THE TEMPERATURE STRUCTURE OF PRIMORDIAL ATMOSPHERES

by

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Abstract

There is a strong possibility that the material out of which the Earth formed was host to prebiotic molecules of varying complexity. The chances that these molecules had in surviving in the early atmosphere are examined by computing a series of models with various effective temperatures and compositions, and seeing whether the atmospheric temperature structure was in the required range to support life as we know it. It was found that the required conditions were satisfied for some of the models, but the majority of them had too high a temperature.

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a	constant of the linearization of B_i
A	Russel-Bond spherical albedo
A_o	Avogadro's number
A_ν	CH_4 absorption coefficient
A_ν	H_2 absorption coefficient
A_i	averaged H_2 absorption coefficient
b	constant of the linearization of B_i
$b(\nu-\nu_\ell, \delta\nu_\ell)$	line shape function
b_i	constant of the linearization of A_i
B_ν	Planck function
B_i	Planck function over waveband i
$\overline{B}_k$	averaged Planck function (at sample point k)
$\mathcal{B}$	equation of transfer solution function
c_{ij}	optical depth power law coefficient
C_i	Planck function coefficient
$C_{\ell k}$	coefficient involved in the atmosphere linearization
C_P	specific heat at constant pressure
C_v	specific heat at constant volume
D_i	Planck function coefficient
E_1, E_2, E_3	Exponential integrals
f	scaling factor for the solar constant
f_k	scaling factor in the linearization of the atmosphere
f_j	fractional abundance of molecule j
F_ν	monochromatic flux
F_i	flux over waveband i

F_k total flux at a given sample point

F_l' linear fluxes without scaling

$\mathcal{F}$ desired flux

g gravitational acceleration

$G_i(T)$ temperature dependence function

G_ν, G_ν' intermediate temperature dependence functions

i frequency point index

I_ν monochromatic specific intensity

I_ν^{out} outgoing monochromatic specific intensity

I_ν^{in} incoming " " "

