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**The Broadening of a Spectrum Line by
Finite Spectrometer Resolution**

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Rolf Engleman, Jr.

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THE BROADENING OF A SPECTRUM LINE BY FINITE SPECTROMETER RESOLUTION

by

Rolf Engleman, Jr.

ABSTRACT

The distortion of a spectrum line by the finite resolving power of a spectrometer is discussed in terms of a mathematical model. Particular attention is given to the case where either a Gaussian or Cauchy slit function broadens an isolated Doppler, Lorentz, or Voigt absorption line. Corrections to the peak absorption, the line width, and the integrated absorption coefficient are calculated and discussed for different combinations of slit functions and line shapes. Several new series expansions for the corrections are derived. Two general FORTRAN IV programs that calculate these corrections are described and some sample correction curves are given.

I. INTRODUCTION

The broadening of a spectrum line by the finite resolving power of a spectrograph or spectrometer is a problem of importance in optical spectroscopy. A spectrometer that cannot resolve the line shape completely causes distortions that must be corrected if the true peak line intensity and the true line shape are to be obtained. The calculation of these corrections is actually an old problem, having been treated by Ladenburg and Reiche¹ in 1913. Other treatments are scattered throughout the literature and no inclusive survey is given here.

The literature contains several general methods with which information about the true spectrum line shape can be obtained from the observed line shape. Some of these methods are primarily experimental techniques^{2,3} and are not discussed here. Another method^{4,5} employs numerical matrix techniques to obtain the true

line shape from the observed line shape and a knowledge of the slit function.* The method is general and does not take into account a priori knowledge of the function form of the true line shape. Methods involving Fourier series^{6,7} and Taylor's series⁸ expansions have been developed, and an integrated approach to the determination of true line shape and the effect of overlapping lines has been given recently.⁹ All of these methods give procedures for treating a set of data and do not lend themselves to a general discussion of the line-distortion problem.

Another general method, developed by Kostkowski and Bass¹⁰ and others¹¹⁻¹⁴ can be called a parametric or mathematical model approach to the problem. It depends on the assumption of specific functional forms for (1) the slit function and (2) the true spectrum line shape. The latter assumption often can be justified; for example, in a low-pressure gas, absorption and emission lines are expected to have a Gaussian shape owing to Doppler broadening. As the gas pressure in the source is increased, Lorentz broadening (also called pressure or collision broadening) contributes and the Voigt function (discussed later) becomes appropriate as the line shape. Although the assumption of a specific form for the slit function usually cannot be justified on theoretical grounds, several workers have found that simple functions such as the Gaussian,^{10,15} Cauchy,¹⁶ and triangular^{12,15,17} will adequately describe several different types of spectrometers and spectrographs. The basic procedure is to assume functional forms for the true line shape and slit function and then to determine the parameters useful in describing the resultant line shape. The adequacy of this approach has been verified by Render and Lovell.¹⁸ This method is examined in detail here. The main objective of this study is to present more complete calculations, particularly on absorption line width corrections, than were available previously and to define FORTRAN computer programs for the evaluation of the required integrals and expressions. Attention is limited to the case of a single isolated spectrum line, a case of importance in high-resolution optical spectroscopy and some other fields, although the method could be adapted to overlapping multiple line spectra.¹⁰

*The slit function is the line shape observed when a sufficiently narrow spectrum line is incident on the spectrometer slit. This spectrum line should be so narrow that it does not affect the shape of the observed line. In practice, the ¹⁹⁸Hg electrodeless discharge lamp can be used for this purpose, although it is not quite narrow enough when used with some of the new high-resolution spectrographs and spectrometers. Various narrow laser light sources are now becoming available, but will not cover all wavelength regions.

II. GENERAL THEORY

The expression governing the broadening of a spectrum line by the finite resolution of a spectrometer can be written in the form of a convolution or folding integral:^{3,10}

$$t(v) = \frac{\int S(v, v') i(v') dv'}{\int S(v, v') dv'} . \quad (1)$$

The function $i(v')$ is the light flux incident on the spectrometer entrance slit as a function of the wave number v ; $t(v)$ is the observed exit flux spectrum; and $S(v, v')$ is the slit function. The integration should extend over all values of v' for which $i(v')$ makes a contribution to $t(v)$. For the purposes of the analytical integration, infinite limits are used and, unless otherwise noted, all integrals in this report are to be taken between $-\infty$ and $+\infty$. The denominator in Eq. (1) normalizes the expression so that if $i(v')$ is a constant with v' , $t(v)$ is the same constant.

For the calculations presented here, only two types of slit functions are used. The Gaussian slit function and the Cauchy slit function, respectively, are given by

$$S(v, v') = \exp \left[-4(\ln_e 2)(v - v')^2/w^2 \right] \quad (2)$$

and

$$S(v, v') = \left[1 + 4(v - v')^2/w^2 \right]^{-1} \quad (3)$$

Both use the parameter w as the width at half peak intensity. Integration of these expressions between $-\infty$ and $+\infty$ yields normalization factors of $(\pi \ln_e 2)^{1/2} w/2$ and $\pi w/2$, respectively, which are used as the denominator of Eq. (1). Notice that neither slit function changes its functional form with wave number. This is a good approximation for most situations encountered in high-resolution spectroscopy. Other functional forms could be used to represent more complicated slit functions, such as those with some asymmetry, by modification of Eq. (2) and (3) and the calculation of a new normalization factor.

No arguments yet made have limited the consideration to either an emission or an absorption line. While the treatment of an absorption line is the major aim of this report, this presentation seems more natural if the well-documented case of an emission line is treated first. The Voigt function, used as the assumed absorption line shape when both Doppler and Lorentz broadening are important, is also the result of a Doppler emission line broadened by a Cauchy slit function.

III. BROADENING OF AN EMISSION LINE

For emission spectra, $i(v')$ is simply the line shape times a constant flux i_0 . Because the three assumed line shape functions will be used later in the absorption line discussion, they are written in terms of $F(v')$, the normalized line shape. Then for an emission line, $i(v') = i_0 F(v')$. For low-pressure spectrum lines where Doppler broadening dominates, a Gaussian line shape of width α at half intensity is used.

$$F(v') = \exp \left[-4(\ln_e 2)(v' - v_0)^2/\alpha^2 \right]. \quad (4)$$

In the case of a Doppler emission line broadened by a Gaussian slit function, Eqs. (2) and (4) should be substituted into Eq. (1). A change of variable and definition of dimensionless constants

$$\begin{aligned} x &= (v - v')/w & \beta &= w/\alpha & \sigma &= 2(v - v_0)/\alpha \\ T(\sigma) &= t(v)/i_0 & \kappa &= 4 \ln_e 2 \end{aligned} \quad (5)$$

gives an expression for the observed line shape:

$$T(\sigma) = \sqrt{\kappa/\pi} \int \exp \left[-\kappa x^2 - \kappa(\sigma/2 - \beta x)^2 \right] dx. \quad (6)$$

Integration produces another Gaussian form:

$$T(\sigma) = (1 + \beta^2)^{-1/2} \exp \left[-\kappa \sigma^2 / 4(1 + \beta^2) \right] \quad (7)$$

which has a width at half intensity of $(\alpha^2 + w^2)^{1/2}$. Thus a Gaussian line shape results from the broadening of a Doppler emission line with a Gaussian slit

function, and the new Gaussian has a width given by the square root of the sum of the slit and line widths squared.

The Cauchy line shape function serves for a spectrum line originating in a source at moderately high pressures. Under such conditions, Lorentz broadening can dominate and the Cauchy function represents the line shape to a first approximation:

$$F(v') = \left[1 + 4 (v' - v_0)^2 / \alpha^2 \right]^{-1} . \quad (8)$$

The width at half intensity is again α . Proceeding as before with Eqs. (3), (8), (1), and (5) and the proper normalization, gives

$$T(\sigma) = 2/\pi \int \frac{dx}{(1 + 4x^2) \left[1 + 4 (\sigma/2 - \beta x)^2 \right]} . \quad (9)$$

This can be integrated* to give another Cauchy function

$$T(\sigma) = \frac{1 + \beta}{\left[\sigma^2 + (1 + \beta)^2 \right]} \quad (10)$$

with a width at half intensity that is just the sum of the line and slit function widths.

The remaining combinations of Eqs. (2), (3), (4), and (8) will now be considered. If (3) and (4) are substituted into (1) and the changes of Eq. (5) are made, a form of the Voigt function results:

$$T(\sigma) = 2/\pi \int \frac{\exp \left[-\kappa (\sigma/2 - \beta x)^2 \right]}{1 + 4x^2} dx . \quad (11)$$

*See Ref. 19. Considerable simplification in this integral results if a common factor is divided out. In Grobner's notation the integral become

$$\int_{-\infty}^{\infty} \frac{dx}{[(x-r_1)^2 + s_1^2][(x-r_2)^2 + s_2^2]} = \frac{\pi(s_1 + s_2)}{s_1 s_2 [(r_1 - r_2)^2 + (s_1 + s_2)^2]} .$$

No analytical integration is possible, but useful compilations of the function and its general properties are available.^{3, 20, 21} The width of the Voigt function is not simply related to the component widths of the Gaussian and Cauchy functions but can be obtained from numerical tables.²² Another form of the Voigt function is obtained by using Eqs. (2) and (8).

$$T(\sigma) = \sqrt{\kappa/\pi} \int \frac{\exp(-\kappa x^2) dx}{1 + 4(\sigma/2 - \beta x)^2} \quad (12)$$

Equation (12) is equivalent to (11) after redefinition of constants, but (11) is used here in numerical calculations.

The Voigt function also describes the case of a spectrum line originating in a system where both Doppler and Lorentz broadening make significant contributions to the width. Thus two more cases should be mentioned to make the emission treatment complete within the framework of the functions described here. Consider the case of a Voigt emission line broadened by either a Cauchy or Gaussian slit function. In either case the resultant line shape is a Voigt function and the individual Gaussian and Cauchy widths involved "add" by the same simple sum rules already shown from Eqs. (7) and (10) (see Ref. 23).

The effects of finite resolution on an emission line can be eliminated if the integral of the area under the line is measured. Consider the slit function $S(v, v')$ in Eq. (1) to be a function only of the difference between v and v' . As mentioned, this form of slit function is usually a good approximation. Then the normalization integral in (1) is readily shown to be only a constant and not a function of v . If this normalization constant is called N and integration is performed over all v ,

$$\int T(v) dv = 1/N \iint S(v - v') i(v') dv' dv \quad (13)$$

If the functions involved are sufficiently regular that the order of integration may be changed,

$$\int T(v) dv = \int i(v') dv' \quad (14)$$

Thus integration of the emission line over wave number eliminates the effect of finite resolution. This is an important general result for emission spectra, but it is not generally true for the most interesting integrated quantity obtained from absorption spectra.

IV. BROADENING OF AN ABSORPTION LINE

The treatment of an absorption line must reflect the fact that a background continuum $i_0(v')$ contributes the observed flux and the absorption removes only selected portions of this flux. The background flux is assumed to be constant over the region of absorption. In general, this is a good approximation in high-resolution spectroscopy. If Lambert's law is assumed valid, the true absorption line shape is

$$i(v') = i_0 \exp [-C F(v')] \quad , \quad (15)$$

where C is the peak absorption coefficient. The quantities $F(v')$ are the same normalized line shape functions as those used in the emission line treatment.

We now develop in detail the equations for the case of a Doppler absorption line broadened by a Gaussian slit function. The other five combinations of line shapes and slit functions can be formulated in an analogous way. Equation (4) is substituted into (15) to obtain the actual form of the flux incident on the spectrometer slit. This flux and Eq. (2) are now substituted into (1) along with the proper normalization. When the transformations of (5) are applied,

$$T(\sigma) = \sqrt{\kappa/\pi} \int \exp(-\kappa x^2) \exp \left\{ -C \exp \left[-\kappa(\sigma/2 - \beta x)^2 \right] \right\} dx \quad . \quad (16)$$

Equation (16) now represents the fractional transmission of light at a given relative wave number as measured by the dimensionless parameter σ . The dimensionless parameter β is a measure of the amount of instrumental broadening. Equation (16) cannot be integrated analytically, but if the second exponential is expanded and the series integrated,

$$T(\sigma) = \sum_{n=0}^{\infty} \frac{(-C)^n}{n! \sqrt{1 + n\beta^2}} \exp \left[-\kappa\sigma^2/4(1 + n\beta^2) \right] \quad . \quad (17)$$

The observed absorption line shape $T(\sigma)$ is not a simple Gaussian but is a superposition of Gaussians of decreasing width and amplitude. For the point of peak absorption ($\sigma = 0$), Eq. (17) gives

$$T(\sigma = 0) = \sum_{n=0}^{\infty} \frac{(-C)^n}{n! \sqrt{1 + n\beta^2}} \quad (18)$$

The comparable quantity as derived from Lambert's law is

$$T(\sigma = 0) = \exp(-C) = \sum_{n=0}^{\infty} \frac{(-C)^n}{n!} \quad (19)$$

As expected when there is no broadening by the slit function ($\beta = 0$), (18) and (19) are identical. Equations (17) and (18) are useful in checking the results of numerical integration of (16).

Equation (16) was integrated numerically by computer codes described later. Successful checks were made between the integration, the evaluation of Eq. (17) for small C , and the work of Kostkowski and Bass¹⁰ where applicable. Figure 1 is a graph* of the observed peak absorption [or $1 - T(\sigma = 0)$] plotted against the true peak absorption coefficient C . Curves for different β 's are given, including the $\beta = 0$ curve which includes no slit broadening and is simply the Lambert's law curve. Notice the progressive flattening of the curves in Fig. 1 at large C and increasing β . In practice this flattening is important because, for example, the $\beta = 2$ curve flattens so that above an absorption of ~ 0.6 little information can be derived about the true value of C . Figure 2 is a graph of the same information given in Fig. 1 but the horizontal scale is the absorption as if there were no broadening or just $[1 - \exp(-C)]$. Figure 2 shows that the observed peak absorption is not a sensitive function of the true peak absorption at high absorption, and this effect becomes rapidly worse with further instrumental broadening. Graphs of this type can be used to correct observed

*All graphs in this report were made from microfilm plotted from computer-processed magnetic tapes with a Stromberg-Carlson 4020 film plotter. Some re-touching was necessary. Dashed lines connect calculated curves to limiting values. Each asterisk on the graph is a calculated point. Calculated points are connected by straight lines.

