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AN EFFICIENT COMPUTATIONAL APPROXIMATION TO THE LORENTZ LINE MOLECULAR ABSORPTION COEFFICIENT

BY

MICHAEL T. POTTER

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Presented to the Faculty of

The Department of Electrical Engineering

The University of Texas at El Paso

In Partial Fulfillment of the

Requirements for Degree of

MASTER OF SCIENCE

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- To My Most Loving Wife -

Patricia

"Love never fails, whereas
prophecies will disappear,
and tongues will cease and
knowledge will be destroyed."

1 Cor. 13, 8

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ABSTRACT

A rapid and accurate approximation to the Lorentz line molecular absorption coefficient has been developed which significantly reduces the time of line-by-line transmittance calculations. By separating computations required for each spectral line, atmospheric level, and absorbing gas under consideration, arithmetical operations are minimized.

Time tests were conducted while computing the monochromatic absorption coefficient for five frequency channels in the 4.3 μm band. The approximation was compared to the evaluation of the Lorentz line shape (standard manner) for a 33 level atmosphere and an average of 1000 absorption lines per region. Water vapor, carbon dioxide, nitrous oxide, and carbon momoxide molecules were considered. The approximation was, in all cases, at least 9 times faster. Absorption coefficient values computed by this approximation agreed to those computed in the standard fashion to at least three decimal places regardless of molecule type, channel, or atmospheric level. Average percent-relative errors were typically: 10^{-4} for H_2O; 10^{-4} for CO_2; 10^{-3} for N_2O; 10^{-8} for CO.

For transmittance calculations over a band, time savings can be predicted by analyzing the required number of arithmetical operations. For 1,000 spectral lines over a bandwidth of 25 cm^{-1} and a step increment of 0.02 cm^{-1}, a reduction in computation time of 450% is anticipated.

TABLE OF CONTENTS

		PAGE
ACKNOWLEDGEMENTS		i
ABSTRACT		iii
TABLE OF CONTENTS		iv
LIST OF FIGURES		vi
LIST OF TABLES		vii
I.	INTRODUCTION	1
II.	GENERAL THEORY OF ATMOSPHERIC TRANSMITTANCE AND ABSORPTION	3
	2.1 Earth's Atmosphere	3
	2.2 Molecular Energy and Spectra	8
	2.3 Line Broadening Mechanisms	12
	2.4 Beer's Law of Molecular Absorption	17
	2.5 The Absorbing Gases	20
III.	A PROPOSED APPROXIMATION TO THE LORENTZ LINE SHAPE	24
	3.1 Preface	24
	3.2 Derivation of the Transmittance Problem	24
	3.3 Derivation of the Approximation	29
	3.4 Selection of Arbitrary Constants and Truncation	34
IV.	TOPICS RELATED TO ATMOSPHERIC ABSORPTION	43
	4.1 Preface	43
	4.2 Line Parameters - AFCRL's Data Tape	43
	4.3 Extracting Data From AFCRL's Tape	47
	4.4 Units of Atmospheric Physics	48
	4.5 The Nimbus - 6 Sounder and the 4.3 μm Band	61
V.	TESTING THE APPROXIMATION	66
	5.1 Preface	66
	5.2 Data File Description	67
	5.3 Data Reorganization	68
	5.4 Evaluation of K	69
	5.5 Execution Time Analysis	70
	5.6 Evaluating the Error	81

Contents

		Page
VI.	RESULTS AND APPLICATIONS	89
	6.1 Preface	89
	6.2 Results of the Time Analysis	89
	6.3 Results of Accuracy Analysis	94
	6.4 Application to the Band Problem	104
VII.	CONCLUDING REMARKS	110
	7.1 Summary	110
	7.2 Use of the Approximation	111
REFERENCES		112
APPENDIX A:	Data Routine for Use With AFCRL's Line Parameter Compilation	114
APPENDIX B:	Lorentz Line Absorption Coefficient Test Routine	123

LIST OF FIGURES

FIGURE		PAGE
2.1-1	Temperature Profile	4
2.1-2	Pressure Profile	6
2.2-1	State Energy Transitions	9
2.2-2	Energy Transition Spectra	11
2.3-1	Lorentz Line Shape	16
2.4-1	Lambert-Beer Law Geometry	18
2.5-1	% Absorption - VS - Wavelength	22
3.2-1	Transmittance Problem Geometry	24
3.2-2	Stratafied Layer Geometry	27
3.4-1	Convergence Areas for Binomial Series	36
4.2-1	Word Format Chart	45
4.3-1	Data Routine Flow Diagram	50
4.5-1	HIRS Weighting Functions and Filter Responses	64
5.4-1	Flow Diagram for the Evaluation of K	71
5.5-1	Timing Routine	79
5.5-2	Time Analysis Methods	83

LIST OF TABLES

TABLE		PAGE
2.1-1	Composition of the Earth's Atmosphere	7
3.1-1	Notation Index	25
3.4-1	Ground State Energy Distribution in the 4.3 μm Band	39
4.2-1	Criterion Intensity Minimum	44
4.2-2	Molecule and Isotope Codes	46
4.3-1	Variable Names for Data Retrieval Routine	49
4.4-1	Gas Amount Table	60
4.5-1	Nimbus-6 Channel Characteristics	62
4.5-2	Number of Lines Per Channel by Molecule Type	65
5.5-1	Time Analysis Chart	82
5.6-1	Bounds on $\lvert\epsilon_A U\rvert$ for $E_A = 5 \times 10^{-4}$	88
6.2-1	"Go-Step" Time Chart	91
6.2-2	"Clock" Time Chart	93
6.2-3	"Assembler" Time Chart	94
6.3-1	Standard 33-Level Atmosphere	96
6.3-2	Computed Gas Amounts	97
6.3-3	Error Analysis - Water Vapor	99
6.3-4	Error Analysis - Carbon Dioxide	100
6.3-5	Error Analysis - Nitrous Oxide	101
6.3-6	Error Analysis - Carbon Monoxide	102
6.3-7	$\lvert K_{MOD} - K_{STD}\rvert$ For Chebyshev and Taylor Expansions	105
6.3-8	Chebyshev Coefficients for EXP[X]	106
6.4-1	Polychromatic Time Chart	109

CHAPTER I

INTRODUCTION

One of the most widely used methods of calculating atmospheric absorption is the line-by-line, direct integration method. With the aid of modern high-speed computers and the availability of accurate line parameters, an ever increasing confidence is being placed in this technique. The adversion to it, however, is that computation time and, consequently cost, tend to excalate beyond feasible limits. Even though larger and faster computers are constantly being developed, the need still exists for a fast and accurate method of calculating the molecular absorption coefficient.

About a year ago, Dr. J. H. Pierluissi [22] and Dr. G. A. Gibson [10], under a research contract from the Atmospheric Sciences Laboratory, WSMR, began investigating a method of reducing the number of required calculations to obtain a molecular absorption coefficient. This work will elaborate on their proposed approximation to the Lorentz line shape which promises to significantly reduce the time and cost of line-by-line calculations. Because application of this approximation to the band problem is not final, only the monochromatic case will be fully developed. However, a discussion of polychromatic radiation is included. Evidence of reduction in the number of required calculations in the standard Lorentz line shape is offered in Chapters 5 and 6.

For the sake of completeness, a chapter has been devoted to the general theory of molecular absorption. Additionally, some space has

been allocated to the "AFCRL Atmospheric Absorption Line Parameters Compilation" data tape [McClatchey[17]], which was used in all calculations and to the units generally used in atmospheric sciences (Chapter 4).

All computer programs presented were written in Fortran IV and designed to be used with the University of Texas at El Paso's IBM-360/65, G-level compiler. Some slight modification of the job-control cards may have to be made if these programs are to be used on another computer.

CHAPTER II

GENERAL THEORY OF ATMOSPHERIC TRANSMITTANCE AND ABSORPTION

This chapter will furnish the reader with a basic review of the fundamentals of atmospheric transmittance of radiant energy. The first section has been devoted to the earth's atmosphere with emphasis placed on its classification methods and composition. Section 2.3 is a discussion of molecular energies and line spectra resulting from state transitions. This is followed by an explanation of the different spectral line broadening mechanisms. Finally, the chapter concludes with the formulation of the Lambert-Beer law for molecular absorption [Brugel[4]] and a discussion of the principle gases involved.

2.1 Earth's Atmosphere

There are many methods for classifying the earth's atmosphere, but the most widely accepted method is based on temperature variations with altitude. One such distribution is presented in Fig. 2.1-1. A region of the atmosphere is characterized by its temperature gradient (either positive or negative) and has the suffix "-sphere." As the variation in temperature begins to change sign, indicating the beginning of a new region, the suffix is changed from "-sphere" to "-pause" (i.e. stratosphere to stratopause).

The lowest region, 0-15 km, is known as the troposphere. It is characterized by a negative vertical temperature gradient. The ceiling, tropopause, may vary as much as 10 km depending on geographical location and season. Temperatures typically decrease $6^{o}K$ per km [Banks[3]].

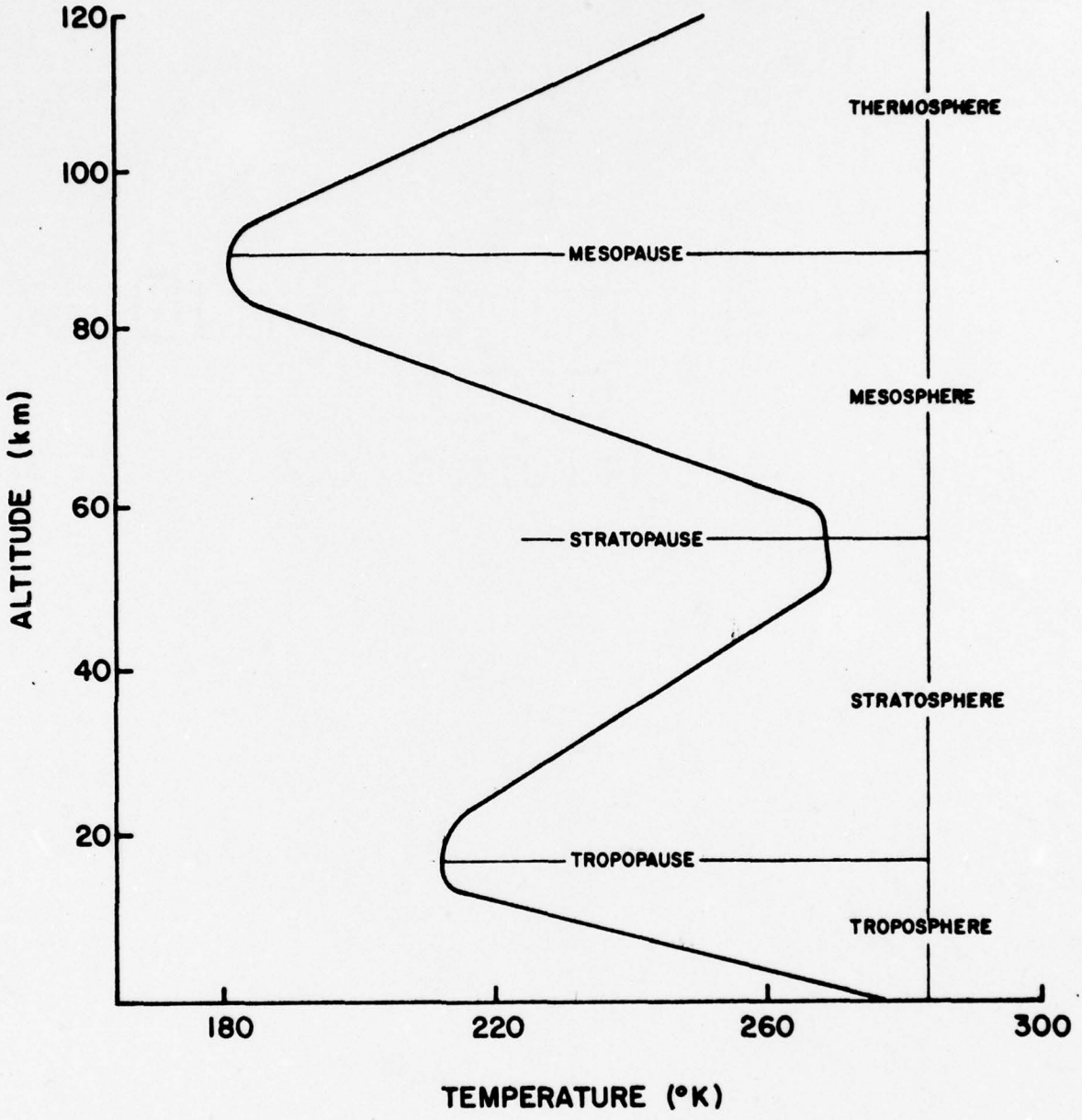


Figure 2.1-1 TEMPERATURE PROFILE
[Adapted from LaRocca[16]]

Temperature in the "stratosphere," 15-50 km, increases to a maximum of about 270°K. The heating effect is due to the absorption of ultraviolet radiation by ozone (O_3) and to atmospheric infrared emissions [Banks[3]].

The "mesosphere" rests above 50 km and reaches to a height of about 100 km. Here the temperature reaches a minimum at 85 $\pm$ 5 km.

The highest region shown in Fig. 2.1-1 is the "thermosphere." It extends beyond 100 km and has a positive temperature gradient. Typically, unless specific requirements dictate otherwise, classification of the atmosphere can stop with the "thermosphere."

While temperatures normally vary up or down with altitude, atmospheric pressure always decreases. Variations in pressure are related to those in altitude by the hydrostatic equation [Whitten[28]]

$$dP = -g(z)\ \rho(z)\ dz, \qquad 2.1\text{-}1$$

where P is the atmospheric pressure, g(z) is the acceleration due to gravity at altitude z, and $\rho(z)$ is the atmospheric density at altitude z. Fig. 2.1-2 illustrates the changes in pressure with respect to altitude.

In terms of gas concentrations, the atmosphere is composed of two groups of molecules. Those which are mixed uniformly in the atmosphere are listed in Table 2.1-1. Those which have a variable mixing ratio are water vapor (H_2O) and ozone (O_3). The densities of these molecules (H_2O, O_3) in the atmosphere are highly dependent on geographical location, season, and even time of day.

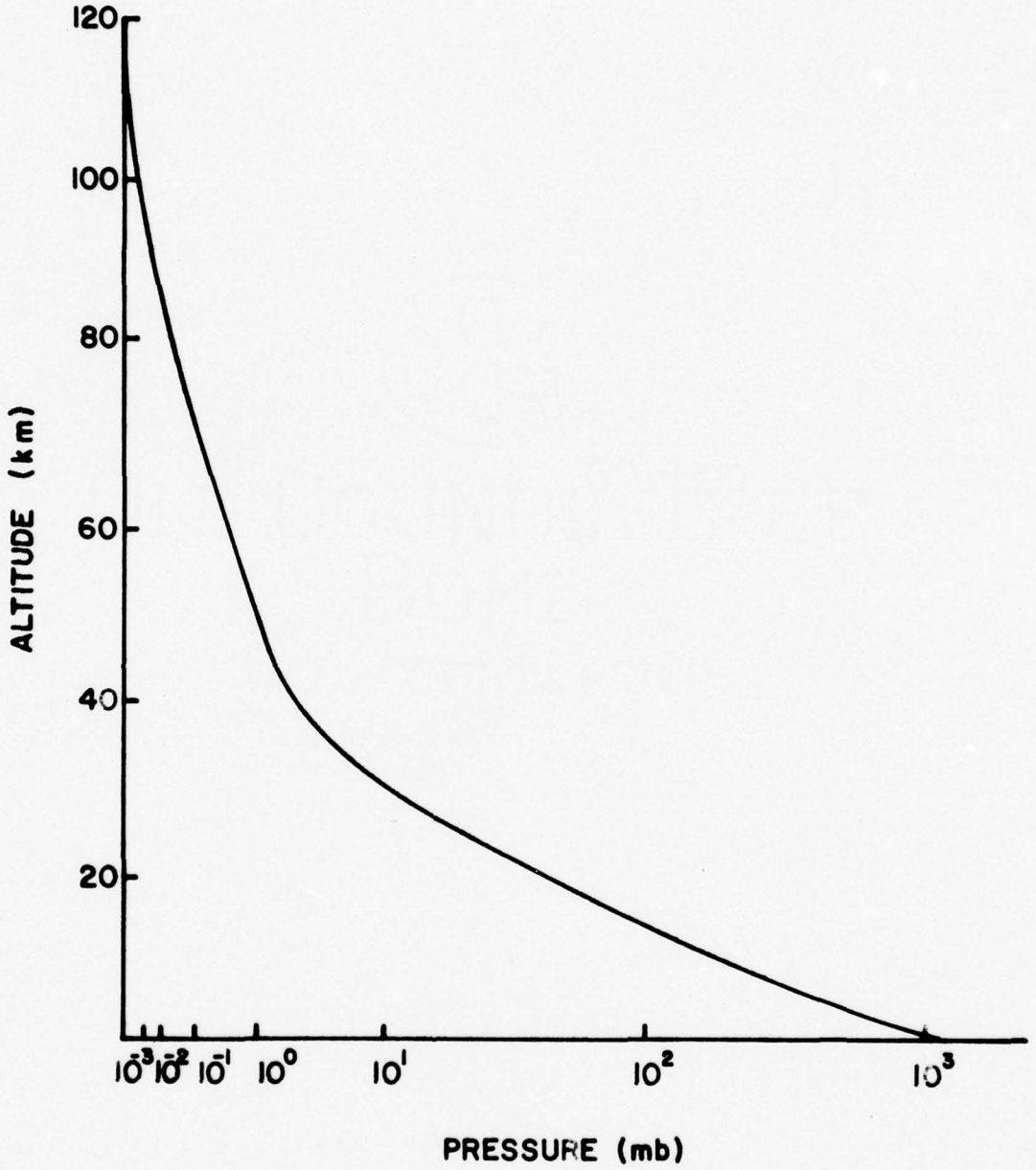


Figure 2.1-2 PRESSURE PROFILE
[Adapted from LaRocca[16]]

ATMOSPHERE CONSTITUENT	CHEMICAL FORMULA	PERCENT BY VOLUME	INFRARED ABSORBER
Nitrogen*	N_2	78.084	No
Oxygen*	O_2	20.946	No**
Argon*	A	0.934	No
Carbon Dioxide*	CO_2	0.032	Yes
Neon	Ne	1.818×10^{-3}	No
Helium	He	5.24×10^{-4}	No
Methane	CH_4	2.0×10^{-4}	Yes
Krypton	Kr	1.14×10^{-4}	No
Nitrous Oxide	N_2O	5.0×10^{-5}	Yes
Hydrogen	H_2	5.0×10^{-5}	No
Xenon	Xe	9.0×10^{-6}	No

*Major atmospheric constituent

**McClatchey, et. al., has included 490 lines of O_2 in AFCRL's data compilation [17].

TABLE 2.1-1 COMPOSITION OF THE EARTH'S ATMOSPHERE (DRY)
[Adapted from Hudson[12]]

Another method for categorizing the contents of the atmosphere is by classifying each component as a major or minor constituent. The major constituents, Nitrogen (N_2), Oxygen (O_2), Argon (A), and Carbon Dioxide (CO_2), make up over 99.9 percent of the atmosphere.

2.2 Molecular Energy and Spectra

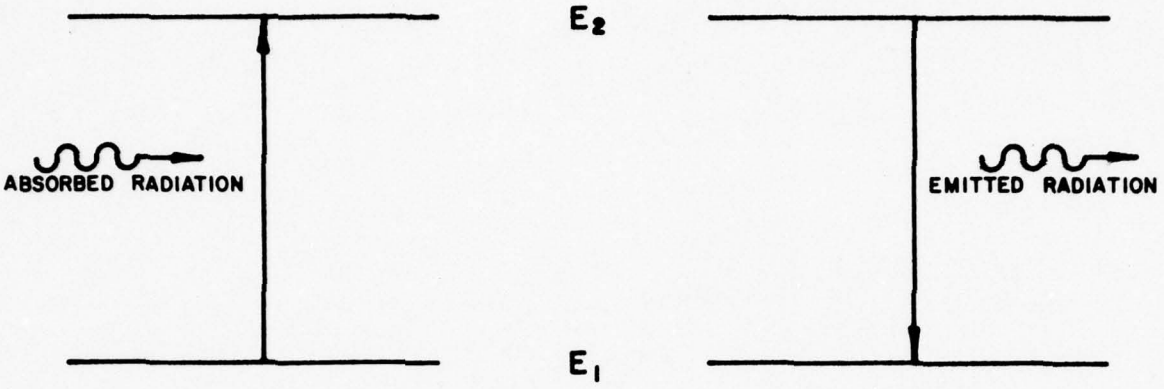
Because molecular and atomic spectra both exhibit discrete energy transitions, the fundamental atomic assumptions made by Niels Bohr in 1913 [Fowles[7]] can be used to illustrate the quantization of molecular energies. In a molecular sense, these assumptions tell us that molecules can possess only certain discrete energy levels. When a transition from one state to another occurs, the frequency at which the transition takes place is governed by Plank's relation. This frequency (ν) is given by

$$\nu = \frac{\Delta E}{h}, \qquad 2.2\text{-}1$$

where ΔE is the energy difference between the two states involved and h is Plank's constant.

Fig. 2.2-1 illustrates two possible transitions between energy states E_1 and E_2. A rise in energy from E_1 to E_2 indicates that the molecule has "absorbed" incident radiation. Similarly, a lowering in energy may be described as an "emission."

In general, the total energy of a molecule is a function of four factors and their combinations. The first is the energy due to translational motion of the molecule which is dependent on velocity. For the purposes of molecular absorption analysis the translational



a. Molecular energy is raised from lower E_1 state to E_2 by absorbing radiant energy.

b. Molecular energy is lowered from higher E_2 state to E_1 by emitting radiant energy.

Figure 2.2-1 STATE ENERGY TRANSITIONS
[Adapted from Fowles[7]]

energy can be ignored [Goody[11]].

Hence, this work only considers three types of energy which contribute to total energy. They are the electronic energy (E_{el}), the rotational energy (E_{rot}), and the energy due to the vibrational modes of motion (E_{vib}). Therefore,

$$E_{tot} = E_{rot} + E_{vib} + E_{el} + E_{comb}, \qquad 2.2\text{-}2$$

where E_{comb} represents the interaction of two or more energy types.

The largest contributor to total energy is that of the electronic type which is typically a few electron-volts. Vibrational energies are a few tenths or hundredths of an electron-volt, and the smallest is due to rotation which is on the order of hundredths, thousandths or ten-thousandths of an electron-volt [Zeuv[29]].

Each of the three energy types are quantized in a different way and hence, by Eq. 2.2-1, may absorb or emit at different frequencies. Transitions that involve rotational energy levels only take place in the far infrared or the microwave region of the spectrum. It is known as the "pure rotation spectrum." A "rotational-vibrational spectrum" is also possible and can be found in the near infrared. The most energetic transitions are due to electronic energy changes. The "electronic spectra" for molecules occur in the visible and ultraviolet region. See Fig. 2.2-2.

The scope of this document will not allow an elaborate explanation of Quantum Theory. It will suffice to state, however, that the frequencies at which a molecule can absorb or emit radiant energy can be predicted from this theory. This is done by assigning

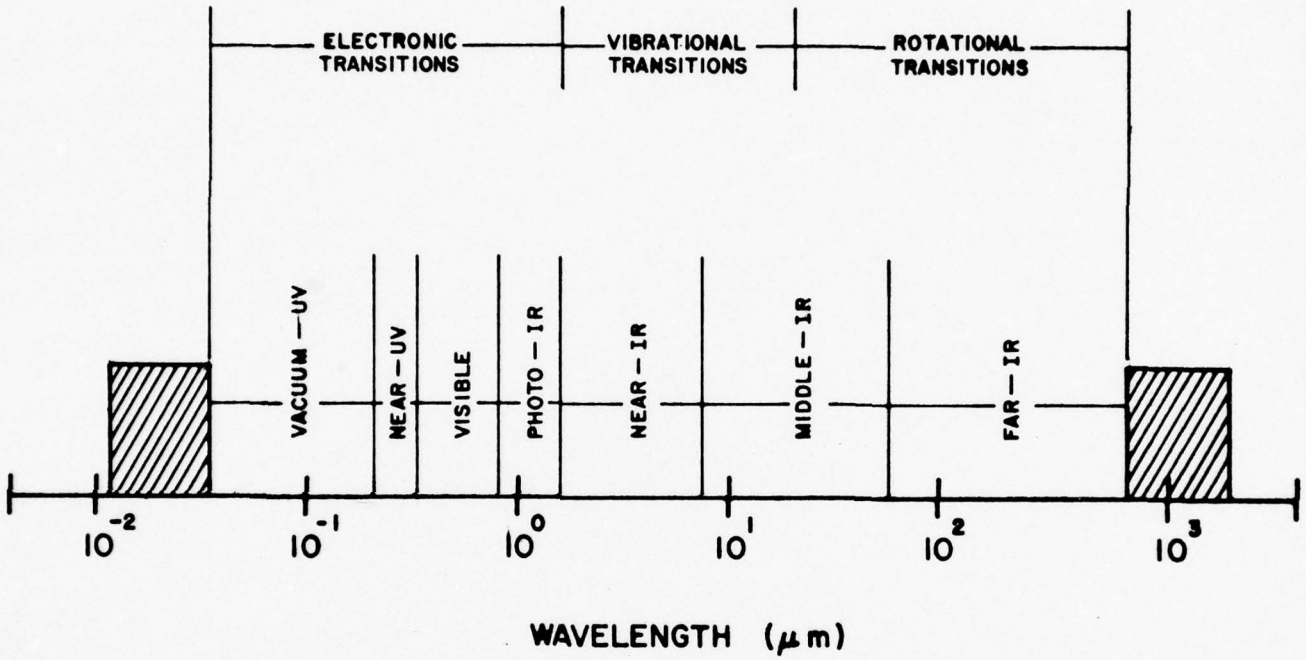


Figure 2.2-2 ENERGY TRANSITION SPECTRA
[Adapted from Fowles[7]]

"quantum numbers" to each of the molecule's energy types. These numbers then describe the allowable energy transitions or allowable frequencies for emission or absorption. The assignment of "quantum numbers" is based on the individual molecule's geometry, modes of motion, and number of atoms.

The absorption or emission frequencies which are predicted by this theory are known as spectral lines. The strength, line width, and energy associated with each spectral line for a given molecule is the subject of much research and study. A widely used compilation of these parameters by R. A. McClatchey, et. al., [17] is discussed in chapter 4.

2.3 Line Broadening Mechanisms

Unfortunately, when a transition between energy states takes place in a molecule the corresponding spectral line can not, in reality, be considered to be purely monochromatic. Depending on atmospheric conditions, spectral lines exhibit a broadened contour shape. The broadening can be attributed to the effects of radiative damping, doppler shifts, and molecular collisions.

Natural spectral-line broadening is a result from the fact that energy transitions take a finite amount of time to occur. Hence, the vibrational process that accompanies the transition gives rise to a spectral interval [Zuev[29]]. Excluding all other disturbances the natural line shape is given by

$$k(\nu) = \frac{\gamma_N}{\pi\left[\gamma_N^2 + (\nu-\nu_o)^2\right]} \qquad 2.3\text{-}1$$

where the line width is given as

$$\gamma_N = \frac{1}{2\pi t} \quad . \qquad 2.3\text{-}2$$

ν_o is the center frequency of the line, and t is the time spent by the molecule in the excited state.

The form of Eq. 2.3-1 will be seen again in the Lorentz line shape and in this sense natural broadening is important. However, the effects are normally ignored in transmittance calculations because of the small line width. Typically γ_N is on the order of 10^{-11} wave numbers [Zeuv[29]].

In the regions of the atmosphere where pressures are around 10 mb and below, the line broadening effects due to the doppler principle are dominant [Drayson[6]]. Assuming a maxwellian velocity distribution among the molecules and ignoring all other effects, the Doppler line shape is predicted by

$$K(\nu) = k_o \, e^{-y^2} \quad , \qquad 2.3\text{-}3$$

where

$$k_o = \frac{S}{\alpha_D} \left[\frac{\ln 2}{\pi} \right]^{1/2} \quad , \qquad 2.3\text{-}4$$

$$y = \frac{[\nu - \nu_o] \, [\ln 2]^{1/2}}{\alpha_D} \quad , \qquad 2.3\text{-}5$$

and α_D is the Doppler half-width.

The line strength, S, is a function of temperature and is expressed as

$$S = S_o \left(\frac{T_o}{T}\right)^b Q_v \, EXP\left[\frac{-E''}{kT_o}\left(\frac{T_o}{T} - 1\right)\right] \qquad 2.3\text{-}6$$

where b is a gas dependent constant, Q_v is the vibrational partition function ratio, E'' is the rest energy, and k is Boltzmann's constant.