I_i^{out} outgoing specific intensity in waveband i

I_i^{in} incoming " " " " i

k Boltzman's constant

k sample point subscript

$K(\nu), K'$ frequency dependence components of optical depth

l a specific sample point index

m_H mass of the atomic mass unit

m_j total mass (in sample) of molecule j

m_i coefficient of the linearization of A_i

M molecular weight

n number density

N_j total number of molecules j

P pressure

P_o initial partial pressure

P_e effective NH_3 pressure

$P_{NH_3}, P_{H_2}, P_{He}$ partial pressures of NH_3, H_2 and He respectively

q_ν', q_ν intermediate pressure exponent

$\bar{q}$ average pressure exponent

r_{ij} power law column density exponent

$R_{\oplus}$ radius of the Earth

s_{ij} power law pressure exponent

S solar constant

$S_{initial}$ solar constants with evolutionary and

S_{cosmol} cosmological effects

S_{ν} monochromatic source function

S_{ℓ} line intensity

t time

t_o age of the Universe

t_E age of the Universe at the Earth's formation

t_b Jean's atmospheric escape time constant

t_e time in which atmosphere reduces to 1/e of original

t_{ij} power law temperature exponent

t_{ν} dummy variable of integration

T temperature

T_{eff} effective temperature

T_{Hart} surface temperature of Hart (1978) models

$T_{Present}$ " " " present models

$\bar{T}$ mean transmission of radiation

u function involved in the NH_3 opacity

$\mathcal{U}$ equation of transfer solution function

v Maxwellian R.M.S. velocity

W column density

x parameter involved in the optical depth regimes

x_1, x_2, x_3 known indept. variables in Lagrangian interpolation

x_k^+, x_k^- coefficients involved in linearization of atmosphere

X_1, X_2, X_3 coefficients in Lagrangian interpolation

y function involved in NH_3 opacity

y_1, y_2, y_3 known dept variables in Lagrangian interpolation

y_k^+, y_k^- coefficients involved in linearization of atmosphere

z physical depth scale

Z physical depth at a specific point within atmosphere

Z_b thickness of atmosphere

$\alpha_\ell(\nu)$ line absorption coefficient

γ constant for cosmological effects

γ abiabatic index

$\delta\nu_\ell$ line half width

Δ half the bandwidth of optical depth scale

$\Delta\nu_i$ frequency bandwidth

$\Delta\nu_j$ NH_3 opacity bandwidth

ΔW column density between two sample points

θ angle between normal to surface and direction of radiation

κ_ν mass absorption coefficient

μ cos θ

ν_ℓ line position

ρ density

σ Stefan-Boltzman constant

Σs_i, $\Sigma\sqrt{s_i\alpha_{oi}}$ parameters involved in NH_3 opacity

τ_ν monochromatic optical depth

τ_b " " " at surface

τ_i frequency averaged optical depth

τ_ν'	central optical depth value
$\overline{\tau}_k$	total frequency averaged optical depth scale
τ_{chg}	lower limit of optical depth regime changeover
τ_{rge}	upper " " " " " "

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I take the opportunity here to gratefully acknowledge the receipt of a University of Victoria Fellowship for the years 77/78 and 78/79.

Dedication

This work is dedicated to my parents. Without their guidance, their sacrifices and many encouragements during my formative years, this work would never have been written.

Preface

In common with present scientific trend, all units in this work are given in their S.I. values. The main S.I. units used in this work are

pressure in kpa (kilopascals)

column density in kpa-m

temperature in (degrees) Kelvin

flux in $Jm^{-2}s^{-1}$

wavelength in μm and nm. Optical depth on the other hand is dimensionless.

It is worth noting here that all tabular values having some power of ten are tabulated in the form

$$3.0\ (8) = 3.0 \times 10^{8}$$

for example.

Chapter 1

THE SETTING

1.1 BACKGROUND AND AIMS

It is generally believed that life on the Earth began from prebiotic molecules created out of the primordial atmosphere by lightning and ultraviolet radiation. However, there is now a possibility that these prebiotic molecules came from a earlier epoch, namely from the interstellar medium out of which the Earth formed. The impetus for this idea comes from the discovery of increasing numbers of interstellar molecules within the last decade. The number of molecules stands at over forty [see for example Hoyle (1978)], and their structure involves up to nine atoms. Two of these molecules are of particular interest: methanimine [Godfrey et al (1973)] and formic acid [Zuckerman et al (1971)]. These two molecules react exothermically to form glycine, the simplest of the amino acids. It is the possible presence of glycine and other complex interstellar molecules which suggests the interstellar origin of life. But have any of these molecules been found in the interstellar medium? The answer is no, not definitely.

Glycine is expected, but the rotational energy of large molecules is spread over many rotational lines, making each line difficult to detect over the background noise with the present detectors [Avery et al (1976)]. Hoyle and Wickramasinghe (1977b) postulate that the interstellar infrared absorbtion bands (2-4 μm, 8-13 μm, and 15-30 μm) are due to cellulose rather than to water-ice and silicates models usually invoked. Certainly, cellulose could quite possibly exist since formaldehye, out of which cellulose is made, is one of the most common of all the interstellar molecules, and by forming polysaccharides like cellulose, formaldehyde is rendered more stable. Even though a mixture of celluloses (with some hydrocarbons added) rather than a single type was later needed to optimize the theoretical fit to the data [Hoyle et al (1978)], the alternative explanation, namely ice-silicate models, is in disagreement with the cosmic abundance criterion in that the required amount of silicon is greater than the presently accepted cosmic abundance [Wickramasinghe et al (1977)].

Another candidate for complex prebiotic molecules is the source of the ultraviolet 220 nm feature observed in interstellar clouds. Hoyle and Wickramasinghe (1977c) postulated a set of bicyclic molecules (empirical formula $C_8H_6N_2$) to explain this feature. Such nitrogenated structures could form in stellar mass flows [Hoyle and Wickramasinghe (1977d)]. However Egan and Hilgeman (1978) simply suggest a nitrile group ($C \equiv N$) or a carbonyl bond ($C=O$) as the source of the UV feature. Certainly, while the nitrile group is consistant with the nitrogenated structures of Hoyle and Wickramasinghe, any of the cyanogen molecules that have been discovered in the interstellar medium also have this group. Moreover, the carbonyl bond is consistent with the presence of formaldehyde, thus offering a simpler explanation of the UV feature than postulating a new set of complex molecules.

