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AN INVESTIGATION OF A MATHEMATICAL MODEL FOR ATMOSPHERIC ABSORPTION SPECTRA

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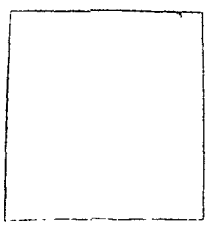

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ABSTRACT

A computer program that calculates absorption spectra for slant paths through the atmosphere is described. The program uses an efficient convolution technique (Romberg integration) to simulate instrument resolution effects. A brief information analysis is performed on a set of calculated spectra to illustrate how such techniques may be used to explore the quality of the information in a spectrum.

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I. INTRODUCTION

Radiation which has passed through and been modified by the atmosphere contains a wealth of information about atmospheric conditions. This includes information about the temperature and density structure of the atmosphere as well as the abundance and distribution of constituent gases and aerosols. In order to retrieve this information, however, an accurate model is needed which describes the dependence of absorption spectra on the atmospheric conditions and on the instrument characteristics. The first dependence has received considerable attention, both theoretical and computational, but the second has received much less. Equivalent width techniques and transmittance averaging are common ways of extracting information from spectra when instrument effects are unknown or poorly understood. However, because these effects mask underlying atmospheric effects, knowledge of the instrument behavior, when properly included in the data analysis, allows extraction of more detailed information than can be obtained in the absence of such knowledge.

Nonlinear least-squares[1] is one data analysis technique which can include all relevant influences on the data. It involves a great deal of computation, however, so efficient computer codes must be developed in order to take advantage of the least-squares techniques. This report describes a program for calculating absorption spectra that was specifically written to efficiently include instrument effects. It is therefore suitable for use in least-squares analysis.

In constructing a model for any experiment it is important to know what type of information the experimental data are likely to contain. Such knowledge allows the level of sophistication for the model to be balanced between computational complexity and interpretative accuracy. The third chapter of this report addresses this question and illustrates a variety of simple techniques for information analysis with a set of atmospheric absorption spectra.

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II. FUNDAMENTALS OF ATMOSPHERIC TRANSMITTANCE

A beam of radiation propagating through the atmosphere is modified through the action of many different processes. Among these are scattering, reflection, refraction, polarization changes, atmospheric emission, and absorption. This report is only concerned with the modifications due to refraction and absorption by gas molecules in the atmosphere, and, in particular, that portion of the absorption due to rotational and vibrational transitions of the molecules. Each transition has associated with it a frequency position, width, intensity and profile. The Voigt profile[2,3,23] is assumed throughout this report, although other shapes can be incorporated if desired.

A. HOMOGENEOUS PATHS

If radiation with a spectral irradiance $E(\nu)$ is incident on a homogeneous gas sample, the spectral radiant exitance $M(\nu)$ is given by[4]

$$M(\nu) = E(\nu) \cdot \tau(\nu) , \tag{1}$$

where ν is the frequency of the radiation measured in cm^{-1}. The modifying factor, $\tau(\nu)$, in Eq. (1) is called the spectral transmittance, which is referred to simply as transmittance in this report, it being understood that the transmittance is a function of frequency.

For a narrow homogeneous sample of thickness $d\ell$, Bouguer's law[5] states that the radiation lost in the sample is linear in $E(\nu)$ and $d\ell$. Beer's law[6] states that the radiation lost is also linear in the concentration N of the absorber, so that

$$dE(\nu,\ell) = -k(\nu)\ E(\nu,\ell)\ N d\ell , \tag{2}$$

where $k(\nu)$ is called the absorption coefficient. When N is measured in molecules/cm^3 and $d\ell$ in cm, $k(\nu)$ is measured in cm^2/molecule. When N is independent of path length, Eq. (2) can be integrated over the entire path length, L, through the sample to give

$$M(\nu) = E(\nu,L) = E(\nu,0)\ \exp[-k(\nu)\ NL] . \tag{3}$$

Consequently, the transmittance is given by

$$\tau(\nu) = \exp[-k(\nu)\ NL] . \tag{4}$$

Equation (2) is based on independent absorption by each absorbing molecule. It does not apply to self-broadening absorption, therefore, in which k can also depend on N. The factor in the exponential of Eq. (4) is called the absorbance.

If there are M different absorbers with concentrations N_1, N_2, ..., N_M independently absorbing in the sample, the total absorbance $A(\nu)$ is

$$A(\nu) = \sum_{m=1}^{M} N_m k_m(\nu)\, L \ , \qquad (5)$$

where $k_m(\nu)$ is the absorption coefficient for the mth absorber. As stated above, this report assumes that the absorption is due to many individual absorption lines, each with absorption coefficient $k_{mj}(\nu)$. Consequently Eq. (5) becomes

$$A(\nu) = L \cdot \sum_{m=1}^{M} N_m \cdot \sum_{j=1}^{J_m} k_{mj}(\nu) \ , \qquad (5b)$$

where J_m is the total number of lines for the mth absorber.

B. ATMOSPHERIC PATHS

Radiation paths in the atmosphere are usually not homogeneous. For such paths, Eq. (2) can still be integrated to give E as a function of path length, provided the variation of k and N with path length is known. The analog of Eq. (5) for atmospheric paths is

$$A(\nu) = \int_0^L \sum_{m=1}^{M} N_m(\ell) \sum_{j=1}^{J_m} k_{mj}(\nu,\ell)\, d\ell \ . \qquad (6)$$

It is convenient to define the mixing ratio $a_m(\ell)$ for the mth absorber as

$$a_m(\ell) = N_m(\ell)/\bar{N}(\ell) \ ,$$

where $\bar{N}(\ell)$ is the mean density of the atmosphere as a function of path length.

Defining a new variable $u(\ell)$, the so-called airmass along the path, by

$$du \equiv \bar{N}(\ell)\, d\ell \ ,$$

Eq. (6) becomes

$$A(\nu) = \int_0^U \sum_{m=1}^{M} a_m(u) \sum_{j=1}^{J_m} k_{mj}(\nu,u)\, du \ , \qquad (7)$$

where

$$U \equiv \int_0^L \bar{N}(\ell)\, d\ell$$

is the total airmass of the path.

C. REFRACTION EFFECTS

This report uses a program written by Treve[7,8] and Snider[9] to determine the path of radiation through the atmosphere. The necessary geometry is shown in Fig. 1, assuming that the sun is the radiation source. The observer is at a height H_{ob} above the surface of the earth at latitude ϕ. The direction of propagation of the radiation makes an angle θ' with the observer's local zenith. A straight line drawn from the observer to the source makes an angle θ with the local zenith and has a minimum height H'_{min} above the surface of the earth. Because of refraction, the true radiation path is not straight and has a different minimum height H_{min}. The actual path taken by the radiation depends on the density profile of the atmosphere as a function of height. This profile is calculated by the program from an imput temperature profile and base level pressure by integrating the hydrostatic equation and assuming an ideal gas law for the relationship between pressure, temperature, and density.[10] The input profile is in the form of many thin atmospheric layers. The program uses Snell's law and the Lorentz-Lorenz relation to perform a ray-tracing through the layers. The output consists of a series of airmass values, effective temperatures, and pressures, one for each layer crossed by the ray.

In order to use these to calculate the spectrum, the integral in Eq. (7) is approximated by a sum according to

$$A(\nu) = \int_0^U \sum_{m=1}^{M} a_m(u) \sum_{j=1}^{J_m} k_{mj}(\nu,u)\, du$$

$$\simeq \sum_{i=1}^{I_L} \sum_{m=1}^{M} \sum_{j=1}^{J_m} \left[\overline{a_m k_{mj}(\nu)}\right]_i \Delta u_i \ , \qquad (8)$$

where I_L is the number of terms in the sum which replaces the integral in Eq. (7).

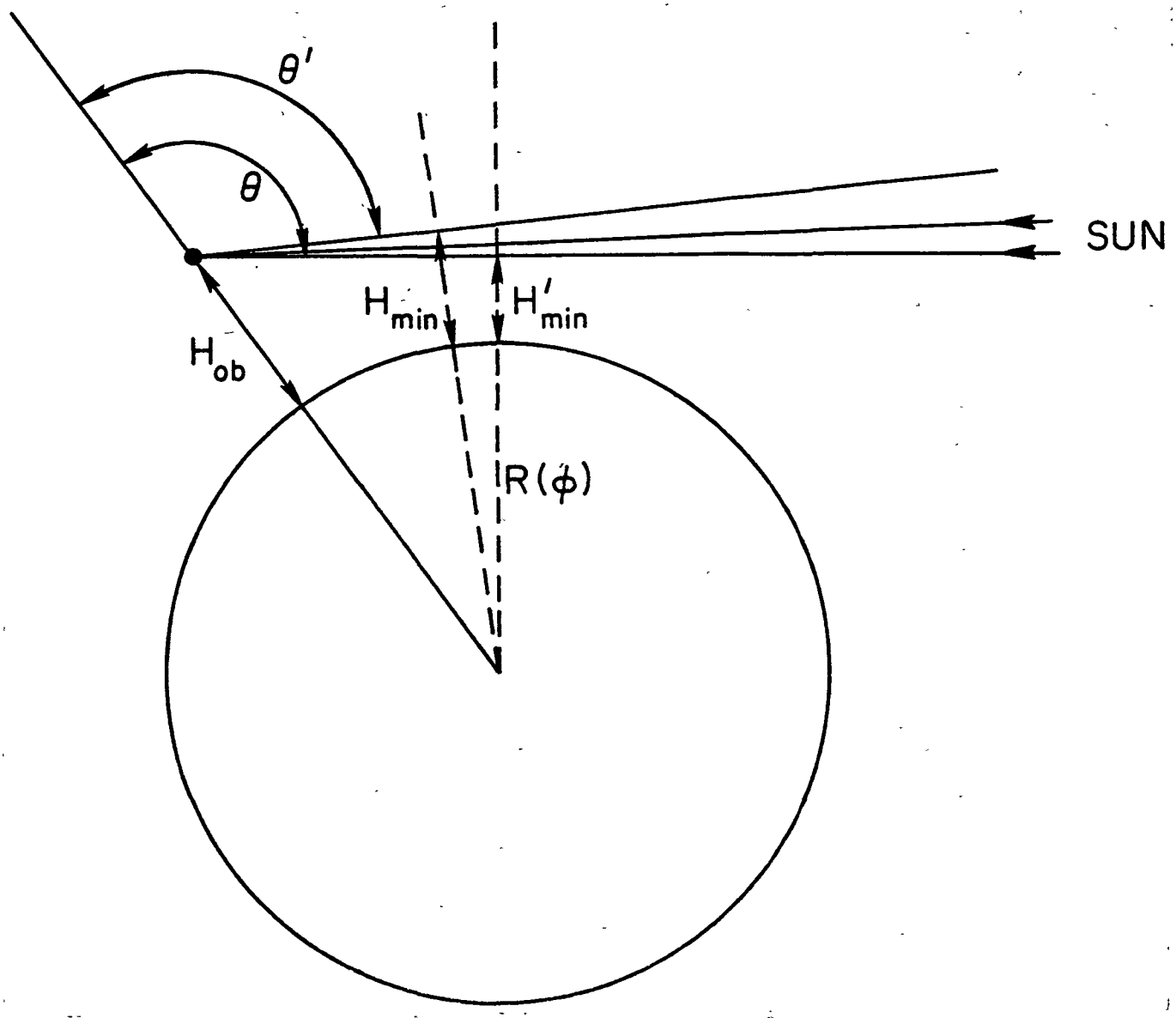
The form of $\left[\overline{a_m k_{mj}(\nu)}\right]_i$ is determined by assuming that the product $a_m(u)\, k_{mj}(\nu,u)$ for fixed ν can be written as a function of the pressure $P(u)$ and temperature $T(u)$ along the path. We therefore write

$$\int a_m(u)\, k_{mj}(\nu,u)\, du = \int f[P(u),T(u)]\, du \ .$$

Expanding f in a Taylor series about some value, P_o, T_o,

$$f(P,T) = f(P_o,T_o) + \left.\frac{\partial f}{\partial P}\right|_{P_o,T_o} (P - P_o) + \left.\frac{\partial f}{\partial T}\right|_{P_o,T_o} (T - T_o) + \{\text{second-order terms}\} \ .$$

Substituting this expression into the integral



θ = "true" or astronomical zenith angle
θ' = apparent zenith angle
H_{ob} = observer height
H'_{min} = unrefracted minimum height
H_{min} = true minimum height
$R(\phi)$ = radius of earth at latitude ϕ

Fig. 1 - Observer-source geometry

$$\int f[P(u),T(u)]\,du = f(P_o,T_o)\int du + \left.\frac{\partial f}{\partial P}\right|_{P_o,T_o}\int (P - P_o)\,du + \left.\frac{\partial f}{\partial T}\right|_{P_o,T_o}\int [T(u) - T_o]\,du$$

$$+ \{\text{second-order terms}\}$$

$$= \left[f(P_o,T_o) + \left.\frac{\partial f}{\partial P}\right|_{P_o,T_o}(\bar{P} - P_o) + \left.\frac{\partial f}{\partial T}\right|_{P_o,T_o}(\bar{T} - T_o)\right.$$

$$\left. + \{\text{second-order terms}\}\right]\int du\ ,$$

where

$$\bar{P} \equiv \int P(u)\,du/\int du$$

and (9)

$$\bar{T} \equiv \int T(u)\,du/\int du\ .$$

But the expression in the brackets, to first-order, is just $f(\bar{P},\bar{T})$. Consequently, provided the variation of $P(u)$ and $T(u)$ is sufficiently small that the first-order terms in the Taylor series are adequate, we may write

$$\int f[P(u),T(u)]\,du \simeq f(\bar{P},\bar{T})\,\Delta u\ , \tag{10}$$

where $\bar{T}$ and $\bar{P}$ are defined as in Eq. (9).

If the atmospheric layers are sufficiently thin, we are therefore justified in replacing the integral in Eq. (7) with the sum in Eq. (8) provided

$$\left[\overline{a_m k_{mj}(\nu)}\right]_i = a_m(\bar{P}_i,\bar{T}_i)\,k_{mj}(\bar{P}_i,\bar{T}_i,\nu)\ , \tag{11}$$

where

$$\bar{P}_i \equiv \int_{\text{layer } i} P(u)\,du/\Delta u_i$$

and (12)

$$\bar{T}_i \equiv \int_{\text{layer } i} T(u)\,du/\Delta u_i\ .$$

Equations (11) and (12) are close to the familiar scaling approximations.[11] The same argument applies to any other variables that effect the $a \cdot k$ product (such as mixing ratio dependence in k). One can therefore approximate the inhomogeneous atmosphere with a series of homogeneous layers whose properties are given by averages over the true inhomogeneous variation.

D. LINE SHAPE

As stated above, this report assumes that the absorption coefficient $k_{mj}(\nu)$ follows the Voigt profile. This profile combines the effects of collision broadening (which is dominant in the troposphere) and Doppler broadening (which is dominant in the upper stratosphere). It is given by

$$k_{mj}(\nu,P,T) = k_{Ojm} \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)\, dt}{y^2 + (x - t)^2} , \tag{13}$$

where

$$k_{Omj} = \frac{S_{jm}}{\alpha_D} \sqrt{\ell n 2/\pi} ,$$

$$y = \frac{\alpha_L}{\alpha_D} \sqrt{\ell n 2} , \text{ and}$$

$$x = \frac{\nu - \nu_{Ojm}}{\alpha_D} \sqrt{\ell n 2} .$$

The line intensity S_{jm} is defined as $S_{jm} = \int_0^{\infty} k_{jm}(\nu)\, d\nu$.

From Quantum Mechanics[12] this quantity is given by

$$S_{jm} = \frac{8\pi^3 \nu_{Ojm}}{3hc} \frac{g''\left(1 - e^{-hc\nu_{Ojm}/kT}\right)}{Q_m(T)} \exp[(-E''_{mj})/kT] \cdot$$
$$\cdot \left| \langle \psi''_{jm} | \bar{\mu} | \psi'_{jm} \rangle \right|^2 . \tag{14}$$

In this expression, ν_{Ojm} is the line center frequency for the mjth line with lower state energy E''_{mj} and upperstate energy $E'_{mj} = hc\nu_{Omj} + E''_{mj}$. g'' is the degeneracy of the lower state and $Q_m(T)$ is the partition function. In the infrared, the expression $\frac{1 - \exp(-hc\nu_{Ojm}/kT)}{Q_m(T)}$ can usually be approximated by $1/Q_{rot}(T)$ where $Q_{rot}(T)$, the rotational partition function, is proportional[13] to T for linear molecules such as CO, N_2O, CO_2, and NO. It is proportional to $T^{3/2}$ for molecules like O_3, H_2O, and CH_4. The term $\left| \langle \psi''_{jm} | \bar{\mu} | \psi'_{jm} \rangle \right|^2$ is the square of the dipole matrix element.

The temperature dependence of S_{jm} is made explicit by writing it as

$$S_{jm} = S_{Ojm} \left(\frac{T_O}{T}\right)^{\beta} \exp[-E''_{mj}(T_O - T)/0.6946TT_O] \ , \qquad (15)$$

where $\beta = 1$ or $3/2$ depending on the molecular structure. The above expression assumes that E is measured in cm^{-1} and T in Kelvin. S_{Ojm} is the value of S_{jm} at some standard temperature, T_O.

The quantities α_L and α_D in Eq. (13) are the Lorentz width and Doppler width of the line, respectively. These are given by

$$\alpha_D = \frac{\nu_{Omj}}{\epsilon} \sqrt{\frac{2kT\ \ell n^2}{M_m}}$$

and (16)

$$\alpha_L = \alpha_{Omj} \left(\frac{T_O}{T}\right)^{\gamma} \frac{P_O}{P} \ .$$

M_m is the mass of molecular species m; α_{Omj} is the Lorentz width at some standard temperature and pressure, T_O and P_O; and γ is an empirical term describing the temperature dependence of α_L. This report makes the standard assumption that $\gamma = 1/2$ although other values are often more accurate for bands of specific molecules. The necessary line parameters were taken from the AFGL line listing.[14]

E. INSTRUMENT EFFECTS

When Eq. (13) and (8) are combined, they constitute a mathematical model for the frequency make-up of a beam of radiation as it propagates through the atmosphere. Since real spectrometers have finite resolution, the signal observed at frequency setting ν is a weighted sum of the radiation incident on the instrument. This is described by writing

$$\tau_{con}(\nu) = \int_0^{\infty} \sigma(\nu,\nu')\ \tau_{mon}(\nu')\ d\nu' \ , \qquad (17)$$

where $\tau_{con}(\nu)$ is the observed transmittance, $\tau_{mon}(\nu')$ is the monochromatic transmittance, and $\sigma(\nu,\nu')$ is the instrument spectral response function (or "slit" function) with

$$\int_0^{\infty} \sigma(\nu,\nu')\ d\nu' = 1 \ .$$

It is often assumed that σ can be written as a function of $(\nu - \nu')$, and many different forms are used. For grating instruments, triangular and Gaussian shapes are common,[15] and for interferometers sinc, $sinc^2$, and various Bessel functions have been tried,[16] depending upon the apodization.

When calculated and observed spectra are to be compared visually, the exact form of σ is often unimportant. However, when more sensitive

techniques, such as least-squares analysis, are used, instrument effects must be modeled with a precision at least better than the precision of the observed spectral values. This imposes an additional set of computational restrictions on spectrum calculation routines, especially when the convolution integral in Eq. (17) must be evaluated numerically, as is usually the case. While considerable effort has gone into devising efficient algorithms for calculating monochromatic transmittances, little work seems to have been done on the special problems associated with calculating convolved transmittances.

Since one of the problems this report seeks to address is the applicability of least-squares data analysis to atmospheric transmission spectra, the precision of convolved transmittances has been a central concern from the start. To see how this concern dictates the overall calculation strategy, consider how Eq. (17) is evaluated in practice. Because of the complex frequency dependence of $\tau(\nu')$, the integral must be evaluated numerically; i.e., replaced by a weighted sum. Each term in the sum requires a value of τ_{mon} and one of σ. If N_c is the number of terms in the sum and N_s is the number of observed spectral values, then $N_c \cdot N_s$ monochromatic transmittance values are needed to calculate the convolved transmittance, τ_{con}.

A typical frequency position may have contributions from 20 different lines and require 20 atmospheric layers to model the atmosphere (Mankin[17] used ~1000 lines over a 10 cm^{-1} region; Snider and Goldman[10] used 197 layers). In addition, if the resolution is $\delta\nu_R$ a typical frequency spacing for observed spectra is $\delta\nu_R/2$. Consequently for a 200 cm^{-1}-long spectrum at moderate resolution, $\delta\nu_R = 0.10$ cm^{-1} (some interferometers have 10 times better resolution), a total of 4000 observed points must be calculated. Assuming that the most time-consuming part of the calculation is the evaluation of the Voigt profile, a total of $N_c \times 20 \times 20 \times 4000 = 1.6 \times 10^6 N_c$ Voigt evaluations must be performed. Running time is dependent on machine characteristics, but Pierluissi and Vanderwood[18] quote a time of ~3 seconds for 100 evaluations on an IBM 360/65. This gives $4.8 \times 10^4 \cdot N_c$ seconds of CPU time in the Voigt routine alone. Clearly N_c must be made as small as possible.