It should be noted here that, in most texts, Eq. 2.3-6 is given without the ratio of partition functions. In this report, the ratio will always be included so that calculations involving S will agree more closely with the line parameter data that was used [McClatchey[17]].

As atmospheric pressure increases, molecular collisions become much more frequent. Hence, it is natural to suspect that the line broadening mechanism in such regions of the atmosphere is heavily dependent on pressure (molecular collisions). The most widely accepted formulation of the pressure broadened line shape is attributed to H. A. Lorentz (1906) although works in this same area were done earlier by A. A. Michelson (1895) and later by W. Lenz (1924) [Goody[28]]. This important line shape is discussed below.

As mentioned in the beginning of this section, the spectral line shape describes how a theoretically single spectral line is actually broadened by various mechanisms. The deviation from monochromatism can be factored into the product of a line strength and a line shape. This line shape is usually normalized so that its integral over infinite limits is unity.

Assuming that the Pressure-broadened line shape could be based

on "strong" encounters between molecules and a statistical function describing the time between collisions, Lorentz developed the well-known formulation

$$f(\nu) = \left(\frac{1}{\pi}\right) \frac{\alpha_L}{\alpha_L^2 + (\nu-\nu_o)^2} \quad . \qquad 2.3\text{-}7$$

Coupling the line shape and line strength (Eq. 2.3-6) we have

$$k(\nu) = \frac{S}{\pi} \frac{\alpha_L}{\alpha_L^2 + (\nu-\nu_o)^2} \quad . \qquad 2.3\text{-}7a$$

The most simplified expression for the Lorentz half-width used in atmospheric applications is

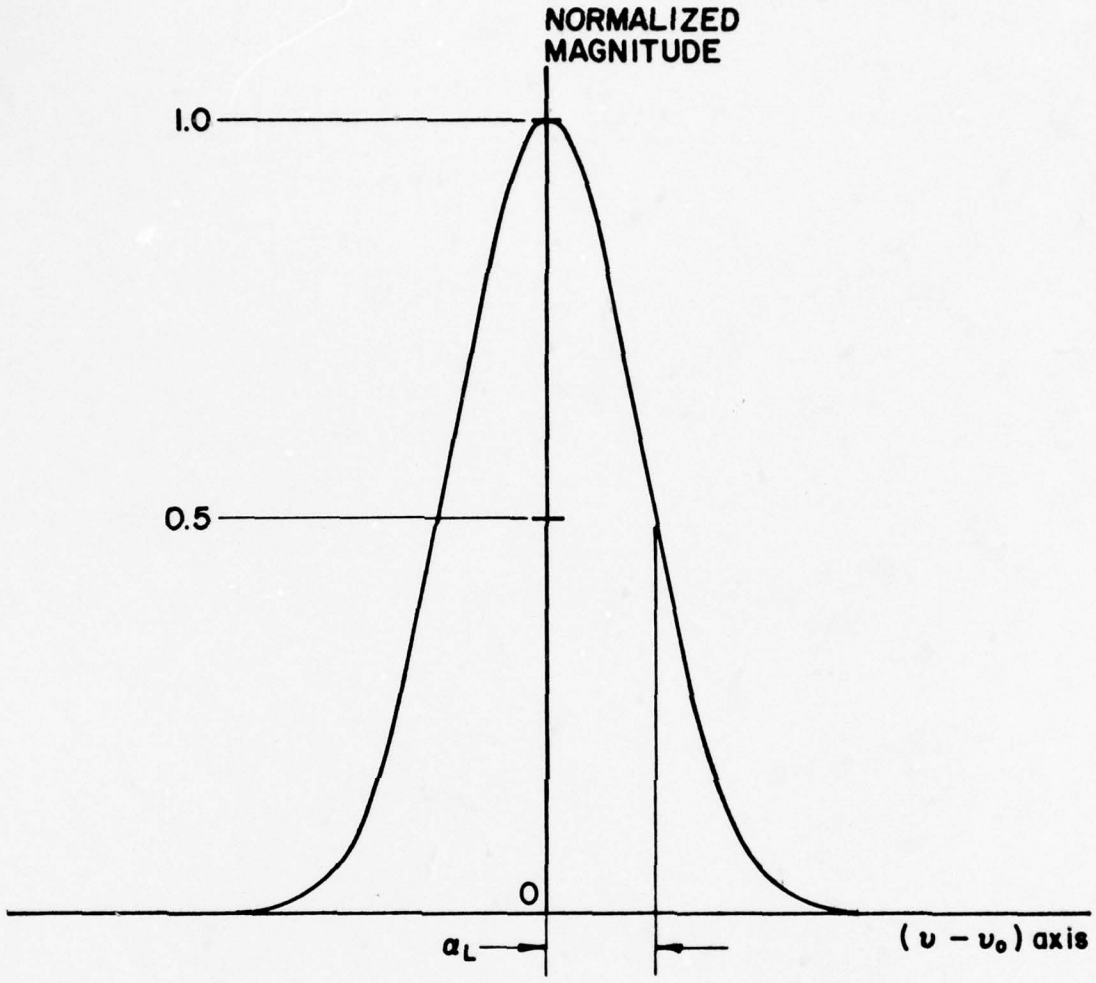
$$\alpha_L = \alpha_{L_o} \left[\frac{P}{Po}\right] \left[\frac{T_o}{T}\right]^{1/2} \quad , \qquad 2.3\text{-}8$$

where α_{L_o} is the half-width value at STP. A contour of the Lorentz profile is shown in Fig. 2.3-1.

When transmittance calculations are to be performed over a wide range of pressure values, a combined Doppler-Lorentz contour is sometimes used to gain better accuracy. The convolution of these two line shapes is known as the Voigt profile [La Rocca[16]]. It is expressed as

$$k(\nu) = \frac{k_o U}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{U^2 + (y-t)^2} \, dt, \qquad 2.3\text{-}9$$

where k_o and y are defined in Eqs. 2.3-4 and 2.3-5 respectively, and



$$f(\nu-\nu_o) = \left(\frac{1}{\pi}\right) \frac{\alpha_L}{\alpha_L^2 + (\nu-\nu_o)^2}$$

Figure 2.3-1 LORENTZ LINE SHAPE

t is a dummy variable. U, a function of the Doppler and Lorentz linewidths, is

$$U = \frac{\alpha_L [\ln 2]^{1/2}}{\alpha_D} \quad . \qquad 2.3\text{-}10$$

It is of interest to note that while the Voigt profile delivers greater accuracy over wide pressure ranges (i.e. 0-1013 mb for earth's atmosphere), it is difficult and time consuming to evaluate. This is due primarily to the integration over infinite limits and the variable characteristics of the Doppler half-width [Goody[11]]. An interesting work in this area has been compiled by Van Derwood [26].

2.4 Beer's Law of Molecular Absorption

Attenuation of radiant energy in the atmosphere can be attributed to the process of scattering and absorption. The latter, because of allowable state transitions, is the primary cause of such abatements in the infrared spectrum. A quantitative analysis of molecular absorption is given by Beer's law (also known as the Lambert-Beer law) which is outlined below.

Referring to Fig. 2.4-1, let $\Delta I_{\nu_o}(z)$ be the amount of radiation which is absorbed by the gas contained within Δz. The subscript indicates monochromatic radiation at frequency ν_o. The gas amount, U(z), between z_1 and z_2 can be computed by

$$U(z) = \rho(z)\Delta z \qquad 2.4\text{-}1$$

if the gas density is known in the layer.

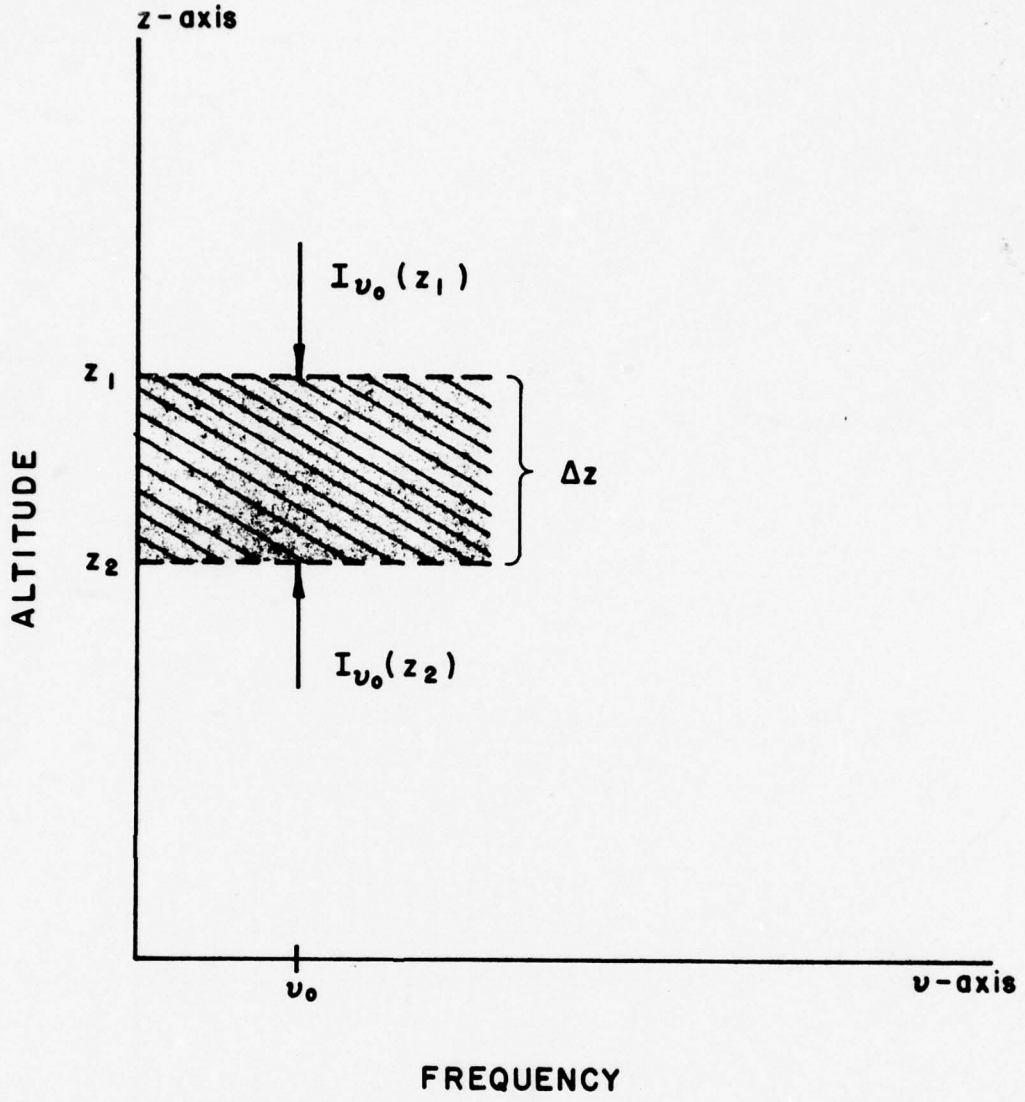


Figure 2.4-1 LAMBERT-BEER LAW GEOMETRY

The absorption law of Beer states that the loss in intensity between z_1 and z_2 is proportional to the path length, Δz, the incoming radiation, $I_{\nu_o}(z_1)$, and the concentration of absorbing gas, $\rho(z)$. If $K_{\nu_o}(z)$ represents the constant of proportionality, then

$$\Delta I_{\nu_o}(z) = -I_{\nu_o}(z_1) K_{\nu_o}(z) \rho(z) \Delta z \ . \qquad 2.4\text{-}2$$

Letting the path length become arbitrarily small, Eq. 2.4-2 can be written in differential form as

$$dI_{\nu_o}(z) = -I_{\nu_o}(z) K_{\nu_o}(z) \rho(z) dz, \qquad 2.4\text{-}3$$

where the negative sign indicates the loss or absorption of radiant intensity. Letting τ_{ν_o} be the ratio of incoming to outgoing intensities, and integrating Eq. 2.4-3 between z_1 and z_2 gives

$$\tau_{\nu_o} = \mathrm{EXP}\left[- \int_{z_1}^{z_2} K_{\nu_o}(z) \rho(z) \, dz \right]. \qquad 2.4\text{-}4$$

If the gas density and constant of proportionality are known, Eq. 2.4-4 becomes

$$\tau_{\nu_o} = \exp\left[-K_{\nu_o} U \right], \qquad 2.4\text{-}4$$

where the gas amount, U, is defined by Eq. 2.4-1.

The constant, K_{ν_o}, is the absorption coefficient. Sometimes K_{ν_o}

is referred to as an "extinction" coefficient, although the term is normally reserved to describe a combination of attenuation mechanisms. K_{ν_o} is formed from the product of a given line shape as described in section 2.3 and a line strength as given by Eq. 2.3-6.

Since τ_{ν_o} measures how well radiant energy passes through a given amount of absorbing gas, it is known as transmittance. Transmittance ranges from values of 1 (indicating no absorption) to 0 (indicating total absorption). Additionally, the term absorptance applies to a medium abating incident radiation and is related to transmittance by $A = 1-\tau$. Therefore, using Eq. 2.4-5, absorptance can be expressed in terms of an absorption coefficient as

$$A = 1 - EXP\left[-K_{\nu_o} U\right]. \qquad 2.4\text{-}6$$

2.5 The Absorbing Gases

As noted earlier, most molecular absorption takes place in the infrared spectrum. This chapter concludes with a brief discussion of the atmospheric constituents which are mainly responsible for this phenomenon.

It is generally accepted that seven molecules contribute to absorption in the infrared and visible regions of the atmosphere [2, 12, 16, 18 & 29]. They are: (1) water vapor - H_2O; (2) carbon dioxide - CO_2: (3) ozone - O_3; (4) nitrous oxide - N_2O; (5) carbon monoxide - CO; (6) methane - CH_4; and (7) oxygen - O_2. McClatchey, et. al., considers only these constitutents in AFCRL's "Line Parameter Compilation" tape which is the source data for all calculations

used in this document.

Of the seven molecules, only CO_2 and O_2 are major atmospheric constituents. Luckily, oxygen is a very minor absorber. The other two major constituents, N_2 and A, are transparent in the spectral region of interest. Carbon dioxide is the only absorber which constitutes any significant portion of the atmosphere (0.032%).

Absorptance calculations are most difficult for H_2O and O_3 due to their variable mixing ratios. Concentrations are dependent on geographical location and time of year. Standard density profiles for these two gases are available for typical latitudes and seasons [McClatchey[18], LaRocca[16]].

The other molecules are considered to be uniformly mixed in the atmosphere. Their parts per million by volume (PPM) ratios are shown below.

Constituent	Ratio in PPM
CO_2	330.0
N_2O	0.28
CO	0.075
CH_4	1.60
O_2	2.10×10^5

[McClatchey[17]]

It is possible to analyze each molecular gas to establish the lines of absorption over a range of frequencies. For the portion of

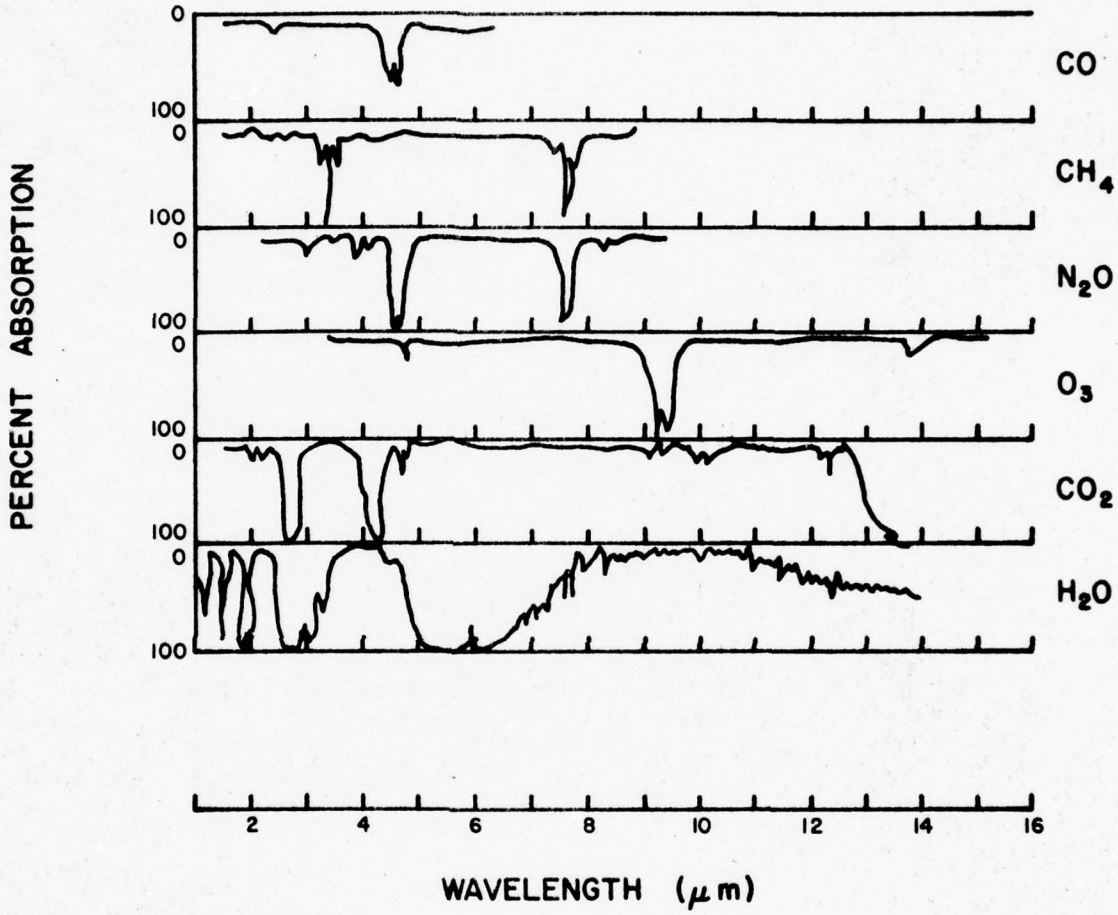


Figure 2.5-1 % ABSORPTION-VS-WAVELENGTH
[Anding^2]

the electromagnetic spectrum from 0-15 μm, Fig. 2.5-1 illustrates the percent absorption for each molecule of interest. Each profile is characterized by discrete bands consisting of a distribution of a large number of overlapping lines of various strengths. The overall contours as shown in Fig. 2.5-1 are dependent on each molecule's distribution of lines, each line's half-width and strength, and proximity to another line.

CHAPTER III

A PROPOSED APPROXIMATION TO THE LORENTZ LINE SHAPE

3.1 Preface

The use of transmittance calculations based on remote radiation measurements to predict temperature and water vapor profiles was first suggested in the late 1950's by Dr. Lewis D. Kaplan [15]. In order to retrieve such information from satellite data in a timely fashion, the solution of the transmittance equation (Eq. 2.4-4) must be accomplished as accurately and as rapidly as possible. A proposed method of calculating an absorption coefficient based on the Lorentz line shape is outlined in this chapter. The approximation presented in Sec. 3-3 was first formulated by Dr. Glenn A. Gibson [9].

Table 3.1-1 is a summary of the notation used in the derivation. Note that the Lorentz half-width is given simply as "α" and the subscript "1" now refers to the atmospheric level under consideration.

3.2 Derivation of the Transmittance Problem

Consider the radiant energies I_1 and I_2 as shown in Fig. 3.2-1. Ray I_1 is attenuated by the molecules in the gas amount labeled U_1. Ray I_2 is incident at zenith angle θ wrt (with respect to) the z-axis and must pass

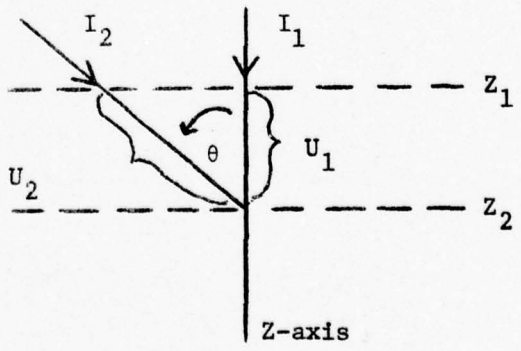


Figure 3.2-1

I. VARIABLE	MEANING
b	gas constant
c	speed of light
E	ground-state energy
g	acceleration due to gravity
h	Planck's constant
K	absorption coefficient
k	Boltzmann's constant
M	gas mixing ratio
P	atmospheric pressure
Q	ratio of vibrational partition functions
S	spectral line strength
T	atmospheric temperature
U	gas amount
α	Lorentz half-width
τ	transmittance
ν	frequency
ρ	gas density
II. SUBSCRIPT	**IDENTIFIER**
i	spectral line
j	*molecular gas*
l	atmospheric level
o	reference or standard

Table 3.1-1 NOTATION INDEX

through a gas amount equal to U_2. If U_1 is known, then the gas amount for any slant-path angle can be calculated by

$$U_2 = (\sec \theta) U_1 \qquad 3.2\text{-}1$$

Therefore, Eq. 2.4-4 can be rewritten to include an arbitrary slant-path angle as

$$\tau_{\nu_o} = \mathrm{EXP}\left[-\sec \theta \int_{z_1}^{z_2} K(z)\, \rho(z)\, dz\right], \qquad 3.2\text{-}2$$

where dz is the vertical path length, and θ is measured as shown in Fig. 3.2-1.

It is normally more convenient to write Eq. 3.2-2 in terms of temperature and pressure. The hydrostatic approximation, as given by Eq. 2.1-1, can also be written as

$$\frac{M(P)dP}{g} = \rho(z)\, dz \qquad 3.2\text{-}2a$$

where M(P) is the gas mixing ratio. Using this form, transmittance is now

$$\tau(\nu,T,P) = \mathrm{EXP}\left[\frac{-\sec \theta}{g} \int_{P_1}^{P_2} K(\nu,T,P)\, M(P)\, dp\right]. \qquad 3.2\text{-}3$$

In order to arrive at an iterative solution to Eq. 3.2-3, it is desirable to express τ as a product of a known transmittance and a "loss" function. Hence, in equation form, we seek

$$\tau_{L+1} = \tau_L\, f(\nu,T,P), \qquad 3.2\text{-}4$$

where $f(\nu,T,P)$ is the "loss" function, and τ_L is known.

As illustrated in Fig. 3.2-2, we would like to express transmittance at any level, τ_{L+1}, in terms of the previous known value, τ_L. To do this we first write τ, as

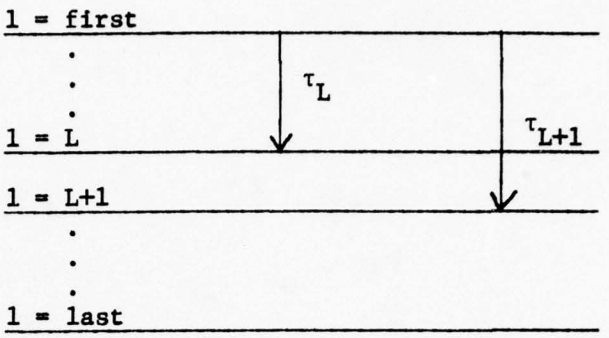


Figure 3.2-2

defined in Eq. 3.2-3, for two successive levels. Hence, for the Lth level

$$\tau_L = \text{EXP}\left[\frac{-\sec\theta}{g}\int_{P_{first}}^{P_L} K(\nu,T,P)\,M(P)\,dP\right], \qquad 3.2\text{-}5a$$

and for the (L+1)th level,

$$\tau_{L+1} = \text{EXP}\left[\frac{-\sec\theta}{g}\int_{P_{first}}^{P_{L+1}} K(\nu,T,P)\,M(P)\,dp\right].$$

Noting that $P_{first} \leq P_L \leq P_{L+1}$ and using a well-known property of definite integrals [Fuller[8]], τ_{L+1} can be expressed as the sum of two integrals as

$$\tau_{L+1} = \text{EXP}\left[\frac{-\sec\theta}{g}\left(\int_{P_{first}}^{P_L} KMdP + \int_{P_L}^{P_{L+1}} KMdP\right)\right], \qquad 3.2\text{-}5b$$

where the terms $K(\nu,T,P)$ and $M(P)$ have been abbreviated. Now we divide Eq. 3.2-5b by Eq. 3.2-5a and solve for τ_{L+1}. This gives

$$\tau_{L+1} = \tau_L \left[\text{EXP} \left(\frac{-\sec\theta}{g} \int_{P_L}^{P_{L+1}} KMdP \right) \right] . \qquad 3.2\text{-}6$$

If we define the "loss" function as the term in brackets, the desired form of Eq. 3.2-4 is achieved.

A number of techniques exist to solve Eq. 3.2-6 in its integral form for τ_{L+1} [Carnahan[5]]. The expression, however, can also be transformed into a differential equation which may be easier to solve numerically.

Taking the natural logarithm of Eq. 3.2-6 we get

$$\ln(\tau_{L+1}) = \ln(\tau_L) + \left[\frac{-\sec\theta}{g} \int_{P_L}^{P_{L+1}} KMdp \right] .$$

Since we assume τ_L is known, $\ln(\tau_L)$ is a constant and its derivative will be zero. Therefore, differentiating wrt pressure gives

$$\frac{1}{\tau_{L+1}} \frac{d\tau_{L+1}}{dP} = \frac{d\left[\frac{-\sec\theta}{g} \int_{P_L}^{P_{L+1}} KMdP \right]}{dP} .$$

From elementary calculus we know that

$$\frac{d\left[\int_x f(x)\,dx\right]}{dx} = f(x).$$

Hence, the above equation can be written as

$$\frac{d\tau_{L+1}}{dp} = \tau_{L+1} \left[\frac{-\sec\theta}{g} KM \right] . \qquad 3.2\text{-}7$$

Equation 3.2-7 is a first order, ordinary differential equation with initial conditions that at $P_1 = P_L$, $\tau_1 = \tau_L$. Many standard solutions exist for the equation in this form [Carnahan[5]] and it is commonly believed to be easier to computerize.

To solve for τ_{L+1} from either equation derived above, it is necessary to know several quantities. They are: (1) slant-path angle - θ; (2) gas mixing ratio - M(P); and (3) absorption coefficient - $K(\nu,T,P)$. Problem geometry will always dictate angle θ and M(P) can be found easily from techniques discussed in Chapter 4. Therefore, for the purpose of this chapter, $K(\nu,T,P)$ is the only remaining unknown. Section 3.3 will formulate a method of calculating the absorption coefficient assuming a Lorentz line shape.

3.3 Derivation of the Approximation

In the pressure regions from 1013 mb to 100 mb, spectral line broadening may be accurately described by the Lorentz contour [McClatchey[17]]. Using the notation of Table 3.1-1, $K(\nu,T,P)$ can be written for the jth absorbing gas, at a given level, as the summation over all contributing lines:

$$K_j(\nu,T,P) = \sum_i \frac{S_{ij}}{\pi} \frac{\alpha_{ij}}{\alpha_{ij}^2 + (\nu-\nu_{oij})^2} . \qquad 3.3\text{-}1$$

Additionally the line strength and half-width can be written as

$$S_{ij} = S_{oij}\, Q_{ij}(T_1)\left(\frac{T_o}{T_1}\right)^{P_j} \mathrm{EXP}\left[\frac{E''_{ij}}{kT_o}\left(1 - \frac{T_o}{T_1}\right)\right] \qquad 3.3\text{-}2$$

and

$$\alpha_{ij} = \alpha_{oij}\left(\frac{P_1}{P_o}\right)\left(\frac{T_o}{T_1}\right)^{1/2} . \qquad 3.3\text{-}3$$

Assuming that a temperature and pressure profile is known and the line parameter data for ν_{oij}, α_{oij}, S_{oij} and E''_{ij} is available, we wish to calculate:

(1) $\tau(\nu,T,P)$ for a fixed frequency ν_o

or

(2) $\overline{\tau}(\Delta\nu,T,P)$ for a band of frequencies $\Delta\nu$.

Regardless of which transmittance is desired, the bulk of calculation time will be spent on evaluating Eq. 3.3-1. The approximation introduced here will shorten this time by separating those arithmetic operations that need computing only once for a given level, gas, or spectral line.