Figure 1 - Observed peak absorption vs true peak absorption coefficient.
Gaussian slit function and Doppler absorption line.

Figure 2 - Observed vs true peak absorption.
Gaussian slit function and Doppler absorption line.

peak absorptions, although a better measure of an absorption line strength is the integrated absorption coefficient. Other combinations of line shape and slit function yield curves similar to those in Figs. 1 and 2.

By proceeding as before with Eqs. (1), (3), (5), (8), and (15), we develop the expression for $T(\sigma)$ for the case of a Lorentz absorption line broadened by a Cauchy slit function:

$$T(\sigma) = 2/\pi \int \exp \left[\frac{-C}{1 + 4 (\sigma/2 - \beta x)^2} \right] \frac{dx}{1 + 4x^2} \quad (20)$$

As before, the second exponential can be expanded, but only the first two terms can be readily integrated.

$$T(\sigma) \doteq 1 - \frac{C(1 + \beta)}{\sigma^2 + (1 + \beta)^2} + \dots \quad (21)$$

The peak transmission can be obtained by placing $\sigma = 0$ in Eq. (20) and integrating the expansion of the exponential. The leading terms are

$$T(\sigma = 0) \doteq 1 - \frac{C}{1 + \beta} + \frac{C^2 (2 + \beta)}{16 \beta^2 (1 + \beta)^2} + \dots \quad (22)$$

Equations (21) and (22) are useful in checking the numerical integration of (20) for small values of C . Figure 3 is a graph similar to that of Fig. 1, although the curves have a somewhat different shape.

The remaining two simple cases can be derived by combining Eqs. (2) and (8) or (3) and (4) with (1), (5), and (15). For a Doppler absorption line broadened by a Cauchy slit function,

$$T(\sigma) = 2/\pi \int \frac{\exp \left\{ -C \exp \left[-\kappa (\sigma/2 - \beta x)^2 \right] \right\}}{1 + 4x^2} dx \quad (23)$$

The case of a Lorentz absorption line broadened by a Gaussian slit function yields

Figure 3 - Observed peak absorption vs true peak absorption coefficient.
Cauchy slit function and Lorentz absorption line.

$$T(\sigma) = \sqrt{\kappa/\pi} \int \exp(-\kappa x^2) \exp\left[\frac{-C}{1 + 4(\sigma/2 - \beta x)^2}\right] dx \quad (24)$$

Neither of these integrals can be solved analytically even if the exponential is expanded as before. Results of their numerical integration are given in Figs. 4 and 6 and indicate the same qualitative behavior as the plots in Figs. 1 and 3. The result of a Doppler line broadened by a Cauchy slit is shown in Fig. 5 plotted in the same way as Fig. 2. Figure 5 shows the differences that appear when only the slit function is changed. Figures 2 and 5 show a nearly straight line for all β and small A (peak observed), indicating that the ratio of the observed peak absorption of two lines is independent of the instrumental broadening if the peak absorption is not too large.

The last two possibilities within the framework of functions to be used here involves use of the Voigt function as the absorption line shape. The Voigt function is arbitrarily taken to be of the form given in Eq. (11). If a new dimensionless parameter ρ is defined as ratio of the Lorentz width to the Doppler width σ , the Voigt function becomes

$$F(v') = 2/\pi \int \frac{\exp\left[-\kappa \left(\frac{v' - v_0}{\alpha} + \rho x'\right)^2\right]}{1 + 4x'^2} dx' \quad (25)$$

Equation (25) may now be substituted into (15) and then into (1) with the appropriate slit function. Even after the use of the definitions in (5), the expression for $T(\sigma)$ is quite complex, and no analytical series solution could be found. The results from numerical integration of an example Voigt case are given in Fig. 7. Results for other values of the parameters β and ρ can be computed by using the codes described in Appendix B.

V. CORRECTIONS TO THE INTEGRATED ABSORPTION COEFFICIENT

The integrated absorption coefficient may be defined as

$$K = \int C'(v) dv = - \int \ln_e [i'(v)/i_0] dv \quad (26)$$

Figure 4 - Observed peak absorption vs true peak absorption coefficient.
Cauchy slit function and Doppler absorption line.

Figure 5 - Observed vs true peak absorption.
Cauchy slit function and Doppler absorption line.

Figure 6 - Observed peak absorption vs true peak absorption coefficient.
Gaussian slit function and Lorentz absorption line.

Figure 7 - Observed peak absorption vs true peak absorption coefficient with $\beta = 0.5$. Gaussian slit function and Voigt absorption line.

where $C'(v)$ is the absorption coefficient obtained by treating the observed absorption as if it were the true absorption and applying Lambert's law. The integration should be carried out over all v that make an appreciable contribution and in the case of the analytical integrations between $-\infty$ and $+\infty$. If there is no instrumental broadening, $i(v)$ is a simple exponential given by Eq. (15). The integrated absorption coefficient for no instrumental broadening K_0 is then

$$K_0 = -\int_{-\infty}^{+\infty} \ln_e \{ \exp[-C F(v)] \} dv = C \int_{-\infty}^{+\infty} F(v) dv \quad . \quad (27)$$

Thus the integrated absorption coefficient is proportional to the absorption coefficient, but only if no instrumental broadening is present. Also, the integral of $F(v)$ in Eq. (27) depends only on the intrinsic line shape and is not affected by line broadening factors such as Lorentz or natural broadening. Mitchell and Zemansky²⁴ express it by saying "Whatever physical processes are responsible for the formation of the absorption line, the integral of the absorption coefficient remains constant when N (number of absorbing atoms) is constant." In the present notation, K_0 calculated for a Doppler line [Eqs. (4) and (27)] is

$$K_0 = C\alpha(\pi/K)^{1/2} \quad . \quad (28)$$

For the pure Lorentz line [Eqs. (8) and (27)] it is

$$K_0 = C\alpha \pi/2 \quad . \quad (29)$$

Equation 28 also will apply to K_0 for the Voigt line shape in the form used here [Eqs. (11) and (25)].

The problem of a Doppler absorption line broadened by a Gaussian slit function (see Sec. IV) is solved by substituting Eq. (16) into (26). The result is not analytically tractable so again, numerical integration is used. However, a series solution is possible. The series expansion of Eq. (16), given by (17), can be substituted into (26). Because the leading term in $T(\sigma)$ is always unity and the following terms are small for small C , the $\ln(1+x) = x - x^2/2 + \dots$ expansion can be used, and the resulting Gaussian-type double integrals can be readily evaluated. Only the first three terms are evaluated here, but any higher order term will yield to perseverance. The integrated absorption coefficient for a

Doppler line with no broadening, given by Eq. (28) is used to calculate the ratio K/K_0 as a measure of the necessary correction:

$$\frac{K}{K_0} = 1 - \frac{C}{2\sqrt{2}} \left[1 - \frac{1}{\sqrt{1+\beta^2}} \right] + \left[\frac{1}{6\sqrt{3}} - \frac{1}{2\sqrt{3+4\beta^2}} + \frac{1}{3\sqrt{3(1+\beta^2)}} \right] C^2 + \dots \quad (30)$$

This expression has the proper behavior so that for no broadening ($\beta = 0$), K/K_0 is not a function of C and is always unity. Equation (30) is useful in checking the numerical integration of (26) for small C .

Figure 8 shows the observed peak absorption coefficient plotted against the ratio K/K_0 for several values of β .^{*} Comparison with Fig. 1 shows that smaller corrections are necessary for the integrated absorption coefficient than for the peak absorption coefficient. Instrumental broadening of an absorption line increases the area in the wings while depressing the peak. Thus the peak absorption decreases rapidly with decreasing resolution but the area decreases much more slowly. Such qualitative behavior also holds true for other line shapes and slit functions.

For the case of a Lorentz absorption line broadened by a Cauchy slit function, the integrated absorption coefficient is found by substituting Eq. (20) into (26). In general, this expression must be numerically integrated, but by expansion of the exponential and logarithm, and by analytical integration (using a table of integrals¹⁹) the first two terms of K/K_0 can be obtained:

$$\frac{K}{K_0} = 1 - \frac{C \beta}{4(1 + \beta)} + \dots \quad (31)$$

The value of K_0 comes from Eq. (29). For small C , K/K_0 from Eq. (31) agrees with the values obtained by numerical integration.

^{10,13}
*Contrary to the common practice of plotting correction quantities against the true peak absorption or true peak absorption coefficient, such quantities are plotted here against observed peak absorption or observed peak absorption coefficient. It is felt that this is of value in reducing experimental data, because the observed (not the true) quantities are obtainable directly from the data.

Figure 8 - Observed peak absorption coefficient vs relative observed integrated absorption coefficient. Gaussian slit function and Doppler absorption line.

The remaining two combinations of Doppler or Lorentz lines with Gaussian or Cauchy slit functions do not lead to any useful series expansions. They were numerically integrated, and the result for a Lorentz line and a Gaussian slit is plotted in Fig. 9.

Still to be discussed are the two combinations between a Voigt line shape and a Gaussian or Cauchy slit function. Here also, there is no simple expansion for K/K_0 and numerical integration is tedious, involving a "nest" of three integrations. The numerical problem was simplified by the use of an approximating function for the innermost Voigt integration.

A second method of integrating an absorption line is that of integrating under the actual observed absorption. The result is independent of the slit function (Ref. 3, p. 61), but it is not directly related to the true integrated absorption coefficient. The latter quantity is the more useful in optical spectroscopy because usually it is proportional to the concentration of absorbing molecules. Because the integral under the absorption line $\bar{A}$ is independent of the slit function, it is tempting to relate this integral to the true integrated absorption coefficient by using the general expression for Lambert's law [Eq. (15)] and expanding the exponential, then interchanging the order of summation and integration:

$$\bar{A} = \int A_{\text{obs}} dv = \int (1 - \exp [-CF(v)]) dv \quad (32)$$

$$\begin{aligned} &= - \int \sum_{n=1}^{\infty} \frac{(-C)^n}{n!} [F(v)]^n dv \\ &= - \sum_{n=1}^{\infty} \frac{(-C)^n}{n!} \int [F(v)]^n dv \quad . \end{aligned} \quad (33)$$

So long as $\bar{A}$ has been measured, the unknowns K_0 and C will be contained in two equations [(33) and (27)]. At least one more unknown resides in the function $F(v)$. In the case of the simple Doppler or Lorentz line shapes it is the width α . C cannot be obtained from the absorption line without a consideration of instrumental broadening effects; consequently, $\bar{A}$ can be usefully related to K_0 only if the values of α and any other parameters in $F(v)$ are specified. If the temperature is defined and known in a low-pressure absorbing gas, the α for a Doppler

Figure 9 - Observed peak absorption coefficient vs relative observed integrated absorption coefficient. Gaussian slit function and Lorentz absorption line.

line shape can be calculated. The quantity C may be eliminated between Eqs. (28) and (33):

$$\bar{A} = - \sum_{n=1}^{\infty} \frac{(-K_0)^n}{n! \sqrt{n}} \left(\frac{\sqrt{K}}{\alpha \sqrt{\pi}} \right)^{n-1} . \quad (34)$$

The above expression may be useful in special circumstances, but in general $\bar{A}$ is not useful. Equation (33) does show that as the absorption becomes small ($C \rightarrow 0$), $\bar{A}$ approaches K_0 . This limiting behavior is exploited in an experimental extrapolation of $\bar{A}$ to zero absorption by reduction of the concentration or path length. The extrapolation then yields the true integrated absorption coefficient.

A result similar to that of Eq. (34) can also be derived for the case of a Lorentz line:

$$\bar{A} = - \sum_{n=1}^{\infty} \frac{(-K_0)^n (2n-3)(2n-5) \dots 1}{n! (n-1)! (\alpha\pi)^{n-1}} . \quad (35)$$

VI. CORRECTIONS TO THE ABSORPTION LINE WIDTH

In a discussion of the absorption line width, two definitions of the width are appropriate. Experimentally, the width of the absorption itself may be most convenient to use. Figure 10 is a diagram of a typical absorption line and the quantity δ (upper figure) is defined as the width at half intensity of the absorption. By inspection of Fig. 10, δ can be obtained in terms of $T(\delta)$ from the expression

$$T(\delta) = 1 - F[1 - T(\sigma = 0)] . \quad (36)$$

The expression is transcendental and is solved by numerical iteration techniques. If $T(\delta_0)$ is the flux for an absorption line with no instrumental broadening, it is given by the ratio of $i(v')/i_0$ from Eq. (15). Equation (36) can then be solved explicitly. If $G = \ln_e \{1 - [1 - \exp(-C)]F\}$ and $F = 1/2$, the Doppler line shape gives

$$\delta_0 = 2\alpha \left[\frac{1}{K} \ln_e (-C/G) \right]^{1/2} \quad (37)$$

Figure 10. Definitions of the absorption line widths δ and Δ .

and the Lorentz line shape yields

$$\delta_0 = \alpha[-1 - C/G]^{1/2} \quad . \quad (38)$$

These are the limiting values of δ for $\beta = 0$. Equation (37) should also be used as the limiting value of δ for the Voigt line shape. Numerical integration and iteration for the $\beta \neq 0$ cases yields the results plotted in Figs. 11 - 15. It was convenient to plot the observed peak absorption against a reduced line width constructed by dividing δ by the true absorption coefficient line width α . In general, the line width corrections are large for even a small value of β . Even in the limits of $\beta \rightarrow 0$ or $C \rightarrow 0$, a width correction usually is required. Only in the limit that both β and C approach zero together is the observed absorption line width equal to the width of the absorption coefficient. Plots of this type can be used to compare experimental data so long as the functional forms for the line shape and slit function are adequate approximations.