1. Convolution Strategies

The numerical evaluation of the integral in Eq. (17) is represented schematically in Fig. 2. To each observed frequency position ν_i there corresponds a set of frequency positions $\{\nu'\}_i$ at which monochromatic transmittances must be calculated. Clearly the number of points ν' can be reduced by making some of the $\{\nu'\}_{i+1}$ points overlap some of the $\{\nu'\}_i$ points. However, because the number of $\{\nu'\}_i$ values needed for a given level of accuracy ϵ in $\tau_{con}(\nu_i)$ depends upon the form of the monochromatic transmittance, the density of $\{\nu'\}_i$ points will be a function of ν_i for a given ϵ. The exact density depends on the numerical integration rule employed, but usually this takes the form of bounds on the magnitude of high-order derivatives of τ_{mon} over the convolution frequency range. The use of an iterative quadrature routine can often eliminate the need for

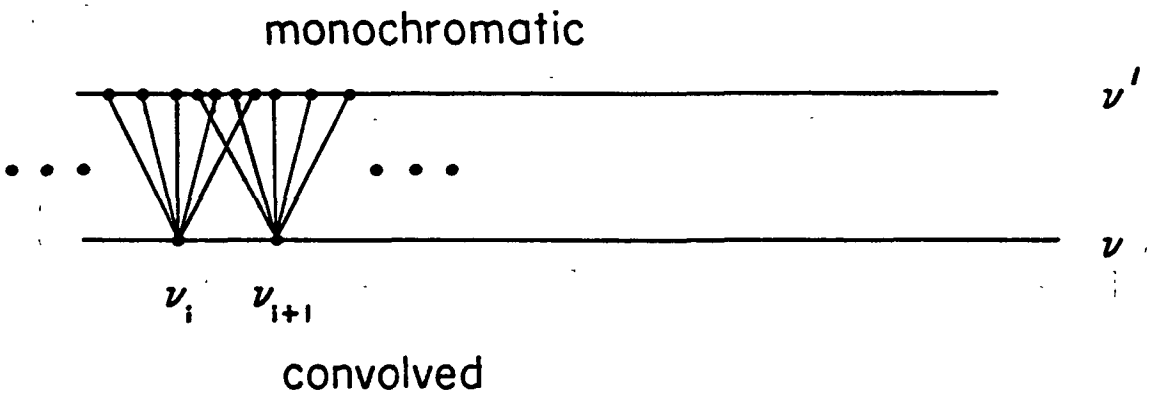


Fig. 2 - Schematic representation of Eq. (17)

evaluating these derivatives. Also, if the $\tau_{con}(\nu_i)$ values are calculated in order of increasing [or decreasing] frequency position, values of τ_{mon} at frequencies lower [higher] than the ith range of ν' values need not be saved. This reduces storage requirements.

Of the many available iterative routines, an equally spaced abscissa Romberg integration algorithm was selected. Gaussian rules require fewer $\{\nu'\}$ points for a given ϵ, but are not well adapted to iterative evaluation. Neither are they well suited for overlapping $\{\nu'\}$ positions for successive ν_i values. Adaptive Simpson's rule techniques are good at varying the ν'-density to meet the accuracy requirements and could be written so as to use overlapping $\{\nu'\}$ positions. Unfortunately they are much more complicated than Romberg schemes, which proved to be complicated enough. Better programmers than the author of this report may wish to use them, however.

2. Romberg Integration

To use classical Romberg integration to evaluate the integral

$$I \equiv \int_a^b f(X)dx$$

the interval [a, b] is divided into 2^{k_o} equal pieces. The function f is evaluated at each of the $2^{k_o} + 1$ points,

$$x_i = a + (i - 1)(b - a)/2^{k_o} \qquad i = 1, \ldots, 2^{k_o} + 1 ,$$

and the sum,

$$T_o^{(k_o)} = \frac{(b - a)}{2^{k_o}} \left[1/2\, f(x_1 = a) + f(x_2) + \ldots \right.$$

$$\left. + f(x_{2^{k_o}}) + 1/2\, f(x_{2^{k_o}+1} = b)\right] , \qquad (18)$$

forms the first element of a table of approximations to I called the Romberg T-table. Equation (18) is easily recognized as the trapezoidal rule. Next, k_o is replaced by $k_1 = k_o + 1$ and $T_o^{(k_1)}$ is calculated from Eq. (18) with k_o replaced by k_1. This value forms a second estimate for I and is written next to $T_o^{(k_o)}$ in the top-most row of the table, as shown in Fig. 3. From these two estimates a third estimate, $T_1^{(k_o)}$, is formed according to

$$T_m^{(k)} = \frac{4^m T_{m-1}^{(k+1)} - T_{m-1}^{(k)}}{4^m - 1} . \qquad (19)$$

$$
\begin{array}{llll}
T_0^{(k_0)} & T_0^{(k_1)} & T_0^{(k_2)} & \cdots \\
 & T_1^{(k_0)} & T_1^{(k_1)} & \cdots \\
 & & T_2^{(k_0)} & \cdots \\
 & & \vdots & \\
 & & \ddots &
\end{array}
$$

Fig. 3 - The Romberg T-table

The values of $T_0^{(k_0)}$ and $T_1^{(k_0)}$ are then compared, and if

$$\left|T_1^{(k_0)} - T_0^{(k_0)}\right| < \epsilon \ , \tag{20}$$

the process stops and outputs $T_1^{(k_0)}$ as the final approximation to I. If the convergence criterion in Eq. (20) is not satisfied, the table construction continues with $T_0^{(k_2)}$, $T_0^{(k_3)}$ and so on until two successive elements along the diagonal of the table do satisfy the convergence criterion.

Davis and Rabinowitz[19] discuss a modification of the classical Romberg scheme which requires calculation of a second table, the Romberg M-table. In this scheme, after $T_0^{(k_0)}$ is calculated, the quantity

$$M_0^{(k_0)} = \frac{b - a}{2^{k_0}} \sum_{j=1}^{2^{k_0}} f\left[a + \left(j - \frac{1}{2}\right)(b - a)/2^{k_0}\right] \tag{21}$$

is calculated. Equation (21) is easily recognized as the midpoint rule. The values of $T_0^{(k_0)}$ and $M_0^{(k_0)}$ are then compared and if

$$\left|M_0^{(k_0)} - T_0^{(k_0)}\right| < \epsilon \ , \tag{22}$$

the process stops and outputs

$$T_0^{(k_1)} = \frac{1}{2}\left(T_0^{(k_0)} + M_0^{(k_0)}\right) \tag{23}$$

as the final approximation to I. If the new convergence criterion [Eq. (22)] is not met, the next diagonal element of the T-table is calculated from

$$T_m^{(k)} = M_{m-1}^{(k)} + \frac{\left(2 \cdot 4^{m-1} - 1\right)\left(T_{m-1}^{(k)} - M_{m-1}^{(k)}\right)}{4^m - 1} \ . \tag{24}$$

The next element of the M-table, $M_0^{(k_1)}$, is calculated from Eq. (21) with k_0 replaced by $k_1 = k_0 + 1$. The two M values are then combined as in Eq. (19) to form $M_1^{(k_0)}$. The convergence criterion is then applied to $M_1^{(k_0)}$ and $T_1^{(k_0)}$. If the criterion is satisfied, these two are combined as in Eq. (23) and output. Otherwise the process continues halving the interval [a,b] and recursively generating the T- and M-tables until two corresponding diagonal elements satisfy the convergence criterion.

Those referring to Davis and Rabinowitz[19] should note that Eq. (6.3.9) in their book is incorrect in some editions, as can be verified from their

Eq. (6.3.8) and the equation below (6.3.2). Also, the FORTRAN version of this technique, incorporated into the program in Appendix A, has a maximum number of interval halvings in the search for convergence. When this limit is exceeded, the output is taken from Eq. (24) rather than Eq. (23).

Incorporating the Romberg Table evaluation in the spectrum calculation routine required less than 15 FORTRAN statements. The logic needed to save τ_{mon} values required nearly 10 times as many statements. The details are given in Appendix A.

F. VERIFYING CALCULATION BEHAVIOR

The program which evaluates Eq. (17), described in Appendix A, is composed of three basic parts: (1) evaluation of the atmospheric path (subroutine SNIDER), (2) setting up approximate layer parameters (subroutine PATHST), and (3) spectrum calculation (subroutine NSPEC). These were first checked individually and then as a whole.

A specific observer-source geometry was selected. This had an observer at 45° N latitude, 45 km height, and an observed zenith angle (θ' in Fig. 1) of 95.2°. The source was assumed to be above the atmosphere. Unfortunately, the atmospheric model used by Snider and Goldman[10] could not be obtained so the January reference atmosphere of Cole and Kantor[20] was used instead. The program's analysis of the path is shown in Table 1 along with the associated results taken from Ref. (10). Also shown are the results using a 190-layer atmosphere taken from the U.S. Standard Atmosphere, 1976.[21] The agreement shown in the table and the proper behavior of the subroutine to changes in zenith angle, observer height, and ground-level pressure indicated that the subroutine was functioning properly.

The output for the 190-layer model included 198 sets of (u_i, $\bar{T}_i$, $\bar{P}_i$) values; 59 values for layers crossed in the portion of the path going from the observer in layer #99 to the minimum height in layer #41, and 139 values for layers crossed in the portion from the minimum height to the top of the atmosphere. The average layer thickness in this model is ~.4 km. Examination of these 198 sets showed that of the 1.200099×10^{26} mol/cm^2 in the path, 3.1341×10^{25}, or 26%, were in the 0.35 km thick portion of layer 41 that contains the lowest segment of the path. This demonstrates the height selective nature of the limb geometry.

Compare this to the result obtained by Schmidt[22] that a uniform error of 0.5 km in the minimum height of a limb emission spectrum produced a 21% rms error in retrieved mixing ratios (using simulated balloon data).

The next highest layer, #42, contained 1.4154×10^{25} mol/cm^2, or 11.8%. A full 60% of the air mass lay between 18.45 and 20.49 km.

Next the Voigt function evaluation routine, due to Hui, Armstrong, and Wray,[23] was checked against the tables of Young.[24] It gave good agreement over the tabulated range of x and y values. A set of sample

Table 1. Comparison of path characteristics.

	Ref. (20)	Ref. (10)	Ref. (21)
Apparent Zenith angle (degrees)	95.2	95.2	95.2
Lower height (m)	45000.0	45000.0	45000.0
Upper height (m)	89999.9	99000.0	82000.0
Minimum height (m)	18454.5	18434.1	18450.0
Chapman airmass	6.168	7.098	6.385
Optical airmass	5.422	6.085	5.573
HDIFF (m)	1000.5	1138.5	1030.0
Refraction (degrees)	0.11255	0.12788	0.11579
Astronomical Zenith angle (degrees)	95.31	95.33	95.32
P(EFF) (N/m^2)	4518.41	5494.93	4999.92
T(EFF) (K)	216.26	219.54	218.93
P(TAN) (N/m^2)	7890.17	9066.33	

line parameters were then chosen. These are shown in Table 2. A uniform mixing ratio of 0.1 ppm was used to calculate the absorbance in each layer.

The total absorbance was 1.231378 at $\nu = \nu_0 = 2090.796$ cm^{-1}, corresponding to a transmittance (no convolution) of 0.29189. The absorbance in layer 41 was 0.197407, or ~16%, and the absorbance between 18.45 and 20.49 km was 0.456708, or 37%. These values show that the absorbance at line center is less peaked with height than the airmass. For Lorentz-like lines, the absorbance at ν_0 is $Su/\alpha\pi$. Consequently the decrease in u with height is offset by the decrease in α (because of decreasing pressure) and the absorbance is "smeared out" with height. The degree of Lorentz-like behavior for Voigt lines is determined by y in Eq. (13). Large y implies a high degree of Lorentz-like behavior; small y implies mainly Doppler-like behavior. The Lorentz-Doppler crossover point, $y \simeq 1$, occurs at layer 63 for the sample line and atmospheric profile used; consequently, the observed "smearing" is reasonable.

The above observations suggest that high-resolution spectra should have better height sensitivity than low-resolution spectra because the same effect which "smears" the line center absorbance sharpens the wing absorbance, which goes as $Su\alpha$. In low-resolution spectra the observed signal is a mix of the two and has intermediate height sensitivity. High-resolution spectra are better to use to study the height-sensitive wing absorbance.

A second consequence of the "smearing" is found when the fine layers are combined into thicker layers. Let consecutive layers $\ell_1, \ell_2, \ldots, \ell_n$ with parameters $(u_1,\bar{T}_1,\bar{P}_2), \ldots, (u_n,\bar{T}_n,\bar{P}_n)$ be combined into one layer with parameters

$$
\begin{aligned}
u &\equiv \sum_{i=1}^{n} u_i \ , \\
\bar{T} &\equiv \sum u_i\bar{T}_i/u \ , \text{ and} \\
\bar{P} &\equiv \sum u_i\bar{P}_i/u \ .
\end{aligned}
\tag{25}
$$

The new layer represents a less accurate approximation to the atmosphere than the original layers. In order to save computation time, it is desirable to use the minimum number of layers to calculate the spectrum. Subroutine SNIDER is sufficiently fast, however, that no such concerns apply to it. To test the sensitivity of the calculated spectrum to the layer coarseness, the original 139 sets of $(u,\bar{T},\bar{P})$, one for each layer crossed, were combined into segments of approximately equal airmass. Each new layer had an airmass as close to, but less than, U/Nge as possible, where Nge is some integer. The calculated absorbances at three different frequencies for several different values of Nge are shown in Table 3. It is clear from these results that more layers are required at line center than in the wings. This is because the result of decreasing Nge is to

Table 2. Sample line parameters*

ν_o = 2090.796 cm^{-1}
S_o = 0.189 × 10^{-20} mol^{-1} cm
α_o = 0.110 cm^{-1}
E" = 272.220 cm^{-1}
m = 48 amu

*corresponding to the (6,13)-(6,14) line of the $\nu_1 + \nu_3$ band of $^{16}O_3$.

Table 3. Effect of different layer thicknesses.

$\nu(cm^{-1})$	Nge	# Layers	A(ν)
2090.796	3	3	1.12296698
2090.796	9	7	1.20571646
2090.796	35	18	1.22967891
2090.796	-	139	1.231378
2090.806	3	3	0.204556963
2090.806	9	7	0.202129669
2090.806	35	18	0.20184368
2090.806	-	139	0.201829374
2090.816	3	3	0.0613707937
2090.816	9	7	0.0616293664
2090.816	35	18	0.0614016373
2090.816	-	139	0.0613723083

produce thicker layers in the upper portions of the atmosphere where the u_i values are small. Since the line center absorbance is more sensitive to these upper layers, the loss of detail has more effect on it than wing absorbance values.

The program in Appendix A includes a subroutine called PATHST which performs the layer combination. The parameter Nge is used to set the fineness of the layers used to calculate the spectrum. As written, however, the subroutine combines the layers in such a way that each has an airmass at least as great as U/Nge but as close to U/Nge as possible. For the spectra in the next section, a value of Nge = 15 was found to be acceptable, but Table 3 indicates that different values may be required for different types of spectra.

The convolution portion of the program was tested on a flat ($\partial\tau/\partial\nu = 0$) spectral region with a Gaussian slit function of the form

$$\sigma_{Gauss}(\nu - \nu') = \frac{\sqrt{\ell n\, 2}}{H\sqrt{\pi}} \exp\left[-\frac{(\nu' - \nu)^2\, \ell n\, 2}{H^2}\right] . \qquad (26)$$

A five-point initial trapezoidal evaluation was used to start the Romberg iterations with a frequency extent of 8H. The T and M table entries calculated for one run are shown in Table 4. A convergence criterion corresponding to 1% between the respective T and M table elements [see Eq. (22)] was used. Only the diagonal of the T-table is shown since the other elements are not calculated in the modified routine. The table elements must be multiplied by 2 to get the corresponding transmittance values. In this example, the routine went two iterations beyond the initial trapezoidal and midpoint evaluations before converging. The final value shows excellent agreement with the true value.

The routine was also tried on a Voigt line with parameters

ν_o = 2875.90 cm^{-1}

S_o = 0.0668 atm^{-1} cm^{-1}/cm

α_{L_o} = 0.023176 cm^{-1}

E" = 400.00 cm^{-1}

m = 36 amu

at a uniform pressure of 1 atm and temperature of 300 K. The total airmass was u = 200 atm cm. Table 5 shows the results for 10 different observed frequency positions spaced 0.2 cm^{-1} apart. The second column gives the calculated transmittance values with ϵ = 0.01, H = 0.083819 cm^{-1}, and an initial five-point trapezoidal evaluation that extended 2-1/2 H on either side of the central position. By comparing values equally spaced around 2875.90 cm^{-1} the consistency is seen to be ~0.001, which is $\epsilon/10$. The

Table 4. A sample T and M table for convolution routine. (Table values must be multiplied by 2 to give transmittance value.)

TRAP	MID	Iteration	
		1	2
0.5284401	0.471553	0.4999984	0.4999976
0.4905153		0.5094798	0.4999971
0.5006297			0.4993649

τ = 0.9999946 (exact = 1.0000000)

Table 5. Convolution results for a sample Voigt line convolved with a Gaussian slit function.

ν (cm^{-1})	τ_{con}	Iterations	Total Points	New Points
2875.00	0.9984500	1	9	9
2875.20	0.9952382	1	9	3
2875.40	0.9944796	1	9	4
2875.60	0.9885907	1	9	4
2875.80	0.8511999	3	33	29
2876.00	0.8508019	2	17	8
2876.20	0.9872358	1	9	3
2876.40	0.9942334	1	9	4
2876.60	0.9960335	1	9	4
2876.80	0.9964244	1	9	4
				TOTAL 72

third column lists the number of iterations required for convergence of the convolution integral. A value of 1 means that the convergence criterion was satisfied on the first try. The fourth column lists the number of monochromatic transmittances required for the convolution, and the fifth column lists the number of new monochromatic transmittance values calculated at each observed frequency. The increased density of points around line center, where the monochromatic transmittance changes most rapidly, is apparent.

Table 6 shows similar results for the identical spectrum except with a smaller frequency spacing. The fifth column shows the larger savings in calculations for more closely spaced observed frequencies. For reference, the 10 points in Table 6 took 0.09 second of cpu time to execute. This corresponds to 1.7 ms per monochromatic transmittance calculation. A later sample spectrum including 55 atmospheric layers and 13 lines, averaged 0.15 ms per monochromatic transmittance calculation on the OSU Amdahl Computer.

Sample spectra for other sets of line parameters produced similar results. It was found that extremely narrow and strong lines required considerably more iterations than broad lines. This can lead to unreasonably high numbers of iterations unless some maximum number of iterations is specified; usually a value of 7 was used. When convergence does not occur on the seventh iteration, the program outputs the most recent element of the T-table, sets an error flag, and proceeds to the next frequency position.

A variety of other tests were performed on the program, including the effect of different convergence criterion values. More is said about this in the next chapter. Overall the behavior was found to be satisfactory but one persistent problem did arise; it was found that the convolution routine would often converge prematurely. An example is shown in Table 7. The rapid decrease in the number of iterations, in a spectral region where the transmittance is not changing much, indicates a premature convergence. This is verified in the T- and M-tables for these two points shown in Table 8. The boxed portions correspond to the values in Table 7 where the convergence criterion was 0.005 (or 0.5%). The larger values in Table 8 correspond to a convergence criterion of 0.0001 (or 0.01%). The premature convergence at 1900.05 cm^{-1} is seen to be due to a misleading resemblence between the first T- and M-values. Subsequent iterations show the true value to be considerably lower than these, which the more stringent convergence criterion has picked up. This type of behavior is often encountered in iterative procedures. This problem was only detected when the slit function width was much larger than the line widths, though in principle it could occur in other situations. It was found that the problem could usually be avoided by adjusting the convergence criterion and the number of points in the first trapezoidal evaluation. The parameters can only be set based on experience and knowledge of the spectral region, and those lacking both these should indicate some caution.

Table 6. Convolution results for sample line with smaller frequency spacing.

$\nu(cm^{-1})$	τ_{con}	Iterations	Total Points	New Points
2875.70	0.9694133	1	9	9
2875.74	0.9396371	1	9	0
2875.78	0.8870856	2	17	10
2875.82	0.8118306	3	33	18
2875.86	0.7381039	3	33	3
2875.90	0.7074896	3	33	3
2875.94	0.7380002	3	33	3
2875.98	0.8117288	3	33	3
2876.02	0.8863926	3	33	3
2876.06	0.9391911	2	17	1
				TOTAL 53

Table 7. An example of a premature convergence.

$\nu(cm^{-1})$	τ_{con}	Iterations
1900.00	0.96867	5
1900.05	0.99230	1

Table 8. The T- and M-tables for convolutions in Table 7. (Boxed portions correspond to a convergence criterion of 0.005. Entire tables for convergence criterion of 0.0001. Multiply table values by 0.0625 to get transmittance.)

TRAP	MID	ν = 1900.00 cm^{-1}				
15.85111	15.72414	14.90784	15.61850	15.52610	15.49732	15.49703
15.77746		14.63574	15.85539	15.49529	15.48772	15.49693
15.16341			15.93670	15.47128	15.48721	15.49755
15.55619				15.46389	15.48746	15.49771
15.50986					15.48755	15.49775
15.49869						15.49775

TRAP	MID	ν = 1900.05 cm^{-1}			
15.87981	15.87390	15.74799	15.85101	15.83745	15.83456
15.87587		15.70601	15.88535	15.83293	15.83359
15.78528			15.89730	15.82943	15.83364
15.84218				15.82835	15.83370
15.83524					15.83372

As a final check on the entire calculation routine, two sample spectra were calculated under conditions similar to those used by Kyle and Goldman.[25] The observer was at a height of 4 km with the sum overhead. The spectra for the 1900-1902 cm^{-1} and 1930-1935 cm^{-1} regions are shown in Figs. 4 and 5, respectively. There are some differences in the conditions between these spectra and the corresponding high-resolution spectra of Kyle. Both have an instrument resolution of 0.1 cm^{-1} but Kyle used a triangular slit function and we used a Gaussian. Also, the values of the CO_2 and H_2O mixing ratios are somewhat different. The calculation routine is currently set up for only constant mixing ratios, whereas Kyle used a decreasing H_2O mixing ratio with height. An attempt was made to fix the CO_2:H_2O ratio in the lowest level. With a CO_2 mixing ratio of 322 ppm (volume), this gave a H_2O = 1080 ppm (volume). Also, it was found that SNIDER will not work with a zenith angle of 0°. In spite of these differences the spectra show good agreement, indicating the two routines are consistent.

In the next chapter, the spectrum calculation routine is used in a brief study that illustrates some information analysis techniques for experimental design.