With this aim in mind, we let

$$X = \left(\frac{P_1}{P_o}\right)\left(\frac{T_o}{T_1}\right)^{1/2}$$

and

$$Y_i = \frac{\nu - \nu_{oi}}{\alpha_{oi}} ,$$

where, for simplicity, the "j" subscript has been omitted as all calculations refer to the jth absorbing gas. From these definitions, Eq. 3.3-1 becomes

$$K(\nu,T,P) = \sum_i \frac{S_i}{\pi\alpha_{oi}} \frac{X_1}{X_1^2 + Y_i^2} . \qquad 3.3\text{-}4$$

The expression $\frac{X_1}{X_1^2 + Y_i^2}$ can be broken up into once-per-level, and once-per-line calculations. For an arbitrary positive constant "a",

$$\frac{X_1}{X_1^2 + Y_i^2} = \frac{X_1}{Y_i^2 + a^2} \frac{1}{1 - \left(\frac{a^2 - X_1^2}{Y_i^2 + a^2}\right)} . \qquad 3.3\text{-}5$$

If $\left| \frac{a^2 - X_1^2}{Y_i^2 + a^2} \right| < 1$, then Eq. 3.3-5 can be expanded by a binomial series [Selby[24]] as

$$\frac{X_1}{X_1^2 + Y_i^2} = \frac{X_1}{Y_i^2 + a^2} \sum_{m=0} \left(\frac{a^2 - X_1^2}{Y_i^2 + a^2}\right)^m .$$

Defining

$$f_m(Y_i) = (Y_i^2 + a^2)^{-(m+1)} \text{ and}$$

$$g_m(X_1) = X_1(a^2 - X_1^2)^m ,$$

Eq. 3.3-4 is now

$$K(\nu,T,P) = \sum_{i} \sum_{m=0}^{\infty} \frac{S_i}{\pi\alpha_{oi}} g_m(X_1)\, f_m(Y_i). \qquad 3.3\text{-}6$$

The next expression to be separated is found in Eq. 3.3-2 as

$$\mathrm{EXP}\left[\frac{E_i}{kT_o}\left(1 - \frac{T_o}{T_1}\right)\right].$$

Let $W_1 = \frac{T_o}{T_1}$, E_a and W_a be constants chosen to be in the middle of their respective ranges of interest. Then

$$\mathrm{EXP}\left[\frac{E_i}{kT_o}\left(1 - \frac{T_o}{T_1}\right)\right] = \mathrm{EXP}\left[\left(\frac{E_a}{kT_o} + \frac{E_i - E_a}{kT_o}\right)\left(1 - W_a - W_1 + W_a\right)\right].$$

If

$$\beta_i = \mathrm{EXP}\left[\frac{E_i(1 - W_a) + E_a W_a}{kT_o}\right] \quad \text{and}$$

$$\eta_1 = \mathrm{EXP}\left[\frac{-E_a W_1}{kT_o}\right] = \mathrm{EXP}\left[\frac{-E_a}{kT_1}\right],$$

then

$$\mathrm{EXP}\left[\frac{E_i}{kT_o}\left(1 - \frac{T_o}{T_1}\right)\right] = \eta_1\beta_i \quad \mathrm{EXP}\left[\left(\frac{E_a - E_i}{kT_o}\right)\left(W_1 - W_a\right)\right].$$

Noting that $E^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$ [Selby[24]], then

$$\text{EXP}\left[\frac{E_i}{kT_o}\left(1 - \frac{T_o}{T_1}\right)\right] = \eta_1 \beta_i \sum_{n=0}^{\infty} \frac{\left[\left(\frac{E_a - E_i}{kT_o}\right)\left(W_1 - W_a\right)\right]^n}{n!} .$$

Using this expression, S_i (from Eq. 3.3-2) is

$$S_i = Q_1 W_1^{bj} \eta_1 \beta_i S_{o_i} \sum_{n=0}^{\infty} \frac{\left[\left(\frac{E_a - E_i}{kT_o}\right)\left(W_1 - W_a\right)\right]^n}{n!} . \qquad 3.3\text{-}7$$

Finally, using Eqs. 3.3-6 and 3.3-7, the Lorentz line absorption coefficient for the 1th level and jth gas is exactly

$$K_{1j} = \frac{1}{\pi} Q_{1j} W_1^{bj} \eta_{1j} \sum_{n=0}^{\infty} \frac{(W_1 - W_a)^n}{n!} \sum_{m=0}^{\infty} g_m (X_1) \cdot$$

$$\sum_i \frac{S_{oij}}{\alpha_{oij}} \beta_{ij} \left(\frac{E_{aj} - E_{ij}}{kT_o}\right)^n f_m(Y_{ij}) \qquad 3.3\text{-}8$$

Equation 3.3-8 is the basis for absorption coefficient calculations in which quantities dependent on atmospheric level, molecular gas, and spectral line have been separated.

3.4 Selection of Arbitrary Constants and Series Truncation

Three decisions involving constants must be made before Eq. 3.3-8 can be used to approximate the Lorentz line absorption coefficient. They are:

(1) selecting appropriate values for E_a and W_a;

(2) fixing the constant "a" in Eq. 3.3-5 to insure convergence of the binomial series; and

(3) truncating the infinite series over "m" and "n" so that a desired degree of accuracy is achieved with the minimum number of terms.

The line parameter data used in this document [McClatchey[17]] was compiled at a standard temperature (T_o) of 296° K. Using T_o = 296° K and choosing T_a to be an average temperature selected from the profile used, we can pick W_a:

$$W_a = \frac{296}{T_a} \quad . \tag{3.4-1}$$

E_{aj} should also use an average value energy for a given gas. For the user's convenience, average energies are computed and furnished by the computer program (see Appendix A) used to extract data from the line parameter tape. These values of E_{aj} are used in all computations throughout this work.

Secondly, the expansion of Eq. 3.3-5 requires the constraint that

$$\left| \frac{a^2-x^2}{y^2+a^2} \right| < 1 \tag{3.4-2}$$

for all real values of x and y. For typical atmospheric profiles from 0 to 100 km [McClatchey[17]], the ranges of temperature and pressure are approximately 300° K to 200° K and 1.4×10^{3} mb to 5.0×10^{-7} mb respectively. Consequently, if $T_o = 296°$ K and $P_o = 1013$ mb are taken to be the standard, x will range from near zero to about 1.3, and Y can vary, theoretically, from 0 to ∞. Using these bounds for x and y we can now choose an "a" and analyze the constraint for regions of convergence and divergence.

Inequality 3.4-2 requires two conditions to be met depending on the sign of $\left(\frac{a^2-x^2}{y^2+a^2}\right)$. When a>x, the inequality reduces to

$$y^2 > -x^2 \ .$$

Since x and y are real, $-x^2$ will always be negative and less than y^2. Hence, the series will always converge for a>x. Next, when a<x the inequality becomes

$$y^2 < x^2 - 2a^2 \ . \qquad 3.4\text{-}3$$

This restriction will be most severe when y = 0. When this occurs, inequality 3.4-3 becomes

$$x^2 < 2a^2 \ . \qquad 3.4\text{-}4$$

Inequality 3.4-3 is plotted in Fig. 3.4-1 using only the I and IV quadrants (regions of interest) for two values of "a". Based on Eq. 3.4-4, convergence can always be assured when

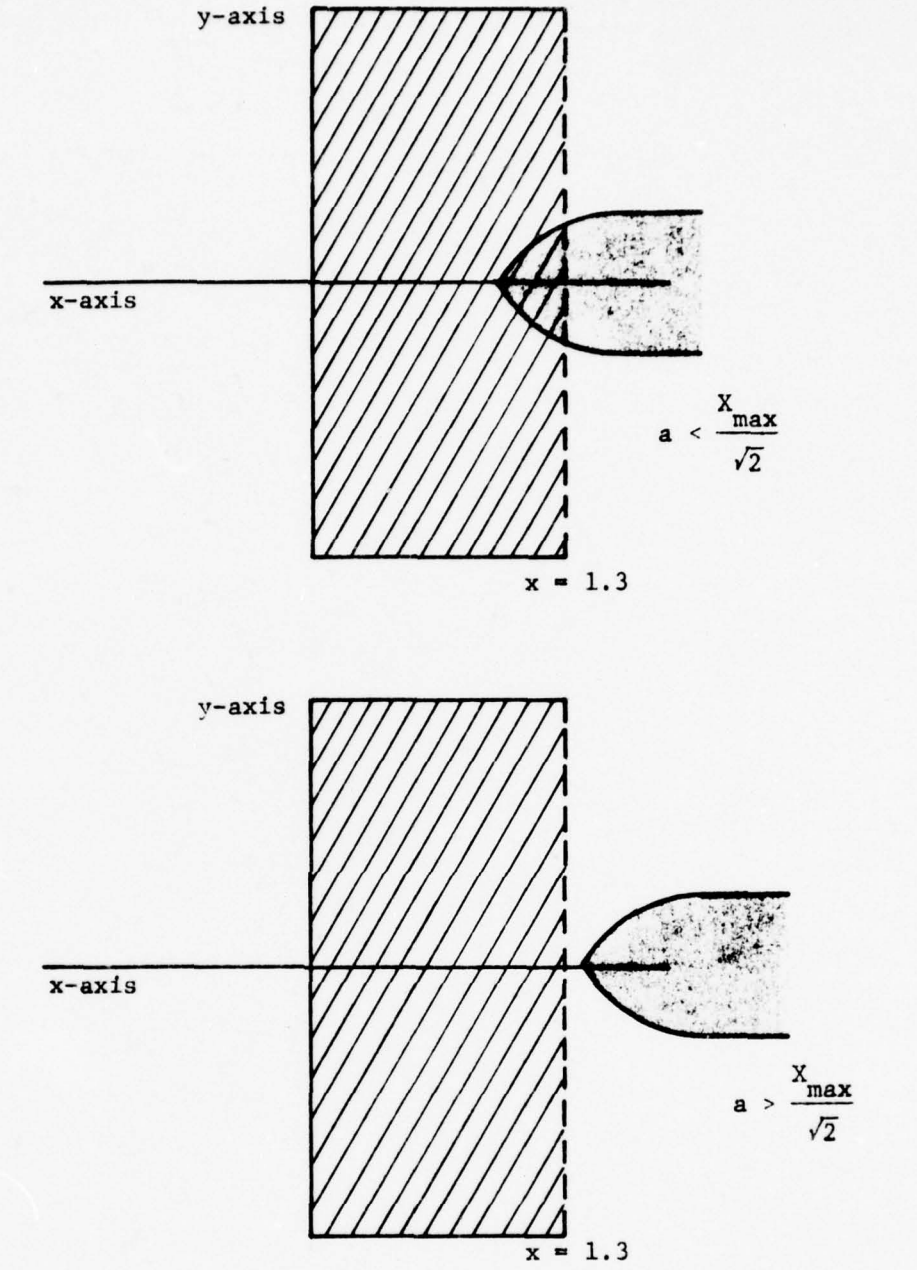


Figure 3.4-1 CONVERGENCE AREAS FOR BINOMIAL SERIES

$$a > \frac{X_{max}}{\sqrt{2}}, \qquad 3.4\text{-}5$$

where X_{max} is the upper bound of x. Satisfying Eq. 3.4-5 will push the region of divergence from the area of valid x and y values. This is illustrated in Fig. 3.4-1.

Insuring the convergence of the binomial series and selecting W_a and E_{aj} have been shown to be straight forward. Truncating the two infinite series in Eq. 3.3-8, however, requires a more complicated approach. Because a finite number of terms must be used, an error is introduced into the approximation. The magnitude of the error can be made arbitrarily small by increasing the number of terms, but this has the adverse effect of increasing calculation time. Care must be taken in keeping the number of terms to a minimum without allowing the resultant error to become larger than desired.

First, consider the Taylor's series expansion used in Eq. 3.3-7 which is repeated here:

$$\text{EXP}\left[\left(\frac{E_a-E_i}{kT_o}\right)\left(W_1-W_a\right)\right] = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\frac{(E_a-E_i)}{kT_o}\left(W_1-W_a\right)\right]^n . \qquad 3.4\text{-}6$$

Let $Z = \left[\left(\frac{E_a-E_i}{kT_o}\right)\left(W_1-W_a\right)\right]$. The average error after n+1 terms is given as

$$R(Z) = \frac{Za^{n+1}}{(n+1)!} \quad \text{EXP} \quad [Z_{max}],$$

where Z_a is the average value of Z and Z_{max} is the maximum value [Carnahan[5]]. Using typical values from line parameters in the 4.3μm band for channels 11-15 we have,

$$(E_a - E_i)_{AVE} \doteq 2204.000 \qquad (E_a - E_i)_{MAX} = 2381.602$$

$$(W - W_a)_{AVE} \doteq 0.199 \qquad (W - W_a)_{MAX} = 0.222$$

(see McClatchey [17] and Table 3.4-1). If the units of $(E_a - E_i)$ are converted properly and if we choose $R(Z) = 5.0 \times 10^{-4}$ to insure three decimal place accuracy, we establish the error bound as

$$5.0 \times 10^{-4} \geq \frac{1}{(n+1)!} \left[1.0\right]^{n+1} \text{EXP}\left[2.500\right]$$

which is satisfied when n = 12. A further reduction in the number of terms needed can be realized through Chebyshev *economization of* EXP[Z]. A reduction to nine terms was obtained in the 4.3μm band.

Lastly, the binomial series of Eq. 3.3-5 must also be truncated. Recall that

$$\frac{X}{Y^2 + X^2} = \frac{X}{Y^2 + a^2} \sum_{m=0}^{\infty} \left(\frac{a^2 - X^2}{Y^2 + a^2} \right)^m . \qquad 3.4\text{-}7$$

Let $V = \left(\frac{a^2 - X^2}{Y^2 + a^2} \right)^m$. Then

$$\frac{1}{1 - V} = \sum_{m=0}^{\infty} V^m = 1 + V + V^2 + \cdots + V^m + \frac{V^{m+1}}{1 - V}, \qquad 3.4\text{-}8$$

Channel #	Molecule	E_{max}	E_{ave}	E_{min}	$\lvert E_a - E \rvert_{max}$
11	H_2O	2734.000	1478.030	222.060	1255.970
	CO_2	4037.079	2884.865	1732.614	1152.233
	N_2O	2299.382	1150.910	2.429	1148.477
	CO	1594.788	883.883	172.977	710.910
12					
	H_2O	2905.420	1804.820	704.220	1100.600
	CO_2	3892.884	2346.357	799.829	1546.528
	N_2O	2938.820	1469.410	0.000	1469.410
	CO	271.29	746.851	522.473	224.378
13					
	H_2O	3101.190	1881.375	661.560	1219.815
	CO_2	4790.563	2408.961	27.359	2381.602
	N_2O	2923.455	1480.583	37.710	1442.873
	CO	2149.372	1747.984	1346.596	401.388
14					
	H_2O	3144.630	1795.670	446.710	1348.960
	CO_2	4587.402	2293.701	0.000	2293.701
	N_2O	2982.590	1817.910	653.221	1164.6845
	CO	2549.953	2549.953	2549.953	0.000
15					
	H_2O	3314.90	1928.905	542.910	1385.995
	CO_2	4669.512	2334.756	0.000	2334.756
	N_2O	1419.607	856.832	294.057	562.775

*Units of E are in cm^{-1}

Table 3.4-1 GROUND STATE ENERGY DISTRIBUTION IN THE 4.3μm BAND

and the exact error is

$$R = \frac{V^{m+1}}{1 - V} = \left[\left(\frac{Y^2 + a^2}{Y^2 + X^2} \right) \left(\frac{a^2 - X^2}{Y^2 + a^2} \right)^{m+1} \right] . \qquad 3.4\text{-}9$$

From Eq. 3.4-9, the absolute fractional error can be formed :

$$R_f = \left| \frac{\frac{V^{m+1}}{1 - V}}{\frac{1}{1 - V}} \right| = \left| V^{m+1} \right| = \left| \left(\frac{a^2 - X^2}{Y^2 + a^2} \right)^{m+1} \right| .$$

Gibson [10] has determined that for a fractional error of one part in ten thousand, the optimum value for the constant "a" will not completely satisfy the convergence criteria of inequality 3.4-5. Divergence of the binomial series takes place whenever $|(\nu - \nu_o)| < 0.4$ wavenumber. Since this occurs often, the series of Eq. 3.4-8 has to be modified to reduce the number of instances in which nonconvergence develops.

In addition to the value defined as V, we add Z:

$$Z = \frac{X}{Y^2 + a^2} .$$

Then from Eq. 3.4-7

$$\frac{X}{X^2 + Y^2} = \frac{Z}{1 - V} = Z \left[1 + V + V^2 + \ldots + V^m + \frac{V^{m+1}}{1 - V} \right] .$$

If the last term in series, $\frac{V^{m+1}}{1 - V}$, is approximated by

$$CV^{m+1} \doteq \frac{V^{m+1}}{1 - V} \quad ,$$

where, for an arbitrary constant "d",

$$C = \frac{d^2 (Y^2 + a^2)}{(X^2 + d^2) Y^2} \quad .$$

For M+1 terms,

$$\frac{X}{X^2 + Y^2} \doteq Z\left[\sum_{m=0}^{M-1} V^m\right] + ZV^M C$$

$$\doteq \sum_{m=0}^{M-1} \frac{X(a^2 - X^2)^m}{(Y^2 + a^2)^{m+1}} + \frac{d^2 X(a^2 - X^2)^M}{(X^2 + d^2)} \cdot \frac{1}{Y^2 (Y^2 + a^2)^M} \quad . \qquad 3.4\text{-}10$$

Equation 3.4-10 has the effect of adding the correction factor $ZV^M C$ to the approximation of Eq. 3.4-8. The error term can now be reduced by selection of constants "a" and "d". Unpublished analysis [Gibson[10]] suggests that, using 7 terms and the same fractional error of .0001, divergence of Eq. 3.4-10 can be avoided unless $|(\nu - \nu_o)| <$ 0.0525 wavenumber. Fortunately, this will happen in less than 0.5% of the spectral lines considered. For these few cases it is not inconvenient to calculate the contribution to the absorption coefficient using the standard formula of Eq. 3.3-1.

It will be shown in Chapter 6 that calculation of transmittance

using Eq. 3.3-8 and the modification explained above is accurate to at least three decimal places. Additionally, it will be seen that because of the separation technique used in the approximation and the small number of terms required for series convergence, a significant amount of computational time is saved.

CHAPTER IV

TOPICS RELATED TO ATMOSPHERIC ABSORPTION

4.1 Preface

This chapter is concerned with developing the tools necessary to apply the theory presented in Chapters 2 and 3. Before Eq. 3.3-8 can be used to calculate the Lorentz line absorption coefficient, spectral line parameters, ν_o, α_o, S_o and E" must be known. Additionally, the various formulae will yield meaningful results only if proper units and conversion factors are employed. Because a working knowledge of units is essential to the atmospheric investigator and the amount of line parameter data one must handle can be overwhelming, this chapter will address some of the practical problems often encountered while working in atmospheric sciences.

4.2 Line Parameters - AFCRL's Data Tape

An excellent source of spectroscopic data is the Air Force Cambridge Research Laboratories' (AFCRL) Atmospheric Absorption Line Parameters Compilation [McClatchey[17]]. The tape includes data on 108,000 spectral lines ranging in wavelength from .828μm to .0325m. Seven molecules are included in the compilation which are found naturally in the earth's atmosphere and considered to be the absorbers in the infrared and visible spectrums. They are: (1) water vapor - H_2O; (2) carbon dioxide - CO_2; (3) ozone - O_3; (4) nitrous oxide - N_2O; (5) carbon monoxide - CO; (6) methane - CH_4; and (7) oxygen - O_2.

To enable the user to implement the equations of Chapters 2 and 3, four essential parameters are included for each data entry along with the molecule's identification information. A spectral line dossier includes: the resonant frequency, ν_o (cm^{-1}); the intensity per absorbing molecule, S_o (cm^{-1}/molecule-cm^{-2}); the Lorentz half-width, α_o (cm^{-1}); the rest-state energy, E" (cm^{-1}); the rotation and vibration identification numbers; date of information; the isotope identification code; and lastly, the molecule identification number. The lines are ordered on the tape in ascending frequency (measured in wavenumbers).

Lines were included in the compilation based on an intensity criteria. The "Criterion Intensity Minimum" for each molecule is shown in Table 4.2-1. The cutoff values were violated in two

Molecule Type	I. D. No.	S_o Minimum*
H_2O	1	3.0×10^{-27}
CO_2	2	2.2×10^{-26}
O_3	3	3.5×10^{-24}
N_2O	4	3.0×10^{-23}
CO	5	8.3×10^{-23}
CH_4	6	3.3×10^{-24}
O_2	7	3.7×10^{-30}

*Units are cm^{-1}/molecule-cm^{-2}

Table 4.2-1 CRITERION INTENSITY MINIMUM
[Adapted from McClatchey[17]]

instances. In regions of very strong absorption, very weak lines above the established minimum were omitted. Also for cases in which weak lines are so closely spaced that their combined effect may contribute significantly to absorption, the minimum criteria was lowered.

Table 4.2-2 is a listing of the coding used to identify each molecule type and isotope. Molecules are identified by a simple numbering system from 1 to 7. Isotope codes are based on the molecule's atomic numbers. For example, the four isotopes of carbon monoxide can be written as: $^{12}C^{16}O$; $^{13}C^{16}O$; $^{12}C^{18}O$; $^{12}C^{27}O$. If the units digit of the atomic numbers are used, the respective isotope codes for carbon monoxide are: 26; 36; 28; and 27.

The spectral data compiled by AFCRL is on a 7-track, 800 BPI, 1/2 in. wide magnetic tape. The format used for each line entry is standardized to an 80 column card and is given below. Data records

Variable	ν_o	S_o	α_o	E"	Rot. & Vib. I. D. No.	Date	Isotope	Molecule
Card Column	1-10	11-20	21-25	26-35	36-70	71-73	74-77	78-80
Format Code	F10.3	E10.3	F5.3	F10.3	5 A6, A5	I3	I4	Ie

Figure 4.2-1 WORD FORMAT CHART

are composed of a number of card-imaged line parameter sets. Each record begins with a number (format I10) indicating how many card-imaged sets are to follow and is separated by a string of alfanumeric characters and symbols which aid in record identification. A full

Molecule Type	Molecule I. D. Number	Isotope I. D. Number
H_2O	1	161 162 181 171
CO_2	2	626 636 628 627 638 637 824
O_3	3	666 668 686
N_2O	4	446 456 546 448 447
CO	5	26 36 28 27
CH_4	6	211 311 212
O_2	7	66 68 67

Table 4.2-2 MOLECULE AND ISOTOPE CODES
[Adapted from McClatchey[17]]

record contains 40 card images in the above format. End of file (EOF) markers are placed on the tape at frequency points: 500, 1000, 2000, 5000, 7500, and 10000 cm^{-1}. A double EOF marker is at the end of the tape.

4.3 Extracting Data from AFCRL's Tape

In the report referenced above [McClatchey[17]], a tape-read program is listed which can be used with a Control Data Corporation 660 computer. Since there is a good chance that some users may not have CDC computer equipment, a data retrieval routine is listed in Appendix A for use with an IBM-360/65.

The routine given in the Appendix was written to perform several tasks:

(1) access AFCRL's tape and extract spectral line data between arbitrary frequency limits (channel limits);

(2) count the number of lines contained within the channel for each molecule type;

(3) segregate line parameters by molecule type into separate arrays;

(4) build a single data file for arbitrary frequency limits with data arranged in ascending frequency and segregated by molecule type; and

(5) compute the mid-point value of energy and the average intensity for each molecule type.

The program is divided into two parts. The main routine initializes variables, selects channel limits and outputs all data. The subroutine,

CHREAD, reads the tape between channel limits, counts the number of lines for each molecule type, segregates the data, writes channel data on a permanent file and computes average values of energy and intensity described in (5) above. The user can easily adapt all or part of the routine for a particular purpose. Flow charts for the main and subroutine programs can be found in Fig. 4.3-1. Table 4.3-1 is a listing of the main variables used in the programs.

4.4 Units of Atmospheric Physics

This section is presented to the novice atmospheric scientist as an aid in understanding the units used in infrared absorption calculations. For the sake of continuity, the subject of units will be discussed as it applies to the basic equation of transmittance. First, however, a clarifying note is in order to explain the term "frequency" which is used rather loosely in atmospheric physics.

In almost all cases, frequency will be synonymous with the term wavenumber (cm^{-1}). The wavelength, λ, and wavenumber, ν, are related by

$$\nu[cm^{-1}] = \frac{10^4}{\lambda\ [\mu m]} ,$$

where λ is given in micrometers. For example,

$$4.3\mu m = 2{,}325.58\ cm^{-1}$$

and

$$15\mu m = 666.67\ cm^{-1}.$$

Recall from Beer's Law that

$$\tau = EXP\ [-KU], \qquad 4.4\text{-}1$$

Variable		Explanation of Variable Name
AN20	-	Data array for nitrous oxide
BWDTH	-	Array containing channel bandwidths
CH4	-	Data array for methane
CNTR	-	Array containing channel center frequencies
CO	-	Data array for carbon monoxide
CO2	-	Data array for carbon dioxide
EAVE	-	Array containing E_a for each molecule type
FHI	-	Channel upper frequency
FLO	-	Channel lower frequency
H_2O	-	Data array for water vapor
ICNT	-	Array containing number of lines per molecule found within channel limits
IFILE	-	Array used to reference a data file
KMOL	-	Molecule identification number
NOFIL	-	Data file reference number
02	-	Data array for oxygen
03	-	Data array for ozone
SAVE	-	Array containing average intensities

Table 4.3-1 VARIABLE NAMES FOR DATA RETRIEVAL ROUTINE

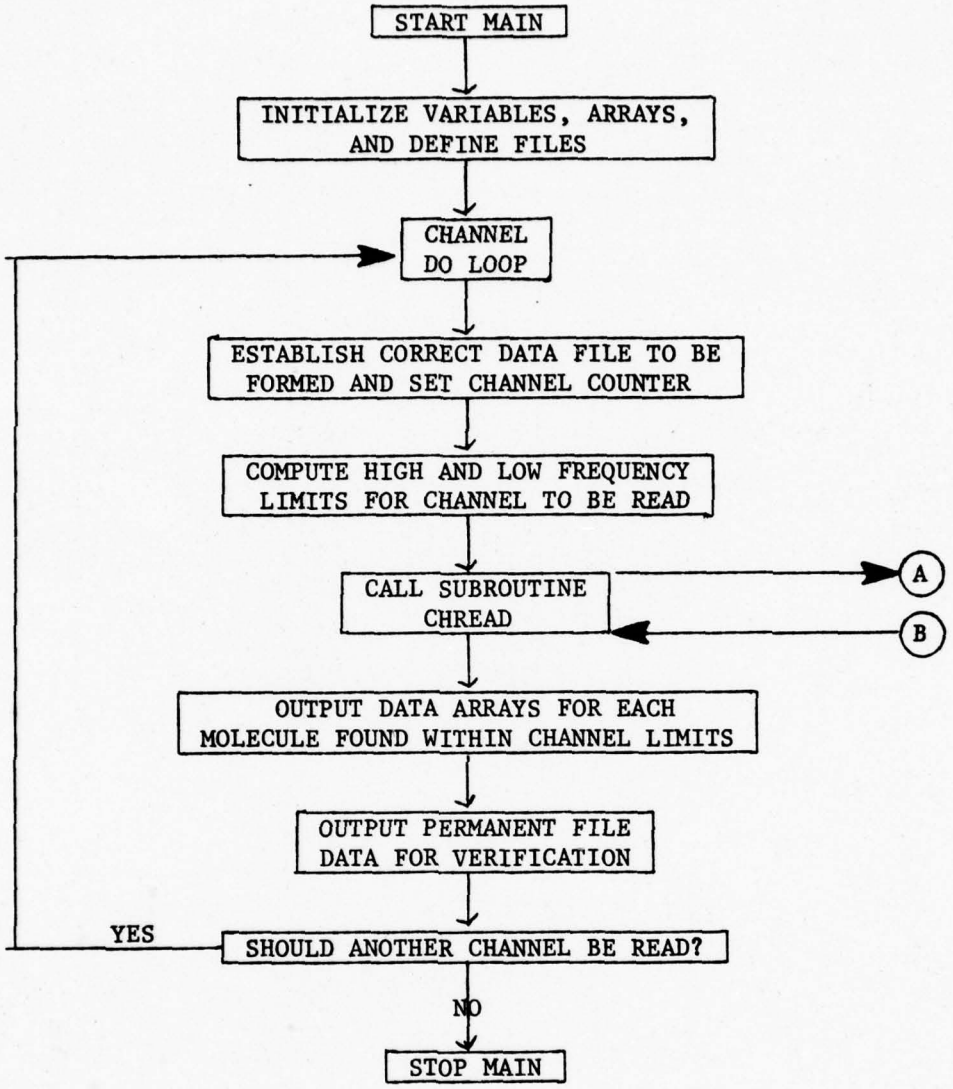


Figure 4.3-1 MAIN DATA ROUTINE FLOW DIAGRAM

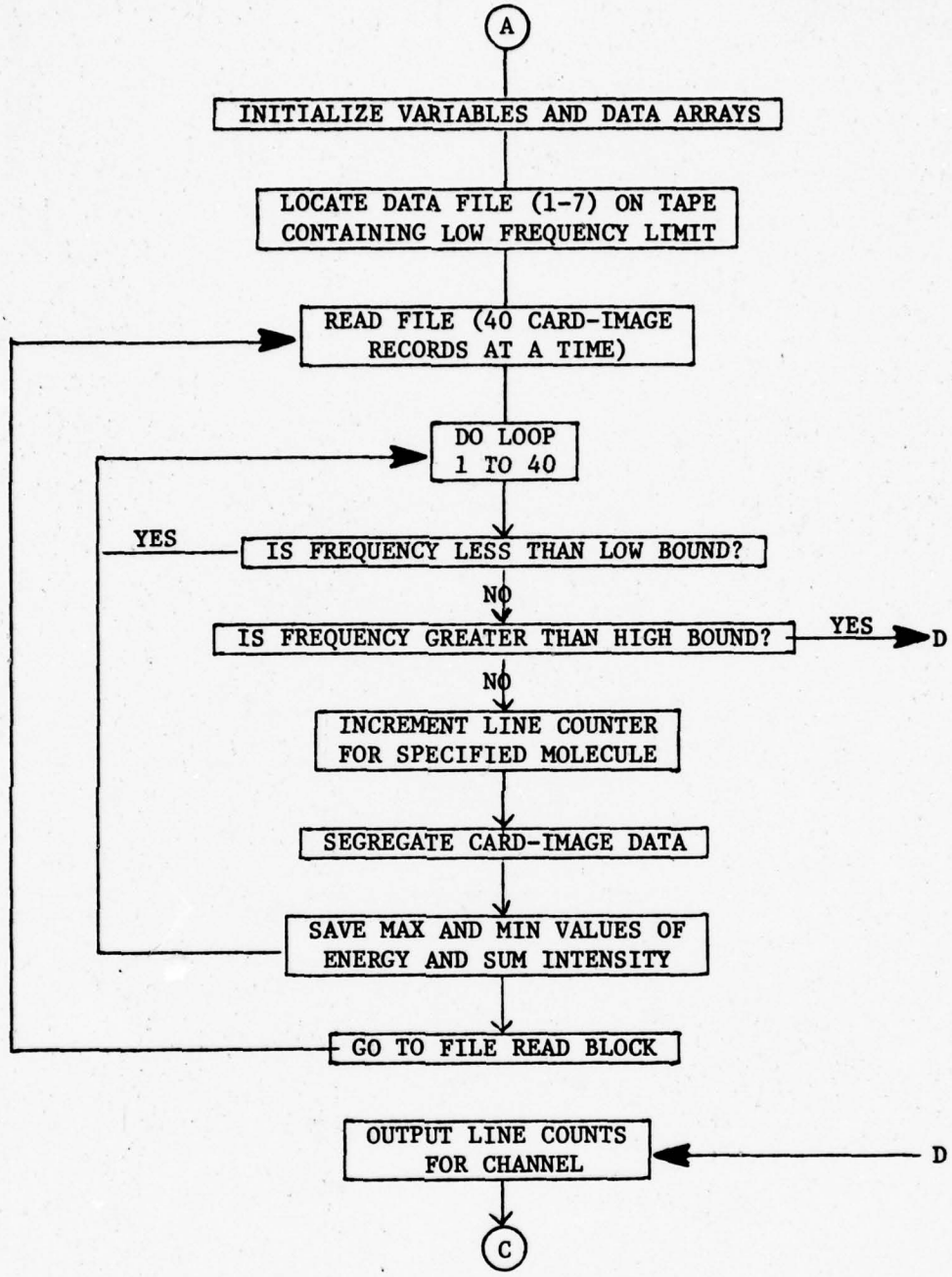


Figure 4.3-1(cont.) CHREAD DATA ROUTINE FLOW DIAGRAM

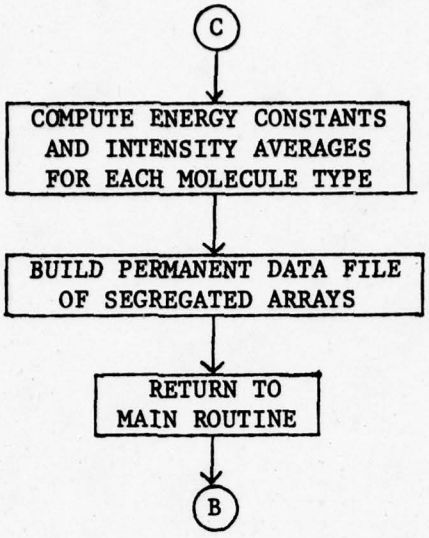


Figure 4.3-1(cont.) CHREAD DATA ROUTINE FLOW DIAGRAM

where τ is the transmittance, K is the attenuation or absorption coefficient, and U is the gas amount defined by Eq. 2.4-1.