There are, of course, non-organic explanations for this UV line. Despite qualms about growth shapes, Edmunds (1978) states that small graphite spheres are still the best explanation for this line. These reservations arise from the fact that the grains must be perfect spheres, a not very likely occurrence. The ice-silicate models fare less well. Not only do they break the cosmic abundance criterion as indicated above, but their evaporation temperature is too high [Cooke and Wickramasinghe (1977)]. The evaporation temperature obtained from comet observations matches that predicted by an organic coating over seed grains, but is some three times lower than that required by silicate grains.

The conclusion is that while prebiotic molecules have not been definitely observed in the interstellar medium, they can be invoked to expain various absorbtion lines equally as effectively as the non-organic models. Certainly the conditions of interstellar space are not unfavourable to their formation as Goldanskii (1976,1977) and Barlow and Silk (1977) have shown.

If such molecules do exist in the interstellar medium, then it is reasonable to assume that they also existed in the protosolar cloud out of which the Sun and the planets formed. Assuming that the molecules survived the formation period, there should be evidence for their existence even now. Such evidence does appear to exist.

Hoyle and Wickramasinghe (1976) postulate that the μm inclusions found in carbonaceous chondrite meteorites are dust grains coated with these primordial organic molecules. Sakata et al (1977) lend support to this idea by noting that spectroscopic measurements made of such inclusions match the interstellar 220 nm absorption line. Furthermore, Knacke (1977) has made infrared observations of this material, and has found good agreement with the interstellar infrared bands mentioned above. It is tempting to speculate, then, that the amino acids found in these meteorites are also of interstellar origin, protected by the matrix of smaller grains in which they are imbedded. Certainly, the meteoritic acids tend seldomly, if ever, to be associated with terrestrial life [Pellegrino and Stoff (1979)], and have too high a proportion of right-handed acids (terrestrial acids are virtually all left-handed). It is safe to assume, therefore, that these acids are not terrestrial, but there is no way of knowing whether they have formed recently within the meteorites, or whether they were already present when the meteorites were formed.

Where is all this leading? Well, if prebiotic molecules exist in the protostellar clouds, and we have attempted to show that there is a good chance that they do, then they could have been incorporated into the primordial Earth right from the beginning, short-circuiting many millions of years of evolution.

Such questions, however, could be academic. Present work on the formation of the solar system indicates that the early temperatures of formation using the cogenic theories (wherein the sun and planets formed at the same time) were too high for these molecules to survive. Cameron (1976) indicates that the surface temperature of the Earth was approximately 800 K when the Sun entered its T-Tauri stage, while Prentice (1976) obtains a surface temperature of around 1000 K. At times, these temperatures will have been higher since the Sun probably went through periods of sporadic brightening during its T-Tauri phase [Herbig (1976)]. However, the non-cogenic theories of Alfven and Arrhenius (1976) predict a black body temperature of only 200 K for the early Earth by the time it reached its present size. It can be seen that these planetary formation theories are still in their infancy, and thus we cannot rule out the possibility that the formation temperatures were quite low. Futhermore, our molecules could have survived as part of an extended atmosphere about the accreting planet, falling back onto the planet as the surface cooled.

So we are still left with our postulate, namely that prebiotic molecules found themselves on the new Earth. The question we wish to answer is whether such molecules could have survived to continue on their evolutionary paths. This is a very complex question, involving the computation of extended chemical reaction schemes. Such schemes are beyond the scope of this work, but all require the computation of the planetary temperature structure. It is to this aspect of the problem, namely the calculation of the temperature structure, that the present work is addressed.

1.2 INITIAL CONDITIONS

1.2.1 The Effective Temperature

We shall assume that all the energy sources driving the Earth's atmosphere are such that the energy is effectively deposited at the Earth's surface (without absorption), and that the surface then re-emits the energy as a black body. This black body will be characterized by an effective temperature T_{eff}. To find this effective temperature, we need to know what the energy sources of the Earth actually are. Apart from the energy released during the Earth's formation, the dominant energy source is solar radiation. In this case, the effective temperature is given by

$$S(1 - A) = f\sigma T_{eff}^4 \qquad (1.1)$$

where S is the solar constant, A is the spherical albedo, f is a geometric scaling factor, and σ is the Stefan-Boltzman constant. The scaling factor enters the equation because the Earth acts like a disc on receiving radiation, but acts like a sphere on reradiating it. Since the ratio of the surface area of a sphere to that of a disc is four, the scaling factor is $f = 4$ (even for a slowly rotating Earth, the atmosphere will ensure a uniform heat flux).