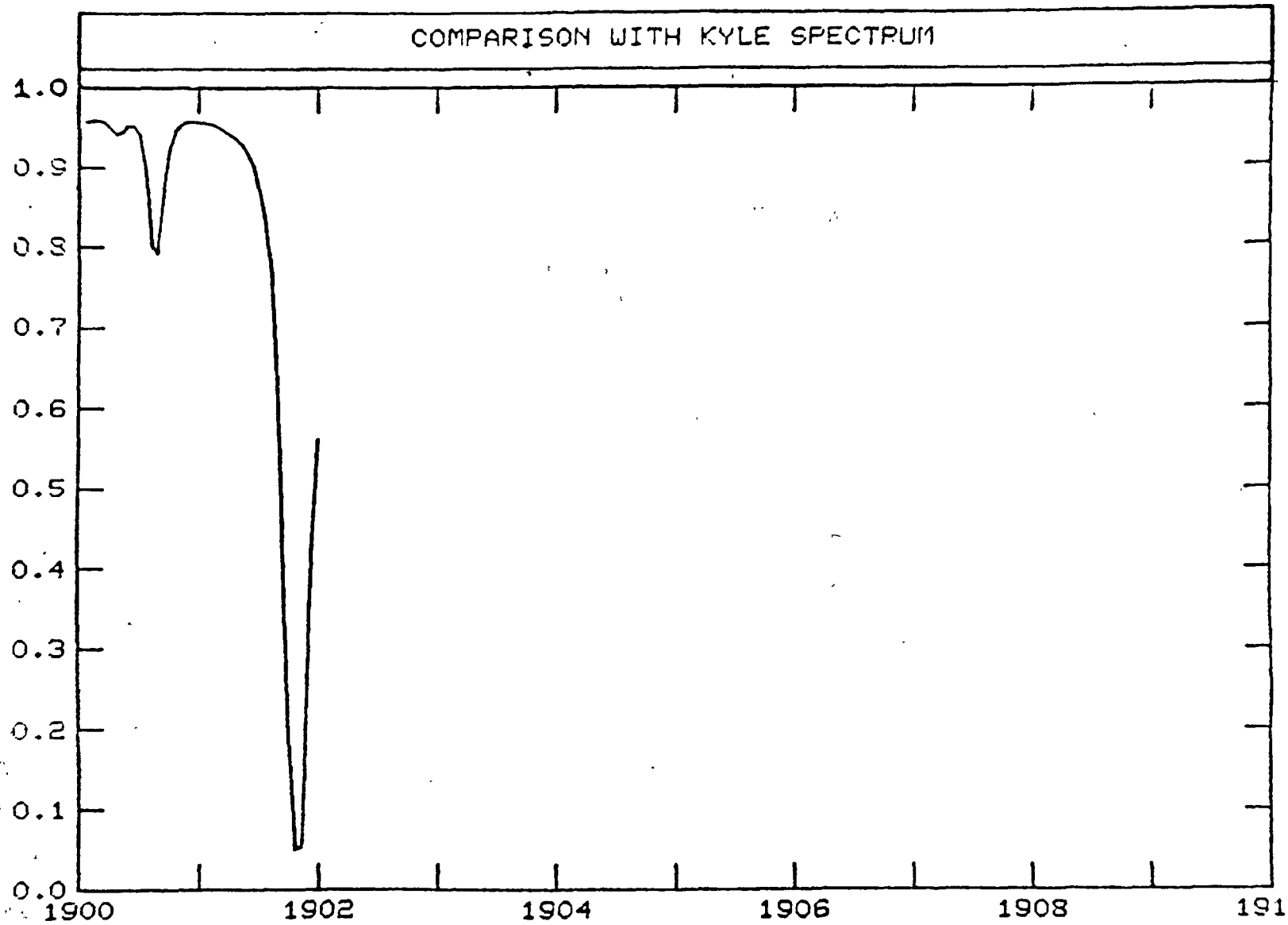


Fig. 4 - Comparison with Kyle[25] spectrum

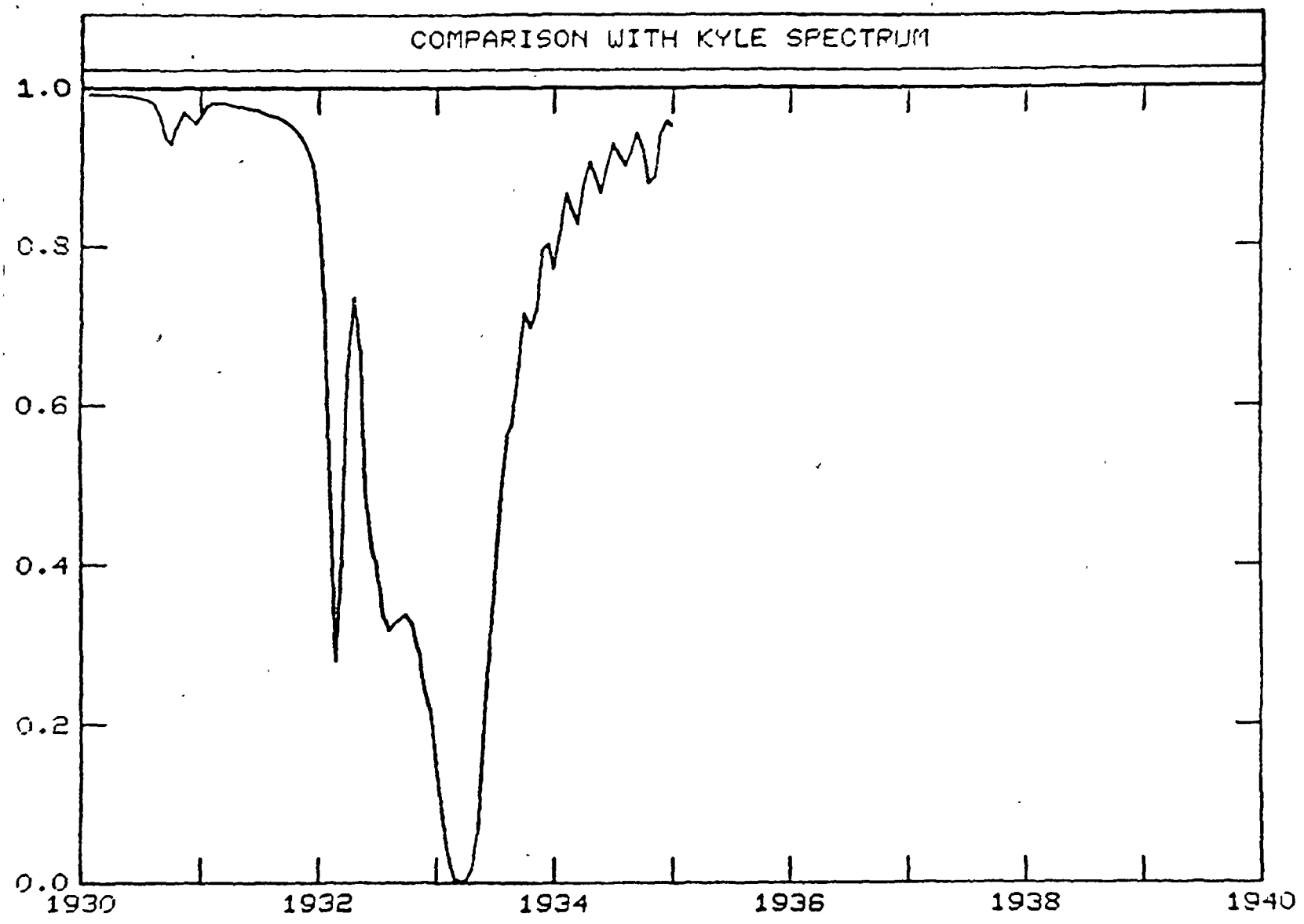


Fig. 5 - Comparison with Kyle[25] spectrum

III. SOME INFORMATION ANALYSIS TECHNIQUES

A. IDENTIFYING "BAD" PARAMETERS

The equations in the previous chapter describe how the appearance of an atmospheric absorption spectrum depends on the physical characteristics of the atmosphere and the molecular properties of the absorbing gases. Assuming that the molecular parameters (line intensity, broadening coefficient, line position, lower state term value) are known, the equations predict what the spectrum will look like, given the atmospheric conditions. This report is concerned with the inverse problem (i.e., inferring the atmospheric conditions given the spectrum). It is clear that those aspects of the atmosphere which have no effect on the spectrum can not be determined from the spectrum. Similarly, those aspects which have only a slight influence on the spectrum will be harder to determine than those aspects with a large influence. For example, consider the calculated spectrum in Fig. 6. This 200-point spectrum corresponds to the same observer-source geometry as in Chapter II-F with the 190-layer model and Nge equal to 15 in Eq. (25). The CO_2 mixing ratio was 322 ppm, and the H_2O mixing ratio was 3.889 ppm. Both were assumed independent of height. The slit function was Gaussian, with a full width at half height of 0.02 cm^{-1}. This particular region contains contributions from nearly 150 CO_2 lines and about a dozen H_2O lines, so it should be sensitive to the mixing ratios of CO_2 and H_2O. It contains no information, however, about the O_3 mixing ratio. A convergence criterion of 0.5% was used with an extent of 0.05 cm^{-1} in the convolution. A more stringent criterion of 0.1% produced an rms change in the transmittance values of 2.89×10^{-4} with a maximum of 0.003, indicating that the accuracy of the convolution is consistent with the convergence criterion. A frequency spacing of 2 points per full width at half height of the slit function was used.

Several atmospheric parameters were selected for investigation. These are listed in Table 9 along with the two different values used to study the influence of the parameter on the spectrum. The spectrum in Fig. 6 corresponds to the upper value for each parameter and is referred to as the reference spectrum. Eight new spectra were then calculated by changing the values of the parameters one at a time. Figure 7 shows the effect on the spectrum of increasing the zenith angle from 95.2° to 95.4°. The difference spectrum is shown in Fig. 8. The sum of the squares of the differences for this pair is 0.44482, which is listed in column 3 of Table 9. The corresponding values are also shown for the other seven parameters. These numbers are one indicator of how much influence a particular parameter has on the spectrum. Of course larger parameter changes produce larger squared differences so the only valid comparisons between parameters are conditioned on specific parameter changes; e.g., a 0.2° change in zenith angle is more influential than a 2 K change in the temperature at layer 41 (18.38 - 18.80 km). It is reasonable, therefore, to scale the difference spectrum by dividing it by the size of the parameter change or step before squaring. Let θ_i denote the ith parameter with step $\Delta\theta_i$. The procedure above produces a set of 8 quantities W_{ii}, i = 1, . . . 8

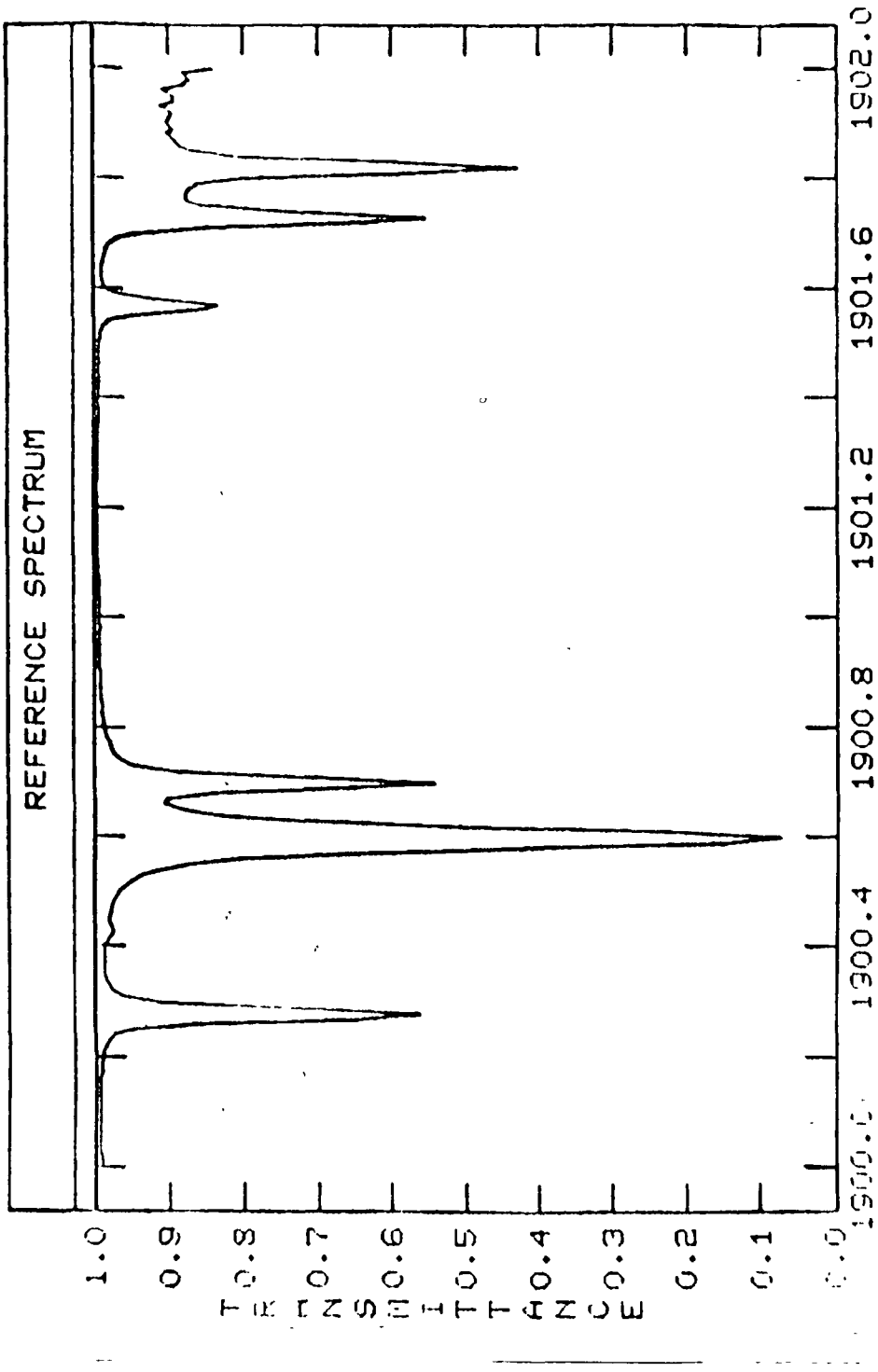


Fig. 6 - Reference spectrum

Table 9. Parameter values used to compute sample spectra.

Parameter	Values	$\sum (\Delta y)^2$
1. CO_2 mixing ratio	322 ppm 354.2 ppm	0.011773
2. Resolution	0.02 cm^{-1} 0.028 cm^{-1}	0.062913
3. Zenith angle	95.2° 95.4°	0.44482
4. Temperature in layer 41	216.65 K 218.65 K	8.4118×10^{-5}
5. Temperature in layer 42	216.65 K 218.65 K	5.4798×10^{-5}
6. Temperature in layer 40	216.65 K 218.65 K	4.888×10^{-7}
7. Ground-level pressure	1013 mb 1063 mb	0.008109
8. Background value	1.0 1.025	0.10954

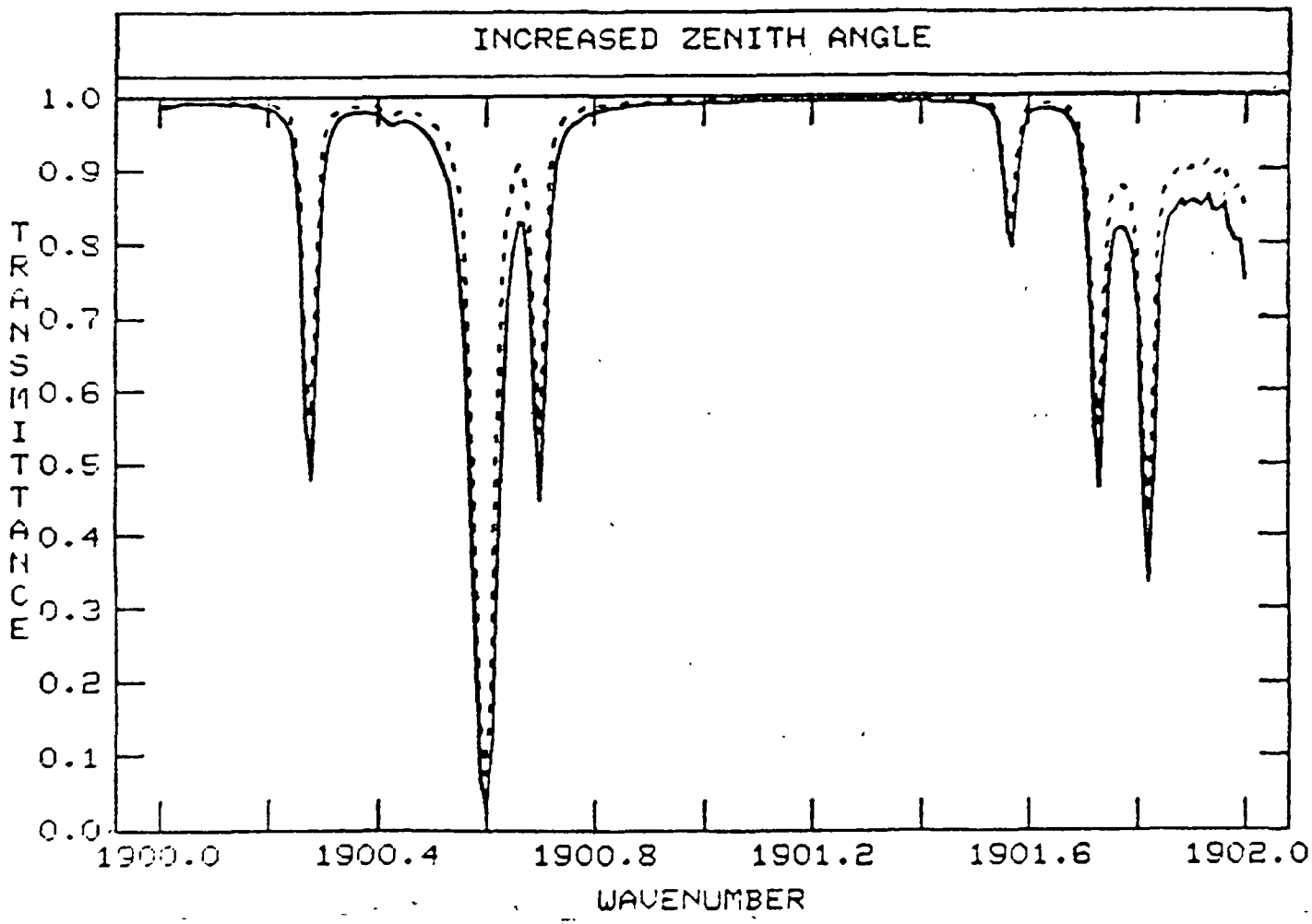


Fig. 7 - Spectrum for increased zenith angle —— 95.4°, ---- 95.2° (reference spectrum)

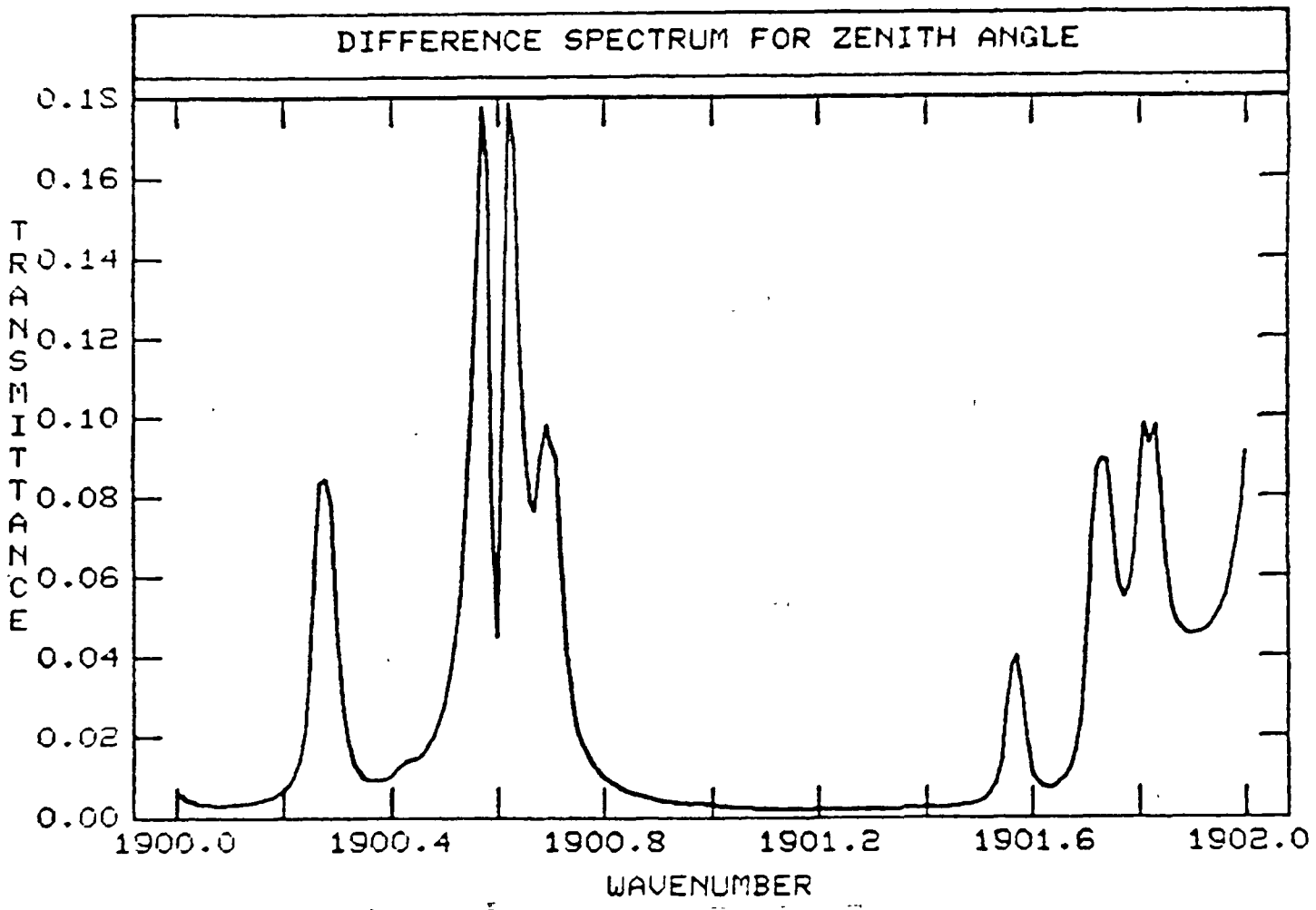


Fig. 8. (Reference spectrum) - (increased zenith angle spectrum)

where

$$W_{ii} \equiv \sum_{j=1}^{N} \left(y_j^{(0)} - y_j^{(i)}\right)^2 \Big/ \Delta\theta_i^2 \ , \tag{27}$$

with N the number of points in the spectrum, $\vec{y}^{(0)} = \left(y_1^{(0)}, \ldots, y_N^{(0)}\right)$ the reference spectrum, and $\vec{y}^{(i)} = \left(y_1^{(i)}, \ldots, y_N^{(i)}\right)$ the spectrum with the ith parameter stepped by $\Delta\theta_i$.

