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Computer Programs for Infrared Spectrophotometry

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Programmes d'ordinateurs pour la spectrophotométrie infrarouge

X-XV

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COMPUTER PROGRAMS FOR INFRARED SPECTROPHOTOMETRY*

VOLUME II

J. Pitha+ and R.N. Jones

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INTRODUCTION TO THE SECOND EDITION

The six programs in this volume were first published in 1968. Their republication here is part of our project to augment and update our total collection of computer programs for infrared spectrophotometry as described in the introduction to the Second Edition of Bulletin 11 which forms Volume I of this series of seven volumes issued as N.R.C.C. Bulletins 11-17.

These programs have been applied by a variety of users to the fitting of band envelopes based on Cauchy and Gauss functions and their sum or product combinations. Though most of the applications have been in the spectroscopic field they have also found application in other areas of science. The versions presented here do not differ significantly from those published previously. In our N.R.C.C. Bulletin 13 we supply three additional variants of the basic program. Two of these versions deal with the system in which all five parameters are free to adjust independently (the "unrestricted Cauchy-Gauss sum function"); another version in Bulletin 13 is arranged for the simplified algorithm for a set of pure Cauchy curves with only three adjustable parameters. This may have advantages where the computer storage facilities and the run time are critical. For most users the basic version given in Program X in this volume is recommended. The subsequent paragraphs of this introduction are reproduced unchanged from the First Edition.

This Bulletin supplements earlier publications from this laboratory dealing with methods of fitting analytical functions to infrared absorption bands of condensed phase systems (1-3). Seven methods of optimization with non-linear least squares approximations were examined, and two have been found to be significantly more effective than the other five (2). These preferred methods were developed by Meiron (4), and by Marquardt (5) for other purposes; they are basically similar and both are modifications of an earlier method of Levenberg (6) which Papoušek and Plivá have also used for fitting infrared band envelopes (7). The programs described in this Bulletin use Method V of our earlier publication; they combine features of both the Meiron and the Marquardt algorithms and use an automated search routine to determine the optimal value of the damping constant.

Three versions of Method V will be presented. All utilize the Cauchy-Gauss product function, while two also permit the alternative use of the Cauchy-Gauss sum function; a floating horizontal baseline is employed. Pure Cauchy or pure Gauss functions can also be fitted by all three programs, but, from the computational point of view, this is not an efficient way of operating with these simpler functions. The development of these programs was initiated on a small S.D.S. Model 920 computer and

several memory conserving procedures were introduced. These have been retained, though the larger storage capacity of the I.B.M. 360(67) computer we are now using diminishes their importance, and their replacement could increase the speed of computation on large computers. In other respects also these programs reflect their piecemeal evolution, and no claim is made for high computational efficiency. The input and output formats interface with the set of modular programs that have been developed in our laboratory to perform the common numerical transformations of absorption spectrophotometry (8).

A. The Basic Version (Program X)

As written, this program will handle a maximum of twenty component bands simultaneously optimizing up to 81 band indices.* It can be expanded by changing the dimensional statement, but the execution time increases rapidly with the number of bands, as also does the demand on the storage capacity.

B. The Moving Subspace Version (Program XI)

This is Method VIII of reference (2). The initial guessed indices are introduced at the beginning of the computation, but the indices of only a limited number of consecutive bands are adjusted at one time. In principle this "moving subspace" program can cope with envelopes containing a very large number of constituent bands. As written the moving subspace can deal with from two to five consecutive bands and twenty bands in all. The total number of bands can be increased by altering the dimension statement with no change in the body of the program. This program operates on the Cauchy-Gauss product function only; a version operating on the unrestrained Cauchy-Gauss sum function is provided by Program XVIII in Bulletin 13.

C. Version with Correction for Spectral Slit Distortion (Program XII)

This version resembles Program X in that it operates on all indices simultaneously and will handle both the product and sum

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*We use the term "band indices" to designate the values of the variables defining the composite band envelope. All three programs described in this Bulletin require 4M+1 indices to define an envelope derived from M overlapping bands.

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functions. The slit function ordinates are introduced (or computed) and the curve generated from the calculated indices is convoluted with the spectral slit function before optimization with the experimental data. In this way a band envelope is generated that conforms with the contour of the "true" spectrum adjusted for the finite spectral slit distortion (9,10).

D. Other Programs

(i) Program XIII. This program evaluates the areas, half-band widths and the Cauchy-Gauss proportionality of the calculated component bands from the band indices.

(ii) Program XIV. This program calculates and lists the individual computed abscissal values of the calculated band envelope from the band indices. It also provides a set of punched cards (or a card image output data set) in the standard 8(I5, I4,1X) format.

(iii) Program XV. When provided with the card decks from the experimental spectrum and the computed spectrum from Program XIV this program first passes a five point quadratic convoluting smoothing function through each and evaluates the following quantities as described in reference (2).

(a) The total error spectrum.

(b) The high frequency component of the error spectrum which is attributed to the misfit arising from the noise component of the experimental curve.

(c) The low frequency component of the error spectrum which is attributed to the mathematical misfit of the computed curve, corrected for noise.

This program also serves as a general purpose program for subtracting one spectrum from another. It will operate on both transmission and absorbance ordinate data and yields a punched card output in our standard formats (8) as well as the printed listing.

For all three band fitting programs the experimental data points are read from Hollerith cards each of which carries eight data points in 8(I5,I4,1X) format. The abscissal units are wavenumber in $cm.^{-1} \times 10$, recorded at constant wavenumber intervals in diminishing sequence. The ordinate units are transmittance×1000; these conditions were dictated by the standardized digital encoding conditions used in our laboratory (11,12). The input and output indices for peak height (x_1) and band center (x_2) are in units of absorbance and $cm.^{-1}$ respectively. A subroutine SORT

checks the sequence of the experimental data cards and will make a limited number of corrections for misplaced cards; all such corrections are noted in the print-out.

The programs are written in FORTRAN IV.* They are listed and described in the main section of this Bulletin with interpretive detail and comment. A set of numerical test data based on a simulated four band spectrum is included. A more critical appraisal with some discussion of the physical significance of the band fits obtained is given on pp. 64-65 of reference (13).

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* IBM System/360 Basic Programming Support FORTRAN IV. (Version 8.1).

ALGEBRAIC STATEMENT OF THE PROBLEM OF SPECTRAL BAND FIT OPTIMIZATION

A. The Cauchy-Gauss Product Function

The experimental band envelope is approximated by the function

$$(T/T_o)_{\nu calc} = \exp - 2.30258 \left\{ \alpha + \sum_{P=1}^{M} x_{1(P)} \left(1+x_{3(P)}^2 \left(\nu - x_{2(P)}\right)^2\right)^{-1} \cdot \exp\left[- x_{4(P)}^2 \left(\nu - x_{2(P)}\right)^2\right] \right\} \quad [1]$$

where $(T/T_o)_{\nu calc}$ is the computed ordinate at the wavenumber ν in transmittance units; α, x_1, x_2, x_3, x_4, are the adjustable indices and M is the number of constituent bands; x_1 is the peak height in absorbance units, x_2 is the wavenumber position of the band center in $cm.^{-1}$; x_3 and x_4 jointly define the half-band width and the Cauchy-Gauss ratio; α is the baseline displacement in absorbance units.

The values of $(x_1 \ldots x_4)_P$ and α are varied to minimize ϕ where

$$\phi = \sum f_i^2 \quad [2]$$

with

$$f_i = (T/T_o)_{\nu obs} - (T/T_o)_{\nu calc} \quad [3]$$

The iteration step is expressed most succinctly in the form developed by Meiron (5)

$$\underline{x}_{m+1} = \underline{x}_m - (\underline{B}_m + p\underline{C}_m)^{-1} \cdot \underline{G}_m \quad [4]$$

where $\underline{x}_m$ is the vector of indices after m iterations and $\underline{B}$ is a matrix equal to $\underline{A}^T\underline{A}$ where $\underline{A}$ is a matrix of the partial derivatives $\partial f_i/\partial x_j$. The diagonal matrix $\underline{C}$ is formed from $\underline{B}$ by setting the off-diagonal terms to zero; p is a scalar damping factor, the value of which is adjusted to minimize ϕ during each iteration cycle; $\underline{G}$ is the gradient vector (grad ϕ).

Equation [4] can be rewritten

$$\underline{x}_{m+1}\underline{C}_m^{\frac{1}{2}} = \underline{x}_m\underline{C}_m^{\frac{1}{2}} - (\underline{C}_m^{-\frac{1}{2}}\underline{B}_m\underline{C}_m^{-\frac{1}{2}}+p\underline{I})^{-1}\underline{G}_m\underline{C}_m^{-\frac{1}{2}} \qquad [5]$$

This is the form of the algorithm developed by Marquardt (5). Our programs compute on this basis, since, from the numerical point of view, it has the advantage that all the diagonal terms are equal to unity. In consequence, no round off difficulties are to be expected, even when the simple Gauss-Jordan procedure is used to solve the system of linear equations (14).

The symbolism used in the above equations conforms with that of our previous publications. Within the computer program it is convenient to handle all the indices in a single array corresponding to the vector $\underline{x}$ and to convert the ordinate scale from decadic to Napierian absorbance. It will simplify the subsequent discussion if we rewrite equation [5] in the form

$$TC_{(W)} = EXP - \left\{X_{(N)} + \sum_{I=1}^{I=M} X_{(I)}\,(1+X^2_{(I+2M)}\,(W-X_{(I+M)})^2)^{-1}\right.$$

$$\left. \cdot\ EXP\left[-\,(X^2_{(I+3M)}\,(W-X_{(I+M)})^2\right]\right\} \qquad [6]$$

where the symbolism conforms more closely with that used in the FORTRAN program.

Equation [2] similarly transposes to

$$FS = \sum_{1}^{NP} F^2 \qquad [7]$$

$$= \sum_{1}^{NP} (Y_{(W)} - TC_{(W)})^2 \qquad [8]$$

B. The Cauchy-Gauss Sum Function

In the symbolism of reference (2) this equation is written

$$(T/T_o)_{\nu calc} = \exp - 2.30258\left\{\alpha + \sum_{P=1}^{M}\left[x_{1(P)}\,(1+x^2_{3(P)}\,(\nu-x^2_{2(P)})^2)^{-1}\right.\right.$$

$$\left.\left. + x_{5(P)} \cdot \exp - (x^2_{4(P)}\,(\nu-x_{2(P)})^2)\right]\right\} \qquad [9]$$

Whereas the product function requires the adjustment of 4M+1 indices, the sum function, as written above, has 5M+1 adjustable parameters, where M is the number of constituent bands. It is used in these programs with the restraint that $x_4 = kx_3$, where k is a constant that is selected by an input card. In this form the sum function has proved superior to the product function in some instances (e.g. for fitting single bands generated by convoluting a Cauchy band with a triangular slit function (3)). Subsequent experience has shown that the sum function will often yield solutions in which x_1 or x_5 assumes negative values, and such solutions can have doubtful physical significance, though they may be acceptable analytically. Provision is included in these programs to restrict x_1 and x_5 to positive values if desired. Values of k in the range 0.4-0.8 are usually satisfactory. An alternative version of the program in which the restraint on x_4/x_3 has been removed is given by Program XVI in Bulletin 13.

In the quasi-FORTRAN symbolism* equation [9] becomes

$$TC_{(W)} = EXP - \left\{ X_{(N)} + \sum_{I=1}^{I=M} \left[X_{(I)} \left(1+X^2_{(I+2M)} \left(W-X_{(I+M)}\right)^2\right)^{-1} + X_{(I+3M)} EXP \left(- X^2_{(I+2M)} CAY^2 \left(W-X_{(I+M)}\right)^2\right)\right]\right\} \qquad [10]$$

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*We apologize for introducing this bastardized mathematical symbolism at several places in this Bulletin, but it is convenient for promoting cross-communication between the FORTRAN programs and the basic mathematical logic. We further admit to inconsistency in the symbolism for the band indices. We have chosen to use the following sets of symbols interchangeably for the band indices, whichever the context would indicate as being the more convenient: (x_1,x_2,x_3,x_4,x_5,α); (X(1),X(2),X(3),X(4), X(5),ALPHA); (X(I),X(J),X(K),X(L),X(L),X(N)): ($X_{(I)}$, $X_{(I+M)}$, $X_{(I+2M)}$, $X_{(I+3M)}$, $X_{(I+3M)}$, $X_{(N)}$) where $CAY = x_4/x_3$, and $X_{(N)}$, $X_{(I)}$ and $X_{(I+3M)}$ have been transposed from decadic absorption to Napierian absorption.

PROGRAM X

PROGRAM X

The Basic Band Fit Optimization Program

(PC-116)

The Input Data

Cards 1 and 2 are heading cards and can carry any desired alphameric indexing, or identification statements (HEAD1,HEAD2). These cards must be included though they may be blank.

Card 3 carries ten fixed point instructions, NDATA, IDECK, NP, M, KURVE, NSEC, NI, MLIST, LIMIT, NONEG, in format 10I5.

NDATA — Use NDATA = 1 to process a single data set or the terminal data set of a series.

Use NDATA = 2 for an initial or intermediate set of a series. After completing the computation, the program will proceed automatically to execute the next computation of the series.

IDECK — Use IDECK = 1 to list the output on the printer only.

Use IDECK = 2 to punch an additional output card deck carrying the optimized indices (one band per card) in the format for input to Programs XIII and XIV. The terminal card of the deck carries the baseline constant ALPHA.

NP — is the number of experimental data points (maximum 2000).

M — is the number of component bands (maximum 20).

KURVE — Use KURVE = 1 for the product function, and for pure Cauchy and pure Gauss functions.

Use KURVE = 2 for the sum function.

NSEC — is the maximum permitted computation time in seconds. This is the time within the iterative cycling routine. If exceeded the program will print the last set of indices obtained and either terminate or proceed to the next data set according to the value of IDECK.

NI — is the maximum permitted number of iteration cycles, a recommended value is 10.

MLIST — Use MLIST = 1 to print the input and output data and a minimal report on the progress of the optimization convergence, as is shown in the numerical examples on pp. 99 and 103.
This will normally suffice unless difficulties are encountered.

Use MLIST = 2 to print additional information about the extreme values of the $\underline{B}$ and $\underline{C}^{-\frac{1}{2}}\underline{B}\underline{C}^{-\frac{1}{2}}$ matrix elements (see p. 6).

Use MLIST = 3 to record the restraints applied by LIMIT and NONEG (see below).

Use MLIST = 4 for a combination of MLIST = 2 and MLIST = 3.

LIMIT — Use LIMIT = 1 to restrict the half-widths of the component bands within the range 1 $cm.^{-1}$ to 50 $cm.^{-1}$.
If LIMIT = 2 no restriction is applied.

NONEG — Use NONEG = 1 with the sum function to restrict both the Cauchy and Gauss bands to zero or positive values.
If NONEG = 2 no restriction is applied.
Always use NONEG = 2 with the product function.

Card 4 carries two floating point instructions for the product function and three for the sum function in formats 2F15.5 or 3F15.5 respectively.

WB — is the highest (starting) wavenumber of the experimental data deck in $cm.^{-1}$.

WI — is the constant wavenumber interval in $cm.^{-1}$. By convention this interval is taken as positive for a diminishing wavenumber sequence.

CAY — is the ratio x_4/x_3 and is required only for the sum function. Suggested trial values are 0.5 or 0.8.

Card 5 carries the instructions DOWN, UP and CHANGE in format 3F15.5 for varying the damping factor (see p. 18).
Recommended values are 0.01 1000.0 0.5

Card Deck 6 is the main data deck carrying the NP experimental data points. These must be sequenced in diminishing order of wavenumber. Subroutine SORT will check this sequence and make a limited number of corrections. It is discussed more fully in Bulletin 11. It is important to make sure that the starting wavenumber of the deck corresponds with WB.
These cards must be punched in format 8(I5, I4,1X) with the wavenumber in units of $cm.^{-1} \times 10$ followed by the intensity in transmittance×1000 (i.e. a transmittance of 0.500 at 1000.0 $cm.^{-1}$ followed by a transmittance of 0.499 at 999.5 $cm.^{-1}$ is encoded as 10000 500 9995 499).

Card Deck 7 — This is a deck of M cards, each of which carries four input indices for one band in format 4F15.5. For the product function these are x_1, x_2, x_3 and x_4 which appear in the FORTRAN symbolism as X(I), X(J), X(K) and X(L). The units of x_1 are absorbance and of x_2 $cm.^{-1}$. For the sum functions x_1, x_2, x_3 and x_5 are listed and they also appear in the FORTRAN symbolism as X(I), X(J), X(K) and X(L). It is important to observe that X(L) has a different connotation for the sum function than for the product function. The units of both x_1 and x_5 are absorbance.

Card 8 — This is the terminating card and carries the input value of the baseline constant α in F15.5 format. It is X(N) in the FORTRAN notation. The units of α are absorbance. The program requires that this card be included, even if $\alpha = 0.0$.

Note that this program calls the library subroutines SETCLK and RDCLK which are discussed in Bulletin 11. If these are not available appropriate alterations have to be made in the program.

B. Description of the Basic Program

The Initial Section, ending at statement 31, accepts the input data, checks the sequence of the abscissal data points by subroutine SORT and transposes the input ordinate data from the fixed point array IY(I) on a scale of transmittance × 1000 to a floating point array Y(I) on a scale of transmittance.

This is followed by the Input Section which continues to statement 154. Here the initial values of several quantities are set. These include the number of completed iterations (NIT), the total number of band indices (N), the starting value of the damping factor (P1), the number of entries (NAL) in the array AQ(IM), and TERM which is needed later for a convergence check. The values of the input indices are then accepted in the DO loop ending at statement 153; they are stored in the array X(I). By this stage the output headings have been printed, including a list of the input indices; the ordinate indices have been converted from a decadic to a Napierian logarithmic scale, as also has the baseline constant X(N). The timing subroutine SETCLK is activated at the beginning of this section.

The central core of the program is the ($\underline{G}$,$\underline{AQ}$,$\underline{F}$) Section, which runs from statement 200 to statement 233. Here, initial values are first set for several quantities; FS is the value of the minimization function within a given iteration cycle (cf. equation [7]). FM is the maximal difference between the observed and computed ordinates, and WFM is the wavenumber position of FM.

The values of FS, the matrix $\underline{B}$ and the vector G are next calculated. The main computation occurs in the double DO loop between statements 203 and 218. For each experimental data point SUBROUTINE POINT determines the ordinate value of the computed curve (cf. equations [6] and [10]). This is compared with the experimental ordinate value to determine F, FM, and FS. The partial differentials are computed in the DO loops beginning at statement 207 for the product function and at statement 210 for the sum function (see p. 17). These comprise one row of the $\underline{A}$ matrix for each data point and are stored for one row at a time in the array AM(I). The matrix $\underline{B}$ and the vector $\underline{G}$ are generated by a storage saving technique which avoids the need to accumulate the complete $\underline{A}$ matrix; the algebra involved is discussed on p. 19. Since $\underline{B}$ is symmetric, only the matrix elements that lie above the diagonal need be calculated. These are stored in the array AQ(IM) at statement 218, and transferred serially to the array A(I,IJ) as required for the subsequent calculations in the DO loop beginning at statement 219.

The diagonal elements of $\underline{B}$ comprise the non-zero terms of $\underline{C}$. The matrix $\underline{C}^{-\frac{1}{2}}$ is formed at statement 226 and stored in the array DIA(I). The upper half of $\underline{B}$ is converted to $\underline{C}^{-\frac{1}{2}}\underline{B}\underline{C}^{-\frac{1}{2}}$ and stored in the array AQ(IM). The vector GAST(I) is formed at the same time at statement 227.

The diagonal terms of $\underline{C}^{-\frac{1}{2}}\underline{B}\underline{C}^{-\frac{1}{2}}$ are unity and the off diagonal terms are correlation coefficients between the indices. If numerical difficulties occur, it is helpful to have a record of the extreme values of these coefficients, and also of the minimal and maximal values of the diagonal elements of $\underline{B}$. When the program is operated with MLIST = 2 or 4, these are located and recorded, using the following terminology:

ADMIN	Value of minimal diagonal element of $\underline{B}$
MINAD	Location of ADMIN
ADMAX	Value of maximal diagonal element of $\underline{B}$
MAXAD	Location of ADMAX
AMIN	Value of minimal off-diagonal element of $\underline{C}^{-\frac{1}{2}}\underline{B}\underline{C}^{-\frac{1}{2}}$
MINA1	Row location of AMIN
MINA2	Column location of AMIN
AMAX	Value of maximal off-diagonal element of $\underline{C}^{-\frac{1}{2}}\underline{B}\underline{C}^{-\frac{1}{2}}$
MAXA1	Row location of AMAX
MAXA2	Column location of AMAX

The absolute values of AMIN and AMAX must be less than unity; an approach to this limiting value implies a strong interaction between the indices involved and may help to locate a source of difficulty in optimization.

This major computational section ends with the evaluation of the gradient length (GL) at statement 233. The time is read (RDCLK) and the accumulated computation time evaluated (ISECS). The values of FS, GI, WFM, FM, NIT, and ISECS are printed. These appear in tabular form and, under normal conditions with MLIST = 1 or 3, they provide all the information needed to demonstrate satisfactory convergence to the m^{th} iteration cycle of equation [5].

The values of FS, $\underline{B}$, G, and $\underline{C}$ having been evaluated above, it is still necessary to select the optimal value of p to complete the $m+1^{th}$ iteration.* The optimal value of FS can be extremely sensitive to the choice of P. For the first approximation P=0.1 is used, but in subsequent cycles the best value of P is sought by an automated, though essentially empirical method which is described in the Appendix to reference (2) and is discussed further on p. 18 of this Bulletin. Four values of P are obtained for each iteration cycle, and the corresponding values of X(I) and FS are calculated; they are designated XP(I) and FSP; if MLIST = 2 or 4 all four values of P and FSP are printed. The value of P associated with the minimal value of FSP is chosen and the corresponding indices in XP(I) are transferred to XB(I), at statement 305, as starting values for the next iteration.

These operations take place in the (P,INVERT,XP) Section, and in the (FSP) Section. Both sections are traversed four times in each iteration cycle; the logical path is controlled by the computed GO TO statement 252. In the first three traversals the

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*Note that p of equation [5] is transposed to P in the FORTRAN notation.

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change in P is controlled by the values of UP, DOWN, and CHANGE. The fourth P value is interpolated by the method discussed in the Appendix to reference (2); this occurs between statements 263 and 270.

The damping factor is added to $\underline{C}^{-\frac{1}{2}}\underline{B}\underline{C}^{-\frac{1}{2}}$ at statement 267 and the linear system of equations is solved by the Gauss-Jordan elimination method in which the diagonal members are used as a pivot (14).

Messages indicating numerical difficulties may be printed at statements 271 and 284. The former will draw attention to difficulty in interpolating a fourth value for P, but the execution of the program will continue. The latter indicates that there are difficulties with the Gauss-Jordan procedure. In that event the computation will output at the end of the current iteration cycle. This is a safety check and is not likely to occur.

The decision whether to continue to the next iteration, or to terminate, is made following statement 312 in the Terminal Section. The number of completed iterations (NIT) is compared with the permitted number (NI), and the elapsed computation time is compared with the permitted time (NSEC). Two checks for slow convergence are also supplied. One is the fractional change in the minimization function (TERM/FSM). The computation terminates if this ratio falls below 1.002. The program will also terminate should GL be reduced below 0.0001. This is also an indication of slow convergence, though normally the TERM/FSM ratio test will terminate the program first. The program will also terminate should FM be reduced below 0.001, which indicates that a maximal significant fit has been achieved; under normal circumstances, the accuracy of the experimental ordinate measurement will not be better than 0.001 transmittance units.

At the end of the computation, the program tabulates the optimized values of the indices, the corresponding values of the error function (FSM), the root-mean-square of the residuals (DIS), the maximal ordinate error (FM), and the wavenumber of FM (WFM).* A check is made against NDATA; if NDATA = 2 the program proceeds to process the next data deck, otherwise it calls the EXIT routine and the calculations are completed.

If LIMIT = 1 or NONEG = 1, restraints are applied to the permitted values of the indices. These boundary conditions are

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*If WFM remains constant throughout the iteration series, it most probably indicates that there is a punch error in the corresponding experimental ordinate, or suggests the need to introduce an additional component band.

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monitored and controlled in the section Boundary Conditions to Limit the Ranges of X(1),X(2),X(4), and X(5). It has been observed that occasionally a band may be virtually eliminated by making the half-width excessively wide, or, more commonly, reducing it to a spike so that it falls almost wholly between two consecutive abscissal data points.* Limits can be set to X(3) and X(4), for the product function, or to X(3) for the sum function which will restrict the half-width within the spectroscopically significant ranges of 1 cm.$^{-1}$ to 50 cm.$^{-1}$. These limiting conditions are summarized in Table I and discussed further in connection with Program XIII on p. 95.

TABLE I

Limiting Values for X(3) and X(4) to Restrain the Half-Band Width in the Approximate Range 1 to 50 cm.$^{-1}$

Product Function

Half-band width < 1 cm.$^{-1}$ if	[X(3)] > 2.0 or [X(4)] > 1.0	
Half-band width < 50 cm.$^{-1}$ if:		
either	[X(3)] > 0.03	
or	[X(3)] ≤ 0.03 but	[X(4)] > 0.0333

Sum Function with CAY in the Range 0.4-0.8

Half-band width < 1 cm.$^{-1}$ if	[X(3)] > 2.0
Half-band width > 50 cm.$^{-1}$ if	[X(3)] < 0.042

Negative values of X(3) and X(4) not infrequently occur for the product function and of X(3) for the sum function. Since these quantities only enter the band shape calculations as squared terms the sign is not significant, and it is the absolute values of these quantities that determine the boundary conditions listed in Table I.

For the sum function, negative values of X(1) and X(5) are also frequently encountered, and indicate that the optimized solution involves a subtraction of a Gauss component from a Cauchy

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*It is also possible for a band to be "lost" by a large abscissal displacement of X(2) out of the computed wavenumber range. We have only rarely encountered this difficulty with this program, though it occurred more frequently with the Method I optimization technique when highly inaccurate starting values were employed (2).

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component, or vice versa. This can be restricted by setting NONEG = 1 which causes a negative X(1) or X(5) ordinate index to be replaced by a positive one, one-tenth of the intensity of that of the preceding iteration. This tends progressively to yield a pure Gauss or Cauchy curve. Generally this gives a solution that converges less efficiently; it can sometimes be circumvented by altering CAY.

C. Subroutine POINT

This small subroutine computes the values of $\ln(T_o/T)_\nu$ for a given set of variables X(I), at a given wavenumber W. It also computes the quantities PC(I) and PG(I) which correspond to

$$x_1(1 + x_3^2(\nu - x_2)^2)^{-1}$$

and

$$x_4^2(\nu - x_2)^2$$

of equations [1] and [6]; these are needed in the evaluation of the arrays of partial derivatives AM(I) at statements 207-209 and 210-212.

D. The Method for Selecting the Damping Factor P

The evaluation of P is crucial to the efficient functioning of the program and some further comment is pertinent.

The technique we use to obtain an optimal P is distinctly an arbitrary one. During the initial development of the program we used an S.D.S. 920 computer with direct access, permitting selected values of P to be introduced on demand from a typewriter. We later used a one-dimensional search by Fibonacci numbers (15), also under the operator's direct control. This would still appear to be the best approach when direct access to the computer is possible. In attempting to achieve a fully automated procedure we first developed a method whereby a succession of preselected damping factors was tested. This was successful in several cases, but often the conditions for rapid convergence were extremely sensitive, and so limited that they might be completely missed. Later we tested the method described by Marquardt (5), but tests on practical examples showed that some efficiency is lost by always accepting the lowest value of P. The method we finally adopted has proved acceptable in most cases: nevertheless it can only be regarded as a compromise solution.

Our method is sensitive to the preselected values of UP, DOWN and CHANGE. In cases where difficulty is encountered, the

values of these quantities should be adjusted. A drawback to the current automatic procedure is that no provision is made to deal with cases where the damping factors must be greatly increased to achieve convergence (i.e. by 10^4 or more). The danger of this situation has been indicated by Marquardt and his article should be consulted (5). We have rarely encountered this difficulty; a more common problem arises with very small damping constants, but here successful convergence can usually be achieved if sufficient iterations are allowed.

E. The Evaluation of the B Matrix

The $\underline{B}$ matrix is constructed from a vector of binary product terms of $\underline{A}$, which is stored in the array AQ(IM). Advantage is taken of the symmetry of $\underline{B}$; only the terms above the diagonal need to be evaluated since $A_{ji} = A_{ij}$. The lower half of $\underline{B}$ can therefore be obtained by interchange of the indices in the $A(\overline{I},IJ)$ array; this reduces the number of B elements to be computed from N^2 to $N(N+1)/2$.

The binary products of the $\underline{A}$ matrix are computed in a sequence that permits all the elements in a single row of $\underline{B}$ to be evaluated simultaneously by a summation procedure which can be illustrated with reference to a 2×3 $\underline{A}$ matrix as follows:

$\underline{A}^T$

$$\begin{matrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \end{matrix}$$

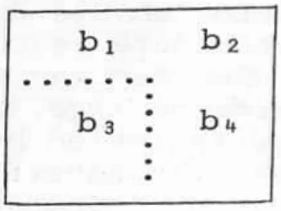
$\underline{A}$

$$\begin{matrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{matrix}$$

$\underline{B}$

$$\begin{matrix} (a_{11}a_{11} + a_{21}a_{21} + a_{31}a_{31}) & (a_{11}a_{12} + a_{21}a_{22} + a_{31}a_{32}) \\ (\text{----------}) & (a_{12}a_{12} + a_{22}a_{22} + a_{32}a_{32}) \end{matrix}$$

On the first passage through the DO loop beginning at statement 203, the three product terms $a_{11}a_{11}$, $a_{11}a_{12}$, and $a_{12}a_{12}$ are evaluated and stored in AQ(1), AQ(2), and AQ(3) at statement 218. The second passage yields $a_{21}a_{21}$, $a_{21}a_{22}$, and $a_{22}a_{22}$ which are added respectively to AQ(1), AQ(2), and AQ(3). The third and final cycle adds $a_{31}a_{31}$ to AQ(1), $a_{31}a_{32}$ to AQ(2) and $a_{32}a_{32}$ to AQ(3), to complete the first, second and fourth elements of $\underline{B}$. The b_3 element, below the diagonal is equal to b_2.



F. The Partial Derivatives

The differential equations $\partial f_i/\partial x_k$ are computed for the product and sum functions in the DO loops beginning at statements 207 and 210 respectively.

From equation [3],

$$f_i = T_{\nu obs} - T_\nu$$
$$= T_{\nu obs} - e^{-A_\nu} \qquad [11]$$

where T_ν and A_ν are the transmittance and Napierian absorbance ordinates for the calculated curve at wavenumber ν.

It follows that

$$\partial f_i/\partial x_k = \partial f_i/\partial A \cdot \partial A/\partial x_k$$
$$= -e^{-A_\nu} \cdot \partial A/\partial x_k$$
$$= -T_\nu \cdot \partial A/\partial x_k \qquad [12]$$

For the product function we may write

$$T = \exp - [x_i' P_c P_g + \alpha'] \qquad [13]$$

where

$$P_c = 1/(1 + R^2 x_3^2) \qquad [14]$$

$$P_g = \exp - [R^2 x_4^2] \qquad [15]$$

$$R = (\nu - x_2) \qquad [16]$$

in which x_2, x_3, x_4 have their usual connotation from equation [1], $x_1' = 2.30258x_1$ and $\alpha' = 2.30258\alpha$.

Differentiation yields the expressions

$$\partial f_i/\partial x_1' = TP_cP_g \quad [17]$$

$$\partial f_i/\partial x_2 = 2x_1'TP_cP_g(x_4^2 + P_cx_3^2)R \quad [18]$$

$$\partial f_i/\partial x_3 = -2x_1'x_3TP_c^2P_gR^2 \quad [19]$$

$$\partial f_i/\partial x_4 = -2x_1'x_4TP_cP_gR^2 \quad [20]$$

$$\partial f_i/\partial \alpha' = T \quad [21]$$

Setting

$$S_p = 2x_1'TP_cP_gR$$

$$= 2x_1'R \cdot \partial f_i/\partial x_1' \quad [22]$$

equations [18 to 20] reduce to

$$\partial f_i/\partial x_2 = S_p(x_4^2 + P_cx_3^2) \quad [23]$$

$$\partial f_i/\partial x_3 = -S_px_3P_cR \quad [24]$$

$$\partial f_i/\partial x_4 = -S_px_4R$$

Likewise, we have for the sum function with $x_5' = 2.30258x_5$

$$A_\nu = x_1'P_c + x_5'P_g + \alpha' \quad [25]$$

and with the restraint that $x_4 = kx_3$

$$P_g = \exp - [R^2k^2x_3^2] \quad [26]$$

The expressions for the derivatives are

$$\partial f_i/\partial x_1' = TP_c \quad [27]$$

$$\partial f_i/\partial x_2 = S_sx_3 \quad [28]$$

$$\partial f_i/\partial x_3 = -S_s R \quad [29]$$

$$\partial f_i/\partial x_5' = TP_g \quad [30]$$

$$\partial f_i/\partial \alpha' = T \quad [31]$$

where

$$S_s = 2x_3 TR(x_1' P_c^2 + x_5 k^2 P_g) \quad [32]$$

$$T = \exp[-(x_1' P_c + x_5' P_g + \alpha')] \quad [32A]$$

THE TEST DATA

As test data for the band fit programs, curves generated from overlapping systems of four bands are used. These are described in connection with Program XIV and are illustrated in Figs. 1 and 2.

Four Band Test Curve for Product Function

X(1)	X(2)	X(3)	X(4)
0.300	970.0	0.200	0.100
0.600	955.0	0.200	0.200
0.300	940.0	0.100	0.100
0.400	920.0	0.200	0.100

Alpha = 0.05

NP = 200 WB = 1000.0 WI = 0.5

Four Band Test Curve for Sum Function

X(1)	X(2)	X(3)	X(5)
0.200	970.0	0.200	0.100
0.400	955.0	0.200	0.200
0.100	940.0	0.100	0.200
0.250	920.0	0.200	0.150

Alpha = 0.05

NP = 200 WB = 100.0 WI = 0.5 CAY = 0.8

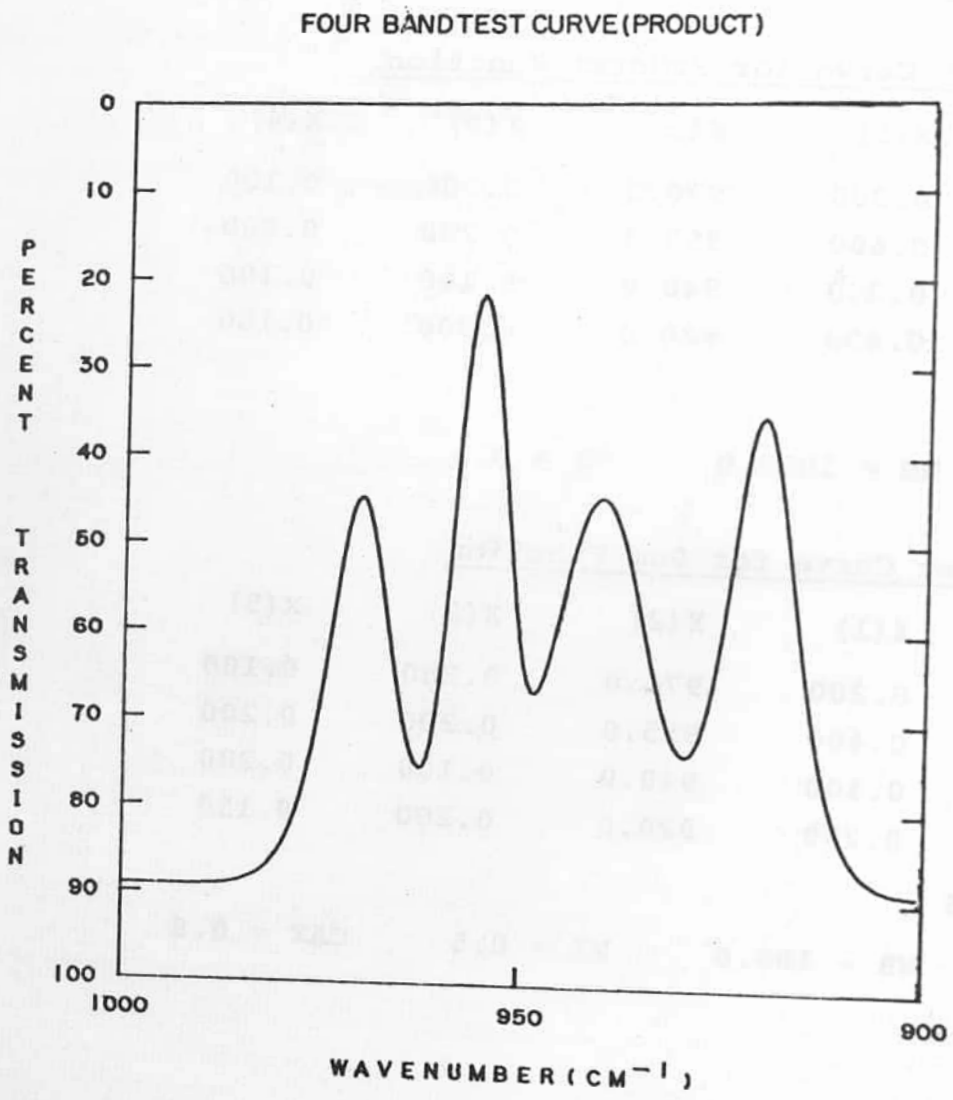


Fig. 1 Four band test curve for the Cauchy-Gauss product function.