There is evidence that the solar constant has increased since the formation period of the Earth [Haselgrove and Hoyle (1959)]; this increase is estimated to be 40-45%. Using an increase of 40%, coupled with the present value of S, we get for the initial value

$$S_{initial} \simeq 991 \ Jm^{-2}s^{-1}$$

Values for the albedo can be obtained from Allen (1963). For the present Earth, the albedo is 0.4. However, as we shall see, the early Earth is Jupiter-like in composition, in which case, the albedo will be 0.58. Substituting these values into (1.1), we get the following effective temperatures

Earth-like	(A = 0.40)	T_{eff} = 226 K
Jupiter-like	(A = 0.58)	T_{eff} = 207 K

Canuto and Hsieh (1978) give an interesting variation to the above results, based on cosmology. In their scale covariant cosmology, S also changes because G, and thus M vary. For the non-matter creation case, which bests fits geological data, S is given by

$$S_{cosmol} = S_{initial} \left(\frac{t_o}{t_E} \right)^{\gamma - 2}$$

where t_o is the age of the Universe ($\sim 1.8 \times 10^{10}$ yrs), while $\gamma = 6.33$. With $t_E = 1.3 \times 10^{10}$ yrs (the age of the Universe at the time of the Earth's formation), we get

$$S_{cosmol} \simeq 4055 \ Jm^{-2}s^{-1}$$

Using this value of S, and the albedos above, the effective temperatures are

Earth-like	(A = 0.40)	T_{eff} = 322 K
Jupiter-like	(A = 0.58)	T_{eff} = 294 K

We will investigate, as much as we're able, the chances our prebiotic molecules had in surviving the formation period of the Earth by characterizing such a period with an effective temperature. For the models of Alfven and Arrhenius (1976), T_{eff} = 200 K. We will characterize Cameron's (1976) models with two effective tenperatures T_{eff} = 400 K and 600 K, the former corresponding to a later period of time after the Earth had cooled a little.

It is also illuminating to investigate the temperature structure of the primordial atmosphere with no incoming solar radiation, corresponding to the very early formation period before the Sun had begun to shine. The power sources for the atmosphere, then, are radoigenic heating, and gravitational collapse of the Earth's core. Elder (1976) gives the early radiogenic flux as 0.53 $Jm^{-2}s^{-1}$. Also from Elder, the total gravitational energy available to the present day is 4 x 10^{31} J. Assuming an exponential decay of the heat flux, with the present flux equal to 0.1% of the initial flux (the present flux is negligible), the gravitational heat source amounts to 3.4 $Jm^{-2}s^{-1}$. The combined non-solar sources, then, give a heat flow of 3.9 $Jm^{-2}s^{-1}$, corresponding to an effective temperature of only 91 K.

In summary, we will investigate models with seven different effective temperatures (Table 1):

Table 1

The Effective Temperatures

91	Pre-solar heat flux	
205	Formation models of Alfven and Arrhenius (1976)	
	Jupiter-like atmosphere	Solar constant with evolutionary effects
225	Earth-like atmosphere	
295	Jupiter-like atmosphere	Solar const.: evolutionary and cosmological effects
320	Earth-like atmosphere	
400	Formation models of Cameron (1976)	
600		

1.2.2 Atmospheric Composition

The composition and size of the primordial atmosphere are completely unknown. However, both Cameron (1968) and Kuiper (1952) give possible initial atmospheric compositions, as shown below (Table 2).

We will take the average of these two compositions as our initial condition; this average is given above. As can be seen, our atmospheres will be rather Jupiter-like, indicating the use of a Jupiter albedo.

Table 2

Atmospheric Compositions

Molecule	Abundance by Number (percent) Kuiper (1952)	Cameron (1968)	Average
H_2	78.2	87.0	82.7
He	21.6	12.8	17.2
Ne	0.074	-	-
H_2O	0.047	0.088	0.067
NH_3	0.029	0.015	0.022
CH_4	0.015	0.062	0.038
Ar	0.009	-	-

We will also try to allow for some gas escape using the expressions given in Jeans (1925). Even though corrections to the Jeans' escape rate do exist [see for example Shizgal (1977)], the uncertainty of the initial conditions render such corrections as merely refinements.