These scaled and summed square difference values alone, however, are insufficient to indicate how well groups of parameters can be determined simultaneously. This is illustrated by Fig. 9. It shows the difference spectra for changes in the temperature values T(41) and T(42) for layers 41 and 42. From the similarity of these spectra and the assumption that the change in the spectrum Δy is linear in $\Delta\theta$, it is clear that a simultaneous increase of 2 K in T(41) and a 2 K decrease in T(42) will produce a much smaller difference spectrum than either one in Fig. 9. Each change tends to cancel out the other. This corresponds to a 2 K change in [T(41) - T(42)]/2, with the average temperature [T(41) + T(42)]/2 held constant. Similarly, a simultaneous 2 K increase in T(41) and T(42) will produce a much larger difference spectrum than either in Fig. 9. This corresponds to a 2 K change in the average temperature, with the difference temperature held constant, and indicates that changes in different linear combinations of the parameters can have significantly different amounts of influence on the spectrum. That, in turn, implies that some combinations are harder to determine from a spectrum than others. Similar observations apply to linear combinations of all 8 different parameters.

The question arises as to whether there exists some linear combination

$$\phi = \sum_{j=1}^{8} u_j \theta_j$$

which has the least influence on the spectrum and hence is the hardest to determine. Lees[26] addressed this question in connection with attempts to analyze methyl alcohol spectra. He found that changes in a particular linear combination of the unknown parameters produced no change in the spectrum, which he called a linear dependence, and he proposed a technique for identifying these as well as "near" linear dependences. In order to adapt this technique to the present problem, form the quantities

$$W_{ik} = \sum_{j=1}^{N} \left(y_j^{(0)} - y_j^{(i)}\right) \cdot \left(y_j^{(0)} - y_j^{(k)}\right) \Big/ \Delta\theta_i \Delta\theta_k \tag{28}$$

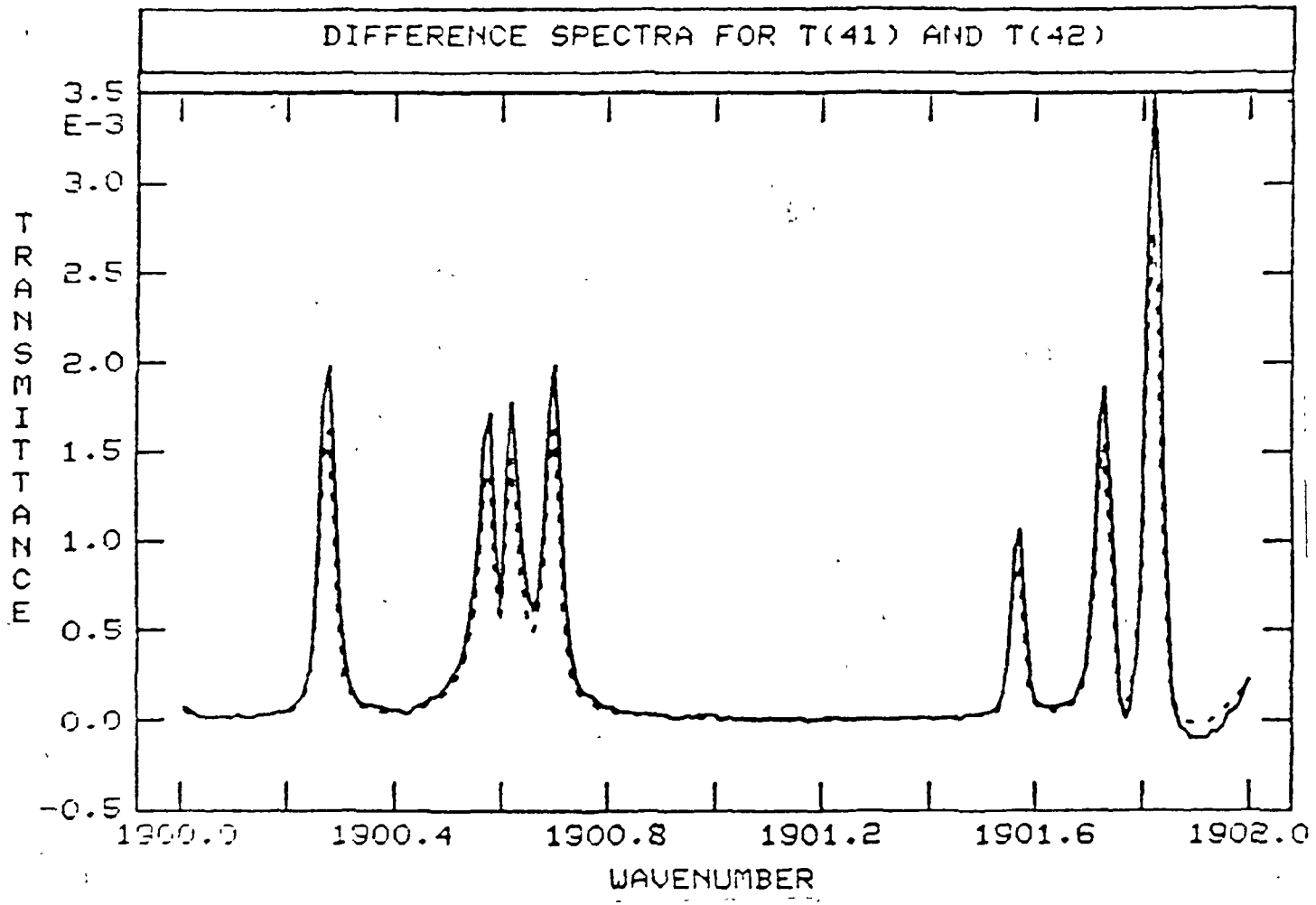


Fig. 9 - Difference spectra for 2 K changes in the temperature in layers 41 and 42. —— $\Delta T(41) = 2$ K, $\Delta T(42) = 0$, ---- $\Delta T(41) = 0$, $\Delta T(42) = 2$ K.

and place these in a matrix W, where the ith diagonal element is W_{ii} from Eq. (27) and the i - kth and k - ith element is W_{ik}. This matrix is often referred to as the information matrix[27] or the curvature matrix.[28]

To be more precise, W becomes the information matrix in the limit as $\Delta\theta \to 0$ and the quantities $y^{(0)} - y^{(i)}/\Delta\theta^i$ become the partial derivative of y with respect to θ_i evaluated at $\vec{\theta}_0$. W is therefore a function of $\vec{\theta}_0$. For small simultaneous changes in the parameters $\vec{\Delta\theta} = \begin{pmatrix} \Delta\theta_1 \\ \vdots \\ \Delta\theta_8 \end{pmatrix}$ the summed squared difference spectrum is given by

$$Q(\vec{\Delta\theta}) = \sum_{ij} \Delta\theta_i W_{ij} \Delta\theta_j = \sum_k \left[y_k^{(0)} - y_k(\vec{\Delta\theta}) \right]^2 \qquad (29)$$

or, in matrix notation,

$$Q(\vec{\Delta\theta}) = \vec{\Delta\theta}' W \vec{\Delta\theta} \ ,$$

where ' denotes transpose. Lees proposes examining the eigenvalues and eigenvectors of a modified information matrix W* given by

$$W^*_{ik} = W_{ik} / \sqrt{W_{ii} W_{kk}} \ .$$

Let the eigenvector $\vec{\lambda}^*$ with elements λ_i^* correspond to the smallest eigenvalue of W^*. The corresponding linear combination of parameters is given by

$$\Phi = \sum_{j=i}^{8} \lambda_i^* \cdot \theta_i \cdot \sqrt{W_{ii}} \ . \qquad (30)$$

When this eigenvalue is much smaller than the others, he says that it indicates a "near" or exact linear dependence. Table 10 lists the information matrix W, and modified matrix W* for the set of 9 spectra already introduced. The eigenvalues and eigenvectors of W* were calculated in SPEAKEASY with the command EIGENVALS. These are listed in Table 11. None of the eigenvalues is significantly lower than the rest, indicating that there are no exact linear dependences among the 8 parameters in Table 9. It is still possible to deduce the "worst" linear combination from these results with the following restriction:

> For each of the 8 parameters θ_i define a parameter step $\Delta\theta_i$ such that $Q(\Delta\theta_i) = 1$. Assuming that Eq. (29) holds, these steps are given by $\Delta\theta_i = 1/\sqrt{W_{ii}}$. The appropriate steps are listed in Table 12. Define new parameters $\{\psi\}$ according to
>
> $$\psi_i \equiv \theta_i / \Delta\theta_i \ .$$

Table 10. Information matrices

W:

ROW 1	1.1355E-5	0.034772	0.010634	1.2303E-5	1.0215E-5
	1.0832E-6	5.7883E-6	-0.020427		
ROW 2	0.034772	3932	-1.6132	-0.090516	-0.072398
	-1.8376E-4	-0.0091847	-70.879		
ROW 3	0.010634	-1.6132	11.12	0.012685	0.010461
	0.0011462	0.0059693	-22.043		
ROW 4	1.2303E-5	-0.090516	0.012685	2.1029E-5	1.6957E-5
	1.3054E-6	7.0995E-6	-0.021157		
ROW 5	1.0215E-5	-0.072398	0.010461	1.6957E-5	1.3699E-5
	1.0741E-6	5.8427E-6	-0.017702		
ROW 6	1.0832E-6	-1.8376E-4	0.0011462	1.3054E-6	1.0741E-6
	1.222E-7	6.2136E-7	-0.0020892		
ROW 7	5.7883E-6	-0.0091847	0.0059693	7.0995E-6	5.8427E-6
	6.2136E-7	3.2436E-6	-0.011075		
ROW 8	-0.020427	-70.879	-22.043	-0.021157	-0.017702
	-0.0020892	-0.011075	175.27		

W*:

1	-0.165	0.946	0.796	0.819	0.920	0.954	-0.458
	1	-0.0077	-0.315	-0.312	-0.0084	-0.081	-0.085
		1	0.829	0.848	0.983	0.994	-0.499
			1	0.999	0.814	0.860	-0.348
				1	0.830	0.876	-0.361
[SYMMETRIC]					1	0.987	-0.451
						1	-0.465
							1

Table 11. Eigenvalues and associated eigenvectors of W^* from Table 10.

Eigenvectors of W^* (as columns):					
ROW 1	-0.02216	0.069408	-0.25559	0.74657	0.46191
	-0.043359	0.015821	-0.39562		
ROW 2	0.0038524	-0.032105	-0.052676	0.18343	-0.32712
	-0.39618	0.83294	0.06913		
ROW 3	-0.008285	0.48954	0.71662	-0.13348	0.17436
	-0.11331	0.14197	-0.40684		
ROW 4	-0.67639	0.08705	-0.093432	0.087113	-0.56248
	-0.048948	-0.23103	-0.38268		
ROW 5	0.7281	-0.032767	-0.0074687	0.12842	-0.50117
	-0.045501	-0.21962	-0.38829		
ROW 6	0.062616	0.23679	-0.59867	-0.57696	0.20514
	-0.17077	0.13061	-0.40051		
ROW 7	-0.088656	-0.83043	0.22346	-0.18346	0.17485
	-0.1211	0.068128	-0.41116		
ROW 8	4.4771E-4	0.013133	0.034914	0.023464	0.095041
	-0.88319	-0.40311	0.21564		

Eigenvalues of W^*:
(1) 1.0655×10^{-4}
(2) 0.0016232
(3) 0.010273
(4) 0.064734
(5) 0.29085
(6) 0.68626
(7) 1.1985
(8) 5.7477

Table 12. Parameter steps producing a summed squared difference spectrum equal to 1, assuming Eq. (29) holds.

(1)	296.76 ppm (CO_2 mixing ratio)
(2)	0.015948 cm^{-1} (resolution)
(3)	0.29988° (zenith angle)
(4)	218.07 K $\Delta T(41)$
(5)	270.18 K $\Delta T(42)$
(6)	2860.6 K $\Delta T(40)$
(7)	555.25 mb $\Delta P(0)$
(8)	0.075535 (background)

For these new parameters, a unit step in ψ_i produces a $Q(\Delta\psi) = 1$. Now consider the set of all linear combinations of steps in the $\{\psi\}$ of the form

$$\vec{\Delta\Phi} = \begin{pmatrix} c_1\Delta\psi_1 \\ c_2\Delta\psi_2 \\ \vdots \\ c_8\Delta\psi_8 \end{pmatrix}$$

such that

$$\sum_k c_i^2 = 1 \ . \tag{31}$$

The set of steps $\vec{\Delta\Phi}_i$, with

$$c_i = 1$$

and

$$c_j = 0 \ ; \quad i \neq j \ ,$$

belongs to this set of $\vec{\Delta\Phi}$ satisfying Eq. (31), and for each $\vec{\Delta\Phi}_i$, $Q(\vec{\Delta\Phi}_i) = 1$. In a sense, steps $\vec{\Delta\Phi}$ satisfying Eq. (31) are all the steps of the same "size," in terms of parameter changes. From the theorems on quadratic forms[29] it can be shown that the extremal values of $Q(\vec{\Delta\Phi})$ for all $\vec{\Delta\Phi}$ correspond to $\vec{\Delta\Phi}$'s whose $\{c_i\}$ values are the elements of the eigenvalues of W^*. Consequently the smallest $Q(\vec{\Delta\Phi})$, and hence smallest change in the spectrum, for all parameter changes of the same "size" as those in Table 12 results from:

$$\vec{\Delta\Phi}_{min} = \begin{pmatrix} -0.02216 & \times & 296.76 \text{ ppm} \\ 0.0038524 & \times & 0.015948 \text{ cm}^{-1} \\ -0.008285 & \times & 0.29988° \\ -0.67639 & \times & 218.07 \text{ K} \\ 0.7281 & \times & 270.18 \text{ K} \\ 0.062616 & \times & 2860.6 \text{ K} \\ -0.088656 & \times & 555.25 \text{ mb} \\ 4.4771 \times 10^{-4} & \times & 0.075535 \end{pmatrix}$$

$$= \begin{pmatrix} -6.576 \text{ ppm} \\ 0.00006144 \text{ cm}^{-1} \\ -0.0024845° \\ -147.5 \text{ K} \\ 196.7 \text{ K} \\ 179.1 \text{ K} \\ -49.23 \text{ mb} \\ 3.382 \times 10^{-5} \end{pmatrix} .$$

The most significant aspect of this set of parameter changes is the temperature steps. The temperature in level 41 is decreased by 147.5 K while the temperatures in the two adjacent layers are increased by approximately the same amount. This zigzagging of the temperature profile is a problem that often occurs in profile retrievals.[30] The summed squared difference spectrum corresponding to this "worst" set of parameter changes is given by the corresponding eigenvalue from Table 11; i.e., 1.0655×10^{-4}. It is seen that this is smaller than most of the values in the third column of Table 9.

The same quadratic forms theorem allows the identification of the set of parameter changes $\vec{\Delta\Phi}_{max}$ leading to the largest change in the spectrum. It is given by the eigenvector associated with the largest eigenvalue of $\underset{\sim}{W}^*$. From the eighth column in Table 12 it is seen that $\vec{\Delta\Phi}_{max}$ corresponds to simultaneous decreases in CO_2 mixing ratio, zenith angle, ground level pressure, and all three temperature values. All of these changes tend to decrease the amount of absorption in the spectrum and hence add together to increase the summed squared difference spectrum. The net change in the spectrum is more than 50,000 times larger than for $\vec{\Delta\Phi}_{min}$.

B. ESTIMATED PARAMETER UNCERTAINTIES

Another useful property of the information matrix W is related to the uncertainties in estimates for the values of the unknown parameters to be determined from an observed spectrum $\vec{y}_{obs}$. If $\vec{y}(\vec{\theta})$ is the calculated

spectrum for the set of parameter values $\vec{\theta}$, then one estimate for the true parameter values corresponding to $\vec{y}_{obs}$ is the well-known least-squares estimate $\hat{\theta}$. This is given by the value of $\vec{\theta}$ which minimizes

$$\sum_{i=1}^{N} \left[y_{obs,i} - y(\vec{\theta})_i \right]^2 .$$

If the rms noise value is σ, then the asymptotic variance-covariance matrix for $\hat{\theta}$ is

$$\S = \sigma^2 W^{-1} ,$$

where W is evaluated at $\hat{\theta}$.

The matrix in Table 10 can therefore be used to estimate, for a given noise level, how precisely the eight parameters in Table 9 could be obtained from a spectrum similar to that in Fig. 6. Attempts to invert W, however, led to warnings by the inversion routine that the matrix is nearly singular and the calculated inverse may not be significant. This implies that numerical difficulties would be encountered while trying to retrieve all eight parameters. If several of the parameters are constrained to given values, this eliminates the corresponding row and column from W. In general this makes retrieval of the other parameters easier. The effect of various sets of constrained parameters were studied by eliminating selected rows and columns and then trying to invert the resulting reduced matrix. Some of the results obtained are listed in Table 13. It is seen from the column labeled 3, that if only the CO_2 mixing ratio, resolution, and zenith angle are determined from a spectrum like Fig. 6 with 1% noise, the respective uncertainties are 10.5 ppm, 0.00018 cm^{-1}, and 0.0105°. If the noise is 2%, the uncertainties would be twice as large. Any attempts to determine more than one temperature value always led to very large uncertainties, as compared to the cases where only one temperature was determined. This is consistent with the conclusions in the previous section. Trying to determine T(41) and T(42) is the same as trying to determine their difference and average. Yet the temperature difference is very hard to determine, and this gives rise to increased uncertainties in T(41) and T(42).

Another way to think of this problem is to consider the addition of a constraint as an injection of information into the analysis. The additional information spreads out over the variance-covariance matrix and leads to smaller uncertainties in the unconstrained parameters. The extent to which the constraint of a θ_i improves the retrieval of θ_j is determined by the correlation coefficient between θ_i and θ_j. This is given by $S_{ij}/\sqrt{S_{ii}S_{jj}}$.

It is also seen in Table 13 that attempts to retrieve the zenith angle and the ground level pressure P(0) produced inversion problems and increased uncertainties. From Table 11 it is seen that this corresponds to the second "worst" parameter combination (column 2 of eigenvectors). Its

Table 13. Parameter uncertainties for various sets of parameter constraints, assuming an rms noise of 1%.

	Parameter	1	3	6	7	8	9
1	CO_2 mix. r.	14.2* ppm	10.5	10.97	10.87	10.87*	10.54*
2	resolution	0.00026* cm^{-1}	0.00018	0.00023	0.00023	0.00018*	0.00023*
3	zenith angle	0.042°*	0.0105	0.0137	0.0138	0.023*	0.040*
4	T(41)	119.5 K*	-	4.91	-	-	-
5	T(42)	157.1 K*	-	-	6.47	-	-
6	T(40)	-	-	-	-	166.2 K*	-
7	P(0)	78.4 mb*	-	-	-	-	72.8*
8	background	0.00094*	-	0.00088	0.00088	0.00091*	0.00094*

*indicates inversion of nearly singular matrix

corresponding eigenvalue, though larger than the smallest, is still 5,000 times smaller than the largest eigenvalue and therefore corresponds to a set of parameter steps having a small effect on the spectrum.

The above techniques of information analysis explore the quality of the information in a proposed set of data. They can be used, therefore, to compare different experimental designs by comparisons of the information in the data produced by the different designs. This function of the techniques was employed to study the effect of decreased instrument resolution on the information in the spectra analyzed above.

C. LOW RESOLUTION INFORMATION ANALYSIS

The calculation steps of the previous two sections were repeated with the parameter values in Table 14. The new reference spectrum is shown in Fig. 10. This spectrum contains 40 points from 1900 - 1902 cm^{-1} which is 2 points per full width at half height of the slit function. Clearly, since there are five times more points in the high-resolution spectra, the summed squared difference spectra should be correspondingly higher. Any deviation from a five-fold change is an indication of differences in the influence of the parameters on the spectrum. The ratios of the summed squared difference spectra are listed in column 4 of Table 14. Only the value for the resolution is less than the expected value of 5. Since both resolution changes were +4%, this implies that the low-resolution spectrum is more sensitive to percent changes in instrument resolution than the high-resolution spectrum. Similarly, the large value (9.23) for T(41) indicates that the low-resolution spectrum is less sensitive to changes in the temperature in layer 41 and hence should yield considerably larger uncertainties in this parameter. Table 15 shows some typical standard deviations for the low-resolution spectrum. It is seen that the uncertainties are larger than for the high-resolution spectrum, especially the temperature uncertainties.

Table 16 shows some of the results of a Lees-type search for the "bad" parameters. The lowest eigenvalue of the modified information matrix corresponds to the zenith angle and P(0) values and the second lowest corresponds to the zigzagging temperature values. This is a reverse in order from the high-resolution case for the two "worst" combinations. Once again, however, the best combination is a simultaneous decrease in CO_2 mixing ratio, zenith angle, ground-level pressure, and all three temperatures. The variation from worst to best corresponds to a change in summed squared difference of better than 100,000.

Table 14. Parameter values used to calculate low-resolution sample spectra. (The fourth column gives the ratio of the $\sum (\Delta y)^2$ values from Table 9 and those in column 3 for each parameter.)