Transmittance, therefore, is dimensionless. This dictates that the units of K and U be inversely proportional. The gas amount, U, is normally measured in atmospheric centimeters, [atm-cm]. Hence, K must be formulated dimensionally to inverse atmospheric centimeters, [atm-cm^{-1}].

Beginning with K, as given by Eq. 2.3-7a, for Lorentz line broadening we have

$$K = \frac{S}{\pi} \frac{\alpha}{\alpha^2 + (\nu-\nu_o)^2} . \qquad 4.4\text{-}2$$

where the half-width is

$$\alpha = \alpha_o \left(\frac{P}{P_o} \right) \left(\frac{T_o}{T} \right)^{1/2} , \qquad 4.4\text{-}3$$

and the line strength is given by

$$S = S_o Q \left(\frac{T_o}{T} \right)^b \text{EXP} \left[\frac{-E''(T_o-T)}{kT_o T} \right] . \qquad 4.4\text{-}4$$

The dimensions of the line parameters (α_o, S_o, E", ν_o), temperature, and pressure are normally established by the data available for use. Typical dimensions for these values are shown below.

Variable	Dimension
T	°K (degrees Kelvin)
P	mb (millibars)
α_o	cm^{-1}/atm (wavenumber/atmosphere)
ν_o	cm^{-1} (wavenumber)
S_o	cm^{-1}/molecule - cm^{-2}
E"	cm^{-1} (wavenumber)

Pressure is also commonly given in atmospheres [atm], and is related to millibars [mb] by

$$1[\text{mb}] = 9.869233 \times 10^{-4}\ [\text{atm}]. \qquad 4.4\text{-}5$$

Since the standard pressure, P_o, used throughout AFCRL's data compilation is one atmosphere (P_o = 1atm ≐ 1013 mb), the numerical value of the half-width is actually α_o/P_o dimensionally. Therefore, the dimensions of α_o are really [cm^{-1}] and will be used as such. Lastly, the partition function ratio, Q, and Boltzmann's constant, k, which appear in Eq. 4.4-4, have dimensions of

$$Q \overset{d}{=} 1$$

and

$$k \overset{d}{=} \text{Joule/°K},$$

where $\overset{d}{=}$ means "dimensionally equal to."

With these facts in mind, Eqs. 4.4-3 and 4.4-4 can be written dimensionally as

$$\alpha \stackrel{d}{=} [cm^{-1}]\left[\frac{mb}{mb}\right]\left[\frac{°K}{°K}\right]^{1/2}$$

$$\stackrel{d}{=} \left[cm^{-1}\right], \qquad 4.4\text{-}5$$

and

$$S \stackrel{d}{=} \left[\frac{cm^{-1}}{molecule\text{-}cm^{-2}}\right]\left[1\right]\left[\frac{°K}{°K}\right]^{b} EXP\left[\frac{cm^{-1}\ °K}{(Joule/°K)(°K^{2})}\right]$$

$$\stackrel{d}{=} \left[\frac{cm^{-1}}{molecule\text{-}cm^{-2}}\right] EXP\left[\frac{cm^{-1}}{Joule}\right]. \qquad 4.4\text{-}6a$$

The dimensions of the exponential in Eq. 4.4-1 must be made equal to unity. This can be accomplished by converting ground-state energy from wavenumbers to Joules. First, note that Planck's constant, h, and the speed of light in a vacuum, c, are given as [Abramowitz[1]]

$$h = 6.626196 \times 10^{-24}[Joule\text{-}sec]$$

and

$$c = 2.997925 \times 10^{10}[cm/sec].$$

If the ground-state energy, E", is multiplied by the factor hc, the dimensions of the expression become

$$\text{EXP}\left[\frac{-E''hc}{kT_o}\left(\frac{T_o-T}{T}\right)\right] \stackrel{d}{=} \left[\frac{(\text{cm}^{-1})(\text{Joule-sec})(\text{cm/sec})(^\circ\text{K})}{(\text{Joule}/^\circ\text{K})(^\circ\text{K})(^\circ\text{K})}\right]$$

$$\stackrel{d}{=} [1],$$

which is the desired result. Therefore, energies which are given in wavenumbers can always be converted to Joules through multiplication with "hc."

With the exponential expression dimensionally equal to unity, Eq. 4.4-6 is finally given as

$$s \stackrel{d}{=} \left[\frac{\text{cm}^{-1}}{\text{molecule-cm}^{-2}}\right]. \qquad 4.4\text{-}6b$$

Now, for α and ν measured in wavenumbers, the Lorentz line shape given by Eq. 2.3-7 is

$$f \stackrel{d}{=} \frac{[\text{cm}^{-1}]}{\left[\text{cm}^{-1}\right]^2 + \left[\text{cm}^{-1}\right]^2}$$

$$\stackrel{d}{=} [\text{cm}]. \qquad 4.4\text{-}7$$

Hence, the absorption coefficient is

$$K \stackrel{d}{=} \left[\frac{\text{cm}^{-1}}{\text{molecule-cm}^{-2}}\right] [\text{cm}]$$

$$\triangleq \left[\frac{1}{\text{molecule-cm}^{-2}} \right] . \qquad 4.4\text{-}8$$

Equation 4.4-8 gives K in terms of units using only AFCRL's data tape and modifying E" as described above. Converting these units to inverse atmospheric centimeters can be accomplished using elementary chemistry [McClatchey[18]].

An [atm-cm] of gas at STP (standard temperature and pressure) is equivalent to a length of 1 cm of gas at STP per cm^2. From Avogadros' hypothesis, the molecular weight (M_t), in grams, of any gas at STP occupies a volume of 22.4×10^{-3} cm^3 (22.4 liters). Therefore,

$$1[\text{atm-cm}] = \frac{M_t}{2.24 \times 10^4} \quad [\text{gm/cm}^2],$$

at STP. From the fact that one mole of gas contains the same number of molecules (Avogadro's constant) and one cubic centimeter would contain $\left(\frac{1}{2.24 \times 10^4}\right)$ moles, it can be deduced that

$$1\ [\text{atm-cm}]_{STP} = 2.6884683 \times 10^{19} [\text{molecules/cm}^2]. \qquad 4.4\text{-}9$$

Therefore, K in Eq. 4.4-8, can be given in inverse atmospheric centimeters using Eq. 4.4-9:

$$K \triangleq C[\text{atm-cm}]^{-1}, \qquad 4.4\text{-}10$$

where C is the conversion factor defined above.

In summary, it is relatively simple to express K in inverse atmospheric centimeters. First E" must be converted to Joules before the line strength equation can be used. Secondly, K must be multiplied by the conversion factor defined in Eq. 4.4-9. Otherwise, for a given atmospheric profile, the AFCRL data tape can be used directly with Eqs. 4.4-2, 4.4-3, and 4.4-4 to calculate K.

The gas amount, U, must now be expressed in terms of atmospheric centimeters. From Eq. 2.4-1, the differential gas amount can be expressed as

$$du \equiv \frac{\rho_g(z)}{\rho_{STP}} \, dz \text{ [atm-cm]}, \qquad 4.4\text{-}12$$

where ρ_{STP} is the density of the gas at STP. Equation 4.4-12 is not commonly used, however, since parameters are normally given in terms of pressure profiles and gas mixing ratios.

If the mixing ratio for a gas is defined in terms of its density to that of dry air, we have

$$M \equiv \frac{\rho_g}{\rho_{air}} \, .$$

Using this definition and multiplying Eq. 4.4-12 by $\frac{\rho_{air}}{\rho_{air}}$, we have

$$dU = \frac{M \, \rho_{air}}{\rho_{STP}} \, . \qquad 4.4\text{-}13a$$

From the hydrostatic equation, the altitude, z, can be expressed in terms of pressure so that the gas amount is now

$$dU = \frac{10^3 \cdot M \cdot dP}{g\ \rho_{STP}} \quad . \qquad 4.4\text{-}13b$$

P is given in [mb]; g is the acceleration due to gravity in [cm/sec^2]; and M is dimensionless.

Equation 4.4-13b is used for gases which have a variable mixing ratio (i.e. H_2O and O_3). Using the definition of M, if the densities of the gas and of dry air are known, a mixing ratio profile can be computed easily.

For the constant mixing ratio gases (see Sec. 2.5), the gas amount is given by

$$dU = \frac{M_{PPM} \cdot M_{tg} \cdot 10^{-3}\ dP}{M_{ta} \cdot g \cdot \rho_{STP}} \qquad 4.4\text{-}14$$

where M_{PPM} is the "parts per million" mixing ratio, and M_{tg} and M_{ta} are the molecular weights of the gas and air respectively. Since these quantities are easily found, Eq. 4.4-14 can be written in terms of a constant times a pressure differential for a given gas:

$$dU = A_g dP,$$

where

$$A_g = \frac{M_{PPM} \cdot M_{tg} \cdot 10^{-3}}{g \cdot M_{ta} \cdot \rho_{STP}} \quad .$$

Table 4.4-1 is a listing of molecular weights, constant parts per million mixing ratios and gas densities at STP. Also listed are computed values of A_g where appropriate.

Molecule Type	Molecular Weight*	Mixing Ratio-PPM*	Gas Density At STP**	A_g Constant of Eq. 4.4-15
H_2O	18	Variable	1.00016	N/A
CO_2	44	330	1.9768441×10^{-3}	$2.58538380 \times 10^{-1}$
O_3	48	Variable	2.1436282×10^{-3}	N/A
N_2O	44	0.28	1.978137×10^{-3}	$2.19222523 \times 10^{-4}$
CO	28	0.075	1.25101×10^{-3}	$5.90866466 \times 10^{-5}$
CH_4	16	1.6	7.1678376×10^{-3}	$1.25713708 \times 10^{-3}$
O_2	32	2.095×10^{-5}	1.4286545×10^{-3}	$1.65172454 \times 10^{+2}$
AIR	28.97	1×10^{6}	N/A	N/A

*[Adapted From McClatchey[18]]

**[Adapted From Nelson[20]] Units in gm/cm^3

Table 4.4-1 GAS AMOUNT TABLE

The discussion of units can be concluded with a few remarks concerning the approximation to K given in Chapter 3. Like the standard, Eq. 3.3-8 will be in units of $\left[\frac{1}{\text{molecule-cm}^{-2}}\right]$ and must be converted to $[\text{atm-cm}]^{-1}$ by Eq. 4.4-10. Additionally the constant E_a must also be expressed in [Joules].

4.5 The Nimbus-6 Sounder And The 4.3μm Band

When the Lorentz line absorption coefficient was developed in Chapter 2, it was stated that the line broadening mechanism was based on molecular collisions or pressure. This suggests that the best accuracy in transmittance calculations using the Lorentz line shape will be attained when atmospheric pressures are relatively high. Commonly, Lorentz line broadening is used in pressure regions from 1013 mb (sea level) to 100 $\pm$ mb (17-20 KM) [McClatchey[17]]. For lower pressures the doppler effect must also be taken into account.

Ultimately, the Lorentz line transmittance calculations are to be used with satellite sounding data for temperature profile retrievals [Kaplan[15]]. One such High Resolution Infrared Radiation Sounder (HIRS) is the Nimbus-6 experiment package [Sissila[25]]. The Nimbus-6 HIRS is a third generation infrared radiation sounding experiment used to monitor the earth's atmosphere from an orbiting satellite. The radiation measurements in 4.3μm and 15μm bands permit high resolution vertical temperature profiles to be calculated from the lower troposphere to the stratopause.

To gather these soundings, the Nimbus-6 has 17 frequency channels from .69μm to 15μm which are listed in Table 4.5-1.

Channel Number	Center Wave No.	Center Wave Length	Channel Bandwidth
	(cm^{-1})	μm	(cm^{-1})
1	668	15.0	2.8
2	679	14.7	13.7
3	690	14.4	12.6
4	702	14.2	15.9
5	716	14.0	17.5
6	733	13.6	17.6
7	749	13.4	18.4
8	900	11.0	34.6
9	1,224	8.2	63.4
10	1,496	6.7	87.6
11	2,190	4.57	20.6
12	2,212	4.52	22.5
13	2,242	4.46	21.6
14	2,275	4.40	35.2
15	2,357	4.24	23.0
16	2,692	3.71	296.9
17	14,443	0.69	892.2

Table 4.5-1 NIMBUS-6 CHANNEL CHARACTERISTICS
[Adapted from Sissila[25]]

Channels 1-7 are used for temperature soundings of the relatively cold regions of the atmosphere and for cloud detection. Channels 8 and 16 are used to measure surface radiances. Water vapor concentrations are monitored through channels 9 and 10. Similar to channels 1-7, temperature soundings and cloud detection of the warmer regions of the atmosphere are accomplished with channels 11-15. Channel 17 is used primarily for cloud detection during daylight hours.

In selecting a frequency region to test the approximation to the Lorentz line absorption coefficient, the Nimbus-6 specifications were studied. Channels 11-15 were chosen because the 4.3μm band is primarily used for temperature soundings for regions in which Lorentz line broadening is valid. This is illustrated in Fig. 4.5-1 which depicts the weighting function curves for channels 11-15. Except for channel 15, all curves are confined to high pressure regions. Also shown is the corresponding channel filter function for the Nimbus-6. The data contained on AFCRL's tape for the 4.3μm band is summarized in Table 4.5-2. The information contained in the table was obtained using the data retrieval program given in Appendix A.

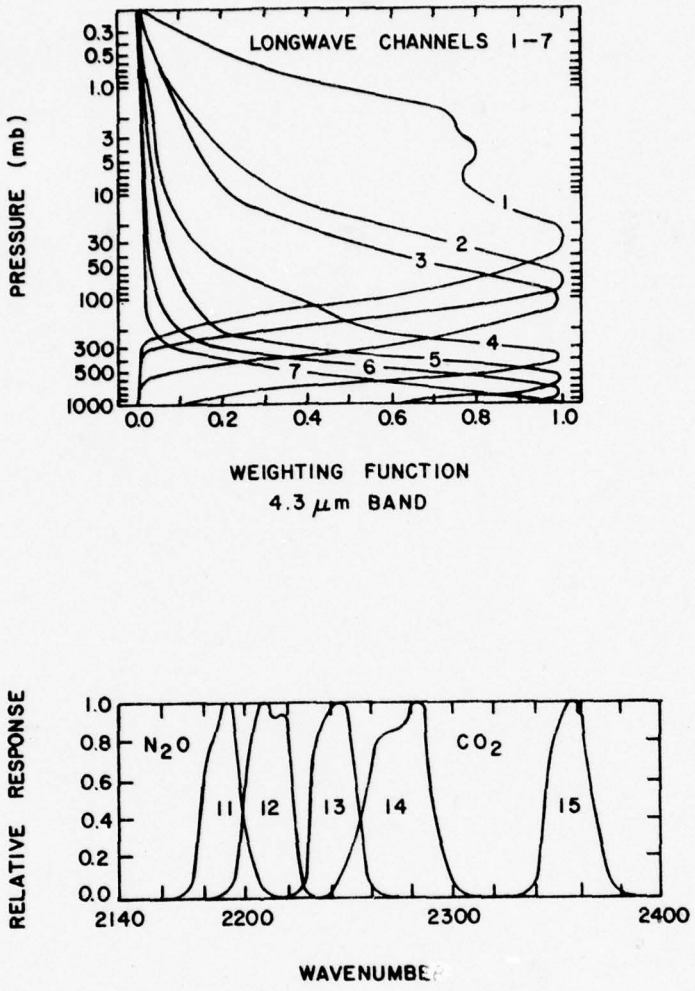


Figure 4.5-1 HIRS WEIGHTING FUNCTIONS AND FILTER RESPONSES

[Adapted from Sissila[25]]

CHANNEL NUMBER → / MOLECULE TYPE ↓	11	12	13	14	15
H_2O	34	53	52	84	42
CO_2	195	208	565	1141	432
O_3	0	0	0	0	0
N_2O	748	790	296	101	30
CO	16	7	8	1	0
CH_4	0	0	0	0	0
O_2	0	0	0	0	0
Totals	993	1058	921	1597	504

Table 4.5-2 NUMBER OF LINES PER CHANNEL BY MOLECULE TYPE

CHAPTER V

TESTING THE APPROXIMATION

5.1 Preface

The standard formula for evaluating the absorption coefficient due to Lorentz line broadening is

$$K = \sum_{i=1}^{I} \frac{S}{\pi} \frac{\alpha}{\alpha^2 + (\nu-\nu_o)^2}, \qquad 5.1\text{-}1$$

where, for a given gas, there are "I" spectral lines contributing to the absorption. The formulas for line intensity, S, and half-width, α, are rewritten here for convenience:

$$S = S_o \, Q \left(\frac{T_o}{T}\right)^b \quad EXP \left[\frac{E''}{kT_o}\left(\frac{T-T_o}{T}\right)\right]$$

and

$$\alpha = \alpha_o \left(\frac{P}{P_o}\right)\left(\frac{T_o}{T}\right)^{1/2}.$$

The approximation to Eq. 5.1-1 was developed in chapter 3 (Eq. 3.3-8). If the infinite series are cut off after (N+1) and (M+1) terms, then the approximation can be written as

$$K \doteq \frac{Q}{\pi} W^b \eta \sum_{n=0}^{N} \frac{(W-W_a)}{n!} \sum_{m=0}^{M} g_m(X). \qquad 5.1\text{-}2$$

$$\sum_{i=1}^{I} \frac{S_o}{\alpha_o} \beta \left(\frac{E_a - E''}{kT_o} \right)^n f_m(Y) ,$$

where "I" is the same as in Eq. 5.1-1 and variables Q, W, η, β, g_m, f_m, X and Y are defined in Chapter 3.

This chapter will discuss a method of computerizing Eq. 5.1-2 for monochromatic radiation. Additionally, several methods of measuring computational times will be presented along with accuracy and error prediction techniques.

5.2 Data File Description

In Chapter 4 the data retrieval program listed in Appendix A was discussed. Not only does the program read AFCRL's data tape between arbitrary frequency limits, but also it creates a permanent data file containing line parameters ν_o, α_o, S_o and E" segregated by gas type. By knowing the number of data records per gas that are contained on a channel's file, the line parameters can easily be retrieved for use in calculating either Eq. 5.1-1 or Eq. 5.1-2. The "line density" counts for channels 11-15 are listed in Table 4.5-2 and were provided by the subroutine "CHREAD" (Appendix A).

For example, channel 11 has a center wavenumber of 2190 cm^{-1} and a bandwidth of 20.6 cm^{-1} with "line densities" of: (1) H_2O with 34 lines; (2) CO_2 with 195 lines; (3) N_2O with 748 lines; (4) CO with 16 lines; (5) O_3, CH_4, and O_2 with 0 lines. Hence, it is easily recognized that record number 34 is the last line entry for H_2O and record number 35 is the first entry for CO_2.

Data files are created in this manner for the following programming considerations:

(1) Only one data file is needed for a given channel; and

(2) gases are segregated by type which eliminates the need to store a molecule identification code, thus keeping required storage space to a minimum.

5.3 Data Reorganization

Chapter 3's development of Eq. 5.1-2 stressed that many calculations needed to compute K could be done once and would never require repeating regardless of the atmospheric level or the molecular gas under consideration. In Eq. 5.1-2, these quantities appear after the summation over spectral lines $\left(\sum_{i=1}^{I} \right)$. For monochromatic radiation, the expression

$$\sum_{i=1}^{I} \frac{S_{oi}}{\alpha_{oi}} \beta_i \left(\frac{E_a - E_i''}{kT_o} \right)^n f_m(Y_i)$$

can be evaluated once and stored in an (N+1) x (M+1) array for each gas. Therefore, for all seven gases, only seven such arrays would contain all the spectral line data to compute K for any number of temperature and pressure profiles.

Reorganizing the data in the form discussed above enables us to "take care of" a problem mentioned in Chapter 3 also. In section 3.4 it was stated that the binomial series would diverge for cases in which

$$|(\nu - \nu_o)| < 0.0525$$

wavenumbers. Experience with AFCRL's data indicates that this takes place in about 0.5% of the spectral lines for a typical channel. By identifying these lines during the data reorganization portion of the program, their contribution to K can be computed in the standard fashion and added in at a later point without a significant addition to the calculation time.

The computer routine used to calculate and compare Eqs. 5.1-1 and 5.1-2 is listed in Appendix B. The data reorganization portion discussed in this section is done in the main routine. It may be prudent to note here that the reorganization of data could just as well be included in the tape read program of Appendix A. This may be a more desirable method if a complete transmittance program is being developed.

5.4 Evaluation of K

The evaluation of K by Eq. 5.1-1, K_{STD}, and by Eq. 5.1-2, K_{MOD}, can be done using the routine listed in Appendix B. Every effort to streamline computation times in both methods has been taken. Some general guidelines which can be used to accomplish this are:

(1) never divide by a constant repeatedly if its inverse can be stored and multiplication can be performed instead;

(2) only read line parameters once from the file and store them in core; and

(3) compute only once and save quantities dependent on atmospheric level or molecular gas.

The routine in Appendix B is initialized for the 4.3μm band

channel 11. Program comments specify which cards must be changed to initialize for a different spectral band. A Flow Diagram for the routine is listed in Fig. 5.4-1. The results obtained from this program are discussed in Chapter 6.

To conclude this section, a brief remark is in order concerning the vibrational partition function ratio Q. In AFCRL's data comilation report, McClatchey [17] gives the ratio as

$$Q = \frac{Q_{vo}(T)}{Q_v(T)} \quad ,$$

where Q_{vo} is the partition function evaluated at $T = T_o = 296°$ K. Data for Q was taken from AFCRL's report which lists values for $Q_v(T)$ for each molecule at seven discrete temperatures ranging from 175°K to 325°K. The subroutine "PART" in Appendix B computes Q based on a 2nd degree least-squares polynomial. Since Q is contained in both Eqs. 5.1-1 and 5.1-2, the relative error induced by this method of computing the partition function ratio is zero.