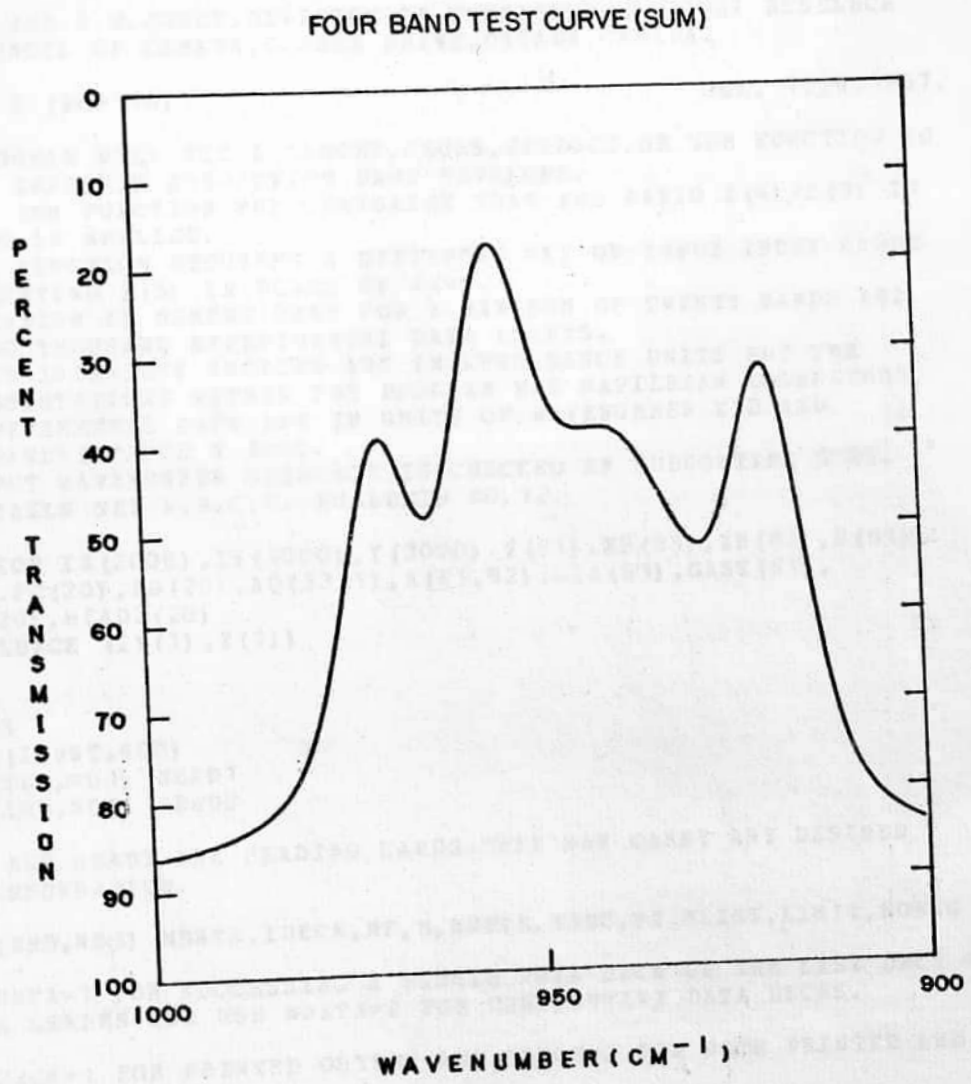


Fig. 2 Four band test curve for the Cauchy-Gauss sum function.

```
C                                                                       10
C     ***********************************************************       20
C     *                                                         *       30
C     *          SPECTRAL BAND FIT OPTIMIZATION PROGRAM         *       40
C     *                                                         *       50
C     *                    BASIC VERSION.                       *       60
C     *                                                         *       70
C     ***********************************************************       80
C                                                                       90
C     J.PITHA AND R.N.JONES,DIVISION OF CHEMISTRY,NATIONAL RESEARCH     100
C          COUNCIL OF CANADA,SUSSEX DRIVE,OTTAWA,CANADA.                110
C                                                                       120
C     PROGRAM X (PC-116)                          JULY 12TH.1967.     130
C                                                                       140
C     THIS PROGRAM WILL FIT A CAUCHY,GAUSS,PRODUCT,OR SUM FUNCTION TO   150
C          AN INFRARED ABSORPTION BAND ENVELOPE.                        160
C     FOR THE SUM FUNCTION THE RESTRAINT THAT THE RATIO X(4)/X(3) IS    170
C     CONSTANT IS APPLIED.                                              180
C     THE SUM FUNCTION REQUIRES A DIFFERENT SET OF INPUT INDEX CARDS    190
C          CARRYING X(5) IN PLACE OF X(4).                              200
C     THIS VERSION IS DIMENSIONED FOR A MAXIMUM OF TWENTY BANDS AND     210
C          TWO THOUSAND EXPERIMENTAL DATA POINTS.                       220
C     THE BAND INTENSITY INDICES ARE IN ABSORBANCE UNITS BUT THE        230
C          COMPUTATIONS WITHIN THE PROGRAM USE NAPIERIAN LOGARITHMS.    240
C     THE EXPERIMENTAL DATA ARE IN UNITS OF WAVENUMBER X10 AND          250
C          TRANSMITTANCE X 1000.                                        260
C     THE INPUT WAVENUMBER SEQUENCE IS CHECKED BY SUBROUTINE SORT.      270
C     FOR DETAILS SEE N.R.C.C. BULLETIN NO.12.                          280
C                                                                       290
      DIMENSION IX(2000),IY(2000),Y(2000),X(81),XP(81),XB(81),G(81),    300
     1AM(81),PC(20),PG(20),AQ(3321),A(81,82),DIA(81),GAST(81),          310
     2HEAD1(20),HEAD2(20)                                               320
      EQUIVALENCE (IY(1),Y(1))                                          330
      IRD=1                                                             340
      IPCH=2                                                            350
      IPRNT=3                                                           360
   11 WRITE (IPRNT,400)                                                 370
      READ (IRD,401) HEAD1                                              380
      READ (IRD,401) HEAD2                                              390
C                                                                       400
C     HEAD1 AND HEAD2 ARE HEADING CARDS.THEY MAY CARRY ANY DESIRED      410
C          INFORMATION.                                                 420
C                                                                       430
      READ (IRD,403) NDATA,IDECK,NP,M,KURVE,NSEC,NI,MLIST,LIMIT,NONEG   440
C                                                                       450
C     USE NDATA=1 FOR PROCESSING A SINGLE DATA DECK OR THE LAST DECK OF  460
C          A SERIES AND USE NDATA=2 FOR CONSECUTIVE DATA DECKS.         470
C                                                                       480
C     USE IDECK=1 FOR PRINTED OUTPUT AND IDECK=2 FOR BOTH PRINTED AND   490
C          CARD OUTPUT.                                                 500
C                                                                       510
C     NP IS THE NUMBER OF DATA POINTS.                                  520
C                                                                       530
C     M IS THE NUMBER OF CALCULATED BANDS.                              540
```

```
C                                                                       550
C     USE KURVE=1 FOR PRODUCT FUNCTION AND KURVE=2 FOR SUM FUNCTION.    560
C                                                                       570
C     NSEC IS THE MAXIMUM PERMITTED COMPUTATION TIME IN SECONDS.        580
C                                                                       590
C     NI IS THE MAXIMUM NUMBER OF PERMITTED ITERATIONS.                 600
C                                                                       610
C     MLIST CONTROLS THE AMOUNT OF INFORMATION REPORTED ABOUT THE       620
C          PROGRESS OF THE COMPUTATION.                                 630
C                                                                       640
C          USE MLIST=1 FOR MINIMUM PROGRESS REPORT AND FINAL OUTPUT     650
C             ONLY.                                                     655
C          USE MLIST=2 FOR ADDITIONAL INFORMATION ON THE EXTREME VALUES 660
C             OF THE B MATRIX ELEMENTS DURING EACH ITERATION.           670
C          USE MLIST=3 TO PRINT RESTRAINTS APPLIED BY LIMIT AND NONEG.  680
C          USE MLIST=4 FOR COMBINATION OF MLIST=2 + MLIST=3.            690
C                                                                       700
      CALL SETCLK                                                       710
C     SETCLK IS A TIMING SUBROUTINE.                                    720
C                                                                       730
C     USE LIMIT=1 TO RESTRICT THE HALF-WIDTHS OF THE COMPONENT BANDS    740
C          WITHIN THE RANGE 1-50 CM.-1                                  750
C          IF LIMIT=2 NO RESTRICTION TO THE HALF-BAND WIDTH IS APPLIED. 760
C                                                                       770
C     USE NONEG=1 WITH THE SUM FUNCTION TO RESTRICT X1 AND X5 TO ZERO   780
C          OR POSITIVE VALUES.                                          790
C          IF NONEG=2 NO RESTRICTION IS APPLIED ----- ALWAYS USE        800
C          NONEG=2  WITH THE PRODUCT FUNCTION.                          810
C                                                                       820
      IF (KURVE.EQ.2) GO TO 13                                          830
      READ (IRD,404) WB,WI                                              840
      GO TO 16                                                          850
   13 READ (IRD,404) WB,WI,CAY                                          860
C                                                                       870
C     CAY DEFINES THE X(4)/X(3) RATIO IN THE SUM FUNCTION CALCULATIONS. 880
C          FOR CHOICE OF VALUE SEE CAN.J.CHEM. VOL.45 PAGE 2347 (1967)  890
C     VALUES OF CAY IN THE RANGE 0.6 - 0.8 ARE SUGGESTED.               900
C                                                                       910
C     WB AND WI ARE THE STARTING WAVENUMBER AND THE WAVENUMBER ENCODING 920
C          INTERVAL IN CM.-1 BY CONVENTION WI IS POSITIVE FOR A          930
C          DIMINISHING WAVENUMBER SEQUENCE.                             940
C                                                                       950
   16 IF (IDECK.EQ.1) GO TO 12                                          960
      WRITE (IPCH,401) HEAD1                                            970
      WRITE (IPCH,401) HEAD2                                            980
   12 WRITE (IPRNT,402) HEAD1                                           990
      WRITE (IPRNT,402) HEAD2                                          1000
      WRITE (IPRNT,408)                                                1010
      READ (IRD,404) DOWN,UP,CHANGE                                    1020
C                                                                      1030
C     DOWN,UP AND CHANGE REGULATE THE SEARCH FOR OPTIMAL DAMPING FACTOR. 1040
C     RECOMMENDED TRIAL VALUES ARE DOWN=0.01  UP=1000.0  CHANGE=0.5    1050
C                                                                      1060
      WRITE (IPRNT,409) DOWN,UP,CHANGE                                 1070
```

```
      WRITE (IPRNT,423) NP,WB,WI                                          1080
      IF (NONEG.EQ.2) GO TO 14                                            1090
      IF (MLIST.LT.3) WRITE (IPRNT,432)                                   1100
   14 IF (LIMIT.EQ.2) GO TO 15                                            1110
      IF (MLIST.LT.3) WRITE (IPRNT,433)                                   1120
   15 READ (IRD,405) (IX(I),IY(I),I=1,NP)                                 1130
      IWB=WB*10.0+0.5                                                     1140
      IWI=WI*10.0+0.5                                                     1150
      CALL SORT1 (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)                    1160
      IF (KLENUP.EQ.1) GO TO 30                                           1170
   20 UP=0.0                                                              1180
      DOWN=0.0                                                            1190
      CHANGE=0.0                                                          1200
      IF (NDATA.EQ.2) GO TO 11                                            1210
      STOP                                                                1220
   30 DO 31 I=1,NP                                                        1230
   31 Y(I)=IY(I)*0.001                                                    1240
C                                                                         1250
C     *************************  INPUT SECTION  ************************  1260
C                                                                         1270
      N=4*M+1                                                             1280
      N1=N+1                                                              1290
      NAL=N*N1/2                                                          1300
      NIT=0                                                               1310
      TERM=1000.0                                                         1320
      P1=0.1                                                              1330
      IF (KURVE.EQ.2) GO TO 151                                           1340
      WRITE (IPRNT,416)                                                   1350
      GO TO 152                                                           1360
  151 WRITE (IPRNT,417)                                                   1370
  152 DO 153 I=1,M                                                        1380
      J=I+M                                                               1390
      K=J+M                                                               1400
      L=K+M                                                               1410
      READ (IRD,404) X(I),X(J),X(K),X(L)                                  1420
C     X(I),X(J),X(K) AND X(L) ARE THE SPECTRAL INDICES FOR EACH BAND.     1430
      IF (KURVE.EQ.2) GO TO 155                                           1440
      WRITE (IPRNT,410) X(I),X(J),X(K),X(L)                               1450
      GO TO 157                                                           1460
  155 XG=X(K)*CAY                                                         1470
      WRITE (IPRNT,406) X(I),X(J),X(K),XG,X(L)                            1480
      X(L)=2.30258*X(L)                                                   1490
  157 X(I)=2.30258*X(I)                                                   1500
  153 CONTINUE                                                            1510
      READ (IRD,404) X(N)                                                 1520
      WRITE (IPRNT,418) X(N)                                              1530
      X(N)=2.30258*X(N)                                                   1540
      DO 154 I=1,N                                                        1550
  154 XB(I)=X(I)                                                          1560
C                                                                         1570
C     ***********************  (G,AQ,F) SECTION  ***********************  1580
C                                                                         1590
  200 DO 201 I=1,N                                                        1600
  201 G(I)=0.0                                                            1610
```

```
      DO 202 I=1,NAL                                                    1620
  202 AQ(I)=0.0                                                         1630
      FS=0.0                                                            1640
      FM=0.0                                                            1650
      FS1=1.0E10                                                        1660
      FS2=1.0E10                                                        1670
      P1L=P1                                                            1680
      IT=1                                                              1690
  203 DO 218 II=1,NP                                                    1700
      W=IX(II)*0.1                                                      1710
      CALL POINT1 (X,PC,PG,W,AC,M,N,CAY,KURVE)                          1720
      TC=EXP(-AC)                                                       1730
      F=Y(II)-TC                                                        1740
      FA=ABS(F)                                                         1750
      IF (FM.GE.FA) GO TO 206                                           1760
      FM=FA                                                             1770
      WFM=W                                                             1780
  206 FS=FS+F*F                                                         1790
      IF (KURVE.EQ.2) GO TO 210                                         1800
  207 DO 209 I=1,M                                                      1810
      J=I+M                                                             1820
      K=J+M                                                             1830
      L=K+M                                                             1840
      AM(I)=TC*PG(I)*PC(I)                                              1850
      R=W-X(J)                                                          1860
      SP=2.0*AM(I)*X(I)*R                                               1870
      AM(J)=SP*(X(L)*X(L)+X(K)*X(K)*PC(I))                              1880
      AM(K)=-SP*R*X(K)*PC(I)                                            1890
  209 AM(L)=-SP*R*X(L)                                                  1900
      GO TO 211                                                         1910
  210 DO 212 I=1,M                                                      1920
      J=I+M                                                             1930
      K=J+M                                                             1940
      L=K+M                                                             1950
      R=W-X(J)                                                          1960
      AM(I)=TC*PC(I)                                                    1970
      SS=2.0*TC*(X(I)*PC(I)*PC(I)+CAY*CAY*X(L)*PG(I))*R*X(K)            1980
      AM(J)=SS*X(K)                                                     1990
      AM(K)=-SS*R                                                       2000
  212 AM(L)=TC*PG(I)                                                    2010
  211 AM(N)=TC                                                          2020
      IM=0                                                              2030
      DO 218 I=1,N                                                      2040
      AMI=AM(I)                                                         2050
      G(I)=G(I)+AMI*F                                                   2060
      DO 218 IJ=I,N                                                     2070
      IM=IM+1                                                           2080
  218 AQ(IM)=AQ(IM)+AMI*AM(IJ)                                          2090
      FSM=FS                                                            2100
      IM=0                                                              2110
      DO 219 I=1,N                                                      2120
      DO 219 IJ=I,N                                                     2130
      IM=IM+1                                                           2140
  219 A(I,IJ)=AQ(IM)                                                    2150
```

```
      ADMIN=1.0E+10                                                          2160
      ADMAX=-1.0E+10                                                         2170
      DO 227 I=1,N                                                           2180
      GO TO (224,220,224,220),MLIST                                          2190
  220 IF (A(I,I).GE.ADMIN) GO TO 221                                         2200
      ADMIN=A(I,I)                                                           2210
      MINAD=I                                                                2220
  221 IF (ADMAX.GE.A(I,I)) GO TO 224                                         2230
      ADMAX=A(I,I)                                                           2240
      MAXAD=I                                                                2250
  224 IF (A(I,I).GT.1.0E-10) GO TO 226                                       2260
      DIA(I)=0.0                                                             2270
      GO TO 227                                                              2280
  226 DIA(I)=1.0/SQRT(A(I,I))                                                2290
  227 GAST(I)=G(I)*DIA(I)                                                    2300
      IM=0                                                                   2310
      AMIN=1.0E+10                                                           2320
      AMAX=-1.0E-10                                                          2330
      DO 228 I=1,N                                                           2340
      DIAI=DIA(I)                                                            2350
      DO 228 IJ=I,N                                                          2360
      IM=IM+1                                                                2370
      AQ(IM)=A(I,IJ)*DIAI*DIA(IJ)                                            2380
      GO TO (228,229,228,229),MLIST                                          2390
  229 IF (I.EQ.IJ) GO TO 228                                                 2400
      IF(AQ(IM).GE.AMIN) GO TO 231                                           2410
      AMIN=AQ(IM)                                                            2420
      MINA1=I                                                                2430
      MINA2=IJ                                                               2440
  231 IF (AMAX.GE.AQ(IM)) GO TO 228                                          2450
      AMAX=AQ(IM)                                                            2460
      MAXA1=I                                                                2470
      MAXA2=IJ                                                               2480
  228 CONTINUE                                                               2490
      GL=0.0                                                                 2500
      DO 233 I=1,N                                                           2510
      GI=G(I)                                                                2520
  233 GL=GL+GI*GI                                                            2530
      SM=-2.0*GL                                                             2540
      GL=SQRT(GL)                                                            2550
C                                                                            2560
C     THERE IS AN APPROXIMATION IN THE EVALUATION OF SM BUT WE FIND NO       2570
C          SIGNIFICANT IMPROVEMENT IN ACCURACY OR CONVERGENCE RATE WHEN      2580
C          THE EXACT FORMULA IS USED. IT HAS NOT BEEN GENERALLY              2590
C          INTRODUCED AS IT OCCASIONALLY CAUSES NUMERICAL DIFFICULTIES.      2600
C                                                                            2610
      CALL RDCLK (TIME)                                                      2620
C                                                                            2630
C     RDCLK IS A TIMING SUBROUTINE.                                          2640
C                                                                            2650
      ISECS=TIME+0.5                                                         2660
      WRITE (IPRNT,407) FS,GL,WFM,FM,NIT,ISECS                               2670
C                                                                            2680
C     ******************  MATRIX DATA OUTPUT SECTION  ******************     2690
```

```
C                                                                       2700
      GO TO (250,249,250,249),MLIST                                     2710
  249 WRITE (IPRNT,424) MINAD,MAXAD,ADMIN,ADMAX,MINA1,MINA2,AMIN,MAXA1, 2720
     1MAXA2,AMAX                                                        2730
C                                                                       2740
C     ********************  (P,INVERT,XP) SECTION  ********************* 2750
C                                                                       2760
  250 IM=0                                                              2770
      DO 251 I=1,N                                                      2780
      DO 251 IJ=I,N                                                     2790
      IM=IM+1                                                           2800
      AQIM=AQ(IM)                                                       2810
      A(I,IJ)=AQIM                                                      2820
  251 A(IJ,I)=AQIM                                                      2830
  252 GO TO (260,261,262,263,311),IT                                    2840
  260 P=P1L                                                             2850
      GO TO 265                                                         2860
  261 IF (FS.LE.FS1) GO TO 266                                          2870
      P=P1L*DOWN                                                        2880
      GO TO 265                                                         2890
  266 P=P1L*UP                                                          2900
      GO TO 265                                                         2910
  262 P=P1*CHANGE                                                       2920
      GO TO 265                                                         2930
  263 X3=1.0/P1                                                         2940
      X4=1.0/P2                                                         2950
      DET=X3*X3*X4*X4*X4-X3*X3*X3*X4*X4                                 2960
      IF (DET.EQ.0.0) GO TO 269                                         2970
      AP1=X3*X3*(FS2-FS-SM*X4)                                          2980
      AP2=X4*X4*(FS1-FS-SM*X3)                                          2990
      AI=6.0*(AP1-AP2)/DET                                              3000
      BI=2.0*(X4*AP2-X3*AP1)/DET                                        3010
      DET=BI*BI-2.0*AI*SM                                               3020
      IF (DET) 269,279,270                                              3030
  270 DET=SQRT(DET)                                                     3040
  279 IF (AI.EQ.0.0) GO TO 269                                          3050
      X3=(-BI+DET)/AI                                                   3060
      X4=(-BI-DET)/AI                                                   3070
      IF (X3.LE.0.0) GO TO 272                                          3080
      IF (X4.LE.0.0) GO TO 275                                          3090
      IF (X4.LE.X3) GO TO 274                                           3100
  275 P=1.0/X3                                                          3110
      GO TO 265                                                         3120
  272 IF (X4.LE.0.0) GO TO 269                                          3130
  274 P=1.0/X4                                                          3140
      GO TO 265                                                         3150
  269 P=10000.0                                                         3160
  271 WRITE (IPRNT,411)                                                 3170
  265 IT=IT+1                                                           3180
  267 DO 278 I=1,N                                                      3190
      A(I,I)=A(I,I)+P                                                   3200
  278 A(I,N1)=-GAST(I)                                                  3210
      DO 282 I=1,N                                                      3220
      AII=A(I,I)                                                        3230
```

```
                                                                      3240
      IF (AII.EQ.0.0) GO TO 284                                       3250
      PIV=1.0/AII                                                     3260
      DO 281 J=I,N1                                                   3270
  281 A(I,J)=PIV*A(I,J)                                               3280
      DO 282 K=1,N                                                    3290
      IF (I.EQ.K) GO TO 282                                           3300
      Q=A(K,I)                                                        3310
      DO 285 J=I,N1                                                   3320
  285 A(K,J)=A(K,J)-Q*A(I,J)                                          3330
  282 CONTINUE                                                        3340
      GO TO 286                                                       3350
  284 WRITE (IPRNT,412)                                               3360
      GO TO 314                                                       3370
  286 DO 288 I=1,N                                                    3380
  288 XP(I)=X(I)+A(I,N1)*DIA(I)                                       3390
C                                                                     3400
CC    * BOUNDARY CONDITIONS TO LIMIT THE RANGES OF X(1),X(3),X(4),X(5) *  3410
C                                                                     3420
      IF (KURVE.EQ.2) GO TO 540                                       3430
C                                                                     3440
CC    THE PRODUCT FUNCTION.                                           3450
C                                                                     3460
      IF (LIMIT.EQ.2) GO TO 299                                       3470
      DO 505 I=1,M                                                    3480
      J=I+M                                                           3490
      K=J+M                                                           3500
      L=K+M                                                           3510
      XPK=ABS(XP(K))                                                  3520
      XPL=ABS(XP(L))                                                  3530
      IF (XPL.LE.1.0) GO TO 500                                       3540
      XPL=1.0                                                         3550
      IF (MLIST.LT.3) GO TO 500                                       3560
      WRITE (IPRNT,427) XP(J)                                         3570
  500 IF (XPK.LE.2.0) GO TO 501                                       3580
      XPK=2.0                                                         3590
      IF (MLIST.LT.3) GO TO 506                                       3600
      WRITE (IPRNT,427) XP(J)                                         3610
      GO TO 506                                                       3620
  501 IF (XPK.GT.0.03) GO TO 506                                      3630
      IF (XPL.GT.0.0333) GO TO 506                                    3640
      XPL=0.0333                                                      3650
      IF (MLIST.LT.3) GO TO 506                                       3660
      WRITE (IPRNT,428) XP(J)                                         3670
  506 IF (XP(K).LT.0.0) GO TO 503                                     3680
      XP(K)=XPK                                                       3690
      GO TO 507                                                       3700
  503 XP(K)=-XPK                                                      3710
  507 IF (XP(L).LT.0.0) GO TO 504                                     3720
      XP(L)=XPL                                                       3730
      GO TO 505                                                       3740
  504 XP(L)=-XPL                                                      3750
  505 CONTINUE                                                        3760
      GO TO 299                                                       3770
C
```

```
C      THE SUM FUNCTION.
C
  540 IF (LIMIT.EQ.1) GO TO 550
      IF (NONEG.EQ.2) GO TO 299
  550 DO 556 I=1,M
      J=I+M
      K=J+M
      L=K+M
      XPI=XP(I)
      XPK=ABS(XP(K))
      XPL=ABS(XP(L))
      IF (LIMIT.EQ.2) GO TO 559
      IF (XPK.LT.2.0) GO TO 551
      XPK=2.0
      IF (MLIST.LT.3) GO TO 552
      WRITE (IPRNT,427) XP(J)
      GO TO 552
  551 IF (XPK.GE.0.042) GO TO 552
      XPK=0.042
      IF (MLIST.LT.3) GO TO 552
      WRITE (IPRNT,428) XP(J)
  552 IF (XP(K).LT.0.0) GO TO 553
      XP(K)=XPK
      GO TO 557
  553 XP(K)=-XPK
  557 IF (XP(L).LT.0.0) GO TO 554
      XP(L)=XPL
      GO TO 558
  554 XP(L)=-XPL
C
  558 IF (NONEG.EQ.2) GO TO 556
  559 IF (XPI.GE.0.0) GO TO 555
      XP(I)=XB(I)*0.1
      IF (MLIST.LT.3) GO TO 555
      WRITE (IPRNT,429) XP(J)
  555 IF (XP(L).GE.0.0) GO TO 556
      XP(L)=XB(L)*0.1
C
C     NOTE THAT IF X1 OR X5 GOES NEGATIVE WE REDUCE IT TO ONE TENTH OF
C          THE VALUE FOUND IN THE PREVIOUS ITERATION.
C
      IF (MLIST.LT.3) GO TO 556
      WRITE (IPRNT,430) XP(J)
  556 CONTINUE
C
C     ************************  (FSP) SECTION  ************************
C
  299 FSP=0.0
      JSKIP=1
      KSKIP=1
      DO 301 II=1,NP
      W=IX(II)*0.1
      CALL POINT1 (XP,PC,PG,W,AC,M,N,CAY,KURVE)
      IF (AC.GT.-2.0) GO TO 304
```

```
      IF (JSKIP.EQ.2) GO TO 300                                          4320
      WRITE (IPRNT,425)                                                  4330
      JSKIP=2                                                            4340
  300 TC=7.3891                                                          4350
      GO TO 310                                                          4360
  304 IF (AC.LT.10.0) GO TO 307                                          4370
      IF (KSKIP.EQ.2) GO TO 302                                          4380
      KSKIP=2                                                            4390
      WRITE (IPRNT,426)                                                  4400
  302 TC=0.000045                                                        4410
      GO TO 310                                                          4420
  307 TC=EXP(-AC)                                                        4430
  310 F=Y(II)-TC                                                         4440
  301 FSP=FSP+F*F                                                        4450
      IF (FSM.LE.FSP) GO TO 303                                          4460
C                                                                        4470
C     NOTE IF RESTRAINTS ARE APPLIED,THE PROGRAM CAN BRANCH BACK HERE ON 4480
C          THE FIRST CYCLE TO REPETITIVELY OUTPUT THE ORIGINAL GUESSED   4490
C          INDICES.THIS INDICATES THAT THE GUESSED INDICES (WITHOUT      4500
C          RESTRAINTS) FIT BETTER THAN THE COMPUTED INDICES (WITH        4510
C          RESTRAINTS). IF IT HAPPENS RERUN WITH MLIST=2 AND CHANGE THE  4520
C          INPUT INDICES.                                                4530
C                                                                        4540
      FSM=FSP                                                            4550
      DO 305 I=1,N                                                       4560
  305 XB(I)=XP(I)                                                        4570
  303 IF (FS1.LE.FSP) GO TO 306                                          4580
      FS2=FS1                                                            4590
      P2=P1                                                              4600
      FS1=FSP                                                            4610
      P1=P                                                               4620
      GO TO 308                                                          4630
  306 IF (FS2.LE.FSP) GO TO 308                                          4640
      P2=P                                                               4650
      FS2=FSP                                                            4660
  308 GO TO (250,309,250,309),MLIST                                      4670
  309 WRITE (IPRNT,414) P,FSP                                            4680
      GO TO 250                                                          4690
  311 DO 312 I=1,N                                                       4700
C     ************************ TERMINAL SECTION ************************ 4710
  312 X(I)=XB(I)                                                         4720
      NIT=NIT+1                                                          4730
      TEST=TERM/FSM                                                      4740
      TERM=FSM                                                           4750
      IF (TEST.GE.1.002) GO TO 315                                       4760
      WRITE (IPRNT,436)                                                  4770
      GO TO 314                                                          4780
  315 IF (NIT.LE.NI) GO TO 316                                           4790
      WRITE (IPRNT,437)                                                  4800
      GO TO 314                                                          4810
  316 IF (GL.GE.0.0001) GO TO 317                                        4820
      WRITE (IPRNT,438)                                                  4830
      GO TO 314                                                          4840
  317 IF (ISECS.LE.NSEC) GO TO 320                                       4850
```

```
      WRITE (IPRNT,439)                                                 4860
      GO TO 314                                                         4870
  320 IF (FM.GT.0.001) GO TO 200                                        4880
      WRITE (IPRNT,440)                                                 4890
  314 DIS=SQRT(FSM/NP)                                                  4900
      WRITE (IPRNT,415)                                                 4910
      WRITE (IPRNT,419) FSM,DIS,FM,WFM                                  4920
      IF (KURVE.EQ.2) GO TO 318                                         4930
      WRITE (IPRNT,416)                                                 4940
      DO 319 I=1,M                                                      4950
      J=I+M                                                             4960
      K=J+M                                                             4970
      L=K+M                                                             4980
      X(I)=0.43429*X(I)                                                 4990
      IF (IDECK.EQ.1) GO TO 319                                         5000
      WRITE (IPCH,420) X(I),X(J),X(K),X(L)                              5010
  319 WRITE (IPRNT,410) X(I),X(J),X(K),X(L)                             5020
      X(N)=0.43429*X(N)                                                 5030
      IF (IDECK.EQ.1) GO TO 322                                         5040
      WRITE (IPCH,434) X(N)                                             5050
  322 WRITE (IPRNT,413) X(N)                                            5060
      GO TO 328                                                         5070
  318 WRITE (IPRNT,417)                                                 5080
      DO 325 I=1,M                                                      5090
      J=I+M                                                             5100
      K=J+M                                                             5110
      L=K+M                                                             5120
      X(I)=0.43429*X(I)                                                 5130
      X(L)=0.43429*X(L)                                                 5140
      XG=X(K)*CAY                                                       5150
      IF (IDECK.EQ.1) GO TO 325                                         5160
      WRITE (IPCH,421) X(I),X(J),X(K),X(L)                              5170
  325 WRITE (IPRNT,406) X(I),X(J),X(K),XG,X(L)                          5180
      X(N)=0.43429*X(N)                                                 5190
      IF (IDECK.EQ.1) GO TO 327                                         5200
      WRITE (IPCH,435) X(N)                                             5210
  327 WRITE (IPRNT,422) X(N),CAY                                        5220
  328 WRITE (IPRNT,431)                                                 5230
      GO TO 20                                                          5240
C                                                                       5250
C                                                                       5260
  400 FORMAT ('1PITHA AND JONES.   PROGRAM X (PC-116)  SPECTRAL BAND FIT 5270
     1 OPTIMIZATION PROGRAM BASIC VERSION.'/)                           5280
  401 FORMAT (20A4)                                                     5290
  402 FORMAT (1X,20A4)                                                  5300
  403 FORMAT (10I5)                                                     5310
  404 FORMAT (4F15.5)                                                   5320
  405 FORMAT (8(I5,I4,1X))                                              5330
  406 FORMAT (1X,5(6X,F15.5))                                           5340
  407 FORMAT (5X,2HFS,E12.4,8X,2HGL,E12.4,7X,3HWFM,F7.1,7X,2HFM,E12.4,7X 5350
     1,3HNIT,I3,4X,5HISECS,I5)                                          5360
  408 FORMAT ('0INPUT PARAMETERS.')                                     5370
  409 FORMAT (20X,4HDOWN,E14.6,7X,2HUP,E14.6,7X,6HCHANGE,E14.6)         5380
  410 FORMAT (1X,4(6X,F15.5))                                           5390
```

```
411 FORMAT (1X,'TROUBLE WITH EVALUATION OF P,CHECK MATRIX DATA OUTPUT.      5400
   1')                                                                     5410
412 FORMAT (1X,'TERMINATED BY TROUBLE WITH SOLUTION OF EQUATIONS.')        5420
413 FORMAT (4X,7HALPHA =F8.5/,'0SOLVED FOR PRODUCT,CAUCHY OR GAUSS FUN    5430
   1CTION.'/' (PURE CAUCHY IF X(4)=0 OR PURE GAUSS IF X(3)=0)')            5440
414 FORMAT (64X,1HP,E14.6,8X,3HFSP,E14.6)                                 5450
415 FORMAT (11X,  '-------------------------------------------------------5460
   1-------------------------'/1X,17HOUTPUT PARAMETERS)                    5470
416 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(4))              5480
417 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(4),17X,4HX(5)    5490
   1)                                                                      5500
418 FORMAT (4X,7HALPHA =,F8.5,/11X,'-------------------------------------5510
   1-----------------------------------------')                           5520
419 FORMAT (18X,3HFSM,E14.6,7X,3HDIS,E14.6,7X,2HFM,E14.6,7X,3HWFM,F7.1    5530
   1)                                                                      5540
420 FORMAT (4F15.5,5X,7HPRODUCT)                                          5550
421 FORMAT (4F15.5,9X,3HSUM)                                              5560
422 FORMAT (4X,7HALPHA =,F8.5/'0SOLVED FOR SUM FUNCTION WITH X4 =',F5.    5570
   12,4H X3.)                                                              5580
423 FORMAT ('0',19X,2HNP,I6,17X,2HWB,F8.1,13X,2HWI,F5.1)                  5590
424 FORMAT (/4X,5HMINAD,I4,13X,5HMAXAD,I4,12X,5HADMIN,E14.6,5X,5HADMAX    5600
   1,E14.6/4X,5HMINA1,I4,1X,5HMINA2,I4,3X,4HAMIN,E14.6,3X,5HMAXA1,I4,     5610
   23X,5HMAXA2,I4,3X,4HAMAX,E14.6)                                         5620
425 FORMAT ('0THE MAXIMAL ALLOWED TRANSMITTANCE HAS BEEN EXCEEDED.')      5630
426 FORMAT ('0THE MINIMAL ALLOWED TRANSMITTANCE HAS BEEN EXCEEDED.')      5640
427 FORMAT ('0MINIMAL HALF-WIDTH FOR BAND AT',F7.1,6H CM.-1)              5650
428 FORMAT ('0MAXIMAL HALF-WIDTH FOR BAND AT',F7.1,6H CM.-1)              5660
429 FORMAT ('0X1 HELD POSITIVE AT',F6.1,6H CM.-1)                         5670
430 FORMAT ('0X5 HELD POSITIVE AT',F6.1,6H CM.-1)                         5680
431 FORMAT ('0FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.'/,           5690
   1'0DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEA    5700
   2N SQUARE OF THE RESIDUALS).'/,'0FM IS THE MAXIMUM ORDINATE DIFFERE    5710
   3NCE.'/,'0WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.    5720
   4')                                                                     5730
432 FORMAT ('0RESTRAINTS TO HOLD X(1) AND X(5) POSITIVE HAVE BEEN APPL    5740
   1IED.')                                                                 5750
433 FORMAT ('0RESTRAINTS TO HOLD THE HALF-WIDTHS BETWEEN 1 AND 50 CM.-    5760
   1-1 HAVE BEEN APPLIED.')                                                5770
434 FORMAT (F15.5,50X,7HPRODUCT)                                          5780
435 FORMAT (F15.5,54X,3HSUM)                                              5790
436 FORMAT ('0TERMINATED BECAUSE OF SLOW CONVERGENCE.'/)                   5800
437 FORMAT ('0TERMINATED BY ITERATION LIMIT.'/)                           5810
438 FORMAT ('0TERMINATED BY LOW VALUE OF GL.'/)                           5820
439 FORMAT ('0TERMINATED BY TIME LIMITATION.'/)                           5830
440 FORMAT ('0TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VA    5840
   1LUE.'/)                                                                5850
    END                                                                    5860
```

```
C                                                                       5870
C                                                                       5880
C     ***************************************************************   5890
C                                                                       5900
C                                                                       5910
      SUBROUTINE SORT1 (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)            5920
C                                                                       5930
C     SUBROUTINE SORT CHECKS FOR ERRORS IN THE INPUT WAVENUMBER DATA.   5940
C     A LIMITED NUMBER OF WAVENUMBER SEQUENCE ERRORS ARE CORRECTED      5950
C          BUT SEQUENCE ERRORS IN EXCESS OF 160 DATA POINTS (20 CARDS)  5960
C          OR ANY OTHER TYPE OF WAVENUMBER ERROR WILL TERMINATE THE     5970
C          COMPUTATION,AS ALSO WILL A DISCREPANCY BETWEEN IWB AND THE   5980
C          STARTING WAVENUMBER.                                         5990
C     THE WAVENUMBER POSITIONS OF THE CORRECTIONS AND OF A TERMINATING  6000
C          ERROR ARE RECORDED.                                          6010
C     IF CORRECTIONS ARE MADE,CORRECTED INPUT DATA ARE LISTED IN FULL.  6020
C     IF A TERMINATING ERROR IS FOUND THE UNCORRECTED INPUT DATA ARE    6030
C          LISTED IN FULL.                                              6040
C                                                                       6050
      DIMENSION IX(2000),IY(2000),ITEMPX(160),X1(160),ITEMPY(160)       6060
      IF (IX(1).EQ.IWB) GO TO 10                                        6070
      WRITE (IPRNT,456)                                                 6080
      KLENUP=2                                                          6090
      RETURN                                                            6100
   10 MM=1                                                              6110
      DO 11 I=2,NP                                                      6120
      IW=IWB-IWI*(I-1)                                                  6130
      IF (IW.EQ.IX(I)) GO TO 11                                         6140
      XX=IX(I)                                                          6150
      TEST=(WB-0.1*XX)/WI                                               6160
      NTEST=TEST+0.005                                                  6170
      IF (ABS(TEST-NTEST).GT.0.005) GO TO 12                            6180
      ITEMPX(MM)=IX(I)                                                  6190
      ITEMPY(MM)=IY(I)                                                  6200
      MM=MM+1                                                           6210
      IF (MM.GT.160) GO TO 13                                           6220
   11 CONTINUE                                                          6230
      IF (MM.GT.1) GO TO 14                                             6240
      WRITE (IPRNT,451)                                                 6250
   15 KLENUP=1                                                          6260
      RETURN                                                            6270
   12 XX1=IX(I-1)*0.1-WI                                                6280
      WRITE (IPRNT,452) XX1                                             6290
   16 KLENUP=2                                                          6300
      RETURN                                                            6310
   13 WRITE (IPRNT,453)                                                 6320
      WRITE (IPRNT,455) (IX(I),IY(I), I=1,NP)                           6330
      GO TO 16                                                          6340
   14 NN=MM-1                                                           6350
      DO 17 MM=1,NN                                                     6360
      K1=1+(IWB-ITEMPX(MM))/IWI                                         6370
      IX(K1)=ITEMPX(MM)                                                 6380
      IY(K1)=ITEMPY(MM)                                                 6390
   17 X1(MM)=IX(K1)*0.1                                                 6400
```

```
      WRITE (IPRNT,450)  (X1(MM),MM=1,NN)                                    6410
      WRITE (IPRNT,454)  (IX(I),IY(I),I=1,NP)                                6420
      GO TO 15                                                               6430
  450 FORMAT ('0WAVENUMBER CORRECTIONS AT'/,12(2X,F6.1,2X))                  6440
  451 FORMAT ('0WAVENUMBER SEQUENCE IS CORRECT.')                            6450
  452 FORMAT ('0TERMINATED BY ERROR AT',F6.1,6H CM.-1)                       6460
  453 FORMAT ('0TERMINATED BY MULTIPLE WAVENUMBER SEQUENCE ERRORS.')         6470
  454 FORMAT ('0REARRANGED INPUT.'/,9(4X,2I5))                               6480
  455 FORMAT ('0UNCORRECTED INPUT.'/,9(4X,2I5))                              6490
  456 FORMAT ('0TERMINATED BY AN ERROR IN THE STARTING WAVENUMBER.')         6500
      END                                                                    6510
```

```
C                                                                       6520
CC                                                                      6530
C     ********************************************************************6540
C                                                                       6550
      SUBROUTINE POINT1 (X,PC,PG,W,AC,M,N,CAY,KURVE)                    6560
C                                                                       6570
CC    SUBROUTINE POINT CALCULATES THE ORDINATES OF THE COMPUTED BAND     6580
C          ENVELOPE.                                                    6590
      DIMENSION X(81),PC(20),PG(20)                                     6600
      AC=0.0                                                            6610
      DO 10 I=1,M                                                       6620
      J=I+M                                                             6630
      K=J+M                                                             6640
      L=K+M                                                             6650
      R=W-X(J)                                                          6660
      RSQ=R*R                                                           6670
      PC(I)=1.0/(1.0+X(K)*X(K)*RSQ)                                     6680
      IF (KURVE.EQ.2) GO TO 12                                          6690
      PG(I)=X(L)*X(L)*RSQ                                               6700
      GO TO 13                                                          6710
   12 PG(I)=CAY*CAY*X(K)*X(K)*RSQ                                       6720
   13 IF (PG(I).LT.10.0) GO TO 14                                       6730
      PG(I)=0.0                                                         6740
      GO TO 16                                                          6750
   14 PG(I)=EXP(-PG(I))                                                 6760
   16 IF (KURVE.EQ.2) GO TO 17                                          6770
      AC= X(I)*PC(I)*PG(I)+AC                                           6780
      GO TO 10                                                          6790
   17 AC=X(I)*PC(I)+X(L)*PG(I)+AC                                       6800
   10 CONTINUE                                                          6810
      AC=AC+X(N)                                                        6820
      RETURN                                                            6830
      END                                                               6840
```

```
PITHA AND JONES.   PROGRAM X (PC-116)  SPECTRAL BAND FIT OPTIMIZATION PROGRAM BASIC VERSION.

FEBRUARY 2ND.1968    PROGRAM X (PC-116)
FOUR BAND TEST DECK.          PRODUCT FUNCTION.

INPUT PARAMETERS.
                  DOWN  0.100000E-01        UP  0.100000E 04        CHANGE  0.500000E 00

                  NP   200                  WB  1000.0              WI  0.5

WAVENUMBER SEQUENCE IS CORRECT.

              X(1)                X(2)                X(3)                X(4)
            0.27000             968.50000           0.18000             0.12000
            0.62000             957.00000           0.22000             0.18000
            0.32000             941.00000           0.12000             0.12000
            0.37000             918.00000           0.22000             0.12000
   ALPHA = 0.02000
   ------------------------------------------------------------------------------
    FS  0.2960E 01        GL  0.1623E 02        WFM  952.5        FM  0.2766E 00        NIT  0    ISECS    2
    FS  0.1804E 00        GL  0.1174E 01        WFM  953.5        FM  0.9665E-01        NIT  1    ISECS    6
    FS  0.8375E-02        GL  0.2064E 00        WFM  957.5        FM  0.2904E-01        NIT  2    ISECS    9
    FS  0.3347E-04        GL  0.1325E-01        WFM  952.0        FM  0.1428E-02        NIT  3    ISECS   13
    FS  0.1748E-04        GL  0.2013E-03        WFM  969.5        FM  0.7316E-03        NIT  4    ISECS   17

TERMINATED BECAUSE OF SLOW CONVERGENCE.

   ------------------------------------------------------------------------------
OUTPUT PARAMETERS
                FSM  0.174846E-04       DIS  0.295674E-03       FM  0.731587E-03       WFM  969.5

              X(1)                X(2)                X(3)                X(4)
            0.29972             969.99951           0.19925             0.10054
            0.59997             954.99902           0.20020             0.19981
            0.29993             939.99756           0.09980             0.10013
            0.39994             920.00098           0.20006             0.09998
   ALPHA = 0.05004

SOLVED FOR PRODUCT,CAUCHY OR GAUSS FUNCTION.
(PURE CAUCHY IF X(4)=0 OR PURE GAUSS IF X(3)=0)

FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.

DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEAN SQUARE OF THE RESIDUALS).

FM IS THE MAXIMUM ORDINATE DIFFERENCE.

WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.
```

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PITHA AND JONES.   PROGRAM X (PC-116)  SPECTRAL BAND FIT OPTIMIZATION PROGRAM BASIC VERSION.

