185.93	1207.83
1225.72	1236.20	1248.26	1262.96	1283.04	1310.60	1346.78	1391.59	1443.61	1501.05	1560.00	1616.73
1667.19	1707.67	1735.26	1748.15	1745.80	1728.83	1698.82	1656.01	1608.87	1553.61	1494.95	1433.95
1372.05	1310.16	1249.03	1189.39	1132.11	1078.26	1029.06	985.81	949.73	921.70	902.19	891.06
887.51	890.18	897.27	906.77	916.84	926.06	933.79	940.29	946.79	955.29	968.29	988.47
1016.24	1059.40	1112.79	1178.08	1253.64	1336.55	1422.79	1507.66	1586.26	1654.15	1707.89	1745.57
1766.99	1775.68	1768.54	1755.39	1738.36	1721.23	1706.95	1697.18	1692.10	1690.38	1689.32	1685.25
1673.97	1651.40	1614.16	1560.14	1488.90	1401.83	1302.05	1194.16	1083.62	976.25	877.52	792.08
723.39	673.59	643.49	632.69	639.67	661.94	696.16	738.30	785.96	828.66	868.29	899.46
919.74	927.78	923.26	906.75	879.46	843.06	799.42	750.45	697.96	643.53	588.51	533.94
480.62	429.14	379.91	333.27	289.45	248.60	210.84	176.42	145.68	118.96	96.05	76.17
57.99	41.33	28.02	21.79	23.80	34.97	42.53					

INTEGRAL = 0.1489E 06 MAXIMUM = 0.1774E 04 AT = 86 MINIMUM = 0.2179E 02 AT = 148

THE EXPERIMENTAL (1) AND GENUINE (2) SPECTRUM

IMPROVEMENT OF RESOLUTION

INPUT PARAMETERS

151	21	10	2	0	20	4	11	1	5	0

1.000	2.500	1.050	1.050

INPUT DATA

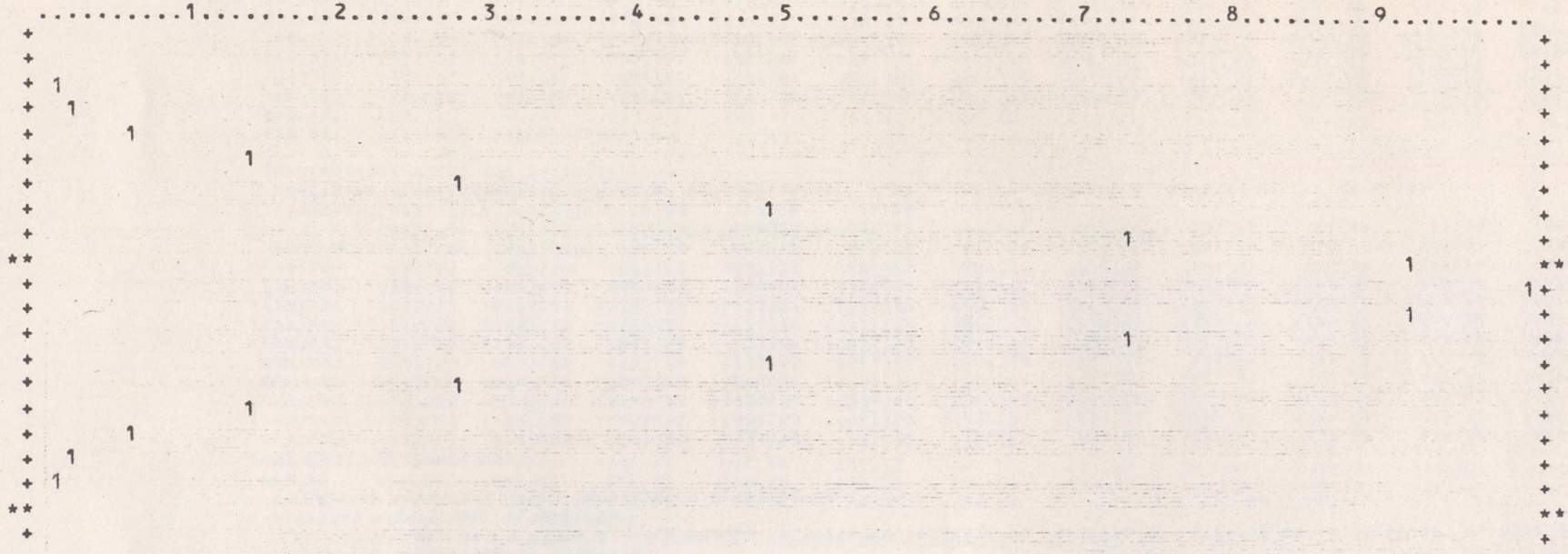
35.94	57.27	81.75	107.90	137.15	170.96	210.84	257.22	309.97	368.58	432.50	501.16
573.75	649.19	726.05	802.65	877.13	947.55	1012.05	1068.99	1117.19	1156.09	1185.93	1207.83
1223.72	1236.20	1248.26	1262.96	1283.04	1310.60	1346.78	1391.59	1443.81	1501.05	1560.00	1616.73
1667.19	1707.67	1735.26	1748.15	1745.80	1728.83	1698.82	1658.01	1608.87	1553.81	1494.95	1433.95
1372.05	1310.16	1249.03	1189.39	1132.11	1078.26	1029.06	985.81	949.73	921.70	902.19	891.06
887.51	890.18	897.27	906.77	916.84	926.06	933.79	940.29	945.79	955.29	968.29	988.47
1018.24	1059.40	1112.79	1178.08	1253.64	1336.55	1422.79	1507.66	1586.26	1654.15	1707.89	1745.57
1766.99	1773.68	1768.54	1755.39	1738.36	1721.23	1706.95	1697.18	1692.10	1690.38	1689.32	1685.25
1673.97	1651.40	1614.16	1560.14	1488.90	1401.83	1302.05	1194.16	1083.62	976.25	877.52	792.08
723.39	673.59	643.49	632.69	639.67	661.94	696.16	738.30	783.96	828.66	868.29	899.46
919.74	927.78	923.26	906.75	879.46	843.06	799.42	750.45	697.96	643.53	588.51	533.94
480.62	429.14	379.91	333.27	289.45	248.60	210.84	176.42	145.68	118.96	96.05	76.17
57.99	41.53	28.02	21.79	23.80	34.97	42.53					