	Parameter	Values	$\sum (\Delta y)^2$	Ratio of $\sum (\Delta y)^2$
(1)	CO_2 mixing ratio	322 ppm 354.2 ppm	0.0016442	7.16
(2)	Resolution	0.10 cm^{-1} 0.14 cm^{-1}	0.014764	4.26
(3)	Zenith angle	95.2° 95.4°	0.070241	6.33
(4)	Temperature in layer 41	216.65 K 218.65 K	9.1177×10^{-6}	9.23
(5)	Temperature in layer 42	216.65 K 218.65 K	6.147×10^{-6}	8.91
(6)	Temperature in layer 40	216.65 K 218.65 K	7.6×10^{-8}	6.43
(7)	Ground-level pressure	1013 mb 1063 mb	0.0012427	6.53
(8)	Background value	1.0 1.025	0.021652	5.06

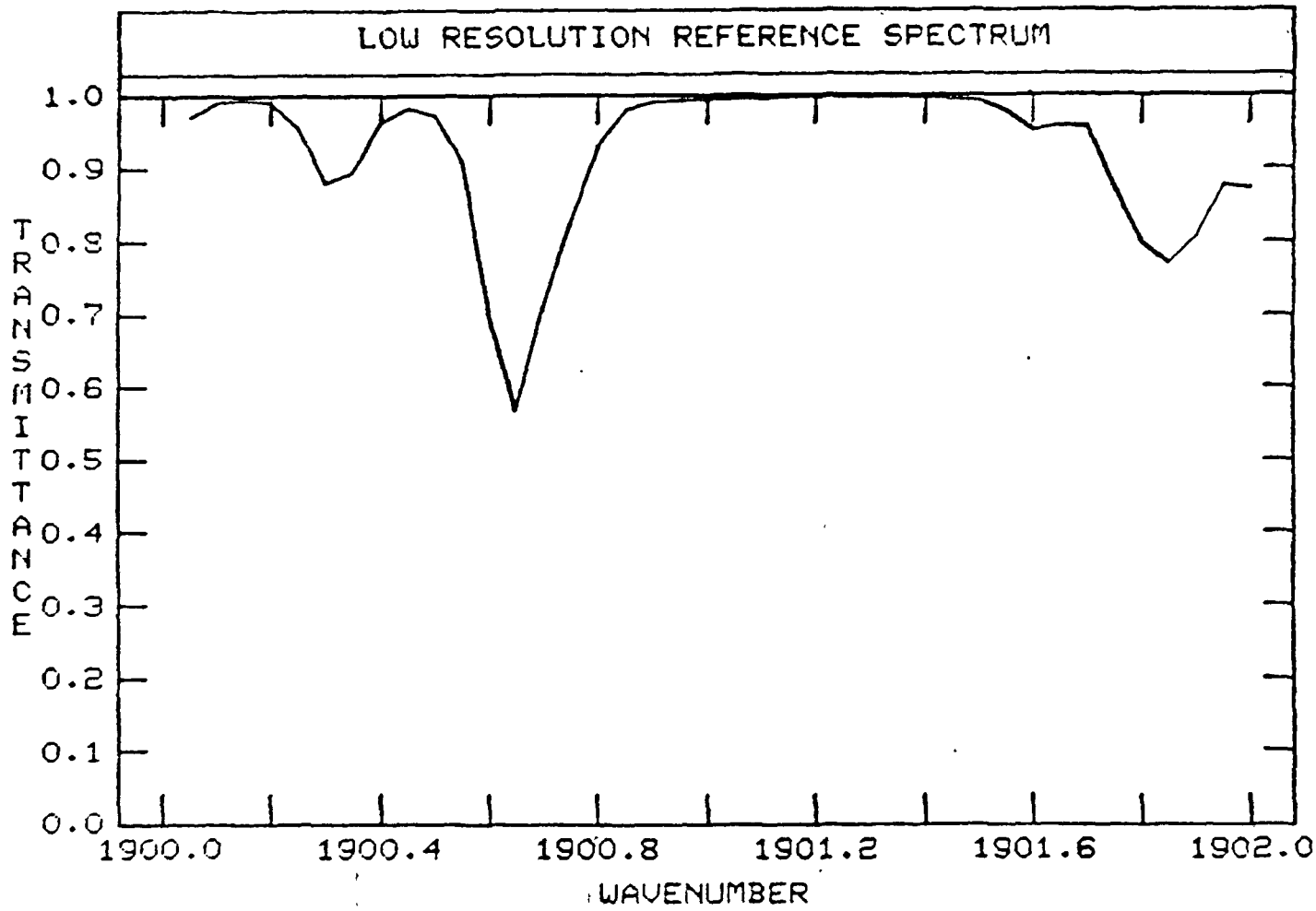


Fig. 10 - Low-resolution reference spectrum

Table 15. Parameter uncertainties for various sets of parameter constraints for low-resolution spectra, assuming an rms noise of 1%.

	Parameter	2	3	6	7	8	9
1	CO_2 mix. r.	61.01 ppm	60.43	61.54	61.93	63.41	64.02*
2	resolution	0.0036 cm^{-1}	0.0034	0.0042	0.0041	0.0038	0.012*
3	zenith angle	0.057°	0.057	0.059	0.059	0.092	0.702*
4	T(41)	-	-	23.03 K	-		
5	T(42)	-	-	-	29.97 K		
6	T(40)	-	-	-	-	531.3 K	
7	P(0)	-	-	-	-		1286* mb
8	background	0.0022	-	0.0023	0.0023	0.0023	0.0027*

*indicates inversion of nearly singular matrix

Table 16. Some eigenvectors and associated eigenvalues of modified information matrix for low-resolution spectra.

Eigenvectors:			
(1)	(2)	. . .	(8)
0.0083607	0.05296		-0.3934
0.025936	0.0074088		0.11675
-0.70477	-0.13512		-0.39486
-0.16379	0.65338		-0.38916
-0.17926	-0.70975		-0.39096
-0.016959	-0.06559		-0.38969
0.66577	0.20956		-0.39544
-0.0071575	0.0028461		0.25133

Eigenvalues:	
(1)	5.3967×10^{-5}
(2)	1.4169×10^{-4}
(3)	0.0062167
(4)	0.020332
(5)	0.12136
(6)	0.45162
(7)	1.134
(8)	6.2663

IV. CONCLUSIONS

This report has described the operation of a computer program for calculating atmospheric absorption spectra for slant paths through the atmosphere, using as input the AFGL line parameter listing. This program, unlike many others, was specifically written to employ an efficient means of including the effects of instrument spectral response functions. In addition the routine is written so that the precision of the convolved or degraded spectral values can be varied to match the noise level of observed spectra. The program was tested and compared to calculated spectra from another source and found to be working correctly.

Some information analysis techniques were then applied to a particular example of slant path spectra. The analysis included an identification of the "bad" parameters and estimated uncertainties for possible sets of unknown parameters. All that was required was a set of spectra and the corresponding conditions for each spectrum. With the aid of a few simple matrix operations the character of the information in the spectra was quickly determined. These techniques are simple and versatile and could be used on many different types of data, both simulated (as in this study) or observed.

The analysis indicated that trying to retrieve closely spaced temperature profile values can lead to large uncertainties in the temperature difference. Problems were also found with simultaneous retrieval of the base level pressure and apparent zenith angle. By analyzing a second set of spectra at a lower spectral resolution, the loss of information with loss of resolution was investigated. In particular, the loss of temperature information was found to be more pronounced than that for the other spectral parameters considered.

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APPENDIX A

THE SPECTRUM CALCULATION PROGRAM

The basic layout of the program is shown in the flow chart (Fig. A-1). The four basic parts are (1) a main program controlling input and output and calculation order; (2) the Snider-Goldman slant path program (subroutine SNIDER and associated subroutines called within SNIDER) for calculating the path of radiation in an inhomogeneous atmosphere; (3) subroutine PATHST for converting the output of SNIDER into a series of layers with specific airmass, temperature, and pressure values; and (4) subroutine NSPEC for calculating the spectrum. All of the source statements for these parts are listed at the end of this appendix.

I. MAIN PROGRAM

There are three basic sets of inputs needed by the main or controlling program; these are listed in Table A-1. The first consists of the input parameters for the Snider-Goldman routine; these specify the observer-source geometry (ALAT, Z, HOBS) and the atmospheric profile (LEVELS, H, T, P). Since SNIDER produces its own pressure profile by integrating the hydrostatic equation and using P(0) and the temperature profile, only the first pressure value is used.

The second set consists of parameters needed by PATHST. These are a value for Nge, which determines the smallest airmass in a layer of [total airmass/Nge], and a set of values, R(1), R(2), . . . , R(5), for calculating the mixing ratios in the layers. As currently written, only constant mixing ratios are allowed, but other types can be easily included by suitably modifying subroutine RMIX. Also, provision has been made for only five absorbing species but others could be included.

The third set of inputs are values needed to control NSPEC. These include the upper and lower frequency positions, VU and VL; the number of observed frequency values, NVO; and the parameters which control the convolution routine. These latter are discussed more fully in Chapter III describing subroutine NSPEC. Also included in this set is the unit number for the line parameters. This parameter must be passed to NSPEC which controls the input of the line parameter data for the spectrum calculation.

The output from the main program is in two parts. First is the calculated transmittance values starting from τ(VL) up to τ(VU). Second is a series of error codes. The subroutine ERROR called in the last statement of the controlling program dumps the stored error code numbers for any errors which may have occurred during execution of previous steps. These code numbers are in the order in which the errors occurred, and may be interpreted by referring to Table A2. No claims for completeness are made for this list of errors. An attempt was made to write self-correcting routines into the program for some of the more simple errors, but there are undoubtedly many which have not been corrected for. The first output

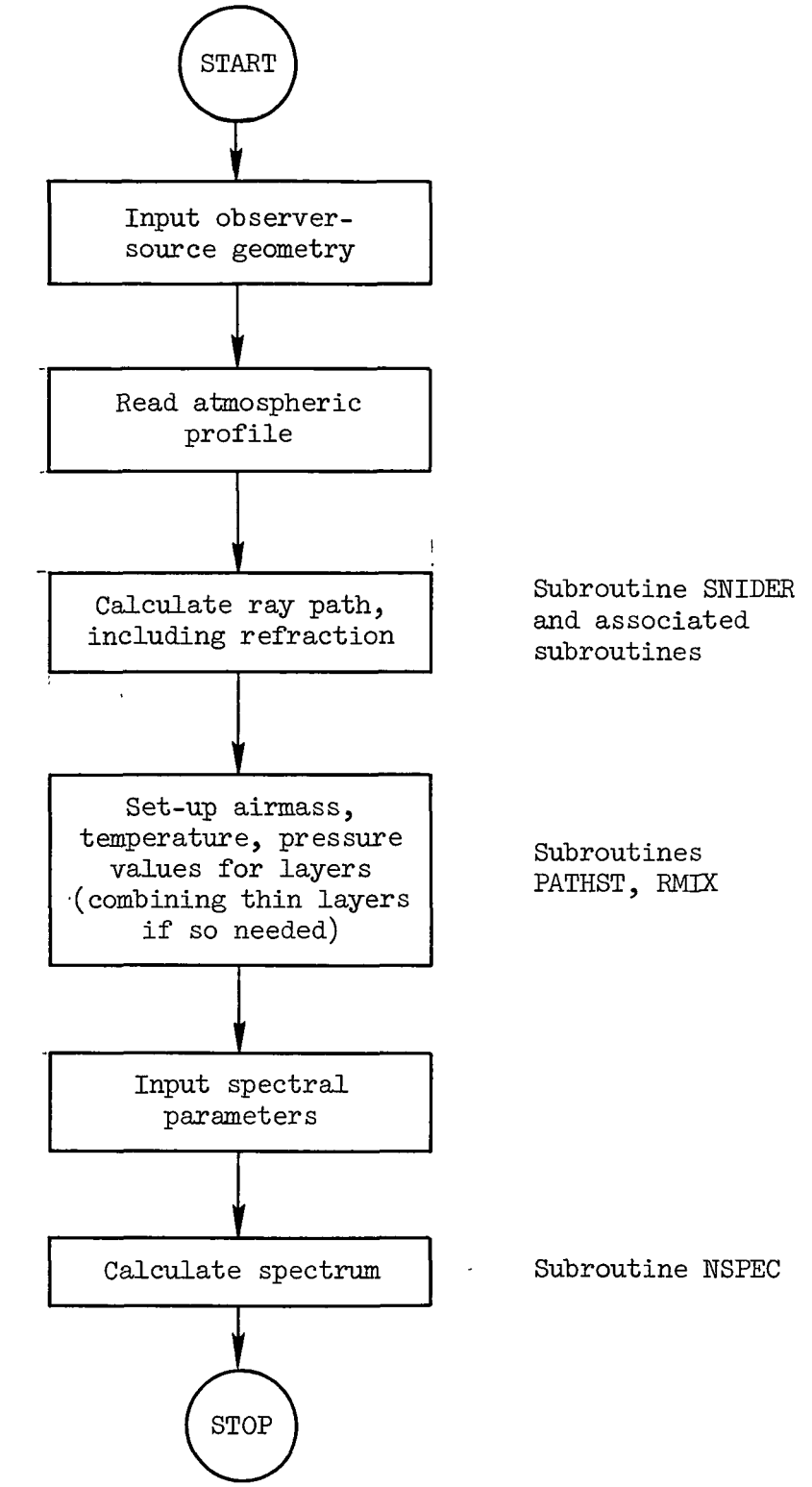

Fig. A1 - Overall program logic

Table A1. Inputs to main program.

LEVELS	Number of levels in atmospheric profile (must be less than 190)
ALAT	Latitude of the observer (in degrees)
Z	Apparent zenith angle of incoming ray (in degrees)
HOBS	Observer height (in kilometers)
NGE	Integer for structuring layers for input to spectrum calculation routine
LUNIT	Unit number of file containing line parameters. This must be the same number as in a JCL DD card; e.g., if LUNIT = 11 then there is a DD card of the form //GO.FT11F001 DD . . . identifying the line parameter file.
H, T, P	Atmospheric profile where H is the height in kilometers, T is the temperature in Kelvin, and P is the pressure in mb. These are on unit 10 (see above).
R	An array of mixing ratio values. As currently written it requires five values R(1), . . , R(5) for the volume mixing ratio of each species; i.e., (molecules of absorber)/(total molecules).
VL	Lower frequency position in cm^{-1}
VU	Upper frequency position in cm^{-1}
NVO	Number of observed frequency values
NM NO	Set convolution iteration limits (see write-up for subroutine NSPEC)
EPA	Convergence criterion. This corresponds to the estimated uncertainty in the transmittance values.
EXTNT	Sets the integration limits for the convolution. It is given as the number of B values (see below) in the integral.
B	Resolution width in cm^{-1}. As currently written this value is half of the full width at half max of a Gaussian slit function.
LIMTOP	Sets the maximum number of lines contributing to any one spectral value (must be less than 200)

Table A1 (continued)

TTOP	Sets the maximum value of the absorption coefficient. When a calculated absorption coefficient exceeds TTOP, the corresponding monochromatic transmittance is set to zero.
NTST	Integer debug flag used to output intermediate convolution results.
	NTST = 0 normal operation
	NTST = 1 the M- and T-table values are printed out on unit 13 for each step of each convolution
	NTST = 2 the monochromatic transmittance values and corresponding frequency positions are printed out on unit 14
	The NTST = 2 function has been removed from the version listed in this appendix.

All input is done with unformated READ statements so that there are no specific format requirements for the input cards.

Table A2. Error codes for subroutine ERROR.

Code No.	Description of Error and Action Taken
1	LEVELS value is greater than 190. LEVELS is set to minimum of 190 and LEVELS.
2	SNIDER could not find index of atmospheric layer containing the observer. Execution terminated.
3	SNIDER could not find index of atmospheric layer containing the source. JHT is set equal to LEVELS, where JHT is the variable labeling the index of the source layer. This is equivalent to assuming the source is at the top of the atmosphere.
4	Zenith angle is incorrect for specified observer-source geometry; e.g., $Z > 90$ but $HOBS > H_{source}$. Execution terminated.
5	SNIDER has looped 10 times trying to find astronomical zenith angle without success to 0.001. Execution terminated [see Ref. (10)].
6	GAMMA = 0 in subroutine OM. Execution continues; results may be in error.
7	Error in OM, not #6 above. Execution continues; results may be in error.
8	Error in subroutine OPT1. Execution continues, results may be in error.
9	FTOT in subroutine PATHST is less than or equal to 0.001, indicating that essentially no airmass is in the path. Execution continues; results may be in error.
10	NM in subroutine NSPEC was specified too large. NM is set to minimum of 7 and NM.
11	Failure to converge in convolution routine of subroutine NSPEC for current value of frequency position and specified maximum number of iterations. Execution continues; current value on T-table main diagonal is used as transmittance value.

Table A2 (continued)

Code No.	Description of Error and Action Taken
12	NLINES equals zero in subroutine NSPEC, indicating that there are no active lines at the current frequency position. Execution continues; transmittance value is set equal to 1.
13	The number of active lines, NLINES, is greater than LINTOP, the capacity of array IACTV. Execution continues; enough lines are kicked out so that NLINES equals LINTOP.
14	VU < VL. Execution terminates.

value from ERROR is the number of type 11 errors which occurred. Since this is a common error and may occur many times, only the number is kept and not the sequence. Use of NTST = 1 may be used to check specific frequency positions.

II. SUBROUTINE SNIDER

Questions about the operation of this part of the program can be answered by referring to Ref. (10). A few minor changes were made in the program listed in that reference in order to run it as a subroutine.

The most important change involved collecting all the error corrections into the error code listing (Table A-2). Also the profile input section was modified.

In addition to these changes, statements were inserted to cause SNIDER to output the individual layer parameters (T,P,u) as it traced the ray through the atmosphere. This is done by calls to subroutine POUT. The layer parameters are stored in the array UED, PED, and TED kept in blank COMMON.

An attempt was made to preserve as much of the flexibility of the Snider-Goldman program as possible. This includes the option of specifying the astronomical zenith angle and having the program find the corresponding apparent zenith angle by an iterative search. To use this facility, the input to SNIDER must be changed so that LSTOP, the 4th input value passed to SNIDER, is equal to 1; see Ref. (10) before using this option.

One minor problem encountered with SNIDER during debugging is that it will not run with an input zenith angle of zero. The associated subroutines are OM, OPT1, ASINX, ZCOMP, QUAD, GETT, and POUT.

III. SUBROUTINE PATHST

This subroutine takes the individual layer parameters stored in UED, PED, and TED and rearranges them into a set of layers with nearly the same airmass values stretching from the lowest layer crossed by the ray up to the highest level.

First it sums all the airmass values to get FTOT, the total airmass. It then folds the parameter arrays to combine contributions from the same layer that occurred during the descending and ascending portions of the path, if the zenith angle is greater than 90°. It next starts from the lowest layer and combines the contributions of the next highest layers until the summed airmass exceeds FTOT/Nge. A call to subroutine RMIX returns a set of mixing ratio values for this composite layer and then the program begins combining the next layers until the airmass again exceeds FTOT/Nge. The recombination continues throughout the entire path. The resulting modified set of atmospheric path parameters is stored in U, PRES, TMP, and RMIXR in blank COMMON.

IV. SUBROUTINE NSPEC

This subroutine takes the path parameters from PATHST, the line parameters from unit LUNIT, and the frequency and convolution parameters from the SUBROUTINE call and calculates the transmittance. The file of line parameters has been created by a separate program BOB listed in Appendix B. These consist of (1) the lowest frequency at which the line has significant absorption, (2) the line intensity, (3) the pressure-broadening coefficient, (4) the lower state term value, (5) the molecule code number, and (6) 1/2 the frequency range of significant absorption by the line. The program has a set of arrays in which the parameter values of the active lines are stored. The input file is sorted on the lowest contributing frequency values and NSPEC proceeds from the lowest observed frequency value, VL, to highest value, VU. The input file is processed in sequence and the active lines are sorted by NSPEC according to the highest frequency at which they have significant absorption. Because of this double sorting (i.e., sorted input file and sorted active list), when the transmittance at a new frequency position is to be calculated, the program needs to check only the first active line to see if any lines need to be removed from the active file. If the first line is still active at the new frequency, all the other lines are also still active. This eliminates the need to check every active line at every frequency position. If the first line is no longer active it is deactivated and the next line is checked. This continues until all lines which are not active at the new frequency position have been removed. The program then checks the next line in the input file. If it is not active at the new frequency, none of the lines below it in the file will be, and the program proceeds to calculate the transmittance. If the new line is active, it is inserted into the active list in the proper sequence and then the next input line is checked. This minimizes the number of checking operations required to maintain a correct list of active lines. Also, by not storing the parameters of inactive lines in core, the overall storage requirements of the program are reduced considerably.

In addition to the input parameters, the program stores the molecular masses (in amu) in the array FMAS. This value is needed to calculate the Doppler width. The active line parameters are stored in the arrays V0, S0, AMAS, ALL, EPP, MOLNM, and CENTW. Instead of sorting the elements of these seven arrays, an array of indices is kept, called IACTV, and these are kept in such a way that the order of the elements in IACTV determines the order in which the lines have to be checked for possible deactivation.

In order to calculate the convolved transmittance, τ_{con}, at observed frequency position, ν_i, the program must calculate the monochromatic transmittance, τ_{mon}, at frequency positions ν_1', . . . , ν_n' (refer to Fig. 2). These are then multiplied by an instrument response (or slit) function value and summed to give τ_{con}. The storage of the τ_{mon} values in array T proved to be the most logically involved aspect of the calculation. The actual values are calculated quite simply using the Hui et al.[23] Voigt routine and summing absorption coefficients by layers and then by active lines in two nested DO-loops. The slit function value, called WT,

is evaluated, multiplied by the τ_{mon} values, and summed in another loop. The problem is how to store the τ_{mon} values so as to be able to retrieve them efficiently. This is all done by proper arrangement of the values in the array T.

First, the maximum number of τ_{mon} values is determined from NO and NM according to NTOT = $2 \cdot 2^{NM} + 1$. The τ_{mon} values will then be stored in the first NTOT elements of T as if each position in T were a frequency position with a spacing between elements of DELVC = EXTNT * $H/2^{NM+1}$. This spacing fits the NTOT values into a total frequency range of EXTNT × H, where H is one-half the full width at half height of the slit function.

To start off the calculation, the first element of the T-table is evaluated using NO to determine the number of points, as shown in Table A-3. Also listed are the number of new points (i.e., τ_{mon} values) used in subsequent iterations. The index n along the left-hand side of the table is used by the program to determine the maximum number of iterations. When the n value exceeds NM, the convolution stops iterating and takes the convergence failure error route.

For example, when NO = 1 and NM = 5, the first trapezoidal rule evaluation is made with five points. The corresponding τ_{mon} values are loaded into T. The next step involves a four-point midpoint rule evaluation. These two values are checked for convergence. If the convergence criterion is satisfied (AMTS.LE.EPA), the convolved transmittance value is loaded into the array TCI. If there is no convergence, an eight-point midpoint rule evaluation is done and the T- and M-table values calculated and compared. The procedure continues until convergence or until the 32-point midpoint rule value is calculated. After this value, the convergence failure route is taken. In this way, up to 65 τ_{mon} values would be calculated and loaded into array T in order of increasing frequency position. When moving to a new observed frequency position (next VI value), the new τ_{mon} values that need to be calculated are written on top of the old τ_{mon} values which are no longer needed. In this way space is conserved and the values of T can be efficiently retrieved.