FEBRUARY 2ND.1968   PROGRAM X (PC-116)
FOUR BAND TEST DECK.          SUM FUNCTION        CAY = 0.8

INPUT PARAMETERS.
                DOWN  0.100000E-01      UP  0.100000E 04      CHANGE  0.500000E 00

                NP  200                 WB  1000.0            WI  0.5

WAVENUMBER SEQUENCE IS CORRECT.

          X(1)            X(2)            X(3)            X(4)            X(5)
        0.18000        968.00000        0.18000         0.14400         0.11000
        0.37000        953.00000        0.22000         0.17600         0.22000
        0.10000        942.00000        0.11000         0.08800         0.18000
        0.26000        919.00000        0.21000         0.16800         0.16000
  ALPHA = 0.02000
  ------------------------------------------------------------------------------
  FS  0.1341E 01    GL  0.1568E 02    WFM  927.5    FM  0.1469E 00    NIT  0   ISECS   2
  FS  0.3667E-01    GL  0.6070E 00    WFM  956.5    FM  0.3637E-01    NIT  1   ISECS   6
  FS  0.2021E-02    GL  0.1412E 00    WFM  968.0    FM  0.8336E-02    NIT  2   ISECS  10
  FS  0.2904E-04    GL  0.3383E-01    WFM  985.5    FM  0.1129E-02    NIT  3   ISECS  13
  FS  0.1548E-04    GL  0.3633E-02    WFM  985.5    FM  0.8870E-03    NIT  4   ISECS  17

TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VALUE.

  ------------------------------------------------------------------------------
OUTPUT PARAMETERS
          FSM  0.153626E-04     DIS  0.277151E-03      FM  0.887036E-03      WFM  985.5

          X(1)            X(2)            X(3)            X(4)            X(5)
        0.20042        970.00488        0.20018         0.16015         0.09910
        0.40776        954.99878        0.19969         0.15975         0.19399
        0.09552        939.97925        0.10035         0.08028         0.20338
        0.25119        920.00195        0.19965         0.15972         0.14941
  ALPHA = 0.04997

SOLVED FOR SUM FUNCTION WITH X4 = 0.80 X3.

FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.

DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEAN SQUARE OF THE RESIDUALS).

FM IS THE MAXIMUM ORDINATE DIFFERENCE.

WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.
```

PROGRAM XI

PROGRAM XI

Band Fit Optimization Program with Moving Subspace

(PC-117)

This program was developed to deal with long sections of spectra. It will probably prove more efficient and economic in computer time than the Basic Version if the number of bands exceeds about twelve, but this has not been systematically examined. When fitting long sections of spectra it is our current practice to break the curve into units of 8 to 12 bands and optimize the sections separately using the Basic Version. The complete curve is then processed through the Multiplet Version using the output indices from the sectionally optimized computations as input indices. Such a "trimmer run" effectively smooths the break points. The program described here is dimensioned for a maximum of 20 bands and 2000 data points.

Equation [6] may be rewritten

$$TC_{(W)} = EXP - \left[\sum_{I=1}^{I=K} \psi_I(\underline{X},W) + \left\{ X_{(N)} + \sum_{I=K+1}^{I=K+MULT} \psi_I(\underline{X},W) \right\} + \sum_{I=K+MULT+1}^{I=M} \psi_I(\underline{X},W) \right] \quad [33]$$

where

$$\psi_I(\underline{X},W) = X_{(I)} \left(1 + X^2_{(I+2M)} \left(W - X_{(I+M)}\right)^2\right)^{-1} \cdot EXP - \left[X^2_{(I+3M)} \left(W - X_{(I+M)}\right)^2 \right] \quad [34]$$

Only the "active subspace" section of the $\underline{X}$ vector within the braces is optimized. As the program is written, this consists of the indices of from two to five consecutive bands together with the baseline variable α. The number of bands in the variable subspace is defined by MULT. The program allows for two iterations within each defined subspace. This number is controlled by the computed GO TO statement following statement 312; it can easily be changed within the program. Having completed the required number of cycles, the subspace shifts by MULT-1 bands so that the terminal band of one subject is carried

as the leading band of the next subset. This process continues until all the bands have been adjusted and the cycle then recommences.

The version of the program published here operates only on the product function; the facility to restrict the half-band widths within the range 1-50 $cm.^{-1}$ under the control of LIMIT=1 is retained, but the NONEG restraint on negative peak heights is not needed.

A multiplet version of the unrestrained sum function is provided in Program XVIII in Bulletin 13.

A. The Input Data

Cards 1 and 2 are the same as for the Basic Version (p. 11).

Card 3 carries nine fixed point instructions in format 9I5; these are consecutively NDATA,IDECK,NP,M,NSEC, NI, MLIST, MULT,LIMIT. The number of bands in the active subspace (range 2-5) is MULT and the other instructions are the same as for the Basic Version (p. 11).

Card 4 carries the two floating point instructions WB and WI in format 2F15.5 (p. 12).

Card 5 carries the floating point instructions for DOWN, UP and CHANGE in format 3F15.5 (p. 12).

Card Deck 6 is the main input data deck carrying the NP experimental data points.

Card Deck 7 is the deck of M cards carrying the 4M input band indices (p. 13).

Card 8 is the input value of the baseline constant α (p. 13).

B. Description of the Multiplet Program

The number of variables in the active subspace, NMULT, is evaluated in the Input Section. The complete set of input indices is read into the array XS(I). N2 and N3 are the index numbers of the initial and terminal bands of the active subspace and ICY is the number of the iteration within the given operational subspace. This may be zero, one or two, under the control of the computed GO TO statement following statement 312.

The major modification from the Basic Version occurs in the Activation Section. This provides for the selection and exchange of the bands in the active subspace. In the first part, ending at statement 180, the values of N2 and N3 are set; N3 is checked against M to determine when a complete cycle has been completed, and in the terminating sequence of the cycle N3 is adjusted to equal M, retaining an increased overlap with the preceding subspace, should this be necessary.

In the DO loop following statement 181, the arrays X(I) and XB(I) of the active subspace are filled from XS(I), and the background index α is added, all ordinate indices have previously been transposed to Napierian absorbance units. In the large DO loop which begins shortly after statement 184, the ordinate contributions from the bands lying outside the active subspace are computed and stored in the array YS(II). They are introduced as needed in Subroutine POINT (X). It should be noted that within the wavenumber range of the active subspace these comprise a wing correction.

The remainder of the program follows that of the Basic Version closely. In the (G,AQ,F) Section, the G vector is calculated along with the elements of the B matrix and of the values of FS for the region within the active subspace. FM and WFM are evaluated over the complete spectrum; a small change in the FORTRAN notation is the replacement of G(I) by PRD(I) for the gradient vector. After the first optimization in a given subspace, the improved values for the indices are transferred to the XB(I) array at statement 312 and the next iteration is initiated. After the second optimization the improved values are transferred to the main array of indices (XS(I)) in the DO loop beginning at statement 330.

The same tests for termination are applied as for the Basic Version, with the exception of the TERM/FSM convergence test which is omitted. The printout lists the active subspace ranges for each iteration cycle so that the regions of the spectrum most sensitive to the optimization process are readily identified. When setting up the program it should be noted that the number of permitted iterations (NI) relates to the total number of iterations, calculated as two for each active subspace for each cycle through the spectrum.

This program calls the library subroutines SETCLK and RDCLK which are discussed in Bulletin 11. If these are not available appropriate alterations have to be made to the program.

The four band test data set (Figure 1) is used with the bands taken two at a time (MULT=2).

```
C                                                                       10
C     ***************************************************************** 20
C     *                                                               * 30
C     *                  SPECTRAL BAND FIT PROGRAM                    * 40
C     *                                                               * 45
C     *              VERSION WITH MOVING SUBSPACE.                    * 50
C     *                                                               * 55
C     ***************************************************************** 60
C                                                                       70
C     J.PITHA AND R.N.JONES,DIVISION OF CHEMISTRY,NATIONAL RESEARCH     80
C        COUNCIL OF CANADA,SUSSEX DRIVE,OTTAWA,CANADA.                  90
C                                                                      100
C     PROGRAM XI (PC-117).                          JULY 12TH.1967   110
C                                                                      120
C     THIS PROGRAM WILL FIT A CAUCHY,GAUSS OR PRODUCT FUNCTION TO AN   130
C        INFRARED ABSORPTION BAND ENVELOPE.IT WILL NOT FIT A SUM       140
C        FUNCTION,BUT COULD BE MODIFIED TO DO THIS.                    150
C     THIS VERSION IS DIMENSIONED FOR A MAXIMUM OF TWO THOUSAND DATA   160
C        POINTS AND A MAXIMAL FIVE BAND SUBSPACE WITH ONE BASELINE     165
C        VARIABLE.                                                     170
C     THE TOTAL NUMBER OF BANDS IN THE SPECTRUM IS LIMITED TO TWENTY.  180
C     THE BAND INTENSITY INDICES ARE IN ABSORBANCE UNITS BUT THE       190
C        COMPUTATIONS WITHIN THE PROGRAM USE NAPIERIAN LOGARITHMS.     200
C     THE EXPERIMENTAL DATA ARE IN UNITS OF WAVENUMBER X10 AND         210
C        TRANSMITTANCE X 1000.                                         220
C     THE INPUT WAVENUMBER SEQUENCE IS CHECKED BY SUBROUTINE SORT.     230
C     FOR DETAILS SEE N.R.C.C. BULLETIN NO.12.                         240
C                                                                      250
C     ************************ INITIAL SECTION ************************ 260
C                                                                      270
      DIMENSION IX(2000),IY(2000),Y(2000),X(21),XP(21),XB(21),PRD(21), 280
     1AM(21),PC(5),PG(5),YS(2000),AQ(231),A(21,22),XS(81),GAST(21),    290
     2DIA(21),HEAD1(20),HEAD2(20)                                      300
      IRD=1                                                            310
      IPCH=2                                                           320
      IPRNT=3                                                          330
   11 WRITE (IPRNT,400)                                                340
      READ (IRD,401) HEAD1                                             350
      READ (IRD,401) HEAD2                                             360
C                                                                      370
C     HEAD1 AND HEAD2 ARE HEADING CARDS.THEY MAY CARRY ANY DESIRED     380
C        INFORMATION.                                                  390
C                                                                      400
      READ (IRD,403) NDATA,IDECK,NP,M,NSEC,NI,MLIST,MULT,LIMIT         410
C                                                                      420
C     USE NDATA=1 FOR PROCESSING A SINGLE DATA DECK OR THE LAST DECK OF 430
C        A SERIES AND USE NDATA=2 FOR CONSECUTIVE DATA DECKS.          440
C                                                                      450
C     USE IDECK=1 FOR PRINTED OUTPUT AND IDECK=2 FOR BOTH PRINTED AND  460
C        CARD OUTPUT.                                                  470
C                                                                      480
C     NP IS THE NUMBER OF DATA POINTS.                                 490
C                                                                      500
C     M IS THE NUMBER OF CALCULATED BANDS.                             510
```

```
C                                                                       520
C     NSEC IS THE MAXIMUM PERMITTED COMPUTATION TIME IN SECONDS.        530
C                                                                       540
C     NI IS THE MAXIMUM NUMBER OF PERMITTED ITERATIONS.                 550
C                                                                       560
C     MLIST CONTROLS THE AMOUNT OF INFORMATION REPORTED ABOUT THE       570
C          PROGRESS OF THE COMPUTATION.                                 580
C                                                                       590
C          USE MLIST=1 FOR MINIMAL PROGRESS REPORT AND FINAL OUTPUT ONLY 600
C          USE MLIST=2 FOR ADDITIONAL INFOPMATION ON THE EXTREME VALUES 610
C             OF THE B MATRIX ELEMENTS DURING EACH ITERATION.           620
C          USE MLIST=3 TO PRINT RESTRAINTS APPLIED BY LIMIT.            630
C          USE MLIST=4 FOR COMBINATION OF MLIST=2 + MLIST=3.            640
C                                                                       650
C     USE LIMIT=1 TO RESTRICT THE HALF-WIDTHS OF THE COMPONENT BANDS    660
C          WITHIN THE RANGE 1-50 CM.-1                                  670
C          IF LIMIT=2 NO RESTRICTION TO THE HALF-BAND WIDTH IS APPLIED. 680
C                                                                       690
C     MULT IS THE NUMBER OF BANDS IN THE VARIABLE SUBSPACE (MAXIMUM 5)  700
C                                                                       710
      READ (IRD,404) WB,WI                                              720
C                                                                       730
C     WB AND WI ARE THE STARTING WAVENUMBER AND THE WAVENUMBER ENCODING 740
C          INTERVAL IN CM.-1   BY CONVENTION WI IS POSITIVE FOR A       750
C          DIMINISHING WAVENUMBER SEQUENCE.                             760
C                                                                       770
      IF (IDECK.EQ.1) GO TO 12                                          780
      WRITE (IPCH,401) HEAD1                                            790
      WRITE (IPCH,401) HEAD2                                            800
   12 WRITE (IPRNT,402) HEAD1                                           810
      WRITE (IPRNT,402) HEAD2                                           820
      WRITE (IPRNT,408)                                                 830
      READ (IRD,404) DOWN,UP,CHANGE                                     840
      WRITE (IPRNT,409) DOWN,UP,CHANGE                                  850
C                                                                       860
C     DOWN,UP AND CHANGE REGULATE SEARCH FOR THE OPTIMAL DAMPING FACTOR.870
C     RECOMMENDED TRIAL VALUES ARE DOWN = 0.01  UP = 1000.0  CHANGE =0.5 880
C                                                                       890
      IF (LIMIT.EQ.2) GO TO 15                                          900
      IF (MLIST.LT.3) WRITE (IPRNT,430)                                 910
   15 READ (IRD,405) (IX(I),IY(I),I=1,NP)                               920
      WRITE (IPRNT,423) NP,WB,WI                                        930
      IWB=WB*10.0+0.5                                                   940
      IWI=WI*10.0+0.5                                                   950
      CALL SORT (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)                   960
      IF (KLENUP.EQ.1) GO TO 30                                         970
   20 IF (NDATA.EQ.2) GO TO 11                                          980
      STOP                                                              990
   30 DO 31 I=1,NP                                                     1000
   31 Y(I)=IY(I)*0.001                                                 1010
C                                                                      1020
C     ************************  INPUT SECTION  ************************1030
C                                                                      1040
      CALL SETCLK                                                      1050
```

```
C                                                                       1060
C     SETCLK IS A TIMING SUBROUTINE.                                    1070
C                                                                       1080
      N=4*M+1                                                           1090
      NIT=0                                                             1100
      P1=0.1                                                            1110
      NMULT=4*MULT+1                                                    1120
      N1MULT=NMULT+1                                                    1130
      NAL=NMULT*N1MULT/2                                                1140
      WRITE (IPRNT,416)                                                 1150
      DO 153 I=1,M                                                      1160
      J=I+M                                                             1170
      K=J+M                                                             1180
      L=K+M                                                             1190
C                                                                       1200
C     XS(I),XS(J),XS(K),XS(L) ARE THE SPECTRAL INDICES OF EACH BAND.    1210
C                                                                       1220
      READ (IRD,404) XS(I),XS(J),XS(K),XS(L)                            1230
      WRITE (IPRNT,410) XS(I),XS(J),XS(K),XS(L)                         1240
      XS(I)=2.30258*XS(I)                                               1250
  153 CONTINUE                                                          1260
      READ (IRD,404) XS(N)                                              1270
      WRITE (IPRNT,418) XS(N)                                           1280
      XS(N)=2.30258*XS(N)                                               1290
C                                                                       1300
C     ONLY THE DIMENSION OF X(S) DEFINES THE MAXIMUM NUMBER OF BANDS    1310
C          IN THE SPECTRUM.                                             1320
C                                                                       1330
C     **********************  ACTIVATION SECTION  **********************1340
C                                                                       1350
      ICY=0                                                             1360
      N2=1                                                              1370
      N3=MULT                                                           1380
      GO TO 175                                                         1390
  176 ICY=0                                                             1400
      IF (N3.NE.M) GO TO 177                                            1410
      N2=-MULT+2                                                        1420
  177 N2=N2+MULT-1                                                      1430
      N3=N2+MULT-1                                                      1440
      IF (N3-M) 175,179,180                                             1450
  180 N2=M-MULT-MULT+2                                                  1460
      GO TO 176                                                         1470
  179 IADBL=1                                                           1480
      GO TO 181                                                         1490
  175 IF (N2-1) 314,182,183                                             1500
  182 IADBL=2                                                           1510
      GO TO 181                                                         1520
  183 IADBL=3                                                           1530
  181 II=0                                                              1540
      DO 184 I=N2,N3                                                    1550
      II=II+1                                                           1560
      JJ=II+MULT                                                        1570
      KK=JJ+MULT                                                        1580
      LL=KK+MULT                                                        1590
```

```
      X(II)=XS(I)                                                        1600
      XB(II)=X(II)                                                       1610
      IPC=I+M                                                            1620
      X(JJ)=XS(IPC)                                                      1630
      XB(JJ)=X(JJ)                                                       1640
      IPC=IPC+M                                                          1650
      X(KK)=XS(IPC)                                                      1660
      XB(KK)=X(KK)                                                       1670
      IPC=IPC+M                                                          1680
      X(LL)=XS(IPC)                                                      1690
  184 XB(LL)=X(LL)                                                       1700
      X(NMULT)=XS(N)                                                     1710
      XB(NMULT)=X(NMULT)                                                 1720
      DO 185 II=1,NP                                                     1730
      W=IX(II)*0.1                                                       1740
      YS(II)=0.0                                                         1750
      IF (IADBL.EQ.2) GO TO 187                                          1760
      IPO=N2-1                                                           1770
      DO 188 I=1,IPO                                                     1780
      IPC=I+M                                                            1790
      R=W-XS(IPC)                                                        1800
      RSQ=R*R                                                            1810
      IPC=IPC+M+M                                                        1820
      PGS=XS(IPC)*XS(IPC)*RSQ                                            1830
      IF (PGS.GE.10.0) GO TO 188                                         1840
      IPC=IPC-M                                                          1850
      PGL=XS(IPC)*XS(IPC)*RSQ                                            1860
      IF (PGL.GE.10000.0) GO TO 188                                      1870
      YS(II)=YS(II)+XS(I)/(1.+PGL)*EXP(-PGS)                             1880
  188 CONTINUE                                                           1890
      IF (IADBL.EQ.1) GO TO 185                                          1900
  187 IPO=N3+1                                                           1910
      DO 189 I=IPO,M                                                     1920
      IPC=I+M                                                            1930
      R=W-XS(IPC)                                                        1940
      RSQ=R*R                                                            1950
      IPC=IPC+M+M                                                        1960
      PGS=XS(IPC)*XS(IPC)*RSQ                                            1970
      IF (PGS.GE.10.0) GO TO 189                                         1980
      IPC=IPC-M                                                          1990
      PGL=XS(IPC)*XS(IPC)*RSQ                                            2000
      IF (PGL.GE.10000.0) GO TO 189                                      2010
      YS(II)=YS(II)+XS(I)/(1.0+PGL)*EXP(-PGS)                            2020
  189 CONTINUE                                                           2030
  185 CONTINUE                                                           2040
C                                                                        2050
CC    ************************  (G,AQ,F) SECTION  ***********************2060
C                                                                        2070
  200 DO 201 I=1,NMULT                                                   2080
  201 PRD(I)=0.0                                                         2090
      DO 202 I=1,NAL                                                     2100
  202 AQ(I)=0.0                                                          2110
      ICY=ICY+1                                                          2120
      FS=0.0                                                             2130
```

```
      FM=0.0                                                            2140
      FS1=1.0E10                                                        2150
      FS2=1.0E10                                                        2160
      P1L=P1                                                            2170
      IT=1                                                              2180
      DO 218 II=1,NP                                                    2190
      W=IX(II)*0.1                                                      2200
      CALL POINT (X,MULT,NMULT,II,W,AC,PC,PG,YS)                        2210
      TC=EXP(-AC)                                                       2220
      F=Y(II)-TC                                                        2230
      FA=ABS(F)                                                         2240
      IF (FM.GE.FA) GO TO 206                                           2250
      FM=FA                                                             2260
      WFM=W                                                             2270
  206 FS=FS+F*F                                                         2280
      DO 209 I=1,MULT                                                   2290
      J=I+MULT                                                          2300
      K=J+MULT                                                          2310
      L=K+MULT                                                          2320
      AM(I)=TC*PG(I)*PC(I)                                              2330
      R=W-X(J)                                                          2340
      SP=2.0*AM(I)*X(I)*R                                               2350
      AM(J)=SP*(X(L)*X(L)+X(K)*X(K)*PC(I))                              2360
      AM(K)=-SP*R*X(K)*PC(I)                                            2370
  209 AM(L)=-SP*R*X(L)                                                  2380
      AM(NMULT)=TC                                                      2390
      IM=0                                                              2400
      DO 218 I=1,NMULT                                                  2410
      AMI=AM(I)                                                         2420
      PRD(I)=PRD(I)+AMI*F                                               2430
      DO 218 IJ=I,NMULT                                                 2440
      IM=IM+1                                                           2450
  218 AQ(IM)=AQ(IM)+AMI*AM(IJ)                                          2460
      FSM=FS                                                            2470
      IM=0                                                              2480
      DO 219 I=1,NMULT                                                  2490
      DO 219 IJ=I,NMULT                                                 2500
      IM=IM+1                                                           2510
  219 A(I,IJ)=AQ(IM)                                                    2520
      ADMIN=1.0E+10                                                     2530
      ADMAX=-1.0E+10                                                    2540
      DO 227 I=1,NMULT                                                  2550
      GO TO (224,220,224,220),MLIST                                     2560
  220 IF (A(I,I).GE.ADMIN) GO TO 221                                    2570
      ADMIN=A(I,I)                                                      2580
      MINAD=I                                                           2590
  221 IF (ADMAX.GE.A(I,I)) GO TO 224                                    2600
      ADMAX=A(I,I)                                                      2610
      MAXAD=I                                                           2620
  224 IF (A(I,I).GT.1.0E-10) GO TO 226                                  2630
      DIA(I)=0.0                                                        2640
      GO TO 227                                                         2650
  226 DIA(I)=1.0/(SQRT(A(I,I)))                                         2660
  227 GAST(I)=PRD(I)*DIA(I)                                             2670
```

```
      IM=0                                                              2680
      AMIN=1.0E+10                                                      2690
      AMAX=-1.0E-10                                                     2700
      DO 228 I=1,NMULT                                                  2710
      DIAI=DIA(I)                                                       2720
      DO 228 IJ=I,NMULT                                                 2730
      IM=IM+1                                                           2740
      AQ(IM)=A(I,IJ)*DIAI*DIA(IJ)                                       2750
      GO TO (228,229,228,229),MLIST                                     2760
  229 IF (I.EQ.IJ) GO TO 228                                            2770
      IF(AQ(IM).GE.AMIN) GO TO 231                                      2780
      AMIN=AQ(IM)                                                       2790
      MINA1=I                                                           2800
      MINA2=IJ                                                          2810
  231 IF (AMAX.GE.AQ(IM)) GO TO 228                                     2820
      AMAX=AQ(IM)                                                       2830
      MAXA1=I                                                           2840
      MAXA2=IJ                                                          2850
  228 CONTINUE                                                          2860
      GL=0.0                                                            2870
      DO 233 I=1,NMULT                                                  2880
      PRDI=PRD(I)                                                       2890
  233 GL=GL+PRDI*PRDI                                                   2900
      SM=-2.0*GL                                                        2910
      GL=SQRT(GL)                                                       2920
C                                                                       2930
CC    SM HAS BEEN APPROXIMATED. SEE COMMENT WRITTEN INTO PROGRAM X.     2940
C                                                                       2950
      CALL RDCLK (TIME)                                                 2960
C                                                                       2970
CC    RDCLK IS A TIMING SUBROUTINE.                                     2980
C                                                                       2990
      ISECS=TIME+0.5                                                    3000
      WRITE (IPRNT,407) FS,GL,WFM,FM,NIT,N2,N3,ISECS                    3010
C                                                                       3020
CC    ******************  MATRIX DATA OUTPUT SECTION  ******************3030
C                                                                       3040
      GO TO (249,248,249,248),MLIST                                     3050
  248 WRITE (IPRNT,424) MINAD,MAXAD,ADMIN,ADMAX,MINA1,MINA2,AMIN,MAXA1, 3060
     1MAXA2,AMAX                                                        3070
C                                                                       3080
CC    **********************  (P,INVEPT,XP) SECTION  ********************3090
C                                                                       3100
  249 ISKIP=1                                                           3110
  250 IM=0                                                              3120
      DO 251 I=1,NMULT                                                  3130
      DO 251 IJ=I,NMULT                                                 3140
      IM=IM+1                                                           3150
      AQIM=AQ(IM)                                                       3160
      A(I,IJ)=AQIM                                                      3170
  251 A(IJ,I)=AQIM                                                      3180
      GO TO (260,261,262,263,311),IT                                    3190
  260 P=P1L                                                             3200
      GO TO 265                                                         3210
```

```
261 IF (FS.LE.FS1) GO TO 266                                        3220
    P=P1L*DCWN                                                      3230
    GO TO 265                                                       3240
266 P=P1L*UP                                                        3250
    GO TO 265                                                       3260
262 P=P1*CHANGE                                                     3270
    GO TO 265                                                       3280
263 X3=1.0/P1                                                       3290
    X4=1.0/P2                                                       3300
    DET=X3*X3*X4*X4*X4-X3*X3*X3*X4*X4                               3310
    IF (DET.EQ.0.0) GO TO 269                                       3320
    AP1=X3*X3*(FS2-FS-SM*X4)                                        3330
    AP2=X4*X4*(FS1-FS-SM*X3)                                        3340
    AI=6.0*(AP1-AP2)/DET                                            3350
    BI=2.0*(X4*AP2-X3*AP1)/DET                                      3360
    DET=BI*BI-2.0*AI*SM                                             3370
    IF (DET) 269,279,270                                            3380
270 DET=SQRT(DET)                                                   3390
279 IF (AI.EQ.0.0) GO TO 269                                        3400
    X3=(-BI+DET)/AI                                                 3410
    X4=(-BI-DET)/AI                                                 3420
    IF (X3.LE.0.0) GO TO 272                                        3430
    IF (X4.LE.0.0) GO TO 275                                        3440
    IF (X4.LE.X3) GO TO 274                                         3450
275 P=1.0/X3                                                        3460
    GO TO 265                                                       3470
272 IF (X4.LE.0.0) GO TO 269                                        3480
274 P=1.0/X4                                                        3490
    GO TO 265                                                       3500
269 P=10000.0                                                       3510
271 WRITE (IPRNT,411)                                               3520
265 IT=IT+1                                                         3530
    DO 278 I=1,NMULT                                                3540
    A(I,I)=A(I,I)+P                                                 3550
278 A(I,N1MULT)=-GAST(I)                                            3560
    DO 282 I=1,NMULT                                                3570
    AII=A(I,I)                                                      3580
    IF (AII.EQ.0.0) GO TO 284                                       3590
    PIV=1.0/AII                                                     3600
    DO 281 J=I,N1MULT                                               3610
281 A(I,J)=PIV*A(I,J)                                               3620
    DO 282 K=1,NMULT                                                3630
    IF (I.EQ.K) GO TO 282                                           3640
    Q=A(K,I)                                                        3650
    DO 280 J=I,N1MULT                                               3660
280 A(K,J)=A(K,J)-Q*A(I,J)                                          3670
282 CONTINUE                                                        3680
    GO TO 286                                                       3690
284 IF (ISKIP.EQ.2) GO TO 285                                       3700
    ISKIP=2                                                         3710
    PIL=100.0                                                       3720
    IT=1                                                            3730
    GO TO 250                                                       3740
285 WRITE (IPRNT,412)                                               3750
```

```
      ISKIP=1                                                          3760
      GO TO 314                                                        3770
  286 DO 288 I=1,NMULT                                                 3780
  288 XP(I)=X(I)+A(I,N1MULT)*DIA(I)                                    3790
C                                                                      3800
C     ********** BOUNDARY CONDITIONS TO LIMIT HALF-BAND WIDTH **********3810
C                                                                      3820
      IF (LIMIT.EQ.2) GO TO 298                                        3830
      DO 505 I=1,MULT                                                  3840
      J=I+MULT                                                         3850
      K=J+MULT                                                         3860
      L=K+MULT                                                         3870
      XPK=ABS(XP(K))                                                   3880
      XPL=ABS(XP(L))                                                   3890
      IF (XPL.LE.1.0) GO TO 500                                        3900
      XPL=1.0                                                          3910
      IF (MLIST.LT.3) GO TO 500                                        3920
      WRITE (IPRNT,427) XP(J)                                          3930
  500 IF (XPK.LE.2.0) GO TO 501                                        3940
      XPK=2.0                                                          3950
      IF (MLIST.LT.3) GO TO 506                                        3960
      WRITE (IPRNT,427) XP(J)                                          3970
      GO TO 506                                                        3980
  501 IF (XPK.GT.0.03) GO TO 506                                       3990
      IF (XPL.GT.0.0333) GO TO 506                                     4000
      XPL=0.0333                                                       4010
      IF (MLIST.LT.3) GO TO 506                                        4020
      WRITE (IPRNT,428) XP(J)                                          4030
  506 IF (XP(K).LT.0.0) GO TO 503                                      4040
      XP(K)=XPK                                                        4050
      GO TO 507                                                        4060
  503 XP(K)=-XPK                                                       4070
  507 IF (XP(L).LT.0.0) GO TO 504                                      4080
      XP(L)=XPL                                                        4090
      GO TO 505                                                        4100
  504 XP(L)=-XPL                                                       4110
  505 CONTINUE                                                         4120
      GO TO 298                                                        4130
C                                                                      4140
C     ************************  (FSP) SECTION  ************************4150
C                                                                      4160
  298 FSP=0.0                                                          4170
      JSKIP=1                                                          4180
      KSKIP=1                                                          4190
      DO 301 II=1,NP                                                   4200
      W=IX(II)*0.1                                                     4210
      CALL POINT (XP,MULT,NMULT,II,W,AC,PC,PG,YS)                      4220
      IF (AC.GT.-2.0) GO TO 304                                        4230
      IF (JSKIP.EQ.2) GO TO 300                                        4240
      WRITE (IPRNT,425)                                                4250
      JSKIP=2                                                          4260
  300 TC=7.3891                                                        4270
      GO TO 310                                                        4280
  304 IF (AC.LT.10.0) GO TO 307                                        4290
```

```
      IF (KSKIP.EQ.2) GO TO 302                                          4300
      WRITE (IPRNT,426)                                                  4310
      KSKIP=2                                                            4320
  302 TC=0.000045                                                        4330
      GO TO 310                                                          4340
  307 TC=EXP(-AC)                                                        4350
  310 F=Y(II)-TC                                                         4360
  301 FSP=FSP+F*F                                                        4370
      IF (FSM.LE.FSP) GO TO 303                                          4380
      FSM=FSP                                                            4390
      DO 305 I=1,NMULT                                                   4400
  305 XB(I)=XP(I)                                                        4410
  303 IF (FS1.LE.FSP) GO TO 306                                          4420
      FS2=FS1                                                            4430
      P2=P1                                                              4440
      FS1=FSP                                                            4450
      P1=P                                                               4460
      GO TO 308                                                          4470
  306 IF (FS2.LE.FSP) GO TO 308                                          4480
      P2=P                                                               4490
      FS2=FSP                                                            4500
  308 GO TO (250,309,250,309),MLIST                                      4510
  309 WRITE (IPRNT,414) P,FSP                                            4520
      GO TO 250                                                          4530
  311 DO 312 I=1,NMULT                                                   4540
  312 X(I)=XB(I)                                                         4550
      GO TO (200,330),ICY                                                4560
C                                                                        4570
C     ICY CONTROLS THE NUMBER OF ITERATIONS WITHIN EACH SUBSPACE.        4580
C          THE ABOVE STATEMENT FIXES THIS AT TWO.                        4590
C          FOR THREE CYCLES USE  GO TO (200,200,330),ICY                 4600
C                                                                        4610
C                                                                        4620
  330 II=0                                                               4630
      DO 331 I=N2,N3                                                     4640
      II=II+1                                                            4650
      J=I+M                                                              4660
      K=J+M                                                              4670
      L=K+M                                                              4680
      XS(I)=XB(II)                                                       4690
      IPC=II+MULT                                                        4700
      XS(J)=XB(IPC)                                                      4710
      IPC=IPC+MULT                                                       4720
      XS(K)=XB(IPC)                                                      4730
      IPC=IPC+MULT                                                       4740
  331 XS(L)=XB(IPC)                                                      4750
C                                                                        4760
C     ************************ TERMINAL SECTION ***********************  4770
C                                                                        4780
      XS(N)=XB(NMULT)                                                    4790
      NIT=NIT+1                                                          4800
      IF (NIT.LT.NI) GO TO 315                                           4810
      WRITE (IPRNT,432)                                                  4820
      GO TO 314                                                          4830
  315 IF (GL.GT.0.00001) GO TO 316
```

```
      WRITE (IPRNT,433)                                                 4840
      GO TO 314                                                         4850
  316 IF (ISECS.LE.NSEC) GO TO 317                                      4860
      WRITE (IPRNT,434)                                                 4870
      GO TO 314                                                         4880
  317 IF (FM.GT.0.001) GO TO 176                                        4890
      WRITE (IPRNT,435)                                                 4900
  314 DIS=SQRT(FSM/NP)                                                  4910
      WRITE (IPRNT,415)                                                 4920
      WRITE (IPRNT,419) FSM,DIS,FM,WFM                                  4930
      WRITE (IPRNT,416)                                                 4940
      DO 319 I=1,M                                                      4950
      J=I+M                                                             4960
      K=J+M                                                             4970
      L=K+M                                                             4980
      XS(I)=0.43429*XS(I)                                               4990
      IF (IDECK.EQ.1) GO TO 319                                         5000
      WRITE (IPCH,404) XS(I),XS(J),XS(K),XS(I)                          5010
  319 WRITE (IPRNT,410) XS(I),XS(J),XS(K),XS(L)                         5020
      XS(N)=0.43429*XS(N)                                               5030
      IF (IDECK.EQ.1) GO TO 322                                         5040
      WRITE (IPCH,404) XS(N)                                            5050
  322 WRITE (IPRNT,413) XS(N)                                           5060
      WRITE (IPRNT,429)                                                 5070
      GO TO 20                                                          5080
C                                                                       5090
C                                                                       5100
  400 FORMAT ('1PITHA AND JONES.  PROGRAM XI (PC-117)  SPECTRAL BAND FIT 5110
     1 OPTIMIZATION PROGRAM,VERSION WITH MOVING SUBSPACE.'/)             5120
  401 FORMAT (20A4)                                                     5130
  402 FORMAT (1X,20A4)                                                  5140
  403 FORMAT (9I5)                                                      5150
  404 FORMAT (4F15.5)                                                   5160
  405 FORMAT (8(I5,I4,1X))                                              5170
  407 FORMAT (3X,2HFS,E12.4,5X,2HGL,E12.4,5X,3HWFM,F7.1,5X,2HFM,E12.4,5X 5180
     1,3HNIT,I3,4X,15HBANDS ADJUSTED ,I3,3H TO,I3,5X,5HISECS,I5)        5190
  408 FORMAT ('0INPUT PARAMETERS.')                                     5200
  409 FORMAT (20X,4HDOWN,E14.6,7X,2HUP,E14.6,7X,6HCHANGE,F14.6)         5210
  410 FORMAT (1X,4(6X,F15.5))                                           5220
  411 FORMAT (1X,'TROUBLE WITH EVALUATION OF P,CHECK MATRIX DATA OUTPUT. 5230
     1')                                                                5240
  412 FORMAT (1X,'TERMINATED BY TROUBLE WITH SOLUTION OF EQUATIONS.')    5250
  413 FORMAT (4X,7HALPHA =F8.5/,'0SOLVED FOR PRODUCT,CAUCHY OR GAUSS FUN 5260
     1CTION.'/' (PURE CAUCHY IF X(4)=0 OR PURE GAUSS IF X(3)=0)')       5270
  414 FORMAT (64X,1HP,E14.6,8X,3HFSP,E14.6)                             5280
  415 FORMAT (11X,  '-------------------------------------------------- 5290
     1----------'/1X,17HOUTPUT PARAMETERS)                              5300
  416 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(4))          5310
  418 FORMAT (4X,7HALPHA =,F8.5,/11X,'-------------------------------- 5320
     1-----------------------------------')                            5330
  419 FORMAT (18X,3HFSM,E14.6,7X,3HDIS,E14.6,7X,2HFM,E14.6,7X,3HWFM,F7.1 5340
     1)                                                                 5350
  423 FORMAT ('0',19X,2HNP,I6,17X,2HWB,F8.1,13X,2HWI,F5.1)              5360
  424 FORMAT (4X,5HMINAD,I4,13X,5HMAXAD,I4,12X,5HADMIN,E14.6,5X,5HADMAX, 5370
```

```
   1E14.6/4X,5HMINA1,I4,1X,5HMINA2,I4,3X,4HAMIN,E14.6,3X,5HMAXA1,I4,      5380
   23X,5HMAXA2,I4,3X,4HAMAX,E14.6)                                        5390
425 FORMAT ('0THE MAXIMAL ALLOWED TRANSMITTANCE HAS BEEN EXCEEDED.')      5400
426 FORMAT ('0THE MINIMAL ALLOWED TRANSMITTANCE HAS BEEN EXCEEDED.')      5410
427 FORMAT ('0MINIMAL HALF-WIDTH FOR BAND AT',F7.1,6H CM.-1)              5420
428 FORMAT ('0MAXIMAL HALF-WIDTH FOR BAND AT',F7.1,6H CM.-1)              5430
429 FORMAT ('0FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.'/,           5440
   1'0DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEA    5450
   2N SQUARE OF THE RESIDUALS).'/,'0FM IS THE MAXIMUM ORDINATE DIFFERE    5460
   3NCE.'/,'0WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.    5470
   4')                                                                    5480
430 FORMAT ('0RESTRAINTS TO HOLD THE HALF-WIDTHS BETWEEN 1 AND 50 CM.-    5490
   1-1 HAVE BEEN APPLIED.')                                               5500
432 FORMAT ('0TERMINATED BY ITERATION LIMIT.'/)                           5510
433 FORMAT ('0TERMINATED BY LOW VALUE OF GI.'/)                           5520
434 FORMAT ('0TERMINATED BY TIME LIMITATION.'/)                           5530
435 FORMAT ('0TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VA    5540
   1LUE.'/)                                                               5550
    END                                                                   5560
```