From Jeans (1925), the escape rate of an atmosphere is given by

$$\frac{dW}{dt} = \frac{n}{t_b} \quad \text{molecules } m^{-2}s^{-1} \quad (1.2)$$

where t_b is given by

$$t_b = \frac{\sqrt{6\pi}}{v} e^{3gR_\oplus/v^2} \frac{1}{(1 + 3gR_\oplus/v^2)} \quad \text{secs}$$

and v is the RMS velocity of the Maxwellian distribution

$$v^2 = \frac{3kT}{m_H M}$$

Here $R_\oplus$ is the radius of the Earth, n is the surface number density, and W is the column density. The latter quantity is defined by

$$dW = \frac{\rho}{Mm_H} dz \qquad \text{molecules/m}^2 \quad (1.3)$$

where M is the molecular weight of the gas species. For an atmosphere in hydrostatic equilibrium (a valid assumption in our case since we will be ignoring convection), the equation of hydrostatic equilibrium yields, for pressures in kpa (kilopascals)

$$dP = \frac{g\rho dz}{1000}$$

Combining these two equations gives

$$dW = 6.1409 \times 10^{28} \frac{dP}{M} \qquad \text{molecules/m}^2 \quad (1.4)$$

From the perfect gas law, we have

$$n = \frac{1000\,P}{kT}$$

for P in kpa.

Substituting the above and (1.4) into (1.2) yields

$$\frac{dP}{dt} = 1.18 \times 10^{-3} \frac{M}{t_b} \frac{P}{T}$$

Solving the above finally yields

$$P = P_o \exp\left[- \frac{1.18 \times 10^{-3} M}{T} \frac{t}{t_b} \right] \qquad (1.5)$$

where P_o is the initial partial pressure of the molecule.

To get an idea of the relative escape rates of the molecules at our various effective temperatures, we can use (1.5) to calculate the time required for an atmosphere to reduce to only 1/e times its initial value. These times, denoted t_e, are given in Table 3 for hydrogen and helium.

Table 3

t_e values for hydrogen

T_{eff}	t_e (yrs) H_2	He
91	5.89 (64)	> 1.(100)
205	1.23 (25)	1.71 (56)
225	1.99 (22)	4.28 (50)
295	3.42 (15)	1.10 (37)
320	6.99 (13)	4.32 (33)
400	7.51 (9)	4.18 (25)
600	4.48 (4)	1.01 (15)

Note: The brackets in the table denote a power of ten, eg
6.26 (64) = 6.26×10^{64}
This notation is used in all tables in this work.

From the t_e values in Table 3, we can see that at only T_{eff}= 600 K do we get any appreciable escape of hydrogen within 10^8 years (later times take us too far away from the formation epoch we are considering), while the helium escape rate is very much slower. Therefore, for this temperature, we will investigate atmospheres which have lost 20%, 40%, 60%, 80%, and all their initial hydrogen, while the remaining constituents remain unchanged (the escape rate for the other molecules is even slower than that of helium). The resulting abundances are given in Table 4. Also in this table is the time t required for the hydrogen to reduce to the tabular value at 600 K, as computed from (1.5).

Table 4

Abundances

Molecule	Abundance by Number (percent)					
H	82.7	79.2	74.1	65.5	48.8	0.0
He	17.2	20.6	25.7	34.2	50.8	99.3
H_2O	0.067	0.080	0.100	0.133	0.198	0.368
NH_3	0.022	0.026	0.033	0.044	0.065	0.127
CH_4	0.038	0.046	0.057	0.075	0.112	0.219
Total	100.0	83.5	66.9	50.4	33.9	17.3
Time	0	1.01(4)	2.31(4)	4.14(4)	7.27(4)	6.56(5)

Note 1. The total row gives the fraction of the initial atmosphere left after each time t.

2. The initial composition (t=0) is applicable for ALL temperatures of Table I, while the remaining compositions are for 600 K only.