INTEGRAL = 0.1487E 06 MAXIMUM = 0.1774E 04 AT = 86 MINIMUM = 0.2179E 02 AT = 148

NORMALISED GAUSSIAN DECONVOLUTING FUNCTION

0.53536E-04	0.24478E-03	0.95370E-03	0.31664E-02	0.89584E-02	0.21598E-01	0.44371E-01	0.77679E-01
0.11588E 00	0.14732E 00	0.15959E 00	0.14732E 00	0.11588E 00	0.77679E-01	0.44371E-01	0.21598E-01
0.89584E-02	0.31664E-02	0.95370E-03	0.24478E-03	0.53536E-04			

INTEGRAL = 0.1000E 01 MAXIMUM = 0.1596E 00 AT = 11 MINIMUM = 0.5354E-04 AT = 21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CALCULATION OF THE 1. DECONVOLUTE

CONVOLUTE:

52.20	70.53	93.18	120.08	151.53	187.72	228.96	275.51	327.42	384.51	446.35	512.28
581.39	652.58	724.54	795.82	864.89	930.23	990.45	1044.44	1091.49	1131.38	1164.47	1191.72
1214.62	1235.06	1255.15	1276.99	1302.41	1332.75	1368.66	1409.97	1455.68	1504.01	1552.56	1598.57
1639.21	1671.86	1694.39	1705.37	1704.16	1690.89	1666.40	1632.02	1589.42	1540.39	1486.67	1429.86
1371.35	1312.38	1254.04	1197.34	1143.28	1092.87	1047.10	1006.88	972.97	945.67	925.77	912.44
905.28	903.33	905.46	910.44	917.22	925.06	933.68	943.39	955.03	969.91	989.61	1015.77
1049.80	1092.64	1144.55	1204.92	1272.26	1344.27	1417.97	1490.01	1557.04	1616.04	1664.70	1701.66
1726.65	1740.48	1744.85	1742.05	1734.64	1724.99	1714.97	1705.64	1697.09	1688.45	1677.96	1663.26
1641.72	1610.82	1568.57	1513.84	1446.60	1368.05	1280.51	1187.31	1092.59	1000.01	914.28	838.86
776.67	729.65	698.74	683.79	685.69	696.44	719.53	749.16	782.45	815.74	845.79	869.86
885.84	892.35	888.77	875.14	852.12	820.78	782.46	738.67	690.88	640.52	588.84	536.91
485.61	435.65	387.57	341.79	298.65	258.41	221.27	187.37	156.79	129.52	105.56	84.83
67.55	53.74	43.62	36.93	32.66	30.45	27.74					