```
C                                                                       5570
CC    ***************************************************************** 5580
C                                                                       5590
      SUBROUTINE SORT (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)             5600
C                                                                       5610
C                                                                       5620
C     SUBROUTINE SORT CHECKS FOR ERRORS IN THE INPUT WAVENUMBER DATA.   5630
C     A LIMITED NUMBER OF WAVENUMBER SEQUENCE ERRORS ARE CORRECTED      5640
C          BUT SEQUENCE ERRORS IN EXCESS OF 160 DATA POINTS (20 CARDS)  5650
C          OR ANY OTHER TYPE OF WAVENUMBER ERROR WILL TERMINATE THE     5660
C          COMPUTATION,AS ALSO WILL A DISCREPANCY BETWEEN IWB AND THE   5670
C          STARTING WAVENUMBER.                                         5680
C     THE WAVENUMBER POSITIONS OF THE CORRECTIONS AND OF A TERMINATING  5690
C          ERROR ARE RECORDED.                                          5700
C     IF CORRECTIONS ARE MADE , CORRECTED INPUT DATA ARE LISTED IN FULL. 5710
C     IF A TERMINATING ERROR IS FOUND THE UNCORRECTED INPUT DATA ARE    5720
C          LISTED IN FULL.                                              5730
C                                                                       5740
      DIMENSION IX(2000),IY(2000),ITEMPX(160),X1(160),ITEMPY(160)       5750
      IF (IX(1).EQ.IWB) GO TO 10                                        5760
      WRITE (IPRNT,456)                                                 5770
      KLENUP=2                                                          5780
      RETURN                                                            5790
   10 MM=1                                                              5800
      DO 11 I=2,NP                                                      5810
      IW=IWB-IWI*(I-1)                                                  5820
      IF (IW.EQ.IX(I)) GO TO 11                                         5830
      XX=IX(I)                                                          5840
      TEST=(WB-0.1*XX)/WI                                               5850
      NTEST=TEST+0.005                                                  5860
      IF (ABS(TEST-NTEST).GT.0.005) GO TO 12                            5870
      ITEMPX(MM)=IX(I)                                                  5880
      ITEMPY(MM)=IY(I)                                                  5890
      MM=MM+1                                                           5900
      IF (MM.GT.160) GO TO 13                                           5910
   11 CONTINUE                                                          5920
      IF (MM.GT.1) GO TO 14                                             5930
      WRITE (IPRNT,451)                                                 5940
   15 KLENUP=1                                                          5950
      RETURN                                                            5960
   12 XX1=IX(I-1)*0.1-WI                                                5970
      WRITE (IPRNT,452) XX1                                             5980
   16 KLENUP=2                                                          5990
      RETURN                                                            6000
   13 WRITE (IPRNT,453)                                                 6010
      WRITE (IPRNT,455) (IX(I),IY(I), I=1,NP)                           6020
      GO TO 16                                                          6030
   14 NN=MM-1                                                           6040
      DO 17 MM=1,NN                                                     6050
      K1=1+(IWB-ITEMPX(MM))/IWI                                         6060
      IX(K1)=ITEMPX(MM)                                                 6070
      IY(K1)=ITEMPY(MM)                                                 6080
   17 X1(MM)=IX(K1)*0.1                                                 6090
      WRITE (IPRNT,450) (X1(MM),MM=1,NN)                                6100
```

```
      WRITE (IPRNT,454) (IX(I),IY(I),I=1,NP)                            6110
      GO TO 15                                                          6120
  450 FORMAT ('0WAVENUMBER CORRECTIONS AT'/,12(2X,F6.1,2X))             6130
  451 FORMAT ('0WAVENUMBER SEQUENCE IS CORRECT.')                       6140
  452 FORMAT ('0TERMINATED BY ERROR AT',F6.1,6H CM.-1)                  6150
  453 FORMAT ('0TERMINATED BY MULTIPLE WAVENUMBER SEQUENCE ERRORS.')    6160
  454 FORMAT ('0REARRANGED INPUT.'/,11(2X,I5,I4))                       6170
  455 FORMAT ('0UNCORRECTED INPUT.'/,11(2X,I5,I4))                      6180
  456 FORMAT ('0TERMINATED BY AN ERROR IN THE STARTING WAVENUMBER.')    6190
      END                                                               6200
```

```
C                                                                       6210
C     ***************************************************************** 6220
C                                                                       6230
      SUBROUTINE POINT (X,MULT,NMULT,II,W,AC,PC,PG,YS)                  6240
C                                                                       6250
C     SUBROUTINE POINT CALCULATES THE ORDINATES OF THE COMPUTED BAND     6260
C          ENVELOPE IN UNITS OF NAPIERIAN ABSORBANCE.                   6270
C                                                                       6280
      DIMENSION X(21),PC(5),PG(5),YS(2000)                              6290
      AC=0.0                                                            6300
      DO 10 I=1,MULT                                                    6310
      J=I+MULT                                                          6320
      K=J+MULT                                                          6330
      L=K+MULT                                                          6340
      R=W-X(J)                                                          6350
      RSQ=R*R                                                           6360
      PC(I)=1.0/(1.0+X(K)*X(K)*RSQ)                                     6370
      PG(I)=X(L)*X(L)*RSQ                                               6380
      IF (PG(I).LT.10.0) GO TO 14                                       6390
      PG(I)=0.0                                                         6400
      GO TO 16                                                          6410
   14 PG(I)=EXP(-PG(I))                                                 6420
   16 AC= X(I)*PC(I)*PG(I)+AC                                           6430
   10 CONTINUE                                                          6440
      AC=AC+X(NMULT)+YS(II)                                             6450
      RETURN                                                            6460
      END                                                               6470
```

PITHA AND JONES. PROGRAM XI (PC-117) SPECTRAL BAND FIT OPTIMIZATION PROGRAM,VERSION WITH MOVING SUBSPACE.

FEBRUARY 5TH.1968. SPECTRAL BAND FIT PROGRAM.
TEST RUN ON FOUR BAND TEST DECK (PRODUCT FUNCTION.) MULT=2.

INPUT PARAMETERS.

DOWN 0.100000E-01 UP 0.100000E 04 CHANGE 0.500000E 00

NP 200 WB 1000.0 WI 0.5

WAVENUMBER SEQUENCE IS CORRECT.

X(1)	X(2)	X(3)	X(4)
0.27000	968.50000	0.18000	0.12000
0.62000	957.00000	0.22000	0.18000
0.32000	941.00000	0.12000	0.12000
0.37000	918.00000	0.22000	0.12000

ALPHA = 0.02000

FS	0.2960E 01	GL	0.1217E 02	WFM	952.5	FM	0.2766E 00	NIT	0	BANDS ADJUSTED	1	TO	2	ISECS	1
FS	0.7930E 00	GL	0.1442E 01	WFM	923.0	FM	0.1917E 00	NIT	0	BANDS ADJUSTED	1	TO	2	ISECS	2
FS	0.6488E 00	GL	0.1948E 01	WFM	923.0	FM	0.1811E 00	NIT	1	BANDS ADJUSTED	2	TO	3	ISECS	4
FS	0.4222E 00	GL	0.1912E 01	WFM	922.5	FM	0.1697E 00	NIT	1	BANDS ADJUSTED	2	TO	3	ISECS	5
FS	0.4145E 00	GL	0.2041E 01	WFM	922.5	FM	0.1686E 00	NIT	2	BANDS ADJUSTED	3	TO	4	ISECS	7
FS	0.4980E-01	GL	0.8782E 00	WFM	921.0	FM	0.5031E-01	NIT	2	BANDS ADJUSTED	3	TO	4	ISECS	8
FS	0.1520E-01	GL	0.3982E 00	WFM	976.5	FM	0.2200E-01	NIT	3	BANDS ADJUSTED	1	TO	2	ISECS	10
FS	0.7260E-02	GL	0.1395E 00	WFM	912.5	FM	0.1416E-01	NIT	3	BANDS ADJUSTED	1	TO	2	ISECS	11
FS	0.6373E-02	GL	0.1589E 00	WFM	912.5	FM	0.1433E-01	NIT	4	BANDS ADJUSTED	2	TO	3	ISECS	13
FS	0.5634E-02	GL	0.2422E-01	WFM	911.5	FM	0.1395E-01	NIT	4	BANDS ADJUSTED	2	TO	3	ISECS	14
FS	0.5549E-02	GL	0.8813E-01	WFM	929.5	FM	0.1398E-01	NIT	5	BANDS ADJUSTED	3	TO	4	ISECS	16
FS	0.4727E-02	GL	0.9772E-02	WFM	929.5	FM	0.1402E-01	NIT	5	BANDS ADJUSTED	3	TO	4	ISECS	17
FS	0.4704E-02	GL	0.1018E 00	WFM	929.5	FM	0.1385E-01	NIT	6	BANDS ADJUSTED	1	TO	2	ISECS	19
FS	0.4346E-02	GL	0.4659E-02	WFM	929.5	FM	0.1292E-01	NIT	6	BANDS ADJUSTED	1	TO	2	ISECS	20
FS	0.4344E-02	GL	0.2231E-01	WFM	929.5	FM	0.1292E-01	NIT	7	BANDS ADJUSTED	2	TO	3	ISECS	22
FS	0.4249E-02	GL	0.6866E-02	WFM	929.5	FM	0.1260E-01	NIT	7	BANDS ADJUSTED	2	TO	3	ISECS	23
FS	0.4237E-02	GL	0.9201E-01	WFM	929.5	FM	0.1230E-01	NIT	8	BANDS ADJUSTED	3	TO	4	ISECS	25
FS	0.3757E-02	GL	0.1337E-01	WFM	929.5	FM	0.1250E-01	NIT	8	BANDS ADJUSTED	3	TO	4	ISECS	26
FS	0.3690E-02	GL	0.1308E 00	WFM	929.5	FM	0.1206E-01	NIT	9	BANDS ADJUSTED	1	TO	2	ISECS	28
FS	0.3187E-02	GL	0.1339E-02	WFM	929.5	FM	0.1116E-01	NIT	9	BANDS ADJUSTED	1	TO	2	ISECS	29
FS	0.3187E-02	GL	0.4029E-01	WFM	929.5	FM	0.1116E-01	NIT	10	BANDS ADJUSTED	2	TO	3	ISECS	30
FS	0.2831E-02	GL	0.1173E-01	WFM	911.5	FM	0.9537E-02	NIT	10	BANDS ADJUSTED	2	TO	3	ISECS	32
FS	0.2799E-02	GL	0.1410E 00	WFM	911.5	FM	0.9668E-02	NIT	11	BANDS ADJUSTED	3	TO	4	ISECS	33
FS	0.1751E-02	GL	0.2589E-01	WFM	929.5	FM	0.7358E-02	NIT	11	BANDS ADJUSTED	3	TO	4	ISECS	35
FS	0.1703E-02	GL	0.1456E 00	WFM	929.5	FM	0.6972E-02	NIT	12	BANDS ADJUSTED	1	TO	2	ISECS	36
FS	0.1130E-02	GL	0.1520E-02	WFM	935.5	FM	0.6287E-02	NIT	12	BANDS ADJUSTED	1	TO	2	ISECS	38
FS	0.1130E-02	GL	0.4343E-01	WFM	935.5	FM	0.6284E-02	NIT	13	BANDS ADJUSTED	2	TO	3	ISECS	39
FS	0.8693E-03	GL	0.1256E-01	WFM	911.5	FM	0.5663E-02	NIT	13	BANDS ADJUSTED	2	TO	3	ISECS	41
FS	0.8650E-03	GL	0.1043E 00	WFM	923.0	FM	0.5736E-02	NIT	14	BANDS ADJUSTED	3	TO	4	ISECS	42
FS	0.3722E-03	GL	0.1918E-01	WFM	952.0	FM	0.3921E-02	NIT	14	BANDS ADJUSTED	3	TO	4	ISECS	44
FS	0.3667E-03	GL	0.7364E-01	WFM	952.0	FM	0.3991E-02	NIT	15	BANDS ADJUSTED	1	TO	2	ISECS	45
FS	0.2228E-03	GL	0.3177E-03	WFM	911.5	FM	0.2708E-02	NIT	15	BANDS ADJUSTED	1	TO	2	ISECS	47
FS	0.2229E-03	GL	0.2690E-01	WFM	911.5	FM	0.2707E-02	NIT	16	BANDS ADJUSTED	2	TO	3	ISECS	48
FS	0.1598E-03	GL	0.3752E-02	WFM	911.5	FM	0.2609E-02	NIT	16	BANDS ADJUSTED	2	TO	3	ISECS	50
FS	0.1582E-03	GL	0.4640E-01	WFM	911.5	FM	0.2608E-02	NIT	17	BANDS ADJUSTED	3	TO	4	ISECS	51
FS	0.6775E-04	GL	0.4838E-02	WFM	952.0	FM	0.1808E-02	NIT	17	BANDS ADJUSTED	3	TO	4	ISECS	53
FS	0.6751E-04	GL	0.2774E-01	WFM	952.0	FM	0.1809E-02	NIT	18	BANDS ADJUSTED	1	TO	2	ISECS	54
FS	0.4615E-04	GL	0.9049E-04	WFM	911.5	FM	0.1258E-02	NIT	18	BANDS ADJUSTED	1	TO	2	ISECS	55
FS	0.4615E-04	GL	0.1200E-01	WFM	911.5	FM	0.1257E-02	NIT	19	BANDS ADJUSTED	2	TO	3	ISECS	57
FS	0.3540E-04	GL	0.7229E-03	WFM	911.5	FM	0.1215E-02	NIT	19	BANDS ADJUSTED	2	TO	3	ISECS	58
FS	0.3540E-04	GL	0.1686E-01	WFM	911.5	FM	0.1215E-02	NIT	20	BANDS ADJUSTED	3	TO	4	ISECS	60
FS	0.2380E-04	GL	0.8310E-03	WFM	952.0	FM	0.9263E-03	NIT	20	BANDS ADJUSTED	3	TO	4	ISECS	61

TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VALUE.

OUTPUT PARAMETERS

FSM 0.237940E-04 DIS 0.344920E-03 FM 0.926316E-03 WFM 952.0

X(1)	X(2)	X(3)	X(4)
0.29957	969.99731	0.19913	0.10058
0.59913	955.00244	0.19529	0.20071
0.30001	940.00171	0.10156	0.09881
0.39981	919.99707	0.19991	0.10038

ALPHA = 0.05009

SOLVED FOR PRODUCT,CAUCHY OR GAUSS FUNCTION.
(PURE CAUCHY IF X(4)=0 OR PURE GAUSS IF X(3)=0)

FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.

DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEAN SQUARE OF THE RESIDUALS).

FM IS THE MAXIMUM ORDINATE DIFFERENCE.

WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.

PROGRAM XII

PROGRAM XII

Spectral Band Fit Optimization Program with Slit Deconvolution Correction

(PC-118)

It is well known that the observed spectrum differs from the true spectrum because of systematic errors of an instrumental nature. An important type of distortion can be expressed by the integral equation

$$T(\nu)_{obs} = \frac{\int \rho\,(\nu,\nu') \cdot T(\nu')_{true} d\nu'}{\int \rho\,(\nu,\nu')\, d\nu'} \qquad [35]$$

where $\rho(\nu,\nu')$ is the instrument function. A major factor contributing to this type of distortion is the finite spectral slit width, which is determined by the spectral slit function.

In this version of the band fit program, the spectral slit function is introduced into the computation and $TC_{(W)}$ of equation [6] is caused to approximate $T(\nu)_{true}$ instead of $T(\nu)_{obs}$. There is an extensive literature dealing with the nature and form of the spectral slit function (16), but it is usually sufficient to approximate it with a symmetric triangular function. Computational methods of dealing with equation [35] from the basis of Program V which is described in Bulletin 11. Program V is incorporated into this version of the band fit program with very little modification; and Bulletin 11 should be consulted for a more detailed discussion of the internal logic of the slit convolution procedure than is included here.

The slit function can be introduced in two ways. If MODE=1, a symmetric triangular slit function is assumed, and it is necessary to supply only the spectral slit width (SSW), expressed in $cm.^{-1}$. The program computes and normalizes the spectral slit ordinates. If MODE=2, the program calls for an odd number of slit ordinates (maximum 25), spaced at the wavenumber encoding interval WI. These are entered into the program from cards and permit the use of slit functions of Gaussian, trapezoidal or non-symmetric contour.

This program will fit both the product and the sum functions and will apply the same restraints to the half-band width (with LIMIT=1) and to the sum function ordinate sign (with NONEG=1) as does the Basic Version.

A. The Input Data

Cards 1 and 2 are the same as for the Basic Version.

Card 3 carries eleven fixed point instructions in format 11I5. The first ten are identical with those used with the Basic Version (p. 11) and the sequence is the same. The eleventh is MODE which determines the manner of introducing the slit function ordinates as discussed above.

Card 4 is the same as for the Basic Version (p. 12).

Card 5 is the same as for the Basic Version (p. 12).

Card 6 If operating with MODE=1 this card carries the spectral slit width in $cm.^{-1}$ in format F15.5. If operating with MODE=2 this card carries the number of slit ordinates (KK) in format I5. KK must be an odd number.

Card Deck 7 is used ONLY WITH MODE = 2 and lists the spectral slit ordinates (which need not be normalized) in format 5F15.9. Note that an odd number of slit ordinates must be supplied, but the terminal values may be zero. It is recommended that not less than 13 ordinates be provided; the maximum number is 25.

Card Deck 8 is the main data deck carrying the NP experimental data points and corresponds to Card Deck 6 of the Basic Version (p. 13).

Card Deck 9 This is a deck of M cards, each carrying four input indices for one band in format 4F15.5. It corresponds to Card Deck 7 of the Basic Version (p. 13).

Card 10 is the terminating card carrying the baseline constant α in format F15.5 and corresponds with Card 8 of the Basic Version (p. 13).

B. Description of the Program

There are only minor changes from the Basic Version in the earlier part of the program where the data are read in. Before entering the Input Section, the slit ordinates are evaluated, normalized, and weighted for quadrature. For MODE=1 Newton-Cotes

weightings are used if the number of ordinates is less than seventeen otherwise Simpson's Rule is applied. Simpson Rule weightings are always used with MODE=2. Between statements 30 and 102 a number of constants are evaluated for MODE=1. These include LL, the spectral slit width expressed in integral multiples of the wavenumber encoding interval (WI), and KK, the total number of slit ordinates. The normalized and weighted ordinates are stored in the array SY(J). These operations are completed in the sections headed Computation of the Slit Ordinates and Slit Ordinates for Mode 2 and for Mode 1 by Simpson's Rule.

In the Input Section two new floating point arrays are created (W(I) and Y(I)), into which the wavenumber positions and the intensity ordinates are transferred from IX(I) and IY(I) respectively. The W(I) array is expanded at each end by LL spaces, and zeroes are entered in the corresponding spaces of the Y(I) array. The need for this expansion of the wavenumber range by m-1 units for an m element slit function vector has been illustrated previously in a numerical example on page 927 of reference (9).

In the calculation of $\underline{A}$, G and FS a difficulty arises because of the integral form of the function. To deal with this an array AP(I,JJ) is introduced in the DO loop ending at statement 206 in the (G,$\underline{A}$Q,F) Section. This contains the row elements of the $\underline{A}$ matrix for KK consecutive terms of the function TC(W); the second index denotes the wavenumber position. Thus the elements AP(I,LL) are identical with the row of the $\underline{A}$ matrix of $T(\nu)_{true}$ for the wavenumber ν, while AP(I,LL-1) is the row corresponding to the wavenumber ν+WI. KK wavenumber positions are first calculated, after which, on multiplication by the SY(I) elements, the row of the $\underline{A}$ matrix corresponding to $T(\nu)_{obs}$ is generated in the DO loop ending at statement 215. The same data in AP(I,JJ) are used also to generate the G vector, and FS in a similar manner. It should be emphasized that it is only necessary to compute all KK wavenumber positions of AP(I,JJ) separately in the initial step. KK-1 of them can be carried forward to the next round of computation for the succeeding values of $T(\nu)_{obs}$ by displacement of their positions, with only one new datum being introduced. These operations are all performed in the (G,$\underline{A}$Q,F) Section and further details should be clear from comparison with the Basic Version. The computation of TC(W) at statement 302 is likewise modified from that in the Basic Version in accord with the requirements of equation [35].

SUBROUTINE POINT is also modified to provide values of the transmittance (T(I)) and the quantities PC and PG for KK consecutive wavenumber values. As above, all KK values need only be evaluated initially; the subsequent values are obtained by increasing the subscripts by unity and computing one additional term at the low wavenumber end.

The other sections of the program resemble the Basic Version closely, and the terminating controls as well as the restraints under LIMIT=1 and NONEG=1 are the same. In the printed output for MODE 1 the normalized and weighted slit elements in the SY(J) array are recorded while in MODE 2 the raw input slit ordinates are also listed.

The Test Data for this program are the four band product and sum function curves of Fig. 1 and Fig. 2 after they have been convolved with appropriate slit functions using Program V of Bulletin 11 for this purpose. The Fig. 1 product curve is initially convolved with a symmetric triangular slit function of half width 5.0 $cm.^{-1}$. The Fig. 2 sum function curve is initially convolved with an asymmetric triangular slit function.

Note that this program calls for the library routines SETCLK and RDCLK which are discussed in Bulletin 11. If they are not available appropriate alterations must be made to the program.

```
C     ****************************************************************      10
C     *                                                              *      20
C     *          SPECTRAL BAND FIT OPTIMIZATION PROGRAM              *      30
C     *                                                              *      35
C     *            WITH SLIT DECONVOLUTION CORRECTION.               *      40
C     *                                                              *      45
C     ****************************************************************      50
C                                                                            60
C     J.PITHA AND R.N.JONES,DIVISION OF CHEMISTRY,NATIONAL RESEARCH          70
C          COUNCIL OF CANADA,SUSSEX DRIVE,OTTAWA,CANADA.                     80
C                                                                            90
C     PROGRAM XII (PC-118)  SLIT DECONVOLUTING VERSION    JULY 12TH.1967     100
C                                                                           110
C     THIS PROGRAM WILL FIT A CAUCHY,GAUSS,PRODUCT,OR SUM FUNCTION TO       120
C          AN INFRARED ABSORPTION BAND ENVELOPE AFTER CORRECTION FOR THE     130
C          SPECTRAL SLIT DISTORTION.                                         140
C     FOR THE SUM FUNCTION THE RESTRAINT THAT THE RATIO X(4)/X(3) IS         150
C          CONSTANT IS APPLIED.                                              160
C     THE SUM FUNCTION REQUIRES A DIFFERENT SET OF INPUT INDEX CARDS         170
C          CARRYING X(5) IN PLACE OF X(4).                                   180
C     THE PROGRAM OPERATES IN TWO MODES.                                     190
C          MODE 1. A SYMMETRICAL TRIANGULAR SLIT FUNCTION IS ASSUMED.        200
C             THE NUMBER OF SLIT ORDINATES IS CALCULATED FROM THE            210
C             SPECTRAL SLIT WIDTH  AND THE ABSCISSAL ENCODING INTERVAL.      220
C             NEWTON-COTES WEIGHTINGS ARE USED FOR QUADRATURE IF THERE       230
C             ARE SEVENTEEN OR LESS SLIT ORDINATES. FOR SEVENTEEN TO         240
C             TWENTY-FIVE SLIT ORDINATES QUADRATURE IS BY SIMPSON'S RULE     250
C             IN THIS MODE ALL THE SLIT ORDINATES AND WEIGHTINGS ARE         260
C             COMPUTED AND STORED WITHIN THE PROGRAM,ONLY THE SLIT WIDTH     270
C             AND THE WAVENUMBER INTERVAL NEED BE SUPPLIED.                  280
C          MODE 2. IN THIS MODE ASYMMETRIC AND NON-TRIANGULAR SLIT           290
C             FUNCTIONS MAY ALSO BE USED.THE RAW SLIT ORDINATES ARE          300
C             SUPPLIED BY CARD INPUT AND ARE NORMALIZED AND WEIGHTED IN      310
C             PROGRAM USING SIMPSON'S RULE. IT IS RECOMMENDED THAT NOT       320
C             LESS THAN THIRTEEN ORDINATES BE PROVIDED.                      330
C     THIS VERSION IS DIMENSIONED FOR A MAXIMUM OF 20 BANDS,2000             340
C          EXPERIMENTAL DATA POINTS,AND ANY ODD NUMBER OF EQUALLY SPACED     350
C          SLIT ORDINATES NOT EXCEEDING TWENTY-FIVE.                         360
C     THE SLIT ORDINATE WAVENUMBER INTERVAL MUST BE THE SAME AS THE DATA     370
C          WAVENUMBER INTERVAL.                                              380
C     THE BAND INTENSITY INDICES ARE IN ABSORBANCE UNITS BUT THE             390
C          COMPUTATIONS WITHIN THE PROGRAM USE NAPIERIAN LOGARITHMS.         400
C     THE EXPERIMENTAL DATA ARE IN UNITS OF WAVENUMBER X 10 AND              410
C          TRANSMITTANCE X 1000.                                             420
C     THE INPUT WAVENUMBER SEQUENCE IS CHECKED BY SUBROUTINE SORT.           430
C     FOR DETAILS SEE N.R.C.C. BULLETIN NO.12.                               440
C                                                                            450
C                                                                            460
C                                                                            470
      DIMENSION IX(2000),W(2000),IY(2000),Y(2000),X(81),XP(81),XB(81),       480
     1G(81),AM(81),PC(20,25),PG(20,25),AQ(3321),A(81,82),DIA(81),            490
     2GAST(81),AP(81,25),T(25),SY(25),HEAD1(20),HEAD2(20)                    500
      IRD=1                                                                  510
      IPCH=2                                                                 520
```

```
      IPRNT=3                                                          530
C                                                                      540
C                                                                      550
   11 READ (IRD,401) HEAD1                                             560
      READ (IRD,401) HEAD2                                             570
C                                                                      580
C     HEAD1 AND HEAD2 ARE HEADING CARDS.THEY MAY CARRY ANY DESIRED     590
C          INFORMATION.                                                600
C                                                                      610
C                                                                      620
C     USE NDATA=1 FOR PROCESSING A SINGLE DATA DECK OR THE LAST DECK OF 630
C          A SERIES AND USE NDATA=2 FOR CONSECUTIVE DATA DECKS.        640
C                                                                      650
C     USE IDECK=1 FOR PRINTED OUTPUT AND IDECK=2 FOR BOTH PRINTED AND  660
C          CARD OUTPUT.                                                670
C                                                                      680
C     NP IS THE NUMBER OF DATA POINTS.                                 690
C                                                                      700
C     M IS THE NUMBER OF CALCULATED BANDS.                             710
C                                                                      720
C     USE KURVE=1 FOR THE PRODUCT FUNCTION,KURVE=2 FOR THE SUM FUNCTION. 730
C                                                                      740
C     NSEC IS THE MAXIMUM PERMITTED COMPUTATION TIME IN SECONDS.       750
C                                                                      760
C     NI IS THE MAXIMUM NUMBER OF PERMITTED ITERATIONS.                770
      WRITE (IPRNT,400)                                                775
C                                                                      780
      READ (IRD,403) NDATA,IDECK,NP,M,KURVE,NSEC,NI,MLIST,LIMIT,NONEG, 790
     1MODE                                                             800
C                                                                      810
C     MLIST CONTROLS THE AMOUNT OF INFORMATION REPORTED ABOUT THE      820
C          PROGRESS OF THE COMPUTATION.                                830
C          USE MLIST=1 FOR MINIMUM PROGRESS REPORT AND FINAL OUTPUT ONLY 840
C          USE MLIST=2 FOR ADDITIONAL INFORMATION ON THE EXTREME VALUES 850
C          OF THE B MATRIX ELEMENTS DURING EACH ITERATION.             860
C          USE MLIST=3 TO PRINT RESTRAINTS APPLIED BY LIMIT AND NONEG. 870
C          USE MLIST=4 FOR COMBINATION OF MLIST=2 + MLIST=3.           880
C                                                                      890
C     USE LIMIT=1 TO RESTRICT THE HALF-WIDTHS OF THE COMPONENT BANDS   900
C          WITHIN THE RANGE 1-50 CM.-1                                 910
C          IF LIMIT=2 NO RESTRICTION TO THE HALF-BAND WIDTH IS APPLIED. 920
C                                                                      930
C     USE NONEG=1 WITH THE SUM FUNCTION TO RESTRICT X1 AND X5 TO ZERO  940
C          OR POSITIVE VALUES.                                         950
C          IF NONEG=2 NO RESTRICTION IS APPLIED ----- ALWAYS USE       960
C          NONEG=2  WITH THE PRODUCT FUNCTION.                         970
C                                                                      980
C                                                                      990
      IF (KURVE.EQ.2) GO TO 13                                         1000
      READ (IRD,404) WB,WI                                             1010
      GO TO 17                                                         1020
   13 READ (IPD,404) WB,WI,CAY                                         1030
C                                                                      1040
C     CAY DEFINES THE X(4)/X(3) RATIO IN THE SUM FUNCTION CALCULATIONS. 1050
```

```
C     VALUES OF CAY IN THE RANGE 0.6 - 0.8 ARE SUGGESTED.                    1060
C                                                                            1070
C     WB AND WI ARE THE STARTING WAVENUMBER AND THE WAVENUMBER ENCODING      1080
C         INTERVAL IN CM.-1                                                  1090
C     BY CONVENTION WI IS POSITIVE FOR A DIMINISHING WAVENUMBER SEQUENCE     1100
C                                                                            1110
   17 IF (IDECK.EQ.1) GO TO 12                                               1120
      WRITE (IPCH,401) HEAD1                                                 1130
      WRITE (IPCH,401) HEAD2                                                 1140
   12 WRITE (IPRNT,402) HEAD1                                                1150
      WRITE (IPRNT,402) HEAD2                                                1160
      WRITE (IPRNT,408)                                                      1170
      READ (IRD,404) DOWN,UP,CHANGE                                          1180
C                                                                            1190
C     DOWN,UP AND CHANGE REGULATE THE SEARCH FOR OPTIMAL DAMPING FACTOR.     1200
C     RECOMMENDED TRIAL VALUES ARE DOWN = 0.01  UP = 1000.0 CHANGE = 0.5     1210
C                                                                            1220
      WRITE (IPRNT,409) DOWN,UP,CHANGE                                       1230
C                                                                            1240
      IF (MODE.EQ.2) GO TO 15                                                1250
   14 READ (IRD,404) SSW                                                     1260
C                                                                            1270
C     SSW IS THE SPECTRAL SLIT WIDTH IN CM.-1                                1280
C                                                                            1290
      WRITE (IPRNT,425) NP,WB,WI,SSW                                         1300
      GO TO 16                                                               1310
   15 READ (IRD,403) KK                                                      1320
C                                                                            1330
C     KK IS THE NUMBER OF SLIT ORDINATES.                                    1340
C                                                                            1350
      LL=(KK-1)/2                                                            1360
      L1=LL+1                                                                1370
      KK1=KK-1                                                               1380
      READ (IRD,426) (SY(J),J=1,KK)                                          1390
C                                                                            1400
C     SY(J) ARE THE SLIT ORDINATE VALUES.THEY NEED NOT BE NORMALIZED.        1410
C     NOTE THAT A CARD LISTING KK IS ONLY NEEDED IF OPERATING IN MODE 2.     1420
C                                                                            1430
      WRITE (IPRNT,427)                                                      1440
      WRITE (IPRNT,428) (SY(J),J=1,KK)                                       1450
      WRITE (IPRNT,423) NP,WB,WI                                             1460
   16 IF (NONEG.EQ.2) GO TO 18                                               1470
      IF (MLIST.LT.3) WRITE (IPRNT,439)                                      1480
   18 IF (LIMIT.EQ.2) GO TO 19                                               1490
      IF (MLIST.LT.3) WRITE (IPRNT,440)                                      1500
   19 READ (IRD,405) (IX(I),IY(I), I=1,NP)                                   1510
      IWB=WB*10.0+0.5                                                        1520
      IWI=WI*10.0+0.5                                                        1530
      CALL SORT3 (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)                       1540
      IF (KLENUP.EQ.1) GO TO 30                                              1550
   20 UP=0.0                                                                 1560
      DOWN=0.0                                                               1570
      CHANGE=0.0                                                             1580
      IF (NDATA.EQ.2) GO TO 11                                               1590
```

```
      STOP                                                              1600
C                                                                       1610
C     ***************** COMPUTATION OF THE SLIT ORDINATES ***************1620
C                                                                       1630
   30 IF (MODE.EQ.2) GO TO 120                                          1640
C                                                                       1650
C     SLIT ORDINATES FOR MODE ONE BY NEWTON-COTES QUADRATURE.           1660
C                                                                       1670
      P=SSW/WI                                                          1680
      LL=P+0.5                                                          1690
      KK=2*LL+1                                                         1700
      L1=LL+1                                                           1710
      KK1=KK-1                                                          1720
      IF (KK.GT.17) GO TO 120                                           1730
      GO TO (102,103,104,105,106,107,108,109),LL                        1740
  102 WRITE (IPRNT,429)                                                 1750
      GO TO 20                                                          1760
  103 KK=5                                                              1770
      SY(1)=0.0                                                         1780
      SY(2)=0.3333333                                                   1790
      SY(3)=SY(2)                                                       1800
      GO TO 110                                                         1810
  104 KK=7                                                              1820
      SY(1)=0.0                                                         1830
      SY(2)=0.125                                                       1840
      SY(3)=0.250                                                       1850
      SY(4)=SY(3)                                                       1860
      GO TO 110                                                         1870
  105 KK=9                                                              1880
      SY(1)=0.0                                                         1890
      SY(2)=0.0888889                                                   1900
      SY(3)=0.0666667                                                   1910
      SY(4)=0.2666667                                                   1920
      SY(5)=0.1555555                                                   1930
      GO TO 110                                                         1940
  106 KK=11                                                             1950
      SY(1)=0.0                                                         1960
      SY(2)=0.0520833                                                   1970
      SY(3)=0.0694444                                                   1980
      SY(4)=0.1041667                                                   1990
      SY(5)=0.2083333                                                   2000
      SY(6)=0.1319444                                                   2010
      GO TO 110                                                         2020
  107 KK=13                                                             2030
      SY(1)=0.0                                                         2040
      SY(2)=0.0428571                                                   2050
      SY(3)=0.0107143                                                   2060
      SY(4)=0.1619043                                                   2070
      SY(5)=0.0214286                                                   2080
      SY(6)=0.2142857                                                   2090
      SY(7)=0.0976190                                                   2100
      GO TO 110                                                         2110
  108 KK=15                                                             2120
      SY(1)=0.0                                                         2130
```

```
      SY(2)=0.0295717                                                    2140
      SY(3)=0.0218750                                                    2150
      SY(4)=0.0741319                                                    2160
      SY(5)=0.0988426                                                    2170
      SY(6)=0.0546875                                                    2180
      SY(7)=0.1774305                                                    2190
      SY(8)=0.0869213                                                    2200
      GO TO 110                                                          2210
  109 KK=17                                                              2220
      SY(1)=0.0                                                          2230
      SY(2)=0.0259620                                                    2240
      SY(3)= -0.0081834                                                  2250
      SY(4)=0.1388359                                                    2260
      SY(5)= -0.0800705                                                  2270
      SY(6)=0.2313932                                                    2280
      SY(7)= -0.0245503                                                  2290
      SY(8)=0.1817284                                                    2300
      SY(9)=0.0697707                                                    2310
  110 JJ=LL+2                                                            2320
      DO 111 K1=1,LL                                                     2330
      J=JJ-2*K1                                                          2340
      SY(JJ)=SY(J)                                                       2350
  111 JJ=JJ+1                                                            2360
      WRITE (IPRNT,430)                                                  2370
      WRITE (IPRNT,428)  (SY(J),J=1,KK)                                  2380
      GO TO 150                                                          2390
C                                                                        2400
C                                                                        2410
C     *** SLIT ORDINATES FOR MODE 2 AND FOR MODE 1 BY SIMPSON RULE. **** 2420
C                                                                        2430
  120 IF (KK.LT.25) GO TO 121                                            2440
      WRITE (IPRNT,431)                                                  2450
      GO TO 20                                                           2460
  121 IF (MODE.EQ.2) GO TO 135                                           2470
      SY(1)=0.0                                                          2480
      S=0.0                                                              2490
      DO 131 J=2,L1                                                      2500
      S=S+1.0                                                            2510
  131 SY(J)=S                                                            2520
      JJ=LL+2                                                            2530
      DO 123 K1=1,LL                                                     2540
      J=JJ-2*K1                                                          2550
      SY(JJ)=SY(J)                                                       2560
  123 JJ=JJ+1                                                            2570
  135 QR=SY(1)                                                           2580
      DO 124 J=2,KK1,2                                                   2590
      SY(J)=SY(J)*4.0                                                    2600
  124 QR=QR+SY(J)                                                        2610
      DO 125 J=3,KK1,2                                                   2620
      SY(J)=SY(J)*2.0                                                    2630
  125 QR=QR+SY(J)                                                        2640
      QR=QR+SY(KK)                                                       2650
      QR=1/QR                                                            2660
      DO 126 J=1,KK                                                      2670
```

```
  126 SY(J)=SY(J)*QP                                                    2680
      IF (MODE.EQ.2) GO TO 128                                          2690
      WRITE (IPRNT,432)                                                 2700
      GO TO 130                                                         2710
  128 WRITE (IPRNT,433)                                                 2720
  130 WRITE (IPRNT,428) (SY(J),J=1,KK)                                  2730
C                                                                       2740
C     ************************  INPUT SECTION  ************************ 2750
C                                                                       2760
  150 CALL SETCLK                                                       2770
C                                                                       2780
C     SETCLK IS A TIMING SUBROUTINE.                                    2790
C                                                                       2800
      N=4*M+1                                                           2810
      N1=N+1                                                            2820
      NAL=N*N1/2                                                        2830
      NIT=0                                                             2840
      TERM=1000.0                                                       2850
      P1=0.1                                                            2860
      IF (KURVE.EQ.2) GO TO 151                                         2870
      WRITE (IPRNT,416)                                                 2880
      GO TO 152                                                         2890
  151 WRITE (IPRNT,417)                                                 2900
  152 DO 153 I=1,M                                                      2910
      J=I+M                                                             2920
      K=J+M                                                             2930
      L=K+M                                                             2940
      READ (IRD,404) X(I),X(J),X(K),X(L)                                2950
C                                                                       2960
C     X(I),X(J),X(K) AND X(L) ARE THE SPECTRAL INDICES FOR EACH BAND.   2970
      IF (KURVE.EQ.2) GO TO 160                                         2980
C                                                                       2990
      WRITE (IPRNT,410) X(I),X(J),X(K),X(L)                             3000
      GO TO 161                                                         3010
  160 XG=X(K)*CAY                                                       3020
      WRITE (IPRNT,406) X(I),X(J),X(K),XG,X(L)                          3030
      X(L)=2.30258*X(L)                                                 3040
  161 X(I)=2.30258*X(I)                                                 3050
  153 CONTINUE                                                          3060
      READ (IRD,404) X(N)                                               3070
      WRITE (IPRNT,418) X(N)                                            3080
      X(N)=2.30258*X(N)                                                 3090
      DO 154 I=1,N                                                      3100
  154 XB(I)=X(I)                                                        3110
      JI=LL                                                             3120
      DO 155 I=1,NP                                                     3130
      JI=JI+1                                                           3140
      W(JI)=IX(I)*0.1                                                   3150
  155 Y(JI)=IY(I)*0.001                                                 3160
      DO 156 I=1,LL                                                     3170
      Y(I)=0.0                                                          3180
  156 W(I)=WB+(L1-I)*WI                                                 3190
      NP=NP+LL                                                          3200
      NP1=NP+1                                                          3210
```