3. The time for hydrogen to completely stream away is infinite. However the abundance of hydrogen is effectively zero after 6.56 (5) years.

The remaining unknown is the size of the primordial atmosphere. Again, this is completely unknown, for outgassing from the Earth's interior has changed the initial composition. If all the present metallic constituents (elements other than hydrogen and helium) came from the primordial atmosphere, then that atmosphere would have had to have been a thousand times the size of the present atmosphere to supply the required metals. However, internal outgassing most likely has added to the primordial metal abundance, and the primitive atmosphere does not have to be as large. We will therefore consider models with ten and a hundred times the present atmosphere (by number).

Chapter 2

THE STAGE

2.1 THE EQUATION OF TRANSFER

Because of the large variation of opacity with frequency for the various molecular components of planetary atmospheres, the grey approximation with its simple temperature distribution is too crude a model. To find the true temperature distribution, we must solve the equation of transfer directly. In our case, the atmosphere is thin compared with the diameter of the planet, justifying the use of the plane parallel approximation for the equation of transfer

$$\mu \frac{dI_\nu(\tau_\nu,\mu)}{d\tau_\nu} = I_\nu(\tau_\nu,\mu) - S_\nu(\tau_\nu,\mu)$$

where I_ν is the specific intensity, and S_ν is the source function at some specific optical depth τ_ν, and direction μ. The parameter μ is defined by

$$\mu \equiv \cos\theta$$

where θ is the angle between the normal to the surface and the direction in which we are looking. The formal solutions to this equation are found by multiplying both sides by $\exp[-\tau_\nu/\mu]$, and integrating. For a bounded atmosphere, the result is

$$I_\nu^{out}(\tau_\nu,\mu) = I_\nu^{out}(\tau_b,\mu)\, e^{-(\tau_b-\tau_\nu)/\mu} + \int_{\tau_\nu}^{\tau_b} S_\nu(t_\nu,\mu)\, e^{-(t_\nu-\tau_\nu)/\mu}\, \frac{dt_\nu}{\mu} \quad (2.1a)$$

and

$$I_\nu^{in}(\tau_\nu,\mu) = -\int_0^{\tau_\nu} S_\nu(t_\nu,\mu)\, e^{-(t_\nu-\tau_\nu)/\mu}\, \frac{dt_\nu}{\mu} \quad (2.1b)$$

where at a given level τ_ν, I_ν^{out} is the outgoing intensity while I_ν^{in} is the incoming intensity. The optical depth at the lower boundary (in this case, the planetary surface itself) is denoted by $\tau_b(\nu)$, while t_ν is a dummy variable of integration. To proceed, we consider a non-scattering atmosphere (at LTE). Under this condition, the source function is the Planck function, and is independent of the angle parameter μ. Thus

$$S_\nu(\tau_\nu,\mu) = B_\nu[T(\tau_\nu)]$$

T is the temperature at the optical depth point τ_ν.

Since the optical depth is a function of frequency, we will rewrite the solutions above in terms of the actual physical depth scale, denoted z. Noting that here, the depth is measured DOWNWARDS, the solutions above become

$$I_\nu^{out}(z,\mu) = I_\nu^{out}(z_b,\mu) \exp\left[-\frac{\tau_b(z_b)-\tau_\nu(z)}{\mu}\right] + \int_{z=z}^{z=z_b} B_\nu[T(z)] \exp\left[-\frac{t_\nu(z)-\tau_\nu(z)}{\mu}\right] \frac{dt_\nu(z)}{\mu}$$

and

$$I_\nu^{in}(z,\mu) = -\int_{z=0}^{z=z} B_\nu[T(z)] \exp\left[-\frac{t_\nu(z)-\tau_\nu(z)}{\mu}\right] \frac{dt_\nu(z)}{\mu}$$

Z_b corresponds to the planetary surface, while Z is the position of the point at which we are evaluating the specific intensity. The flux at Z is given by the sum over all angles

$$F_\nu(z) = 2\pi \int_0^1 I_\nu^{out}(z,\mu)\mu d\mu + 2\pi \int_{-1}^0 I_\nu^{in}(z,\mu)\mu d\mu \qquad (2.2)$$

while the total flux is found by integrating F_ν over all frequencies.