INFORMATIONS ABOUT THE DECONVOLUTION

NUMBER OF DECONV ITERATIONS= 7 NR: 1

STANDARD DEVIATIONS OF DECONVOLUTION

0.2313E 02 0.5667E 01 0.2427E 01 0.1933E 01 0.1646E 01 0.1332E 01 0.1214E 01

DECONVOLUTE BEFORE SMOOTHING

10.82	41.05	76.13	105.32	125.37	150.87	186.87	234.02	289.82	351.22	417.24	487.84
563.37	645.07	725.47	808.46	889.82	967.15	1038.00	1099.93	1150.88	1189.55	1215.75	1230.68
1236.88	1237.99	1238.34	1242.40	1254.22	1276.98	1312.62	1361.52	1422.56	1492.05	1565.98	1638.40
1703.21	1754.18	1788.83	1805.02	1797.16	1772.98	1733.65	1683.00	1624.90	1562.66	1496.75	1434.66
1371.05	1308.04	1245.52	1183.61	1122.86	1064.46	1010.13	961.91	921.84	891.57	872.12	863.62
865.20	875.00	890.28	907.74	924.04	936.45	943.49	945.32	946.81	942.20	944.53	954.96
977.26	1014.34	1067.93	1138.29	1223.94	1321.47	1425.61	1529.58	1625.89	1707.46	1766.78	1806.83
1821.65	1816.02	1795.14	1765.35	1733.25	1704.65	1683.91	1673.42	1675.47	1682.13	1695.50	1708.05
1713.31	1704.72	1678.62	1625.17	1549.13	1450.14	1332.73	1205.70	1071.26	943.82	828.86	732.10
657.12	605.55	577.48	571.95	587.24	620.76	668.91	726.88	788.88	848.69	900.56	939.96
964.12	972.17	964.34	942.50	908.72	865.45	815.13	760.08	702.59	643.79	585.64	528.86
474.02	421.31	371.59	324.69	280.63	239.21	199.57	162.68	130.24	106.93	90.44	77.00
54.28	22.28	-.64	0.97	2.59	19.15	110.63					

STANDARD DEVIATIONS OF SMOOTHING

0.4879E 01 0.1318E 01 0.7198E 00 0.5024E 00 0.3853E 00 0.3097E 00 0.2563E 00 0.2164E 00 0.1855E 00

0.1611E 00 0.1670E 00

STANDARD DEVIATION AFTER SMOOTHING = 0.29299E 02

NORMALISED DECONVOLUTE:

26.35	45.61	70.25	97.25	125.18	155.24	190.75	234.68	287.93	349.22	416.50	488.31
564.04	643.72	725.26	808.14	889.63	967.09	1037.90	1099.66	1150.41	1188.93	1215.10	1230.11
1236.43	1237.69	1238.14	1242.25	1254.10	1276.90	1312.60	1361.58	1422.46	1492.09	1565.83	1637.96
1702.45	1753.80	1787.79	1802.10	1796.47	1772.57	1733.46	1682.96	1624.91	1562.66	1496.67	1434.47
1370.74	1307.60	1245.00	1183.05	1122.35	1064.06	1009.86	961.75	921.75	891.53	872.13	863.68
865.31	875.09	890.24	907.46	923.49	935.72	942.74	944.72	946.45	942.05	944.48	954.90
977.14	1014.21	1067.89	1138.41	1224.20	1321.76	1425.72	1529.31	1625.18	1706.37	1767.50	1805.62
1820.67	1815.42	1794.86	1765.29	1733.27	1704.67	1683.89	1673.40	1675.47	1682.13	1695.43	1707.82
1712.65	1704.30	1675.67	1624.09	1548.04	1449.21	1332.11	1203.50	1071.48	944.32	829.38	732.38
657.04	605.35	576.98	571.62	587.23	621.05	669.27	727.04	788.95	848.09	899.76	939.21
965.60	971.60	964.24	942.46	908.66	865.34	815.00	759.98	702.34	643.76	585.51	528.60
475.76	421.72	372.05	325.10	280.25	237.47	197.76	162.99	134.55	111.69	91.13	69.19
45.20	23.10	10.28	9.54	17.90	26.29	28.24					

INTEGRAL = 0.1487E 06 MAXIMUM = 0.1821E 04 AT = 85 MINIMUM = 0.9538E 01 AT = 148

CALCULATION OF THE 2. DECONVOLUTE

CONVOLUTE:

43.73	60.62	81.90	107.32	137.25	171.91	211.93	257.84	309.95	368.22	432.17	501.04
573.65	649.74	726.19	802.74	877.19	947.58	1012.04	1068.93	1117.96	1155.90	1183.73	1207.64
1225.56	1238.13	1248.27	1263.04	1283.19	1310.81	1347.04	1391.67	1444.07	1501.24	1560.07	1616.64
1668.96	1707.14	1734.90	1747.85	1745.61	1728.77	1698.90	1656.19	1604.10	1544.04	1485.13	1434.05