```
      NPL1=NP+LL                                                                3220
      DO 157 I=NP1,NPL1                                                         3230
      Y(I)=0.0                                                                  3240
  157 W(I)=WB-WI*(I-L1)                                                         3250
      NP1=NP+15                                                                 3260
                                                                                3270
C     ************************  (G,AQ,F) SECTION  **********************        3280
C                                                                               3290
C                                                                               3300
  200 DO 201 I=1,N                                                              3310
  201 G(I)=0.0                                                                  3320
      DO 202 I=1,NAL                                                            3330
  202 AQ(I)=0.0                                                                 3340
      FS=0.0                                                                    3350
      FM=0.0                                                                    3360
      FS1=1.0E10                                                                3370
      FS2=1.0E10                                                                3380
      P1L=P1                                                                    3390
      IT=1                                                                      3400
  203 DO 218 II=L1,NP                                                           3410
      CALL POINT3 (X,PC,PG,T,W,II,IK,KK,KK1,L1,M,N,IPRNT,CAY,KURVE,IJ)          3420
      IF(II.EQ.L1) GO TO 204                                                    3430
      DO 206 JJ=1,KK1                                                           3440
      DO 206 I=1,N                                                              3450
  206 AP(I,JJ)=AP(I,JJ+1)                                                       3460
  204 DO 211 JJ=IJ,KK                                                           3470
            LL1=II+JJ-L1                                                        3475
            WP=W(LL1)                                                           3480
      IF (KURVE.EQ.2) GO TO 210                                                 3490
      DO 209 I=1,M                                                              3500
      J=I+M                                                                     3510
      K=J+M                                                                     3520
      L=K+M                                                                     3530
      AP(I,JJ)=T(JJ)*PG(I,JJ)*PC(I,JJ)                                         3540
      R=WP-X(J)                                                                 3550
      SP=2.0*AP(I,JJ)*X(I)*R                                                    3560
      AP(J,JJ)=SP*(X(L)*X(L)+X(K)*X(K)*PC(I,JJ))                                3570
      AP(K,JJ)=-SP*R*X(K)*PC(I,JJ)                                              3580
      AP(L,JJ)=-SP*R*X(L)                                                       3590
  209 GO TO 211                                                                 3600
      DO 212 I=1,M                                                              3610
  210 J=I+M                                                                     3620
      K=J+M                                                                     3630
      L=K+M                                                                     3640
      R=WP-X(J)                                                                 3650
      AP(I,JJ)=T(JJ)*PC(I,JJ)                                                   3660
      SS=2.0*T(JJ)*(X(I)*PC(I,JJ)*PC(I,JJ)+CAY*CAY*X(L)*PG(I,JJ))*R*X(K)       3670
      AP(J,JJ)=SS*X(K)                                                          3680
      AP(K,JJ)=-SS*R                                                            3690
      AP(L,JJ)=T(JJ)*PG(I,JJ)                                                   3700
  212 AP(N,JJ)=T(JJ)                                                            3710
  211 DO 216 I=1,N                                                              3720
      AMI=0.0                                                                   3730
      DO 215 JJ=1,KK                                                            3740
  215 AMI=AMI+SY(JJ)*AP(I,JJ)
```

```
216 AM(I)=AMI                                                          3750
    TC=AM(N)                                                           3760
    F=Y(II)-TC                                                         3770
    FA=ABS(F)                                                          3780
    I3=L1+3                                                            3790
    I4=NP-2                                                            3800
    IF (II.LT.I3) GO TO 220                                            3810
    IF (II.GT.I4) GO TO 220                                            3820
    IF (FM.GE.FA) GO TO 217                                            3830
    FM=FA                                                              3840
    WFM=W(II)                                                          3850
217 FS=FS+F*F                                                          3860
220 IM=0                                                               3870
    DO 218 I=1,N                                                       3880
    AMI=AM(I)                                                          3890
    G(I)=G(I)+AMI*F                                                    3900
    DO 218 IJ=I,N                                                      3910
    IM=IM+1                                                            3920
218 AQ(IM)=AQ(IM)+AMI*AM(IJ)                                           3930
    FSM=FS                                                             3940
    IM=0                                                               3950
    DO 219 I=1,N                                                       3960
    DO 219 IJ=I,N                                                      3970
    IM=IM+1                                                            3980
219 A(I,IJ)=AQ(IM)                                                     3990
    ADMIN=+1.E+10                                                      4000
    ADMAX=-1.E+10                                                      4010
    DO 227 I=1,N                                                       4020
    GO TO (224,222,224,222),MLIST                                      4030
222 IF (A(I,I).GE.ADMIN) GO TO 221                                     4040
    ADMIN=A(I,I)                                                       4050
    MINAD=I                                                            4060
221 IF (ADMAX.GE.A(I,I)) GO TO 224                                     4070
    ADMAX=A(I,I)                                                       4080
    MAXAD=I                                                            4090
224 IF (A(I,I).GT.1.0E-10) GO TO 226                                   4100
    DIA(I)=0.0                                                         4110
    GO TO 227                                                          4120
226 DIA(I)=1.0/SQRT(A(I,I))                                            4130
227 GAST(I)=G(I)*DIA(I)                                                4140
    IM=0                                                               4150
    AMIN=1.0E+10                                                       4160
    AMAX=-1.0E-10                                                      4170
    DO 228 I=1,N                                                       4180
    DIAI=DIA(I)                                                        4190
    DO 228 IJ=I,N                                                      4200
    IM=IM+1                                                            4210
    AQ(IM)=A(I,IJ)*DIAI*DIA(IJ)                                        4220
    IF (MLIST.EQ.1) GO TO 228                                          4230
229 IF (I.EQ.IJ) GO TO 228                                             4240
    IF (AQ(IM).GE.AMIN) GO TO 231                                      4250
    AMIN=AQ(IM)                                                        4260
    MINA1=I                                                            4270
    MINA2=IJ                                                           4280
```

```
  231 IF (AMAX.GE.AQ(IM)) GO TO 228                                      4290
      AMAX=AQ(IM)                                                        4300
      MAXA1=I                                                            4310
      MAXA2=IJ                                                           4320
  228 CONTINUE                                                           4330
      GL=0.0                                                             4340
      DO 233 I=1,N                                                       4350
      GI=G(I)                                                            4360
  233 GL=GL+GI*GI                                                        4370
      SM=-2.0*GL                                                         4380
      GL=SQRT(GL)                                                        4390
C                                                                        4400
C     SM HAS BEEN APPROXIMATED. SEE COMMENT WRITTEN INTO PROGRAM X.      4410
C                                                                        4420
      CALL RDCLK (TIME)                                                  4430
C                                                                        4440
C     RDCLK IS A TIMING SUBROUTINE.                                      4450
C                                                                        4460
      ISECS=TIME+0.5                                                     4470
      WRITE (IPRNT,407) FS,GL,WFM,FM,NIT,ISECS                           4480
C                                                                        4490
C     ******************  MATRIX DATA OUTPUT SECTION  ******************  4500
C                                                                        4510
      GO TO (250,249,250,249),MLIST                                      4520
  249 WRITE (IPRNT,424) MINAD,MAXAD,ADMIN,ADMAX,MINA1,MINA2,AMIN,MAXA1,  4530
     1MAXA2,AMAX                                                         4540
C                                                                        4550
C                                                                        4560
C     **********************  (P,INVERT,XP) SECTION  ********************  4570
C                                                                        4580
  250 IM=0                                                               4590
      DO 251 I=1,N                                                       4600
      DO 251 IJ=I,N                                                      4610
      IM=IM+1                                                            4620
      AQIM=AQ(IM)                                                        4630
      A(I,IJ)=AQIM                                                       4640
  251 A(IJ,I)=AQIM                                                       4650
      GO TO (260,261,262,263,311),IT                                     4660
  260 P=P1L                                                              4670
      GO TO 265                                                          4680
  261 IF (FS.LE.FS1) GO TO 266                                           4690
      P=P1L*DOWN                                                         4700
      GO TO 265                                                          4710
  266 P=P1L*UP                                                           4720
      GO TO 265                                                          4730
  262 P=P1*CHANGE                                                        4740
      GO TO 265                                                          4750
  263 X3=1.0/P1                                                          4760
      X4=1.0/P2                                                          4770
      DET=X3*X3*X4*X4*X4-X3*X3*X3*X4*X4                                  4780
      IF (DET.EQ.0.0) GO TO 269                                          4790
      AP1=X3*X3*(FS2-FS-SM*X4)                                           4800
      AP2=X4*X4*(FS1-FS-SM*X3)                                           4810
      AI=6.0*(AP1-AP2)/DET                                               4820
```

```
      BI=2.0*(X4*AP2-X3*AP1)/DET                                        4830
      DET=BI*BI-2.0*AI*SM                                               4840
      IF (DET) 269,279,270                                              4850
  270 DET=SQRT(DET)                                                     4860
  279 IF (AI.EQ.0.0) GO TO 269                                          4870
      X3=(-BI+DET)/AI                                                   4880
      X4=(-BI-DET)/AI                                                   4890
      IF (X3.LE.0.0) GO TO 272                                          4900
      IF (X4.LE.0.0) GO TO 275                                          4910
      IF (X4.LE.X3) GO TO 274                                           4920
  275 P=1.0/X3                                                          4930
      GO TO 265                                                         4940
  272 IF (X4.LE.0.0) GO TO 269                                          4950
  274 P=1.0/X4                                                          4960
      GO TO 265                                                         4970
  269 P=10000.0                                                         4980
  271 WRITE (IPRNT,411)                                                 4990
  265 IT=IT+1                                                           5000
      DO 278 I=1,N                                                      5010
      A(I,I)=A(I,I)+P                                                   5020
  278 A(I,N1)=-GAST(I)                                                  5030
      DO 282 I=1,N                                                      5040
      AII=A(I,I)                                                        5050
      IF (AII.EQ.0.0) GO TO 284                                         5060
      PIV=1.0/AII                                                       5070
      DO 281 J=I,N1                                                     5080
  281 A(I,J)=PIV*A(I,J)                                                 5090
      DO 282 K=1,N                                                      5100
      IF (I.EQ.K) GO TO 282                                             5110
      Q=A(K,I)                                                          5120
      DO 285 J=I,N1                                                     5130
  285 A(K,J)=A(K,J)-Q*A(I,J)                                            5140
  282 CONTINUE                                                          5150
      GO TO 286                                                         5160
  284 WRITE (IPRNT,412)                                                 5170
      GO TO 314                                                         5180
  286 DO 288 I=1,N                                                      5190
  288 XP(I)=X(I)+A(I,N1)*DIA(I)                                         5200
C                                                                       5210
CC    * BOUNDARY CONDITIONS TO LIMIT THE RANGES OF X(1),X(3),X(4),X(5) *5220
C                                                                       5230
      IF (KURVE.EQ.2) GO TO 540                                         5240
C                                                                       5250
CC    THE PRODUCT FUNCTION.                                             5260
C                                                                       5270
      IF (LIMIT.EQ.2) GO TO 299                                         5280
      DO 505 I=1,M                                                      5290
      J=I+M                                                             5300
      K=J+M                                                             5310
      L=K+M                                                             5320
      XPK=ABS(XP(K))                                                    5330
      XPL=ABS(XP(L))                                                    5340
      IF (XPL.LE.1.0) GO TO 500                                         5350
      XPL=1.0                                                           5360
```

```
      IF (MLIST.LT.3) GO TO 500                                         5370
      WRITE (IPRNT,435) XP(J)                                           5380
  500 IF (XPK.LE.2.0) GO TO 501                                         5390
      XPK=2.0                                                           5400
      IF (MLIST.LT.3) GO TO 506                                         5410
      WRITE (IPRNT,435) XP(J)                                           5420
      GO TO 506                                                         5430
  501 IF (XPK.GT.0.03) GO TO 506                                        5440
      IF (XPL.GT.0.0333) GO TO 506                                      5450
      XPL=0.0333                                                        5460
      IF (MLIST.LT.3) GO TO 506                                         5470
      WRITE (IPRNT,436) XP(J)                                           5480
  506 IF (XP(K).LT.0.0) GO TO 503                                       5490
      XP(K)=XPK                                                         5500
      GO TO 507                                                         5510
  503 XP(K)=-XPK                                                        5520
  507 IF (XP(L).LT.0.0) GO TO 504                                       5530
      XP(L)=XPL                                                         5540
      GO TO 505                                                         5550
  504 XP(L)=-XPL                                                        5560
  505 CONTINUE                                                          5570
      GO TO 299                                                         5580
C                                                                       5590
C     THE SUM FUNCTION.                                                 5600
C                                                                       5610
  540 IF (LIMIT.EQ.1) GO TO 550                                         5620
      IF (NONEG.EQ.2) GO TO 299                                         5630
  550 DO 556 I=1,M                                                      5640
      J=I+M                                                             5650
      K=J+M                                                             5660
      L=K+M                                                             5670
      XPI=XP(I)                                                         5680
      XPK=ABS(XP(K))                                                    5690
      XPL=ABS(XP(L))                                                    5700
      IF (LIMIT.EQ.2) GO TO 559                                         5710
      IF (XPK.LT.2.0) GO TO 551                                         5720
      XPK=2.0                                                           5730
      IF (MLIST.LT.3) GO TO 552                                         5740
      WRITE (IPRNT,435) XP(J)                                           5750
      GO TO 552                                                         5760
  551 IF (XPK.GE.0.042) GO TO 552                                       5770
      XPK=0.042                                                         5780
      IF (MLIST.LT.3) GO TO 552                                         5790
      WRITE (IPRNT,436) XP(J)                                           5800
  552 IF (XP(K).LT.0.0) GO TO 553                                       5810
      XP(K)=XPK                                                         5820
      GO TO 557                                                         5830
  553 XP(K)=-XPK                                                        5840
  557 IF (XP(L).LT.0.0) GO TO 554                                       5850
      XP(L)=XPL                                                         5860
      GO TO 558                                                         5870
  554 XP(L)=-XPL                                                        5880
C                                                                       5890
  558 IF (NONEG.EQ.2) GO TO 556                                         5900
```

```
  559 IF (XPI.GE.0.0) GO TO 555                                          5910
      XP(I)=XB(I)*0.1                                                    5920
      IF (MLIST.LT.3) GO TO 555                                          5930
      WRITE (IPRNT,437) XP(J)                                            5940
  555 IF (XP(L).GE.0.0) GO TO 556                                        5950
      XP(L)=XB(L)*0.1                                                    5960
C                                                                        5970
C     NOTE THAT IF X1 OR X5 GOES NEGATIVE WE REDUCE IT TO ONE TENTH OF   5980
C          THE VALUE FOUND IN THE PREVIOUS ITERATION.                    5990
C                                                                        6000
      IF (MLIST.LT.3) GO TO 556                                          6010
      WRITE (IPRNT,438) XP(J)                                            6020
  556 CONTINUE                                                           6030
C                                                                        6040
C                                                                        6050
C     ************************  (FSP) SECTION  ************************  6060
C                                                                        6070
  299 FSP=0.0                                                            6080
      DO 301 II=L1,NP                                                    6090
      CALL POINT3 (XP,PC,PG,T,W,II,IK,KK,KK1,L1,M,N,IPRNT,CAY,KURVE,IJ)  6100
      TC=0.0                                                             6110
      DO 302 JJ=1,KK                                                     6120
  302 TC=TC+T(JJ)*SY(JJ)                                                 6130
      F=Y(II)-TC                                                         6140
  301 FSP=FSP+F*F                                                        6150
      IF (FSM.LE.FSP) GO TO 303                                          6160
C                                                                        6170
C     NOTE IF RESTRAINTS ARE APPLIED,THE PROGRAM CAN BRANCH BACK HERE ON 6180
C          THE FIRST CYCLE TO REPETITIVELY OUTPUT THE ORIGINAL GUESSED   6190
C          INDICES.THIS INDICATES THAT THE GUESSED INDICES (WITHOUT      6200
C          RESTRAINTS) FIT BETTER THAN THE COMPUTED INDICES (WITH        6210
C          RESTRAINTS). THIS IS ONLY LIKELY FOR SINGLE BANDS,BUT IF SO   6220
C          RERUN WITH MLIST=4 AND CHANGE THE INITIAL INPUT INDICES.      6230
      FSM=FSP                                                            6240
      DO 305 I=1,N                                                       6250
  305 XB(I)=XP(I)                                                        6260
  303 IF (FS1.LE.FSP) GO TO 306                                          6270
      FS2=FS1                                                            6280
      P2=P1                                                              6290
      FS1=FSP                                                            6300
      P1=P                                                               6310
      GO TO 308                                                          6320
  306 IF (FS2.LE.FSP) GO TO 308                                          6330
      P2=P                                                               6340
      FS2=FSP                                                            6350
  308 GO TO (250,309,250,309),MLIST                                      6360
  309 WRITE (IPRNT,414) P,FSP                                            6370
      GO TO 250                                                          6380
  311 DO 312 I=1,N                                                       6390
C                                                                        6400
C     ************************ TERMINAL SECTION ************************ 6410
C                                                                        6420
  312 X(I)=XB(I)                                                         6430
                                                                         6440
```

```
      NIT=NIT+1                                                          6450
      TEST=TERM/FSM                                                      6460
      TERM=FSM                                                           6470
      IF (TEST.GE.1.002) GO TO 315                                       6480
      WRITE (IPRNT,441)                                                  6490
      GO TO 314                                                          6500
  315 IF (NIT.LE.NI) GO TO 316                                           6510
      WRITE (IPRNT,442)                                                  6520
      GO TO 314                                                          6530
  316 IF (GL.GE.0.0001) GO TO 317                                        6540
      WRITE (IPRNT,443)                                                  6550
      GO TO 314                                                          6560
  317 IF (ISECS.LE.NSEC) GO TO 320                                       6570
      WRITE (IPRNT,444)                                                  6580
      GO TO 314                                                          6590
  320 IF (FM.GT.0.001) GO TO 200                                         6600
      WRITE (IPRNT,445)                                                  6610
  314 DIS=SQRT(FSM/NP)                                                   6620
      WRITE (IPRNT,415)                                                  6630
      WRITE (IPRNT,419) FSM,DIS,FM,WFM                                   6640
      IF (KURVE.EQ.2) GO TO 318                                          6650
      WRITE (IPRNT,416)                                                  6660
      DO 319 I=1,M                                                       6670
      J=I+M                                                              6680
      K=J+M                                                              6690
      L=K+M                                                              6700
      X(I)=0.43429*X(I)                                                  6710
      IF (IDECK.EQ.1) GO TO 319                                          6720
      WRITE (IPCH,420) X(I),X(J),X(K),X(L)                               6730
  319 WRITE (IPRNT,410) X(I),X(J),X(K),X(L)                              6740
      X(N)=0.43429*X(N)                                                  6750
      IF (IDECK.EQ.1) GO TO 322                                          6760
      WRITE (IPCH,420) X(N)                                              6770
  322 WRITE (IPRNT,413) X(N)                                             6780
      GO TO 328                                                          6790
  318 WRITE (IPRNT,417)                                                  6800
      DO 325 I=1,M                                                       6810
      J=I+M                                                              6820
      K=J+M                                                              6830
      L=K+M                                                              6840
      X(I)=0.43429*X(I)                                                  6850
      X(L)=0.43429*X(L)                                                  6860
      XG=X(K)*CAY                                                        6870
      IF (IDECK.EQ.1) GO TO 325                                          6880
      WRITE (IPCH,421) X(I),X(J),X(K),X(L)                               6890
  325 WRITE (IPRNT,406) X(I),X(J),X(K),XG,X(L)                           6900
      X(N)=0.43429*X(N)                                                  6910
      IF (IDECK.EQ.1) GO TO 327                                          6920
      WRITE (IPCH,421) X(N)                                              6930
  327 WRITE (IPRNT,422) X(N),CAY                                         6940
  328 WRITE (IPRNT,434)                                                  6950
      GO TO 20                                                           6960
C                                                                        6970
C                                                                        6980
```

```
400 FORMAT ('1PITHA AND JONES.  PROGRAM XII (PC-118)  SPECTRAL BAND FI    6990
   1T OPTIMIZATION PROGRAM WITH SLIT FUNCTION CORRECTION.'/)              7000
401 FORMAT (20A4)                                                        7010
402 FORMAT (1X,20A4)                                                     7020
403 FORMAT (11I5)                                                        7030
404 FORMAT (4F15.5)                                                      7040
405 FORMAT (8(I5,I4,1X))                                                 7050
406 FORMAT (1X,5(6X,F15.5))                                              7060
407 FORMAT (5X,2HFS,E12.4,8X,2HGL,E12.4,7X,3HWFM,F6.1,7X,2HFM,E12.4,7X   7070
   1,3HNIT,I3,4X,5HISECS,I5)                                             7080
408 FORMAT ('0INPUT PARAMETERS.')                                        7090
409 FORMAT (20X,4HDOWN,E14.6,7X,2HUP,E14.6,7X,6HCHANGE,E14.6)            7100
410 FORMAT (1X,4(6X,F15.5))                                              7110
411 FORMAT (1X,'TROUBLE WITH EVALUATION OF P,CHECK MATRIX DATA OUTPUT.    7120
   1')                                                                   7130
412 FORMAT (1X,'TERMINATED BY TROUBLE WITH SOLUTION OF EQUATIONS.')      7140
413 FORMAT (4X,7HALPHA =F8.5/,'0SOLVED FOR PRODUCT,CAUCHY OR GAUSS FUN   7150
   1CTION.'/' (PURE CAUCHY IF X(4)=0 OR PURE GAUSS IF X(3)=0)')          7160
414 FORMAT (64X,1HP,E14.6,8X,3HFSP,E14.6)                                7170
415 FORMAT (11X,  '-------------------------------------------------------7180
   1------------------------'/1X,17HOUTPUT PARAMETERS)                   7190
416 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(4))             7200
417 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(4),17X,4HX(5)   7210
   1)                                                                    7220
418 FORMAT (4X,7HALPHA =,F8.5,/11X,'-----------------------------------  7230
   1-------------------------------------------')                       7240
419 FORMAT (18X,3HFSM,E14.6,7X,3HLIS,E14.6,7X,2HFM,E14.6,7X,3HWFM,F7.1   7250
   1)                                                                    7260
420 FORMAT (4F15.5,5X,7HPRODUCT)                                         7270
421 FORMAT (4F15.5,9X,3HSUM)                                             7280
422 FORMAT (4X,7HALPHA =,F8.5/'0SOLVED FOR SUM FUNCTION WITH X4=',F5.2   7290
   1,4H X3.)                                                             7300
423 FORMAT ('0',19X,2HNP,I6,17X,2HWB,F8.1,13X,2HWI,F5.1)                 7310
424 FORMAT (/4X,5HMINAD,I4,13X,5HMAXAD,I4,12X,5HADMIN,E14.6,5X,5HADMAX   7320
   1,E14.6/4X,5HMINA1,I4,1X,5HMINA2,I4,3X,4HAMIN,E14.6,3X,5HMAXA1,I4,    7330
   23X,5HMAXA2,I4,3X,4HAMAX,E14.6)                                       7340
425 FORMAT ('0',9X,2HNP,I6,15X,2HWB,F8.1,11X,2HWI,F5.1,11X,3HSSW,F6.2)   7350
426 FORMAT (5F15.9)                                                      7360
427 FORMAT ('0INPUT SLIT ORDINATES.')                                    7370
428 FORMAT (5X,10F12.8)                                                  7380
429 FORMAT ('0COMPUTATION TERMINATED--INSUFFICIENT SLIT ORDINATES.')      7390
430 FORMAT ('0SYMMETRIC TRIANGULAR SLIT FUNCTION--NEWTON COTES WEIGHTI   7400
   1NGS.')                                                               7410
431 FORMAT ('0COMPUTATION TERMINATED-TOO MANY SLIT ORDINATES.')           7420
432 FORMAT ('0SYMMETRIC TRIANGULAR SLIT FUNCTION--SIMPSON RULE WEIGHTI   7430
   1NGS.')                                                               7440
433 FORMAT ('0COMPUTATION BY MODE 2--NORMALIZED SLIT ELEMENTS WITH SIM   7450
   1PSON RULE WEIGHTINGS.')                                              7460
434 FORMAT ('0FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.'/,          7470
   1'0DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEA   7480
   2N SQUARE OF THE RESIDUALS).'/,'0FM IS THE MAXIMUM ORDINATE DIFFERE   7490
   3NCE.'/,'0WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.   7500
   4')                                                                   7510
435 FORMAT ('0MINIMAL HALF-WIDTH FOR BAND AT',F7.1,6H CM.-1)             7520
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436 FORMAT ('0MAXIMAL HALF-WIDTH FOR BAND AT',F7.1,6H CM.-1)                    7530
437 FORMAT ('0X1 HELD POSITIVE AT',F7.1,6H CM.-1)                              7540
438 FORMAT ('0X5 HELD POSITIVE AT',F7.1,6H CM.-1)                              7550
439 FORMAT ('0RESTRAINTS TO HOLD X(1) AND X(5) POSITIVE HAVE BEEN APPL         7560
   1IED.')                                                                     7570
440 FORMAT ('0RESTRAINTS TO HOLD THE HALF-WIDTHS BETWEEN 1 AND 50 CM.-         7580
   1-1 HAVE BEEN APPLIED.')                                                    7590
441 FORMAT ('0TERMINATED BECAUSE OF SLOW CONVERGENCE.'/)                       7600
442 FORMAT ('0TERMINATED BY ITERATION LIMIT.'/)                                7610
443 FORMAT ('0TERMINATED BY LOW VALUE OF GL.'/)                                7620
444 FORMAT ('0TERMINATED BY TIME LIMITATION.'/)                                7630
445 FORMAT ('0TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VA         7640
   1LUE.'/)                                                                    7650
    END                                                                        7660
```

```
C                                                                       7670
CC    ***************************************************************** 7680
C                                                                       7690
      SUBROUTINE SORT3 (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)            7700
C                                                                       7710
CC                                                                      7720
CC    SUBROUTINE SORT CHECKS FOR ERRORS IN THE INPUT WAVENUMBER DATA.   7730
CC    A LIMITED NUMBER OF WAVENUMBER SEQUENCE ERRORS ARE CORRECTED      7740
CC         BUT SEQUENCE ERRORS IN EXCESS OF 160 DATA POINTS (20 CARDS)  7750
CC         OR ANY OTHER TYPE OF WAVENUMBER ERROR WILL TERMINATE THE     7760
CC         COMPUTATION,AS ALSO WILL A DISCREPANCY BETWEEN IWB AND THE   7770
CC         STARTING WAVENUMBER.                                         7780
CC    THE WAVENUMBER POSITIONS OF THE CORRECTIONS AND OF A TERMINATING  7790
CC         ERROR ARE RECORDED.                                          7800
CC    IF CORRECTIONS ARE MADE,CORRECTED INPUT DATA ARE LISTED IN FULL.  7810
CC    IF A TERMINATING ERROR IS FOUND THE UNCORRECTED INPUT DATA ARE    7820
CC         LISTED IN FULL.                                              7830
C                                                                       7840
      DIMENSION IX(2000),IY(2000),ITEMPX(160),X1(160),ITEMPY(160)       7850
      IF (IX(1).EQ.IWB) GO TO 10                                        7860
      WRITE (IPRNT,456)                                                 7870
      KLENUP=2                                                          7880
      RETURN                                                            7890
   10 MM=1                                                              7900
      DO 11 I=2,NP                                                      7910
      IW=IWB-IWI*(I-1)                                                  7920
      IF (IW.EQ.IX(I)) GO TO 11                                         7930
      XX=IX(I)                                                          7940
      TEST=(WB-0.1*XX)/WI                                               7950
      NTEST=TEST+0.005                                                  7960
      IF (ABS(TEST-NTEST).GT.0.005) GO TO 12                            7970
      ITEMPX(MM)=IX(I)                                                  7980
      ITEMPY(MM)=IY(I)                                                  7990
      MM=MM+1                                                           8000
      IF (MM.GT.160) GO TO 13                                           8010
   11 CONTINUE                                                          8020
      IF (MM.GT.1) GO TO 14                                             8030
      WRITE (IPRNT,451)                                                 8040
   15 KLENUP=1                                                          8050
      RETURN                                                            8060
   12 XX1=IX(I-1)*0.1-WI                                                8070
      WRITE (IPRNT,452) XX1                                             8080
   16 KLENUP=2                                                          8090
      RETURN                                                            8100
   13 WRITE (IPRNT,453)                                                 8110
      WRITE (IPRNT,455) (IX(I),IY(I), I=1,NP)                           8120
      GO TO 16                                                          8130
   14 NN=MM-1                                                           8140
      DO 17 MM=1,NN                                                     8150
      K1=1+(IWB-ITEMPX(MM))/IWI                                         8160
      IX(K1)=ITEMPX(MM)                                                 8170
      IY(K1)=ITEMPY(MM)                                                 8180
   17 X1(MM)=IX(K1)*0.1                                                 8190
      WRITE (IPRNT,450) (X1(MM),MM=1,NN)                                8200
```

```
      WRITE (IPRNT,454) (IX(I),IY(I),I=1,NP)                                    8210
      GO TO 15                                                                  8220
  450 FORMAT ('0WAVENUMBER CORRECTIONS AT'/,12(2X,F6.1,2X))                     8230
  451 FORMAT ('0WAVENUMBER SEQUENCE IS CORRECT.')                               8240
  452 FORMAT ('0TERMINATED BY ERROR AT',F6.1,6H CM.-1)                          8250
  453 FORMAT ('0TERMINATED BY MULTIPLE WAVENUMBER SEQUENCE ERRORS.')            8260
  454 FORMAT ('0REARRANGED INPUT.'/,9(4X,2I5))                                  8270
  455 FORMAT ('0UNCORRECTED INPUT.'/,9(4X,2I5))                                 8280
  456 FORMAT ('0TERMINATED BY AN ERROR IN THE STARTING WAVENUMBER.')            8290
      END                                                                       8300
```

```
C                                                                       8310
C     ***************************************************************** 8320
C                                                                       8330
      SUBROUTINE POINT3 (PX,PC,PG,T,W,II,IK,KK,KK1,L1,M,N,IPRNT,CAY,KURV 8340
     1E,IJ)                                                             8350
C                                                                       8360
C     SUBROUTINE POINT CALCULATES THE ORDINATES OF THE COMPUTED BAND    8370
C          ENVELOPE IN UNITS OF NAPIERIAN ABSORBANCE.                   8380
C                                                                       8390
      DIMENSION PX(81),PC(20,25),PG(20,25),T(25),W(2000)                8400
      JSKIP=1                                                           8410
      KSKIP=1                                                           8420
      IJ=1                                                              8430
      IF (II.GT.L1) GO TO 102                                           8440
      IK=KK                                                             8450
      GO TO 103                                                         8460
  102 DO 104 JJ=1,KK1                                                   8470
      T(JJ)=T(JJ+1)                                                     8480
      DO 104 I=1,M                                                      8490
      PC(I,JJ)=PC(I,JJ+1)                                               8500
  104 PG(I,JJ)=PG(I,JJ+1)                                               8510
      IJ=KK                                                             8520
      IK=KK                                                             8530
  103 DO 105 JJ=IJ,IK                                                   8540
          LL1=II+JJ-L1                                                  8550
          WP=W(LL1)                                                     8555
      AC=0.0                                                            8560
      DO 106 I=1,M                                                      8570
      J=I+M                                                             8580
      K=J+M                                                             8590
      L=K+M                                                             8600
      R=WP-PX(J)                                                        8610
      RSQ=R*R                                                           8620
      PC(I,JJ)=1.0/(1.0+PX(K)*PX(K)*RSQ)                                8630
      IF (KURVE.EQ.2) GO TO 108                                         8640
      PG(I,JJ)=PX(L)*PX(L)*RSQ                                          8650
      IF (PG(I,JJ).LT.10.0) GO TO 109                                   8660
      PG(I,JJ)=0.0                                                      8670
      GO TO 111                                                         8680
  109 PG(I,JJ)=EXP(-PG(I,JJ))                                           8690
  111 AC=PX(I)*PC(I,JJ)*PG(I,JJ)+AC                                     8700
      GO TO 106                                                         8710
  108 PG(I,JJ)=CAY*CAY*PX(K)*PX(K)*RSQ                                  8720
      IF (PG(I,JJ).LT.10.0) GO TO 112                                   8730
      PG(I,JJ)=0.0                                                      8740
      GO TO 114                                                         8750
  112 PG(I,JJ)=EXP(-PG(I,JJ))                                           8760
  114 AC=PX(I)*PC(I,JJ)+PX(L)*PG(I,JJ)+AC                               8770
  106 CONTINUE                                                          8780
      AC=AC+PX(N)                                                       8790
      IF (AC.GT.-2.0) GO TO 116                                         8800
      IF (JSKIP.EQ.2) GO TO 107                                         8810
      WRITE (IPRNT,470)                                                 8820
      JSKIP=2                                                           8830
```

```
107 T(JJ)=2.7184                                                                8840
    GO TO 105                                                                   8850
116 IF (AC.LE.10.0) GO TO 117                                                   8860
    IF (KSKIP.EQ.2) GO TO 117                                                   8870
    WRITE (IPRNT,471)                                                           8880
    KSKIP=2                                                                     8890
118 T(JJ)=0.0                                                                   8900
    GO TO 105                                                                   8910
117 T(JJ)=EXP(-AC)                                                              8920
105 CONTINUE                                                                    8930
    RETURN                                                                      8940
470 FORMAT ('0THE MAXIMAL ALLOWED TRANSMITTANCE HAS BEEN EXCEEDED.')            8950
471 FORMAT ('0THE MINIMAL ALLOWED TRANSMITTANCE HAS BEEN EXCEEDED.')            8960
    END                                                                         8970
```

```
PITHA AND JONES.  PROGRAM XII (PC-118)  SPECTRAL BAND FIT OPTIMIZATION PROGRAM WITH SLIT FUNCTION CORRECTION.

MARCH 13TH.1968.  BAND FIT PROGRAM WITH SLIT DECONVOLUTION.
FOUR BAND TEST DECK (PRODUCT)     SYMMETRIC TRIANG SLIT WITH SSW 5.0 CM.-1

INPUT PARAMETERS.
                DOWN  0.100000E-01       UP  0.100000E 04       CHANGE  0.500000E 00

        NP   180                 WB   995.0           WI  0.5          SSW  5.00

WAVENUMBER SEQUENCE IS CORRECT.

SYMMETRIC TRIANGULAR SLIT FUNCTION--SIMPSON RULE WEIGHTINGS.
      0.00000000  0.01333333  0.01333333  0.04000000  0.02666666  0.06666666  0.04000000  0.08333330  0.05333333  0.119
      0.06666666  0.11999995  0.05333333  0.09333330  0.04000000  0.06666666  0.02666666  0.04000000  0.01333333  0.013
      0.00000000

            X(1)              X(2)              X(3)              X(4)
          0.27000          968.50000          0.18000          0.12000
          0.62000          957.00000          0.22000          0.18000
          0.32000          941.00000          0.12000          0.12000
          0.37000          918.00000          0.22000          0.12000
   ALPHA = 0.02000
   ------------------------------------------------------------------------------
    FS  0.2276E 01      GL  0.1444E 02      WFM 924.0      FM  0.2241E 00      NIT  0    ISECS    8
    FS  0.8185E-01      GL  0.8244E 00      WFM 953.5      FM  0.5457E-01      NIT  1    ISECS   22
    FS  0.1825E-02      GL  0.1597E 00      WFM 917.0      FM  0.8025E-02      NIT  2    ISECS   37
    FS  0.2109E-04      GL  0.1196E-01      WFM 961.5      FM  0.8969E-03      NIT  3    ISECS   51

TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VALUE.

   ------------------------------------------------------------------------------
OUTPUT PARAMETERS
              FSM  0.138526E-04       DIS  0.270015E-03       FM  0.896871E-03       WFM  961.5

            X(1)              X(2)              X(3)              X(4)
          0.29997          969.99951          0.19999          0.09992
          0.60066          954.99707          0.20223          0.19879
          0.29994          939.99390          0.09928          0.10058
          0.39958          920.00391          0.19950          0.10005
   ALPHA = 0.04999

SOLVED FOR PRODUCT,CAUCHY OR GAUSS FUNCTION.
(PURE CAUCHY IF X(4)=0 OR PURE GAUSS IF X(3)=0)

FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.

DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEAN SQUARE OF THE RESIDUALS).

FM IS THE MAXIMUM ORDINATE DIFFERENCE.

WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.
```

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PITHA AND JONES.  PROGRAM XII (PC-118)  SPECTRAL BAND FIT OPTIMIZATION PROGRAM WITH SLIT FUNCTION CORRECTION.

MARCH 13TH.1968.  BAND FIT PROGRAM WITH SLIT DECONVOLUTION.
FOUR BAND TEST DECK (SUM)    ASYM.TRIANG. SLIT BY MODE 2.

INPUT PARAMETERS.
                DOWN  0.100000E-01        UP  0.100000E 04        CHANGE  0.500000E 00

INPUT SLIT ORDINATES.
     0.00000000  0.09999996  0.19999999  0.29999995  0.39999998  0.50000000  0.59999996  0.69999999  0.79999995  0.899
     1.00000000  0.75000000  0.50000000  0.25000000  0.00000000

                NP   186                  WB   596.5              WI  0.5

WAVENUMBER SEQUENCE IS CORRECT.

COMPUTATION BY MODE 2--NORMALIZED SLIT ELEMENTS WITH SIMPSON RULE WEIGHTINGS.
     0.00000000  0.01904763  0.01904763  0.05714289  0.03809526  0.09523815  0.05714289  0.13333338  0.07619047  0.171
     0.09523815  0.14285719  0.04761908  0.04761908  0.00000000

            X(1)              X(2)              X(3)              X(4)              X(5)
          0.18000           968.00000         0.18000           0.14400           0.11000
          0.37000           953.00000         0.22000           0.17600           0.22000
          0.10000           942.00000         0.11000           0.08800           0.18000
          0.26000           919.00000         0.21000           0.16800           0.16000
  ALPHA = 0.02000
     ------------------------------------------------------------------------------

  FS  0.1185E 01      GL  0.1469E 02      WFM 928.5      FM  0.1450E 00      NIT  0    ISECS    6
  FS  0.2678E-01      GL  0.4360E 00      WFM 957.0      FM  0.3184E-01      NIT  1    ISECS   18
  FS  0.1328E-02      GL  0.1157E 00      WFM 953.0      FM  0.6925E-02      NIT  2    ISECS   30
  FS  0.1643E-04      GL  0.1055E-01      WFM 967.5      FM  0.7808E-03      NIT  3    ISECS   42

TERMINATED BECAUSE FM HAS REACHED MINIMAL SIGNIFICANT VALUE.

     ------------------------------------------------------------------------------
OUTPUT PARAMETERS
          FSM  0.140989E-04      DIS  0.270280E-03      FM  0.780761E-03      WFM  967.5

            X(1)              X(2)              X(3)              X(4)              X(5)
          0.19999           970.00684         0.20051           0.16041           0.09940
          0.39874           954.99780         0.20004           0.16003           0.19916
          0.11103           939.99902         0.09926           0.07941           0.19002
          0.24609           919.99365         0.20055           0.16044           0.15183
  ALPHA = 0.04957

SOLVED FOR SUM FUNCTION WITH X4= 0.80 X3.

FSM IS THE VALUE OF THE MINIMIZATION FUNCTION.

DIS IS THE DISCREPANCE IN THE TRANSMITTANCE DIFFERENCE (ROOT MEAN SQUARE OF THE RESIDUALS).

FM IS THE MAXIMUM ORDINATE DIFFERENCE.

WFM IS THE WAVENUMBER OF THE MAXIMUM ORDINATE DIFFERENCE.
```

PROGRAM XIII

PROGRAM XIII

Calculation of Cauchy-Gauss Shape Ratio and Half-band Widths

(PC-121)

This program retabulates the values of the indices and adds x_4 for the sum program; it also evaluates the following additional parameters for each component band:

1. The Cauchy-Gauss shape ratio
2. The half-band widths

A. The Cauchy-Gauss Shape Ratio

For the product function the shape ratio is defined as

$$SHAPP = ABS(X(3))/[ABS(X(3)) + ABS(X(4))] \quad [36]$$

It should be noted that X(3) and X(4) indices of negative sign are not uncommon, but the sign is immaterial to the computation of the ordinates as these indices occur in equations [1] and [6] only as squared terms. SHAPP takes a value of unity for a pure Cauchy curve and zero for a pure Gauss curve.

For the sum function the shape ratio is defined as

$$SHAPS = AREAC/[AREAC + AREAG] \quad [37]$$

where

$$AREAC = 1.570796\ X(1) \cdot (HLFWC) \quad [38]$$

and

$$AREAG = 1.0645\ X(5) \cdot (HLFWG) \quad [39]$$

in which HLFWC and HLFWG are the half-band widths of the Cauchy and Gauss component curves respectively in $cm.^{-1}$.

B. The Half-Band Widths

There are no simple algebraic expressions for the half-band widths and it is necessary to evaluate them by an iteration method.