A second way of defining the width is to assume that the observed absorption follows Lambert's law and to derive a pseudo-absorption coefficient C' . The width Δ of C' at half intensity is then defined as shown in Fig. 10 (lower figure). The appropriate expression used to obtain Δ is then

$$C'(\Delta) = F C' (\sigma = 0) \quad . \quad (39)$$

For the case of no instrumental broadening, Δ is equal to the width of the absorption coefficient α regardless of the value of C . For the $\beta \neq 0$ case, numerical integration and iteration must be used. Figures 16 - 20 are graphs of the observed absorption coefficient plotted against a reduced width made by dividing Δ by the true absorption coefficient width α . Again, the width corrections can be substantial for only small amounts of instrumental broadening.

Comparison of the two methods of width definition indicates that in general the corrections are smaller for Δ (β and C being the same). In practice, experimental limitations may play a larger role than these calculated differences between Δ and δ corrections.

Satisfactory agreement with the width corrections of Kostkowski and Bass¹⁰ (see Table I) was obtained except for the case of a Gaussian slit function and a Lorentz absorption line. As C approaches zero, limiting values of Δ/α and δ/α are reached. These values can be calculated and are numerically the same.

Figure 11 - Observed peak absorption vs reduced absorption width.
Gaussian slit function and Doppler absorption line.

Figure 12 - Observed peak absorption vs reduced absorption width.
Cauchy slit function and Lorentz absorption line.

Figure 13 - Observed peak absorption vs reduced absorption width.
Cauchy slit function and Doppler absorption line.

Figure 14 - Observed peak absorption vs reduced absorption width.
Gaussian slit function and Lorentz absorption line.

Figure 15 - Observed peak absorption vs reduced absorption width with $\beta = 0.5$. Gaussian slit function and Voigt absorption line.

Figure 16 - Observed peak absorption coefficient vs reduced absorption coefficient width. Gaussian slit function and Doppler absorption line.

Figure 17 - Observed peak absorption coefficient vs reduced absorption coefficient width. Cauchy slit function and Lorentz absorption line.

Figure 18 - Observed peak absorption coefficient vs reduced absorption coefficient width. Cauchy slit function and Doppler absorption line.

Figure 19 - Observed peak absorption coefficient vs reduced absorption coefficient width. Gaussian slit function and Lorentz absorption line.

Figure 20 - Observed peak absorption coefficient vs reduced absorption coefficient width with $\beta = 0.5$. Gaussian slit function and Voigt absorption line.

TABLE I

VALUES OF VARIOUS CORRECTION FACTORS

(All numbers for 30% true peak absorption or $C = 0.355$. Kostkowski and Bass¹⁰ numbers in parentheses.)

β	Δ/α				$A(\text{obs})/A(\text{true})$				K/K_o				Line Shape
	Cauchy		Gauss		Cauchy		Gauss		Cauchy		Gauss		
0.219	1.220	(1.21)	1.047	(1.04)	0.833	(0.84)	0.973	(0.97)	0.982	(0.99)	0.995	(1.00)	Lorentz
0.438	1.440	(1.44)	1.166	(1.14)	0.714	(0.70)	0.911	(0.91)	0.972	(0.97)	0.992	(0.99)	Lorentz
0.876	1.880	(1.88)	1.510	(1.46)	0.555	(0.53)	0.768	(0.76)	0.961	(0.95)	0.982	(0.98)	Lorentz
0.438	1.247	(1.25)	1.079	(1.08)	0.707	(0.70)	0.927	(0.91)	0.941	(0.96)	0.989	(0.99)	Doppler

For the Gaussian slit function and Doppler line, Δ/α and δ/α both approach $(1 + \beta^2)^{1/2}$ for small C ; for the Cauchy slit function and Lorentz line, they both approach $1 + \beta$. For the other combinations of slit functions and line shapes, the width approaches the width of an appropriate Voigt function obtainable from tables.²² When the width corrections of Kostkowski and Bass¹⁰ are extrapolated to small C , agreement is obtained except for the case of the Gaussian slit function and Lorentz line, where a 10% discrepancy remains. Similar results calculated here agree well with the small C expectations.

The quantity F was included in the expressions for Δ and δ [Eqs. (36) and (39)] because F is just that fraction of the peak intensity at which the width is measured. Thus the computer program (Appendix B) can calculate widths at a quarter of peak intensity ($F = 0.25$) or any other fractional width between 0 and 1.

VII. NUMERICAL CALCULATIONS

The various expressions were evaluated on a digital computer using basically standard techniques. Because the integration to obtain the normalization for Eq. (1) always was carried out analytically from $-\infty$ to $+\infty$, the integral over the absorption line should also be carried out over the same limits. Numerically this is accomplished by integration with Simpson's rule between $-L$ and $+L$ and the addition of a contribution for the analytic integration between $-L$ and $-\infty$ and $+L$ and $+\infty$, assuming negligible absorption in that region. For example, the $T(\alpha)$ for the Lorentz absorption line broadened by a Cauchy slit function can be written

$$T(\sigma) \doteq \frac{2}{\pi} \int_{-L}^{+L} I \, dx + \frac{2}{\pi} \int_{+L}^{+\infty} \frac{dx}{1 + 4x^2} + \frac{2}{\pi} \int_{-\infty}^{-L} \frac{dx}{1 + 4x^2}, \quad (40)$$

where the integrand of the first integral is the same as in Eq. (20). The second and third integrals are obtained by neglecting any absorption over the region of integration. The second and third integrals are equal and can be analytically integrated; consequently,

$$T(\sigma) \doteq \frac{2}{\pi} \int_{-L}^{+L} I \, dx + 1 - \frac{2}{\pi} \tan^{-1} 2L. \quad (41)$$

This correction term applies to any integral of the $T(\sigma)$ type when the Cauchy slit function is used and is important in the numerical calculations.

A similar correction term can be obtained for $T(\sigma)$ integrals when the Gaussian slit function is used.

$$T(\sigma) \doteq \sqrt{\frac{K}{\pi}} \int_{-L}^{+L} I \, dx + 1 - \operatorname{erf}(\sqrt{K} L) \quad , \quad (42)$$

where the integrand I is as in Eq. (16) or as in any similar expression that uses a Gaussian slit function. Although this correction was included in the numerical calculations, it was of only minor importance in contrast to the Cauchy slit correction -- a difference that may be related to the more rapid decrease in amplitude of the Gaussian slit function as one moves away from the maximum. In actual calculations the value of L was increased to the point where further increases made no significant change in calculated integral values. In general, the use of the correction terms allowed smaller values of L to be used in obtaining the required accuracy in the numerical integrations. In some cases already noted certain expressions over certain ranges of parameters had valid analytical solutions that could be checked against the numerical results.

Iteration was necessary to solve Eqs. (36) and (39) and a modified Ralphson-Newton method was used. The iteration converged rapidly with the initial approximation that δ/α or Δ/α equals 1.8β .

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APPENDIX A

A VOIGT FUNCTION APPROXIMATION

Several approximations to the Voigt function have been described.^{3,20,21} The form used here in the numerical integrations is actually two functions with an appropriate "crossover" between them. For any value of p and not too far from the Voigt maximum, the expression given by Penner²⁵ is used after the substitution

of an approximation function for the error integral.²⁶ This substitution allows the calculation of one less exponential and somewhat shortens the calculation time.

$$F(v') = \left(U E + \frac{1-U}{2\pi a} \right) \exp(-\epsilon^2) - \frac{2a}{\pi} \sum_{n=1}^{\infty} [2U \exp(W) - \exp(n\epsilon + W) - \exp(-n\epsilon + W)] / (n^2 + 4a^2) \quad (A-1)$$

where

$$U = \cos(2a\epsilon)$$

$$W = -\epsilon^2 - n^2/4$$

$$a = p(K)^{1/2}/2$$

$$E = \sum_{i=1}^5 c_i T^i$$

$$T = 1/(1 + ap)$$

$$\epsilon = \sigma(K)^{1/2}/2$$

The coefficients for the error function approximation, c_i and p , are the ones given by Hastings²⁶ multiplied by $2/(\pi)^{1/2}$. For large distances from the Voigt function maximum, too many terms are required in the summation of Eq. (A-1) to give sufficient accuracy, so an asymptotic form taken from Born²⁷ is used. The first two terms as given by Penner (Ref. 3, P. 46) are

$$F(v') = \frac{a}{(\pi)^{1/2} (a^2 + \epsilon^2)} \left[1 - \frac{a^2 - 3\epsilon^2}{2(a^2 + \epsilon^2)^2} \right] \quad (A-2)$$

Evaluation of Eq. (A-1) to an accuracy of 1 part in 10^5 requires no more than 41 terms if $\sigma < 10$. This combination of functions requires far less time to compute than a Simpson's rule integration and is accurate to at least 1 part in 10^5 for all values of p and σ if the crossover is set at $\sigma = 10$. Later calculations indicate that 1 part in 10^4 is sufficient accuracy in the approximating function, so the crossover becomes $\sigma = 7$.

APPENDIX B

COMPUTER PROGRAMS

Two computer programs are available to evaluate the expressions developed here. They are written in the FORTRAN IV language and are designed for operation on a CDC 7600 digital computer, although, except for the plotting feature, they should be adaptable to any FORTRAN-compatible machine. Both programs contain comment cards by which the plotting feature can be removed.

Both programs have in common the options given in Table B-I. The option number specifies the combination of slit function and absorption line shape to be used in the calculation. Option numbers 7, 8, and 9 provide for the use of some slit function other than a Gaussian or Cauchy. In that case, several modifications must be made, mainly in programming the new integrand and normalization factors.

Table B-II gives the input data card format for the SAL program, which does all the computations outlined in this report with the exception of integrated absorption coefficient corrections. Table B-III gives the input data card format for the KAL program, whose only purpose is to calculate and plot the integrated absorption coefficient corrections. Input and output constants are labeled in notation similar to that used in this report.

Computation time for these programs varies greatly with the problem to be solved. For one value of β and C , the CDC 7600 can do one SAL calculation in about 1 s if the option number does not ask for a Voigt function line shape. If the Voigt function approximation is used, it takes longer by an order of magnitude. The KAL program requires an additional integration, and takes considerably more time than SAL. These running times are greatly influenced by the value of L and

TABLE B-I

SLIT FUNCTION AND ABSORPTION LINE SHAPE OPTIONS

<u>Option Number</u>	<u>Slit Function</u>	<u>Absorption Line Shape</u>
1	Gaussian	Doppler
2	Gaussian	Lorentz
3	Cauchy	Doppler
4	Cauchy	Lorentz
5	Gaussian	Voigt
6	Cauchy	Voigt
7	Unspecified	Doppler
8	Unspecified	Lorentz
9	Unspecified	Voigt

the integration error. A good compromise between accuracy and running time can be achieved with $L = 10.0$ and the error at 0.001. Increasing L or decreasing the error does not change results significantly.

TABLE B-II

DATA INPUT CARDS FOR THE SAL PROGRAM

Card	Column	Contents
1	5	Option number. See Table I.
	10*	If 1, plot A(peak observed) vs A(peak true).
	15*	If 1, plot A(peak observed) vs C(true).
	20*	If 1, plot C(observed) vs C(true).
	25*	If 1, plot A(peak observed) vs reduced line width.
	30*	If 1, plot C(observed) vs reduced line width.
	35	If 0, reduce width by dividing by α . If 1, reduce width by dividing by w .
	40	If 0, calculate Voigt function expressions as a function of β . If 1, calculate as a function of ρ .
	45	If 0, calculate widths (δ) of absorption. If 1, calculate widths (Δ) of absorption coefficient.
	50	If 0, use Simpson's rule integration to evaluate Voigt function. If 1, use Voigt approximation function.
2†	1-10	Initial value of β .
	11-20	Increment to be added to β .
	21-30	Maximum value of β .
	31-40	Initial value of C.
	41-50	Increment to be added to C.
	51-60	Maximum value of C.
	61-70	Fraction of peak at which to calculate width (F in Sec. VI).
3†	Card needed only if option number is 5, 6, or 9 (See Table I).	
	1-10	Initial value of ρ .
	11-20	Increment to be added to ρ . (Not needed if column 40, card 1, is 0).
	21-30	Maximum value of ρ . (Not needed if column 40, card 1, is 0).

*If 0, do not plot this type of graph.

†All numbers on these cards have a FORTRAN F10.5 format.

TABLE B-II (continued)

DATA INPUT CARDS FOR THE SAL PROGRAM

<u>Card</u>	<u>Column</u>	<u>Contents</u>
4†	1-10	Limits on numerical integration (L of Sec. VII).
	11-20	Error in integration procedure.
5†	Card needed only if column 10, 15, 20, 25, and 30, card 1, are not all blank.	
	1-10	Upper limit on plot when C (observed) vs C(true) is a coordinate.
	11-20	Upper limit on plot when reduced line width is a coordinate.

TABLE B-III

DATA INPUT CARDS FOR THE KAL PROGRAM

Card	Column	Contents
1	5	Option number. See Table I.
	10*	If 1, plot A(peak observed) vs K/K_0 .
	15*	If 1, plot C(observed) vs K/K_0 .
	20	If 0, use Simpson's rule integration to evaluate Voigt function. If 1, use Voigt approximation function.
	25	If 0, calculate Voigt function expression as a function of β . If 1, calculate as a function of ρ .
	30	If 0, calculate Voigt function expressions as a function of β . If 1, calculate as a function of ρ .
2†	1-10	Initial value of β .
	11-20	Increment to be added to β .
	21-30	Maximum value of β .
	31-40	Initial value of C.
	41-50	Increment to be added to C.
	51-60	Maximum value of C.
3†	Card needed only if option number is 5, 6, or 9 (see Table I).	
	1-10	Initial value of ρ .
	11-20	Increment to be added to ρ . (Not needed if column 25, card 1, is 0).
	21-30	Maximum value of ρ . (Not needed if column 25, card 1, is 0).
4†	1-10	Limits on numerical integration (L of Sec. VII). Outer K integral.
	11-20	Error in integration procedure. Outer K integral.
	21-30	Limits on numerical integration. Inner T(σ) integral.
	31-40	Error in integration procedure. Inner T(σ) integral.
5†	Card needed only if columns 10 and 15, cards 1, are not both blank.	