887.69	890.31	897.30	906.68	916.65	925.78	933.50	940.06	946.65	953.24	960.32	968.56
1016.38	1059.59	1113.04	1178.39	1253.97	1336.83	1422.95	1507.63	1586.03	1653.75	1707.41	1745.11
1766.65	1773.50	1768.53	1755.54	1738.61	1721.54	1707.28	1697.50	1692.40	1690.62	1689.48	1685.29
1673.87	1651.15	1613.80	1559.72	1488.48	1401.49	1301.86	1194.16	1083.41	976.57	877.87	792.36
725.54	673.61	643.46	632.69	639.75	662.10	696.32	738.38	783.90	828.46	866.02	894.19
919.55	927.09	923.26	906.80	879.53	843.13	799.48	750.50	698.00	643.57	588.54	533.98
480.67	429.18	379.90	333.13	289.17	248.34	210.90	177.03	146.65	119.53	95.58	74.14
56.09	41.78	31.45	25.13	21.55	20.05	18.46					

INFORMATIONS ABOUT THE DECONVOLUTION
NUMBER OF DECONV ITERATIONS= 6 NR: 1
STANDARD DEVIATIONS OF DECONVOLUTION
0.2947E 02 0.6154E 01 0.3536E 01 0.2528E 01 0.2200E 01 0.2046E 01
DECONVOLUTE BEFORE SMOOTHING

4.74	23.09	60.75	102.66	125.75	139.78	159.95	198.63	257.09	328.97	404.23	478.17
552.80	632.40	718.65	809.54	900.92	988.59	1069.00	1138.97	1195.58	1239.54	1258.15	1264.11
1256.82	1241.63	1225.01	1213.46	1212.82	1227.68	1261.11	1314.29	1386.36	1473.18	1569.00	1665.12
1751.84	1819.98	1862.63	1876.53	1862.42	1824.49	1769.05	1702.99	1632.47	1562.03	1494.27	1429.54
1368.28	1307.69	1246.45	1183.44	1118.75	1053.85	991.43	934.67	887.51	852.59	831.28	825.97
834.52	855.14	883.84	915.14	942.94	961.85	968.65	963.35	949.21	931.83	917.81	913.46
924.04	953.60	1004.93	1079.41	1176.52	1293.12	1422.79	1555.67	1688.42	1784.50	1857.75	1895.55
1898.19	1871.43	1824.65	1768.72	1713.97	1668.82	1639.07	1627.72	1635.82	1658.43	1692.75	1730.31
1761.54	1776.11	1764.38	1719.11	1637.12	1520.24	1375.54	1214.30	1050.01	895.75	761.80	654.37
575.70	525.19	501.02	501.40	524.96	570.25	634.59	712.94	794.56	878.92	947.74	997.11
1023.75	1027.99	1012.57	981.28	937.88	885.72	827.65	766.22	705.51	648.79	579.57	520.12
463.90	412.39	365.92	322.21	276.77	226.88	176.74	136.57	114.15	109.22	108.60	78.26
24.72	1.75	0.03	0.04	4.14	38.05	58.29					

STANDARD DEVIATIONS OF SMOOTHING
0.2450E 01 0.9282E 00 0.5967E 00 0.4803E 00 0.4188E 00 0.3755E 00 0.3407E 00 0.3110E 00 0.2851E 00
0.2622E 00 0.2419E 00 0.2239E 00 0.2077E 00 0.1931E 00 0.1801E 00 0.1683E 00 0.1577E 00 0.1481E 00
0.1394E 00 0.1315E 00
STANDARD DEVIATION AFTER SMOOTHING = 0.38795E 02

NORMALISED DECONVOLUTE:

21.01	58.47	61.16	86.44	112.27	138.99	169.92	209.58	261.01	324.12	396.08	473.31
555.46	636.01	721.47	809.84	899.50	987.09	1068.27	1138.64	1194.62	1233.95	1256.05	1262.14
1255.50	1241.03	1224.77	1213.18	1212.30	1227.04	1260.68	1314.37	1386.28	1473.92	1569.22	1664.20
1759.55	1846.03	1858.99	1873.42	1860.40	1823.64	1769.06	1703.39	1632.85	1562.16	1494.07	1429.35
1367.28	1306.79	1244.76	1181.72	1117.27	1052.81	990.82	934.53	887.54	852.51	831.62	826.16
835.14	855.94	884.23	914.52	941.09	959.14	965.95	961.51	948.59	932.14	918.32	913.47
923.30	952.43	1004.00	1079.38	1177.61	1294.88	1424.24	1555.90	1678.40	1780.44	1855.00	1891.23
1895.31	1870.27	1824.80	1769.38	1714.40	1668.67	1638.45	1627.00	1635.56	1658.36	1692.95	1730.38
1760.99	1774.52	1761.59	1715.34	1632.99	1516.70	1373.54	1214.37	1051.92	898.51	764.10	655.17
574.67	522.42	498.40	499.73	525.00	571.93	636.95	714.56	792.32	876.69	944.41	994.05
1021.92	1027.56	1012.97	981.77	938.05	885.60	827.44	765.85	702.62	639.49	578.23	520.33
463.38	415.47	366.45	317.26	268.30	222.00	181.91	150.28	126.19	105.64	84.19	60.15
36.17	17.36	7.68	6.39	9.03	9.64	6.91					