5.5 Execution Time Analysis

One of the primary reasons for developing the approximation was the hope that the calculation time of K could be significantly reduced. There are several methods of estimating in a quantitative measure just how significant of a reduction can be realized. However, there is no absolute measuring device widely available for time analysis. Most timing "clocks" cannot distinguish the times during program

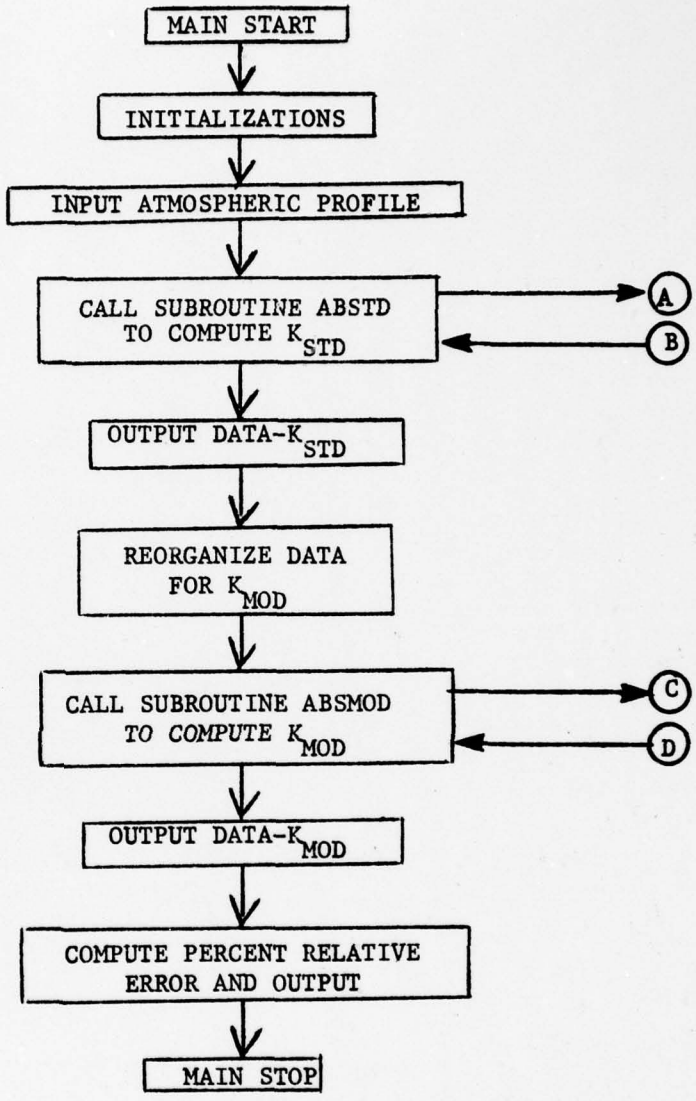


Figure 5.4-1 FLOW DIAGRAM FOR THE EVALUATION OF K-MAIN ROUTINE

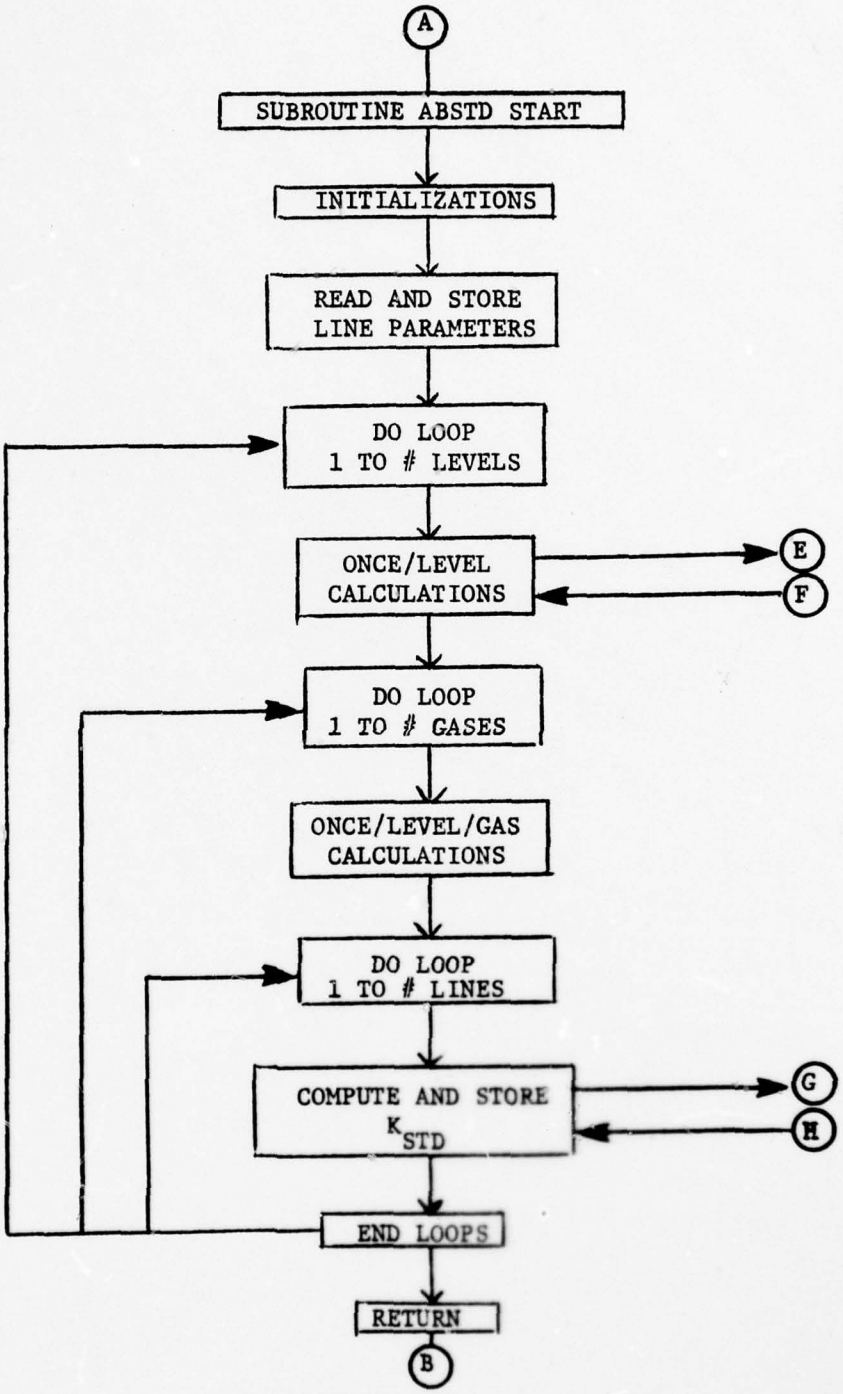


Figure 5.4-1 (cont.) EVALUATION OF K-SUBROUTINE ABSTD

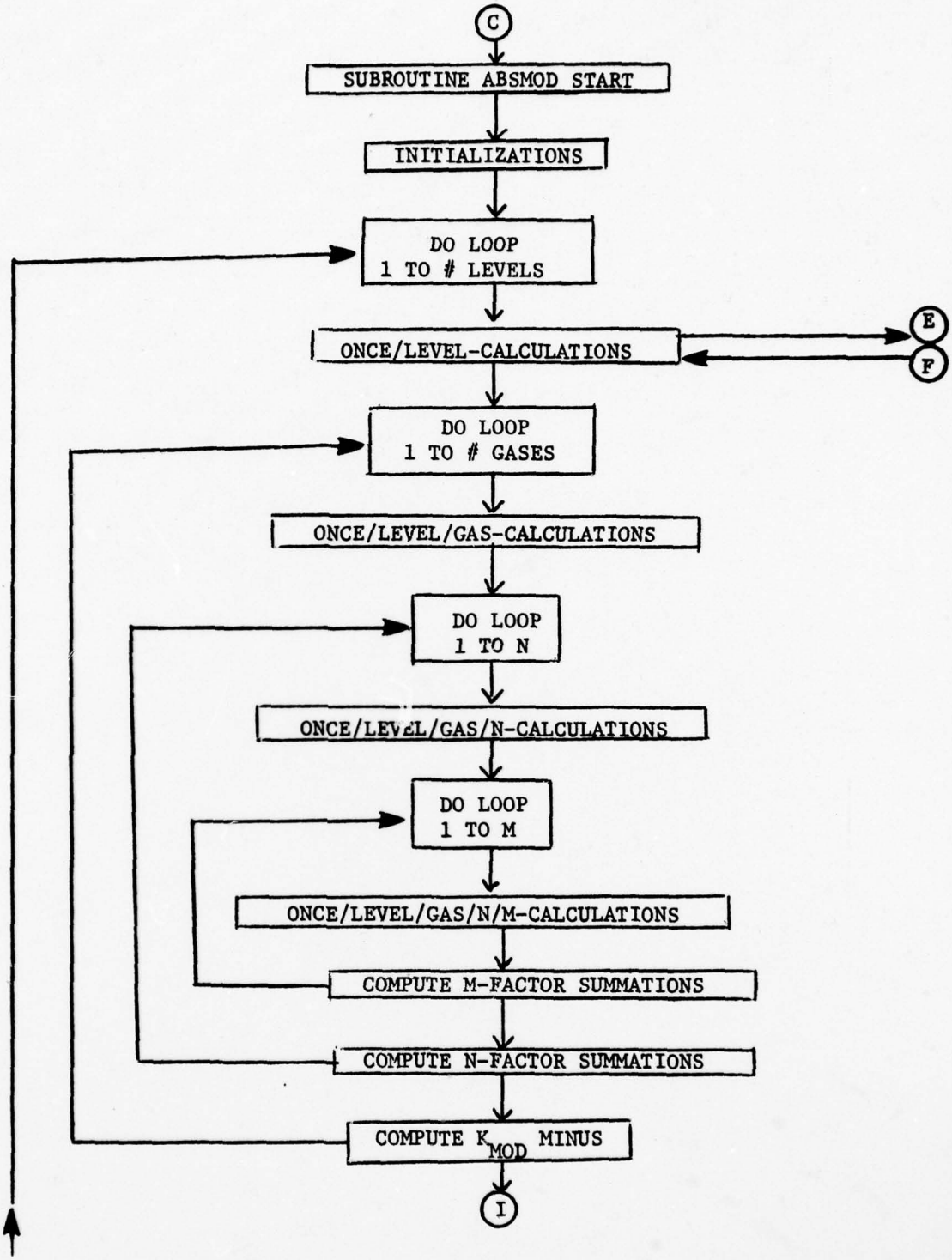


Figure 5.4-1 (cont.) EVALUATION OF K-SUBROUTINE ABSMOD

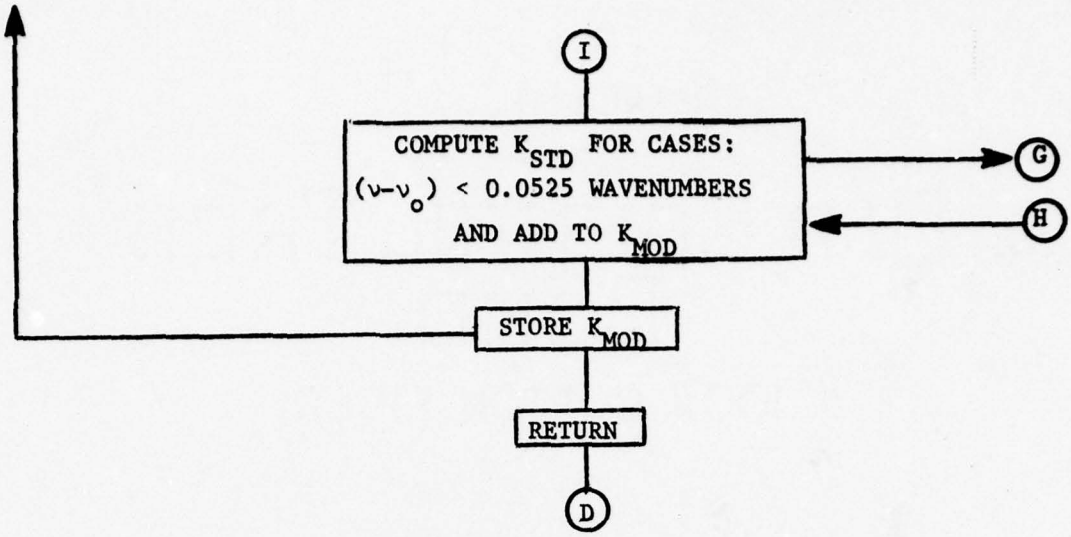


Figure 5.4-1 (cont.) EVALUATION OF K-SUBROUTINE ABSMOD

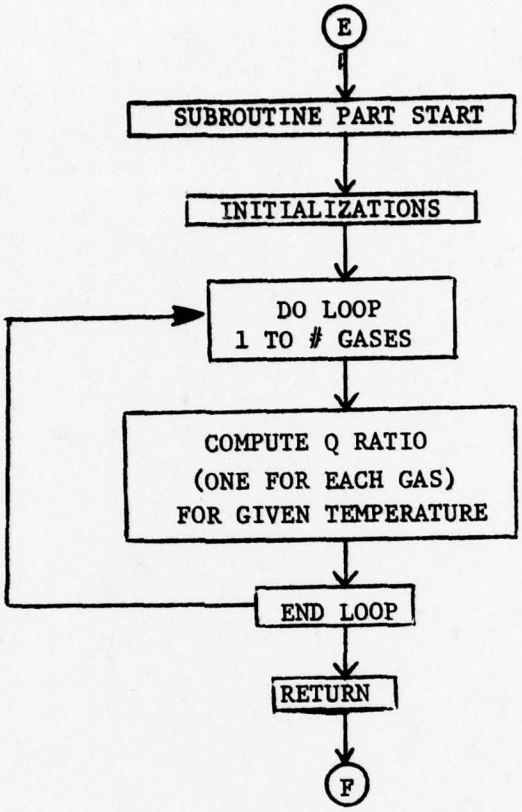


Figure 5.4-1 (cont.) EVALUATION OF K-SUBROUTINE PART

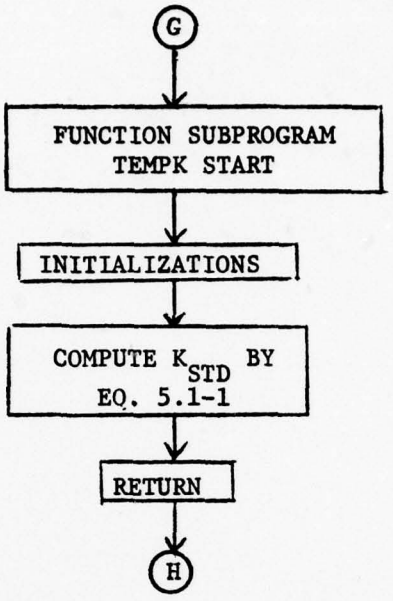


Figure 5.4-1 (cont.) EVALUATION OF K-FUNCTION SUBPROGRAM TEMPK

execution in which the routine is put in a "wait" state for some reason or another. Hence, the "execution" times for two identical program runs will very seldom be the same, much less be an accurate measure of the true execution time.

Even assuming that the routine to be analyzed is the only one being compiled in the computer, it is highly doubtful that two consecutive runs would now produce the same execution times. This is due to the fact that machine instruction times can vary because the physical location of the data being used does not necessarily remain the same from run to run. Therefore, it should be understood that any time comparison figures presented here are not absolute and are intended to measure only in a relative fashion.

One method that is normally used to measure total computation time is to use the GO-STEP time which is used in figuring the number of CPU seconds used by the routine during execution. This time is taken to be fairly accurate, especially since it is directly related to money. Most computer listings show the GO-STEP execution time in the documentation section. For the University of Texas at El Paso's IBM 360/65 system, the time can be found by requesting a "MSGLEVEL = (1,1)" resource and using the "//GO EXECUTION" time which will be listed separately.

The second method for timing a program is to use "clock" routines which are available as internal software to the system. The "clock" is similar to the one which measures the GO-STEP time, but it has the versatility of being initialized and read during any portion of the program. Therefore, instead of measuring total run times only, the

programmer can "clock" individual sections of his routine. Start and stop commands can be obtained through the computer facility having these internal subroutines.

In case such a routine is not available, one is provided in Fig. 5.5-1. This routine is written in Assembler and is linked to the Fortran program by the Job Control Language (JCL) provided. Output is given in microseconds (μsec). In step 5 of Fig. 5.5-1 an example of using the clock to time the subroutine "ABSTD" is given. The clock is initialized by calling "STIMER" and when the program returns from the subroutine the clock is stopped and read by using the "TTIMER" call statement. The output will be the elapsed time in CPU μsec plus any time injected while the routine was in a "wait" state.

Lastly, a different method which does not use a "clock" to compare computation times, is presented here. A relative time analysis can be done by counting every arithmetic operation and assigning it a normalized time based on average Assembler instruction times for the system. This method assumes the following:

(1) the relative times between different Assembler and Fortran instructions are about the same (i.e. a division takes about 5.8 times as long as an addition regardless of the code used); and

(2) the time involved in transfer of control, variable initializations and other overhead are small compared to the time required to perform arithmetic operations.

STEP	CARD LISTING
1	//** (Resource Card if Needed) (Charge Card)
2	//_EXEC_FORTGC
3	//FORT. SYSLIN_DD_SPACE = (CYL, (2,1))
4	(FIRST CARD IN FORTRAN DECK) . . . CALL STIMER (initialize clock) CALL SUBROUTINE ABSTD (to be timed) CALL TTIMER (ITIME) (stops clock) TIME = ITIME*26.04116 (in μsec) WRITE (6,XX) TIME XX FORMAT (output) (LAST CARD IN FORTRAN DECK)
5	//*
6	//_EXEC_ASMFCLG, PARM. ASM = 'NO DECK, LOAD', PARM.LKED = 'LIST, LET, XREF, CALL'
7	STIMER CSECT BASRG 12 STIMER TASK, TUINTVL = BIG BYE ENTRY TTIMER TTIMER BASRG 12 L 2, Ø(1) TTIMER L 1, BIG SR 1, Ø ST 1, Ø(2) BYE BIG DC ØF'Ø', X'ØFFFFFFF' END
8	//LKED.SYSLMOD_DD_SPACE = (CYL, (5,5,1))
9	//LKED.SYSUTI_DD_SPACE = (CYL, (5,5,1))

Figure 5.5-1 TIMING ROUTINE
[Adapted From Weismann[27]]

STEP	CARD LISTING

10	//LKED.SYSLIB DD DSN = SYS1.FORTLIB, DISP=SHR
	// DD DSN = UTEP, FORTLIB, DISP=SHR
	// DD DSN = UTEP, CALCOMP.LOAD, DISP=SHR

11	//GO.FT06F001 DD SYSOUT = A
12	//GO.FT05F001 DD *
13	(FORTRAN DATA CARDS IF NEEDED)
14	//*
15	(FORTRAN JCL CARDS IF NEEDED)
16	//

Figure 5.5-1 (Cont.) TIMING ROUTINE

Table 5.5-1 is a list of typical arithmetic operations and the average Assembler instruction time in μsec for the IBM 360/65 system with H-level compiler. Instruction times are based on double-precision real variable operations. Column 4 lists the times normalized to that required by addition (T_A). Times which had to be estimated are indicated.

In summary, three types of timing schemes can be used to indicate which routine is computationally faster than another. The advantages and disadvantages of each method are presented in Fig. 5.5-2. All three methods were used in timing the routines for computing K_{STD} by Eq. 5.1-1 and K_{MOD} by Eq. 5.1-2. Results of the time analyses are presented in Chapter 6.

5.6 Evaluating The Error

Not only must the approximation of Eq. 5.1-1 be computationally fast, it also must be accurate. To determine how accurate it is, the error must be analyzed. In this text, three error terms will be mentioned. Because they apply to any quantity the definitions are presented in general terms:

(1) Absolute Error - E_A

$$E_A = |Q_1 - Q_2| \; ; \qquad 5.6\text{-}1a$$

(2) Absolute Relative Error - E_r

$$E_r = \left|\frac{Q_1 - Q_2}{Q_1}\right| \; ; \text{ and} \qquad 5.6\text{-}1b$$

	OPERATION	SYMBOL	TIME(μsec)	NORMALIZED TIME
*	Addition	+	2.45	1 T_A
*	Subtraction	-	2.45	1 T_A
*	Division	÷	14.10	5.8 T_A
*	Multiplication	*	7.60	3.1 T_A
**	Exponentiation	DEXP	145.00	59.2 T_A
**	Square Root	DSQRT	5.85	2.4 T_A
***	Integer Power	**INT	(7.6)INT	(3.1)(INT) T_A
***	Real Power	**REAL	145.00	59.2 T_A
***	Logical Branch	IF	5.85	2.4 T_A
***	Loop	DO	92	37.6 T_A

Note: (1) Symbol INT represents the integer power to which a real # is raised.

(2) T_A is the time for 1 addition in μsec. T_A = 2.45 μsec for Assembler.

* [IBM[13]]

** [IBM[14]]

*** ESTIMATED

Table 5.5-1 TIME ANALYSIS CHART
[Adapted from IBM[13,14]]

1	GO-STEP TIMER	
	Advantage -	Good overall accuracy, easy to use, directly related to computer usage costs.
	Disadvantage -	Only measures complete program, fluctuates.
2	CLOCK-TYPE TIMER	
	Advantage -	Good accuracy, can time selected portion(s) of routine, can be used more than once in a given run.
	Disadvantage -	Requires some programming knowledge, fluctuates from run to run.
3	ASSEMBLY-COMPARISON	
	Advantage -	Good relative measure, requires no programming, measures only arithmetic operations.
	Disadvantage -	Not accurate in computer time sense, requires estimates, excludes overhead times.

Figure 5.5-2 TIME ANALYSIS METHODS

(3) Percent Absolute Relative Error - $E_{\%}$

$$E_{\%} = 100\ E_r. \qquad 5.6\text{-}1c$$

The quantity Q_1 represents the standard and Q_2 represents the approximation. Absorption coefficient K, and transmittance τ, calculations computed in the standard fashion are subscripted "STD"; those done by the approximate method are subscripted "MOD."

Absolute error, E_A, is sometimes called a "deviation." It measures the difference between two quantities. Because transmittance is always between 0 and 1, the order of magnitude of E_A will also indicate the number of decimal digits of accuracy obtained with τ_{MOD}. Relative error, E_r, measures the fractional part an estimate calculation is "off" from the standard. Percent absolute relative error, $E_{\%}$, is simply stating E_r is terms of a percentage.

To illustrate the concept of E_A and E_r as they could apply to transmittance calculations consider the two cases below:

(1) Case I Let

$$\tau_{STD} = .9999 \text{ and } \tau_{MOD} = .99985.$$

Therefore,

$$E_A = 5 \times 10^{-5},$$

and

$$E_r = 5.0005 \times 10^{-5}.$$

(2) Case II Let

$$\tau_{STD} = .0001 \text{ and } \tau_{MOD} = .00005$$

Again

$$E_A = 5 \times 10^{-5}$$

but

$$E_r = 5 \times 10^{-1},$$

which is an increase of 4 orders of magnitude in absolute relative error, even though absolute error has remained the same.

Conversely, if the desire had been to keep relative error the same as in Case I, the absolute error in Case II would have to be on the order of 10^{-9} which is an increase of 4 orders of magnitude.

Caution must be exercised in error predictions for the reasons illustrated above. Error must be evaluated within the total context in which calculations are to be used. Because the ultimate use of absorption coefficient calculations are to compute transmittances, it will be within this scope that error for the approximation will be analyzed.

Beer's Law (Chapter 2) states that, for monochromatic radiation, transmittance is

$$\tau = \text{EXP } [-KU], \qquad 5.6\text{-}2$$

where U is the amount of gas that the radiation must pass through. Hence, the absolute error is

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$$E_A = \left|\tau_{STD} - \tau_{MOD}\right| \qquad 5.6\text{-}3$$

$$= \left|EXP[-K_{STD}U] - EXP[-K_{MOD}U]\right|.$$

K_{STD} and K_{MOD} are related by their absolute error:

$$\varepsilon_A = \left|K_{STD} - K_{MOD}\right|, \qquad 5.6\text{-}4$$

where the symbol ε_A will distinguish absorption coefficient error from transmittance error, E_A. Combining Eqs. 5.6-3 and 5.6-4, E_A can be expressed in terms of τ_{STD}, U, and ε_A as follows:

$$E_A = \tau_{STD}\left|1 - EXP[\mp\varepsilon_A U]\right|. \qquad 5.6\text{-}5$$

Note that

$$\frac{E_A}{\tau_{STD}} = \left|1 - EXP[\mp\varepsilon_A U]\right| = E_r. \qquad 5.6\text{-}6$$

It can be seen from Eq. 5.6-5 that E_A will vary depending on the value of τ_{STD} as well as the quantity $(\varepsilon_A U)$.

If three digits of accuracy (rounded) are desired in transmittance then a bound can be placed on the value of E_A:

$$E_A \leq 5 \times 10^{-4}.$$

Then Eq. 5.6-6 can be written to reflect this upper limit as

$$\frac{5 \times 10^{-4}}{\tau_{STD}} \geq \left|1 - EXP[\mp\varepsilon_A U]\right|. \qquad 5.6\text{-}7$$

It can be seen that the inequality will be most stringent for transmittance values close to unity and most relaxed for values near zero. Table 5.6-1 is a listing of the limits placed on the quantity $(\varepsilon_A U)$ for various values of τ_{STD}. Computed values of $(\varepsilon_A U)$ for the 4.3μm band are given in Chapter 6.

Value of τ_{STD}	Limits on $\lvert\epsilon_A U\rvert$	
	Positive	Negative
1.0	4.999×10^{-4}	5.001×10^{-4}
0.1	4.988×10^{-3}	5.013×10^{-3}
0.01	4.880×10^{-2}	5.130×10^{-2}
0.001	4.055×10^{-1}	6.932×10^{-1}
0.0001	1.792	NONE

$$\frac{5 \times 10^{-4}}{\tau_{STD}} \geq \left|1 - \text{EXP}[\mp\epsilon_A U]\right|$$

Table 5.6-1 Bounds on $\lvert\epsilon_A U\rvert$ for

$E_A = 5 \times 10^{-4}$

CHAPTER VI

RESULTS AND APPLICATIONS

6.1 Preface

The various methods of quantifying computation speed and accuracy for the approximation to the Lorentz line absorption coefficient were outlined in Chapter 5. Sections 6.2 and 6.3 of this chapter present the time and accuracy measurements obtained by testing the subroutines "ABSTD" and "ABSMOD" listed in Appendix B. All test runs were conducted on the University of Texas at El Paso's IBM 360/65 computer. Results using Chebyshev economization to replace the Taylor series expansion (discussed in Section 3.4) is also contained in this chapter. Finally, a brief section is included on the expected results of applying the approximation to a transmittance "band" problem.

6.2 Results of the Time Analysis

To calculate the time involved in executing subroutines "ABSTD" and "ABSMOD" (Appendix B) for monochromatic radiation, each timing method discussed in Section 5.5 was used. In all cases a significant time savings was measured when the absorption coefficient due to Lorentz broadening was calculated by the approximation express in Eq. 5.1-2.

All timing methods sought to measure only the calculation time involved in computing K. Every effort was made to subtract out the time involved in data retrieval, routine initializations, and other programming overheads.

The "GO-STEP" computation times were obtained by making computer runs with and without different sections of the absorption coefficient program and subtracting the CPU "GO-STEP" times. The types of runs timed were:

(1) Program without subroutines "ABSTD" and "ABSMOD";

(2) Program without subroutines "ABSTD" and "ABSMOD" and also without the "DATA REORGANIZATION" portion of the main routine;

(3) Program containing only subroutine "ABSTD";

(4) Program using only subroutine "ABSTD" modified to return control as soon as line parameters were read into core; and finally,

(5) Program containing only subroutine "ABSMOD".

If T_1 - T_5 are defined as the "GO-STEP" times for (1) - (5) above and T_{STD} and T_{MOD} represent the time required to calculate K_{STD} and K_{MOD} respectively, then

$$T_{STD} \equiv T_3 - T_2.$$

and

$$T_{MOD} \equiv T_5 - T_2.$$

The time involved in reorganizing the line parameter data for use with subroutine "ABSMOD" is given by

$$T_{DATA} = T_1 - T_2.$$

Using the above definitions, timing runs were made using a standard 33 - level atmosphere (see Table 6.3-1) for channels 11-15

[Sissila[25]]. Representative times are given in Table 6.2-1. The times listed for T_{STD} and T_{MOD} represent the best estimates of CPU time required to compute K_{STD} and K_{MOD} respectively.

CHANNEL NUMBER	LINE DENSITY	T_{STD} (sec)	T_{MOD} (sec)	T_{DATA} (sec)	$\frac{T_{STD}}{T_{MOD}}$
11	993	15.38	1.59	5.18	9.67
12	1058	16.04	1.72	6.02	9.32
13	921	12.82	1.44	5.10	8.90
14	1597	44.14	2.83	10.68	15.59
15	504	5.15	1.01	3.42	5.09
NOTE: Subroutine "ABSMOD" used 7 terms in both Binomial and Taylor Series.					

Table 6.2-1 "GO-STEP" TIME CHART

Note that the numbers of spectral lines which contribute to the absorption are listed also.

For channels 11, 12, and 13 which all contain around 1000 spectral lines, K_{MOD} was calculated about 9 times faster than K_{STD}. As the number of lines in the channel increase (decrease) the ratio increases (decreases). A ratio of over 15 was achieved in channel 14 where the number of lines exceed 1500.

If the user is willing to make a small study of the line parameters contained in the spectral band of interest and compute the "DATA REORGANIZATION" portion of the routine separately, a significant savings in computer time can be realized in calculating

K. A lesser savings will be attained if the data is reorganized in the same routine that K_{MOD} is calculated. For monochromatic radiation, it is always possible to reorganize the line parameter data separately. Unfortunately, for polychromatic considerations, only a portion of the data can be reorganized this way. Section 6.4 will address this case.

Measurements using the "GO-STEP" timer are difficult to adapt to a particular portion of a computer program (i.e. subroutines "ABSTD" and "ABSMOD"). This method requires numerous program executions with and without selected sections which are to be timed. Because of this, the "GO-STEP" method is awkward and inconvenient to implement, and hence, not convincingly accurate.

In an effort to measure the execution times of subroutines "ABSMOD" and "ABSTD" more precisely, the "CLOCK" timer (see Fig. 5.5-1) was also used. The execution time of each subroutine was measured independently from the main program because the "CLOCK" timer enables the user to start and stop the clock whenever desired. Using the "CLOCK" timer routine presented in Chapter 5, similar timing runs were made to those in Table 6.2-1. The "CLOCK" times for each subroutine and the "DATA REORGANIZATION" section are given in Table 6.2-2. T_{MOD} was found to be about 14 times faster than T_{STD} for 1000 spectral lines considered. As the number of lines approached 1600 the ratio of computation times (column 6, Table 6.6-2) exceeded 16.

CHANNEL NUMBER	LINE DENSITY	T_{STD} (sec.)	T_{MOD} (sec.)	T_{DATA} (sec.)	$\frac{T_{STD}}{T_{MOD}}$
11	993	16.15	1.08	5.53	14.95
12	1058	16.35	1.13	6.13	14.46
13	921	16.04	1.10	5.06	14.58
14	1597	30.12	1.88	9.86	16.02
15	504	5.51	0.62	3.35	8.89
NOTE: Subroutine "ABSMOD" used 7 terms in both Binomial and Taylor Series.					