(i) The Product Function

If 2b is the half-band width in cm.$^{-1}$ we may write from equation [1]

$$0.5 = (1+x_3^2b^2)^{-1} \cdot \exp - [x_4^2b^2] \qquad [40]$$

On inversion and expansion of the exponential term

$$2.0 = (1 + x_3^2b^2)(1 + x_4^2b^2 + ...) \qquad [41]$$

This provides a first approximation to b^2 in the form

$$b^4/2 + (WP)b^2 - 1/2x_3^2x_4^2 \approx 0 \qquad [42]$$

in which

$$WP = (x_3^2 + x_4^2)/2x_3^2x_4^2 \qquad [43]$$

In the program WP is evaluated following statement 13, and the quadratic equation [42] is solved to yield WX as an initial approximation for b^2; both roots are computed if they are real and positive, though there will normally be only one real and positive root; the two half-widths so found are designated HLFW1 and HLFW2. WX will differ from b^2 by an amount WF, where

$$WF = 2.0 - [1 + x_3^2(WX)] \cdot \exp x_4^2(WX) \qquad [44]$$

The gradient dWF/dWX is next calculated; this reduces to the expression

$$dWF/dWX = -P_5(P_3(1+P_6) + P_2) \qquad [45]$$

$$= WFD$$

where $P_2=x_3^2$; $P_3=x_4^2$; $P_5=\exp P_3\,(WX)$; $P_6=P_2(WX)$.

A correction term WF/WFD is subtracted from WX to provide WXN, the second approximation to b^2. This iterative process is continued until an acceptable agreement is obtained.

(ii) The Sum Function

For the sum function the treatment is similar, we have initially, with $x_4=kx_3$

$$0.5(x_1+x_5) = x_1(1+x_3^2b^2)^{-1}+x_5 \cdot \exp - [k^2x_3^2b^2] \qquad [46]$$

Inversion of equation [46] does not simplify the algebra (cf. equation [42]): the expansion of equation [46] and collection of terms yields

$$b^4[2x_5x_3^2k^2] + b^2[x_1-x_5+2x_5k^2] - (x_1+x_5)/x_3^2 = 0 \qquad [47]$$

which may be written

$$b^4S_3 + b^2S_5 + S_6 = 0 \qquad [48]$$

where $S_1=x_3^2$; $S_2=S_1k^2$; $S_3=2S_2x_5$; $S_4=1/S_1$;

$S_5= S_3S_4+x_1-x_5$; $S_6= -S_4(x_1+x_5)$.

Equation [48] is solved to obtain the first approximation of the composite half-band width (WX) following statement 128 in the program. The iterative process resembles that described for the product function with

$$WF = 0.5(x_1+x_5) - S_8x_1 + S_2S_{10} \qquad [49]$$

and

$$WFD = x_1S_1S_8^2 + S_2S_{10} \qquad [50]$$

where $S_8=1/(1+S_1(WX))$; $S_9=-S_2(WX)$; $S_{10}=x_5 \cdot \exp S_9$.

The half-band widths of the separate component Cauchy and Gauss curves (HLFWC) and (HLFWG) are also evaluated and recorded.

C. The Input Data

Cards 1 and 2 are heading cards HEAD1,HEAD2 (see Program X).

Card 3 carries four fixed point instructions in format 4I5. The instructions are NDATA, M, KURVE and NSEC which have the same connotations as for Program X.

Card 4 carries the ratio CAY in format F15.5. This CARD IS NEEDED ONLY FOR THE SUM FUNCTION AND MUST BE OMITTED WHEN WORKING WITH THE PRODUCT FUNCTION.

Card Deck 5 is a deck of M cards, each carrying the four band indices of a single band in format 4F15.5. The indices are x_1, x_2, x_3 and x_4 for the product function and x_1, x_2, x_3, x_5 for the sum function. The output data cards from the optimization programs X, XI, XIII can be used directly after removing the introductory and heading cards (see also Card Deck 7 on p. 13).

Card 6 This is a terminal card carrying the baseline constant α in format F15.5. This quantity does not enter into the computations, but it is stored and relisted with the output. When processing data not derived from the optimization programs α is liable to be zero, and should be entered as such. Failure to include this card will cause the program to terminate when attempting to process multiple decks with NDATA=2.

No detailed account of the internal logic of the program is called for. In the output of both the product and sum function computations the column headed HLFW-2 will normally be blank, indicating that only one real root of the quadratic equation [42] has been obtained.

The values computed by this program for the half-band widths and shape ratios for a range of values of x_3 and x_4 for the product function are listed in Table II. Similar data for the sum function for a range of values of x_3 with CAY=0.2 to CAY=0.8 are recorded in Table III. These tables will be found useful in selecting appropriate initial values for use with the band fit optimization programs. The boundary conditions limiting x_3 and x_4 in Table I were selected on the basis of these data.

TABLE II

Dependence of the Shape and Half-Band Width on X(3) and X(4) for the Cauchy-Gauss Product Curve*

SHAPE RATIO	X(3)	X(4)	HALF-WIDTH ($cm.^{-1}$)
0.0	0.0	0.017	100.3
		0.021	80.1
		0.028	60.1
		0.042	40.0
		0.083	20.0
		0.111	15.0
		0.166	10.0
		0.208	8.0
		0.277	6.0
		0.416	4.0
		0.555	3.0
		0.833	2.0
		1.166	1.4
		1.665	1.0
		3.330	0.5
0.1	0.002	0.018	91.9
	0.003	0.027	61.3
	0.004	0.036	46.0
	0.005	0.045	36.8
	0.006	0.054	30.6
	0.008	0.072	23.0
	0.010	0.090	18.4
	0.020	0.180	9.2
	0.030	0.270	6.1
	0.040	0.360	4.6
	0.050	0.450	3.7
	0.060	0.540	3.1
	0.080	0.720	2.3
	0.100	0.900	1.8
	0.150	1.350	1.2
	0.200	1.800	0.92
0.2	0.004	0.016	101.0
	0.005	0.020	80.8
	0.010	0.040	40.4
	0.020	0.080	20.2
	0.030	0.120	13.5
	0.040	0.160	10.1
	0.050	0.200	8.1
	0.060	0.240	6.7
	0.080	0.320	5.1
	0.100	0.400	4.0
	0.140	0.560	2.9
	0.200	0.800	2.0
	0.300	1.200	1.3
	0.400	1.600	1.0

Table II - ii.

SHAPE RATIO	X(3)	X(4)	HALF-WIDTH ($cm.^{-1}$)
0.3	0.005	0.012	128.5
	0.010	0.023	66.7
	0.020	0.047	32.7
	0.030	0.070	22.0
	0.040	0.093	16.5
	0.050	0.117	13.1
	0.060	0.140	11.0
	0.080	0.187	8.2
	0.100	0.233	6.6
	0.150	0.350	4.4
	0.200	0.467	3.3
	0.400	0.932	1.6
	0.600	1.400	1.1
0.4	0.01	0.015	93.8
	0.02	0.030	46.9
	0.03	0.045	31.3
	0.04	0.060	23.4
	0.05	0.075	18.8
	0.06	0.090	15.6
	0.08	0.120	11.7
	0.10	0.150	9.4
	0.15	0.225	6.3
	0.20	0.300	4.7
	0.30	0.450	3.1
	0.40	0.60	2.3
	0.70	1.05	1.3
	1.00	1.50	0.9
0.5	0.01	0.01	122.4
	0.02	0.02	61.2
	0.03	0.03	40.8
	0.04	0.04	30.6
	0.05	0.05	24.5
	0.06	0.06	20.4
	0.08	0.08	15.3
	0.10	0.10	12.2
	0.14	0.14	8.7
	0.20	0.20	6.1
	0.30	0.30	4.1
	0.40	0.40	3.1
	0.60	0.60	2.0
	1.00	1.00	1.2
	2.00	2.00	0.6

Table II - iii.

SHAPE RATIO	X(3)	X(4)	HALF-WIDTH ($cm.^{-1}$)
0.6	0.015	0.010	99.7
	0.02	0.013	74.9
	0.03	0.020	49.9
	0.04	0.027	37.4
	0.05	0.033	29.9
	0.06	0.040	24.9
	0.08	0.053	18.7
	0.10	0.067	15.0
	0.14	0.093	10.7
	0.20	0.133	7.5
	0.30	0.200	5.0
	0.40	0.267	3.7
	0.60	0.400	2.5
	1.00	0.667	1.5
	2.00	1.333	0.75
0.7	0.015	0.006	115.2
	0.02	0.009	86.2
	0.03	0.013	57.6
	0.04	0.017	43.2
	0.05	0.021	34.5
	0.06	0.026	28.8
	0.08	0.034	21.6
	0.10	0.043	17.3
	0.15	0.064	11.5
	0.20	0.086	8.6
	0.30	0.129	5.7
	0.40	0.171	4.3
	0.60	0.257	2.9
	1.00	0.429	1.7
	2.00	0.857	0.9
0.8	0.02	0.005	94.4
	0.03	0.007	62.9
	0.04	0.010	47.2
	0.05	0.012	37.8
	0.06	0.015	31.5
	0.08	0.020	23.6
	0.10	0.025	18.9
	0.20	0.050	9.4
	0.30	0.075	6.3
	0.40	0.100	4.7
	0.60	0.150	3.1
	1.00	0.250	1.9
	2.00	0.500	0.9

Table II - iv.

SHAPE RATIO	X(3)	X(4)	HALF-WIDTH ($cm.^{-1}$)
0.9	0.02	0.0022	98.8
	0.03	0.0033	65.9
	0.05	0.0056	39.5
	0.10	0.0111	19.8
	0.15	0.0167	13.1
	0.20	0.0222	9.9
	0.25	0.0278	7.9
	0.30	0.0333	6.6
	0.40	0.0444	4.9
	0.60	0.0667	3.3
	1.00	0.1111	2.0
	1.50	0.1667	1.3
	2.00	0.2222	1.0
1.0	0.017	0.0	119.8
	0.025		80.0
	0.050		40.0
	0.100		20.0
	0.200		10.0
	0.300		6.7
	0.400		5.0
	0.600		3.3
	1.000		2.0
	2.000		1.0

---

*Note that these figures have been rounded for tabulation; they are intended to be used only as a guide to the selection of appropriate starting values for X(3) and X(4).

TABLE III

Dependence of the Half-Width on X(3) and CAY for the Cauchy-Gauss Sum Function*

		HALF-WIDTH ($cm.^{-1}$)			
X(1)/X(5)=0.1	X(3)	CAY=0.8	CAY=0.6	CAY=0.4	CAY=0.2
	0.02	103.8	135.8	199.2	390.0
	0.04	51.9	67.9	99.6	195.1
	0.06	34.6	45.3	66.4	130.1
	0.08	26.0	33.9	49.8	97.6
	0.10	20.8	27.2	39.8	78.0
	0.20	10.4	13.6	19.9	39.0
	0.30	6.9	9.1	13.3	26.0
	0.40	5.2	6.8	10.0	19.5
	0.60	3.5	4.5	6.6	13.0
	1.00	2.1	2.7	4.0	7.8
	2.00	1.0	1.4	2.0	3.9
X(1)/X(5)=0.5					
	0.02	103.0	127.1	171.8	298.8
	0.04	51.5	63.6	85.9	149.4
	0.06	34.3	42.4	57.3	99.6
	0.08	25.7	31.7	43.0	74.7
	0.10	20.6	25.4	34.4	59.8
	0.20	10.3	12.7	17.2	29.9
	0.30	6.9	8.5	11.4	19.9
	0.40	5.1	6.4	8.6	14.9
	0.60	3.4	4.2	5.7	10.0
	1.00	2.1	1.7	3.4	6.0
	2.00	1.0	1.3	1.7	3.0
X(1)/X(5)=1.0					
	0.02	102.3	120.6	150.9	218.3
	0.04	51.1	60.3	75.4	109.1
	0.06	34.1	40.2	50.3	72.7
	0.08	25.6	30.1	37.7	54.6
	0.10	20.5	24.1	30.1	43.7
	0.20	10.2	12.1	15.1	21.8
	0.30	6.8	8.0	10.1	14.6
	0.40	5.1	6.0	7.5	10.9
	0.60	3.4	4.0	5.0	7.3
	1.00	2.0	2.4	3.0	4.4
	2.00	1.0	1.2	1.5	2.2

Table III - ii.

X(1)/X(5)=10.0 X(3)	HALF-WIDTH ($cm.^{-1}$) CAY=0.8	CAY=0.6	CAY=0.4	CAY=0.2
0.02	100.5	103.7	106.9	109.5
0.04	50.2	51.8	53.4	54.8
0.06	33.5	34.6	35.6	36.5
0.08	25.1	25.9	26.7	27.4
0.10	20.1	20.7	21.4	21.9
0.20	10.0	10.4	10.7	11.0
0.30	6.7	6.9	7.1	7.3
0.40	5.0	5.2	5.3	5.5
0.60	3.3	3.5	3.6	3.6
1.00	2.0	2.1	2.1	2.2
2.00	1.0	1.0	1.1	1.1

---

* Note that these figures have been rounded for tabulation; they are intended to be used only as a guide to the selection of appropriate starting values for X(3).

Most absorption bands are closer to the Cauchy than the Gauss shape and, in our experience an initial ratio of X(1)/X(5)= 10.0 is usually acceptable. Under these conditions the half-band width is not very sensitive to the value chosen for CAY, but it becomes increasingly so as X(1)/X(5) diminishes and the band becomes more Gaussian.

```
C                                                                       10
C     ***********************************************************       20
C     *                                                         *       30
C     *          CALCULATION OF CAUCHY-GAUSS SHAPE RATIO AND    *       40
C     *                                                         *       50
C     *                    HALF-BAND WIDTHS.                    *       60
C     *                                                         *       70
C     ***********************************************************       80
C                                                                       90
C     R.N.JONES AND J.PITHA,DIVISION OF CHEMISTRY,NATIONAL RESEARCH     100
C          COUNCIL OF CANADA,SUSSEX DRIVE,OTTAWA,CANADA.                110
C                                                                       120
C                                                                       130
C     PROGRAM XIII (PC-121) SHAPE AND HALF-WIDTH CALCULATOR.            140
C          JULY 22ND.1967.                                              145
C                                                                       150
C     FOR THE SUM FUNCTION THE HALF-WIDTHS AND SHAPES OF THE CAUCHY     160
C          AND GAUSS COMPONENT BANDS ARE SEPARATELY EVALUATED.          170
C     THESE CALCULATIONS DO NOT INVOLVE THE BASELINE CONSTANT,ALPHA,    180
C          BUT,FOR COMPLETENESS,IT IS INCLUDED IN THE OUTPUT TABULATION.190
C     FOR DETAILS SEE N.R.C.C. BULLETIN NO.12.                          200
C                                                                       210
C     ========= DON'T FORGET THE CAY CARD FOR THE SUM FUNCTION.=========220
C                                                                       230
C     THE CAY CARD IMMEDIATELY PRECEEDS THE DATA DECK.                  240
C                                                                       250
C     ============== DON'T FORGET THE TERMINAL ALPHA CARD.==============260
C                                                                       270
      DIMENSION HEAD1(20),HEAD2(20)                                     280
      IRD=1                                                             290
      IPRNT=3                                                           300
   10 WRITE (IPRNT,400)                                                 310
      READ (IRD,401) HEAD1                                              320
      READ (IRD,401) HEAD2                                              330
      READ (IRD,402) NDATA,M,KURVE,NSEC                                 340
C                                                                       350
C     M IS THE NUMBER OF BANDS TO BE CALCULATED.                        360
C                                                                       370
C     USE KURVE=1 FOR A PRODUCT FUNCTION; KURVE=2 FOR A SUM FUNCTION.   380
C                                                                       390
      WRITE (IPRNT,403) HEAD1                                           400
      WRITE (IPRNT,403) HEAD2                                           410
      ISKIP=1                                                           420
      IF (KURVE.EQ.2) GO TO 100                                         430
C                                                                       440
C     ******************  PRODUCT FUNCTION SECTION  ******************450
C                                                                       460
      WRITE (IPRNT,404)                                                 470
      CALL SETCLK                                                       480
      DO 50 J=1,M                                                       490
      IT=0                                                              500
      X1=0.0                                                            510
      X2=0.0                                                            520
      X3=0.0                                                            530
```

```
      X4=0.0                                                            540
      HLFW1=0.0                                                         550
      HLFW2=0.0                                                         560
      READ (IRD,405)  X1,X2,X3,X4                                       570
C                                                                       580
C                                                                       590
      IF (ABS(X4).LT.0.0001) GO TO 11                                   600
      IF (ABS(X3).LT.0.0001) GO TO 12                                   610
      GO TO 13                                                          620
C                                                                       630
C     CALCULATION OF SHAPE AND HALF-WIDTH FOR THE PURE CAUCHY CURVE.    640
C                                                                       650
   11 HLFW1=2.0/X3                                                      660
      SHAPP=1.000                                                       670
      GO TO 40                                                          680
C                                                                       690
C     CALCULATION OF THE SHAPE AND HALF-WIDTH FOR THE PURE GAUSS CURVE. 700
C                                                                       710
   12 HLFW1=1.665109/X4                                                 720
      SHAPP = 0.000                                                     730
      GO TO 40                                                          740
C                                                                       750
C     CALCULATION OF THE HALF-WIDTH OF THE PRODUCT CURVE BY ITERATION.  760
C                                                                       765
C     THE SOLUTION OF THE QUADRATIC EQUATION GIVES TWO VALUES,          770
C          BOTH ARE COMPUTED IF THEY ARE REAL AND POSITIVE, BUT NORMALLY 780
C          ONLY HLFW1 WILL BE OBTAINED.                                 790
C                                                                       800
   13 P2=X3*X3                                                          810
      P3=X4*X4                                                          820
      WP=(P2+P3)/(2.0*P2*P3)                                            830
      P4=WP*WP+1.0/(P2*P3)                                              840
      IF (P4.LT.0.0) GO TO 17                                           850
      P4=SQRT(P4)                                                       860
      IF (ISKIP.EQ.2) GO TO 16                                          870
      WX=P4-WP                                                          880
      GO TO 27                                                          890
   17 WRITE (IPRNT,415)                                                 900
      GO TO 49                                                          910
   16 WX=-WP-P4                                                         920
   27 IF (WX.GT.0.0) GO TO 21                                           930
      IF (ISKIP.EQ.2) GO TO 30                                          940
      ISKIP=2                                                           950
      GO TO 16                                                          960
   21 P5=EXP(P3*WX)                                                     970
      P6=P2*WX                                                          980
      WF=2.0-P5*(1.0+P6)                                                990
      WFD=-P5*(P3*(1.0+P6)+P2)                                         1000
      WXN=WX-WF/WFD                                                    1010
      WDIF=ABS(WX-WXN)                                                 1020
      IF (WDIF.LE.(WXN*0.0001)) GO TO 22                               1030
      WX=WXN                                                           1040
      IT=IT+1                                                          1050
      IF (IT.LT.5) GO TO 21                                            1060
```

```
      WRITE (IPRNT,417)                                                 1070
      GO TO 22                                                          1080
   22 WX=SQRT(WXN)                                                      1090
      IF (ISKIP.EQ.2) GO TO 25                                          1100
      HLFW1=2.0*WX                                                      1110
      ISKIP=2                                                           1120
      GO TO 16                                                          1130
   25 HLFW2=2.0*WX                                                      1140
   30 ISKIP=1                                                           1150
C                                                                       1160
C     CALCULATION OF THE SHAPE RATIO OF THE PRODUCT CURVE.              1170
C                                                                       1180
      SHAPP= ABS(X3)/(ABS(X3)+ABS(X4))                                  1190
   40 IF (HLFW2.EQ.0.0) GO TO 41                                        1200
      WRITE (IPRNT,406) X1,X2,X3,X4,SHAPP,HLFW1,HLFW2                   1210
      GO TO 49                                                          1220
   41 WRITE (IPRNT,407) X1,X2,X3,X4,SHAPP,HLFW1                         1230
   49 CALL RDCLK (TIME)                                                 1240
      ISECS=TIME+0.5                                                    1250
      IF (ISECS.GT.NSEC) GO TO 52                                       1260
   50 CONTINUE                                                          1270
      GO TO 53                                                          1280
   52 WRITE (IPRNT,414)                                                 1290
   53 WRITE (IPRNT,408)                                                 1300
C                                                                       1310
C     *************  TERMINAL SECTION FOR BOTH FUNCTIONS  **************1320
C                                                                       1330
   51 READ (IRD,405) XN                                                 1340
      WRITE (IPRNT,409) XN                                              1350
      IF (NDATA.EQ.2) GO TO 10                                          1360
      STOP                                                              1370
C                                                                       1380
C     **********************  SUM FUNCTION SECTION  **********************1390
C                                                                       1400
  100 WRITE (IPPNT,410)                                                 1410
      READ (IRD,405) CAY                                                1420
      CALL SETCLK                                                       1430
  101 DO 150 J=1,M                                                      1440
      IT=0                                                              1450
      X1=0.0                                                            1460
      X2=0.0                                                            1470
      X3=0.0                                                            1480
      X5=0.0                                                            1490
      HLFW1=0.0                                                         1500
      HLFW2=0.0                                                         1510
      READ (IRD,405) X1,X2,X3,X5                                        1520
      XX1=X1                                                            1530
      XX3=X3                                                            1540
      XX5=X5                                                            1550
      X1=ABS(X1)                                                        1560
      X3=ABS(X3)                                                        1570
      X5=ABS(X5)                                                        1580
      X4=X3*CAY                                                         1590
      XX4=XX3*CAY                                                       1600
```

```
C                                                                       1610
C     CALCULATION OF THE HALF-WIDTH OF THE CAUCHY COMPONENT CURVE.      1620
C                                                                       1630
      HLFWC=2.0/X3                                                      1640
C                                                                       1650
C     CALCULATION OF THE HALF-WIDTH OF THE GAUSS COMPONENT CURVE.       1660
C                                                                       1670
      HLFWG=1.665109/X4                                                 1680
C                                                                       1690
C     CALCULATION OF THE HALF-WIDTH OF THE COMPOSITE CURVE.             1700
C                                                                       1710
C     FIRST CHECK FOR ZERO X1 OR X5                                     1720
C     THIS SIGNIFIES A PURE GAUSS OR PURE CAUCHY CURVE, RESPECTIVELY.   1730
C                                                                       1740
      IF (X1.NE.0.0) GO TO 112                                          1750
      HLFW1=HLFWG                                                       1760
      HLFW2=0.0                                                         1770
      GO TO 130                                                         1780
  112 IF (X5.NE.0.0) GO TO 114                                          1790
      HLFW1=HLFWC                                                       1800
      HLFW2=0.0                                                         1810
      GO TO 130                                                         1820
  114 S1=X3*X3                                                          1830
      S2=X4*X4                                                          1840
      S3=2.0*X5*S2                                                      1850
      S4=1.0/S1                                                         1860
      S5=S3*S4+X1-X5                                                    1870
      S6=-S4*(X1+X5)                                                    1880
      S7=S5*S5-4.0*S3*S6                                                1890
      IF (S7.GE.0.0) GO TO 128                                          1900
      WRITE (IPRNT,415)                                                 1910
      GO TO 150                                                         1920
  128 S7=SQRT(S7)                                                       1930
      IF (ISKIP.EQ.2) GO TO 116                                         1940
      WX=S7-S5                                                          1950
      GO TO 127                                                         1960
  116 WX=-S5-S7                                                         1970
  127 WX=WX/(2.0*S3)                                                    1980
      IF (WX.GT.0.0) GO TO 121                                          1990
      IF (ISKIP.EQ.2) GO TO 130                                         2000
      ISKIP=2                                                           2010
      GO TO 116                                                         2020
  121 S8=1.0/(1.0+S1*WX)                                                2030
      S9=-S2*WX                                                         2040
      S10=X5*EXP(S9)                                                    2050
      WF=0.5*(X1+X5)-X1*S8-S10                                          2060
      WFD=X1*S1*S8*S8+S2*S10                                            2070
      WXN=WX-WF/WFD                                                     2080
      WDIF=ABS(WX-WXN)                                                  2090
      IF (WDIF.LE.WXN*0.0001) GO TO 122                                 2100
      WX=WXN                                                            2110
      IT=IT+1                                                           2120
      IF (IT.LT.5) GO TO 121                                            2130
      WRITE (IPRNT,417)                                                 2140
```

```
      GO TO 122                                                          2150
  122 IF (WXN.GE.0.0) GO TO 129                                          2160
      WRITE (IPRNT,416)                                                  2170
      IF (ISKIP.EQ.1) GO TO 123                                          2180
      GO TO 150                                                          2190
  129 WX=SQRT(WXN)                                                       2200
      IF (ISKIP.EQ.2) GO TO 125                                          2210
      HLFW1=2.0*WX                                                       2220
  123 ISKIP=2                                                            2230
      GO TO 116                                                          2240
  125 HLFW2=2.0*WX                                                       2250
  130 ISKIP=1                                                            2260
C                                                                        2270
C     CALCULATION OF THE CAUCHY-GAUSS SHAPE RATIO FOR THE SUM BAND.      2280
C                                                                        2290
      AREAC=1.570796*XX1*HLFWC                                           2300
      AREAG=1.0645*XX5*HLFWG                                             2310
      SHAPS=AREAC/(AREAC+AREAG)                                          2320
      IF (HLFW2.EQ.0.0) GO TO 141                                        2330
      WRITE (IPRNT,411) XX1,X2,XX3,XX4,XX5,SHAPS,HLFWC,HLFWG,HLFW1,HLFW2 2340
      GO TO 149                                                          2350
  141 WRITE (IPRNT,411) XX1,X2,XX3,XX4,XX5,SHAPS,HLFWC,HLFWG,HLFW1       2360
  149 CALL RDCLK (TIME)                                                  2370
      ISECS=TIME+0.5                                                     2380
      IF (ISECS.GT.NSEC) GO TO 152                                       2390
  150 CONTINUE                                                           2400
      GO TO 153                                                          2410
  152 WRITE (IPRNT,414)                                                  2420
  153 WRITE (IPRNT,413) CAY                                              2430
      GO TO 51                                                           2440
C                                                                        2450
C                                                                        2460
  400 FORMAT ('1PITHA AND JONES.   PROGRAM XIII (PC-121)   BAND FIT PROG 2470
     1RAM--SHAPES AND HALF-WIDTHS.'/)                                    2480
  401 FORMAT (20A4)                                                      2490
  402 FORMAT (4I5)                                                       2500
  403 FORMAT (1X,20A4)                                                   2510
  404 FORMAT ('0',10X,4HX(1),8X,4HX(2),7X,4HX(3),7X,4HX(4),7X,5HSHAPE,   2520
     16X,6HHLFW-1,5X,6HHLFW-2)                                           2530
  405 FORMAT (4F15.5)                                                    2540
  406 FORMAT ('0',5X,F10.6,2X,F10.3,2F11.6,3F12.6)                       2550
  407 FORMAT ('0',5X,F10.6,2X,F10.3,2F11.6,2F12.6,7X,1H-)                2560
  408 FORMAT ('0THESE DATA ARE FOR THE PRODUCT FUNCTION.')               2570
  409 FORMAT (/8X,7HALPHA = ,E14.6)                                      2580
  410 FORMAT ('0',10X,4HX(1),6X,4HX(2),7X,4HX(3),7X,4HX(4),7X,4HX(5),6X, 2590
     15HSHAPE,6X,6HHLFW-C,6X,6HHLFW-G,6X,6HHIFW-1,5X,6HHLFW-2)           2600
  411 FORMAT ('0',5X,F10.6,F10.3,4F11.6,4F12.6)                          2610
  412 FORMAT ('0',5X,F10.6,F10.3,4F11.6,3F12.6,7X,1H-)                   2620
  413 FORMAT ('0THESE DATA ARE FOR THE SUM FUNCTION WITH CAY =',F5.2)    2630
  414 FORMAT ('0TERMINATED BY PROGRAM TIME CONTROL.')                    2640
  415 FORMAT ('0ROOTS OF THE QUADRATIC EQUATION ARE IMAGINARY.')         2650
  416 FORMAT ('0HALF-WIDTH OF THE COMPOSITE CURVE IS IMAGINARY.')        2660
  417 FORMAT ('0FIVE ITERATION LIMIT ON NEXT BAND.')                     2670
      END                                                                2680
```

PITHA AND JONES. PROGRAM XIII (PC-121) BAND FIT PROGRAM--SHAPES AND HALF-WIDTHS.

APRIL 3RD. 1968. FOUR BAND TEST DECK FOR PRODUCT FUNCTION.
TRUE VALUES FROM CALCULATED CURVE.

X(1)	X(2)	X(3)	X(4)	SHAPE	HLFW-1	HLFW-2
0.300000	970.000	0.200000	0.100000	0.666667	8.277420	-
0.600000	955.000	0.200000	0.200000	0.500000	6.122278	-
0.300000	940.000	0.100000	0.100000	0.500000	12.244562	-
0.400000	920.000	0.200000	0.100000	0.666667	8.277420	-

THESE DATA ARE FOR THE PRODUCT FUNCTION.

ALPHA = 0.500000E-01

PITHA AND JONES. PROGRAM XIII (PC-121) BAND FIT PROGRAM--SHAPES AND HALF-WIDTHS.

APRIL 3RD.1968. FOUR BAND TEST DECK FOR SUM FUNCTION.
TRUE VALUES FROM CALCULATED CURVE.

X(1)	X(2)	X(3)	X(4)	X(5)	SHAPE	HLFW-C	HLFW-G	HLFW-1	HLFW-2
0.200000	970.000	0.200000	0.160000	0.100000	0.739301	10.000000	10.406931	10.163906	
0.400000	955.000	0.200000	0.160000	0.200000	0.739301	10.000000	10.406931	10.163906	
0.100000	940.000	0.100000	0.080000	0.200000	0.414848	20.000000	20.813873	20.594498	
0.250000	920.000	0.200000	0.160000	0.150000	0.702664	10.000000	10.406931	10.182089	

THESE DATA ARE FOR THE SUM FUNCTION WITH CAY = 0.80

ALPHA = 0.500000E-01

PROGRAM XIV

PROGRAM XIV

Calculation of the Ordinates of Cauchy-Gauss Band Envelopes

(PC-122)

When supplied with the indices of either the product or sum functions, this program generates a set of ordinates for the overlapping band envelope. The calculated ordinates are spaced at equal abscissal intervals determined by the selected value of WI.

This program is dimensioned for a maximum of twenty overlapping bands and two thousand calculated ordinates. The output can be either in units of absorbance or transmittance × 1000, and a card deck in the standard punched format can be obtained as well as the printed listing. When operated in the absorbance mode, the Cauchy and Gauss components of the sum function are listed separately in parallel columns while a third column lists the summed value, included in which is the baseline constant α. On the transmittance × 1000 scale only the summed value, including α, is listed.

This program may also be used to generate a set of ordinates for single bands of pure Cauchy, pure Gauss, product, or sum contour, but a more versatile program that will generate single band of any requisite contour, based on a single valued function, is described in Bulletin 11 (Program VIII).

A. The Input Data

Cards 1 and 2 are heading cards HEAD1,HEAD2 (see Program X).

Card 3 carries six fixed point instructions NDATA,IDECK,NP,M, KURVE,IXIT in format 6I5. The first five have the same connotation as for Program X.
Use IXIT = 1 for ordinate output in units of transmittance × 1000.
Use IXIT = 2 for ordinate output in absorbance units.

Card 4 carries two floating point instructions for the product function and three for the sum function in formats 2F15.5 or 3F15.5 respectively. They are WB, WI and CAY as described for Program X.

Card Deck 5 This is a set of M cards carrying the input ordinate indices x_1, x_2, x_3, x_4 for the product function and x_1, x_2, x_3, x_5 for the sum function. (See Card Deck 7 on p. 13).

Card 6 is the terminal card carrying the baseline constant α. (See Card 8 on p. 13.)

No detailed account of the internal logic of the program is required beyond the comment statements that are incorporated in the program.

The test data sets are for the four band product and sum band enveloped illustrated in Figs. 1 and 2 on pp. 24,25 of this volume.

```
C                                                                       10
C     ***************************************************************** 20
C     *                                                               * 30
C     *          CALCULATION OF THE ORDINATES OF CAUCHY-GAUSS         * 40
C     *                                                               * 50
C     *                        BAND ENVELOPES.                        * 60
C     *                                                               * 70
C     ***************************************************************** 80
C                                                                       90
C     J.PITHA AND R.N.JONES,DIVISION OF CHEMISTRY,NATIONAL RESEARCH     100
C          COUNCIL OF CANADA,SUSSEX DRIVE,OTTAWA,CANADA.                110
C                                                                       120
C     PROGRAM XIV (PC-122)                              JULY 20TH.1967. 130
C                                                                       140
C     THE ORDINATES CAN BE EVALUATED IN TRANSMITTANCE X 1000 OR IN      150
C          ABSORBANCE.                                                  160
C     FOR THE SUM FUNCTION THE ABSORBANCE OF THE GAUSS AND CAUCHY       170
C          COMPONENTS ARE LISTED SEPARATELY. THEY ARE ALSO SUMMED       180
C          TOGETHER WITH THE BASELINE CONSTANT. THE SUMMED ORDINATES MAY 190
C          BE LISTED IN EITHER ABSORBANCE OR TRANSMITTANCE X 1000.      200
C     THIS PROGRAM IN DIMENSIONED FOR 2000 DATA POINTS AND 20 COMPONENT 210
C     BANDS. IN THE PRODUCT MODE THE PROGRAM WILL GENERATE A PURE CAUCHY 220
C          CURVE IF X(4)=0 AND PURE GAUSS CURVE IF X(3)=0.              230
C                                                                       235
C     FOR DETAILS SEE N.R.C.C. BULLETIN NO.12.                          240
C                                                                       250
      DIMENSION PC(20), PG(20), X(81), IW(2000), WW(2000),ORD1(2000),   260
     1ORD2(2000), SUM(2000), HEAD1(20), HEAD2(20),IT(2000)              270
      EQUIVALENCE (SUM(1),IT(1))                                        280
      IRD=1                                                             290
      IPCH=2                                                            300
      IPRNT=3                                                           310
   10 WRITE (IPRNT,400)                                                 320
      READ (IRD,401) HEAD1                                              330
      READ (IRD,401) HEAD2                                              340
      READ (IRD,402) NDATA,IDECK,NP,M,KURVE,IXIT                        350
      IF (KURVE.EQ.2) GO TO 12                                          360
      READ (IRD,407) WB,WI                                              370
      GO TO 13                                                          380
   12 READ (IRD,407) WB,WI,CAY                                          390
C                                                                       400
C     USE KURVE=1 FOR PRODUCT FUNCTION AND KURVE=2 FOR SUM FUNCTION.    410
C     REMEMBER THAT IF KURVE=2 CAY MUST BE DEFINED.                     420
C     USE IXIT=1 FOR OUTPUT IN CM.-| X 10 AND TRANSMITTANCE X 1000.     430
C     USE IXIT=2 FOR OUTPUT IN CM.-1 AND ABSORBANCE UNITS.              440
C                                                                       450
   13 IF (IDECK.EQ.1) GO TO 11                                          460
      WRITE (IPCH,401) HEAD1                                            470
      WRITE (IPCH,401) HEAD2                                            480
   11 WRITE (IPRNT,404) HEAD1                                           490
      WRITE (IPRNT,404) HEAD2                                           500
      IF (KURVE.EQ.2) GO TO 14                                          510
      WRITE (IPRNT,405)                                                 520
      GO TO 15                                                          530
```

```
   14 WRITE (IPRNT,406)                                                  540
   15 N=4*M+1                                                            550
      DO 16 I=1,M                                                        560
      J=I+M                                                              570
      K=J+M                                                              580
      L=K+M                                                              590
      READ (IRD,407) X(I),X(J),X(K),X(L)                                 600
      WRITE (IPRNT,408) X(I),X(J),X(K),X(L)                              610
   16 CONTINUE                                                           620
      READ (IRD,407) X(N)                                                630
      WRITE (IPRNT,409) X(N)                                             640
      WRITE (IPRNT,410) NP,WB,WI                                         650
      IF (KURVE.EQ.2) GO TO 120                                          660
C                                                                        670
C     ****** COMPUTATION OF THE ORDINATES OF THE PRODUCT FUNCTION ******  680
C                                                                        690
      DO 21 II=1,NP                                                      700
      FII=II-1                                                           710
      W=WB-WI*FII                                                        720
      AC=0.0                                                             730
      DO 22 I=1,M                                                        740
      J=I+M                                                              750
      K=J+M                                                              760
      L=K+M                                                              770
      R=W-X(J)                                                           780
      RSQ=R*R                                                            790
      PC(I)=1.0/(1.0+X(K)*X(K)*RSQ)                                      800
      PG(I)=X(L)*X(L)*RSQ                                                810
      IF (PG(I).LT.10.0) GO TO 23                                        820
      PG(I)=0.0                                                          830
      GO TO 22                                                           840
   23 PG(I)=EXP(-PG(I))                                                  850
   22 AC=X(I)*PC(I)*PG(I)+AC                                             860
      AC=AC+X(N)                                                         870
      IF (AC.LE.0.0006) GO TO 26                                         880
      IF (AC.LT.10.0) GO TO 30                                           890
      AC=10.0                                                            900
      GO TO 30                                                           910
   26 AC=0.0                                                             920
   30 ORD1(II)=AC                                                        930
      WW(II)=W                                                           940
   21 IW(II)=W*10.0+0.5                                                  950
      WRITE (IPRNT,420)                                                  960
      IF (IXIT.EQ.2) GO TO 34                                            970
      DO 31 I=1,NP                                                       980
   31 IT(I)=EXP(-ORD1(I)*2.30258)*1000.0+0.5                             990
      WRITE (IPRNT,411)                                                 1000
      WRITE (IPRNT,412) (IW(I),IT(I),I=1,NP)                            1010
      IF (IDECK.EQ.1) GO TO 32                                          1020
      WRITE (IPCH,413) (IW(I),IT(I),I=1,NP)                             1030
   32 IF (NDATA.EQ.1) GO TO 33                                          1040
      GO TO 10                                                          1050
   33 STOP                                                              1060
   34 WRITE (IPRNT,414)                                                 1070
```

```
      WRITE (IPRNT,415) (WW(I),ORD1(I),I=1,NP)                          1080
      IF (IDECK.EQ.1) GO TO 32                                          1090
      WRITE (IPCH,416) (WW(I),ORD1(I),I=1,NP)                           1100
      GO TO 32                                                          1110
C                                                                       1120
C     ******** COMPUTATION OF THE ORDINATES OF THE SUM FUNCTION ********1130
C                                                                       1140
C     IN THIS SECTION, ORDINATES OF THE CAUCHY COMPONENT ARE EVALUATED. 1150
C                                                                       1160
  120 DO 121 II=1,NP                                                    1170
      FII=II-1                                                          1180
      W=WB-WI*FII                                                       1190
      AC=0.0                                                            1200
      DO 122 I=1,M                                                      1210
      J=I+M                                                             1220
      K=J+M                                                             1230
      L=K+M                                                             1240
      R=(W-X(J))*X(K)                                                   1250
      RSQ=R*R                                                           1260
      PC(I)=1.0/(1.0+RSQ)                                               1270
  122 AC=X(I)*PC(I)+AC                                                  1280
      ORD1(II)=AC                                                       1290
  121 IW(II)=W*10.0+0.5                                                 1300
C                                                                       1310
C     IN THIS SECTION, ORDINATES OF THE GAUSS COMPONENT ARE EVALUATED.  1320
C                                                                       1330
      DO 221 II=1,NP                                                    1340
      FII=II-1                                                          1350
      W=WB-WI*FII                                                       1360
      AC=0.0                                                            1370
      DO 222 I=1,M                                                      1380
      J=I+M                                                             1390
      K=J+M                                                             1400
      L=K+M                                                             1410
      R=(W-X(J))*CAY*X(K)                                               1420
      PG(I)=R*R                                                         1430
      IF (PG(I).LT.10.0) GO TO 223                                      1440
      PG(I)=0.0                                                         1450
      GO TO 222                                                         1460
  223 PG(I)=EXP(-PG(I))                                                 1470
  222 AC=X(L)*PG(I)+AC                                                  1480
      IF (AC.LT.4.6) GO TO 221                                          1490
      AC=4.6                                                            1500
  221 ORD2(II)=AC                                                       1510
C                                                                       1520
C     ************************* OUTPUT SECTION *************************1530
C                                                                       1540
      XN=X(N)                                                           1550
      WRITE (IPRNT,421) CAY                                             1560
      IF (IXIT.EQ.1) GO TO 234                                          1570
      WRITE (IPRNT,414)                                                 1580
      DO 236 I=1,NP                                                     1590
      WW(I)=IW(I)*0.1                                                   1600
  236 SUM(I)=ORD1(I)+ORD2(I)+XN                                         1610
```

```
      WRITE (IPRNT,417) (WW(I),ORD1(I),ORD2(I),SUM(I),I=1,NP)                1620
      WRITE (IPRNT,418)                                                      1630
      IF (IDECK.EQ.1) GO TO 32                                               1640
      WRITE (IPCH,422) (WW(I),SUM(I),I=1,NP)                                 1650
      GO TO 32                                                               1660
  234 WRITE (IPRNT,411)                                                      1670
      DO 237 I=1,NP                                                          1680
      SUM(I)=ORD1(I)+ORD2(I)+XN                                              1690
  237 IT(I)=0.5+EXP(-SUM(I)*2.30258)*1000.0                                  1700
      WRITE (IPRNT,412) (IW(I),IT(I), I=1,NP)                                1710
      WRITE (IPRNT,419)                                                      1720
      IF (IDECK.EQ.1) GO TO 32                                               1730
      WRITE (IPCH,413) (IW(I),IT(I), I=1,NP)                                 1740
      GO TO 32                                                               1750
C                                                                            1760
  400 FORMAT ('1PITHA AND JONES,INFRARED BAND FIT---COMPUTATION OF THE O     1770
     1RDINATES OF CAUCHY-GAUSS BAND ENVELOPES.'/)                            1780
  401 FORMAT (20A4)                                                          1790
  402 FORMAT (6I5)                                                           1800
  403 FORMAT (2(4X,1H1),3I5)                                                 1810
  404 FORMAT (1X,20A4)                                                       1820
  405 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(4))               1830
  406 FORMAT ('0',15X,4HX(1),17X,4HX(2),17X,4HX(3),17X,4HX(5))               1840
  407 FORMAT (4F15.5)                                                        1850
  408 FORMAT (1X,4(6X,F15.5))                                                1860
  409 FORMAT (4X,7HALPHA =,F8.5)                                             1870
  410 FORMAT (10X,2HNP,I6,15X,2HWB,F8.1,11X,2HWI,F5.1)                       1880
  411 FORMAT ('0ORDINATES IN TRANSMITTANCE X 1000. ----------------------    1890
     1-------------------------------- '/)                                   1900
  412 FORMAT (11(2X,I5,I4))                                                  1910
  413 FORMAT (8(I5,I4,1X))                                                   1920
  414 FORMAT ('0ORDINATES IN ABSORBANCE UNITS. -------------------------     1930
     1-------------------------------- '/)                                   1940
  415 FORMAT (8(1X,F6.1,F6.3,2X))                                            1950
  416 FORMAT (6(F6.1,F6.3,1X))                                               1960
  417 FORMAT (4(3X,F6.1,3F6.3))                                              1970
  418 FORMAT ('0','CAUCHY,GAUSS, AND THE SUMMED ORDINATES ARE LISTED CON     1980
     1SECUTIVELY.')                                                          1990
  419 FORMAT ('0THE SUMMED ORDINATES ONLY ARE LISTED.')                      2000
  420 FORMAT ('0CALCULATIONS FOR THE PRODUCT FUNCTION.')                     2010
  421 FORMAT ('0CALCULATIONS FOR THE SUM FUNCTION WITH CAY=',F4.2)           2020
  422 FORMAT (6(F6.1,F6.3,1X))                                               2030
      END                                                                    2040
```

PITHA AND JONES,INFPARFD BAND FIT---COMPUTATION OF THE ORDINATES OF CAUCHY-GAUSS BAND ENVELOPES.