As currently written, NSPEC generates its own observed frequency positions at which to calculate τ_{con} values. This can be easily changed to calculate τ_{con} values at specified nonuniformly spaced frequencies by passing the array of frequency positions to NSPEC and changing the scalar VI to an array V(I) of these frequency positions.

Table A3. The number of points in the first trapezoidal evaluation for different values of NO.

n \ NO	0	1	2	3	4	5
0	3					
1	2	5				
2	4	4	9			
3	8	8	8	17		
4	16	16	16	16	33	
5	32	32	32	32	32	65 . . .
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.

```
//      TIME=4,REGION=512K
/*JOBPARM  LINES=4000,DISKIO=3000
//NPL   EXEC  FORTXCG,PARM=(FORMAT,GOSTMT,
//      MAP,XREF,'OPT(2)'),TIME=4,REGION=512K
//FORT.SYSLIN  DD  DSN=TSO462.NSPEC.OBJ,DISP=(OLD,PASS),
//    SPACE=(TRK,(1,1))
//FORT.SYSIN  DD  *
      DIMENSION UIN(300),PU(300),TU(300),U(50),PRES(50),TMP(50),
     * RMIXR(5,50),H(200),P(200),T(200),R(5)
      DIMENSION TCI(300)
      REAL*8 VL,VU
      COMMON H,P,T,UIN,PU,TU,IED,U,PRES,TMP,RMIXR
      READ(5,*) LEVELS,ALAT,Z,HOBS,NGE,LUNIT
      DO 100 I=1,LEVELS
      READ(10,*) H(I),T(I),P(I)
  100 CONTINUE
      CALL SNIDER(LEVELS,ALAT,0,0,7,5.0,HOBS,82.0,1)
      READ(5,*) R(1),R(2),R(3),R(4),R(5)
      CALL PATHST(NGE,R,LEVTOP)
      READ(5,*) VL,VU,NVC,NM,NO,EPA,EXTNT,B,LINTOP,TTOP,NTST
      CALL NSPEC(VL,VU,NVC,NM,NO,EPA,EXTNT,B,LINTOP,LEVTOP,TTOP,
     * NTST,LUNIT,TCI)
      DO 500 I=1,NVC
      WRITE(12,110) TCI(I)
  110 FORMAT(F8.5,1X,F11.5,1X,I3)
  500 CONTINUE
      CALL ERROR(1,1)
      STOP
      END
      SUBROUTINE SNIDER(LEVELS,ALAT,NOPT,LSTOP,DD1,DD2,DD3,DD4,NLOPT)
      DIMENSION VARCOM(200)                                          00000010
      DIMENSION P(200)                                               00000020
      DIMENSION H(200),T(200),GRAD(200),GAMMA(200)                   00000030
      DIMENSION Z(200)                                               00000040
      DIMENSION THETAS(200),DELTH(200)                               00000050
      DIMENSION OMSTRA(200)                                          00000060
      DIMENSION   AIRS(200)                                          00000070
      DIMENSION   ESTR(200)                                          00000080
      DIMENSION RHO(200), ZRHO(200)                                  00000090
      DIMENSION XPTS(6),WGHT(6)                                      00000100
      REAL*8 TITLE(13)                                               00000110
      COMMON /SLANT/ VARCOM                                          00000120
      COMMON H,P,T                                                   00000125
      EQUIVALENCE (VARCOM(1),G),   (VARCOM(2),AIRWT), (VARCOM(3),    00000130
     1  RSTAR),  (VARCOM(4),RADIUS), (VARCOM(5),CONST1),(VARCOM(6)    00000140
     2,XPTS(1)),(VARCOM(12),WGHT(1)),(VARCOM(18),FAKE)
      EQUIVALENCE (VARCOM(20),REFAM)                                 00000160
      REAL IP                                                        00000170
      FCNA(Q000FL)=(1.0+Q000FL/2.0)*(1.0+2.0*Q000FL*(1.0+Q000FL/2.0)/3.000000180
     1)/(1.0+Q000FL)**2                                              00000190
      FCNB(Q001FL)=2.0*Q001FL*(1.0+Q001FL/2.0)/3.0                   00000200
      FCNC(Q002FL,Q003FL,Q004FL,Q005FL)=2.0*Q004FL*Q005FL*Q002FL/(1.0+Q000000210
     1Q3FL*Q005FL)                                                   00000220
      FCNE(Q006FL,Q007FL)=Q006FL*(1.0-Q007FL)*(1.0-Q007FL*Q006FL/6.0) 00000230
      FHC(X)=GPHI * X/(RADIUS + X)                                   00000240
      FZC(Y)=RADIUS*Y/(GPHI - Y)                                     00000250
      NTAPA2=5                                                       00000260
      NERROR=6                                                       00000270
      NTAPA3=6                                                       00000280
      RADSEC=.2062648066E+06                                         00000290
      RADCON=.174532925E-01                                          00000300
      FAKE=-10000000.0                                               00000310
```

```
      XPTS(1)=-.466234757E+00                                          00000320
      XPTS(2)=-.330604693E+00                                          00000330
      XPTS(3)=-.119309593E+00                                          00000340
      XPTS(4)=-.119309593E+00                                          00000350
      XPTS(5)=.330604693E+00                                           00000360
      XPTS(6)=+.466234757E+00                                          00000370
      WGHT(1)=.056622491E-01                                           00000380
      WGHT(2)=.180380786E+00                                           00000390
      WGHT(3)=.233956967E+00                                           00000400
      WGHT(4)=.233956967E+00                                           00000410
      WGHT(5)=.180380786E+00                                           00000420
      WGHT(6)=.356622491E-01                                           00000430
      AVNMB= 6.02257 E26                                               00000440
      IF (LEVELS.GT.190) CALL ERROR(1,0)
      LEVELS=MIN0(LEVELS,190)
 1000 CONTINUE                                                         00000450
C1000 READ (NTATA2,1021) (TITLE(I),I=1,13)                             00000460
 1021 FORMAT(13A6)                                                     00000470
      ALTORH=1.0                                                       00000510
      PHI = ALAT * RADCON                                              00000530
      A = 6378160.0                                                    00000540
      B = 6356775.0                                                    00000550
      R = SQRT((A**4*(COS(PHI))**2  + B**4*(SIN(PHI))**2)/             00000560
     1 ( A**2*(COS(PHI))**2  + B**2*(SIN(PHI))**2))                    00000570
      X = COS(2.0 * PHI)                                               00000610
      Y = COS(4.0 * PHI)                                               00000620
      G = 980.6160 * ( 1.0 -( 0.0026373 * X ) + ( 0.0000059 *X**2))    00000630
      G = G/100.0                                                      00000640
      PARTGZ = 3.085462 E-06  + 2.27 E-09 * X  - 2.0 E-12 * Y          00000650
C     RADIUS = 2.0 * G / PARTGZ                                        00000660
      RADIUS =R                                                        00000670
      RSTAR=8314.39                                                    00000680
      AIRWT=28.966                                                     00000690
      CONST1=G*AIRWT/RSTAR                                             00000700
      GEE  = 9.80665                                                   00000710
      GPHI = RADIUS * G / GEE                                          00000720
      DO 1 I=1,LEVELS                                                  00000800
      P(I)=P(I)*100.                                                   00000810
      H(I)=H(I)*1000.                                                  00000820
    1 CONTINUE                                                         00000830
 1051 CONTINUE                                                         00000840
      IF(P(1).EQ.0.)  P(1)= 101325.0                                   00000850
      DO 1090  I=2,LEVELS                                              00000860
      CALL GETT(H(I-1),H(I),P(I-1),P(I),T(I-1),T(I))                   00000870
 1090 CONTINUE                                                         00000880
      IF(ALTORH) 1100,1150,1100                                        00000890
 1100 CONTINUE                                                         00000900
      DO 1125  I=1,LEVELS                                              00000910
      H(I) = FHG(H(I))                                                 00000920
 1125 CONTINUE                                                         00000930
 1150 CONTINUE                                                         00000940
      DO 1175  I=2,LEVELS                                              00000950
      GRAD(I-1)=(T(I)-T(I-1))/(H(I)-H(I-1))                            00000960
      GAMMA(I-1)=(CONST1)/(GRAD(I-1)+CONST1)                           00000970
      DELTH (I-1)= H(I) -H(I-1)                                        00000980
 1175 CONTINUE                                                         00000990
      GAMMA(LEVELS) = 1.                                               00001000
      GRAD(LEVELS) = 0.                                                00001010
      DELTH( LEVELS ) = 0.0                                            00001020
      SUMRHO = 0.0                                                     00001030
      DO 1190 I = 1,LEVELS                                             00001040
      ZRHO(I) = AVNMB * P(I) /(RSTAR * T(I))                           00001050
```

```
      SUMRHO = SUMRHO + ZRHO(I) * DELTH (I)                              00001060
 1190 CONTINUE                                                           00001070
      RHO(1) = ZRHO(1)                                                   00001080
      OMSTRO = 1.0 -( RHO(1) / 2.5475521 E25 )                           00001090
      DO 1200    I=2,LEVELS                                              00001100
      CALL OM (H(I),H(I-1),H(I-1),T(I-1),GAMMA(I-1),OMEGA, DUMMY)        00001110
      NLC =I-1                                                           00001120
      OMSTRA(NLC)=OMEGA                                                  00001130
      RHO(I)=RHO(I-1)*(1.0-OMEGA)                                        00001140
      CALL OPTI(H(I-1),H(I),T(I-1),GAMMA(I-1),RHO(I-1),OMEGA,AIRS(I-1)   00001150
     1)                                                                  00001160
 1200 CONTINUE                                                           00001170
      AIRS(LEVELS)=0.0                                                   00001180
      DO 1225  I=2,LEVELS                                                00001190
      IND=LEVELS+1-I                                                     00001200
      AIRS(IND)=AIRS(IND)+AIRS(IND+1)                                    00001210
 1225 CONTINUE                                                           00001220
      STARD = AIRS(1)                                                    00001230
C     REFAM = AIRS(1)                                                    00001240
      REFAM = 2.15335 E29                                                00001250
 1243 FORMAT(1H1)                                                        00001420
      LINC=-1                                                            00001430
      ALTORH=1.0                                                         00001470
      CALL POUT(-1.0,1.0,1.0)                                            00001475
 1250 CONTINUE
      DD3=DD3*1000.0                                                     00001490
      DD4 = DD4*1000.0                                                   00001500
      NLOP = 0                                                           00001510
      JMP=LSTOP+1                                                        00001520
      NTF=0                                                              00001530
      LINC=-1                                                            00001540
      GO TO (1257,1257,1257,1256,1000), JMP
 1256 GO TO 1400                                                         00001560
 1257 DO 4150 IN=1,50                                                    00001570
      NTF=0
      NLOP = NLOP + 1                                                    00001610
      IF (NLOP.GT.NLOPT) GO TO 1400                                      00001620
 1297 CONTINUE                                                           00001630
      ZO=DD1                                                             00001640
      ZOS=ZO                                                             00001650
      OHGHT=DD3                                                          00001660
      HGHT=DD4                                                           00001670
 1258 WAVEL=DD2                                                          00001680
      ZO=ZOS                                                             00001690
 1270 IF(ALTORH) 1280,1290,1280                                          00001700
 1280 OHGHT=FHC(OHGHT)                                                   00001710
      HGHT =FHC( HGHT)                                                   00001720
 1290 CONTINUE                                                           00001730
      ZOS=ZO                                                             00001740
      ZT=ZOS                                                             00001750
 1295 CONTINUE                                                           00001760
      NTF=NTF+1
      IF (NTF-10) 1296,1296,4700                                         00001770
 1296 CONTINUE                                                           00001780
      SECT2=0.                                                           00001790
      SECT3 = 0.0                                                        00001800
      SECT4 = 0.0                                                        00001810
      RSAVE=0.                                                           00001820
      OSAVE=0.                                                           00001830
      PSAVE= 0.0                                                         00001840
      TSAVE= 0.0                                                         00001850
      HDIFF = 0.0                                                        00001860
```

```
      HTAN = 0.0                                                        00001870
      TP   = 273.15                                                     00001880
       TG=TP                                                            00001890
      ZG=ZO*RADCON                                                      00001900
      UTEMP=1.0/WAVEL**2                                                00001910
      E1 = 0.0                                                          00001920
      E1=.CC00643280+.0294981/(146.0-UTEMP)+.0002554/(41.0-UTEMP)       00001930
      DO 1300 IHT=2,LEVELS                                              00001940
      IF(H(IHT)-OHGHT)  1300,1325,1325                                  00001950
 1300 CONTINUE                                                          00001960
      CALL ERROR(2,0)
      RETURN
 1325 IHT=IHT-1                                                         00001990
      CALL GETT ( H(IHT), OHGHT, P(IHT), POB, T(IHT), T(IHT) )          00002000
      RHOP = AVNMB * POB/( RSTAR*T(IHT))                                00002010
      RHOMIN = RHOP                                                     00002020
      TP = T( IHT )                                                     00002030
      DO 1335  IND= 2,LEVELS                                            00002040
      JHT=IND                                                           00002050
      IF(H(JHT)-HGHT)  1335,1340,1340                                   00002060
 1335 CONTINUE                                                          00002070
      CALL ERROR(3,0)
 1337 FORMAT(20H  UPPER HEIGHT RESET)                                   00002090
 1330 JHT=IND                                                           00002100
 1340 CONTINUE                                                          00002110
      ESTR (1) = FCNE (E1 , OMSTRO )                                    00002120
      DO 1350 I=2,LEVELS                                                00002130
      ESTR(I)=FCNE(ESTR(I-1),OMSTRA(I-1))                               00002140
 1350 CONTINUE                                                          00002150
      JNS=1                                                             00002160
      HMINA=OHGHT                                                       00002170
      IF (ZOS.LE.90.) IF (HGHT-OHGHT+.05) 4500,4600,1373                00002180
      CALL OM(OHGHT,H(IHT),H(IHT),T(IHT),GAMMA(IHT),OME,XXX)            00002190
      EC=FCNE(ESTR(IHT),OME)                                            00002200
      ZCRIT = ASIN ((1.0 + ESTR (1) ) * ( 1.0 - OHGHT / RADIUS ) / ( 1.000002210
     1 + EO ))                                                          00002220
      ZCRIT=3.141592653-ZCRIT                                           00002230
      IF (ZO.GT.ZCRIT+.00001) IF(OHGHT-HGHT+.05) 4500,4600,1357         00002240
      FVAL =SIN(ZG)*(1.+EO)/(RADIUS-OHGHT)                              00002250
      F1=(1.+ESTR(1))/ RADIUS - FVAL                                    00002260
      DO 1351 I=2,LEVELS                                                00002270
      K=I-1                                                             00002280
      F2=(1.+ESTR(I))/(RADIUS-H(I))-FVAL                                00002290
      IF(F2*F1) 1352,1352,1351                                          00002300
 1351 F1=F2                                                             00002310
      GO TO 4500                                                        00002320
 1352 H1=H(K)                                                           00002330
      H2=H(K+1)                                                         00002340
      H3=H1-(H2-H1)*F1/(F2-F1)                                          00002350
 1353 CALL OM(  H3,H(K),H(K),T(K),GAMMA(K),W,XXX)                       00002360
      F3=(1.+FCNE(ESTR(K),W))/(RADIUS-H3)-FVAL                          00002370
      HM=H3-F3*((H3-H2)/(F3-F2)+ (H3-H1)/(F3-F1)-(H2-H1)/(F2-F1))       00002380
      IF(ABS(HM-H3).LE.1.)  GO TO 1354                                  00002390
      H1=H2                                                             00002400
      H2=H3                                                             00002410
      H3=HM                                                             00002420
      F1=F2                                                             00002430
      F2=F3                                                             00002440
      GO TO 1353                                                        00002450
 1354 IF (HM.GT.HGHT+.05) GO TO 4500                                    00002460
      HMINA=HM                                                          00002470
      ZGSAVE=ZG                                                         00002480
```

```
      HOSAVE=OHGHT                                                          00002490
      HSSAVE=HGHT                                                           00002500
      ZO=1.570796326                                                        00002510
      OHGHT=HH                                                              00002520
      HGHT=HOSAVE                                                           00002530
      TG=T (K)                                                              00002540
      JSAV=JHT                                                              00002550
      JHT=IHT+1                                                             00002560
      IHT=K                                                                 00002570
      INS=2                                                                 00002580
      GO TO 1374                                                            00002590
 1355 RSAVE=REFRS                                                           00002600
      OSAVE=SECT2                                                           00002610
      PSAVE = SECT3                                                         00002620
      TSAVE = SECT4                                                         00002630
      HGHT=HSSAVE                                                           00002640
      JHT=JSAV                                                              00002650
      INS=3                                                                 00002660
      GO TO 1374                                                            00002670
 1356 IF(HSSAVE.LT.HOSAVE)  JNS=2                                           00002680
      OHGHT=HOSAVE                                                          00002690
      GO TO 3950                                                            00002700
 1357 CALL OM(HGHT,H(JHT),H(JHT),T(JHT),GAMMA(JHT),W,XXX)                   00002710
      ZSAVE=ASIN((1.+EO)/(1.+FCNE(ESTR(JHT),W))*(RADIUS-HGHT)/(RADIUS-      00002720
     1OHGHT))                                                               00002730
      IHT=JHT                                                               00002740
      ZZ=ZO                                                                 00002750
      ZO=ZSAVE                                                              00002760
      HOSAVE=OHGHT                                                          00002770
      HSSAVE=HGHT                                                           00002780
      OHGHT=HSSAVE                                                          00002790
      HGHT=HOSAVE                                                           00002800
      ZO=ZZ                                                                 00002810
      INS=4                                                                 00002820
      GO TO 1374                                                            00002830
 1358 JNS=1                                                                 00002840
      OHGHT=HOSAVE                                                          00002850
      HGHT=HSSAVE                                                           00002860
      GO TO 3950                                                            00002870
 1373 INS=1                                                                 00002880
 1374 CONTINUE                                                              00002890
      CALL OM(OHGHT,H(IHT),H(IHT),T(IHT),GAMMA(IHT),OME,DUMMY)              00002900
      CALL OM(H(IHT+1),OHGHT,H(IHT),T(IHT),GAMMA(IHT),OMO,TOO)              00002910
      EO=FCNE(ESTR(IHT),OME)                                                00002920
      VARCOM(19)=RHO(IHT)*(1.-OME)                                          00002930
      IF(JHT.EQ.IHT+1)  GO TO 1380                                          00002940
      US=FCNU(FCNA(EO),FCNB(EO),EC,OMO)                                     00002950
      CALL ZCOMP(ZO,Z(IHT+1),OHGHT,H(IHT+1),US,DELZ,THETAS(IHT+1)           00002960
     1)                                                                     00002970
      CALL QUAD(THETAS(IHT+1),ZO,OHGHT,TOO,P(IHT+1),GAMMA(IHT),EO,SECT1,    00002980
     1SECT2,SECT3,SECT4)                                                    00002990
      CALL POUT(SECT2,SECT3,SECT4)                                          00002994
      REFR =(DELZ +SECT1)                                                   00003000
      REFRS=REFR*RADSEC                                                     00003010
 2010 DELRS=REFRS                                                           00003020
 2060 INDU=JHT-2                                                            00003030
      IHT1=IHT+1                                                            00003040
      IF(INDU.LT.IHT1)  GO TO 1376                                          00003050
 1360 CONTINUE                                                              00003060
      DO 1375 I=IHT1,INDU                                                   00003070
      U=FCNU(FCNA(ESTR(I)),FCNB(ESTR(I)),ESTR(I),OMSTRA(I))                 00003080
      CALL ZCOMP(Z(I),Z(I+1),H(I),H(I+1),U,DELZ,THETAS(I+1))                00003090
```

```
      DELZT=DELZT+DELZ                                                  00003100
      VARCOM(19)=RHO(I)                                                 00003110
      CALL QUAD(THETAS(I+1),Z(I),H(I),T(I),P(I),GAMMA(I),ESTR(I),ADD1,  00003120
     1ADD2,ADD3,ADD4)                                                   00003130
      CALL POUT(ADD2,ADD3,ADD4)                                         00003135
      SECT2=SECT2+ADD2                                                  00003140
      SECT3 = SECT3 + ADD3                                              00003150
      SECT4 = SECT4 + ADD4                                              00003160
      DELR =(DELZ+ADD1)                                                 00003170
      REFR = DELR+REFR                                                  00003180
      REFRS=REFR*RADSEC                                                 00003190
      DELD=DELR*RADSEC                                                  00003200
 1375 CONTINUE                                                          00003210
 1376 CONTINUE                                                          00003220
      RHOLAST=RHO(JHT-1)                                                00003230
      ZLAST=Z(JHT-1)                                                    00003240
      ELAST=ESTR(JHT-1)                                                 00003250
      PLAST = P(JHT -1)                                                 00003260
      TLAST=T(JHT-1)                                                    00003270
      GLAST=GAMMA(JHT-1)                                                00003280
      HLAST=H(JHT-1)                                                    00003290
 1377 CONTINUE                                                          00003300
      CALL OM(HGHT,HLAST,H(JHT-1),TLAST,GLAST,OLAST,XXX)                00003310
      U=FCNU(FCNA(ELAST),FCNB(ELAST),ELAST,OLAST)                       00003320
      CALL ZCUMP(ZLAST,ZFIN,HLAST,HGHT,U,DELZ,THFIN)                    00003330
      VARCOM(19)=RHOLAST                                                00003340
      CALL QUAD(THFIN,ZLAST,HLAST,TLAST,PLAST,GLAST,ELAST,ADD1,ADD2,ADD300003350
     1,ADD4)                                                            00003360
      CALL POUT(ADD2,ADD3,ADD4)                                         00003365
      SECT3 = SECT3 + ADD3                                              00003370
      SECT4 = SECT4 + ADD4                                              00003380
      DELR=DELZ+ADD1                                                    00003390
      REFR=DELR+REFR                                                    00003400
      REFRS=REFR*RADSEC                                                 00003410
      SECT2=SECT2+ADD2                                                  00003420
      DELD=DELR*RADSEC                                                  00003430
      IF (INS.EQ.2)  GO TO 1355                                         00003440
      KJHT=JHT-1                                                        00003450
      GO TO (3950,1355,1356,1358),INS                                   00003460
 1380 RHOLAST=VARCOM(19)                                                00003470
      ZLAST=ZO                                                          00003480
      ELAST=EO                                                          00003490
      HLAST=OHGHT                                                       00003500
      TLAST=T(JHT-1)                                                    00003510
      PLAST = P(JHT -1)                                                 00003520
      GLAST=GAMMA(JHT-1)                                                00003530
      REFR=0.                                                           00003540
      GO TO 1377                                                        00003550
 3950 CONTINUE                                                          00003560
      SECT3 = SECT3 + PSAVE                                             00003570
      SECT4 = SECT4 + TSAVE                                             00003580
      REFRS=REFRS+RSAVE                                                 00003590
      SECT2=SECT2+QSAVE                                                 00003600
      DERF=REFRS/3600.                                                  00003610
      ZEND=ZOS+DERF                                                     00003620
      PEFF = SECT3/SECT2                                                00003630
      TEFF = SECT4/SECT2                                                00003640
      IF(JUMP.EQ.2)  GO TO 4100                                         00003650
 3960 CONTINUE                                                          00003660
      IF (LINC) 3990,3999,3999                                          00003670
 3990 CONTINUE                                                          00003680
C3990 WRITE(NTAPA3,3991) TITLE                                          00003690
```

```
 3991 FORMAT(1H1,5X25HREFRACTION AIRMASS TABLES,5X13A6,/,                00003700
     340X38HALL HEIGHTS ARE IN GEOMETRIC METERS    /,40X,'ALL TEMPERATUR00003710
     3ES ARE IN DEGREES KELVIN'/,40X,'ALL PRESSURES ARE IN N/SQ M '/    00003720
     440X40HTHE APPARENT AND ASTRONOMICAL ANGLES ARE/                    00003730
     540X34HIN DECIMAL DEGREES FROM THE ZENITH/)                        00003740
C      WRITE ( 6 , 3993 ) WAVEL
 3993 FORMAT ( 40X 'THE WAVELENGTH FOR THIS TABLE IS ',F5.2,' MICROMETER00003760
     1S.'//)                                                            00003770
C      WRITE(6,3992)
 3992 FORMAT(11X5HLOWER,5X5HUPPER,5X4HMIN.,  7 X7HCHAPMAN ,  5X7HOPTICAL)00003790
C      WRITE(6,3995)
 3995 FORMAT(1X5HAPP. Z,4X5HHEIGHT,4X6HHEIGHT,4X6HHEIGHT,5X8HAIR MASS,4X00003810
     18HAIR MASS,4X5HHDIFF,3X10HREFRACTION,  4X6HAST. Z,6X 6HP(EFF),4X6H00003820
     1T(EFF),6X6HP(TAN)  )                                              00003830
C      WRITE(6,3996)                                                   00003840
 3996 FORMAT(5X3H(1),7X3H(2),7X3H(3),7X3H(4),8X3H(5),  8X3H(6),10X3H(7), 00003850
     1 6X3H(8),9X3H(9),9X4H(10),6X4H(11),  8X4H(12) ,/,1X )             00003860
      LINC=42                                                           00003870
 3999 LINC=LINC-1                                                       00003880
      ZFIN = ZEND * RADCON                                              00003890
      OHGHT = FZC (OHGHT )                                              00003900
      HGHT = FZC (HGHT )                                                00003910
      HMINA = FZC (HMINA)                                               00003920
      SCALHP = RSTAR * TP  /AIRWT / G                                   00003930
      XP = ( RADIUS + OHGHT ) / SCALHP                                  00003940
      WHY = SQRT ( 0.5 * XP ) * ABS (COS(ZFIN))                         00003950
      FERF = EXP((WHY)**2.0) * ( 1.0 - ERF (WHY))                       00003960
 4040 CONTINUE                                                          00004210
 4150 CONTINUE                                                          00004270
      LSTOP = 3                                                         00004275
      GO TO (1250,4100,1250,1256,1000),JMP                              00004280
 4160 CONTINUE                                                          00004290
      IF (ABS(ZT-ZEND).LT.0.0001) GOTO 4200
      ZOS=ZT-DERF                                                       00004310
      ZO=ZOS                                                            00004320
      GO TO 1295                                                        00004330
 4200 JMP=1                                                             00004340
      GO TO 3980                                                        00004350
 4500 CALL ERROR(4,0)
 4510 FORMAT(1XF14.5, 60X20H *** NO SOLUTION ***)                       00004370
      LINC=LINC-1                                                       00004380
      RETURN
 4600 REFRS=0.                                                          00004400
      SECT2=0.                                                          00004410
      SECT3=0.                                                          00004420
      SECT4=0.                                                          00004430
      GO TO 3950                                                        00004440
 4700 IF (ABS(ZT-ZEND).LT..001) GO TO 4200                              00004450
      LINC=LINC-2                                                       00004460
      CALL ERROR(5,0)
 4705 FORMAT(1H ,37H***NO GCOL SOLUTION FOR LINE ABOVE***)              00004500
 4003 FORMAT( 1H '                UNREFRACTED RAY STRIKES DISC    ' )   00004520
      RETURN
 1400 CONTINUE                                                          00004540
      RETURN
      END                                                               00004560
      SUBROUTINE UM(H,HC,HN,TN,GAMMA,OMEGA,TO)                          00004610
      COMMON /SLANT/ G,AIRWT,RSTAR,RADIUS,CONST1                        00004620
      GM=ABS(GAMMA)                                                     00004630
      IF(GM.LT.0.000001)GO TO 801                                       00004640
      ONEG=1.0-GAMMA                                                    00004650
      ONG=ONEG                                                          00004660
```

```
      IF(RADIUS+HN)  500,500,600                                        00004670
  500 CONTINUE                                                          00004680
      X=CONST1*H*(RADIUS-HO)/TN                                         00004690
      GO TO 700                                                         00004700
  600 CONTINUE                                                          00004710
      A=CONST1*(H-HO)                                                   00004720
      TO=TN+CONST1*(HO-HN)*(ONG)/GAMMA                                  00004730
      X=A/TO                                                            00004740
  700 CONTINUE                                                          00004750
      Y=-X/GAMMA                                                        00004760
      IF(ONEG.EQ.0.) GO TO 800                                          00004770
      IF(1.0-ONEG*Y) 803,803,400                                        00004780
  400 IF(1.0-(1.0-ONEG*Y)) 800,800,300                                  00004790
  300 OMEGA=1.-(1.-ONEG*Y)**(-1./ONEG)                                  00004800
      RETURN                                                            00004810
  800 CONTINUE                                                          00004820
      IF(Y.LT.(-30.0))Y=0.0                                             00004830
    1 FORMAT ( 1H  ,5E20.8)                                             00004840
      IF(  ABS(Y ) .GT. 25.0 )  GO TO 10                                00004850
      OMEGA=1.0- EXP(Y)                                                 00004860
   10 CONTINUE                                                          00004870
      RETURN                                                            00004880
  801 CALL ERROR(6,0)
  802 FORMAT(1X,8H GAMMA=0)                                             00004900
  803 CALL ERROR(7,0)
  804 FORMAT(' BOGBGO ',4E20.8 )                                        00004920
      RETURN                                                            00004950
      END                                                               00004960
      SUBROUTINE OPT1(HO,H,TO,GAMMA,RHOO,OMEGA,AIRM)                    00004970
      COMMON /SLANT/ G,AIRWT,RSTAR,RADIUS,CONST1                        00004980
      RAD=RADIUS-HO                                                     00004990
      XK=CONST1*RAD/(TO*GAMMA)                                          00005000
      SMALLH=(H-HO)/(RADIUS-HO)                                         00005010
      ONEH=1.0-SMALLH                                                   00005020
      ONEG=GAMMA-1.0                                                    00005030
      XK2=(1.0-ONEG*SMALLH*XK)/ONEH                                     00005040
      SUMU=0.0                                                          00005050
      SUMV=0.0                                                          00005060
      XN=0.0                                                            00005070
      DENOM=1.0                                                         00005080
      TERMU=1.0                                                         00005090
      TERMV=1.0                                                         00005100
      TEST=.00000001/(XK*GAMMA)                                         00005110
      KOUNT=0                                                           00005120
 1000 CONTINUE                                                          00005130
      KOUNT=KOUNT+1                                                     00005140
      XN=XN+1.0                                                         00005150
      DENOM=DENOM+ONEG                                                  00005160
      FACT=XN/(XK*DENOM)                                                00005170
      TERMU=TERMU*FACT                                                  00005180
      TERMV=TERMV*FACT*XK2                                              00005190
      SUMU=SUMU+TERMU                                                   00005200
      SUMV=SUMV+TERMV                                                   00005210
      IF (KOUNT-31) 1040,1040,1080                                      00005220
 1040 IF(ABS(TEST)-ABS(TERMV)) 1000,1000,1050                           00005230
 1050 IF(ABS(TEST)-ABS(TERMU)) 1000,1000,1075                           00005240
 1075 IF (KOUNT-30)             1100,1100,1080                         00005250
 1080 WRITE(6,1085)                                                     00005260
 1085 FORMAT(17H0  SOGBOO IN OPT1)                                      00005270
 1100 AIRM=(RADIUS**2/RAD)*RHOO*(SUMU-(1.0-OMEGA)*SUMV/ONEH)            00005280
      RETURN                                                            00005290
      END                                                               00005300
```

```
      FUNCTION ASINX(X)                                                 00005310
      Z=X**2                                                            00005320
      ASINX=X*(1.+Z/6.+.075*Z**2)                                       00005330
      RETURN                                                            00005340
      END                                                               00005350
      SUBROUTINE ZCOMP(ZO,ZS,HO,HS,US,DELZ,THETA)                       00005360
      COMMON /SLANT/ G,AIRWT,RSTAR,RADIUS,CONST1                        00005370
      SMALLH=(HS-HO)/(RADIUS-HO)                                        00005380
      ONEH=1.0-SMALLH                                                   00005390
      TWOH=SMALLH*(2.0-SMALLH)                                          00005400
      C=COS(ZO)                                                         00005410
      S=SIN(ZO)                                                         00005420
      CONE=C*ONEH                                                       00005430
      CPLUS=CONE**2+TWOH                                                00005440
      DELZ=S*(US-TWOH)                                                  00005450
      DEL3=SQRT(1.0-US)*(CONE+SQRT(CPLUS-US))                           00005460
      DEL=S*TWOH/(CONE+SQRT(CPLUS))                                     00005470
      DELZ=ASINX(DEL2/DEL3)                                             00005480
      ZS=ZO+DELZ                                                        00005490
      THETA=ASINX(DEL)                                                  00005500
      RETURN                                                            00005510
      END                                                               00005520
      SUBROUTINE QUAD(THETA,ZO,HO,T,P,GAMMA,EO,SUM,VALM,PBAR,TBAR)      00005530
      DIMENSION VALUEA(6)                                               00005540
      DIMENSION VARCOM(50)                                              00005550
      DIMENSION HINT(6)                                                 00005560
      DIMENSION XPTS(6),THTPTS(6),WGHT(6),VALUES(6)                     00005570
      COMMON /SLANT/ VARCOM                                             00005580
      EQUIVALENCE (VARCOM(1),G),   (VARCOM(2),AIRWT), (VARCOM(3),       00005590
     1  RSTAR),  (VARCOM(4),RADIUS), (VARCOM(5),CONST1),(VARCOM(6)       00005600
     2,XPTS(1)),(VARCOM(12),WGHT(1)),(VARCOM(18),FAKE)
      EQUIVALENCE (VARCOM(20),REFAM)                                    00005620
      EQUIVALENCE (VARCOM(19),RHO)                                      00005630
      FCNA(Q000FL)=(1.0+Q000FL/2.0)*(1.0+2.0*Q000FL*(1.0+Q000FL/2.0)/3.000005650
     1)/(1.0+Q000FL)**2                                                 00005660
      FCNB(Q001FL)=2.0*Q001FL*(1.0+Q001FL/2.0)/3.0                      00005670
      FCNJ(Q002FL,Q003FL,Q004FL,Q005FL)=2.0*Q004FL*Q005FL*Q002FL/(1.0+Q000005680
     1Q3FL*Q005FL)                                                      00005690
      FCNH(Q008FL,Q009FL)=2.0*SIN(Q008FL/2.0)**2+COTAN(Q009FL)*SIN(Q008F00005700
     2L)                                                                00005710
      SMALLR=RADIUS+HO+HO**2/(RADIUS-HO)                                00005720
      VALC=RHO*SMALLR*SIN(ZO)*THETA/REFAM                               00005730
      A=FCNA(EO)                                                        00005740
      B=FCNB(EO)                                                        00005750
      DO  1000 I=1,6                                                    00005760
      THTPTS(I)=THETA*(.5+XPTS(I))                                      00005770
      HINT(I)=FCNH(THTPTS(I),ZO)                                        00005780
 1000 CONTINUE                                                          00005790
      DO 2000 I=1,6                                                     00005800
      CALL GM(HINT(I),HO,FAKE,T,GAMMA, OMEGA,DUMMY)                     00005810
      U=FCNJ(A,B,EO,OMEGA)                                              00005820
      ARG1=1.0-U/COS(ZO-THTPTS(I))**2                                   00005830
      VALUES(I)=1./SQRT(ARG1)                                           00005840
      VALUEA(I)=VALUES(I)*(1.-OMEGA)*SQRT(1.-U)/SIN(ZO-THTPTS(I))**2    00005850
 2000 CONTINUE                                                          00005860
      SUM=0.0                                                           00005870
      VALM=0.                                                           00005880
      DO 3000 I=1,6                                                     00005890
      SUM=VALUES(I)*WGHT(I)+SUM                                         00005900
      VALM=VALM+VALUEA(I)*WGHT(I)                                       00005910
 3000 CONTINUE                                                          00005920
      SUM=SUM*THETA                                                     00005930
```