*If 0, do not plot this type of graph.

†All numbers on these cards have a FORTRAN F10.5 format.

TABLE B-III (continued)

DATA INPUT CARDS FOR THE KAL PROGRAM

<u>Card</u>	<u>Column</u>	<u>Contents</u>
	1-10	Upper limit on plot when $C(\text{observed})$ is a coordinate.
	11-20	Lower limit on plot of K/K_0 coordinate.

LASL Identification No. LP-949

```

PROGRAM SAL(INP,OUT,FILM,FSET1=INP,FSET9=OUT,FSET12=FILM)
EXTERNAL SIMPS2,FGAG,FGAL,FLAG,FLAL,FGAV,FLAV,FHAG,FHAL,FHAV
DIMENSION ATRUE(50),CTRUE(50),YMT(50),A0BS(10,50),
1YM(10,50),ALP(2),ALPP(2),Y(50),TP(50)
DIMENSION AC(9),KC(2)
EQUIVALENCE (KC(1),AC(A))
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
1,ERF
C NTYPE DETERMINES SLIT AND LINE SHAPE PAIR USED
C NTYPE = 1 SLIT = GAUSS LINE = DOPPLER
C NTYPE = 2 SLIT = GAUSS LINE = LORENTZ
C NTYPE = 3 SLIT = CAUCHY LINE = DOPPLER
C NTYPE = 4 SLIT = CAUCHY LINE = LORENTZ
C NTYPE = 5 SLIT = GAUSS LINE = VOIGT
C NTYPE = 6 SLIT = CAUCHY LINE = VOIGT
C NTYPE = 7 SLIT = OTHER LINE = DOPPLER
C NTYPE = 8 SLIT = OTHER LINE = LORENTZ
C NTYPE = 9 SLIT = OTHER LINE = VOIGT
C BETA=RATIO OF SLIT TO LINE WIDTH
C BETAM=INCREMENT OF BETA
C BETAM=MAX. VALUE OF BETA
C C=PEAK ABSORPTION COEFFICIENT
C CD=INCREMENT OF C
C CM=MAX. VALUE OF C
C RHO=RATIO OF LORENTZ TO DOPPLER WIDTH
C RHO=INCREMENT OF RHO IF USED
C RHO=MAX. VALUE OF RHO
C ALIM=LIMIT ON INTEGRALS
C ERROR=MEASURE OF ERROR IN NUMERICAL INTEGRATION
C NPX (X=ANY NUMBER) =0 NO PLOT
C NP1=1 PLOT A(0BS) VS. A(TRUE)
C NP2=1 PLOT A(0BS) VS. C(TRUE)
C NP3=1 PLOT C(0BS) VS. C(TRUE)
C NP4=1 PLOT A(0BS) VS. REDUCED LINE WIDTH
C NP5=1 PLOT C(0BS) VS. REDUCED LINE WIDTH
C NDI=0 CALC. WIDTH/ALPHA
C NDI=1 CALC. WIDTH/W
C NRHO=1 CALC. VOIGT AS FUNCTION OF RHO
C NRHO=0 CALC. VOIGT AS FUNCTION OF BETA
C NWID=0 CALC. WIDTHS OF ABSORPTION/ NWID=1 CALC. WIDTH ABS. COEF.
C NINT=0 INTEGRATE VOIGT BY SIMPSON RULE
C NINT=1 USE FUNCTION FOR VOIGT
C CONSTANTS USED
B1=4.0*ALOG(2.0)
B2=2.0/3.1415926536
B3=SQRT(B1/3.1415926536)
B4=SQRT(B1)
B5=3.1415926536
B6=SQRT(B5)
1 READ(10,500) NTYPE,NP1,NP2,NP3,NP4,NP5,NDI,NRHO,NWID,NINT
500 FORMAT (10I5)
IF(NTYPE.EQ.0) CALL EXIT
WRITE(9,510)
510 FORMAT(1H1,23HCONVOLUTION INTEGRATION,
131H VERSION 1, 8/15/78, R.ENGLEMAN)
READ(10,530)BETA,BETAD,BETAM,C,CD,CM,FRACT
530 FORMAT(7(F10.5))
540 FORMAT(6H BETA=F10.5,2(6X,F10.5), 3H C=F10.5,2(6X,F10.5))
IF(NRHO.EQ.0)WRITE( 9,540)BETA,BETAD,BETAM,C,CD,CM
540 FORMAT(15H BETA CONSTANT=F10.5,3H C=F10.5,2(6X,F10.5))

```

```

      IF(NRHO, EQ, 1) WRITE( 9, 542) BETA, C, CD, CM
      GO TO (11, 12, 13, 14, 15, 16, 17, 18, 19), NTYPE
11  WRITE( 9, 521)
521 FORMAT(25H SLIT=GAUSS  LINE=DOPPLER)
      GO TO 20
12  WRITE( 9, 522)
522 FORMAT(25H SLIT=GAUSS  LINE=LORENTZ)
      GO TO 20
13  WRITE( 9, 523)
523 FORMAT(26H SLIT=CAUCHY  LINE=DOPPLER)
      GO TO 20
14  WRITE( 9, 524)
524 FORMAT(26H SLIT=CAUCHY  LINE=LORENTZ)
      GO TO 20
15  READ(10, 530) RHO, RHOD, RHOM
      IF(NRHO, EQ, 0) WRITE( 9, 525) RHO
525 FORMAT(29H SLIT=GAUSS  LINE=VOIGT  RHO=, F10, 5)
      IF(NRHO, EQ, 1) WRITE( 9, 535) RHO, RHOD, RHOM
535 FORMAT(29H SLIT=GAUSS  LINE=VOIGT  RHO=, F10, 5, 2(6X, F10, 5))
      GO TO 20
16  READ(10, 530) RHO, RHOD, RHOM
      IF(NRHO, EQ, 0) WRITE( 9, 526) RHO
526 FORMAT(30H SLIT=CAUCHY  LINE=VOIGT  RHO=, F10, 5)
      IF(NRHO, EQ, 1) WRITE( 9, 536) RHO, RHOD, RHOM
536 FORMAT(30H SLIT=CAUCHY  LINE=VOIGT  RHO=, F10, 5, 2(6X, F10, 5))
      GO TO 20
17  WRITE( 9, 527)
527 FORMAT(25H SLIT=OTHER  LINE=DOPPLER)
      GO TO 20
18  WRITE( 9, 528)
528 FORMAT(25H SLIT=OTHER  LINE=LORENTZ)
      GO TO 20
19  READ(10, 530) RHO, RHOD, RHOM
      IF(NRHO, EQ, 0) WRITE( 9, 529) RHO
529 FORMAT(29H SLIT=OTHER  LINE=VOIGT  RHO=, F10, 5)
      IF(NRHO, EQ, 1) WRITE( 9, 539) RHO, RHOD, RHOM
539 FORMAT(29H SLIT=OTHER  LINE=VOIGT  RHO=, F10, 5, 2(6X, F10, 5))
20  READ(10, 530) ALIM, ERROR
      IF((NTYPE, EQ, 5, OR, NTYPE, EQ, 6, OR, NTYPE, EQ, 9), AND, NINT, EQ, 0)
1  WRITE ( 9, 700)
700 FORMAT(35H SIMPSON INTEGRATION USED FOR VOIGT)
      IF((NTYPE, EQ, 5, OR, NTYPE, EQ, 6, OR, NTYPE, EQ, 9), AND, NINT, EQ, 1)
1  WRITE ( 9, 701)
701 FORMAT(24H FUNCTION USED FOR VOIGT)
      WRITE( 9, 560) ALIM, ERROR
560 FORMAT(19H INTEGRATION LIMIT=, F10, 5, 2X,
119H INTEGRATION ERROR=, F10, 5)
      J=1
      SB=BETA
      SR=RHO
      SC=C
70  ATRUE(J)=1.0-EXP(-C)
      CTRUE(J)=C
      IF (NDIV, EQ, 1, OR, NWID, EQ, 1) GO TO 75
      GO TO (71, 72, 71, 72, 71, 71, 71, 72, 71), NTYPE
71  YMT(J)=2.*SQRT(ALOG(-C/ALOG(1.-(1.-EXP(-C))*FRACT) )/B1)
      GO TO 75
72  YMT(J)=SQRT(-C/ALOG(1.-(1.-EXP(-C))*FRACT) -1.)
75  C=C+CD
      J=J+1

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      IF (C.LT.CM) GO TO 70
      C=SC
      ALIMP=ALIM
      I=1
      IF (NWID.EQ.0) WRITE(9,585)
585  FORMAT(28H WIDTH IS THAT OF ABSORPTION)
      IF (NWID.EQ.1) WRITE(9,586)
586  FORMAT(28H WIDTH IS THAT OF ABS. COEF.)
      WRITE(9,589) FRACT
589  FORMAT(16H WIDTH CALC. AT ,F10.5,18H OF PEAK INTENSITY)
      IF (NWID.EQ.1) GO TO 76
      IF (NDIV.EQ.0.AND.NRHO.EQ.0) WRITE(9,580)
580  FORMAT(/,/,7H BETA,10X,1HC,11X,5HATRUE,10X,
        14HA0BS, 8X,7HY/ALPHA,10X,3HYMT,/)
      IF (NDIV.EQ.1.AND.NRHO.EQ.0) WRITE(9,581)
581  FORMAT(/,/,7H BETA,10X,1HC,11X,5HATRUE,10X,
        14HA0BS,10X,3HY/W,/)
      IF (NDIV.EQ.0.AND.NRHO.EQ.1) WRITE(9,582)
582  FORMAT(/,/,7H RHO,10X,1HC,11X,5HATRUE,10X,
        14HA0BS, 8X,7HY/ALPHA,10X,3HYMT,/)
      IF (NDIV.EQ.1.AND.NRHO.EQ.1) WRITE(9,583)
583  FORMAT(/,/,7H RHO,10X,1HC,11X,5HATRUE,10X,
        14HA0BS,10X,3HY/W,/)
      GO TO 60
76  IF (NDIV.EQ.0.AND.NRHO.EQ.0) WRITE(9,584)
584  FORMAT(/,/,7H BETA,10X,1HC,11X,5HATRUE,10X,
        14HA0BS, 8X,7HY/ALPHA,/)
      IF (NDIV.EQ.1.AND.NRHO.EQ.0) WRITE(9,581)
      IF (NDIV.EQ.0.AND.NRHO.EQ.1) WRITE(9,587)
587  FORMAT(/,/,7H RHO,10X,1HC,11X,5HATRUE,10X,
        14HA0BS, 8X,7HY/ALPHA,/)
      IF (NDIV.EQ.1.AND.NRHO.EQ.1) WRITE(9,583)
60  J=1
      IF (NINT.EQ.0) GO TO 51
      AL=RH0*84/2.0
      U=1.0/(1.0+0.3275011*AL)
      ERF=U*(0.254029502+U*(-0.284496736+U*
        1(1.421413741+U*(-1.453152027+U*1.061405429)))
51  YM(1,1)=0.0
C  FOR PEAK ABSORPTION Y=0.0
50  Y=0.0
      GO TO (101,102,103,104,105,106,107,108,109), NTYPE
101  A0BS(I,J)=ERR169(B4*ALIM)-2.*SIMP82(FGAG,0.0,ALIM,ERROR)*B3
      GO TO 100
102  A0BS(I,J)=ERR169(B4*ALIM)-2.*SIMP82(FGAL,0.0,ALIM,ERROR)*B3
      GO TO 100
103  A0BS(I,J)=B2*(ATAN(2.*ALIM)-2.*SIMP82(FLAG,0.0,ALIM,ERROR))
      GO TO 100
104  A0BS(I,J)=B2*(ATAN(2.*ALIM)-2.*SIMP82(FLAL,0.0,ALIM,ERROR))
      GO TO 100
105  A0BS(I,J)=ERR169(B4*ALIM)-2.*SIMP82(FGAV,0.0,ALIM,ERROR)*B3
      GO TO 100
106  A0BS(I,J)=B2*(ATAN(2.*ALIM)-2.*SIMP82(FLAV,0.0,ALIM,ERROR))
      GO TO 100
C  MUST ADD NTYPE EQ 7 8 9 IF OTHER SLOTS USED
107  A0BS(I,J)=0.0
      GO TO 100
108  A0BS(I,J)=0.0
      GO TO 100
109  A0BS(I,J)=0.0