MARCH 12TH.1968. PROGRAM XIV (PC-122) MULTIPLE CURVE GENERATION.
FOUR BAND TEST DECK FOR PRODUCT FUNCTION. IXIT=1

X(1)	X(2)	X(3)	X(4)
0.30000	970.00000	0.20000	0.10000
0.60000	955.00000	0.20000	0.20000
0.30000	940.00000	0.10000	0.10000
0.40000	920.00000	0.20000	0.10000

ALPHA = 0.05000
NP 200 WB 1000.0 WI 0.5

CALCULATIONS FOR THE PRODUCT FUNCTION.

ORDINATES IN TRANSMITTANCE X 1000. ----------

10000 891	9995 891	9990 891	9985 891	9980 891	9975 891	9970 891	9965 891	9960 891	9955 891	9950 891
9945 891	9940 891	9935 891	9930 891	9925 891	9920 891	9915 891	9910 891	9905 891	9900 891	9895 890
9890 890	9885 890	9880 890	9875 889	9870 889	9865 888	9860 887	9855 886	9850 885	9845 883	9840 881
9835 879	9830 877	9825 874	9820 870	9815 866	9810 860	9805 854	9800 847	9795 839	9790 829	9785 818
9780 805	9775 790	9770 773	9765 753	9760 732	9755 707	9750 681	9745 653	9740 622	9735 591	9730 560
9725 530	9720 503	9715 480	9710 462	9705 451	9700 447	9695 450	9690 462	9685 480	9680 503	9675 530
9670 560	9665 591	9660 621	9655 650	9650 677	9645 702	9640 722	9635 738	9630 749	9625 754	9620 753
9615 743	9610 724	9605 695	9600 655	9595 606	9590 550	9585 488	9580 426	9575 366	9570 315	9565 273
9560 242	9555 224	9550 217	9545 223	9540 240	9535 268	9530 307	9525 355	9520 409	9515 466	9510 520
9505 569	9500 608	9495 638	9490 657	9485 667	9480 668	9475 662	9470 651	9465 636	9460 617	9455 597
9450 577	9445 556	9440 535	9435 516	9430 499	9425 484	9420 471	9415 460	9410 453	9405 448	9400 446
9395 449	9390 452	9385 459	9380 470	9375 482	9370 497	9365 514	9360 533	9355 553	9350 574	9345 595
9340 616	9335 637	9330 656	9325 675	9320 691	9315 705	9310 718	9305 727	9300 733	9295 737	9290 737
9285 734	9280 727	9275 717	9270 702	9265 684	9260 663	9255 637	9250 609	9245 577	9240 544	9235 510
9230 475	9225 443	9220 413	9215 388	9210 369	9205 358	9200 354	9195 358	9190 370	9185 390	9180 415
9175 446	9170 480	9165 516	9160 552	9155 588	9150 623	9145 655	9140 685	9135 712	9130 737	9125 758
9120 778	9115 794	9110 809	9105 822	9100 833	9095 842	9090 850	9085 857	9080 863	9075 868	9070 872
9065 875	9060 878	9055 881	9050 883	9045 884	9040 886	9035 887	9030 888	9025 888	9020 889	9015 889
9010 890	9005 890									

PITHA AND JONES,INFRARED BAND FIT---COMPUTATION OF THE ORDINATES OF CAUCHY-GAUSS BAND ENVELOPES.

MARCH 12TH.1968. PROGRAM XIV (PC-122) MULTIPLE CURVE GENERATION.
FOUR BAND TEST DECK FOR SUM FUNCTION. IXIT=1

X(1)	X(2)	X(3)	X(5)
0.20000	970.00000	0.20000	0.10000
0.40000	955.00000	0.20000	0.20000
0.10000	940.00000	0.10000	0.20000
0.25000	920.00000	0.20000	0.15000

ALPHA = 0.05000
NP 200 WB 1000.0 WI 0.5

CALCULATIONS FOR THE SUM FUNCTION WITH CAY=0.80

ORDINATES IN TRANSMITTANCE X 1000. ----------

10000 863	9995 862	9990 862	9985 861	9980 860	9975 859	9970 859	9965 858	9960 857	9955 856	9950 855
9945 854	9940 853	9935 851	9930 850	9925 849	9920 848	9915 846	9910 845	9905 843	9900 842	9895 840
9890 838	9885 836	9880 834	9875 832	9870 829	9865 827	9860 824	9855 821	9850 818	9845 814	9840 810
9835 806	9830 801	9825 796	9820 790	9815 783	9810 776	9805 767	9800 757	9795 746	9790 734	9785 720
9780 705	9775 688	9770 669	9765 649	9760 627	9755 605	9750 581	9745 556	9740 532	9735 507	9730 483
9725 461	9720 440	9715 423	9710 409	9705 400	9700 395	9695 394	9690 398	9685 405	9680 415	9675 427
9670 439	9665 452	9660 463	9655 473	9650 480	9645 484	9640 485	9635 482	9630 475	9625 464	9620 449
9615 431	9610 410	9605 386	9600 361	9595 335	9590 308	9585 283	9580 258	9575 236	9570 217	9565 201
9560 189	9555 180	9550 176	9545 176	9540 180	9535 188	9530 199	9525 212	9520 227	9515 244	9510 261
9505 278	9500 296	9495 312	9490 327	9485 340	9480 352	9475 362	9470 370	9465 376	9460 381	9455 384
9450 386	9445 387	9440 387	9435 387	9430 387	9425 386	9420 386	9415 386	9410 386	9405 387	9400 388
9395 391	9390 394	9385 397	9380 402	9375 407	9370 413	9365 420	9360 427	9355 435	9350 441	9345 452
9340 460	9335 469	9330 478	9325 486	9320 494	9315 502	9310 508	9305 514	9300 518	9295 521	9290 522
9285 521	9280 518	9275 512	9270 504	9265 494	9260 482	9255 467	9250 451	9245 434	9240 415	9235 397
9230 379	9225 361	9220 346	9215 334	9210 325	9205 320	9200 320	9195 324	9190 334	9185 348	9180 366
9175 383	9170 413	9165 440	9160 468	9155 497	9150 526	9145 554	9140 582	9135 608	9130 633	9125 657
9120 678	9115 697	9110 715	9105 730	9100 744	9095 756	9090 767	9085 776	9080 784	9075 791	9070 797
9065 803	9060 808	9055 812	9050 816	9045 820	9040 823	9035 826	9030 829	9025 831	9020 834	9015 836
9010 838	9005 840									

THE SUMMED ORDINATES ONLY ARE LISTED.

PITHA AND JONES,INFRARED BAND FIT---COMPUTATION OF THE ORDINATES OF CAUCHY-GAUSS BAND ENVELOPES.

MARCH 12TH.1968. PROGRAM XIV (PC-122) MULTIPLE CURVE GENERATION.
FOUR BAND TEST DECK FOR SUM FUNCTION. IXIT=2

X(1)	X(2)	X(3)	X(5)
0.20000	970.00000	0.20000	0.10000
0.40000	955.00000	0.20000	0.20000
0.10000	940.00000	0.10000	0.20000
0.25000	920.00000	0.20000	0.15000

ALPHA = 0.05000
NP 200 WB 1000.0 WI 0.5

CALCULATIONS FOR THE SUM FUNCTION WITH CAY=0.80

ORDINATES IN ABSORBANCE UNITS. ----------

1000.0 0.014 0.000 0.064	999.5 0.014 0.000 0.064	999.0 0.015 0.000 0.065	998.5 0.015 0.000 0.065
998.0 0.015 0.000 0.065	997.5 0.016 0.000 0.066	997.0 0.016 0.000 0.066	996.5 0.017 0.000 0.067
996.0 0.017 0.000 0.067	995.5 0.018 0.000 0.068	995.0 0.018 0.000 0.068	994.5 0.019 0.000 0.069
994.0 0.019 0.000 0.069	993.5 0.020 0.000 0.070	993.0 0.020 0.000 0.070	992.5 0.021 0.000 0.071
992.0 0.022 0.000 0.072	991.5 0.022 0.000 0.072	991.0 0.023 0.000 0.073	990.5 0.024 0.000 0.074
990.0 0.025 0.000 0.075	989.5 0.026 0.000 0.076	989.0 0.027 0.000 0.077	988.5 0.028 0.000 0.078
988.0 0.029 0.000 0.079	987.5 0.030 0.000 0.080	987.0 0.031 0.000 0.081	986.5 0.032 0.000 0.083
986.0 0.034 0.000 0.084	985.5 0.035 0.000 0.086	985.0 0.037 0.000 0.087	984.5 0.039 0.000 0.089
984.0 0.041 0.001 0.091	983.5 0.043 0.001 0.094	983.0 0.045 0.001 0.096	982.5 0.047 0.002 0.099
982.0 0.050 0.003 0.102	981.5 0.053 0.003 0.106	981.0 0.056 0.005 0.110	980.5 0.059 0.006 0.115
980.0 0.063 0.008 0.121	979.5 0.067 0.010 0.127	979.0 0.072 0.013 0.134	978.5 0.077 0.016 0.143
978.0 0.083 0.019 0.152	977.5 0.089 0.024 0.163	977.0 0.096 0.029 0.174	976.5 0.104 0.034 0.188
976.0 0.113 0.040 0.202	975.5 0.122 0.046 0.218	975.0 0.133 0.053 0.236	974.5 0.145 0.060 0.255
974.0 0.158 0.067 0.274	973.5 0.172 0.073 0.295	973.0 0.186 0.080 0.316	972.5 0.201 0.086 0.337
972.0 0.215 0.091 0.356	971.5 0.229 0.095 0.374	971.0 0.240 0.098 0.388	970.5 0.248 0.100 0.398
970.0 0.252 0.101 0.404	969.5 0.253 0.101 0.404	969.0 0.251 0.100 0.400	968.5 0.245 0.097 0.393
968.0 0.238 0.094 0.382	967.5 0.230 0.090 0.370	967.0 0.221 0.086 0.357	966.5 0.213 0.082 0.345
966.0 0.206 0.078 0.334	965.5 0.201 0.075 0.325	965.0 0.197 0.072 0.319	964.5 0.195 0.070 0.315
964.0 0.194 0.070 0.314	963.5 0.196 0.071 0.317	963.0 0.199 0.074 0.323	962.5 0.205 0.079 0.333
962.0 0.212 0.086 0.347	961.5 0.221 0.094 0.365	961.0 0.233 0.104 0.387	960.5 0.247 0.116 0.413
960.0 0.264 0.129 0.442	959.5 0.283 0.143 0.475	959.0 0.304 0.157 0.511	958.5 0.327 0.172 0.549
958.0 0.352 0.186 0.588	957.5 0.377 0.200 0.627	957.0 0.401 0.213 0.664	956.5 0.423 0.225 0.697
956.0 0.440 0.234 0.725	955.5 0.452 0.242 0.744	955.0 0.456 0.248 0.753	954.5 0.452 0.251 0.753
954.0 0.441 0.252 0.744	953.5 0.425 0.251 0.726	953.0 0.404 0.248 0.702	952.5 0.380 0.244 0.674
952.0 0.355 0.238 0.644	951.5 0.331 0.232 0.613	951.0 0.308 0.225 0.583	950.5 0.287 0.218 0.555
950.0 0.269 0.211 0.529	949.5 0.252 0.204 0.506	949.0 0.237 0.199 0.486	948.5 0.224 0.194 0.468
948.0 0.214 0.190 0.453	947.5 0.204 0.187 0.441	947.0 0.197 0.185 0.432	946.5 0.190 0.184 0.424
946.0 0.185 0.184 0.419	945.5 0.181 0.185 0.415	945.0 0.177 0.186 0.413	944.5 0.174 0.188 0.412
944.0 0.172 0.190 0.412	943.5 0.170 0.192 0.412	943.0 0.169 0.194 0.413	942.5 0.167 0.196 0.413
942.0 0.166 0.198 0.414	941.5 0.165 0.199 0.414	941.0 0.163 0.200 0.413	940.5 0.162 0.201 0.412
940.0 0.160 0.201 0.411	939.5 0.158 0.200 0.408	939.0 0.156 0.199 0.405	938.5 0.153 0.197 0.401
938.0 0.151 0.195 0.396	937.5 0.148 0.192 0.390	937.0 0.145 0.189 0.384	936.5 0.142 0.185 0.377
936.0 0.139 0.181 0.369	935.5 0.136 0.176 0.362	935.0 0.133 0.171 0.353	934.5 0.130 0.165 0.345
934.0 0.127 0.160 0.337	933.5 0.125 0.154 0.329	933.0 0.123 0.148 0.321	932.5 0.121 0.142 0.313
932.0 0.119 0.137 0.306	931.5 0.118 0.131 0.299	931.0 0.118 0.126 0.294	930.5 0.118 0.121 0.289
930.0 0.118 0.117 0.286	929.5 0.120 0.114 0.283	929.0 0.121 0.111 0.282	928.5 0.124 0.109 0.283
928.0 0.127 0.109 0.286	927.5 0.131 0.109 0.291	927.0 0.137 0.111 0.297	926.5 0.143 0.113 0.306
926.0 0.150 0.117 0.317	925.5 0.159 0.121 0.330	925.0 0.169 0.126 0.345	924.5 0.180 0.132 0.363
924.0 0.193 0.138 0.381	923.5 0.207 0.145 0.401	923.0 0.221 0.151 0.422	922.5 0.236 0.156 0.442
922.0 0.250 0.161 0.461	921.5 0.263 0.164 0.477	921.0 0.273 0.166 0.489	920.5 0.279 0.167 0.495
920.0 0.280 0.165 0.495	919.5 0.276 0.163 0.489	919.0 0.268 0.158 0.476	918.5 0.256 0.152 0.458
918.0 0.242 0.144 0.436	917.5 0.225 0.136 0.411	917.0 0.208 0.126 0.384	916.5 0.191 0.115 0.357
916.0 0.175 0.105 0.330	915.5 0.160 0.094 0.304	915.0 0.147 0.083 0.279	914.5 0.134 0.072 0.256
914.0 0.123 0.062 0.235	913.5 0.113 0.053 0.216	913.0 0.104 0.045 0.198	912.5 0.096 0.037 0.183
912.0 0.088 0.030 0.169	911.5 0.082 0.025 0.157	911.0 0.076 0.020 0.146	910.5 0.071 0.016 0.137

910.0	0.066	0.012	0.128	909.5	0.062	0.009	0.121	909.0	0.058	0.007	0.115	908.5	0.055	0.005	0.110
908.0	0.052	0.004	0.106	907.5	0.049	0.003	0.102	907.0	0.046	0.002	0.098	906.5	0.044	0.002	0.095
906.0	0.042	0.001	0.093	905.5	0.040	0.001	0.090	905.0	0.038	0.001	0.088	904.5	0.036	0.000	0.086
904.0	0.034	0.000	0.085	903.5	0.033	0.000	0.083	903.0	0.031	0.000	0.082	902.5	0.030	0.000	0.080
902.0	0.029	0.000	0.079	901.5	0.028	0.000	0.078	901.0	0.027	0.000	0.077	900.5	0.026	0.000	0.076

CAUCHY,GAUSS, AND THE SUMMED ORDINATES ARE LISTED CONSECUTIVELY.

PROGRAM XV

PROGRAM XV

Spectrum Subtraction and Band Fit Error Analysis Program

(PC-128)

This program can be used as a general purpose program to obtain difference spectra by subtracting the ordinates of one spectral curve from those of another. Should the two curves be the experimentally measured spectrum and the band envelope computed by one of the band fit optimization programs, the difference is the error spectrum, showing the mismatch of the calculated curve.

Two factors contribute to this mismatch; one is the true mismatch and the second is a random component resulting from the fact that the noise level on the calculated curve is low, being derived only from the round-off error, whereas the peak-to-peak noise level on the experimental curve will normally be of the order of 0.005 to 0.010 transmittance units. A method of separating these error components has been described in a previous publication (2) and is illustrated in Figs. 3-5 taken from simulation studies on part of the spectrum of cyclohexanone in carbon disulfide solution. These calculations which separate "true" misfit error from misfit error due to the greater random noise level on the experimentally measured curve are activated when NOISAN = 2.

When operating the program in this mode, both the experimental ordinates and the calculated ordinates are convolved with a five point quadratic smoothing function. Subtraction of the smoothed experimental curve from the unsmoothed experimental curve extracts the high-frequency noise elements, and this difference curve provides a measure of the mismatch contributed by the higher noise level of the experimental curve (Fig. 4). Subtraction of the smoothed calculated curve from the smoothed experimental curves (Fig. 5) gives a measure of the mathematical mismatch of the calculated curve, after allowance for noise. In doing this it is assumed that the smoothing convolution induces negligible distortion of the computed curve, or of the spectral band structure in the experimental curve.* Another example based on an

---

*It would be more correct to say that the effect of the smoothing function on these two curves is comparable, so that the difference curve is not significantly affected. If desired this distortion can be evaluated by subtracting the spectrum of the smoothed calculated curve from that of the unsmoothed calculated curve, but this is not incorporated in the program since previous studies have shown it is not necessary (see reference (10)).

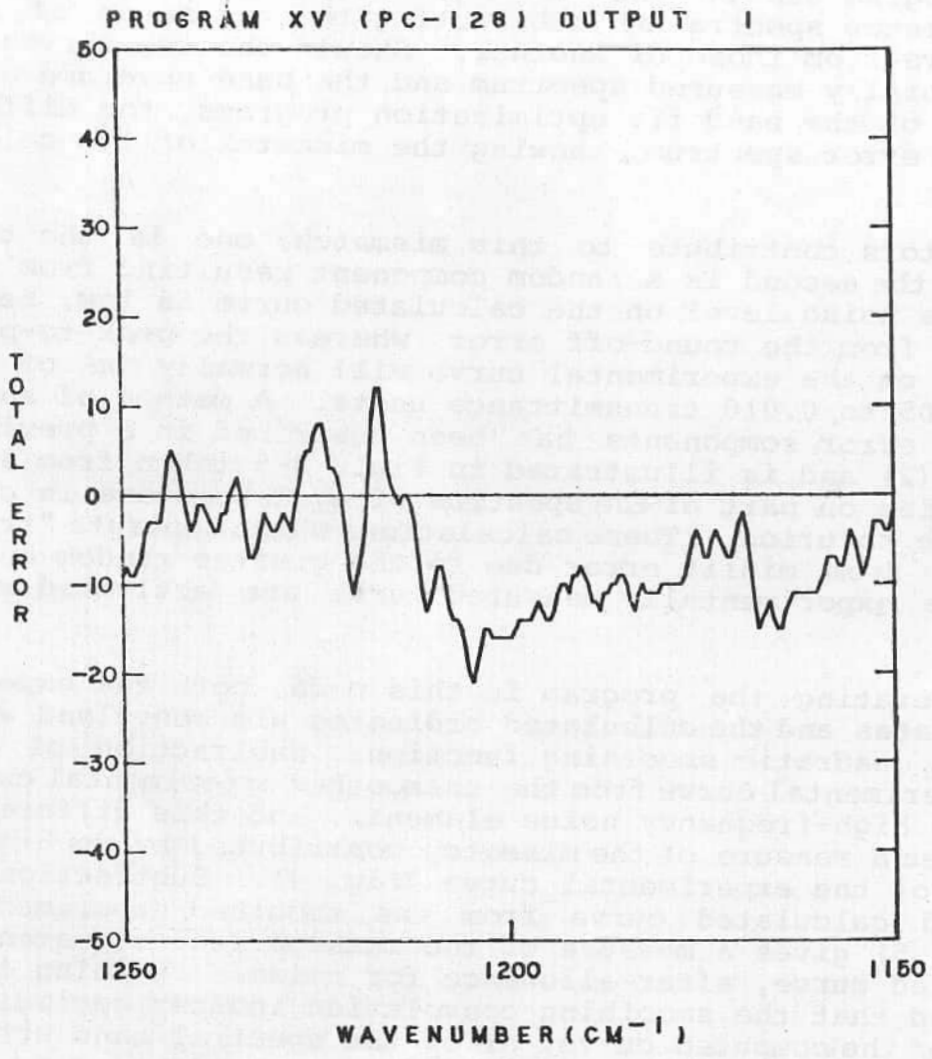

Fig. 3 Total error spectrum obtained by subtraction of the computed ordinates from the measured ordinates. The tabulated data are listed on p. 146.

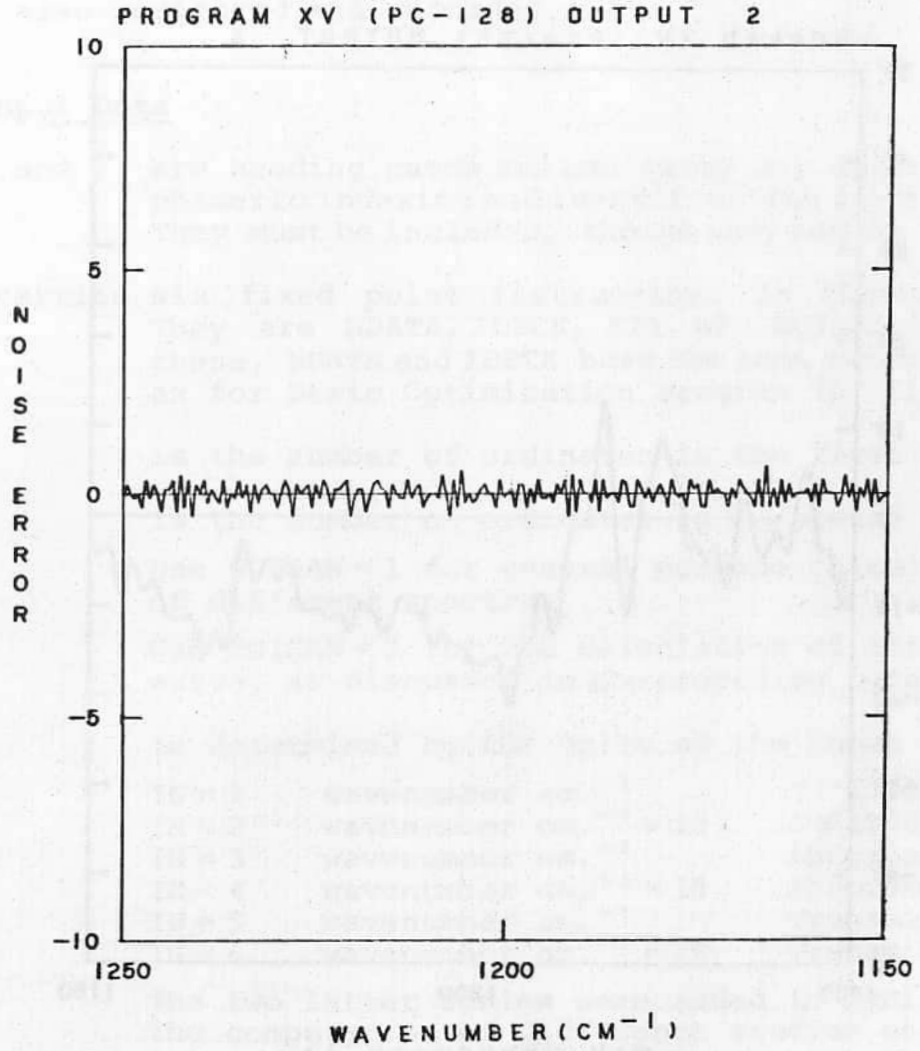

Fig. 4 High frequency noise error obtained by subtraction of the smoothed experimental ordinates from the measured experimental ordinates. The tabulated data are listed on p. 147.

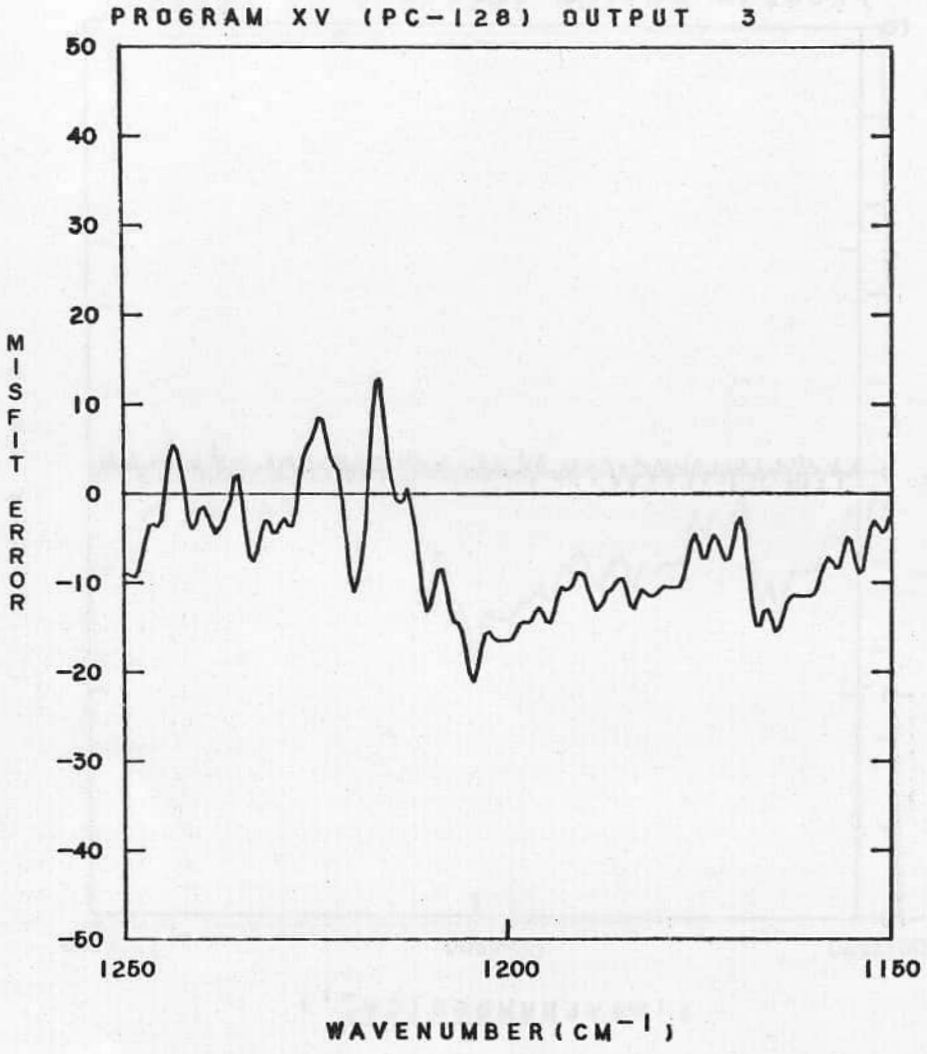

Fig. 5 "True" mismatch error obtained by subtraction of the smoothed computed ordinates from the smoothed measured ordinates. The tabulated data are listed on p. 148.

experimental curve with much higher noise level is given on p. 3045 of reference (2).

These statistical differences are also evaluated numerically in terms of the root-mean-square of the residuals (the discrepance) and the algebraic sum of the residuals (the average); the ordinate value and the wavenumber of the maximum absolute residual is also monitored and recorded.

A. The Input Data

Cards 1 and 2 are heading cards and can carry any desired alphameric indexing and identification statements. They must be included, though they may be blank.

Card 3 carries six fixed point instructions in format 6I5. They are NDATA, IDECK, NP1, NP2, NOISAN, IN. Of these, NDATA and IDECK have the same connotation as for Basic Optimization Program (p. 11).

NP1 is the number of ordinates in the first curve.

NP2 is the number of ordinates in the second curve.

Use NOISAN = 1 for general purpose calculations of different spectra.

Use NOISAN = 2 for the calculation of the error curve, as discussed in the preceding paragraph.

IN is determined by the units of the input data:

IN = 1	wavenumber $cm.^{-1}$	T × 1000
IN = 2	wavenumber $cm.^{-1}$ × 10	T × 1000
IN = 3	wavenumber $cm.^{-1}$	Absorbance
IN = 4	wavenumber $cm.^{-1}$ × 10	Absorbance
IN = 5	wavenumber $cm.^{-1}$	Transmittance
IN = 6	wavenumber $cm.^{-1}$ × 10	Transmittance

The two latter scales were added to facilitate the computation of difference studies on first and second differential spectra which are discussed in Bulletin 11 in connection with Program IV.

Card 4 carries three floating point instructions in format 3F15.5.

WB1 is the starting wavenumber of the first curve in $cm.^{-1}$.

WB2 is the starting wavenumber of the second curve in $cm.^{-1}$.

WI is the constant wavenumber interval in $cm.^{-1}$. This is positive for a diminishing wavenumber sequence.

WB1 and WB2 must be chosen so that the absolute value of WB1-WB2 does not exceed 100 × WI.

Card Deck 5 is the data deck of the first spectrum consisting of NP1 points; the format depends on the value of IN and is listed in Table I of Bulletin 11.

Card 6 carries the fixed point instruction IXIT in format I5. IXIT determines the format of the output and is discussed in the following section.

Card Deck 7 is the data deck of the second spectrum consisting of NP2 points; the format depends on the value of IN, as for Card Deck 5. When operating in the error mode it is important that the experimental spectrum be listed as Card Deck 5 and the calculated spectrum as Card Deck 7.

B. Description of the Program

The six input formats have been summarized in the preceding section, they are under the control of IN. There are four output formats under the control of IXIT. In all cases the abscissal units are $cm.^{-1} \times 10$. With IXIT = 1 the ordinates are direct ordinate differences in units of transmittance × 1000. If IXIT = 2 the ordinate differences are in absorbance units. With IXIT = 3 the ordinate scale is transmittance normalized to make the maximum residual ±1000, while with IXIT = 4 the ordinate range is adjusted so that all residuals lie between +200 and +800. This scale is useful for plotting purposes where the ordinate grid range is 0 to 1000 and the main interest is in the graphical display of the error curve. All four IXIT formats can be used for the general purpose recording of difference spectra, but only IXIT = 1 and IXIT = 3 are available in the error analysis mode.

The initial section of the program, ending at statement 125, is concerned with the input and reformulation of the data. All data are converted to $cm.^{-1} \times 10$ and transmittance × 1000 prior to numerical analysis. Between statements 13 and 19 the starting wavenumber is adjusted to the spectrum beginning at the lower wavenumber. The consecutive abscissal data points on the two curves are then checked against one another. If a mismatch is

detected, SUBROUTINE SORT is called to monitor and correct both data decks. The two decks are again compared, and if a mismatch still exists the calculation is terminated. The program branches at the computed GO TO statement 45, in accordance with the selected value of IXIT. The ordinates are next subtracted, the residuals stored in the arrays IY3 and Y3, and the difference spectrum printed out; when operating under IXIT = 3 or IXIT = 4 the residuals are appropriately scaled in the sections beginning at statements 210 or 220 respectively. A punched card version is also obtained if IDECK = 2.