TABLE 6.2-2 "CLOCK" TIME CHART

Tables 6.2-1 and 6.2-2 suggest that T_{STD} and T_{MOD} are strongly dependent on the number of spectral lines present within the band limits. This dependence can be quantized using the method of "ASSEMBLER" time comparison which was outlined in section 5.5. If it is assumed that 0.5% of the spectral lines will be:

$$(\nu - \nu_o) \leq 0.0525$$

wave numbers, and only 7 terms of the Binomial and Taylor Series are used, then for the program in Appendix B,

$$T_{STD} = [38204.1 + 10490.86\ I]\ T_A$$

and

$$T_{MOD} = [1325982.2 + 23.8978\ I]\ T_A,$$

Where I is the total number of spectral lines considered, and T_A is the time in μ sec to complete one assembler addition instruction. The ratio of T_{STD} to T_{MOD} for I values of 500, 1000, and 1500 are listed in Table 6.2-3. Values for T_{STD} and T_{MOD} are given as functions of T_A. T_{MOD} is predicted to be 7.8 times faster than T_{MOD} for the 1000 line case.

I VALUE	T_{STD} (sec.)	T_{MOD} (sec.)	$\frac{T_{STD}}{T_{MOD}}$
500	5.28 T_A	1.34 T_A	3.94
1000	10.53 T_A	1.35 T_A	7.80
1500	15.77 T_A	1.36 T_A	11.59

TABLE 6.2-3 "ASSEMBLER" TIME CHART

6.3 Results of Accuracy Analysis

In section 5.6 various definitions of error were defined. Table 5.6-1 lists typical bounds on the absolute error in K, ε_A, times the gas amount, U. These bounds assure 3 place accuracy in transmittance (when rounded to the nearest ten-thousandths). The inequality which must be satisfied is rewritten here for convenience as

$$\frac{5.0 \times 10^{-4}}{\tau_{STD}} \geq \left| 1 - \text{EXP} \left[\mp \varepsilon_A U \right] \right| \qquad 6.3\text{-}1$$

where τ_{STD} is the transmittance through gas amount U calculated using the standard Lorentz line absorption coefficient, and ε_A is the absolute error in absorption coefficients as defined by Eq. 5.6-4.

To calculate K, U, and ε_A, a standard atmospheric profile containing 33 levels was used. The profile which represents typical temperatures and pressures for a midlattitude - summer climate is listed in Table 6.3-1. Altitude ranges from sea-level to 100 KM. Pressures are listed in both millibars and atmospheres.

Gas amounts were calculated for every layer between each level of the profile. All seven gas amounts were computed, however, Table 6.3-2 only lists the most important layers for the four gases found in the 4.3 μm band (H_2O, CO_2, N_2O, CO). It should be noted that for all gases listed, the maximum gas amount is found in layer #1 (0 to 1 km). The only exception in all seven gases analyzed was ozone which had its maximum concentration occur between 21 to 22 km (layer 22). Column 2 of Table 6.3-2 lists the lower and upper altitude limits for each layer given.

Using the program in Appendix B values for K_{STD} and K_{MOD} were computed for all channels in the 4.3 μm band. Using 7 terms in the Binomial and Taylor Series expansions for computation of K_{MOD}, three place accuracy in transmittance was more than assured in all cases. To insure this result the following analysis was performed.

Let

$$\left[\varepsilon_A U\right]_{MAX} \leq \ln\left[1 + \frac{5 \times 10^{-4}}{\tau_{STD}}\right], \qquad 6.3\text{-}2$$

(KM)	PRESSURE (mb)	(ATM)	TEMPERATURE (°K)
0	1013.0	0.999	294
1	902.0	0.890	290
2	802.0	0.791	285
3	710.0	0.700	279
4	628.0	0.619	273
5	554.0	0.546	267
6	487.0	0.480	261
7	426.0	0.420	255
8	372.0	0.367	248
9	324.0	0.319	242
10	281.0	0.277	235
11	243.0	0.239	229
12	209.0	0.206	222
13	179.0	0.176	216
14	153.0	0.151	216
15	130.0	0.128	216
16	111.0	0.109	216
17	95.0	0.093	216
18	81.2	0.080	216
19	69.5	0.068	217
20	59.5	0.058	218
21	51.0	0.050	219
22	43.7	0.043	220
23	37.6	0.037	222
24	32.2	0.031	223
25	27.7	0.027	224
30	13.2	0.013	234
35	6.52	0.643×10^{-2}	245
40	3.33	0.328×10^{-2}	258
45	1.76	0.173×10^{-2}	270
50	0.951	0.938×10^{-3}	276
70	0.061	0.662×10^{-4}	218
100	0.0003	0.296×10^{-6}	210

TABLE 6.3-1 STANDARD 33-LEVEL ATMOSPHERE [Adapted from La Rocca[16]]

Layer No.	Alt ΔZ (KM)	H_2O	CO_2	N_2O	CO
1	0-1	1.152	28.697	.024	.006
2	1-2	.747	25.853	.022	.005
3	2-3	.458	23.785	.020	.005
4	3-4	.255	21.200	.017	.004
5	4-5	.141	19.131	.016	.004
6	5-6	.079	17.322	.014	.004
7	6-7	.048	15.770	.013	.003
8	7-8	.028	13.961	.011	.003
9	8-9	.016	12.409	.010	.002
10	9-10	.009	11.117	.009	.002
15	14-15	8.9×10^{-5}	5.946	.005	.001
20	19-20	4.6×10^{-5}	2.585	.002	5.9×10^{-4}
25	24-25	6.3×10^{-5}	1.163	9.8×10^{-4}	2.6×10^{-4}
30	45-50	7.1×10^{-6}	.209	1.7×10^{-4}	4.7×10^{-5}
31	50-70	3.9×10^{-6}	.228	1.9×10^{-4}	5.2×10^{-5}
32	70-100	1.3×10^{-7}	.017	1.4×10^{-5}	3.9×10^{-6}

Note: Units of gas amounts are (ATM-CM).

TABLE 6.3-2 COMPUTED GAS AMOUNTS

which is the most restrictive case of Eq. 6.3-1. In all cases the maximum value of $\varepsilon_A U$ was obtained between 0 and 1 km. Values for $\left[\varepsilon_A U\right]_{MAX}$ and

$$\ell n \left[1 + \frac{5 \times 10^{-4}}{\tau_{STD}} \right]$$

are given in Table 6.3-3 to 6.3-6. The transmittance, τ_{STD}, was computed for the same layer in which the gas amount was found to be maximum.

Even though the error tolerances in transmittance were not breached, Table 6.3-4 shows a definite decrease in accuracy for channels 13-15 (CO_2). This is caused by the Taylor series expansion of EXP[X] and the variations of the magnitude of X. The use of Chebyshev economization will correct the skewed error distribution.

Recall the Taylor series used in the approximation (Eq. 3.4-6):

$$EXP[X] = EXP\left[\frac{(E_a - E_i)(W_1 - W_a)}{kT_o} \right] - \sum_{n=0}^{N} \frac{\left[\frac{(E_a - E_i)(W_1 - W_a)}{kT_o} \right]^n}{n!} \qquad 6.6\text{-}3$$

where the bracketed term, X, is approximated using (N+1) terms. When X becomes large, more terms are needed to approximate EXP[X] to keep the same degree of accuracy. To keep the magnitude of X small, strict restrictions have to be placed on constants E_a and W_a.

The value of X is determined by two primary factors:

Channel No.	$\left[\varepsilon_A U_{H_2O}\right]^*_{MAX}$	ERROR BOUND	τ_{STD}
11	3.439×10^{-10}	4.999×10^{-4}	.9999929
12	3.228×10^{-10}	4.999×10^{-4}	.9999690
13	1.013×10^{-9}	4.999×10^{-4}	.9999750
14	7.756×10^{-5}	4.999×10^{-4}	.9999224
15	3.067×10^{-10}	4.999×10^{-4}	.9999926

*U_{MAX} = 1.152 atm-cm of H_2O

TABLE 6.3-3 ERROR ANALYSIS - WATER VAPOR

TABLE 6.3-4 ERROR ANALYSIS - CARBON DIOXIDE

CHANNEL NO.	$\left[\epsilon_A U_{CO_2}\right]^*_{MAX}$	ERROR BOUND	τ_{STD}
11	2.323×10^{-8}	5.000×10^{-4}	.9996881
12	2.547×10^{-7}	5.095×10^{-4}	.9810430
13	2.130×10^{-4}	1.225×10^{-3}	.4078124
14	1.935×10^{-3}	2.509×10^{-1}	.0019920
15	3.600×10^{-1}	$\rightarrow \infty$	0.0×10^{-99}

*U_{MAX} = 28.697 atm -cm of CO_2

Table 6.3-4 ERROR ANALYSIS-CARBON DIOXIDE

CHANNEL NO.	$\left[\varepsilon_A \, U_{N_2O}\right]^*_{MAX}$	ERROR BOUND	τ_{STD}
11	8.522×10^{-6}	5.354×10^{-4}	.9336696
12	6.295×10^{-5}	6.746×10^{-4}	.7409964
13	6.514×10^{-5}	7.255×10^{-4}	.6890441
14	1.413×10^{-9}	4.999×10^{-4}	.9999888
15	1.865×10^{-9}	4.999×10^{-4}	.9999779

*U_{MAX} = .024 atm-cm of N_2O

Table 6.3-5 ERROR ANALYSIS-NITROUS OXIDE

CHANNEL NO.	$\left[\varepsilon_A U_{CO}\right]^*_{MAX}$	ERROR BOUND	τ_{STD}
11	0.0	6.58×10^{-4}	.8117192
12	7.263×10^{-9}	5.001×10^{-4}	.9995790
13	6.617×10^{-10}	$.4999 \times 10^{-4}$	.9999809
14	1.242×10^{-15}	4.999×10^{-4}	1.0
15	N/A	N/A	N/A

*U_{MAX} = .006 atm-cm of CO

Table 6.3-6 ERROR ANALYSIS-CARBON MONOXIDE

$$X = AX_1X_2,$$

where A is a constant, and

$$X_1 = |E_a - E_i|,$$

$$X_2 = |W_1 - W_a|.$$

Values of E_i range from a low of 0 to a maximum in excess or 4700 wavenumbers. If E_a is picked to minimize X_1, variations may still exceed 2000 wavenumbers. Based on a standard temperature profile, X_2 will vary from -0.3 to +0.3. This implies that X, using appropriate conversion factors in A, will fall between $\pm$4.5 depending on energy and temperature values. Values of X which reach this magnitude may require up to 20 terms in the Taylor expansion and this undermines the inherent quickness of the approximation.

A study of the line parameter data revealed the fact that high energy values are associated with low line intensity values. Hence it is possible to limit the value of X, by placing a maximum on the ground-state energy. Analysis indicates that 7 decimal place accuracy in K_{STD} is maintained when the maximum energy value is limited to 3250 wavenumbers. Using this maximum, X can be reduced to values in the range of -2.5 to +2.5. Using Chebyshev coefficients to equally distribute the error, a greater stability in the approximation is attained.

Table 6.3-7 lists the absolute error in absorption coefficients, $|K_{MOD} - K_{STD}|$, where K_{MOD} is calculated by both Chebyshev and Taylor expansions. Note that the Chebyshev error in K, expressed in atmos-

pharic centimeters, is as good or better than the Taylor error. The best correction occurs in channel 15 for CO_2.

In Table 6.3-8, Chebyshev coefficients for the EXP[X] expansion are given for reference. Coefficients are listed for various ranges in X and for different numbers of terms. The standard form of the Chebyshev expansion is

$$EXP[X] = C_0 + C_1X + C_2X^2 + C_3X^3 + ... + C_nX^n,$$

where (n + 1) terms are used.

6.4 Application to the Band Problem

The inherent importance of a fast and accurate approximation to the Lorentz line absorption coefficient is illustrated more in the light of transmittance calculations. Thus far transmittance has been discussed in terms of only monochromatic radiation which, in reality, can not actually be measured. Because present instrumentation is restricted to opeating in a spectral band regardless of the resolution achieved, transmittance is often desired over a range of frequencies.

The polychromatic transmittance is normally expressed as an average of the monochromatic values taken over a band. Mathematically,

$$\bar{\tau} = \frac{1}{\nu_o} \int_{\nu_o} \tau(\nu,T,P)d\nu, \qquad 6.4\text{-}1$$

where ν_o is the spectral band width and $\tau(\nu,T,P)$ is the monochromatic transmittance. Regardless of the transmittance desired, the Lorentz line absorption coefficient can be calculated by the approximation defined in Eq. 3.3-8. Accuracy of $\bar{\tau}$ will be similar to that of τ.

Channel/Gas	Chebyshev Error*	Taylor Error
11/H_2O	2.2×10^{-11}	2.9×10^{-10}
12/H_2O	3.0×10^{-10}	3.2×10^{-10}
13/H_2O	8.9×10^{-12}	8.6×10^{-10}
14/H_2O	1.3×10^{-9}	6.7×10^{-5}
15/H_2O	3.5×10^{-12}	6.3×10^{-6}
11/CO_2	1.1×10^{-10}	8.0×10^{-10}
12/CO_2	9.0×10^{-9}	8.8×10^{-9}
13/CO_2	7.0×10^{-8}	7.4×10^{-6}
14/CO_2	6.6×10^{-5}	6.7×10^{-5}
15/CO_2	8.9×10^{-5}	1.2×10^{-2}
11/N_2O	1.3×10^{-5}	3.4×10^{-4}
12/N_2O	2.6×10^{-3}	2.6×10^{-3}
13/N_2O	3.2×10^{-4}	2.7×10^{-3}
14/N_2O	5.8×10^{-8}	5.8×10^{-8}
15/N_2O	5.7×10^{-9}	7.7×10^{-8}
11/CO	1.9×10^{-7}	2.6×10^{-6}
12/CO	1.2×10^{-6}	1.2×10^{-6}
13/CO	7.1×10^{-9}	1.1×10^{-7}
14/CO	2.0×10^{-13}	2.0×10^{-13}

Note: Chebyshev expansion used 9 terms for X on the interval [-2.7 to +2.7]

Table 6.3-7. $\left|K_{MOD}-K_{STD}\right|$ FOR CHEBYSHEV AND TAYLOR EXPANSIONS

[X]	(n+1)	MAX ABS DIFF		
±2.7	9	1.13×10^{-4}		
C_0	C_1	C_2	C_3	C_4
1.00001	0.999679	0.499912	0.167249	0.0417623
C_5	C_6	C_7	C_8	C_9
8.05045×10^{-3}	1.35271×10^{-3}	2.4848×10^{-4}	3.03078×10^{-5}	

[X]	(n+1)	MAX ABS DIFF		
±2.0	8	6.79789×10^{-5}		
C_0	C_1	C_2	C_3	C_4
0.999945	0.99997	0.500437	0.166765	.0411259
C_5	C_6	C_7	C_8	C_9
8.2475×10^{-3}	1.60055×10^{-3}	2.25779×10^{-4}		

[X]	(n+1)	MAX ABS DIFF		
±3.0	9	3.10035×10^{-4}		
C_0	C_1	C_2	C_3	C_4
1.00004	0.999225	0.499789	0.167802	0.0418524
C_5	C_6	C_7	C_8	C_9
7.88829×10^{-3}	1.33215×10^{-3}	2.61742×10^{-4}	3.17493×10^{-5}	

[X]	(n+1)	MAX ABS DIFF		
±2.7	7	4.824322×10^{-3}		
C_0	C_1	C_2	C_3	C_4
0.999344	1.01021	0.502848	0.155694	0.0397489
C_5	C_6	C_7	C_8	C_9
1.12204×10^{-2}	1.7946×10^{-3}			

Table 6.3-8 CHEBYSHEV COEFFICIENTS FOR EXP[X]
[Adapted from Gibson[10]]

The method of calculation, and hence, the speed of the approximation, will change however.

In the monochromatic case, the approximation achieves its great speed advantage by allowing those quantities dependent on line parameters ν_{oi}, α_{oi}, S_{oi} and E_i'' to be calculated separate from K. For a band transmittance, on the otherhand, quantities dependent on ν_{oi} can not be calculated prior to the calculation of K because of the frequency stepping that must be done.

For example, the monochromatic "DATA REORGANIZATION" routine computes

$$\sum_{i=1}^{I} \frac{S_{oi}}{\alpha_{oi}} \beta_i \left(\frac{E_a - E_i''}{kT_o} \right)^n f_m(Y_i), \qquad 6.4\text{-}2$$

where I is the number of lines. The results are stored in a (NxM) array for each gas and need be computed only once for a channel. For the polychromatic instance, the term

$$f_m(Y_i) \equiv (Y_i^2 + a^2)^{-(m+1)},$$

where

$$Y_i = \frac{\nu - \nu_{oi}}{\alpha_{oi}}$$

and a^2 is defined in Chapter 3, can not be computed once and forgotten. Because the values of ν are stepped across the spectral band in small increments, $f_m(Y_i)$ will change in value each time a new ν is used.

Gibson [9] has estimated the predicted T_{STD} and T_{MOD} times for

the polychromatic case. The estimates are based on the "ASSEMBLER" method explained previously and projected calculations which will be required. At the time of this writing the approximation has not actually been applied to the polychromatic problem and verified by computational analysis.

Letting P represent the number of frequency increments taken within a band of width ν_o, the estimated times are given by Gibson as

$$T_{MOD} \doteq (113\ PI + 1245L + 415\ PL)T_A$$

and

$$T_{STD} \doteq (15\ PIL + 906\ L + 62\ IL)T_A,$$

where there are "I" lines considered within the band and "L" is the number of stratified levels of the atmosphere. T_A is the time required to perform an assembler addition instruction.

Using these predictors for T_{MOD} and T_{STD}, Table 6.4-1 was developed. The frequency increment (P) used was based on a band width of 25 wavenumbers and a step size of 0.02 cm^{-1}.

I value	T_{STD} (sec)	T_{MOD} (sec)	$\frac{T_{STD}}{T_{MOD}}$
500	310.43	87.78	3.53
1000	620.83	158.40	3.92
1500	931.22	229.03	4.06
2000	1241.62	299.65	4.14
P = 1250 L = 33			

$$T_{MOD} = (113\ PI + 1245\ L + 415\ PL)T_A$$

$$T_{STD} = (15\ PIL + 906\ L + 62\ IL)T_A$$

Table 6.4-1 POLYCHROMATIC TIME CHART

CHAPTER VII

CONCLUDING REMARKS

7.1 Summary

Attenuation of radiant energy by the earth's atmosphere can be described mathematically by the Lambert-Beer Law (see Sec. 2.4). In the infrared spectrum, the attenuation is due to molecular absorption by water vapor, carbon dioxide, ozone, nitrous oxide, methane, carbon monoxide, and sometimes, oxygen. The absorption coefficient, K, is composed of a strength and a line shape. The line shape in the lower regions of the atmosphere is primarily due to pressure broadening. The standard formula for the absorption coefficient is given by Eq. 2.3-7a.

The Lorentz line absorption coefficient can be written in an alternate form as given by Eq. 3.3-8 and approximated using Eq. 5.1-2. Using this approximation, K can be computed about 9 times faster than the standard method, while retaining at least three digits of accuracy in corresponding transmittance calculations. Accuracy can be improved even more by replacing the Taylor series coefficients with those of Chebyshev. The approximation's development and its testing are presented in Chapters 3, 5, and 6.

Chapters 2 and 4 are intended to lend emphasis to the problem of atmospheric transmittance as a whole. Often the theoretical developer neglects the mundane problems of atmospheric units and data. Hopefully, these chapters will enable the novice atmospheric scientist to better understand the complexities with which he is dealing.

7.2 Use of the Approximation

The approximation to the Lorentz line absorption coefficient will sufficiently retain the high resolution calculations of the standard line-by-line method and simultaneously, greatly reduce the computational time required. Continued investigation is needed into applying the approximation to a polychromatic transmittance problem. From results obtained thus far, the adversion of using line-by-line methods to calculate "band" transmittances may be eliminated.

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APPENDIX A

DATA ROUTINE FOR USE WITH AFCRL'S LINE PARAMETER COMPILATION

```
C
C                                   4.3 MICRON BAND
C                                  MICHAEL T. POTTER
C
C
C     THIS PROGRAM USES SUBROUTINE "CHREAD" AND "MCCLATCHEY'S" TAPE
C     TO OUTPUT SPECTRAL LINE DATA WITHIN SELECTED BANDWIDTHS.
C     IN ADDITION, THIS PROGRAM WILL ALSO BUILD PERMANENT DATA FILES.
C     PRESENT PROGRAM INITIALIZATIONS ARE FOR CHANNELS 11-15 IN THE
C     4.3 MICRON BAND.  TO USE THIS PROGRAM FOR ANY SELECTED CHANNEL(S)
C     CHANGE THE FOLLOWING INITIALIZATIONS*****
C        1.) FILL ARRAYS "CNTR" & "BWDTH" WITH DESIRED CHANNEL CENTER
C            WAVE NO. AND BANDWIDTH,RESPECTIVELY.
C        2.) MOLECULE ARRAYS (H2O,CO2,O3,AN2O,CO,CH4,&O2) SHOULD BE DIM-
C            ENSIONED SO THAT THE FIRST ELEMENT REFLECTS THE HIGHEST
C            MOLECULE NUMBER DENSITY FOR ANY CHANNEL BEING CONSIDERED.
C            THE SECOND ELEMENT REMAINS AT 4.
C        3.) ARRAY "MOLBND" SHOULD REFLECT THE SAME UPPER BOUND AS DE-
C            SCRIBED IN NO. 2 ABOVE.
C        4.) THE DATA IN EACH MOLECULE ARRAY BY COLUMNS IS*****
C              1___ WAVE NUMBER
C              2___ LINE INTENSITY
C              3___ HALF WIDTH
C              4___ ENERGY
C
C     FOR EACH CHANNEL(S) TO BE READ, ONLY THOSE MOLECULES PRESENT
C     WITHIN THE BANDWIDTH ARE WRITTEN INTO THE MOLUCULE ARRAY(S).
C     THE MAIN PROGRAM WILL NOT PRINT A MOLECULE HEADING IF THERE ARE NO
C     MOLECULES FOUND ON THE TAPE BETWEEN THE SPECIFIED LIMITS.
C     BEFORE EACH CHANNEL OUTPUT THE CHANNEL NO.,CENTER WAVE NO., AND
C     THE CHANNEL BANDWIDTH ARE DISPLAYED.  AFTER EACH CHANNEL OUTPUT,
C     THE ENERGY CONSTANT AND INTENSITY AVERAGE FOR THE CHANNEL ARE ALSO
C     DISPLAYED.
C
C
C  INITIALIZATIONS
C
0001          DIMENSION CNTR(5),ICNT(7),SAVE(7),EAVE(7)
0002          DIMENSION ISUM(7),BWDTH(5),MOLBND(7),TEMOL(4)
0003          COMMON  H2O( 85,4),CO2(1415,4),O3(1,4),AN2O( 800,4),CO(20,4),
             1 CH4(1,4),O2(1,4)
0004          DIMENSION IFILE(5)
0005          DATA IFILE/81,82,83,84,85/
0006          DATA MOLBND/85,1415,1,800,20,1,1/
0007          DATA CNTR/2190.0,2212.0,2242.0,2275.0,2357.0/
0008          DATA ISUM/7*0/
0009          DATA BWDTH/ 20.6,22.5,21.6,35.2,23.0/
0010          DEFINE FILE 81(1000, 16,L,IA1)
0011          DEFINE FILE 82(1075,16,L,IB2)
0012          DEFINE FILE 83(1000,16,L,IC3)
0013          DEFINE FILE 84(1600,16,L,ID4)
0014          DEFINE FILE 85(550,16,L,IE5)
0015          JR=0
C
C  SETTING UP CHANNEL COUNTER AND CHANNEL LIMITS
C
0016          DO 10 I1=1,5
0017          JR=JR+1
```


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```
0018                JJ=IFILE(I1)
0019                ICHAN= 10 + I1
0020                FHI= CNTR(I1) + (BWDTH(I1)/2.0)
0021                FLO= FHI - BWDTH(I1)
0022                WRITE(6,100) ICHAN,CNTR(I1),BWDTH(I1)
                C
                C  CALLING CHANNEL READ SUBPROGRAM
                C
0023                CALL CHREAD(FHI,FLO,MOLBND,JR,ICNT,SAVE,EAVE,ITOTAL)
0024                DO 111 L=1,7
0025              111 ISUM(L)= ISUM(L) + ICNT(L)
                C
                C  OUTPUT
                C
0026                ISTOP=ICNT(1)
0027                IF(ISTOP.EQ.0) GO TO 31
0028                WRITE(6,11)
0029                WRITE(6,12)
0030                DO 200 I20=1,ISTOP
0031                WRITE(6,14) I20,(H2O(I20,N),N=1,4)
0032              200 CONTINUE
0033               31 CONTINUE
0034                ISTOP=ICNT(2)
0035                IF(ISTOP.EQ.0) GO TO 32
0036                WRITE(6,15)
0037                WRITE(6,12)
0038                DO 300 I30=1,ISTOP
0039                WRITE(6,14) I30,(CO2(I30,N),N=1,4)
0040              300 CONTINUE
0041               32 CONTINUE
0042                ISTOP=ICNT(3)
0043                IF(ISTOP.EQ.0) GO TO 33
0044                WRITE(6,16)
0045                WRITE(6,12)
0046                DO 400 I40=1,ISTOP
0047                WRITE(6,14) I40,(O3(I40,N),N=1,4)
0048              400 CONTINUE
0049               33 CONTINUE
0050                ISTOP=ICNT(4)
0051                IF(ISTOP.EQ.0) GO TO 34
0052                WRITE(6,17)
0053                WRITE(6,12)
0054                DO 500 I50=1,ISTOP
0055                WRITE(6,14) I50,(AN2O(I50,N),N=1,4)
0056              500 CONTINUE
0057               34 CONTINUE
0058                ISTOP=ICNT(5)
0059                IF(ISTOP.EQ.0) GO TO 35
0060                WRITE(6,45)
0061                WRITE(6,12)
0062                DO 600 I60=1,ISTOP
0063                WRITE(6,14) I60,(CO(I60,N),N=1,4)
0064              600 CONTINUE
0065               35 CONTINUE
0066                ISTOP=ICNT(6)
0067                IF(ISTOP.EQ.0) GO TO 36
0068                WRITE(6,46)
0069                WRITE(6,12)
```

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```
0070              DO 700 I70=1,ISTOP
0071              WRITE(6,14) I70,(CH4(I70,N),N=1,4)
0072            700 CONTINUE
0073             36 CONTINUE
0074              ISTOP=ICNT(7)
0075              IF(ISTOP.EQ.0) GO TO 37
0076              WRITE(6,47)
0077              WRITE(6,12)
0078              DO 800 I80=1,ISTOP
0079              WRITE(6,14) I80,(O2(I80,N),N=1,4)
0080            800 CONTINUE
0081             37 CONTINUE
0082              WRITE(6,25)
0083              DO 65 I9=1,7
0084             65 WRITE(6,66) I9,EAVE(I9),SAVE(I9)
0085              WRITE(6,112) (ISUM(L),L=1,7)
0086              ISTOP=0
                C
                C     OUTPUT PERMANENT FILE DATA FOR VERIFICATION
                C
0087              WRITE(6,12)
0088              DO 900 K=1,7
0089              IF(ICNT(K).EQ.0) GO TO 900
0090              ISTART=ISTOP + 1
0091              ISTOP=ISTOP + ICNT(K)
0092              DO 910 L=ISTART,ISTOP
0093              READ(JJ'L) (TEMOL(N),N=1,4)
0094              KK=L+1
0095              FIND(JJ'KK)
0096              WRITE(6,14) L,(TEMOL(M),M=1,4)
0097            910 CONTINUE
0098            900 CONTINUE
0099              WRITE (6,42) ITOTAL
0100             10 CONTINUE
0101             42 FORMAT(1X, 'ITOTAL IS',I10)
0102            112 FORMAT(///,25X,'ICOUNT TOTALS FOR ALL CHANNELS ARE',/,25X,7(I5,1
                   1)
0103             11 FORMAT(1H1,25X,25HWATER VAPOR MOLECULE DATA,/,26X,25(1H*))
0104             12 FORMAT(2X,10HRECORD NO.,7X,8HWAVE NO.,3X,14HLINE INTENSITY,4X,
                   1 10HHALF WIDTH,7X,6HENERGY,/,2X,69(1H=))
0105             14 FORMAT(5X,I5,8X,F10.3,5X,E10.3,7X,F5.3,8X,F10.3)
0106             25 FORMAT(///,6X,29HENERGY AND INTENSITY AVERAGES,/,6X,29(1H=),//,5
                   17HMOL NO.,5X,10HENERGY AVE,5X,13HINTENSITY AVE,/,5X,40(1H?))
0107             15 FORMAT(1H1,23X,28HCARBON DICXIDE MOLECULE DATA,/,24X,28(1H*))
0108             16 FORMAT(1H1,28X,19HOZONE MOLECULE DATA,/,29X,19(1H*))
0109             17 FORMAT(1H1,24X,27HNITROUS OXIDE MOLECULE DATA,/,25X,27(1H*))
0110             45 FORMAT(1H1,22X,29HCARBON MONOXIDE MOLECULE DATA,/,23X,29(1H*))
0111             46 FORMAT(1H1,27X,21HMETHANE MOLECULE DATA,/,28X,21(1H*))
0112             47 FORMAT(1H1,28X,20HOXYGEN MOLECULE DATA,/,29X,20(1H*))
0113             66 FORMAT(8X,I1,8X,F10.3,8X,E10.3)
0114            100 FORMAT(///,5X,14HCHANNEL NO. IS,I4,3X,25HFOR CENTER WAVE NUMBER
                   1,3X,F6.1,2X,21HCHANNEL BANDWIDTH IS:,F6.1)
0115              STOP
0116              END
```