```

```

100 Y=YM(I,J)
    AC(1)=0.0
    AC(4)=Y
    AC(2)=AC(4)+0.1
    KC(1)=0
220 CALL FROOT(AC)
    KE=KC(2)
    IF (ABS(AC(2)-AC(4)).LT.0.00005) KE=1
    GO TO (102,240, 90, 90),KE
102 Y=AC(2)
    IF (NDIV.EQ.0) YM(I,J)=2.*Y
    IF (NDIV.EQ.1) YM(I,J)=2.*Y/BETA
    IF (NRHO.EQ.1) GO TO 197
    IF (NDIV.EQ.0.AND.NRHO.EQ.0) WRITE( 9,590) BETA,C,ATRUE(J),AOBS(I,J),
    1YM(I,J),YMT(J)
590 FORMAT(6(F10,5,4X))
    IF (NDIV.EQ.1.AND.NRHO.EQ.0) WRITE( 9,591) BETA,C,ATRUE(J),AOBS(I,J),
    1YM(I,J)
591 FORMAT(5(F10,5,4X))
    IF (NDIV.EQ.0.AND.NRHO.EQ.1) WRITE( 9,590) RHO,C,ATRUE(J),AOBS(I,J),
    1YM(I,J),YMT(J)
    IF (NDIV.EQ.1.AND.NRHO.EQ.1) WRITE( 9,591) RHO,C,ATRUE(J),AOBS(I,J),
    1YM(I,J)
    GO TO 198
197 IF (NRHO.EQ.0) WRITE ( 9,591) BETA,C,ATRUE(J),AOBS(I,J),YM(I,J)
    IF (NRHO.EQ.1) WRITE ( 9,591) RHO,C,ATRUE(J),AOBS(I,J),YM(I,J)
198 C=C+CD
    J=J+1
    YM(I,J)=Y
    IF(C.LT.CM) GO TO 50
    C=BC
    I=I+1
    IF(NRHO.EQ.1) GO TO 194
    BETA=BETA+BETAD
    IF(BETA.LT.BETAM) GO TO 60
    BETA=SB
    GO TO 195
194 RHO=RHO+RHOD
    IF (RHO.LT.RHOM) GO TO 60
    RHO=SR
195 CONTINUE
C FOLLOWING CARDS CAN BE REMOVED IF NO 4020 PLOT USED *****
    IMAX=J+1
    JMAX=J+1
    IF (NP1+NP2+NP3+NP4+NP5.EQ.0) GO TO 1
    READ(10,530) CMAX,YMAX
    IF (NP1.EQ.0) GO TO 420
C PLOT A(OBS) VS. A(TRUE)
    CALL ADV (1)
    CALL LINCNT (59)
    WRITE(12,601)
601 FORMAT(19H A(OBS) VS. A(TRUE))
    WRITE (12,511)
511 FORMAT( 24H CONVOLUTION INTEGRATION,
    131H VERSION 1, 5/12/66, R.ENGLEMAN)
    IF(NRHO.EQ.0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
    IF(NRHO.EQ.1)WRITE(12,542)BETA,C,CD,CM
    GO TO (301,302,303,304,305,306,307,308,309),NTYPE
301 WRITE(12,521)
    GO TO 300.

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```

302 WRITE(12,522)
   GO TO 300
303 WRITE(12,523)
   GO TO 300
304 WRITE(12,524)
   GO TO 300
305 IF(NRHO.EQ.0)WRITE(12,525)RHO
   IF(NRHO.EQ.1)WRITE(12,535)RHO,RHOD,RHOM
   GO TO 300
306 IF(NRHO.EQ.0)WRITE(12,526)RHO
   IF(NRHO.EQ.1)WRITE(12,536)RHO,RHOD,RHOM
   GO TO 300
307 WRITE(12,527)
   GO TO 300
308 WRITE(12,528)
   GO TO 300
309 IF(NRHO.EQ.0)WRITE(12,529)RHO
   IF(NRHO.EQ.1)WRITE(12,539)RHO,RHOD,RHOM
300 WRITE(12,560) ALIM,ERROR
   CALL DGA (120,900,50,910,0.0,1.0,1.0,0.0)
   CALL DLNIN (20,20)
   CALL SBLIN (5,2)
   CALL SLLIN (5,2)
   ALP(1)=0.0
   ALP(2)=1.0
   ALPP(1)=0.0
   ALPP(2)=1.0
   CALL PLOT (2,ALP,1,ALPP,1,42,1)
   DO 415 I=1,IMAX
   DO 416 J=1,JMAX
416 T(J)=A0BS(I,J)
415 CALL PLOT(JMAX,ATRUE,1,T,1,44,1)
420 IF (NP2.EQ.0) GO TO 430
C PLOT A(OBS) VS. C(TRUE)
   CALL ADV (1)
   CALL LINCNT (59)
   WRITE(12,602)
602 FORMAT(19H A(OBS) VS. C(TRUE))
   WRITE (12,511)
   IF(NRHO.EQ.0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
   IF(NRHO.EQ.1)WRITE(12,542)BETA,C,CD,CM
   GO TO (321,322,323,324,325,326,327,328,329),NTYPE
321 WRITE(12,521)
   GO TO 320
322 WRITE(12,522)
   GO TO 320
323 WRITE(12,523)
   GO TO 320
324 WRITE(12,524)
   GO TO 320
325 IF(NRHO.EQ.0)WRITE(12,525)RHO
   IF(NRHO.EQ.1)WRITE(12,535)RHO,RHOD,RHOM
   GO TO 320
326 IF(NRHO.EQ.0)WRITE(12,526)RHO
   IF(NRHO.EQ.1)WRITE(12,536)RHO,RHOD,RHOM
   GO TO 320
327 WRITE(12,527)
   GO TO 320
328 WRITE(12,528)
   GO TO 320

```

```

329 IF(NRHO,EQ.0)WRITE(12,529)RHO
    IF(NRHO,EQ.1)WRITE(12,539)RHO,RHOD,RHOM
320 WRITE(12,560) ALIM,ERROR
    CALL DGA (120,980,50,910,0.0,CMAX,1,0,0,0)
    CALL DLNLN (20,20)
    CALL SLLIN (5,2)
    CALL SBLIN (5,2)
    CALL PLOT(JMAX,CTRUE,1,ATRUE,1,63,1)
    DO 425 I=1,JMAX
    DO 426 J=1,JMAX
426 T(J)=A0BS(I,J)
425 CALL PLOT(JMAX,CTRUE,1,T,1,44,1)
430 IF (NP3,EQ.0) GO TO 440
C PLOT C(OBS) VS. C(TRUE)
    CALL ADV (1)
    CALL LINCNT (59)
    WRITE(12,603)
603 FORMAT(19H C(OBS) VS. C(TRUE))
    WRITE (12,511)
    IF(NRHO,EQ.0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
    IF(NRHO,EQ.1)WRITE(12,542)BETA,C,CD,CM
    GO TO (341,342,343,344,345,346,347,348,349),NTYPE
341 WRITE(12,521)
    GO TO 340
342 WRITE(12,522)
    GO TO 340
343 WRITE(12,523)
    GO TO 340
344 WRITE(12,524)
    GO TO 340
345 IF(NRHO,EQ.0)WRITE(12,525)RHO
    IF(NRHO,EQ.1)WRITE(12,535)RHO,RHOD,RHOM
    GO TO 340
346 IF(NRHO,EQ.0)WRITE(12,526)RHO
    IF(NRHO,EQ.1)WRITE(12,536)RHO,RHOD,RHOM
    GO TO 340
347 WRITE(12,527)
    GO TO 340
348 WRITE(12,528)
    GO TO 340
349 IF(NRHO,EQ.0)WRITE(12,529)RHO
    IF(NRHO,EQ.1)WRITE(12,539)RHO,RHOD,RHOM
340 WRITE(12,560) ALIM,ERROR
    CALL DGA (120,980,50,910,0.0,CMAX,CMAX,0,0)
    CALL DLNLN (20,20)
    CALL SLLIN (5,2)
    CALL SBLIN (5,2)
    ALP(1)=0.0
    ALP(2)=CMAX
    ALPP(1)=0.0
    ALPP(2)=CMAX
    CALL PLOT (2,ALP,1,ALPP,1,42,1)
    DO 435 I=1,JMAX
    DO 436 J=1,JMAX
436 T(J)=-ALOG(1.0-A0BS(I,J))
435 CALL PLOT(JMAX,CTRUE,1,T,1,44,1)
440 IF (NP4,EQ.0) GO TO 460
C PLOT A(OBS) VS. REDUCED LINE WIDTH (Y)
    CALL ADV (1)
    CALL LINCNT (59)

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      IF(NDIV,EQ.0.AND.NWID,EQ.0)WRITE(12,604) FRACT
604  FORMAT(27H A(OBS) VS. WIDTH/ALPHA AT ,F10.5,15H PEAK INTENSITY)
      IF(NDIV,EQ.1.AND.NWID,EQ.0)WRITE(12,605) FRACT
605  FORMAT(23H A(OBS) VS. WIDTH/W AT ,F10.5,15H PEAK INTENSITY)
      IF(NDIV,EQ.0.AND.NWID,EQ.1)WRITE(12,606) FRACT
606  FORMAT(34H A(OBS) VS. WIDTH(ABS,COEF.)/ALPHA AT ,F10.5,
      15H PEAK INTENSITY)
      IF(NDIV,EQ.1.AND.NWID,EQ.1)WRITE(12,607) FRACT
607  FORMAT(34H A(OBS) VS. WIDTH(ABS,COEF.)/W AT ,F10.5,
      15H PEAK INTENSITY)
      WRITE (12,511)
      IF(NRHO,EQ.0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
      IF(NRHO,EQ.1)WRITE(12,542)BETA,C,CD,CM
      GO TO (361,362,363,364,365,366,367,368,369),NTYPE
361  WRITE(12,521)
      GO TO 360
362  WRITE(12,522)
      GO TO 360
363  WRITE(12,523)
      GO TO 360
364  WRITE(12,524)
      GO TO 360
365  IF(NRHO,EQ.0)WRITE(12,525)RHO
      IF(NRHO,EQ.1)WRITE(12,535)RHO,RHOD,RHOM
      GO TO 360
366  IF(NRHO,EQ.0)WRITE(12,526)RHO
      IF(NRHO,EQ.1)WRITE(12,536)RHO,RHOD,RHOM
      GO TO 360
367  WRITE(12,527)
      GO TO 360
368  WRITE(12,528)
      GO TO 360
369  IF(NRHO,EQ.0)WRITE(12,529)RHO
      IF(NRHO,EQ.1)WRITE(12,539)RHO,RHOD,RHOM
360  WRITE(12,560) ALIM,ERROR
      CALL DGA (120,980,50,910,1.0,YMAX,1.0,0.0)
      CALL DLNLN (20,20)
      CALL SLLJN (5,2)
      CALL SBLJN (5,2)
      IF (NDIV,EQ.1.OR.NWID,EQ.1) GO TO 370
      CALL PLOT (JMAX,YMT,1,ATRUE,1.63,1)
370  DO 445 J=1,JMAX
      DO 446 J=1,JMAX
      TP(J)=AABS(1,J)
446  T(J)=YM(T,J)
445  CALL PLOT (JMAX,T,1,TP,1.44,i)
460  IF (NP5,EQ.0) GO TO 1
C  PLOT C(OBS) VS. REDUCED LINE WIDTH (Y)
      CALL ADV (1)
      CALL LJNCNT (50)
      IF(NDIV,EQ.0.AND.NWID,EQ.0)WRITE(12,624) FRACT
624  FORMAT(27H C(OBS) VS. WIDTH/ALPHA AT ,F10.5,15H PEAK INTENSITY)
      IF(NDIV,EQ.1.AND.NWID,EQ.0)WRITE(12,625) FRACT
625  FORMAT(23H C(OBS) VS. WIDTH/W AT ,F10.5,15H PEAK INTENSITY)
      IF(NDIV,EQ.0.AND.NWID,EQ.1)WRITE(12,626) FRACT
626  FORMAT(34H C(OBS) VS. WIDTH(ABS,COEF.)/ALPHA AT ,F10.5,
      15H PEAK INTENSITY)
      IF(NDIV,EQ.1.AND.NWID,EQ.1)WRITE(12,627) FRACT
627  FORMAT(34H C(OBS) VS. WIDTH(ABS,COEF.)/W AT ,F10.5,
      15H PEAK INTENSITY)