If NOISAN = 1 the program now terminates or returns to process another pair of data decks under the control of NDATA. If NOISAN = 2 the error calculation routine is entered at statement 310. This mode requires that IXIT = 1 or 3, the experimental and calculated ordinates are stored in units of transmittance × 1000 in the fixed point arrays IY1 and IY2 respectively. They are first transferred to the floating point arrays Y1 and Y2 and convolved with a five point quadratic smoothing function (16,17) to yield the smoothed ordinates which are stored in the floating point arrays Y3 and Y4. The total error curve has already been evaluated and recorded before entering the error analysis routine. The noise component is Y1-Y3 and the noise corrected mismatch Y3-Y4. These are calculated in the DO loop ending at statement 311 and are stored in the arrays Y1 and Y2 respectively. The program branches following statement 311; if IXIT = 1 it proceeds directly to calculate the statistical parameters AVE and DIS and output the tables of differences. If IXIT = 3 it transfers to statement 350 and scales the ordinates to the range ±1000. The quantities AVE and DIS are always evaluated in transmittance units so that they can be compared directly with the corresponding quantities obtained in the band fit optimization programs.

```
C                                                                       10
C   ************************************************************        20
C   *                                                          *        30
C   *              SPECTRUM SUBTRACTION AND BAND FIT           *        40
C   *                                                          *        50
C   *                   ERROR ANALYSIS PROGRAM.                *        60
C   *                                                          *        70
C   ************************************************************        80
C                                                                       90
C   J.PITHA AND R.N.JONES,DIVISION OF CHEMISTRY,NATIONAL RESEARCH      100
C        COUNCIL OF CANADA,SUSSEX DRIVE,OTTAWA,CANADA.                 110
C                                                                      120
C   PROGRAM XV (PC-128)                          JULY 29TH.1967        130
C                                                                      140
C   THIS IS A PROGRAM FOR SUBTRACTING ONE SPECTRUM FROM ANOTHER.       150
C                                                                      160
C   IN CURVE FITTING STUDIES IT CAN ALSO BE USED TO EVALUATE           170
C        THE ERROR BETWEEN THE REAL SPECTRUM AND THE COMPUTED BAND     180
C        ENVELOPE.                                                     190
C                                                                      200
C        IT CONTAINS A BRANCH WHICH WILL SEPARATE THE ERROR COMPONENT  210
C        ORIGINATING IN THE NOISE ON THE REAL SPECTRUM FROM THE        220
C        MATHEMATICAL MISFIT OF THE SYNTHESIZED CURVE.                 230
C                                                                      240
C   THE INPUT ABSCISSAL SCALE CAN BE EITHER CM.-1 OR CM.-1 X 10.       250
C   THE INPUT ORDINATES CAN BE TRANSMITTANCE,TRANSMITTANCE X 1000      260
C        OR ABSORBANCE.THE TRANSMITTANCE SCALE WAS ADDED TO FACILITATE 270
C        DIFFERENCE STUDIES ON FIRST AND SECOND DERIVATIVE SPECTRA     280
C        (COMPARE PROGRAM IV).                                         290
C                                                                      300
C   FOR THE ERROR ANALYSIS THE TRUE DATA SPECTRUM MUST PRECEED THE     310
C        CALCULATED SPECTRUM.                                          320
C                                                                      330
C   INPUT CONTROL                                                      340
C        IN=1        X IN CM.-1              Y IN T X 1000.            350
C        IN=2        X IN CM.-1 X 10.        Y IN T X 1000.            360
C        IN=3        X IN CM.-1              Y IN ABSORBANCE UNITS.    370
C        IN=4        X IN CM-1 X 10.         Y IN ABSORBANCE UNITS.    380
C        IN=5        X IN CM-1               Y IN TRANSMITTANCE.       390
C        IN=6        X IN CM-1 X 10.         Y IN TRANSMITTANCE.       400
C                                                                      410
C                                                                      420
C   FOUR OUTPUT FORMATS ARE PROVIDED.                                  430
C   OUTPUT CONTROL                                                     440
C      IXIT=1    X IN CM.-1 X 10.     Y AS DIFFERENCE IN T X 1000.     450
C      IXIT=2    X IN CM.-1           Y AS DIFFERENCE IN ABSORBANCE.   460
C      IXIT=3    X IN CM.-1 X 10.     Y AS RELATIVE DIFFERENCE IN      470
C                                        TRANSMITTANCE UNITS X 1000.   480
C                                        NORMALIZED FOR A MAXIMAL      490
C                                        VALUE OF + OR - 1000.         500
C      IXIT=4    X IN CM.-1 X 10.     Y AS RELATIVE DIFFERENCE IN      510
C                                        TRANSMITTANCE UNITS X 1000.   520
C                                        NORMALIZED WITHIN THE RANGE   530
C                                        +200 TO +800.                 540
```

```
C                                                                       550
C     NOTE THAT THE SAME SCALES MUST BE USED FOR BOTH SPECTRA.          560
C                                                                       570
C     NOTE THAT FOR THE ERROP ANALYSIS ONLY IXIT=1 OR IXIT=3 IS ALLOWED.580
C                                                                       590
C     NOTE THAT THE IXIT SPECIFICATION CARD IS INSERTED BETWEEN THE TWO 600
C          DATA DECKS. THIS IS A CONVENIENCE TO PREVENT THE OVER-RUN OF 610
C          DATA IN THE EVENT THAT NP1 HAS BEEN PUNCHED INCORRECTLY.     620
C                                                                       630
C     IT IS HELPFUL TO LIST IXIT ON A CARD OF DIFFERENT COLOR.          640
C                                                                       650
C     THIS PROGRAM IS DIMENSIONED FOR 2000 DATA POINTS ON EACH CURVE.   660
C     THE INPUT WAVENUMBER SEQUENCES ARE CHECKED BY SUBROUTINE SORT AND 670
C          THE WAVENUMBER SCALES ALIGNED.                               680
C     FOR DETAILS SEE N.R.C.C. BULLETIN NO.12.                          690
C                                                                       700
      DIMENSION IX1(2000),IX2(2000),X1(2000),X2(2000),Y1(2000),Y2(2000),710
     1Y3(2000),Y4(2000),IY1(2000),IY2(2000),IY3(2000),HEAD1(20),HEAD2(20720
     2)                                                                730
      EQUIVALENCE (X1(1),IX2(1),Y3(1)),(X2(1),IY3(1),Y4(1))             740
      IRD=1                                                             750
      IPCH=2                                                            760
      IPRNT=3                                                           770
   10 WRITE (IPRNT,400)                                                 780
      READ (IRD,401) HEAD1                                              790
      READ (IRD,401) HEAD2                                              800
      READ (IRD,402) NDATA,IDECK,NP1,NP2,NOISAN,IN                      810
C                                                                       820
C     USE NOISAN=1 FOR SIMPLE CURVE SUBTRACTION AND NOISAN=2 FOR        830
C          BAND FIT ERROR ANALYSIS.                                     840
      READ (IRD,403) WB1,WB2,WI                                         850
C                                                                       860
C     NOTE THAT THE STARTING WAVENUMBER OF EACH CURVE (WB1),(WB2) AND   870
C          THE NUMBER OF POINTS ON EACH CURVE  (NP1,NP2) MUST BE GIVEN. 880
C     THE STARTING WAVENUMBERS FOR THE TWO DECKS MUST AGREE WITHIN ONE  890
C          HUNDRED TIMES THE WAVENUMBER INTERVAL.                       900
   11 GO TO (100,12,110,120,110,120),IN                                 910
   12 READ (IRD,404) (IX1(I),IY1(I),I=1,NP1)                            920
      READ (IRD,402) IXIT                                               930
      READ (IRD,404) (IX2(I),IY2(I), I=1,NP2)                           940
      GO TO 13                                                          950
C                                                                       960
  100 READ (IRD,425) (X1(I),IY1(I),I=1,NP1)                             970
      READ (IRD,402) IXIT                                               980
      READ (IRD,425) (X2(I),IY2(I),I=1,NP2)                             990
      DO 101 I=1,NP1                                                   1000
  101 IX1(I)=X1(I)*10.0+0.5                                            1010
      DO 102 I=1,NP2                                                   1020
  102 IX2(I)=X2(I)*10.0+0.5                                            1030
      GO TO 13                                                         1040
C                                                                      1050
  110 READ (IRD,426) (X1(I),Y1(I),I=1,NP1)                             1060
      READ (IRD,402) IXIT                                              1070
      READ (IRD,426) (X2(I),Y2(I),I=1,NP2)                             1080
```

```
      IF (IN.EQ.5) GO TO 113                                            1090
      DO 111 I=1,NP1                                                    1100
      IX1(I)=X1(I)*10.0+0.5                                             1110
  111 IY1(I)=EXP(-2.30258*Y1(I))*1000.0+0.5                             1120
      DO 112 I=1,NP2                                                    1130
      IX2(I)=X2(I)*10.0+0.5                                             1140
  112 IY2(I)=EXP(-2.30258*Y2(I))*1000.0+0.5                             1150
      GO TO 13                                                          1160
  113 DO 114 I=1,NP1                                                    1170
      IX1(I)=X1(I)*10.0+0.5                                             1180
  114 IY1(I)=Y1(I)*1000.0+0.5                                           1190
      DO 115 I=1,NP2                                                    1200
      IX2(I)=X2(I)*10.0+0.5                                             1210
  115 IY2(I)=Y2(I)*1000.0+0.5                                           1220
      GO TO 13                                                          1230
C                                                                       1240
  120 READ (IRD,420) (IX1(I),Y1(I),I=1,NP1)                             1250
      READ (IRD,402) IXIT                                               1260
      READ (IRD,420) (IX2(I),Y2(I),I=1,NP2)                             1270
      IF (IN.EQ.6) GO TO 123                                            1280
      DO 121 I=1,NP1                                                    1290
  121 IY1(I)=EXP(-2.30218*Y1(I))*1000.0+0.5                             1300
      DO 122 I=1,NP2                                                    1310
  122 IY2(I)=EXP(-2.30218*Y2(I))*1000.0+0.5                             1320
      GO TO 13                                                          1330
  123 DO 124 I=1,NP1                                                    1340
  124 IY1(I)=Y1(I)*1000.0+0.5                                           1350
      DO 125 I=1,NP2                                                    1360
  125 IY2(I)=Y2(I)*1000.0+0.5                                           1370
C                                                                       1380
   13 IF (WB2.GT.WB1) GO TO 14                                          1390
      WB=WB2                                                            1400
      GO TO 15                                                          1410
   14 WB=WB1                                                            1420
   15 IF (NP2.LE.NP1) GO TO 17                                          1430
      NP=NP1                                                            1440
      GO TO 18                                                          1450
   17 NP=NP2                                                            1460
   18 IF (IDECK.EQ.1) GO TO 19                                          1470
      WRITE (IPCH,401) HEAD1                                            1480
      WRITE (IPCH,401) HEAD2                                            1490
   19 WRITE (IPRNT,405) HEAD1                                           1500
      WRITE (IPRNT,405) HEAD2                                           1510
      WRITE (IPRNT,406) NP,WB,WI                                        1520
C                                                                       1530
C     IN THIS SECTION THE WAVENUMBER SEQUENCES OF THE TWO CARD DECKS ARE 1540
C          CHECKED AGAINST ONE ANOTHER. IF A MISMATCH IS DETECTED,EACH  1550
C          CARD DECK IS SEQUENCED BY THE SUBROUTINE SORT. THE TWO DECKS 1560
C          ARE RECHECKED AGAINST  EACH OTHER AND IF ANY INCONSISTANCY   1570
C          REMAINS THE COMPUTATION IS TERMINATED.                       1580
C                                                                       1590
      IWI=WI*10.0+0.5                                                   1600
      IWB=WB*10.0+0.5                                                   1610
      K2=1                                                              1620
```

```
   21 IF (IX1(K2)-IWB) 22,23,24                                          1630
   22 WRITE (IPRNT,407)                                                  1640
   32 IF (NDATA.EQ.2) GO TO 10                                           1650
      STOP                                                               1660
   24 IF (K2.GT.100) GO TO 22                                            1670
      K2=K2+1                                                            1680
      GO TO 21                                                           1690
   23 IF (K2.EQ.1) GO TO 28                                              1700
      DO 30 I=1,NP                                                       1710
      IX1(I)=IX1(K2)                                                     1720
      IY1(I)=IY1(K2)                                                     1730
   30 K2=K2+1                                                            1740
      WRITE (IPRNT,408)                                                  1750
   28 K2=1                                                               1760
   35 IF (IX2(K2)-IWB) 31,36,33                                          1770
   31 WRITE (IPRNT,409)                                                  1780
      GO TO 32                                                           1790
   33 IF (K2.GT.100) GO TO 31                                            1800
      K2=K2+1                                                            1810
      GO TO 35                                                           1820
   36 IF (K2.EQ.1) GO TO 40                                              1830
      DO 39 I=1,NP                                                       1840
      IX2(I)=IX2(K2)                                                     1850
      IY2(I)=IY2(K2)                                                     1860
   39 K2=K2+1                                                            1870
      WRITE (IPRNT,410)                                                  1880
   40 ISKIP=1                                                            1890
   50 DO 44 I=1,NP                                                       1900
      IF (IX1(I).NE.IX2(I)) GO TO 45                                     1910
   44 CONTINUE                                                           1920
   46 MAX=0                                                              1930
      AMAY=0.0                                                           1940
      SUM=0.0                                                            1950
      DIS=0.0                                                            1960
      GO TO (160,200,210,210),IXIT                                       1970
   45 IF (ISKIP.EQ.2) GO TO 47                                           1980
      WRITE (IPRNT,411)                                                  1990
      CALL SORT4 (IX1,IY1,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)                 2000
      IF (KLENUP.EQ.2) GO TO 32                                          2010
      WRITE (IPRNT,412)                                                  2020
      WRITE (IPRNT,413)                                                  2030
      CALL SORT4 (IX2,IY2,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)                 2040
      IF (KLENUP.EQ.2) GO TO 32                                          2050
      WRITE (IPRNT,414)                                                  2060
      ISKIP=2                                                            2070
      GO TO 50                                                           2080
   47 WRITE (IPRNT,415)                                                  2090
      GO TO 32                                                           2100
C                                                                        2110
C     ** EVALUATION OF THE DIFFERENCE IN UNITS OF TRANSMITTANCE X 1000.  2120
C                                                                        2130
  160 WRITE (IPRNT,416)                                                  2140
      DO 161 I=1,NP                                                      2150
      IY3(I)=IY1(I)-IY2(I)                                               2160
```

```
      YY=FLOAT(IY3(I))                                                  2170
      IF (ABS(YY).LE.ABS(AMAY)) GO TO 162                               2180
      AMAY=YY                                                           2190
      MAX=IX1(I)                                                        2200
  162 SUM=SUM+YY                                                        2210
  161 DIS=DIS+YY*YY                                                     2220
  163 AVE=0.001*SUM/NP                                                  2230
      DIS=0.000001*DIS/NP                                               2240
      DIS=SQRT(DIS)                                                     2250
      AMAX=MAX*0.1                                                      2260
      AMAY=0.001*AMAY                                                   2270
  164 IF (IDECK.EQ.1) GO TO 165                                         2280
      WRITE (IPCH,404) (IX1(I),IY3(I), I=1,NP)                          2290
  165 WRITE (IPRNT,436)                                                 2300
      WRITE (IPRNT,418) (IX1(I),IY3(I), I=1,NP)                         2310
      WRITE (IPRNT,417) AVE,DIS,AMAX,AMAY                               2320
      WRITE (IPRNT,434)                                                 2330
      GO TO 300                                                         2340
C                                                                       2350
C     ******** EVALUATION OF THE DIFFERENCES IN ABSORBANCE UNITS *******2360
C                                                                       2370
  200 WRITE (IPRNT,419)                                                 2380
      DO 202 I=1,NP                                                     2390
      YY=ALOG10(FLOAT(IY2(I)))-ALOG10(FLOAT(IY1(I)))                    2400
      Y3(I)=YY                                                          2410
      IF (ABS(YY).LE.ABS(AMAY)) GO TO 201                               2420
      AMAY=YY                                                           2430
      MAX=IX1(I)                                                        2440
  201 SUM=SUM+YY                                                        2450
  202 DIS=DIS+YY*YY                                                     2460
      AVE=SUM/NP                                                        2470
      DIS=DIS/NP                                                        2480
      DIS=SQRT(DIS)                                                     2490
      AMAX=MAX*0.1                                                      2500
      IF (KLENUP.EQ.1) GO TO 204                                        2510
      DO 205 I=1,NP                                                     2520
      X2(I)=IX1(I)*0.1                                                  2530
  205 CONTINUE                                                          2540
  204 IF (IDECK.EQ.1) GO TO 203                                         2550
      WRITE (IPCH,420) (X2(I),Y3(I),I=1,NP)                             2560
  203 WRITE (IPRNT,436)                                                 2570
      WRITE (IPRNT,421) (X2(I),Y3(I),I=1,NP)                            2580
      WRITE (IPRNT,417) AVE,DIS,AMAX,AMAY                               2590
      WRITE (IPRNT,435)                                                 2600
      GO TO 300                                                         2610
C                                                                       2620
C     ****** EVALUATION OF NORMALIZED TRANSMITTANCE DIFFERENCES WITH THE 2630
C          MAXIMUM OR MINIMUM = 1000. **********************************2640
C                                                                       2650
  210 NMIN=100                                                          2660
      NMAX=-100                                                         2670
      DO 211 I=1,NP                                                     2680
      IY3(I)=IY1(I)-IY2(I)                                              2690
      NMIN=MIN0(NMIN,IY3(I))                                            2700
```

```
  211 NMAX=MAX0(NMAX,IY3(I))                                          2710
      IF (IXIT.EQ.4) GO TO 220                                        2720
      WRITE (IPRNT,422)                                               2730
      IF ((NMAX+NMIN).GT.0) GO TO 213                                 2740
      SLOPE =-1000.0/NMIN                                             2750
      GO TO 214                                                       2760
  213 SLOPE=1000.0/NMAX                                               2770
  214 DO 216 I=1,NP                                                   2780
      YY=FLOAT(IY3(I))                                                2790
      IF (ABS(YY).LE.ABS(AMAY)) GO TO 215                             2800
      MAX=IX1(I)                                                      2810
      AMAY=YY                                                         2820
  215 SUM=SUM+YY                                                      2830
      DIS=DIS+YY*YY                                                   2840
  216 IY3(I)=IY3(I)*SLOPE                                             2850
      GO TO 163                                                       2860
C                                                                     2870
C     ****** EVALUATION OF TRANSMITTANCE DIFFERENCES NORMALIZED TO A   2880
C          SCALE OF + 200 TO + 800.    **********************************2890
C                                                                     2900
C     THIS ORDINATE RANGE IS CONVENIENT FOR PLOTTING DIFFERENCE SPECTRA 2910
C          FOR VISUAL DISPLAY ON A GRID SCALED FROM ZERO TO 1000.     2920
C                                                                     2930
  220 WRITE (IPRNT,423)                                               2940
      SLOPE=600.0/(NMAX-NMIN)                                         2950
      CEPT=200.5-SLOPE*NMIN                                           2960
      WRITE (IPRNT,424)NP,NMIN,NMAX,CEPT,SLOPE                        2970
      DO 230 I=1,NP                                                   2980
      YY=FLOAT(IY3(I))                                                2990
      IF (ABS(YY).LE.ABS(AMAY)) GO TO 221                             3000
      MAX=IX1(I)                                                      3010
      AMAY=YY                                                         3020
  221 SUM=SUM+YY                                                      3030
      DIS=DIS+YY*YY                                                   3040
  230 IY3(I)=CEPT+SLOPE*IY3(I)                                        3050
      GO TO 163                                                       3060
C                                                                     3070
C     ************************* ERROR ANALYSIS **************************3080
C                                                                     3090
C     BOTH THE EXPERIMENTAL AND THE CALCULATED CURVES ARE SMOOTHED    3100
C          WITH A FIVE POINT QUADRATIC CONVOLUTE FUNCTION.            3110
C     THE HIGH FREQUENCY COMPONENTS ELIMINATED FROM THE TRUE CURVE BY 3120
C          SMOOTHING ARE OBTAINED FROM THE ORDINATE DIFFERENCES IN THE 3130
C          TRUE CURVE BEFORE AND AFTER SMOOTHING. THESE ARE EQUATED WITH3140
C          THE NOISE ERROR.                                           3150
C     THE NOISE-CORRECTED CURVE MISFIT EPROR IS EQUATED WITH THE      3160
C          DIFFERENCE BETWEEN THE TRUE AND CALCULATED CURVES AFTER EACH3170
C          HAS BEEN SUBJECTED TO THE SMOOTHING ROUTINE.FOR A GRAPHICAL 3180
C          ILLUSTRATION AND DISCUSSION SEE CANADIAN J.CHEM. FIG.7     3190
C          PAGE 3045 VOL.44 (1966).                                   3200
  300 IF (NOISAN.EQ.1) GO TO 32                                       3210
      ISKIP = 1                                                       3220
      GO TO (310,305,310,305),IXIT                                    3230
  305 WRITE (IPRNT,427)                                               3240
```

```
      GO TO 32                                                          3250
  310 NNP=NP-2                                                          3260
      DO 311 I=3,NNP                                                    3270
      IYS=-3*(IY1(I-2)+IY1(I+2))+12*(IY1(I-1)+IY1(I+1))+17*IY1(I)       3280
      Y3(I)=0.285714E-1*IYS                                             3290
      IYS=-3*(IY2(I-2)+IY2(I+2))+12*(IY2(I-1)+IY2(I+1))+17*IY2(I)       3300
      Y4(I)=0.285714E-1*IYS                                             3310
      Y1(I)=IY1(I)                                                      3320
      Y2(I)=IY2(I)                                                      3330
      Y1(I)=Y1(I)-Y3(I)                                                 3340
      Y2(I)=Y3(I)-Y4(I)                                                 3350
  311 CONTINUE                                                          3360
  321 MAX=0                                                             3370
      AMAY=0.0                                                          3380
      SUM=0.0                                                           3390
      DIS=0.0                                                           3400
      IF (IXIT.EQ.3) GO TO 350                                          3410
      DO 325 I=3,NNP                                                    3420
      YY=Y1(I)                                                          3430
      IF (ABS(YY).LE.ABS(AMAY)) GO TO 322                               3440
      AMAY=YY                                                           3450
      MAX = IX1(I)                                                      3460
  322 SUM=SUM+YY                                                        3470
  325 DIS=DIS+YY*YY                                                     3480
      AVE=0.001*SUM/NNP                                                 3490
      DIS=0.000001*DIS/NNP                                              3500
      DIS=SQRT(DIS)                                                     3510
      AMAX=MAX*0.1                                                      3520
      AMAY=0.001*AMAY                                                   3530
      GO TO (330,340),ISKIP                                             3540
  330 WRITE (IPRNT,428)                                                 3550
      WRITE (IPRNT,438)                                                 3560
      WRITE (IPRNT,437) (IX1(I),Y1(I),I=3,NNP)                          3570
      WRITE (IPRNT,417) AVE,DIS,AMAX,AMAY                               3580
      IF (IDECK.EQ.1) GO TO 333                                         3590
      WRITE (IPCH,432)                                                  3600
      WRITE (IPCH,439) (IX1(I),Y1(I),I=3,NNP)                           3610
  333 ISKIP=2                                                           3620
      DO 334 I=3,NNP                                                    3630
  334 Y1(I)=Y2(I)                                                       3640
      GO TO 321                                                         3650
  340 WRITE (IPRNT,429)                                                 3660
      WRITE (IPRNT,438)                                                 3670
      WRITE (IPRNT,437) (IX1(I),Y2(I),I=3,NNP)                          3680
      WRITE (IPRNT,417) AVE,DIS,AMAX,AMAY                               3690
      IF (IDECK.EQ.1) GO TO 32                                          3700
      WRITE (IPCH,433)                                                  3710
      WRITE (IPCH,439) (IX1(I),Y2(I),I=3,NNP)                           3720
      GO TO 32                                                          3730
C                                                                       3740
C     **** ERPOR ANALYSIS WITH NORMALIZATION OF MAX.ORDINATE = 1000. ***3750
C                                                                       3760
  350 DO 356 I=3,NNP                                                    3770
      YY=Y1(I)                                                          3780
```

```
      IF (ABS(YY).LE.ABS(AMAY)) GO TO 355                                3790
      AMAY=YY                                                            3800
      MAX=IX1(I)                                                         3810
  355 SUM=SUM+YY                                                         3820
      DIS=DIS+YY*YY                                                      3830
  356 IY1(I)=Y1(I)*SLOPE+0.5                                             3840
      AVE=0.001*SUM/NNP                                                  3850
      DIS=0.000001*DIS/NNP                                               3860
      DIS=SQRT(DIS)                                                      3870
      AMAX=MAX*0.1                                                       3880
      AMAY=0.001*AMAY                                                    3890
      GO TO (360,370),ISKIP                                              3900
  360 WRITE (IPRNT,430)                                                  3910
      WRITE (IPRNT,418) (IX1(I),IY1(I),I=3,NNP)                          3920
      WRITE(IPRNT,417) AVE,DIS,AMAX,AMAY                                 3930
      IF (IDECK.EQ.1) GO TO 365                                          3940
      WRITE (IPCH,432)                                                   3950
      WRITE (IPCH,404) (IX1(I),IY1(I),I=3,NNP)                           3960
  365 GO TO (361,370),ISKIP                                              3970
  361 ISKIP=2                                                            3980
      DO 363 I=3,NNP                                                     3990
  363 Y1(I)=Y2(I)                                                        4000
      MAX=0                                                              4010
      AMAY=0.0                                                           4020
      SUM=0.0                                                            4030
      DIS=0.0                                                            4040
      GO TO 350                                                          4050
  370 WRITE (IPRNT,431)                                                  4060
      WRITE (IPRNT,418) (IX1(I),IY1(I),I=3,NNP)                          4070
      WRITE (IPRNT,417) AVE,DIS,AMAX,AMAY                                4080
      IF (IDECK.EQ.1) GO TO 32                                           4090
      WRITE (IPCH,433)                                                   4100
      WRITE (IPCH,404) (IX1(I),IY1(I),I=3,NNP)                           4110
      GO TO 32                                                           4120
C                                                                        4130
  400 FORMAT ('1PITHA AND JONES,BAND FIT ERROR ANALYSIS AND CURVE SUBTRA  4140
     1CTION.'/)                                                          4150
  401 FORMAT (20A4)                                                      4160
  402 FORMAT (6I5)                                                       4170
  403 FORMAT (3F15.5)                                                    4180
  404 FORMAT (8(I5,I4,1X))                                               4190
  405 FORMAT (1X,20A4)                                                   4200
  406 FORMAT ('0',10X,2HNP,I5,15X,2HWB,F8.1,11X,2HWI,F5.1)               4210
  407 FORMAT ('0ERROR IN STARTING WAVENUMBER OF FIRST CURVE.')           4220
  408 FORMAT ('0STARTING WAVENUMBER OF FIRST CURVE ADJUSTED.')           4230
  409 FORMAT ('0ERROR IN STARTING WAVENUMBER OF SECOND CURVE.')          4240
  410 FORMAT ('0STARTING WAVENUMBER OF SECOND CURVE ADJUSTED.')          4250
  411 FORMAT ('0FIRST CARD DECK.')                                       4260
  412 FORMAT ('0FIRST CARD DECK HAS BEEN CHECKED.')                      4270
  413 FORMAT ('0SECOND CARD DECK.')                                      4280
  414 FORMAT ('0SECOND CARD DECK HAS BEEN CHECKED.')                     4290
  415 FORMAT ('0SUBROUTINE SORT HAS FAILED TO ALIGN THE INPUT DATA.')    4300
  416 FORMAT ('0ORDINATES ARE ABSOLUTE TRANSMITTANCE X 1000'/)           4310
  417 FORMAT (//5X,9HAVERAGE =,E13.5,5X,13HDISCREPANCE =,E13.5,5X,7HMAX  4320
```

```
   1X =,F7.1,5X,7HMAX Y =,F8.5/)                                          4330
418 FORMAT (9(4X,2I5))                                                    4340
419 FORMAT ('0ORDINATES ARE ABSORBANCE DIFFERENCES.'/)                    4350
420 FORMAT (6(F6.1,F6.3,1X))                                              4360
421 FORMAT (9(1X,F6.1,F7.3))                                              4370
422 FORMAT ('0ORDINATES NORMALIZED TO MAX.ERROR=1000.'/)                  4380
423 FORMAT ('0ORDINATES NORMALIZED TO RANGE +800 TO +200'/)               4390
424 FORMAT (10X,3HNP=,I5,5X,5HNMIN=,I5,5X,5HNMAX=,I5,5X,5HCEPT=,F6.2,     4400
   15X,6HSLOPE=,F6.2)                                                     4410
425 FORMAT (7(F6.1,I4,1X))                                                4420
426 FORMAT (6(F6.1,F6.3,1X))                                              4430
427 FORMAT ('0ERROR ANALYSIS DOES NOT OPERATE ON THIS ORDINATE SCALE.'     4440
   1/)                                                                    4450
428 FORMAT ('1 NOISE ERROR.----------------------------------------------  4460
   1---------------------------------------------------------- '/)        4470
429 FORMAT ('1 CURVE MISFIT ERROR.---------------------------------------  4480
   1---------------------------------------------------------- '/)        4490
430 FORMAT ('1 NOISE ERROR ON SCALE OF MAX.TOTAL ERROR = 1000.---------   4500
   1-----------------------------------------------------------'/)        4510
431 FORMAT ('1 CURVE MISFIT ERROR ON SCALE OF MAX. TOTAL ERROR = 1000.    4520
   1-----------------------------------------------------------'/)        4530
432 FORMAT ('NOISE ERROR COMPONENT')                                      4540
433 FORMAT ('NOISE CORRECTED CURVE MISFIT ERROR').                        4550
434 FORMAT (/5X,'AVERAGE,DISCREPANCE,AND MAX Y ARE IN UNITS OF TRANSMI    4560
   1TTANCE.')                                                             4570
435 FORMAT (/5X,'AVERAGE,DISCREPANCE,AND Y MAX ARE IN ABSORBANCE UNITS    4580
   1.')                                                                   4590
436 FORMAT (//' DIFFERENCE SPECTRUM. -------------------------------     4600
   1------------------------------- '/)                                   4610
437 FORMAT (8(2X,I5,1X,F6.1))                                             4620
438 FORMAT ('0ORDINATES ARE ABSOLUTE TRANSMITTANCE X 1000.0'/)            4630
439 FORMAT (6(I5,F7.2,1X))                                                4640
    END                                                                   4650
```

```
C                                                                       4660
C     ***************************************************************   4670
      SUBROUTINE SOFT4 (IX,IY,WB,WI,NP,IPRNT,KLENUP,IWB,IWI)            4680
C                                                                       4690
C     SUBROUTINE SORT CHECKS FOR ERRORS IN THE INPUT WAVENUMBER DATA.   4700
C     A LIMITED NUMBER OF WAVENUMBER SEQUENCE ERRORS ARE CORRECTED      4710
C          BUT SEQUENCE ERRORS IN EXCESS OF 160 DATA POINTS (20 CARDS)  4720
C          OR ANY OTHER TYPE OF WAVENUMBER ERROR WILL TERMINATE THE     4730
C          COMPUTATION,AS ALSO WILL A DISCREPANCY BETWEEN IWB AND THE   4740
C          STARTING WAVENUMBER.                                         4750
C     THE WAVENUMBER POSITIONS OF THE CORRECTIONS AND OF A TERMINATING  4760
C          ERROR ARE RECORDED.                                          4770
C     IF CORRECTIONS ARE MADE THE CORRECTED INPUT DATA ARE LISTED IN FUL 4780
C     IF A TERMINATING ERROR IS FOUND THE UNCORRECTED INPUT DATA ARE    4790
C          LISTED IN FULL.                                              4800
      DIMENSION IX(2000),IY(2000),ITEMPX(160),X1(160),ITEMPY(160)       4810
      MM=1                                                              4820
      DO 11 I=2,NP                                                      4830
      IW=IWB-IWI*(I-1)                                                  4840
      IF (IW.EQ.IX(I)) GO TO 11                                         4850
      XX=IX(I)                                                          4860
      TEST=(WB-0.1*XX)/WI                                               4870
      NTEST=TEST+0.005                                                  4880
      IF (ABS(TEST-NTEST).GT.0.005) GO TO 12                            4890
      ITEMPX(MM)=IX(I)                                                  4900
      ITEMPY(MM)=IY(I)                                                  4910
      MM=MM+1                                                           4920
      IF (MM.GT.160) GO TO 13                                           4930
   11 CONTINUE                                                          4940
      IF (MM.GT.1) GO TO 14                                             4950
      WRITE (IPRNT,451)                                                 4960
   15 KLENUP=1                                                          4970
      RETURN                                                            4980
   12 XX1=IX(I-1)*0.1-WI                                                4990
      WRITE (IPRNT,452) XX1                                             5000
   16 KLENUP=2                                                          5010
      RETURN                                                            5020
   13 WRITE (IPRNT,453)                                                 5030
      WRITE (IPRNT,455) (IX(I),IY(I), I=1,NP)                           5040
      GO TO 16                                                          5050
   14 NN=MM-1                                                           5060
      DO 17 MM=1,NN                                                     5070
      K1=1+(IWB-ITEMPX(MM))/IWI                                         5080
      IX(K1)=ITEMPX(MM)                                                 5090
      IY(K1)=ITEMPY(MM)                                                 5100
   17 X1(MM)=IX(K1)*0.1                                                 5110
      WRITE (IPRNT,450) (X1(MM),MM=1,NN)                                5120
      WRITE (IPRNT,454) (IX(I),IY(I),I=1,NP)                            5130
      GO TO 15                                                          5140
C                                                                       5150
  450 FORMAT ('0WAVENUMBER CORRECTIONS AT'/,12(2X,F6.1,2X))             5160
  451 FORMAT ('0NO ERRORS.')                                            5170
  452 FORMAT ('0TERMINATED BY ERROR AT',F6.1,6H CM-1.)                  5180
  453 FORMAT ('0TERMINATED BY MULTIPLE WAVENUMBER SEQUENCE ERRORS.')     5190
```

```
454 FORMAT ('0REARRANGED INPUT.'/,9(4X,2I5))                          5200
455 FORMAT ('0UNCORRECTED INPUT.'/,9(4X,2I5))                         5210
    END                                                               5220
```

PITHA AND JONES,BAND FIT ERROR ANALYSIS AND CURVE SUBTRACTION.

APRIL 28TH 1969 PROGRAM IV (PC-128) IXIT=1 NOISAM=2
TEST RUN ON CYCLOHEXANONE SPECTRUM AS COMPUTED BY THE PRODUCT FUNCTION.

NP 208 NB 1251.0 NI 0.5

ORDINATES ARE ABSOLUTE TRANSMITTANCE X 1000

DIFFERENCE SPECTRUM. ----------

12510	-9	12505	-9	12500	-9	12495	-8	12490	-9	12485	-9	12480	-8	12475	-7	12470	-8
12465	-3	12460	-3	12455	-3	12450	-3	12445	0	12440	4	12435	5	12430	4	12425	3
12420	0	12415	-2	12410	-4	12405	-3	12400	-1	12395	-1	12390	-2	12385	-3	12380	-4
12375	-4	12370	-2	12365	-2	12360	0	12355	1	12350	2	12345	0	12340	-4	12335	-7
12330	-7	12325	-6	12320	-4	12315	-2	12310	-3	12305	-4	12300	-4	12295	-3	12290	-2
12285	-3	12280	-4	12275	-1	12270	1	12265	4	12260	5	12255	5	12250	7	12245	6
12240	8	12235	6	12230	3	12225	3	12220	2	12215	0	12210	-4	12205	-9	12200	-11
12195	-9	12190	-7	12185	-4	12180	2	12175	9	12170	12	12165	12	12160	8	12155	3
12150	1	12145	0	12140	-1	12135	0	12130	0	12125	-1	12120	-3	12115	-7	12110	-11
12105	-13	12100	-12	12095	-10	12090	-8	12085	-8	12080	-10	12075	-13	12070	-14	12065	-14
12060	-15	12055	-17	12050	-20	12045	-21	12040	-19	12035	-17	12030	-15	12025	-15	12020	-16
12015	-16	12010	-16	12005	-16	12000	-16	11995	-16	11990	-15	11985	-14	11980	-14	11975	-14
11970	-14	11965	-13	11960	-12	11955	-13	11950	-14	11945	-14	11940	-13	11935	-11	11930	-10
11925	-10	11920	-11	11915	-9	11910	-9	11905	-8	11900	-9	11895	-10	11890	-12	11885	-12
11880	-13	11875	-11	11870	-11	11865	-10	11860	-10	11855	-9	11850	-9	11845	-10	11840	-12
11835	-13	11830	-11	11825	-10	11820	-11	11815	-11	11810	-11	11805	-11	11800	-10	11795	-10
11790	-10	11785	-10	11780	-10	11775	-10	11770	-9	11765	-7	11760	-5	11755	-4	11750	-5
11745	-7	11740	-7	11735	-5	11730	-4	11725	-5	11720	-6	11715	-7	11710	-7	11705	-5
11700	-3	11695	-2	11690	-4	11685	-8	11680	-12	11675	-15	11670	-14	11665	-13	11660	-12
11655	-14	11650	-15	11645	-15	11640	-13	11635	-12	11630	-11	11625	-11	11620	-11	11615	-11
11610	-11	11605	-11	11600	-11	11595	-10	11590	-9	11585	-7	11580	-7	11575	-7	11570	-8
11565	-8	11560	-6	11555	-4	11550	-5	11545	-7	11540	-9	11535	-8	11530	-6	11525	-3
11520	-3	11515	-3	11510	-4	11505	-4	11500	-2	11495	-1	11490	-1	11485	-3	11480	-4
11475	-3																

AVERAGE = -0.66827E-02 DISCREPANCE = 0.91368E-02 MAX X = 1204.5 MAX Y =-0.02100

AVERAGE,DISCREPANCE,AND MAX Y ARE IN UNITS OF TRANSMITTANCE.

NOISE ERROR.----------

ORDINATES ARE ABSOLUTE TRANSMITTANCE X 1000.0

12500	0.0	12495	0.2	12490	0.0	12485	-0.1	12480	0.0	12475	-0.3	12470	0.3	12465	-0.1
12460	0.2	12455	0.0	12450	-0.4	12445	0.1	12440	0.1	12435	0.3	12430	-0.4	12425	0.4
12420	-0.3	12415	0.3	12410	-0.5	12405	0.2	12400	0.0	12395	0.3	12390	-0.2	12385	0.1
12380	-0.1	12375	-0.2	12370	0.3	12365	-0.3	12360	0.0	12355	-0.1	12350	0.3	12345	-0.1
12340	0.2	12335	-0.4	12330	0.2	12325	-0.2	12320	0.1	12315	0.2	12310	0.0	12305	0.0
12300	-0.3	12295	0.0	12290	0.3	12285	0.1	12280	-0.5	12275	0.2	12270	0.0	12265	0.1
12260	0.2	12255	-0.3	12250	0.2	12245	-0.1	12240	0.3	12235	0.1	12230	-0.3	12225	0.1
12220	0.1	12215	0.2	12210	0.3	12205	-0.5	12200	-0.1	12195	0.1	12190	0.1	12185	-0.4
12180	-0.1	12175	0.2	12170	0.3	12165	0.1	12160	0.1	12155	-0.3	12150	0.2	12145	0.0
12140	-0.1	12135	-0.1	12130	0.3	12125	-0.1	12120	0.1	12115	0.2	12110	-0.3	12105	-0.1
12100	0.0	12095	0.0	12090	-0.1	12085	0.4	12080	0.0	12075	-0.5	12070	0.3	12065	-0.3
12060	0.5	12055	-0.2	12050	0.0	12045	-0.2	12040	-0.1	12035	0.1	12030	0.2	12025	0.0
12020	0.0	12015	-0.3	12010	0.3	12005	-0.1	12000	0.0	11995	0.1	11990	-0.3	11985	0.2
11980	0.2	11975	-0.3	11970	0.1	11965	-0.2	11960	0.3	11955	-0.1	11950	-0.1	11945	0.0
11940	-0.2	11935	0.2	11930	0.0	11925	0.3	11920	-0.5	11915	0.4	11910	-0.4	11905	0.3
11900	0.0	11895	0.0	11890	-0.2	11885	0.3	11880	-0.4	11875	0.3	11870	-0.1	11865	0.0
11860	0.0	11855	-0.2	11850	0.3	11845	0.2	11840	-0.3	11835	-0.3	11830	0.3	11825	0.1
11820	-0.1	11815	0.1	11810	-0.2	11805	0.0	11800	0.2	11795	0.0	11790	-0.3	11785	0.3
11780	0.0	11775	-0.1	11770	0.0	11765	-0.3	11760	0.3	11755	0.1	11750	0.2	11745	-0.3
11740	-0.3	11735	0.3	11730	0.0	11725	0.1	11720	0.0	11715	0.0	11710	-0.3	11705	0.1
11700	-0.1	11695	0.3	11690	0.1	11685	0.0	11680	-0.1	11675	-0.3	11670	0.3	11665	-0.3
11660	0.6	11655	-0.3	11650	0.1	11645	-0.3	11640	0.3	11635	-0.2	11630	0.2	11625	-0.1
11620	0.0	11615	0.0	11610	0.0	11605	0.1	11600	-0.2	11595	0.2	11590	-0.3	11585	0.3
11580	0.0	11575	0.0	11570	0.0	11565	-0.3	11560	-0.1	11555	0.4	11550	-0.1	11545	0.2
11540	-0.4	11535	0.1	11530	-0.1	11525	0.3	11520	-0.3	11515	0.3	11510	-0.2	11505	-0.1
11500	0.0	11495	0.0	11490	0.3	11485	0.1								

AVERAGE = 0.27460E-05 DISCREPANCE = 0.22315E-03 MAX X = 1166.0 MAX Y = 0.00060

CURVE MISFIT ERROR.----------

ORDINATES ARE ABSOLUTE TRANSMITTANCE X 1000.0

12500	-8.7	12495	-8.5	12490	-8.7	12485	-8.9	12480	-8.3	12475	-6.5	12470	-4.4	12465	-3.0
12460	-2.9	12455	-3.3	12450	-2.6	12445	0.2	12440	3.6	12435	4.9	12430	4.3	12425	2.6
12420	0.3	12415	-2.3	12410	-3.6	12405	-2.9	12400	-1.3	12395	-1.0	12390	-1.9	12385	-3.1
12380	-4.0	12375	-3.6	12370	-2.7	12365	-1.4	12360	-0.3	12355	1.3	12350	1.7	12345	-0.2
12340	-3.9	12335	-6.7	12330	-7.2	12325	-5.9	12320	-3.8	12315	-2.5	12310	-2.8	12305	-3.9
12300	-3.9	12295	-2.9	12290	-2.3	12285	-3.2	12280	-3.2	12275	-1.6	12270	1.4	12265	3.7
12260	4.8	12255	5.5	12250	6.7	12245	8.1	12240	7.8	12235	5.7	12230	3.7	12225	2.7
12220	2.1	12215	-0.2	12210	-4.3	12205	-8.7	12200	-10.6	12195	-9.4	12190	-7.1	12185	-3.7
12180	2.3	12175	8.5	12170	12.2	12165	11.7	12160	7.9	12155	3.5	12150	0.9	12145	-0.3
12140	-0.6	12135	-0.3	12130	0.0	12125	-0.9	12120	-3.3	12115	-7.0	12110	-10.9	12105	-12.7
12100	-12.1	12095	-9.9	12090	-8.2	12085	-8.1	12080	-10.2	12075	-12.7	12070	-13.9	12065	-14.2
12060	-15.0	12055	-17.3	12050	-19.8	12045	-20.7	12040	-19.3	12035	-16.8	12030	-15.3	12025	-15.1
12020	-15.7	12015	-16.1	12010	-16.0	12005	-16.0	12000	-16.1	11995	-15.8	11990	-15.0	11985	-14.2
11980	-13.9	11975	-14.1	11970	-13.8	11965	-12.9	11960	-12.3	11955	-12.9	11950	-13.9	11945	-14.0
11940	-12.8	11935	-11.2	11930	-10.0	11925	-10.3	11920	-10.2	11915	-9.7	11910	-8.5	11905	-8.4
11900	-8.7	11895	-10.3	11890	-11.5	11885	-12.6	11880	-12.2	11875	-11.7	11870	-10.6	11865	-10.3
11860	-9.7	11855	-9.2	11850	-9.0	11845	-10.2	11840	-12.0	11835	-12.5	11830	-11.3	11825	-10.3
11820	-10.7	11815	-11.1	11810	-11.1	11805	-10.7	11800	-10.3	11795	-9.9	11790	-10.0	11785	-10.0
11780	-10.1	11775	-9.9	11770	-8.9	11765	-7.0	11760	-5.0	11755	-4.2	11750	-5.2	11745	-6.7
11740	-6.7	11735	-5.2	11730	-4.3	11725	-4.8	11720	-6.1	11715	-7.0	11710	-6.7	11705	-5.1
11700	-2.9	11695	-2.3	11690	-4.1	11685	-7.9	11680	-12.2	11675	-14.4	11670	-14.3	11665	-12.7
11660	-12.6	11655	-13.7	11650	-15.1	11645	-14.7	11640	-13.3	11635	-11.8	11630	-11.2	11625	-10.9
11620	-11.0	11615	-11.0	11610	-11.0	11605	-11.1	11600	-10.8	11595	-10.2	11590	-8.7	11585	-7.4
11580	-6.7	11575	-7.3	11570	-7.9	11565	-7.7	11560	-5.9	11555	-4.4	11550	-4.9	11545	-7.2
11540	-8.6	11535	-8.2	11530	-5.7	11525	-3.6	11520	-2.7	11515	-3.3	11510	-3.9	11505	-3.7
11500	-2.3	11495	-0.9	11490	-1.3	11485	-2.8								

AVERAGE = -0.66262E-02 DISCREPANCE = 0.91124E-02 MAX X = 1204.5 MAX Y =-0.02066

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SUMMARY

Three computer programs for fitting infrared band contours are described and listed. These programs utilize Cauchy (Lorentz), Gauss, Cauchy-Gauss product, and Cauchy-Gauss sum functions, and will optimize the parameters for fitting single bands or multiple overlapping band systems using a non-linear least squares algorithm.

Supplementary programs are included for the evaluation of the half-widths and shape characteristics of the synthesized component bands, also for the computation of the ordinates of the synthesized band envelope, and for an analysis of the misfit with the true spectrum. This latter program also serves as a general purpose program for subtracting spectral ordinates.

The programs are written in FORTRAN IV. They are designed for card input and output in a standardized format that facilitates their interfacing with other programs developed in our laboratory for the numerical analysis of infrared and ultraviolet spectrophotometric absorption curves.