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```
C
C                                   SUBROUTINE CHREAD
C                                   MICHAEL T. POTTER
C
C     SUBROUTINE "CHREAD" WILL EXTRACT DATA FROM THE "MCCLATCHEY" TAPE
C     BETWEEN ANY TWO WAVENUMBER LIMITS, AND BUILD PERMANENT DATA FILES.
C     DATA IS ALSO SEGRAGATED BY MOLECULE TYPE.  MOLECULE CODES ARE
C     NUMBERED FROM 1-7 AND ARE GIVEN BELOW*****
C        1.  WATER VAPOR
C        2.  CARBON DIOXIDE
C        3.  OZONE
C        4.  NITROUS OXIDE
C        5.  CARBON MONOXIDE
C        6.  METHANE
C        7.  OXYGEN
C     PARAMETERS PASSED TO "CHREAD" ARE THE HI & LO WAVE NO LIMITS OF
C     THE DESIRED BAND AND THE ARRAY CONTAINING THE UPPER BOUND FOR
C     MOLECULE DENSITIES.  CHREAD WILL PLACE THE FOLLOWING
C     DATA IN THE FOLLOWING ARRAYS*****
C        1. ICNT-- 7D VECTOR WITH TOTAL MOLECULE NUMBER DENSITY FOR
C           EACH OF THE 7 MOLECULES.
C        2. SAVE,EAVE-- 7D VECTORS CONTAINING THE AVERAGE INTENSITY AND
C           ENERGY FOR EACH MOLECULE.
C        3.H2O,CO2,.... -- MOLECULE ARRAYS WHICH MUST BE IN COMMON WITH
C           THE MAIN PROGRAM.  DATA CONTAINED IN THE 4 COLUMNS ARE*****
C              1___ WAVE NUMBER
C              2___ LINE INTENSITY
C              3___ HALF WIDTH
C              4___ ENERGY
C     THE FOLLOWING ERROR FORMAT WILL BE PRINTED BY "CHREAD" IN THE
C     GIVEN CIRCUMSTANCES*****
C        1. FORMAT 97- DATA FILE ON TAPE DOES NOT CONTAIN LOW BOUND OF
C                      BANDWIDTH.
C        2. FORMAT 96- THERE ARE MORE RECORDS BETWEEN LIMITS THAN THE
C                      MOLECULE ARRAY(S) WERE DIMENSIONED FOR .
C     AN OPTION EXISTS TO HAVE THE ROUTINE PRINT OUT MOLECULE DENSITY
C     COUNTS FOR EACH TYPE PRESENT.    SEE COMMENT CARD AFTER FORMAT 999
C     ADDITIONALLY, PERMANENT FILES 81 - 85 ARE PRODUCED AND CONTAIN ALL
C     LINE DATA ARRANGED BY TYPE IN ASCENDING WAVE NO.  START AND STOP
C     POINTS FOR DATA TYPES CAN BE FOUND BY USING ARRAY ICNT.  EACH
C     RECORD CONTAINS FOUR ELEMENTS CORRESPONDING TO THE COLUMNS IN
C     THE MOLECULE ARRAYS.
C
0001          SUBROUTINE CHREAD(FHI,FLO,MOLBND,JOE,ICNT,SAVE,EAVE,ITOTAL)
C
C  CLEARING MOLECULE ARRAYS AND INITIALIZING
C
0002          DIMENSION WAV(40),STRGH(40),WDTH(40),ENGY(40),ROTID(40,5),VIB(40)
0003          DIMENSION IDATE(40),ISO(40),MOL(40),GBG(23),ICNT(7)
0004          DIMENSION EAVE(7),SAVE(7),MOLBND(7)
0005          DIMENSION IFILE(5)
0006          COMMON  H2O( 85,4),CO2(1415,4),O3(1,4),AN2O( 800,4),CO(20,4),
             1 CH4( 1,4),O2(1,4)
0007          DATA  MH2O,MCO2,MO3,MAN2O,MCO,MCH4,MO2/ 85,1415,1, 800,20,1,1/
0008          DATA IFILE/81,82,83,84,85/
0009          DATA EAMAX,EAMIN/0.0,1.0E10/
0010           DO 87 MM=1,7
0011           ICNT(MM)=0
```


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```
0012                SAVE(MM)=0.0
0013                EAVE(MM)=0.0
0014             87 CONTINUE
0015                DO 70 II=1,4
0016                DO 71 KA=1,MH2O
0017             71 H2O(KA,II)=0.0
0018                DO 72 KB=1,MCO2
0019             72 CO2(KB,II)=0.0
0020                DO 73 KC=1,MO3
0021                O3(KC,II)=0.0
0022                CH4(KC,II)=0.0
0023             73 O2(KC,II)=0.0
0024                DO 74 KD=1,MAN2O
0025             74 AN2O(KD,II)=0.0
0026                DO 75 KE=1,MCO
0027             75 CO(KE,II)=0.0
0028             70 CONTINUE
0029                JO=IFILE(JOE)
                 C
                 C  LOCATING BEGINNING WAVE NUMBER ON APPROPRIATE FILE
                 C
0030                NOFIL=10
0031                IF(FLO  .GT.00500.0) NOFIL=20
0032                IF(FLO  .GT.01000.0) NOFIL=30
0033                IF(FLO  .GT.02000.0) NOFIL=40
0034                IF(FLO  .GT.05000.0) NOFIL=50
0035                IF(FLO  .GT.07500.0) NOFIL=60
0036                IF(FLO  .GT.10000.0) NOFIL=70
0037             05 READ(NOFIL,91,END=99) INUM,FR
0038                IF(FR.LT.FLO) GO TO 05
0039                BACKSPACE NOFIL
0040                BACKSPACE NOFIL
                 C
                 C  READ TAPE FROM LOWER LIMIT TO HIGHER ONE
                 C
0041             13 READ(NOFIL,21,END=33)INUM,(WAV(K),STRGH(K),WDTH(K),ENGY(K),
                    1  (ROTID(K,J),J=1,5),VIB(K),IDATE(K),ISO(K),
                    2   MOL(K),K=1,40),(GBG(M),M=1,23)
0042                DO 20 I2=1,INUM
0043                KMOL=MOL(I2)
0044                IF(WAV(I2).LT.FLO) GO TO 20
0045                IF(WAV(I2).GT.FHI) GO TO 15
0046                ICNT(KMOL)=ICNT(KMOL)+1
0047                JJ=ICNT(KMOL)
0048                IF (ICNT(KMOL) .GT. MOLBND(KMOL))  GO TO 95
                 C
                 C      DATA SEGREGATION
                 C
0049                IF(KMOL.EQ.1) GO TO 101
0050                IF(KMOL.EQ.2) GO TO 102
0051                IF(KMOL.EQ.3) GO TO 103
0052                IF(KMOL.EQ.4) GO TO 104
0053                IF(KMOL.EQ.5) GO TO 105
0054                IF(KMOL.EQ.6) GO TO 106
0055                GO TO 107
0056             101 H2O(JJ,1)=WAV(I2)
0057                H2O(JJ,2)=STRGH(I2)
0058                H2O(JJ,3)=WDTH(I2)
```

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```
0059                H2O(JJ,4)=ENGY(I2)
0060                GO TO 110
0061              102 CO2(JJ,1)=WAV(I2)
0062                CO2(JJ,2)=STRGH(I2)
0063                CO2(JJ,3)=WDTH(I2)
0064                CO2(JJ,4)=ENGY(I2)
0065                GO TO 110
0066              103 O3(JJ,1)=WAV(I2)
0067                O3(JJ,2)=STRGH(I2)
0068                O3(JJ,3)=WDTH(I2)
0069                O3(JJ,4)=ENGY(I2)
0070                GO TO 110
0071              104 AN2O(JJ,1)=WAV(I2)
0072                AN2O(JJ,2)=STRGH(I2)
0073                AN2O(JJ,3)=WDTH(I2)
0074                AN2O(JJ,4)=ENGY(I2)
0075                GO TO 110
0076              105 CO(JJ,1)=WAV(I2)
0077                CO(JJ,2)=STRGH(I2)
0078                CO(JJ,3)=WDTH(I2)
0079                CO(JJ,4)=ENGY(I2)
0080                GO TO 110
0081              106 CH4(JJ,1)=WAV(I2)
0082                CH4(JJ,2)=STRGH(I2)
0083                CH4(JJ,3)=WDTH(I2)
0084                CH4(JJ,4)=ENGY(I2)
0085                GO TO 110
0086              107 O2(JJ,1)=WAV(I2)
0087                O2(JJ,2)=STRGH(I2)
0088                O2(JJ,3)=WDTH(I2)
0089                O2(JJ,4)=ENGY(I2)
0090              110 CONTINUE
                C
                C  SUMMING ENERGY AND INTENSITY
                C
0091                SAVE(KMOL)=SAVE(KMOL) + STRGH(I2)
0092                EAVE(KMOL)=EAVE(KMOL) + ENGY(I2)
0093               20 CONTINUE
0094                GO TO 13
0095               15 CONTINUE
0096                REWIND NOFIL
0097                GO TO 999
0098               99 WRITE(6,97) NOFIL,FR
0099                REWIND NOFIL
0100                GO TO 999
0101               33 REWIND NOFIL
0102                IF(NOFIL.EQ.70) GO TO 99
0103                NOFIL=NOFIL + 10
0104                GO TO 13
0105               95 WRITE(6,96) (ICNT(J),J=1,7),WAV(I2)
0106                REWIND NOFIL
0107              999 CONTINUE
0108                WRITE(6,755) (ICNT(66),LL=1,7)
                C
                C  AVERAGING ENERGY AND INTENSITY
                C
0109                DO 172 I9=1,7
0110                IF(ICNT(I9).EQ.0) GO TO 55
```


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```
0111                SAVE(I9)=SAVE(I9)/ICNT(I9)
0112                EAVE(I9)=EAVE(I9)/ICNT(I9)
0113                GO TO 172
0114             55 SAVE(I9)=0.0
0115                EAVE(I9)=0.0
0116            172 CONTINUE
0117                K=1
0118                ITOTAL = 0
                C
                C       BUILD PERMANENT DATA FILES FOR CHANNEL
                C
0119                DO 500 I50=1,7
0120                IF (ICNT(I50) .EQ.0) GO TO 500
0121                KK=ICNT(I50)
0122                DO 550 M=1,KK
0123                GO TO (561,562,563,564,565,566,567),I50
0124            561 WRITE(JO'K) (H2O (M,N),N=1,4)
0125                GO TO 550
0126            562 WRITE(JO'K) (CO2 (M,N),N=1,4)
0127                GO TO 550
0128            563 WRITE(JO'K) (O3  (M,N),N=1,4)
0129                GO TO 550
0130            564 WRITE(JO'K) (AN2O(M,N),N=1,4)
0131                GO TO 550
0132            565 WRITE(JO'K) (CO  (M,N),N=1,4)
0133                GO TO 550
0134            566 WRITE(JO'K) (CH4 (M,N),N=1,4)
0135                GO TO 550
0136            567 WRITE(JO'K) (O2  (M,N),N=1,4)
0137            550 K=K+1
0138                ITOTAL= ITOTAL + ICNT(I50)
0139            500 CONTINUE
0140             21 FORMAT(I10,40(F10.3,E10.3,   F5.3,F10.3,5A6,A5,I3,I4,I3),23A30)
0141             91 FORMAT(I10,F10.3)
0142             96 FORMAT(1H1,23HDIMENSION SIZE EXCEEDED,/,1X,7(I6,2X),/,1X,
                   1 20HLAST WAVE NUMBER IS:,2X,F10.3)
0143             97 FORMAT(1H2,5X,9H FILE NO:,2X,I2,2X,25HDOES NOT CONTAIN WAVE NO:
                   12X,F10.3)
0144            755 FORMAT(1X,'ICOUNT FOR ABOVE CHANNEL NO. IS',/,7(I8,2X))
0145                RETURN
0146                END
```

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```
     XXSYSLIN     DD       DSNAME=&LOADSET,DISP=(MOD,PASS),UNIT=SYSSQ,          X28000020
     XX              SPACE=(80,(200,100)),RLSE),DCB=BLKSIZE=80)                 X35000020
//FORT.SYSIN DD *
          IEF236I ALLOC. FOR JOBN7840 FORT      STEPNAME
          IEF237I 443    ALLOCATED TO SYSPRINT
          IEF237I 431    ALLOCATED TO SYSPUNCH
          IEF237I 232    ALLOCATED TO SYSLIN
          IEF237I 411    ALLOCATED TO SYSIN -
          IEF142I - STEP WAS EXECUTED - COND CODE 0000
          IEF285I   SYS77108.T065922.RV00)).JOBN7840.LOADSET       PASSED
          IEF285I   VOL SER NOS= UTEP84.
          UTEP111 STEP FORT      EXECUTION TIME =    010.17 SEC.
          UTEP131 STEP FORT      REGION = 0128K  MAX CORE USED = 0102K
     XXGO         EXEC     PGM=LOADER,PARM=(MAP,LET,PRINT),COND=(4,LT,FORT)    42000020
     XXSYSLIB     DD       DSNAME=SYS1.FORTLIB,DISP=SHR                        49000020
     XX           DD  DSN=UTEP.FORTLIB,DISP=SHR                 FORTGCLD    49000035
     XX           DD  DSN=UTEP.CALCOMP.LOAD,DISP=SHR            FORTGCLD    49000040
     XXSYSLOUT    DD       SYSOUT=A                                           56000020
     XXSYSLIN     DD       DSNAME=*.FORT.SYSLIN,DISP=(OLD,DELETE)             63000020
     XXFT05F001   DD       DDNAME=SYSIN                                       70000020
//GO.FT06F001 DD SYSOUT=(A,,6410)
     X/FT06F001   DD       SYSOUT=A                                           77000020
     XXFT07F001   DD       SYSOUT=B                                           84000020
//GO.FT10F001 DD UNIT=2400,DSN=DATA10,LABEL=(02,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT20F001 DD UNIT=2400,DSN=DATA20,LABEL=(05,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT30F001 DD UNIT=2400,DSN=DATA30,LABEL=(08,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT40F001 DD UNIT=2400,DSN=DATA40,LABEL=(11,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT50F001 DD UNIT=2400,DSN=DATA50,LABEL=(14,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT60F001 DD UNIT=2400,DSN=DATA60,LABEL=(17,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT70F001 DD UNIT=2400,DSN=DATA70,LABEL=(20,BLP,,IN),
// DISP=OLD,VOL=SER=T00388,DCB=(RECFM=F,BLKSIZE=3900)
//GO.FT81F001 DD DSN=USER.EEE02947.POTMOL,DISP=(NEW,CATLG,DELETE),
// VOL=SER=UTEP33,UNIT=2314,SPACE=(CYL,(02,01),RLSE)
//GO.FT82F001 DD DSN=USER.EEE02947.POT888,DISP=(NEW,CATLG,DELETE),
// VOL=SER=UTEP33,UNIT=2314,SPACE=(CYL,(02,01),RLSE)
//GO.FT83F001 DD DSN=USER.EEE02947.POTCCC,DISP=(NEW,CATLG,DELETE),
// VOL=SER=UTEP33,UNIT=2314,SPACE=(CYL,(02,01),RLSE)
//GO.FT84F001 DD DSN=USER.EEE02947.POTDDD,DISP=(NEW,CATLG,DELETE),
// VOL=SER=UTEP33,UNIT=2314,SPACE=(CYL,(02,01),RLSE)
//GO.FT85F001 DD DSN=USER.EEE02947.POTEEE,DISP=(NEW,CATLG,DELETE),
// VOL=SER=UTEP33,UNIT=2314,SPACE=(CYL,(01,01),RLSE)
//GO.SYSIN DD *
//
          IEF253I JOBN7840 GO       FT81F001 DIRECT ACCESS-DUPLICATE NAME ON VOLUME
          IEF285I   SYSL.FORTLIB                                        KEPT
          IEF285I   VOL SER NOS= LNK218.
          IEF285I   UTEP.FORTLIB                                        KEPT
          IEF285I   VOL SER NOS= UTEP11.
          IEF285I   UTEP.CALCOMP.LOAD                                   KEPT
          IEF285I   VOL SER NOS= UTEP11.
          IEF285I   SYS77108.T065922.RV000.JOBN7840.LOADSET             DELETED
          IEF285I   VOL SER NOS= UTEP84.
          IEF285I   DATA10                                              KEPT
          IEF285I   VOL SER NOS= T00388.
          IEF285I   DATA20                                              KEPT
```


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APPENDIX B

LORENTZ LINE ABSORPTION

COEFFICIENT TEST ROUTINE

```
C
C                          ABSORPTION COEFFICIENT TEST ROUTINE
C
C                                                MICHAEL T. POTTER
C
C  MAIN ROUTINE INITIALIZATIONS
C
0001        REAL *8 ABMCD(33,7)/231*0.00000000/,STDK(33,7)/231*0.00000000/,
           1 PERDIF(7)/7*0.00000000/
0002        REAL*8 ABDIF(7)/7*0.00000000/
0003        REAL *8 P(33),PR(33),T(33)
0004        REAL*8 SPEC1(1600)/1600*0.00000000/,SPEC2(1600)/1600*0.00000000/,
           1 SPEC3(1600)/1600*0.00000000/,SPEC4(1600)/1600*0.00000000/,
           2 SAVIT(7, 9,7)/441*0.00000000/
0005        REAL * 8 AA,ALFA,AMARG,BB,BLTZ,CNVRT1,CNVRT2,ENG,ONE,PIE,PIV,
           1 PLK,POV,PO,SPDL,TEST,TO,WA,WA2
0006        REAL *8 ENGA(7)/2.936C8275E-20,5.73070102E-20,0.00000000,
           1 2.28626414E-20,1.75581932E-20,0.00000000,0.00000000/
0007        DIMENSION HGT(33),ICNT( 7),CNSTG(7),MOLNAM(7)
0008        DIMENSION NEW1(7),NEW2(7),FE(100),FA(100),FW(100),FS(100)
0009        DATA LEVEL,ITOTAL/33,993/
0010        DATA CNSTG/1.5,1.0,1.5,1.0,1.0,1.5,1.0/
0011        DATA NEW1,NEW2/7*0,7*0/
0012        DATA BLTZ,PLK,SPDL/1.38062200E-23,6.62619600E-34,2.99792500E+10/
0013        DATA WA,TO,PO,PIE,AA,BB/1.18400000,2.96000000E02,1.00000000,
           1 3.14159265,.65000000,.70000000/
0014        DATA ONE,AMARG ,MCNT,NCNT/1.00000000,0.05250000,7,9/
0015        DATA ICNT/ 34,195,0,743,16,0,0/
0016        DEFINE FILE 81(2500,16,L,IA)
0017        WAV=2190.0
0018        CNVRT1=SPDL*PLK
0019        CNVRT2= ONE/(BLTZ*TO)
0020        PIV=ONE/PIE
0021        POV=ONE/PO
0022        WA2= ONE -WA
C
C  INPUT ATMOSPHERE PROFILE
C
0023        DO 10 I1=1,LEVEL
0024        READ( 5,01) HGT(I1),PR(I1),T(I1)
C  CONVERT PRESSURE FROM MILLIBARS TO ATMOSPHERES
0025        P(I1)=PR(I1)*9.87E-04
0026     10 CONTINUE
0027        READ(5,02) (MOLNAM(K),K=1,7)
C
C  COMPUTATION OF STANDARD LORENTZ LINE ABSORPTION COEFFICIENT
C
0028        CALL ABSTD(ICNT,WAV,LEVEL,T,P,CNSTG,ITOTAL,STDK)
C
C  OUTPUT OF COEFFICIENTS
C
0029        WRITE(6,03)
0030        WRITE(6,04)
0031        WRITE(6,05) (MOLNAM(K),K=1,7)
0032        DO 30 I3=1,LEVEL
0033        WRITE(6,06) HGT(I3),(STDK(I3,N),N=1,7)
0034     30 CONTINUE
0035        WRITE(6,19)
```


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```
C
C
C  COMPUTATION OF MODIFIED LORENTZ LINE ABSORPTION COEFFICIENT
C
0036        IHALT=0
0037        N1=0
0038        N2=0
0039        DO 90 I9=1,7
0040        IF(ICNT(I9) .EQ. 0) GO TO 90
0041        IGO=1 + IHALT
0042        IHALT= IHALT + ICNT(I9)
0043        DO 100 I10= IGO, IHALT
0044        READ(81'I10) WNUM,ST,ALFAC,EY
0045        JK=I10 + 1
0046        FIND(81'JK)
0047        TEST=ONE*(WAV-WNUM)
0048        IF(DABS(TEST) .LT. AMARG) GO TO 101
0049        ALFA=ONE/ALFAO
0050        ENG=CNVRT1*EY
0051        N1= N1 + 1
0052        SPEC1(N1)=TEST*ALFA
0053        SPEC2(N1) = (ENG-ENGA(I9))*CNVRT2
0054        SPEC3(N1) = ALFA*ST*DEXP(((ENG*WA2)+(ENGA(I9)*WA))*CNVRT2)
0055        SPEC4(N1) = ONE/(SPEC1(N1)*SPEC1(N1) + AA)
0056        NEW1(I9) = NEW1(I9) + 1
0057        GO TO 100
0058      101 N2= N2 + 1
0059        NEW2(I9)= NEW2(I9) + 1
0060        FW(N2)=WNUM
0061        FS(N2)= ST
0062        FA(N2)=ALFAO
0063        FE(N2)= EY
0064      100 CONTINUE
0065       90 CONTINUE
0066        IQUIT=0
0067        DO 200 I20=1,7
0068        IF(NEW1(I20).EQ.0) GO TO 200
0069        ISTART=1 + IQUIT
0070        IQUIT= IQUIT + NEW1(I20)
0071        DO 300 I30=1,NCNT
0072        NPO=I30 - 1
0073        DO 400 I40=1,MCNT
0074        M= I40 - 1
0075        IF(I40 .EQ. MCNT) GO TO 501
0076        DO 500 I50=ISTART,IQUIT
0077        SAVIT(I40,I30,I20)= SAVIT(I40,I30,I20) + (SPEC4(I50)**I40)*
           1 (SPEC2(I50)**NPO)*SPEC3(I50)
0078      500 CONTINUE
0079        GO TO 400
0080      501 DO 502 I52=ISTART,IQUIT
0081        SAVIT(I40,I30,I20)=SAVIT(I40,I30,I20) + (SPEC4 (I52)**M)*
           1 (SPEC2(I52)**NPO)*(SPEC3(I52))/(SPEC1(I52)*SPEC1(I52))
0082      502 CONTINUE
0083      400 CONTINUE
0084      300 CONTINUE
0085      200 CONTINUE
0086        CALL ABSMOD(NEW1,NEW2,TO,POV,T,P,LEVEL,AA,BB,MCNT,NCNT,ENGA,CNVRT2
           1,PIV,FW,FS,FA,FE,SAVIT,CNSTG,WA,WAV,ABMOD)
```


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```
0087                  WRITE(6,03)
0088                  WRITE(6,07)
0089                  WRITE(6,05) (MOLNAM(K),K=1,7)
0090                  DO 40 I4=1,LEVEL
0091                  WRITE(6,06) HGT(I4),(ABMOD(I4,M),M=1,7)
0092               40 CONTINUE
0093                  WRITE(6,19)
                   C
                   C  CALCULATION AND OUTPUT OF PERCENT RELATIVE ERROR
                   C
0094                  WRITE(6,09)
0095                  WRITE(6,11) (MOLNAM(N),N=1,7)
0096                  DO 50 I5=1,LEVEL
0097                  DO 60 I6=1,7
0098                  IF(STDK(I5,I6) .EQ. 0.00000000) GO TO 60
0099                  PERDIF(I6)=100.0*DABS((STDK(I5,I6)-ABMOD(I5,I6))/STDK(I5,I6))
0100               60 CONTINUE
0101                  WRITE(6,06) HGT(I5),(PERDIF(L),L=1,7)
0102               50 CONTINUE
                   C
                   C     CALCULATE ABSOLUTE ERROR IN INVERSE ATM-CMS
                   C
0103                  WRITE(6,18)
0104                  WRITE(6,11) (MOLNAM(MMM),MMM=1,7)
0105                  DO 51 I51=1,LEVEL
0106                  DO 61 I61=1,7
0107               61 ABDIF(I61)=2.69E+19*DABS(STDK(I51,I61)-ABMOD(I51,I61))
0108               51 WRITE (6,06) HGT(I51),(ABDIF(I),I=1,7)
0109               01 FORMAT(F5.1,1X,E9.3,F5.1)
0110               02 FORMAT(7A4)
0111               03 FORMAT(1H1,52X,26HABSORPTION COEFFICIENT FOR)
0112               04 FORMAT(1H ,51X,27HSTANDARD LORENTZ LINE SHAPE)
0113               05 FORMAT(1H ,51X,28(1H*),//,3X,7HALT(KM),1X,7(5X,A4,6X),/,1X,115
                     1(1H-))
0114               06 FORMAT(1H ,2X,F5.1,3X,7(1X,E13.7,1X))
0115               07 FORMAT(1H ,51X,27HMODIFIED LORENTZ LINE SHAPE)
0116               09 FORMAT(1H1,54X,22HPERCENT RELATIVE ERROR,2(/,55X,22(1H*)))
0117               11 FORMAT(1H ,2X,7HALT(KM),1X,7(5X,A4,6X),/,1X,115(1H-))
0118               18 FORMAT(1H1,48X,33HABSOLUTE ERROR IN INVERSE ATM-CMS,/,2(49X,33(1H*
                     1),/))
0119               19 FORMAT(//,1H ,44HUNITS ARE IN SQUARE CENTIMETERS PER MOLECULE)
0120                  STOP
0121                  END
```


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```
C            SUBROUTINE ABSTD
C            MICHAEL T. POTTER
C      THIS SUBROUTINE USES THE STANDARD LORENTZ LINE SHAPE AND
C      COMPUTES ABSORPTION COEFFICIENTS LINE-BY-LINE.
C      COEFFICIENTS ARE PRODUCED FOR EACH GAS AT EVERY LEVEL.  THEY ARE
C      PASSED BACK TO THE MAIN ROUTINE IN ARRAY STDK.
C
0001         SUBROUTINE ABSTD(ICNT,CTRFRQ,LEVEL,TEMP,PRESS,CNSTG,ITOTAL,STDK)
0002         IMPLICIT REAL*8(A-H,O-Z)
0003         REAL CNSTG,CTRFRQ,WAVO,STRO,ALFAC,ENGO
0004         DIMENSION ALFAO(1600),ENGO(1600),WAVO(1600),STRO(1600)
0005         DIMENSION ICNT(7),STDK(33,7),QRTO(7),TEMP(33),PRESS(33),CNSTG(7)
0006         DATA BLTZ,PLK,SPDL/1.38062200E-23,6.62619600E-34,2.99792500E+10/
0007         DATA PIE,TO,PO/3.14159265,2.96000000E02,1.00000000/
0008         PIEE=1.0/PIE
C
C      ATMOSPHERIC LEVEL LOOP
0009         DO 5 I5=1,ITOTAL
0010         READ(81'I5) WAVO(I5),STRO(I5),ALFAO(I5),ENGO(I5)
0011         JA=I5+1
0012         FIND(81'JA)
0013       5 CONTINUE
0014         DO 10 I1=1,LEVEL
C
C  ONCE PER LEVEL CALCULATIONS
0015         T1=TO/TEMP(I1)
0016         P1=PRESS(I1)/PO
0017         RTO=P1*DSQRT(T1)
0018         DENOM=(1.0/(BLTZ*TO))
0019         DO 15 I5=1,7
0020      15 STDK(I1,I5)=0.00000000
0021         TP=TEMP(I1)
0022         CALL PART(TP,QRTO)
0023         ISTOP=0
C  MOLECULE GAS LOOP
0024         DO 20 I2=1,7
0025         IF(ICNT(I2).EQ.0) GO TO 20
0026          ISTART=1 + ISTOP
0027         ISTOP= ISTOP+ICNT(I2)
0028         TPWR=T1**CNSTG(I2)
0029         VIB=QRTO(I2)
0030         DO 300 I3=ISTART,ISTOP
0031         STDK(I1,I2)=STDK(I1,I2) + TEMPK(WAVO(I3),STRO(I3),ALFAO(I3),ENGO(I
            13),DENOM,TPWR,T1,RTO,CTRFRQ)
0032     300 CONTINUE
0033         STDK(I1,I2)=STDK(I1,I2)*VIB*PIEE
0034      20 CONTINUE
0035      10 CONTINUE
0036         RETURN
0037         END
```