```



```

WRITE (12,511)
IF(NRHO.EQ.0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
IF(NRHO.EQ.1)WRITE(12,542)BETA,C,CD,CM
GO TO (381,382,383,384,385,386,387,388,389),NTYPE
381 WRITE(12,521)
GO TO 380
382 WRITE(12,522)
GO TO 380
383 WRITE(12,523)
GO TO 380
384 WRITE(12,524)
GO TO 380
385 IF(NRHO.EQ.0)WRITE(12,525)RHO
IF(NRHO.EQ.1)WRITE(12,535)RHO,RHOD,RHOM
GO TO 380
386 IF(NRHO.EQ.0)WRITE(12,526)RHO
IF(NRHO.EQ.1)WRITE(12,536)RHO,RHOD,RHOM
GO TO 380
387 WRITE(12,527)
GO TO 380
388 WRITE(12,528)
GO TO 380
389 IF(NRHO.EQ.0)WRITE(12,529)RHO
IF(NRHO.EQ.1)WRITE(12,539)RHO,RHOD,RHOM
390 WRITE(12,560) ALIM,ERROR
CALL DGA (120,980,50,910,1,0,YMAX,CMAX,0,0)
CALL DLNLN (20,20)
CALL SLLIN (5,2)
CALL SBLIN (5,2)
IF (NDIV.EQ.1.OR.NWID.EQ.1) GO TO 390
CALL PLOT (JMAX,YMT,1,CTRUE,1,63,1)
390 DO 465 J=1,IMAX
DO 466 J=1,JMAX
TP(J)=ALOG(1.0-AOBS(I,J))
466 T(J)=YMT(I,J)
465 CALL PLOT (JMAX,T,1,TP,1,44,1)
C ABOVE CARDS CAN BE REMOVED IF NO 4020 PLOT USED *****
GO TO 1
90 WRITE( 9,578)
578 FORMAT(17H TROUBLE IN FRONT)
GO TO 192
240 Y=AC(2)
GO TO (201,202,203,204,205,206,207,208,209),NTYPE
201 S=SIMPS2(FGAG,ALIMP,ALIM,ERROR)*B3+1.0-ERR169(B4*ALIM)
GO TO 200
202 S=SIMPS2(FGAL,ALIMP,ALIM,ERROR)*B3+1.0-ERR169(B4*ALIM)
GO TO 200
203 S=1.0-B2*(ATAN(2.*ALIM)-SIMPS2(FLAG,ALIMP,ALIM,ERROR))
GO TO 200
204 S=1.0-B2*(ATAN(2.*ALIM)-SIMPS2(FLAL,ALIMP,ALIM,ERROR))
GO TO 200
205 S=SIMPS2(FGAV,ALIMP,ALIM,ERROR)*B3+1.0-ERR169(B4*ALIM)
GO TO 200
206 S=1.0-B2*(ATAN(2.*ALIM)-SIMPS2(FLAV,ALIMP,ALIM,ERROR))
GO TO 200
207 S=0.0
GO TO 200
208 S=0.0
GO TO 200
209 S=0.0

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200 IF (NWD, EQ, 0) AC(3) = S - (2, -ANBS(I, J)) * FRAC
IF (NWD, EQ, 1) AC(3) = S - (1, -ANBS(I, J)) * FRAC
GO TO 220
END
FUNCTION FGAG (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
FGAG = EXP(-B1 * V ** 2) * C * EXP(-B1 * (BETA * V + Y) ** 2)
RETURN
END
FUNCTION FGAL (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
FGAL = EXP(-B1 * V ** 2) * EXP(-C / (1, 0 + 4, 0 * (BETA * V + Y) ** 2))
RETURN
END
FUNCTION FLAG (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
FLAG = EXP(-C * EXP(-B1 * (BETA * V + Y) ** 2)) / (1, 0 + 4, 0 * V ** 2)
RETURN
END
FUNCTION FLAL (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
FLAL = EXP(-C / (1, 0 + 4, 0 * (BETA * V + Y) ** 2)) / (1, 0 + 4, 0 * V ** 2)
RETURN
END
FUNCTION FGAV (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
EXTERNAL SIMPS3, FSAV1, VOIGT
VV = BETA * V
IF (NINT, EQ, 1) GO TO 2
FGAV = EXP(-C * B2 * SIMPS3(FSAV1, ALIMP, ALIM, ERROR) - B1 * V ** 2)
RETURN
2 FGAV = EXP(-C * VOIGT(VV) - B1 * V ** 2)
RETURN
END
FUNCTION FLAV (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
EXTERNAL SIMPS3, FSAV1, VOIGT
VV = BETA * V
IF (NINT, EQ, 1) GO TO 2
FLAV = EXP(-C * B2 * SIMPS3(FSAV1, ALIMP, ALIM, ERROR)) / (1, 0 + 4, 0 * V ** 2)
RETURN
2 FLAV = EXP(-C * VOIGT(VV)) / (1, 0 + 4, 0 * V ** 2)
RETURN
END
FUNCTION FHAG (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
FHAG = 0, 0
RETURN
END
FUNCTION FHAL (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
FHAL = 0, 0
RETURN
END
FUNCTION FHAV (V)
COMMON ALIMP, ALIM, ERROR, B1, B2, B3, B4, Y, C, BETA, RHO, VV, B5, B6, AL, NINT
EXTERNAL SIMPS3, FSAV1, VOIGT
VV = BETA * V
FHAV = 0, 0
RETURN

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<pre> DIMENSION C(12) EQUIVALENCE (IC8,CA),(IC9,C9) INTEGER EXIT CA=C(8) C E00 IC9=2 IF(C(8),NE,0.0) GO TO 100 XP=C(4) GO TO 600 100 IF(ABS(C(3)),GT,C(1)) GO TO 120 IC9=1 GO TO 900 120 IF(IC8,NE,1) GO TO 140 XP=C(4) GO TO 600 C E1 140 X=C(4) F=C(5) ASSIGN 200 TO EXIT GO TO 1000 200 IF (IC8,EQ,2) GO TO 600 C (C10,C11* + C12,C13*,C14) IF(C(3),NE,C(5)) GO TO 300 IF(C(3),NE,C(7)) GO TO 400 300 IF(C(3)*C(5),LT,0.0) GO TO 500 IF(C(3)*C(7),GT,0.0) GO TO 500 IF((XP=C(2))*C(6)),LT,0.0) GO TO 500 400 X=C(6) F=C(7) ASSIGN 450 TO EXIT GO TO 1000 450 CONTINUE C (C12* + C13) ... 500 IF (C(3)*C(5),LT,0.0) GO TO 550 IF (C(3)*C(7),LT,0.0) GO TO 700 550 IF (C(3),NE,C(5)) GO TO 600 IF (C(3),NE,C(7)) GO TO 700 C H1+E20 600 C(6)=C(4) C(7)=C(5) C E21 700 C(4)=C(2) C(5)=C(3) C(2)=XP IC8=IC8+1 C H2 = RETURN 900 C(8)=CA C(9)=C9 RETURN C T1 1000 E1=C(3)=F IF(E),NE,0.0) GO TO 1030 XP=0.5*(C(2)+C(4)) IC9=4 GO TO 1000 1030 XP=C(2)+C(3)*((C(2)+X)/E1) IF(XP,NE,C(2)) GO TO 1000 IC9=3 1090 GO TO EXIT,(200,450) END </pre>	<pre> 850 FRO 851 FRO 852 FRO C10 FRO D10 FRO D11 FRO D12 FRO D13 FRO D14 FRO D20 FRO D21 FRO D22 FRO D30 FRO D31 FRO D32 FRO E10 FRO E11 FRO E12 FRO E20 FRO E21 FRO E30 FRO E31 FRO E32 FRO E33 FRO E34 FRO E35 FRO E36 FRO E37 FRO E38 FRO E40 FRO E41 FRO F10 FRO F11 FRO F12 FRO F13 FRO F14 FRO F15 FRO G10 FRO G11 FRO G12 FRO H10 FRO H11 FRO H12 FRO H13 FRO H14 FRO I10 FRO I11 FRO I12 FRO I20 FRO J10 FRO J11 FRO J12 FRO J13 FRO J14 FRO J15 FRO J20 FRO J21 FRO J22 FRO J23 FRO Z10 FRO </pre>
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FUNCTION STMP2(ARG,Y1,Y2,FERR)
DIMENSION F2T(20),FMT(20),F3T(20),F4T(20),F8T(20),
DXT(20),X1T(20),X2T(20),ART(20),EPST(20),EST2T(20),
EST3T(20),LEG(20),SUM1(20),SUM2(20)
C INITIAL SET-UP
A=Y1
EPS=FERR
B=Y2
DA=B-A
FA=ARG(A)
FM=4.*ARG((A+B)*.5)
FB=ARG(B)
AREA=1.0
EST=1.0
L=1
C BEGIN SIMPSON
1 DX=DA/3,
X1=A+DX
X2=X1+DX
F1=4.*ARG(A+.5*DX)
F2=ARG(X1)
F3=ARG(X2)
F4=4.*ARG(A+2.5*DX)
DX6=DX/6.
EST1=(F1+F2)*DX6
EST2=(F2+FM+F3)*DX6
EST3=(F3+F4+FB)*DX6
AREA=AREA+ABS(EST)+ABS(EST1)+ABS(EST2)+ABS(EST3)
SUM=EST1+EST2+EST3
C TEST FOR CONVERGENCE
IF(ABS(EST-SUM)*EPS*AREA)2,2,3
2 IF(EST=1.0)6,3,6
3 IF(L=20)5,6,6
5 L=L+1
LEG(L)=3
C STORE PARAMETERS FOR SIMPSON II AND III
F2T(L)=F2
FMT(L)=FM
F3T(L)=F3
F4T(L)=F4
F8T(L)=FB
DXT(L)=DX
X1T(L)=X1
X2T(L)=X2
ART(L)=AREA
EPST(L)=EPS/1.7
EST2T(L)=EST2
EST3T(L)=EST3
C RETURN TO SIMPSON I
DA=DX
FM=F1
FB=F2
EST=EST1
EPS=EPST(L)
GO TO 1
6 IF(LEG(L)=2)9,8,7
7 SUM1(L)=SUM
LEG(L)=2
C RETURN TO SIMPSON II
A=X1T(L)

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      DA=DXT(L)
      FA=F2T(L)
      FM=FM1(L)
      FB=F3T(L)
      AREA=ART(L)
      EST=ES2T(L)
      EPS=EPST(L)
      GO TO 1
A SUM2(L)=SUM
  LEG(L)=1
C RETURN TO SIMPSON III
  A=X2T(L)
  DA=DXT(L)
  FA=F3T(L)
  FM=F4T(L)
  FB=F5T(L)
  AREA=ART(L)
  EST=ES3T(L)
  EPS=EPST(L)
  GO TO 1
O SUM=SUM1(L)+SUM2(L)+SUM
  L=L+1
  IF(L=1)11,11,6
11 SIMPS2=SUM
  RETURN
  END
  FUNCTION SIMPS3(ARG,Y1,Y2,FERR)
  DIMENSION F2T(20),FM1(20),F3T(20),F4T(20),F5T(20),
1 DXT(20),X1T(20),X2T(20),ART(20),EPST(20),ES2T(20),
2 ES3T(20),LEG(20),SUM1(20),SUM2(20)
C INITIAL SET=UP
  A=Y1
  EPS=FERR
  B=Y2
  DA=B-A
  FA=ARG(A)
  FM=4.*ARG((A+B)*.5)
  FB=ARG(B)
  AREA=1.0
  EST=1.0
  L=1
C BEGIN SIMPSON
1 DX=DA/3,
  X1=A+DX
  X2=X1+DX
  F1=4.*ARG(A+.5*DX)
  F2=ARG(X1)
  F3=ARG(X2)
  F4=4.*ARG(A+2.5*DX)
  DX6=DX/6,
  EST1=(FA+F1+F2)*DX6
  EST2=(F2+FM+F3)*DX6
  EST3=(F3+F4+FB)*DX6
  AREA=AREA-ABS(EST)+ABS(EST1)+ABS(EST2)+ABS(EST3)
  SUM=EST1+EST2+EST3
C TEST FOR CONVERGENCE
  IF(ABS(EST-SUM)-EPS*AREA)2,2,3
2 IF(EST-1.0)6,3,6
3 IF(L=20)5,6,6
5 L=L+1

```

```

      LEG(L)=3
C     STORE PARAMETERS FOR SIMPSON II AND III
      F2T(L)=F2
      FMT(L)=FM
      F3T(L)=F3
      F4T(L)=F4
      FBT(L)=FB
      DXT(L)=DX
      X1T(L)=X1
      X2T(L)=X2
      ART(L)=AREA
      EPS1(L)=EPS/1.7
      ES2T(L)=EST2
      ES3T(L)=EST3
C     RETURN TO SIMPSON I
      DA=DX
      FM=F1
      FB=F2
      EST=EST1
      EPS=EPS1(L)
      GO TO 1
6     IF(LEG(L)-2)9,8,7
7     SUM1(L)=SUM
      LEG(L)=2
C     RETURN TO SIMPSON II
      A=X1T(L)
      DA=DXT(L)
      FA=F2T(L)
      FM=FMT(L)
      FB=F3T(L)
      AREA=ART(L)
      EST=ES2T(L)
      EPS=EPS1(L)
      GO TO 1
8     SUM2(L)=SUM
      LEG(L)=1
C     RETURN TO SIMPSON III
      A=X2T(L)
      DA=DXT(L)
      FA=F3T(L)
      FM=F4T(L)
      FB=FBT(L)
      AREA=ART(L)
      EST=ES3T(L)
      EPS=EPS1(L)
      GO TO 1
9     SUM=SUM1(L)+SUM2(L)+SUM
      L=L+1
      IF(L=1)11,11,6
11    SIMP33=SUM
      RETURN
      END