INTEGRAL = 0.1487E 06 MAXIMUM = 0.1895E 04 AT = 85 MINIMUM = 0.6393E 01 AT = 148

CALCULATION OF THE 3. DECONVOLUTE
CONVOLUTE:

57.97	53.13	72.38	95.53	123.02	155.27	193.22	237.78	289.61	348.82	414.92	486.98
563.75	644.93	726.33	809.04	890.18	967.38	1038.06	1099.71	1150.31	1188.67	1214.76	1229.82
1236.32	1237.80	1238.47	1242.73	1254.70	1277.65	1313.54	1362.70	1425.66	1495.18	1566.56	1638.16
1706.10	1768.04	1786.92	1801.44	1796.27	1772.92	1734.30	1684.12	1626.17	1563.81	1499.58	1435.05
1370.97	1307.54	1244.74	1182.74	1122.10	1063.95	1009.93	962.01	922.17	892.11	872.86	864.54
866.20	875.64	890.66	907.42	923.01	934.96	941.99	944.23	943.36	942.31	944.91	955.35
977.55	1014.68	1068.59	1139.47	1225.59	1323.22	1426.87	1529.82	1624.88	1705.38	1766.18	1804.42
1819.99	1815.44	1795.53	1766.38	1734.53	1705.89	1685.01	1674.46	1674.51	1683.18	1696.41	1708.57
1713.19	1703.50	1674.93	1622.96	1546.82	1448.28	1331.83	1204.06	1072.79	946.01	830.94	733.36
657.24	604.74	576.39	571.35	587.57	621.95	670.37	727.86	788.85	847.62	898.89	938.35
963.09	971.80	964.68	943.12	909.32	865.85	815.31	760.12	702.38	643.82	585.79	529.16
474.16	421.89	371.59	323.76	278.83	237.34	199.78	166.31	136.70	110.45	87.09	66.46
48.78	34.46	23.70	16.30	11.59	8.68	6.82					

INFORMATIONS ABOUT THE DECONVOLUTION
NUMBER OF DECONV ITERATIONS= 6 NR: 1
STANDARD DEVIATIONS OF DECONVOLUTION
0.3926E 02 0.1192E 02 0.4764E 01 0.2656E 01 0.2080E 01 0.1906E 01
DECONVOLUTE BEFORE SMOOTHING

3.10	16.46	49.53	93.98	120.75	130.11	138.29	163.37	213.96	290.48	381.69	471.75
552.39	627.33	706.56	796.97	898.48	1004.48	1105.28	1191.98	1258.39	1301.06	1316.80	1312.84
1287.37	1249.62	1208.77	1174.34	1154.69	1156.42	1184.20	1240.73	1326.20	1437.17	1565.64	1698.87
1820.85	1915.50	1970.59	1980.87	1949.13	1884.74	1800.52	1709.28	1621.17	1542.34	1474.77	1416.88
1364.70	1313.21	1257.73	1195.31	1125.54	1050.71	975.24	904.66	844.37	799.88	774.36	770.35
788.18	825.50	876.53	932.05	980.69	1011.81	1018.92	1002.03	967.52	925.70	887.44	861.81
855.25	872.31	916.73	991.38	1100.01	1240.29	1406.40	1585.03	1756.60	1899.00	1993.39	2029.82
2009.92	1945.78	1855.61	1758.58	1670.80	1603.46	1562.83	1551.32	1568.42	1611.60	1673.98	1747.71
1819.56	1873.49	1892.30	1861.07	1771.36	1624.72	1433.76	1219.84	1007.56	818.27	665.30	552.89
475.20	435.06	417.58	422.79	451.32	505.61	586.72	691.07	808.51	923.41	1018.84	1082.12
1108.45	1100.92	1067.70	1018.27	960.52	899.27	836.10	770.43	701.51	630.74	562.61	502.90
454.80	415.48	375.69	324.69	260.36	194.68	144.84	119.20	115.47	119.93	105.08	55.85
12.21	0.79	0.03	0.10	4.43	37.56	4.60					

STANDARD DEVIATIONS OF SMOOTHING
0.2272E 01 0.6218E 00 0.4870E 00 0.4427E 00 0.4127E 00 0.3882E 00 0.3667E 00 0.3475E 00 0.3301E 00
0.3143E 00 0.2998E 00
STANDARD DEVIATION AFTER SMOOTHING = 0.54978E 02

NORMALISED DECONVOLUTE:

13.56	30.02	55.13	83.23	106.98	124.95	143.30	172.88	222.08	291.60	375.16	462.38
546.82	628.16	711.08	800.87	899.12	1002.05	1101.75	1189.11	1256.55	1299.49	1316.77	1310.40
1285.17	1248.16	1207.94	1173.53	1153.37	1154.57	1182.54	1239.56	1326.05	1437.70	1565.85	1697.58
1817.44	1910.33	1964.85	1975.97	1945.95	1883.27	1800.11	1709.11	1620.70	1541.41	1473.42	1415.19
1362.68	1310.34	1255.18	1192.87	1123.55	1049.32	974.33	903.89	843.65	798.72	773.28	769.83
788.53	826.45	877.15	931.21	977.85	1007.58	1014.81	999.51	967.07	926.59	888.32	861.53
853.46	869.51	913.99	990.35	1100.38	1242.26	1403.59	1585.47	1763.81	1892.99	1985.81	2023.05
2005.73	1944.46	1856.10	1759.30	1670.55	1601.84	1560.21	1548.42	1565.99	1609.72	1673.52	1747.84
1819.38	1871.89	1888.46	1855.04	1764.36	1618.81	1430.85	1220.53	1010.78	821.91	667.48	552.72
475.84	431.32	413.70	420.14	450.91	507.60	590.12	693.47	808.69	920.23	1013.50	1076.86
1105.07	1099.89	1068.37	1019.63	961.67	899.40	834.50	766.96	697.54	628.22	563.85	507.67
459.77	415.61	368.51	314.25	255.05	199.28	156.45	130.57	116.92	105.00	85.79	57.92
28.30	6.61	-1.46	1.58	8.30	10.48	7.35					

INTEGRAL = 0.1488E 06 MAXIMUM = 0.2023E 04 AT = 84 MINIMUM = -0.1461E 01 AT = 147

CALCULATION OF THE 4. DECONVOLUTE
CONVOLUTE:

51.86	46.03	63.92	84.84	109.20	137.63	171.90	215.65	264.95	325.49	394.58	470.50
551.47	636.10	723.41	812.44	901.56	988.12	1066.47	1138.56	1194.04	1234.17	1256.40	1262.61
1256.08	1241.73	1225.56	1213.98	1213.07	1227.89	1261.61	1315.94	1388.76	1476.03	1571.04	1665.32
1749.82	1816.24	1858.39	1873.15	1860.84	1824.92	1771.01	1705.68	1635.10	1564.08	1495.50	1430.27
1367.78	1306.50	1244.86	1181.85	1117.55	1053.24	991.35	935.10	887.93	853.01	832.57	827.44
836.65	857.40	885.26	914.84	940.70	958.36	965.31	961.46	949.28	933.34	919.55	914.28
923.57	952.44	1004.32	1080.52	1179.72	1297.60	1426.84	1557.62	1678.61	1779.67	1851.69	1890.22
1895.29	1871.47	1826.96	1771.90	1716.68	1670.35	1639.53	1627.82	1635.55	1659.85	1694.92	1732.54
1762.85	1775.58	1761.56	1714.36	1631.58	1515.67	1373.63	1215.96	1054.78	901.84	766.84	656.45
574.21	521.13	496.52	498.75	525.55	573.88	639.50	716.68	798.24	876.27	943.14	992.73
1021.36	1028.10	1014.49	983.74	939.82	886.59	827.47	765.21	702.09	639.88	579.83	522.52
467.62	415.17	364.07	314.62	267.67	224.58	186.56	154.00	126.27	102.11	80.35	60.57
43.17	29.85	18.76	12.25	8.69	6.89	5.93					

INFORMATIONS ABOUT THE DECONVOLUTION
NUMBER OF DECONV ITERATIONS= 6 NR: -1
STANDARD DEVIATIONS OF DECONVOLUTION
0.5566E 02 0.1953E 02 0.9351E 01 0.5217E 01 0.3164E 01 0.4717E 01
DECONVOLUTE BEFORE SMOOTHING

0.23	4.60	36.11	115.68	157.94	132.28	97.94	96.20	157.07	251.27	366.98	497.66
563.99	632.54	673.00	750.10	859.75	996.31	1143.11	1266.76	1337.96	1404.93	1411.82	1384.45
1359.76	1461.15	1587.93	1723.46	1876.01	1959.27	1973.34	1925.90	1821.68	1761.79	1539.61	1737.29
1926.11	2072.15	2150.10	2147.27	2073.11	1951.36	1811.04	1677.65	1566.12	1485.91	1426.72	1393.01