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```
C
C              SUBROUTINE ABSMOD
C              MICHAEL T. POTTER
C
C      THIS SUBROUTINE COMPUTES AN ABSORPTION COEFFICIENT USING A
C      MODIFIED LORENTZ LINE SHAPE.  COEFFICIENTS ARE PRODUCED FOR EACH
C      MOLECULE TYPE EVERY ATMOSPHERIC LEVEL.
C
0001          SUBROUTINE ABSMOD(NEW1,NEW2,TO,POV,T,P,LEVEL,AA,BB,MCNT,NCNT,ENGA,
             1CNVRT2,PIV,FW,FS,FA,FE,SAVIT,CNSTG,WA,WAV,ABMOD)
C
C      INITIALIZATIONS
C
0002          IMPLICIT REAL*8(A-H,O-Z)
0003          REAL WNUM,ST,EY,ALFAO,CNSTG,FW,FS,FE,FA,WAV,FAC
0004          REAL*8 CHEBY(9)/1.00000000,.99997000,.49999100,.16676500,
             1 .41683400E-1,.10824750,.00137756,.22577900E-3,.27374800E-4/
0005          DIMENSION NEW1(7),NEW2(7),SAVIT(7, 9,7),FE(100),FS(100),FA(100),
             1 FW(100),CNSTG(7),T(33),P(33),ABMOD(33,7),QRTO(7),FAC(11)
0006          DIMENSION ENGA(7)
0007          DATA FAC/1.0,1.0,2.0,6.0,24.0,120.0,720.0,5040.0,40320.0,
             1  362880.0,3628800.0/
C
C      ATMOSPHERIC LEVEL LOOP
C
0008          DO 200 I20=1,LEVEL
C  CALCULATE PARTITION FUNCTION VALUES
0009          CALL PART(T(I20),QRTO)
0010          TCNST=TO/T(I20)
0011          PCNST=P(I20)*POV
0012          WATA=TCNST*CNVRT2
0013          X=PCNST*DSQRT(TCNST)
0014          GM=(AA-(X*X))
C
C      ABSORPTION GAS LOOP
C
0015          DO 250 I25=1,7
0016          IF(NEW1(I25) .EQ.0) GO TO 250
0017          SAVEX=0.00000000
0018          WAT=PIV*QRTO(I25)*(TCNST**CNSTG(I25))*DEXP(-ENGA(I25)*WATA)
C      N COUNTER LOOP
0019          DO 300 I30=1,NCNT
0020          NPO=I30-1
0021          SAVGEE=0.00000000
0022          EXPON=((WA-TCNST)**NPO)*CHEBY(I30)
C      M COUNTER LOOP
0023          DO 400 I40=1,MCNT
0024          M=I40-1
0025          GEE=(GM**M)*X
0026          IF(I40 .EQ.MCNT) GO TO 502
0027          SAVI=SAVIT(I40,I30,I25)
0028          GO TO 503
0029        502 GEE=BB*GEE/(X*X+ BB)
0030          SAVI=SAVIT(I40,I30,I25)
0031        503 CONTINUE
0032          SAVGEE=SAVGEE + SAVI*GEE
0033        400 CONTINUE
0034          SAVEX=SAVEX+ EXPON*SAVGEE
```


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```
0035          300 CONTINUE
0036              ABMOD(I20,I25)= WAT*SAVEX
0037          250 CONTINUE
0038          255 ISTOP=0
0039              DO 45 I=1,7
0040              HOLD=0.00000000
0041              IF(NEW2(I) .EQ. 0) GO TO 45
0042              IBEGIN = 1 + ISTOP
0043              ISTOP = ISTOP + NEW2(I)
0044              TPW=TCNST**CNSTG(I)
0045              DO 35 I3=IBEGIN,ISTOP
0046              WNUM=FW(I3)
0047              ST=FS(I3)
0048              ALFAO=FA(I3)
0049              EY=FE(I3)
0050              STD=TEMPK(WNUM,ST,ALFAO,EY,CNVRT2,TPW,TCNST,X,WAV)
0051              HOLD=HOLD+STD*CRTG(I)*PIV
0052           35 CONTINUE
0053              ABMOD(I20,I)=ABMOD(I20,I) + HOLD
0054          45  CONTINUE
0055          200 CONTINUE
0056              RETURN
0057              END
```

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```
C
C            FUNCTION SUBPROGRAM FOR THE
C            COMPUTATION OF ABSORPTION COEFFICIENTS
C            USING STANDARD LORENTZ LINE SHAPES
C               MICHAEL T. POTTER
0001          REAL FUNCTION TEMPK*8(WAVO,STRO,ALFAO,ENGO,DENOM,TPWR,TL,RTO,
             1 CTRFRQ)
0002          IMPLICIT REAL *8(A-H,C-Z)
0003          REAL  WAVO,STRO,ALFAO,ENGO,CTRFRQ
0004          DATA BLTZ,PLK,SPDL/1.38052200E-23,6.62619600E-34,2.99792500E+10/
0005          EHCKT=(ENGO*SPDL*PLK*DENOM)
0006          STNGTH=STRO*TPWR*DEXP(EHCKT*(1.0-TL))
0007          ALFA=ALFAO*RTO
0008          DIF=CTRFRQ-WAVO
0009          SHAPE= ALFA/((ALFA*ALFA) + (DIF*DIF))
0010          TEMPK=SHAPE*STNGTH
0011          RETURN
0012          END
```

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```
C
C            SUBROUTINE PART
C            MICHAEL T. POTTER
C
C     THIS SUBROUTINE COMPUTES VIBRATIONAL PARTITION FUNCTION
C     VALUES FOR EACH MOLECULE TYPE.   ARRAYS A,B,C ARE DATA FROM A
C     LEAST SQUARES 2ND DEGREE POLYNOMIAL.  DEPENDENT VARIABLE IS
C     TEMPERATURE.
C
0001        SUBROUTINE PART (T,QRTO)
0002        IMPLICIT REAL*8(A-H,O-Z)
0003        DIMENSION A(7),B(7),C(7),QRTO(7)
0004        DATA A/-.93896039E-07,-.25483461E-05,-.21673751E-05,-.28101372E-05
           1,.00000000,-.60069938E-06,-.98896C39E-07/
0005        DATA B/.44933103E-04,.51691420E-03,.67787503E-03,.42823000E-03,
           1.00000000,.22756513E-03,.44933103E-04/
0006        DATA C/.99504424,.1070761 3E01,.98969448,.11201483E01,.10000000E01,
           1.98548537,.99504424/
0007        DO 10 I1=1,7
0008        QRTO(I1)=A(I1)*T*T + B(I1)*T + C(I1)
0009     10 CONTINUE
0010        RETURN
0011        END
```

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```
     XX               SPACE=(80,(200,100),RLSE),DCB=BLKSIZE=80                    00100014
//FORT.SYSIN DD *
          IEF236I ALLOC. FOR JOBN7838 FORT      STEPNAME
          IEF237I 449    ALLOCATED TO SYSPRINT
          IEF237I 432    ALLOCATED TO SYSPUNCH
          IEF237I 236    ALLOCATED TO SYSLIN
          IEF237I 411    ALLOCATED TO SYSIN
          IEF142I - STEP WAS EXECUTED - COND CODE 0000
          IEF285I   SYS77108.T065922.RV000.JOBN7838.LOADSET       PASSED
          IEF285I   VOL SER NOS= UTEP33.
          UTEP111I STEP FORT      EXECUTION TIME =    012.92 SEC.
          UTEP113I STEP FORT      REGION = 0192K   MAX CORE USED = 0094K
     XXLKED EXEC PGM=IEWL,REGION=96K,PARM=(XREF,LET,LIST),COND=(4,LT,FORT)    00120000
     XXSYSLIB   DD  DSNAME=SYS1.FORTLIB,DISP=SHR                              00140000
     XX         DD  DSN=UTEP.FORTLIB,DISP=SHR                  FORTGCLG      00140020
     XX         DD  DSN=UTEP.CALCOMP.LOAD,DISP=SHR             FORTGCLG      00140040
//LKED.SYSLMOD DD SPACE=(CYL,(5,5,1))
     X/SYSLMOD  DD  DSNAME=&GOSET(MAIN),DISP=(NEW,PASS),UNIT=SYSDA,           X00160000
     XX             SPACE=(1024,(20,10,1),RLSE),DCB=BLKSIZE=1024              00180014
     XXSYSPRINT DD  SYSOUT=A                                                  00200000
     XXSYSUT1   DD  UNIT=SYSDA,SPACE=(1024,(100,10),RLSE),DCB=BLKSIZE=1024,  X00210018
     XX             DSNAME=&SYSUT1                                            00220018
     XXSYSLIN   DD  DSNAME=&LOADSET,DISP=(OLD,DELETE)                         00240000
     XX         DD  DDNAME=SYSIN                                              00260000
          IEF236I ALLOC. FOR JOBN7838 LKED      STEPNAME
          IEF237I 131    ALLOCATED TO SYSLIB
          IEF237I 136    ALLOCATED TO
          IEF237I 136    ALLOCATED TO
          IEF237I 237    ALLOCATED TO SYSLMOD
          IEF237I 440    ALLOCATED TO SYSPRINT
          IEF237I 232    ALLOCATED TO SYSUT1
          IEF237I 236    ALLOCATED TO SYSLIN
          IEF142I - STEP WAS EXECUTED - COND CODE 0000
          IEF285I   SYS1.FORTLIB                                  KEPT
          IEF285I   VOL SER NOS= LNK218.
          IEF285I   UTEP.FORTLIB                                  KEPT
          IEF285I   VOL SER NOS= UTEP11.
          IEF285I   UTEP.CALCOMP.LOAD                             KEPT
          IEF285I   VOL SER NOS= UTEP11.
          IEF285I   SYS77108.T065922.RV000.JOBN7838.GOSET         PASSED
          IEF285I   VOL SER NOS= UTEP32.
          IEF285I   SYS77108.T065922.RV000.JOBN7838.SYSUT1        DELETED
          IEF285I   VOL SER NOS= DTEST1.
          IEF285I   SYS77108.T065922.RV000.JOBN7838.LOADSET       DELETED
          IEF285I   VOL SER NOS= UTEP33.
          UTEP111I STEP LKED      EXECUTION TIME =    002.04 SEC.
          UTEP113I STEP LKED      REGION = 0192K   MAX CORE USED = 0132K
     XXGO EXEC PGM=*.LKED.SYSLMOD,COND=((4,LT,FORT),(4,LT,LKED))              00280000
     XXFT05F001 DD  DDNAME=SYSIN                                              00300000
//GO.FT06F001 DD SYSOUT=(A,,6410)
     X/FT06F001 DD  SYSOUT=A                                                  00320000
     XXFT07F001 DD  SYSOUT=B                                                  00340000
//GO.FT91F001 DD DSN=USER.EEE02947.POTMGL,DISP=OLD
//GO.SYSIN DD *
//
          IEF236I ALLOC. FOR JOBN7838 GO        STEPNAME
          IEF237I 237    ALLOCATED TO PGM=*.DD
          IEF237I 413    ALLOCATED TO FT05F001
          IEF237I 470    ALLOCATED TO FT06F001
          IEF237I 433    ALLOCATED TO FT07F001
          IEF237I 236    ALLOCATED TO FT91F001
```

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ABSORPTION COEFFICIENT FOR
STANDARD LORENTZ LINE SHAPE
****

ALT (KM)	H2O	CO2	O3	N2O	CO	CH4	O2
0.0	0.2261326D-24	0.4041435D-24	0.0	0.1063083D-18	0.1292446D-17	0.0	0.0
1.0	0.1923712D-24	0.3470447D-24	0.0	0.9422905D-19	0.1399635D-17	0.0	0.0
2.0	0.1425556D-24	0.2845242D-24	0.0	0.8283990D-19	0.1504721D-17	0.0	0.0
3.0	0.1073850D-24	0.2215603D-24	0.0	0.7198997D-19	0.1607016D-17	0.0	0.0
4.0	0.8022145D-25	0.1697156D-24	0.0	0.6230477D-19	0.1703489D-17	0.0	0.0
5.0	0.5930997D-25	0.1276122D-24	0.0	0.5361398D-19	0.1791675D-17	0.0	0.0
6.0	0.4334448D-25	0.9399994D-25	0.0	0.4583266D-19	0.1867072D-17	0.0	0.0
7.0	0.3125766D-25	0.6767493D-25	0.0	0.3887027D-19	0.1924408D-17	0.0	0.0
8.0	0.2154866D-25	0.4542722D-25	0.0	0.3258857D-19	0.1948622D-17	0.0	0.0
9.0	0.1517684D-25	0.3115563D-25	0.0	0.2733649D-19	0.1948736D-17	0.0	0.0
10.0	0.1015236D-25	0.1975124D-25	0.0	0.2259410D-19	0.1908608D-17	0.0	0.0
11.0	0.6355313D-26	0.1282744D-25	0.0	0.1869399D-19	0.1840540D-17	0.0	0.0
12.0	0.4503409D-26	0.7834886D-26	0.0	0.1520666D-19	0.1732947D-17	0.0	0.0
13.0	0.2992774D-26	0.4666879D-26	0.0	0.1237677D-19	0.1603555D-17	0.0	0.0
14.0	0.2558297D-26	0.4067628D-26	0.0	0.1058972D-19	0.1486460D-17	0.0	0.0
15.0	0.2173862D-26	0.3508635D-26	0.0	0.9004654D-20	0.1348963D-17	0.0	0.0
16.0	0.1856232D-26	0.3028340D-26	0.0	0.7692759D-20	0.1209727D-17	0.0	0.0
17.0	0.1588721D-26	0.2612296D-26	0.0	0.6586485D-20	0.1074236D-17	0.0	0.0
18.0	0.1357972D-26	0.2245947D-26	0.0	0.5631357D-20	0.9443545D-18	0.0	0.0
19.0	0.1213334D-26	0.2052999D-26	0.0	0.4864150D-20	0.8274371D-18	0.0	0.0
20.0	0.1084076D-26	0.1873812D-26	0.0	0.4201896D-20	0.7211806D-18	0.0	0.0
21.0	0.9594968D-27	0.1709865D-26	0.0	0.3633726D-20	0.6266783D-18	0.0	0.0
22.0	0.8665168D-27	0.1557922D-26	0.0	0.3141016D-20	0.5427249D-18	0.0	0.0
23.0	0.8105440D-27	0.1509881D-26	0.0	0.2749426D-20	0.4718028D-18	0.0	0.0
24.0	0.7234692D-27	0.1371620D-26	0.0	0.2374652D-20	0.4067259D-18	0.0	0.0
25.0	0.6434908D-27	0.1250652D-26	0.0	0.2061037D-20	0.3517252D-18	0.0	0.0
30.0	0.4594302D-27	0.1032324D-26	0.0	0.1063218D-20	0.1716955D-18	0.0	0.0
35.0	0.3404687D-27	0.8841527D-27	0.0	0.5687850D-21	0.8612480D-19	0.0	0.0
40.0	0.2700016D-27	0.8136743D-27	0.0	0.3161472D-21	0.4449644D-19	0.0	0.0
45.0	0.2067962D-27	0.7033856D-27	0.0	0.1791574D-21	0.2366379D-19	0.0	0.0
50.0	0.1329440D-27	0.4788034D-27	0.0	0.9996310D-22	0.1280933D-19	0.0	0.0
70.0	0.1222591D-29	0.2131449D-29	0.0	0.4740663D-23	0.8495318D-21	0.0	0.0
100.0	0.3857354D-32	0.5760260D-32	0.0	0.1970347D-25	0.3725637D-23	0.0	0.0

UNITS ARE IN SQUARE CENTIMETERS PER MOLECULE

ABSORPTION COEFFICIENT FOR
MODIFIED LORENTZ LINE SHAPE
****

ALT(KM)	H2O	CO2	O3	N2O	CO	CH4	O2
0.0	0.2261317D-24	0.4041473D-24	0.0	0.1063088D-18	0.1292446D-17	0.0	0.0
1.0	0.1823705D-24	0.3470456D-24	0.0	0.9422954D-19	0.1399635D-17	0.0	0.0
2.0	0.1425551D-24	0.2845251D-24	0.0	0.8284042D-19	0.1504721D-17	0.0	0.0
3.0	0.1073846D-24	0.2215611D-24	0.0	0.7199046D-19	0.1607016D-17	0.0	0.0
4.0	0.8022114D-25	0.1697163D-24	0.0	0.6231519D-19	0.1703489D-17	0.0	0.0
5.0	0.5930978D-25	0.1276130D-24	0.0	0.5361430D-19	0.1791675D-17	0.0	0.0
6.0	0.4334439D-25	0.9400890D-25	0.0	0.4583288D-19	0.1867072D-17	0.0	0.0
7.0	0.3125763D-25	0.6767600D-25	0.0	0.3887039D-19	0.1924408D-17	0.0	0.0
8.0	0.2154867D-25	0.4542817D-25	0.0	0.3258859D-19	0.1948622D-17	0.0	0.0
9.0	0.1517687D-25	0.3115140D-25	0.0	0.2733646D-19	0.1948736D-17	0.0	0.0
10.0	0.1015239D-25	0.1975175D-25	0.0	0.2259404D-19	0.1908608D-17	0.0	0.0
11.0	0.6955345D-26	0.1282777D-25	0.0	0.1869393D-19	0.1840540D-17	0.0	0.0
12.0	0.4503431D-26	0.7635065D-26	0.0	0.1520662D-19	0.1732947D-17	0.0	0.0
13.0	0.2992786D-26	0.4666976D-26	0.0	0.1237695D-19	0.1603555D-17	0.0	0.0
14.0	0.2558307D-26	0.4067696D-26	0.0	0.1058970D-19	0.1486460D-17	0.0	0.0
15.0	0.2173871D-26	0.3533681D-26	0.0	0.9004637D-20	0.1348963D-17	0.0	0.0
16.0	0.1856239D-26	0.3028370D-26	0.0	0.7692743D-20	0.1209727D-17	0.0	0.0
17.0	0.1588727D-26	0.2612314D-26	0.0	0.6586471D-20	0.1074236D-17	0.0	0.0
18.0	0.1357978D-26	0.2245958D-26	0.0	0.5631344D-20	0.9435450-18	0.0	0.0
19.0	0.1213339D-26	0.2053006D-26	0.0	0.4864138D-20	0.8274371D-18	0.0	0.0
20.0	0.1034081D-26	0.1873816D-26	0.0	0.4201884D-20	0.7211806D-18	0.0	0.0
21.0	0.9695012D-27	0.1709866D-26	0.0	0.3633715D-20	0.6266783D-18	0.0	0.0
22.0	0.8665209D-27	0.1557922D-26	0.0	0.3141006D-20	0.5427249D-18	0.0	0.0
23.0	0.8105479D-27	0.1502879D-26	0.0	0.2749416D-20	0.4718028D-18	0.0	0.0
24.0	0.7234727D-27	0.1371618D-26	0.0	0.2374642D-20	0.4067259D-18	0.0	0.0
25.0	0.6484939D-27	0.1250650D-26	0.0	0.2060029D-20	0.3517252D-18	0.0	0.0
30.0	0.4594320D-27	0.1032322D-26	0.0	0.1063214D-20	0.1716955D-18	0.0	0.0
35.0	0.3404691D-27	0.8841519D-27	0.0	0.5687840D-21	0.8612480D-19	0.0	0.0
40.0	0.2700011D-27	0.8136756D-27	0.0	0.3161482D-21	0.4449644D-19	0.0	0.0
45.0	0.2067955D-27	0.7038879D-27	0.0	0.1791585D-21	0.2366379D-19	0.0	0.0
50.0	0.1329434D-27	0.4788052D-27	0.0	0.9996376D-22	0.1280933D-19	0.0	0.0
70.0	0.1222597D-29	0.2131445D-29	0.0	0.4740649D-23	0.8495318D-21	0.0	0.0
100.0	0.3857362D-32	0.5760255D-32	0.0	0.1970345D-25	0.3725637D-23	0.0	0.0

UNITS ARE IN SQUARE CENTIMETERS PER MOLECULE

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PERCENT RELATIVE ERROR
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ALT (KM)	H2O	CO2	O3	N2O	CO	CH4	O2
0.0	0.3730980D-03	0.1069895D-02	0.0	0.4811396D-03	0.5477035D-06	0.0	0.0
1.0	0.3959634D-03	0.2593587D-03	0.0	0.5186002D-03	0.5514273D-06	0.0	0.0
2.0	0.4129686D-03	0.3370911D-03	0.0	0.6186047D-03	0.5267756D-06	0.0	0.0
3.0	0.4123502D-03	0.3908148D-03	0.0	0.6820346D-03	0.4619175D-06	0.0	0.0
4.0	0.3844473D-03	0.4364968D-03	0.0	0.6739316D-03	0.3643236D-06	0.0	0.0
5.0	0.3250079D-03	0.6132351D-03	0.0	0.5996689D-03	0.2549099D-06	0.0	0.0
6.0	0.2360626D-03	0.1017022D-02	0.0	0.4715437D-03	0.1496605D-06	0.0	0.0
7.0	0.1169253D-03	0.1587532D-02	0.0	0.3020873D-03	0.5930317D-07	0.0	0.0
8.0	0.4978779D-04	0.2097282D-02	0.0	0.6458147D-04	0.1987882D-07	0.0	0.0
9.0	0.2021607D-03	0.2471842D-02	0.0	0.1211349D-03	0.6381177D-07	0.0	0.0
10.0	0.3642818D-03	0.2601982D-02	0.0	0.2789099D-03	0.8892553D-07	0.0	0.0
11.0	0.4610486D-03	0.2546933D-02	0.0	0.3244596D-03	0.8798226D-07	0.0	0.0
12.0	0.4843709D-03	0.2347246D-02	0.0	0.2691485D-03	0.6984318D-07	0.0	0.0
13.0	0.3982453D-03	0.2065544D-02	0.0	0.1585360D-03	0.4355472D-07	0.0	0.0
14.0	0.3982618D-03	0.1684929D-02	0.0	0.1725842D-03	0.4016110D-07	0.0	0.0
15.0	0.3982743D-03	0.1302510D-02	0.0	0.1876368D-03	0.3760206D-07	0.0	0.0
16.0	0.3982831D-03	0.9779262D-03	0.0	0.2003304D-03	0.3580176D-07	0.0	0.0
17.0	0.3982894D-03	0.7131382D-03	0.0	0.2120519D-03	0.3450589D-07	0.0	0.0
18.0	0.3982941D-03	0.4999612D-03	0.0	0.2211607D-03	0.3354985D-07	0.0	0.0
19.0	0.4202674D-03	0.3228644D-03	0.0	0.2527912D-03	0.3586891D-07	0.0	0.0
20.0	0.4391452D-03	0.1851801D-03	0.0	0.2925231D-03	0.3812399D-07	0.0	0.0
21.0	0.4549525D-03	0.7951986D-04	0.0	0.3103082D-03	0.4028877D-07	0.0	0.0
22.0	0.4577349D-03	0.1979775D-05	0.0	0.3361687D-03	0.4232964D-07	0.0	0.0
23.0	0.4844916D-03	0.7218202D-04	0.0	0.3799199D-03	0.4615261D-07	0.0	0.0
24.0	0.4886378D-03	0.1196210D-03	0.0	0.4000150D-03	0.4761992D-07	0.0	0.0
25.0	0.4900953D-03	0.1549047D-03	0.0	0.4178154D-03	0.4888825D-07	0.0	0.0
30.0	0.3841547D-03	0.2176403D-03	0.0	0.4500751D-03	0.4790882D-07	0.0	0.0
35.0	0.1261085D-03	0.9081805D-04	0.0	0.1359826D-03	0.1905266D-07	0.0	0.0
40.0	0.1900129D-03	0.1598416D-03	0.0	0.3061733D-03	0.3183557D-07	0.0	0.0
45.0	0.3596087D-03	0.3359356D-03	0.0	0.6178265D-03	0.6833596D-07	0.0	0.0
50.0	0.4025815D-03	0.3731090D-03	0.0	0.6619581D-03	0.7655277D-07	0.0	0.0
70.0	0.4391535D-03	0.1837617D-03	0.0	0.2996132D-03	0.3649799D-07	0.0	0.0
100.0	0.2032996D-03	0.8483052D-04	0.0	0.1021742D-03	0.1194822D-07	0.0	0.0

BEST AVAILABLE COPY

ABSOLUTE ERROR IN INVERSE ATM-CMS

ALT(KM)	H2O	CO2	O3	N2O	CO	CH4	O2
0.0	0.2269541D-10	0.1162044D-09	0.0	0.1375911D-04	0.1904189D-06	0.0	0.0
1.0	0.1942510D-10	0.2421242D-10	0.0	0.1314527D-04	0.2076132D-06	0.0	0.0
2.0	0.1583628D-10	0.2579993D-10	0.0	0.1378494D-04	0.2132229D-06	0.0	0.0
3.0	0.1191137D-10	0.2329243D-10	0.0	0.1320877D-04	0.1996809D-06	0.0	0.0
4.0	0.8296196D-11	0.1992759D-10	0.0	0.1129508D-04	0.1669516D-06	0.0	0.0
5.0	0.5201251D-11	0.2105093D-10	0.0	0.8648515D-05	0.1228565D-06	0.0	0.0
6.0	0.2752409D-11	0.2571638D-10	0.0	0.5813653D-05	0.7516580D-07	0.0	0.0
7.0	0.9831436D-12	0.2890029D-10	0.0	0.3158654D-05	0.3069921D-07	0.0	0.0
8.0	0.2885992D-12	0.2552860D-10	0.0	0.5661418D-06	0.1042006D-07	0.0	0.0
9.0	0.8253346D-12	0.2071283D-10	0.0	0.8907671D-06	0.3345074D-07	0.0	0.0
10.0	0.9948470D-12	0.1382454D-10	0.0	0.1695162D-05	0.4565571D-07	0.0	0.0
11.0	0.8626119D-12	0.8788394D-11	0.0	0.1631603D-05	0.4356045D-07	0.0	0.0
12.0	0.5867748D-12	0.4820734D-11	0.0	0.1100976D-05	0.3255827D-07	0.0	0.0
13.0	0.3206096D-12	0.2594318D-11	0.0	0.5278301D-06	0.1878758D-07	0.0	0.0
14.0	0.2740764D-12	0.1843634D-11	0.0	0.4916290D-06	0.1605871D-07	0.0	0.0
15.0	0.2323983D-12	0.1229338D-11	0.0	0.4545033D-06	0.1364469D-07	0.0	0.0
16.0	0.1988731D-12	0.7966412D-12	0.0	0.4157955D-06	0.1165048D-07	0.0	0.0
17.0	0.1702152D-12	0.5011273D-12	0.0	0.3757057D-06	0.9971148D-08	0.0	0.0
18.0	0.1454945D-12	0.3020562D-12	0.0	0.3350218D-06	0.8522709D-08	0.0	0.0
19.0	0.1371697D-12	0.1783040D-12	0.0	0.3307661D-06	0.7983718D-08	0.0	0.0
20.0	0.1230619D-12	0.9334099D-13	0.0	0.3193385D-06	0.7395958D-08	0.0	0.0
21.0	0.1186491D-12	0.3657404D-13	0.0	0.3033175D-06	0.6791734D-08	0.0	0.0
22.0	0.1093257D-12	0.8296855D-15	0.0	0.2840400D-06	0.6179827D-08	0.0	0.0
23.0	0.1056367D-12	0.2931728D-13	0.0	0.2809129D-06	0.5857452D-08	0.0	0.0
24.0	0.9509531D-13	0.4413601D-13	0.0	0.2555220D-06	0.5210056D-08	0.0	0.0
25.0	0.8549413D-13	0.5211394D-13	0.0	0.2315323D-06	0.4625514D-08	0.0	0.0
30.0	0.4747638D-13	0.6043761D-13	0.0	0.1287240D-06	0.2212719D-08	0.0	0.0
35.0	0.1154977D-13	0.2159938D-13	0.0	0.2845590D-07	0.4414036D-09	0.0	0.0
40.0	0.1307441D-13	0.3498586D-13	0.0	0.2603807D-07	0.3810569D-09	0.0	0.0
45.0	0.2000437D-13	0.6360775D-13	0.0	0.2977510D-07	0.4349964D-09	0.0	0.0
50.0	0.1439709D-13	0.4805571D-13	0.0	0.1780009D-07	0.2627785D-09	0.0	0.0
70.0	0.1444274D-15	0.1053615D-15	0.0	0.3820780D-09	0.8340664D-11	0.0	0.0
100.0	0.2109493D-18	0.1314456D-18	0.0	0.5415466D-12	0.1197446D-13	0.0	0.0