These equations are not directly soluble, especially due to the large variation of opacity with frequency. To get around this frequency dependence, Pollack (1969a) devised an opacity averaging procedure, which he used in greenhouse models for Venus [Pollack (1969b)], and which has also been used in models for Jupiter [Graboske et al (1975), Bodenheimer (1976)], and Saturn [Pollack et al (1977)]. His method involves dividing the frequency range into a series of bands each of width $\Delta\nu_i$, such that the black body function $B_\nu[T]$ is effectively constant over each band; we can do this since B_ν is slowly varying at its maximum values, which contribute most to the flux. Then the total specific intensity within a band i, $I_i(Z,\mu)$, is found by integrating I_ν over the range $\Delta\nu_i$, yielding

$$I_i^{out}(z,\mu) = B_\nu[T(z_b)] \int_{\Delta\nu_i} \exp\left[-\frac{\tau_\nu(z_b)-\tau_\nu(z)}{\mu}\right] d\nu$$

$$+\int_{\Delta\nu_i}\int_{z=Z}^{z=Z_b} B_\nu[T(z)]\exp\left[-\frac{t_\nu(z)-\tau_\nu(Z)}{\mu}\right]\frac{dt_\nu}{\mu}\,d\nu \qquad (2.3)$$

[Note: For the present, we shall consider I_i^{out} only; I_i^{in} is obtained in exactly the same manner.]

Here we have assumed that the surface of the Earth is radiating as a black body, so that

$$I_\nu^{out}(Z_b,\mu) = B_\nu[T(Z_b)]$$

Defining the average optical depth τ_i within a band i by

$$\exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] \equiv \int_{\Delta\nu_i}\exp\left[-\frac{\tau_\nu(z)-\tau_\nu(Z)}{\mu}\right]\frac{d\nu}{\Delta\nu_i} \qquad (2.4)$$

equation (2.3) becomes

$$I_i^{out}(Z,\mu) = B_\nu[T(Z_b)]\exp\left[-\frac{\tau_i(Z_b,Z)}{\mu}\right]\Delta\nu_i$$

$$+\int_{z=Z}^{z=Z_b} B_\nu[T(z)]\Delta\nu_i\exp\left[-\frac{\tau_i(z,Z)}{\mu}\right]\frac{d\tau_i}{\mu}$$

By further defining

$$B_i(z) \equiv B_\nu[T(z)]\,\Delta\nu_i \qquad (2.5)$$

we can finally write

$$I_i^{out}(Z,\mu) = B_i(Z_b)\exp\left[-\frac{\tau_i(Z_b,Z)}{\mu}\right]$$

$$+\int_{z=Z}^{z=Z_b} B_i(z)\exp\left[-\frac{\tau_i(z,Z)}{\mu}\right]\frac{d\tau_i}{\mu} \qquad (2.6a)$$

and similarly

$$I_i^{in}(Z,\mu) = -\int_{z=0}^{z=Z} B_i(z) \exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] \frac{d\tau_i}{\mu} \qquad (2.6b)$$

Rewriting (2.2), the flux over each band $\Delta\nu_i$ is

$$F_i(Z) = 2\pi\int_0^1 I_i^{in}(Z,\mu)\mu d\mu \; + \; 2\pi\int_{-1}^0 I_i^{in}(Z,\mu)\mu d\mu$$

Substituting for the I_i's from (2.6) gives

$$F_i(Z) = \int_0^1 B_i(Z_b) \exp\left[-\frac{\tau_i(Z_b,Z)}{\mu}\right]\mu d\mu$$

$$+ \; 2\pi\int_{z=Z}^{z=Z_b}\int_0^1 B_i(z) \exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] d\mu \, d\tau_i$$

$$- \; 2\pi\int_{z=0}^{z=Z}\int_{-1}^0 B_i(z) \exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] d\mu \, d\tau_i$$

noting that the order of the double integral is unimportant. Since $B_i(z)$ is isotropic, it can come outside the angular integration. In addition, we have by definition

$$E_2(\tau_i) \equiv \int_0^1 e^{-\tau_i/\mu} \, d\mu$$

$$E_2(-\tau_i) \equiv \int_{-1}^0 e^{-\tau_i/\mu} \, d\mu$$

and

$$E_3(\tau_i) \equiv \int_0^1 e^{-\tau_i/\mu} \, \mu d\mu$$

where E_2 is the second exponential integral, and E_3 is the third. Approximate expressions for E_1 can be found in Abramowitz and Stegun (1964), and Mewe (1972). These expressions are given in the appendix. The recursion relation