1303.78	1336.18	1293.33	1232.70	1133.47	1001.04	903.74	870.71	887.74	727.47	670.48	662.66
708.67	769.29	858.84	962.27	1055.81	1113.88	1120.26	1076.51	999.73	915.08	842.98	794.61
772.48	775.54	804.07	865.33	970.30	1129.29	1344.18	1609.73	1863.05	2089.42	2228.45	2257.89
2184.45	2040.65	1869.34	1707.89	1579.71	1493.90	1449.81	1442.68	1469.39	1528.18	1618.95	1738.09
1873.81	2002.78	2090.98	2100.89	2004.88	1799.61	1512.76	1195.29	901.39	669.30	510.88	418.76
375.31	359.61	353.53	351.45	363.60	406.80	494.95	632.97	809.93	995.43	1148.09	1234.50
1245.08	1195.43	1114.58	1029.96	957.74	899.89	846.47	782.57	709.08	606.33	522.11	466.68
445.08	442.11	422.10	350.41	237.45	137.85	85.76	78.20	109.75	158.24	142.78	45.86
2.38	0.00	-0.00	0.00	1.90	58.77	2.80					

STANDARD DEVIATIONS OF SMOOTHING

0.4829E 01 0.1518E 01 0.1191E 01 0.1081E 01 0.1014E 01 0.9616E 00 0.9181E 00

STANDARD DEVIATION AFTER SMOOTHING = 0.84898E 02

NORMALISED DECONVOLUTE:

1.50	22.20	60.47	102.52	126.22	123.38	107.19	107.41	150.56	241.36	360.74	477.18
567.77	631.42	687.02	759.41	863.17	994.61	1134.95	1260.48	1352.48	1402.05	1409.48	1381.24
1327.00	1257.96	1185.74	1121.56	1075.29	1055.28	1068.75	1122.05	1219.69	1362.23	1540.63	1735.98
1920.11	2062.24	2158.02	2187.37	2067.42	1949.27	1810.32	1675.95	1565.56	1480.48	1425.06	1389.33
1362.05	1331.65	1288.78	1228.27	1150.08	1058.88	962.38	869.32	787.85	725.04	687.25	680.28
708.33	771.23	861.26	961.82	1050.19	1104.36	1111.42	1071.75	1000.31	918.20	845.23	793.85
768.44	769.18	797.69	860.63	968.90	1131.93	1349.28	1603.83	1863.11	2076.94	2211.49	2243.37
2177.11	2040.20	1871.83	1709.21	1577.90	1489.12	1443.24	1435.87	1463.14	1523.65	1616.86	1738.47
1875.27	2002.19	2084.73	2087.78	1988.34	1786.52	1508.61	1199.77	909.11	674.17	511.64	416.98
371.65	353.55	346.67	346.85	362.34	408.81	500.37	639.91	813.13	990.28	1135.67	1221.22
1257.13	1194.43	1118.02	1034.51	960.82	899.20	840.21	771.96	690.21	605.41	528.52	479.40
455.04	437.38	400.42	331.12	238.73	152.22	106.84	93.34	111.80	125.04	111.22	71.55
26.04	-3.65	-8.67	2.96	16.51	19.05	11.96					

INTEGRAL = 0.1490E 06 MAXIMUM = 0.2243E 04 AT = 84 MINIMUM = -0.8670E 01 AT = 147

CALCULATION OF THE 5. DECONVOLUTE

CONVOLUTE:

28.78	44.12	62.46	81.31	100.66	121.46	147.71	183.93	235.77	297.73	375.12	455.40
540.56	626.93	715.40	807.38	905.11	1004.85	1101.59	1187.75	1255.73	1299.99	1318.39	1312.54
1287.37	1250.18	1209.63	1174.71	1154.01	1154.98	1185.21	1241.62	1329.58	1442.24	1570.27	1700.69
1818.58	1909.79	1963.74	1975.62	1947.29	1886.44	1804.50	1715.78	1624.31	1544.49	1475.43	1416.36
1363.32	1311.29	1255.73	1193.76	1124.84	1050.87	975.80	904.94	844.17	799.07	774.10	771.69
791.51	829.39	879.92	932.28	977.01	1005.66	1013.34	999.85	969.64	930.53	891.96	863.31
852.83	867.34	912.17	990.82	1104.05	1248.47	1415.34	1590.39	1755.89	1891.37	1982.72	2020.88
2006.38	1948.38	1862.21	1765.62	1675.22	1603.95	1569.10	1547.42	1565.76	1611.53	1677.70	1753.63
1825.17	1875.56	1889.38	1852.95	1760.77	1616.09	1431.22	1224.96	1018.40	830.31	673.74	554.71
473.16	425.57	407.75	416.91	452.06	512.82	597.28	700.05	811.60	919.25	1009.89	1073.08
1103.51	1101.79	1075.28	1025.65	966.32	900.77	832.39	763.21	695.05	629.93	569.58	514.45
463.14	413.00	361.62	308.60	256.21	208.45	168.92	138.88	116.58	98.47	81.20	63.46
46.06	31.15	20.37	14.10	11.26	10.10	9.49					