```

```

SPM. 6           1           1           1           1           1           1
3.5           2.0           30.0           1.0           1.0           10.0           0.5
5.0           0.000075
15.0          30.0
2.0
SEJ.

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```

PROGRAM KAL(INP,OUT,FILM,FSET10=INP,FSET9=OUT,FSET12=FILM)
EXTERNAL SIMPSN,FGAG,FGAL,FLAG,FLAL,FGAV,FLAV,PHAG,PHAL,PHAV,
1BKAG,BKAL,BKLAG,BKIAL,BKGAV,BKIALV,BKHAG,BKHAL,BKHAV
DIMENSION ATRUE(50), AOB(50,50),BKOBS(50,50),
IT(50),TP(50),BKTRUE(50)
DIMENSION CORR(50)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
1,ERF
C NTYPE DETERMINES SLIT AND LINE SHAPE PAIR USED
C NTYPE = 1 SLIT = GAUSS LINE = DOPPLER
C NTYPE = 2 SLIT = GAUSS LINE = LORENTZ
C NTYPE = 3 SLIT = CAUCHY LINE = DOPPLER
C NTYPE = 4 SLIT = CAUCHY LINE = LORENTZ
C NTYPE = 5 SLIT = GAUSS LINE = VOIGT
C NTYPE = 6 SLIT = CAUCHY LINE = VOIGT
C NTYPE = 7 SLIT = OTHER LINE = DOPPLER
C NTYPE = 8 SLIT = OTHER LINE = LORENTZ
C NTYPE = 9 SLIT = OTHER LINE = VOIGT
C BETA=RATIO OF SLIT TO LINE WIDTH
C BETAD=INCREMENT OF BETA
C BETAM=MAX. VALUE OF BETA
C C=PEAK ABSORPTION COEFFICIENT
C CD=INCREMENT OF C
C CM=MAX. VALUE OF C
C ALIM=LIMIT ON INTEGRALS
C ERROR=MEASURE OF ERROR IN NUMERICAL INTEGRATION
C RHO=RATIO IF LORENTZ TO DOPPLER WIDTH
C NP1=1 PLOT A(OBS) VS. K(OBS)/K(TRUE)
C NP2=1 PLOT C(OBS) VS. K(OBS)/K(TRUE)
C NINT=0 INTEGRATE VOIGT BY SIMPSN RULE
C NINT=1 USE FUNCTION FOR VOIGT
C NRHO=0 CALC. VOIGT AS FUNCTION OF BETA
C NRHO=1 CALC. VOIGT AS FUNCTION OF RHO
C CONSTANTS USED
B1=4.0*ALOG(2.0)
B2=2.0/3.1415926536
B3=80RT(B1/3.1415926536)
B4=80RT(B1)
B5=3.1415926536
B6=80RT(B5)
1 READ(10,500) NTYPE,NP1,NP2,NINT,NRHO
500 FORMAT(5I5)
WRITE(9,510)
510 FORMAT(1H1,32HINTEGRATE ABSORPTION COEFFICIENT,
131H VERSION 1, 8/15/78, R.ENGLEMAN)
READ(10,530)BETA,BETAD,BETAM,C,CD,CM
530 FORMAT(6(F10.5))
IF(NRHO.EQ.0)WRITE( 9,540)BETA,BETAD,BETAM,C,CD,CM
540 FORMAT(6H BETA=F10.5,2(6X,F10.5), 3H C=F10.5,2(6X,F10.5))
IF(NRHO.EQ.1)WRITE( 9,542)BETA,C,CD,CM
542 FORMAT(15H BETA CONSTANT=F10.5,3H C=F10.5,2(6X,F10.5))
GO TO (11,12,13,14,15,16,17,18,19),NTYPE
11 WRITE( 9,521)
521 FORMAT(25H SLIT=GAUSS LINE=DOPPLER)
GO TO 20
12 WRITE( 9,522)
522 FORMAT(25H SLIT=GAUSS LINE=LORENTZ)
GO TO 20
13 WRITE( 9,523)
523 FORMAT(26H SLIT=CAUCHY LINE=DOPPLER)

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      GO TO 20
14  WRITE( 9,524)
524  FORMAT(26H SLIT=CAUCHY  LINE=LORENTZ)
      GO TO 20
15  READ(10,530)RHO,RHOD,RHOM
      IF(NRHO.EQ.0)WRITE( 9,525)RHO
525  FORMAT(20H SLIT=GAUSS  LINE=VOIGT  RHO=F10.5)
      IF(NRHO.EQ.1)WRITE( 9,535)RHO,RHOD,RHOM
535  FORMAT(20H SLIT=GAUSS  LINE=VOIGT  RHO=F10.5,2(6X,F10.5))
      GO TO 20
16  READ(10,530)RHO,RHOD,RHOM
      IF(NRHO.EQ.0)WRITE( 9,526)RHO
526  FORMAT(30H SLIT=CAUCHY  LINE=VOIGT  RHO=F10.5)
      IF(NRHO.EQ.1)WRITE( 9,536)RHO,RHOD,RHOM
536  FORMAT(30H SLIT=CAUCHY  LINE=VOIGT  RHO=F10.5,2(6X,F10.5))
      GO TO 20
17  WRITE( 9,527)
527  FORMAT(25H SLIT=OTHER  LINE=DOPPLER)
      GO TO 20
18  WRITE( 9,528)
528  FORMAT(25H SLIT=OTHER  LINE=LORENTZ)
      GO TO 20
19  READ(10,530)RHO,RHOD,RHOM
      IF(NRHO.EQ.0)WRITE( 9,529)RHO
529  FORMAT(20H SLIT=OTHER  LINE=VOIGT  RHO=F10.5)
      IF(NRHO.EQ.1)WRITE( 9,539)RHO,RHOD,RHOM
539  FORMAT(20H SLIT=OTHER  LINE=VOIGT  RHO=F10.5,2(6X,F10.5))
20  READ(10,530)ALIN,ERR0S,ALIM,ERROR
      IF((NTYPE.EQ.5.OR,NTYPE.EQ.6.OR,NTYPE.EQ.9).AND,NINT.EQ.0)
      WRITE ( 9,700)
700  FORMAT(35H SYMPSON INTEGRATION USED FOR VOIGT)
      IF((NTYPE.EQ.5.OR,NTYPE.EQ.6.OR,NTYPE.EQ.9).AND,NINT.EQ.1)
      WRITE ( 9,701)
701  FORMAT(24H FUNCTION USED FOR VOIGT)
      WRITE( 9,560) ALIN,ALIM,ERR0S,ERROR
560  FORMAT(19H INTEGRATION LIMIT=.2F10.5,2X,
119H INTEGRATION ERROR=.2F10.5)
      ALIMP=ALIM
      ALINP=ALIN
      JM=1
      SB=BETA
      SR=RHO
      TM=1
C  CORRECTION TERMS FOR INTEGRATION OF K
900  GO TO (901,902,903,904,905,906,907,908,909),NTYPE
C 901  CORR(1)=1,-ERR  (SQRT(B1/(1.+BETA**2)))*ALIN)
901  CORR(1)=0,0
      GO TO 910
902  CORR(1)=0,0
      GO TO 910
903  CORR(1)=0,0
      GO TO 910
904  CORR(1)=1,0-B2*ATAN( ALIN/(1.+BETA))
      GO TO 910
905  CORR(1)=0,0
      GO TO 910
906  CORR(1)=0,0
      GO TO 910
907  CORR(1)=0,0
      GO TO 910

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908 CORR(I)=0.0
GO TO 910
909 CORR(I)=0.0
910 I=I+1
IF (NRHO.EQ.1) GO TO 920
BETA=BETA+RETAD
IF (BETA.LT.BETAM) GO TO 900
BETA=SB
GO TO 930
920 RHO=RHO+RHOD
IF (RHO.LT.RHOM) GO TO 900
RHO=SR
930 SC=C
70 ATRUE(J)=1.0-EXP(-C)
GO TO (71,72,71,72,71,71,71,72,71),NTYPE
71 BKTRUE(J)=C/B3
GO TO 75
72 BKTRUE(J)=C/B2
75 C=C*CD
J=J+1
IF (C.LT.CM) GO TO 70
C=SC
I=I
IF (NRHO.EQ.0) WRITE(9,580)
580 FORMAT(/,/,7H BETA,10X,1HC,11X,7HA(TRUE),8X,6HA(NBS),4X,
114HK(NBS)/K(TRUE),4X,7HK(TRUE),/)
IF (NRHO.EQ.1) WRITE(9,581)
581 FORMAT(/,/,7H RHO,10X,1HC,11X,7HA(TRUE),8X,6HA(NBS),4X,
114HK(NBS)/K(TRUE),4X,7HK(TRUE),/)
60 J=1
IF (NINT.EQ.0) GO TO 50
AL=RHOB4/2.0
U=1.0/(1.0+0.3275911*AL)
ERF=U*(0.254829592+U*(-0.284496736+U*
1(1.421413741+U*(-1.453152027+U*1.061405429))))
C FOR PEAK ABSORPTION Y=0.0
50 Y=0.0
GO TO (101,102,103,104,105,106,107,108,109),NTYPE
101 A0BS(I,J)=ERR (B4*ALIM)-2.*SIMP52(FGAG,0.0,ALIM,ERROR)*B3
BK0BS(I,J)=-B3*SIMP52(BKGAG,ALINP,ALIN,ERRORS)/C+CORR(I)
GO TO 100
102 A0BS(I,J)=ERR (B4*ALIM)-2.*SIMP52(FGAL,0.0,ALIM,ERROR)*B3
BK0BS(I,J)=-B2*SIMP52(BKGL,ALINP,ALIN,ERRORS)/C+CORR(I)
GO TO 100
103 A0BS(I,J)=B2*(ATAN(2.*ALIM)-2.*SIMP52(FLAG,0.0,ALIM,ERROR))
BK0BS(I,J)=-B3*SIMP52(BKLAG,ALINP,ALIN,ERRORS)/C+CORR(I)
GO TO 100
104 A0BS(I,J)=B2*(ATAN(2.*ALIM)-2.*SIMP52(FLAL,0.0,ALIM,ERROR))
BK0BS(I,J)=-B2*SIMP52(BKLAL,ALINP,ALIN,ERRORS)/C+CORR(I)
GO TO 100
105 A0BS(I,J)=ERR (B4*ALIM)-2.*SIMP52(FGAV,0.0,ALIM,ERROR)*B3
BK0BS(I,J)=-B3*SIMP52(BKGAV,ALINP,ALIN,ERRORS)/C+CORR(I)
GO TO 100
106 A0BS(I,J)=B2*(ATAN(2.*ALIM)-2.*SIMP52(FLAV,0.0,ALIM,ERROR))
BK0BS(I,J)=-B3*SIMP52(BKLAV,ALINP,ALIN,ERRORS)/C+CORR(I)
GO TO 100
C MUST ADD NTYPE EQ 7 8 9 IF OTHER SLITS USED
107 A0BS(I,J)=0.0
BK0BS(I,J)=0.0
GO TO 100

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```

100 A(OBS(I,J))=0.0
   B(OBS(I,J))=0.0
   GO TO 100
100 A(OBS(I,J))=0.0
   B(OBS(I,J))=0.0
100 IF (NRHO.EQ.0) WRITE( 9,590) BETA,C,ATRU(J),
   I(A(OBS(I,J)),B(OBS(I,J)),B(TRUE(J))
590 FORMAT (6(F10.5,4X))
   IF (NRHO.EQ.1) WRITE( 9,590) RHO ,C,ATRU(J),
   I(A(OBS(I,J)),B(OBS(I,J)),B(TRUE(J))
   C=C*CD
   J=J+1
   IF(C.LT.CM) GO TO 50
   C=SC
   I=I+1
   IF (NRHO.EQ.1) GO TO 194
   BETA=BETA+BETAD
   IF(BETA.LT.BETAM) GO TO 60
   BETA=SB
   GO TO 195
194 RHO=RHO+RHOD
   IF (RHO.LT.RHOM) GO TO 60
   RHO=SR
195 CONTINUE
C FOLLOWING CARDS CAN BE REMOVED IF NO 4020 PLOT USED *****
   IMAX=I-1
   JMAX=J-1
   IF (NP1+NP2.EQ.0) GO TO 1
   READ(10,530) CMAX,BKMIN
   IF (NP1.EQ.0) GO TO 420
C PLOT A(OBS) VS. K(OBS)/K(TRUE)
   CALL ADV (1)
   CALL LINCNT (59)
   WRITE (12,601)
401 FORMAT(26H A(OBS) VS. K(OBS)/K(TRUE))
   WRITE (12,511)
511 FORMAT(33H INTEGRATE ABSORPTION COEFFICIENT,
   131H VERSION 1, 5/12/66, R.ENGLEMAN)
   IF(NRHO.EQ.0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
   IF(NRHO.EQ.1)WRITE(12,542)BETA,C,CD,CM
   GO TO (301,302,303,304,305,306,307,308,309),NTYPE
301 WRITE(12,521)
   GO TO 300
302 WRITE(12,522)
   GO TO 300
303 WRITE(12,523)
   GO TO 300
304 WRITE(12,524)
   GO TO 300
305 IF(NRHO.EQ.0)WRITE(12,525)RHO
   IF(NRHO.EQ.1)WRITE(12,535)RHO,RHOD,RHOM
   GO TO 300
306 IF(NRHO.EQ.0)WRITE(12,526)RHO
   IF(NRHO.EQ.1)WRITE(12,536)RHO,RHOD,RHOM
   GO TO 300
307 WRITE(12,527)
   GO TO 300
308 WRITE(12,528)
   GO TO 300
309 IF(NRHO.EQ.0)WRITE(12,529)RHO

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      IF(NRHO,EO,1)WRITE(12,539)RHO,RHOD,RHOM
300 WRITE(12,560) ALIN,ALIM,ERROS,ERROR
      CALL DGA (120,980,50,910,BKMTN,1.0,1.0,0.0)
      CALL DINLN (20,20)
      CALL SBLIN (5,2)
      CALL SLLIN (5,2)
      DO 415 J=1,JMAX
      DO 416 J=1,JMAX
      TP(J)=BKOB8(I,J)
416 T(J)=AOBS(T,J)
415 CALL PLOT (JMAX,TP,1,T,1,44,1)
420 IF (NP2,EO,0) GO TO 1
C PLOT C(OBS) VS. K(OBS)/K(TRUE)
      CALL ADV (1)
      CALL LYNCHY (59)
      WRITE (12,602)
402 FORMAT(26H C(OBS) VS. K(OBS)/K(TRUE))
      WRITE (12,511)
      IF(NRHO,EO,0)WRITE(12,540)BETA,BETAD,BETAM,C,CD,CM
      IF(NRHO,EO,1)WRITE(12,542)BETA,C,CD,CM
      GO TO (321,322,323,324,325,326,327,328,329),NTYPE
321 WRITE(12,521)
      GO TO 320
322 WRITE(12,522)
      GO TO 320
323 WRITE(12,523)
      GO TO 320
324 WRITE(12,524)
      GO TO 320
325 IF(NRHO,EO,0)WRITE(12,525)RHO
      IF(NRHO,EO,1)WRITE(12,535)RHO,RHOD,RHOM
      GO TO 320
326 IF(NRHO,EO,0)WRITE(12,526)RHO
      IF(NRHO,EO,1)WRITE(12,536)RHO,RHOD,RHOM
      GO TO 320
327 WRITE(12,527)
      GO TO 320
328 WRITE(12,528)
      GO TO 320
329 IF(NRHO,EO,0)WRITE(12,529)RHO
      IF(NRHO,EO,1)WRITE(12,539)RHO,RHOD,RHOM
320 WRITE(12,560) ALIN,ALIM,ERROS,ERROR
      CALL DGA (120,980,50,910,BKMTN,1.0,CMAX,0.0)
      CALL DINLN (20,20)
      CALL SBLIN (5,2)
      CALL SLLIN (5,2)
      DO 425 J=1,JMAX
      DO 426 J=1,JMAX
      TP(J)=ALOG(1.-AOBS(I,J))
426 T(J)=BKOB8(I,J)
425 CALL PLOT (JMAX,T,1,TP ,1,44,1)
C ABOVE CARDS CAN BE REMOVED IF NO 4020 PLOT USED *****
      GO TO 1
      END
      FUNCTION BKGAG(W)
      COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
      EXTERNAL STPSM,FGAG
      Y=W
      BKGAG=ALOG(STPSM(FGAG,ALIMP,ALIM,ERROR)*B3+1,-ERR (B4*ALIM))
      RETURN