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      VALM=VALC*VALM                                                    00005940
      PBAR = VALM*P                                                     00005950
      TBAR = VALM*T                                                     00005960
      RETURN                                                            00005970
      END                                                               00005980
      SUBROUTINE GETT(H1,H2,P1,P2,T1,T2)                                00005990
      COMMON /SLANT/ G,AIRWT,RSTAR,RADIUS,CONST1                        00006000
      IF(T2.GT.0.) GO TO 1700                                           00006010
      K=0                                                               00006020
      X=P2/P1                                                           00006030
      XL=ALOG(X)                                                        00006040
      A1=CONST1*(H2-H1)/T1                                              00006050
      CRIT=EXP(-A1)                                                     00006060
      A1=1./A1                                                          00006070
      IF(ABS(X-CRIT).GT..000001)  GO TO 1000                            00006080
       T2=T1                                                            00006090
      RETURN                                                            00006100
 1000 XC=A1*XL+ALOG(A1)                                                 00006110
      ACRIT=-1./XL                                                      00006120
      A2=.000011                                                        00006130
      IF(A1.LT.ACRIT)  A2=A2+ACRIT                                      00006140
 1100 F=A2*XL+ALOG(A2)-XC                                               00006150
      FP=XL+1./A2                                                       00006160
      A3=A2-F/FP                                                        00006170
      IF(K.LT.3)  GO TO 1200                                            00006180
      IF(ABS(A3-A2).LT..0000001)  GO TO 1300                            00006190
 1200 A2=A3                                                             00006200
      K=K+1                                                             00006210
      GO TO 1100                                                        00006220
 1300 T2=T1*A2/A1                                                       00006230
      RETURN                                                            00006240
 1700 IF(T1.EQ.T2)  GO TO 1800                                          00006250
      P2=P1*(T2/T1)**((CONST1*(H2-H1))/(T1-T2))                         00006260
      RETURN                                                            00006270
 1800 P2=P1*EXP(CONST1*(H1-H2)/T1)                                      00006280
      RETURN                                                            00006290
      END                                                               00006300
      SUBROUTINE POUT(A1,A2,A3)                                         00006310
      DIMENSION UED(300),TED(300),PED(300),H(200),P(200),T(200)
      COMMON H,P,T,UED,PED,TED,IED
      IF (A1.EQ.-1.0) GO TO 100
      IED=IED+1
      UED(IED)=A1*0.215335E26
      PED(IED)=A2*0.215335E26
      TED(IED)=A3*0.215335E26
      RETURN
  100 IED=0
      RETURN
      END
      SUBROUTINE PATHST(NOE,ZN,LEVTOP)
      DIMENSION UIN(300),PU(300),TU(300),U(50),PRES(50),TMP(50),
     * RMIXR(5,50),HT(200),PP(200),TP(200),RN(5)
      COMMON HT,PP,TP,UIN,PU,TU,IED,U,PRES,TMP,RMIXR
      FTOT=0.0
      DO 50 I=1,IED
   50 FTOT=FTOT+UIN(I)
      DO 100 I=2,IED
      IF (ABS(UIN(I)-UIN(1)).LE.0.001) GOTO 120
  100 CONTINUE
      NFOLD=0
      GO TO 220
  120 NFOLD=I-1
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```
      DO 200 J=1,NFOLD
      K=NFOLD+J
      UIN(K)=UIN(J)+UIN(K)
      PU(K)=PU(J)+PU(K)
      TU(K)=TU(J)+TU(K)
  200 CONTINUE
  220 J1=NFOLD+1
      K=0
      IF (FTOT.LE.0.001) CALL ERROR(9,0)
      SUMU=0.0
      SUMPU=0.0
      SUMTU=0.0
      DO 400 J=J1,IED
      SUMU=SUMU+UIN(J)
      SUMPU=SUMPU+PU(J)
      SUMTU=SUMTU+TU(J)
      IF (SUMU.GT.FTOT/NGE) GO TO 390
      GO TO 400
  390 K=K+1
      U(K)=SUMU
      PRES(K)=SUMPU/SUMU
      TMP(K)=SUMTU/SUMU
      SUMU=0.0
      SUMPU=0.0
      SUMTU=0.0
      IF (J.EQ.IED) GO TO 420
  400 CONTINUE
      K=K+1
      U(K)=SUMU
      PRES(K)=SUMPU/SUMU
      TMP(K)=SUMTU/SUMU
  420 CONTINUE
      DO 600 J=1,K
      DO 500 IJ=1,5
      RMIXR(IJ,J)=RMIX(IJ,PRES(J),RN)
  500 CONTINUE
  600 CONTINUE
      LEVTOP=K
      RETURN
      END
      FUNCTION RMIX(I,P,RN)
      DIMENSION RN(5)
      RMIX=RN(I)
      RETURN
      END
      SUBROUTINE NSPEC(VL,VU,NVO,NM,NO,EPA,EXTNT,H,LINTOP,NLEVLS,      00000010
     *TTOP,NTST,IUNIT,TCI)                                             00000020
      COMPLEX*16 AO/(1.2260793177710432600D2,0.0D0)/,A1/               00000030
     +(2.1438238869470642500D2,0.0D0)/,A2/(1.8192853309218154900D2,    00000040
     +0.0D0)/,A3/(9.3155580458138441001,0.0D0)/,A4/                    00000050
     +(3.0160142196210589001,0.0D0)/,A5/(5.9126262097731530D0,0.0D0)/  00000060
     +,A6/(0.5641895835626150D0,0.0D0)/,B0/(1.2260793177387535000D2,   00000070
     +0.0D0)/,B1/(3.5273062511096355800D2,0.0D0)/,B2/                  00000080
     +(4.5733447878589773700D2,0.0D0)/,B3/(3.4870391771949579200D2,    00000090
     +0.0D0)/,B4/(1.7035400182109147200D2,0.0D0)/,B5/                  00000100
     +(5.3992906912940267001,0.0D0)/,B6/(1.0479857114260399001,       00000110
     +0.0D0)/,ZM,F,DCMPLX                                              00000120
      DIMENSION HX(200),PX(200),TX(200),UINX(300),PUX(300),TUX(300)    00000130
      REAL*8 ZVOIGT,X,Y,ABSK,V0,V1,VK,VIK,VL,VU,VBH,VONXT,VOL,VUP,D2ABS 00000140
      DIMENSION VG(200),SG(200),ALL(200),EPP(200),TCI(300),
     2 MOLNM(200),NH(7),NST(7),T(260),AMK(8),PRES(50),TMP(50),         00000160
     3 U(50),RMIXR(5,50),IACTV(200),AMAS(200),CENTW(200)               00000170
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      REAL FMAS(5)/18.0,44.0,48.0,40.0,28.0/                            00000180
      INTEGER NPART(5)/3,2,3,2,2/                                       00000190
      COMMON HX,PA,TX,UINX,PUX,TUX,IEDX,U,PRES,TMP,RMIXR                00000200
      CALL UNDEFL                                                       00000210
      ASSIGN 137 TO ISWT                                                00000220
      IF(VU.LE.VL) GOTO 1350
      NLINES=0                                                          00000230
      ITAIL=1                                                           00000240
      DO 20 JL=1,200                                                    00000250
   20 IACTV(JL)=JL                                                      00000260
      PO=101330.                                                        00000270
      TO=273.                                                           00000280
      CONST2=ALOG(2.)                                                   00000290
      ALN2=SQRT(CONST2)                                                 00000300
      PI=3.14159254                                                     00000310
      CONST1=ALN2/SQRT(PI)                                              00000320
      IF (NM.GT.7) CALL ERROR(10,0)
      NM=MINO(NM,7)
      WID=EXTNT*H/2.                                                    00000340
      NTOT=2*2**NM + 1                                                  00000350
      READ(IUNIT,9010,END=1340) VONXT,SONXT,ALLNXT,EPPNXT,MOLNXT,CWNXT  00000360
 9010 FORMAT(F9.3,E10.3,F6.3,F9.3,I2,F6.3)                              00000370
      VONXT=VONXT+CWNXT                                                 00000380
      DELVC=EXTNT*H/FLOAT(2**(NM+1))                                    00000390
  110 I=1                                                               00000400
      VI=VL                                                             00000410
  120 NBH=1                                                             00000420
      VBH=VI-DELVC*FLOAT(NTOT-1)/FLOAT(2)                               00000430
      NH(1)=-2**(NM-NO)                                                 00000440
      NSTW(1)=2**(NM-NO)                                                00000450
      MTOP=NM-NO+1                                                      00000460
      DO 125 M=2,MTOP                                                   00000470
      NH(M)=-2**(NM+1-NO-M)                                             00000480
      NSTW(M)=2**(NM+2-NO-M)                                            00000490
  125 CONTINUE                                                          00000500
      EPA=EPA/FLOAT(NSTW(1))/DELVC                                      00000510
  130 NWL=1                                                             00000520
      NST=NSTW(NWL)                                                     00000530
      K=NH(1)+NST                                                       00000540
      NOUT=0                                                            00000550
      IF(NLINES.LE.0) GOTO 132                                          00000560
  131 IF(VO(IACTV(ITAIL))+CENTV(IACTV(ITAIL)).GT.VI-WID) GOTO 132       00000570
      ITAIL=MOD(ITAIL,LINTOP)+1                                         00000580
      NOUT=NOUT+1                                                       00000590
      IF(NOUT.LT.NLINES) GOTO 131                                       00000600
  132 NLINES=MAX0(0,NLINES-NOUT)                                        00000610
  133 IF(VONXT-CWNXT.GT.VI+WID) GOTO 138                                00000620
      IF(VONXT+CWNXT.LT.VI-WID) GOTO 136                                00000630
      ILOAD=IACTV(MOD(ITAIL+NLINES-1,LINTOP)+1)                         00000640
      VO(ILOAD)=VONXT                                                   00000650
      SO(ILOAD)=SONXT*CONST1                                            00000660
      AMAS(ILOAD)=VONXT*3.58133E-07/SQRT(FMAS(MOLNXT))                  00000670
      ALL(ILOAD)=ALLNXT*ALN2/PO*SQRT(TO)/AMAS(ILOAD)                    00000680
      EPP(ILOAD)=-EPPNXT/0.6946/TO                                      00000690
      MOLNM(ILOAD)=MOLNXT                                               00000700
      CENTW(ILOAD)=CWNXT                                                00000710
      VOP=VONXT+CWNXT                                                   00000720
      J=NLINES-1                                                        00000730
      NLINES=NLINES+1                                                   00000740
      IF(NLINES.GT.LINTOP) GOTO 1340                                    00000750
      IF(NLINES.EQ.1) GOTO 136                                          00000760
  134 K1=MOD(ITAIL+J-1,LINTOP)+1                                        00000770
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      INXT=IACTV(K1)                                                    00000780
      IF(VUP.GE.VO(INXT)+CENTW(INXT)) GOTO 136                          00000790
      K2=MOD(ITAIL+J,LINTUP)+1                                          00000800
      IACTV(K2)=INXT                                                    00000810
      IACTV(K1)=ILOAD                                                   00000820
      IF(J.EQ.0) GOTO 136                                               00000830
      J=J-1                                                             00000840
      GO TO 134                                                         00000850
  136 CONTINUE                                                          00000860
      GO TO ISNT,(137,138)                                              00000870
  137 READ(IUNIT,9010,END=1330) VCNXT,SCNXT,ALLNXT,EPPNXT,MOLNXT,CWNXT  00000880
      VONXT=VCNXT+CWNXT                                                 00000890
      GO TO 133                                                         00000900
  138 CONTINUE                                                          00000910
      IF(NLINES.LE.0) GOTO 1320                                         00000920
  140 VK=VBH+DELVC*FLOAT(K)                                             00000930
      IF(K.GE.NTOT) GOTO 410                                            00000940
      ABSK=0.                                                           00000950
      DO 200 L1=1,NLINES                                                00000960
      L=IACTV(MOD(ITAIL+L1-2,LINTOP)+1)                                 00000970
      MOLNML=MOLNM(L)                                                   00000980
      SOL=SO(L)                                                         00000990
      VOL=(VK-VO(L))*ALN2                                               00001000
      ALLL=ALL(L)                                                       00001010
      AMASL=AMAS(L)                                                     00001020
      EPPL=EPP(L)                                                       00001030
      NPARTL=NPART(MOLNML)                                              00001040
      DO 300 IAT=1,NLEVLS                                               00001050
      TEMP=TMP(IAT)                                                     00001060
      RT=T0/TEMP                                                        00001070
      ALD=AMASL*SQRT(TEMP)                                              00001080
      BOLT=SQRT(RT**NPARTL)*EXP(EPPL*(RT-1.))                           00001090
      AKO=U(IAT)*SOL*BOLT/ALD*RMIXR(MOLNML,IAT)                         00001100
      Y=ALLL*PRES(IAT)/TEMP                                             00001110
      X=VOL/ALD                                                         00001120
      ZH=DCMPLX(Y,-X)                                                   00001130
      F=(((((((A6*ZH+A5)*ZH+A4)*ZH+A3)*ZH+A2)*ZH+A1)*ZH+A0)            00001140
     2/(((((((ZH+B6)*ZH+B5)*ZH+B4)*ZH+B3)*ZH+B2)*ZH+B1)*ZH+B0)          00001150
      ZVOIGT=F                                                          00001160
      D2ABS=AKO*ZVOIGT                                                  00001170
      ABSK=ABSK+D2ABS                                                   00001180
  300 CONTINUE                                                          00001190
      IF(ABSK.GT.TTOP) GOTO 210                                         00001200
  200 CONTINUE                                                          00001210
  210 NK=MOD(NBH+K-1,NTOT)+1                                            00001220
      T(NK)=DEXP(-ABSK)                                                 00001230
C     IF(NTST.EQ.2) WRITE(14,9014) T(NK),VK                             00001240
 9014 FORMAT(' ',F8.5,1X,F11.5)                                         00001250
      K=K+NST                                                           00001260
  400 GO TO 140                                                         00001270
  410 NHC=K-NST                                                         00001280
      CONVT=0.                                                          00001290
      SUMWT=0.                                                          00001300
      NH(I)=NHC                                                         00001310
  420 NIK=MOD(NBH+NHC-1,NTOT)+1                                         00001320
      VIK=VBH+DELVC*FLOAT(NHC)                                          00001330
      WT=CONST1/H*EXP(-SNGL(VI-VIK)**2*CONST2/H**2)                     00001340
      CONVT=CONVT+WT*T(NIK)                                             00001350
      SUMWT=SUMWT+WT                                                    00001360
      NHC=NHC-NST                                                       00001370
      IF(NHC.LT.0) GOTO 510                                             00001380
  500 GO TO 420                                                         00001390
```