INFORMATIONS ABOUT THE DECONVOLUTION

NUMBER OF DECONV ITERATIONS= 7 NR: -1

STANDARD DEVIATIONS OF DECONVOLUTION

0.3664E 02 0.3833E 02 0.2443E 02 0.1945E 02 0.1703E 02 0.1558E 02 0.1464E 02

DECONVOLUTE BEFORE SMOOTHING

0.00	0.05	14.38	178.39	370.54	142.73	23.62	6.30	15.40	88.40	336.35	666.30
786.89	699.13	592.15	580.36	690.28	911.55	1187.26	1425.87	1562.70	1593.93	1551.99	1469.93
1368.26	1259.48	1154.74	1064.72	996.41	952.33	933.40	955.76	1032.55	1186.52	1430.18	1749.65
2091.94	2370.92	2503.66	2456.54	2263.27	2000.30	1744.25	1543.75	1415.74	1355.22	1345.85	1366.37
1393.67	1405.05	1382.01	1315.72	1210.69	1082.79	951.48	831.41	728.85	643.51	578.43	543.92
557.19	635.66	788.47	1000.92	1217.83	1354.61	1349.30	1212.32	1017.11	843.28	734.25	694.20
700.45	715.97	714.66	709.74	746.22	872.58	1126.68	1519.93	2004.74	2457.61	2725.42	2719.87
2475.74	2117.32	1773.94	1522.20	1380.72	1330.58	1334.85	1356.24	1376.12	1404.66	1472.72	1611.24
1855.90	2128.37	2418.67	2586.73	2510.28	2149.52	1598.49	1036.06	605.86	358.96	251.25	242.10
306.13	395.91	415.15	336.44	249.61	222.31	277.11	440.52	735.51	1120.01	1457.24	1602.42
1519.59	1299.05	1069.30	914.32	856.30	881.55	923.76	893.30	741.16	535.15	381.44	336.20
404.97	562.11	650.50	457.35	150.02	24.10	4.61	8.98	24.26	315.72	287.06	30.08
0.08	0.30	0.00	0.00	5.76	129.21	1.26					

STANDARD DEVIATIONS OF SMOOTHING

0.2125E 02 0.8214E 01 0.4117E 01 0.3536E 01 0.3334E 01 0.3154E 01 0.3011E 01

STANDARD DEVIATION AFTER SMOOTHING = 0.1540E 03

STANDARD DEVIATION AFTER SMOOTHING = 0.1380E 03

NORMALISED DECONVOLUTE:

-11.84	25.33	100.28	180.73	211.30	165.88	69.68	-5.15	15.42	157.78	377.36	582.71
692.97	691.08	634.67	617.01	706.23	905.74	1159.14	1368.72	1536.87	1585.80	1551.73	1465.97
1357.96	1247.61	1145.99	1058.86	989.61	941.52	920.96	941.20	1022.81	1186.39	1437.68	1753.71
2077.25	2333.33	2457.06	2421.67	2249.68	2000.87	1745.39	1537.62	1405.28	1341.31	1353.88	1356.27
1383.11	1392.03	1367.00	1301.70	1200.85	1077.91	949.34	828.48	722.57	633.70	566.73	533.15
552.38	642.46	804.29	1008.91	1199.64	1313.42	1311.37	1199.87	1027.49	859.02	745.00	692.29
686.90	694.27	694.12	695.29	737.20	874.05	1145.50	1545.24	2005.81	2412.91	2652.53	2661.61
2458.39	2130.48	1790.17	1525.14	1370.87	1313.65	1313.99	1333.79	1355.25	1387.62	1461.51	1611.45
1849.63	2145.06	2406.58	2531.06	2432.61	2099.69	1605.51	1076.06	655.96	351.93	237.54	247.28
313.73	371.65	379.97	331.50	258.30	219.26	226.73	466.13	778.94	1117.96	1402.22	1534.65
1467.41	1308.26	1093.36	934.46	872.10	860.66	891.38	839.23	706.85	538.64	416.98	386.52
449.29	526.08	527.63	415.21	229.75	62.99	-6.76	35.72	129.45	200.59	197.73	128.22
40.98	-14.53	-19.36	8.42	37.40	41.61	25.52					

INTEGRAL = 0.1493E 06 MAXIMUM = 0.2662E 04 AT = 84 MINIMUM = -0.1936E 02 AT = 147

(THE TIME IS NOW 13/24/15)
* * * * AXIS USED ON 10/07/73 AT 24/00/33
IMPROVEMENT OF RESOLUTION
THE NUMBER 1 IN THE PLOT IS THE GENUINE SPECTRUM, THE OTHERS DENOTE THE SEQUENTIAL DECONVOLUTES
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