```

```

END
FUNCTION FGAG (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FGAG=EXP(-B1*V**2+C*EXP(-B1*(BETA*V+Y)**2))
RETURN
END
FUNCTION BKGAL (W)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FGAL
Y=W
BKGAL=ALOG(SIMPSM(FGAL,ALIMP,ALIM,ERROR)*B3+1,-ERR (B4*ALIM))
RETURN
END
FUNCTION FGAL (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FGAL=EXP(-B1*V**2+C/(1.0+4.0*(BETA*V+Y)**2))
RETURN
END
FUNCTION BKLAG(W)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FLAG
Y=W
BKLAG=ALOG(1.+B2*(SIMPSM(FLAG,ALIMP,ALIM,ERROR)-ATAN(2.*ALIM)))
RETURN
END
FUNCTION FLAG (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FLAG=EXP(-C*EXP(-B1*(BETA*V+Y)**2))/(1.0+4.0*V**2)
RETURN
END
FUNCTION BKLAG(W)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FLAL
Y=W
BKLAG=ALOG(1.+B2*(SIMPSM(FLAL,ALIMP,ALIM,ERROR)-ATAN(2.*ALIM)))
RETURN
END
FUNCTION FLAL (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FLAL=EXP(-C/(1.0+4.0*(BETA*V+Y)**2))/(1.0+4.0*V**2)
RETURN
END
FUNCTION BKGAV(W)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FGAV
Y=W
BKGAV=ALOG(SIMPSM(FGAV,ALIMP,ALIM,ERROR)*B3+1,-ERR (B4*ALIM))
RETURN
END
FUNCTION FGAV (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FSAV1,VOIGT
VV=BETA*V
IF (NINT.EQ.1) GO TO 2
FGAV=EXP(-C*B2*SIMPSP(FSAV1,ALIMP,ALIM,ERROR)-B1*V**2)
RETURN
2 FGAV=EXP(-C*VOIGT(VV)-B1*V**2)
RETURN
END
FUNCTION BKLAG(W)

```

```

COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FLAV
Y=W
BKLA V =ALOG(1.+B2*(SIMPSM(FLAV ,ALIMP,ALIM,ERROR)*ATAN(2.*ALIM)))
RETURN
END
FUNCTION FLAV (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSP,FSAV1,VOIGT
VV=BETA*V
IF (NINT.EQ.1) GO TO 2
FLAV=EXP(-C*B2*SIMPSP(FSAV1,ALIMP,ALIM,ERROR))/(1.0+4.0*V**2)
RETURN
2 FLAV=EXP(-C*VOIGT(VV))/(1.0+4.0*V**2)
RETURN
END
FUNCTION BKHAG(W)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FHAG
Y=W
BKHAG=0.0
RETURN
END
FUNCTION FHAG (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FHAG=0.0
RETURN
END
FUNCTION BKHAL(W)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FHAL
Y=W
BKHAL=0.0
RETURN
END
FUNCTION FHAL (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FHAL=0.0
RETURN
END
FUNCTION BKHAV(V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSM,FHAV
Y=W
BKHAV=0.0
RETURN
END
FUNCTION FHAV (V)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
EXTERNAL SIMPSP,FSAV1,VOIGT
VV=BETA*V
FHAV=0.0
RETURN
END
FUNCTION FSAV1(X)
COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
FSAV1=EXP(-B1*(Y+RHO*(X+VV)**2))/(1.0+4.0*X**2)
RETURN
END
FUNCTION VOIGT(X)

```

```

COMMON ALIMP,ALIM,ERROR,B1,B2,B3,B4,Y,C,BETA,RHO,VV,B5,B6,AL,NINT
1,ERF
EP=(X+Y)*B4
EL=(EP/AL)**2
IF (ABS(EP).GT. 7.0) GO TO 20
U=COS(2.0*AL*EP)
IF (ABS(EP).LT.1.0E-05) GO TO 7
VOJGT=(U*ERF+(1.-U)/(2.*AL*B5))*EXP(-EP**2)
AN=1.0
2 W=-AN**2/4.0-EP**2
Z=2.0*AL*(2.0*U*EXP(W)-EXP(AN*EP+W))
J=EXP(-AN*EP+W))/(B5*(AN**2+4.*AL**2))
VOJGT=VOJGT-Z
IF (ABS(Z/VOJGT).LT.1.0E-04) RETURN
AN=AN+1.0
IF (AN.GT.999.0) GO TO 5
GO TO 2
5 WRITE (9,102)
102 FORMAT (16H TOO MANY CYCLES)
RETURN
7 VJGT=ERF
RETURN
20 VJGT=(1.-(1.-3.*EL)/(2.*(1.+EL)**2*AL**2))/(B6*(1.+EL)*AL)
RETURN
END
FUNCTION SIMPS2(ARG,Y1,Y2,FERR)
DIMENSION F2T(20),FMT(20),F3T(20),F4T(20),FRT(20),
1DXT(20),X1T(20),X2T(20),ART(20),EPST(20),ES2T(20),
2ES3T(20),LEG(20),SUM1(20),SUM2(20)
C INITIAL SET-UP
A=Y1
EPS=FERR
B=Y2
DA=B-A
FA=ARG(A)
FM=4.*ARG((A+B)*.5)
FB=ARG(B)
AREA=1.0
EST=1.0
L=1
C BEGIN SIMPSON
1 DX=DA/3.
X1=A+DX
X2=X1+DX
F1=4.*ARG(A+.5*DX)
F2=ARG(X1)
F3=ARG(X2)
F4=4.*ARG(A+2.5*DX)
DX6=DX/6.
EST1=(FA+F1+F2)*DX6
EST2=(F2+FM+F3)*DX6
EST3=(F3+F4+FB)*DX6
AREA=AREA-ABS(EST1)+ABS(EST2)+ABS(EST3)
SUM=EST1+EST2+EST3
C TEST FOR CONVERGENCE
IF (ABS(EST-SUM)*EPS*AREA)2,2,3
2 IF (EST=1.0)6,3,6
3 IF (L=20)5,6,6
5 L=L+1
LEG(L)=3

```

```

C   STORE PARAMETERS FOR SIMPSON II AND III
      F2T(L)=F2
      FMT(L)=FM
      F3T(L)=F3
      F4T(L)=F4
      FBT(L)=FB
      DXT(L)=DX
      X1T(L)=X1
      X2T(L)=X2
      ART(L)=AREA
      EPST(L)=EPS/1.7
      ES2T(L)=EST2
      ES3T(L)=EST3
C   RETURN TO SIMPSON I
      DA=DX
      FM=F1
      FB=F2
      EST=EST1
      EPS=EPST(L)
      GO TO 1
6   IF(LEG(L)-2)9,8,7
7   SUM1(L)=SUM
      LEG(L)=2
C   RETURN TO SIMPSON II
      A=X1T(L)
      DA=DXT(L)
      FA=F2T(L)
      FM=FMT(L)
      FB=F3T(L)
      AREA=ART(L)
      EST=ES2T(L)
      EPS=EPST(L)
      GO TO 1
8   SUM2(L)=SUM
      LEG(L)=1
C   RETURN TO SIMPSON III
      A=X2T(L)
      DA=DXT(L)
      FA=F3T(L)
      FM=F4T(L)
      FB=FBT(L)
      AREA=ART(L)
      EST=ES3T(L)
      EPS=EPST(L)
      GO TO 1
9   SUM=SUM1(L)+SUM2(L)+SUM
      L=L+1
      IF(L-1)11,11,6
11  SIMPS2=SUM
      RETURN
      END
      FUNCTION SIMPSM(ARG,Y1,Y2,FERR)
      DIMENSION F2T(20),FMT(20),F3T(20),F4T(20),FBT(20),
      1DXT(20),X1T(20),X2T(20),ART(20),EPST(20),ES2T(20),
      2ES3T(20),LEG(20),SUM1(20),SUM2(20)
C   INITIAL SET-UP
      A=Y1
      EPS=FERR
      B=Y2
      DA=B-A

```



```

FA=ARG(A)
FM=4.*ARG((A+B)*.5)
FB=ARG(B)
AREA=1.0
EST=1.0
L=1
C BEGIN SIMPSON
1 DX=DA/3.
X1=A+DX
X2=X1+DX
F1=4.*ARG(A+.5*DX)
F2=ARG(X1)
F3=ARG(X2)
F4=4.*ARG(A+2.5*DX)
DX6=DX/6.
EST1=(FA+F1+F2)*DX6
EST2=(F2+FM+F3)*DX6
EST3=(F3+F4+FB)*DX6
AREA=AREA+ABS(EST)+ABS(EST1)+ABS(EST2)+ABS(EST3)
SUM=EST1+EST2+EST3
C TEST FOR CONVERGENCE
1F(ABS(EST-SUM)-EPS*AREA)2,2,3
2 1F(EST=1.0)6,3,6
3 1F(L=20)5,6,6
5 L=L+1
LEG(L)=3
C STORE PARAMETERS FOR SIMPSON II AND III
F2T(L)=F2
FMT(L)=FM
F3T(L)=F3
F4T(L)=F4
FBT(L)=FB
DXT(L)=DX
X1T(L)=X1
X2T(L)=X2
ART(L)=AREA
EPST(L)=EPS/1.7
ES2T(L)=EST2
ES3T(L)=EST3
C RETURN TO SIMPSON I
DA=DX
FM=F1
FB=F2
EST=EST1
EPS=EPST(L)
GO TO 1
6 1F(LEG(L)=2)9,8,7
7 SUM1(L)=SUM
LEG(L)=2
C RETURN TO SIMPSON II
A=X1T(L)
DA=DXT(L)
FA=F2T(L)
FM=FMT(L)
FB=FBT(L)
AREA=ART(L)
EST=ES2T(L)
EPS=EPST(L)
GO TO 1
8 SUM2(L)=SUM

```

```

      LEG(L)=1
C     RETURN TO SIMPSON III
      A=X2T(L)
      DA=DXT(L)
      FA=F3T(L)
      FM=F4T(L)
      FB=FBT(L)
      AREA=ART(L)
      EST=ES3T(L)
      EPS=EPST(L)
      GO TO 1
9     SUM=SUM1(L)+SUM2(L)+SUM
      L=L-1
      IF(L-1)11,11,6
11    SIMPSH=SUM
      RETURN
      END
      FUNCTION SIMPSP(ARG,Y1,Y2,FERR)
      DIMENSION F2T(20),FMT(20),F3T(20),F4T(20),FBT(20),
1DXT(20),X1T(20),X2T(20),ART(20),EPST(20),ES2T(20),
2ES3T(20),LEG(20),SUM1(20),SUM2(20)
C     INITIAL SET-UP
      A=Y1
      EPS=FERR
      B=Y2
      DA=B-A
      FA=ARG(A)
      FM=4.*ARG((A+B)*.5)
      FB=ARG(B)
      AREA=1.0
      EST=1.0
      L=1
C     BEGIN SIMPSON
1     DX=DA/3.
      X1=A+DX
      X2=X1+DX
      F1=4.*ARG(A+.5*DX)
      F2=ARG(X1)
      F3=ARG(X2)
      F4=4.*ARG(A+2.5*DX)
      DX6=DX/6.
      EST1=(FA+F1+F2)*DX6
      EST2=(F2+FM+F3)*DX6
      EST3=(F3+F4+FB)*DX6
      AREA=AREA-ABS(EST)+ABS(EST1)+ABS(EST2)+ABS(EST3)
      SUM=EST1+EST2+EST3
C     TEST FOR CONVERGENCE
      IF(ABS(EST-SUM)-EPS*AREA)2,2,3
2     IF(EST=1.0)6,3,6
3     IF(L=20)5,6,6
5     L=L+1
      LEG(L)=3
C     STORE PARAMETERS FOR SIMPSON II AND III
      F2T(L)=F2
      FMT(L)=FM
      F3T(L)=F3
      F4T(L)=F4
      FBT(L)=FB
      DXT(L)=DX
      X1T(L)=X1

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```

      X2T(L)=X2
      ART(L)=AREA
      FPST(L)=EPS/1.7
      ES2T(L)=EST2
      ES3T(L)=EST3
C     RETURN TO SIMPSON I
      DA=DX
      FM=F1
      FB=F2
      EST=EST1
      EPS=FPST(L)
      GO TO 1
6     IF(LEG(L)-2)9,8,7
7     SUM1(L)=SUM
      LEG(L)=2
C     RETURN TO SIMPSON II
      A=X1T(L)
      DA=DXT(L)
      FA=F2T(L)
      FM=FMT(L)
      FB=FS1T(L)
      AREA=ART(L)
      EST=ES2T(L)
      EPS=EPST(L)
      GO TO 1
8     SUM2(L)=SUM
      LEG(L)=1
C     RETURN TO SIMPSON III
      A=X2T(L)
      DA=DXT(L)
      FA=FS1T(L)
      FM=FS4T(L)
      FB=FS1T(L)
      AREA=ART(L)
      EST=ES3T(L)
      EPS=EPST(L)
      GO TO 1
9     SUM=SUM1(L)+SUM2(L)+SUM
      L=L+1
      IF(L-1)11,11,6
11    SIMPSP=SUM
      RETURN
      END
C     ERROR FUNCTION APPROXIMATION (ACCURATE WITHIN .00000015)
      FUNCTION ERR (X)
1     IF(X.NE.0.0) GO TO 4
2     ERR = 0.0
3     RETURN
4     E = 1.0/(1.0 + .3275911*X)
5     S = (((((.940646070*E)-1.287822453)*E+1.259695130)*E+.252128668)*E
1     +.225036806)*E
6     S = S * EXP (-X**2 )*(1.1283791679551)
7     ERR = 1.0 * S
8     RETURN
9     END
SFH,
3
0.25      0.5      2.0      0.5      2.0      10.0
10.0      0.001     10.0      0.001
5.0       0.0
SEI,

```