```
  510 SUMWT2=SUMWT                                                      00001400
      TKO=CONVT                                                         00001410
      IF(NTST.EQ.1) WRITE(13,9013) TKO                                  00001420
 9013 FORMAT(' ',5(E14.7,1X))                                           00001430
      NWL=2                                                             00001440
  520 IF(NWL-1+NO.GT.NM) GOTO 1310                                      00001450
      NST=NSTW(NWL)                                                     00001460
      K=NH(NWL)+NST                                                     00001470
  530 VK=VBH+DELVC*FLOAT(K)                                             00001480
      IF(K.GE.NTOT) GOTO 810                                            00001490
      ABSK=0.                                                           00001500
      DO 600 L1=1,NLINES                                                00001510
      L=IACTV(MOD(ITAIL+L1-2,LINTOP)+1)                                 00001520
      MOLNML=MOLNM(L)                                                   00001530
      SOL=SO(L)                                                         00001540
      VOL=(VK-VO(L))*ALN2                                               00001550
      ALLL=ALL(L)                                                       00001560
      AMASL=AMAS(L)                                                     00001570
      EPPL=EPP(L)                                                       00001580
      NPARTL=NPART(MOLNML)                                              00001590
      DO 700 IAT=1,NLEVLS                                               00001600
      TEMP=TMP(IAT)                                                     00001610
      RT=TO/TEMP                                                        00001620
      ALD=AMASL*SQRT(TEMP)                                              00001630
      BOLT=SQRT(RT**NPARTL)*EXP(EPPL*(RT-1.))                           00001640
      AKO=U(IAT)*SOL*BOLT/ALD*RMIXR(MOLNML,IAT)                         00001650
      Y=ALLL*PRES(IAT)/TEMP                                             00001660
      X=VOL/ALD                                                         00001670
      ZH=DCMPLX(Y,-X)                                                   00001680
      F=((((((A6*ZH+A5)*ZH+A4)*ZH+A3)*ZH+A2)*ZH+A1)*ZH+A0)             00001690
     2/(((((((ZH+B6)*ZH+B5)*ZH+B4)*ZH+B3)*ZH+B2)*ZH+B1)*ZH+B0)          00001700
      ZVOIGT=F                                                          00001710
      DZABS=AKO*ZVOIGT                                                  00001720
      ABSK=ABSK+DZABS                                                   00001730
  700 CONTINUE                                                          00001740
      IF(ABSK.GT.TTOP) GOTO 610                                         00001750
  600 CONTINUE                                                          00001760
  610 NK=MOD(NBH+K-1,NTOT)+1                                            00001770
      T(NK)=DEXP(-ABSK)                                                 00001780
C     IF(NTST.EQ.2) WRITE(14,9014) T(NK),VK                             00001790
      K=K+NST                                                           00001800
  800 GO TO 530                                                         00001810
  810 NHC=K-NST                                                         00001820
      CONVT=0.                                                          00001830
      SUMWT=0.                                                          00001840
      NH(NWL)=NHC                                                       00001850
  820 NIK=MOD(NBH+NHC-1,NTOT)+1                                         00001860
      VIK=VBH+DELVC*FLOAT(NHC)                                          00001870
      WT=CONST1/H*EXP(-SNGL(VI-VIK)**2*CONST2/H**2)                     00001880
      CONVT=CONVT+WT*T(NIK)                                             00001890
      SUMWT=SUMWT+WT                                                    00001900
      NHC=NHC-NST                                                       00001910
      IF(NHC.LT.0) GOTO 910                                             00001920
  900 GO TO 820                                                         00001930
  910 SUMWT2=SUMWT2+SUMWT                                               00001940
      CONVT=CONVT/FLOAT(2**(NWL-2))                                     00001950
      IF(NWL.LE.2) GOTO 1010                                            00001960
      NSTOPR=NWL-2                                                      00001970
      DO 1000 NCR=1,NSTOPR                                              00001980
      FNCR=FLOAT(4**NCR)                                                00001990
      AMKN=(FNCR*CONVT-AMK(NCR))/(FNCR-1.)                              00002000
      AMK(NCR)=CONVT                                                    00002010
```

```
      CONVT=AMKN                                                        00002020
1000  CONTINUE                                                          00002030
1010  AMK(NWL-1)=CONVT                                                  00002040
      AMTS=ABS(TKO-CONVT)                                               00002050
      IF(AMTS.LE.EPA) GOTO 1110                                         00002060
      DAVF=FLOAT(2**4**(NWL-2)-1)/FLOAT(4**(NWL-1)-1)                   00002070
      TKO=CONVT+DAVF*(TKO-CONVT)                                        00002080
      IF(NTST.EQ.1) WRITE(13,9013) AMK,TKO                              00002090
      NWL=NWL+1                                                         00002100
1160  GO TO 529                                                         00002110
1110  TCI(I)=FLOAT(NSTW(1)/2)*DELVC*(CONVT+TKO)                         00002120
      IF(NTST.EQ.1) WRITE(13,9013) AMK                                  00002130
1120  IF(I.GE.NVO) RETURN                                               00002140
      I=I+1                                                             00002150
      VI=VL+FLOAT(I-1)*(VU-VL)/FLOAT(NVC-1)                             00002160
      VDBH=(VI-VBH)/DELVC-FLOAT((NTOT-1)/2)                             00002170
      IF(VDBH.GE.FLOAT(NTOT-1)) GOTO 120                                00002180
      NDBH=INT(VDBH)                                                    00002190
      NBH=MOD(NBH+NDBH-1,NTOT)+1                                        00002200
      VBH=VBH+DELVC*FLOAT(NDBH)                                         00002210
      JSTOP=NM-NO+1                                                     00002220
      DO 1200 J=1,JSTOP                                                 00002230
      NH(J)=NH(J)-NDBH                                                  00002240
1200  CONTINUE                                                          00002250
      NCH=1                                                             00002260
      NST=NSTW(1)                                                       00002270
1490  NHH=NH(NCH)                                                       00002280
1500  IF(NHH.GE.NST) GOTO 1510                                          00002290
      NHH=NHH+NST                                                       00002300
      GO TO 1500                                                        00002310
1510  NH(NCH)=NHH                                                       00002320
1520  NCH=NCH+1                                                         00002330
      IF(NCH.GT.(NM-NO+1)) GOTO 1600                                    00002340
      NST=NSTW(NCH)                                                     00002350
      GO TO 1490                                                        00002360
1600  CONTINUE                                                          00002370
      GO TO 130                                                         00002380
1310  TCI(I)=TKO*DELVC*FLOAT(NSTW(1))                                   00002390
      CALL ERROR(11,0)
      GO TO 1120                                                        00002400
1320  TCI(I)=1.0                                                        00002410
      CALL ERROR(12,0)
      GO TO 1120                                                        00002420
1330  ASSIGN 138 TO ISWT                                                00002430
      VONXT=CANXT+VU+10.*H*EXTNT                                        00002440
      GO TO 138                                                         00002450
1340  CALL ERROR(13,0)
      ITAIL=MOD(ITAIL+LINTOP-NLINES-1,LINTOP)+1
      NLINES=LINTOP
9912  FORMAT(' ERROR IN LINE SORTER')                                   00002470
      GO TO 134
1350  CALL ERROR(14,0)
      RETURN                                                            00002480
      END                                                               00002490
      SUBROUTINE ERROR(I,J)
      DIMENSION IER(50)
      COMMON /ERR/ N,M11,IER
      IF (J.NE.0) GOTO 1009
      IF (I.EQ.11) GOTO 500
      N=N+1
      IER(N)=I
      RETURN
```

```
  500 M11=M11+1
      RETURN
 1000 WRITE(6,*) M11,IER
      RETURN
      END
/*
//GO.SYSLIN  DD  DSN=TSO462.NSPEC.OBJ,DISP=SHR
//GO.FT10F001  DD  DSN=TSO462.SNIDER.DATA(SAVE),DISP=SHR
//GO.FT11F001  DD  DSN=TSO462.LINPAR.DATA,DISP=SHR
//GO.FT12F001  DD  SYSOUT=A
//GO.FT13F001  DD  SYSOUT=A
//GO.SYSIN  DD  *
 190 45.0 95.0 45.0 15 11
 3.89E-06 322.0E-06 0.0 0.0 0.0
 1900.0 1900.05 2 7 1 0.005 5.5 0.05 200 10.0 0
/*
//
```

APPENDIX B

THE LINE PARAMETER SETUP PROGRAM

This program reads the AFGL line listing tape and creates a file of selected line parameters. The two-step JCL routine runs the FORTRAN program to read and select the line parameters and then calls for an all core sort using the IBM system sort routine to put the lines in increasing order of the lowest frequency value at which they have significant absorption. A sample of the line parameter output after sorting is also included. As written, the program selects N_2O lines from 2550 - 2560 cm^{-1} for a ground-based observer looking straight up at the sun. The line parameter listing example is for a different case.

```
00010 //     REGION=192K,TIME=2
00020 /*SETUP   UNIT=TAPE9,ID=(AFCRL,J229,READ)
00030 //NTAPE  EXEC FORTRUN,TIME=2,REGION=192K
00035 //CMP.SYSPRINT  DD  SYSOUT=X
00040 //CMP.SYSIN  DD  DSN=TS0462.BOB.FORT,DISP=SHR
00045 //GO.SYSLOUT  DD  SYSOUT=X
00050 //GO.FT09F001  DD  LABEL=(1,BLP,,IN),
00060 //  UNIT=TAPE9,VOL=SER=AFCRL,DISP=(OLD,KEEP),DCB=(LRECL=3200,RECFM
=FB,
00070 //    BLKSIZE=3200)
00080 //GO.FT10F001  DD  LABEL=(2,BLP,,IN),
00090 //  UNIT=TAPE9,VOL=SER=AFCRL,DISP=(OLD,KEEP),DCB=(LRECL=3200,RECFM
=FB,
00100 //  BLKSIZE=3200)
00110 //GO.FT11F001  DD  LABEL=(3,BLP,,IN),
00120 //  UNIT=TAPE9,VOL=SER=AFCRL,DISP=(OLD,KEEP),DCB=(LRECL=3200,RECFM
=FB,
00130 //  BLKSIZE=3200)
00140 //GO.FT12F001  DD  LABEL=(4,BLP,,IN),
00150 //  UNIT=TAPE9,VOL=SER=AFCRL,DISP=(OLD,KEEP),DCB=(LRECL=3200,RECFM
=FB,
00160 //  BLKSIZE=3200)
00170 //GO.FT13F001  DD  LABEL=(5,BLP,,IN),
00180 //  UNIT=TAPE9,VOL=SER=AFCRL,DISP=(OLD,KEEP),DCB=(LRECL=3200,RECFM
=FB,
00190 //  BLKSIZE=3200)
00200 //GO.FT14F001  DD  DSN=&&LINE,DISP=(MOD,PASS),UNIT=SYSDA,
00210 //    SPACE=(TRK,(1,1)),DCB=(RECFM=FB,LRECL=42,BLKSIZE=2100)
00220 //S  EXEC  SORT
00230 //S.SORTIN  DD  DSN=&&LINE,DISP=(OLD,DELETE)
00240 //S.SORTOUT  DD  DSN=TS0462.L2.DATA,DISP=SHR
00250 //S.SYSIN  DD  *
00260    SORT  FIELDS=(1,9,CH,A),SIZE=E200
END OF DATA
```

```
00010       DIMENSION G(40), SS(40), AP(40),A(9, 40), ISOT(40), MOL(40),
00020      #  ID(40), EE(40), UM(6),EPSLON(2)
00030       INTEGER TOPE
00040        REAL*8  G
00050       DATA VINIT, VFINAL, BOUND, H, DEPTH
00060      # /2550.0, 2560.0, 2.0, .30, 0.010/
00070       KOUNT = 0
00080       VBOT = VINIT - (BOUND + H)
00090       VTOP = VFINAL + (BOUND + H)
00110       UM(4)=5.80E18
00120       P=1.0
00130       EPSLON(1)=DEPTH/UM(1)*3.1415927*P
00140       EPSLON(2)=DEPTH/UM(2)*3.1415927*P
00150       MF = 9
00160       IF (VBOT .GT. 500.0) MF = 10
00170       IF (VBOT .GT. 1000.0) MF = 11
00180       IF (VBOT .GT. 2000.0) MF = 12
00190       IF (VBOT .GT. 5000.0) MF = 13
00200     3 REWIND MF
00210     1 CONTINUE
00220       READ (MF, 2, END=6, ERR=4) (G(I), SS(I), AP(I), EE(I), (A(J,
I),
00230      @  J = 1, 9), ID(I), ISOT(I), MOL(I), I = 1, 40)
00240     2 FORMAT (40(F10.3, E10.3, F5.3, F10.3, 8A4, A3, I3, I4, I3))
00250       IF(G(40) .LT. VBOT) GO TO 1
00260       IF (G(1) .GT. VTOP) GO TO 9
00270          DO 2002 I = 1, 40
00280       IF(MOL(I).NE.4) GOTO 2002
00290       IF(SS(I)/AP(I).LT.EPSLON(MOL(I))) GOTO 2002
00300       KOUNT = KOUNT + 1
00310       CENTW=SQRT(SS(I)*UM(MOL(I))*AP(I)*P/3.1415927/0.0001
00320      #-(AP(I)*P)**2)
00321       IG=G(I)*1.0D3
00331       IC=CENTW*1000.0
```

```
00341         G(I)=DFLOAT(IG-IC)/1.0D3
00351         CENTW=FLOAT(IC)/1000.0
00352         WRITE(14,100) G(I),SS(I),AP(I),EE(I),MOL(I),CENTW
00353   100 FORMAT(F9.3,E10.3,F6.3,F9.3,I2,F6.3)
00354         IF (KOUNT .GE.  200) GO TO 9
00355  2002 CONTINUE
00360            GO TO 1
00370     6 MF = MF + 1
00380            GO TO 3
00390     4 WRITE (6, 605) MF
00400   605 FORMAT( '0 ERROR ON UNIT #', I3)
00410     9 CONTINUE
00420         STOP
00430         END
```

1878.393	0.815E-20	0.077	504.000	116.277	
1888.333	0.121E-21	0.041	1216.200	1	1.446
1892.945	0.403E-22	0.041	1216.200	1	0.834
1893.308	0.913E-22	0.044	1411.650	1	1.301
1893.417	0.494E-23	0.063	994.190	2	1.301
1893.530	0.557E-25	0.075	48.596	2	0.150
1893.545	0.116E-22	0.007	2661.050	1	0.185
1893.624	0.392E-23	0.007	2661.050	1	0.106
1893.775	0.388E-25	0.074	1429.125	2	0.124
1893.854	0.122E-23	0.069	1054.764	2	0.677
1893.859	0.303E-22	0.044	1411.680	1	0.751
1893.932	0.680E-23	0.050	2144.120	1	0.378
1893.999	0.126E-23	0.069	1031.127	2	0.688
1894.205	0.715E-25	0.070	2764.710	1	0.045
1894.271	0.484E-25	0.075	40.497	2	0.140
1894.291	0.466E-22	0.047	1631.410	1	0.959
1894.456	0.919E-25	0.074	2398.390	1	0.053
1894.468	0.301E-24	0.053	2337.700	1	0.082
1894.492	0.315E-22	0.059	1843.020	1	0.887
1894.535	0.349E-25	0.074	1417.376	2	0.118
1894.586	0.249E-23	0.099	221.234	1	0.322
1894.678	0.648E-23	0.064	917.056	2	1.502
1894.823	0.991E-25	0.053	2337.530	1	0.047
1894.838	0.155E-22	0.046	1631.270	1	0.551
1894.855	0.207E-24	0.073	786.903	2	0.286
1894.868	0.640E-23	0.049	1875.530	1	0.362
1894.894	0.864E-26	0.010	2952.700	1	0.005
1894.970	0.107E-26	0.075	2046.403	2	0.020
1894.991	0.115E-26	0.075	2055.035	2	0.021
1895.012	0.412E-25	0.075	33.134	2	0.129
1895.015	0.121E-26	0.074	2064.452	2	0.021
1895.040	0.126E-26	0.074	2074.654	2	0.022
1895.069	0.129E-26	0.074	2085.640	2	0.022

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