$$E_{j+1}(\tau) = \frac{1}{j}\left[e^{-\tau} - \tau E_j(\tau)\right]$$

gives the higher exponential integrals. With these definitions, the flux integral becomes

$$\begin{aligned} F_i(\text{z}) = {} & 2\pi B_i(\text{z}_b) E_3\left[\tau_i(\text{z}_b, \text{z})\right] \\ & + 2\pi \int_{z=\text{z}}^{z=\text{z}_b} B_i(z) E_2\left[\tau_i(z,\text{z})\right] d\tau_i \\ & - 2\pi \int_{z=0}^{z=\text{z}} B_i(z) E_2\left[-\tau_i(z,\text{z})\right] d\tau_i \end{aligned} \tag{2.7}$$

The integrals in (2.7) can be solved by following a method suggested by Gingerich (1963), involving the lineri-zation of $B_i(T)$. We subdivide the range in τ_i into a series of layers over each of which B_i can be approximated as a linear function of τ_i. Consider one such layer, centred at a value of $\tau_i = \tau_i'$, and of thickness (in τ_i) of 2Δ. Then the integrals of (2.7) become a sum of integrals of the form

$$\int_{\tau_i'-\Delta}^{\tau_i'+\Delta} \left[a + b(\tau_i - \tau_i')\right] E_2(\tau_i)\, d\tau_i$$

where a and b are the

constants of the linearization of B_i. The solution of these approximate integrals are

$$\int_{\tau_i'-\Delta}^{\tau_i'+\Delta} [a + b(\tau_i - \tau_i')] E_2(\tau_i) d\tau_i = a\,\mathcal{U}(\tau_i') + b\,\mathcal{B}(\tau_i') \tag{2.8}$$

where the functions $\mathcal{U}$ and $\mathcal{B}$ are defined by

$$\mathcal{U}(\tau_i) = E_3(\tau_i'-\Delta) - E_3(\tau_i'+\Delta) \tag{2.9a}$$

$$\mathcal{B}(\tau_i) = -\Delta\left[E_3(\tau_i-\Delta) + E_3(\tau_i+\Delta)\right] - E_4(\tau_i'-\Delta) + E_4(\tau_i'+\Delta) \tag{2.9b}$$

The expressions for a and b are given by

$$a = B_i[T(\tau_i')] \quad \text{and} \quad b = \frac{dB_i[T(\tau_i')]}{d\tau_i}$$

which become

$$a = \frac{B_i[T(\tau_i'+\Delta)] + B_i[T(\tau_i'-\Delta)]}{2} \tag{2.10a}$$

and

$$b = \frac{B_i[T(\tau_i'+\Delta)] - B_i[T(\tau_i'-\Delta)]}{2\Delta} \tag{2.10b}$$

These two constants, coupled with equations (2.7), (2.8), and (2.9) enable us to compute $F(z)$, the solution to the equation of transfer, using

$$F(z) = \sum_i F_i(z) \tag{2.11}$$

2.2 TEMPERATURE CORRECTION SCHEMES

It is essential to note that equations (2.7) to (2.11) do not solve the planetary temperature structure directly in that they will only enable the computation of the flux at each point z to be performed once a temperature structure is given. Thus, we must solve the planetary atmosphere indirectly by modifying a given temperature structure until the computed flux equals the desired flux throughout the atmosphere. There are several iteration schemes available for doing this. The most powerful of these is due to Avrett and Krook (1963), but unfortunately, this scheme is not amenable to the problem at hand as it involves the manipulation of the optical depth distribution, something we cannot readily do due to the power law nature of the averaged optical depth (Section 3.1). Another scheme is the Ünsold-Lucy method [described in Mihalas (1978)], but this method was found to be too slowly converging. A simpler, and perhaps more naive approach was suggested by Pollack and Ohring (1973). This method assumes that we have a temperature distribution evaluated at several points throughout the atmosphere. These points are labelled with a subscript k. Equations (2.7) to (2.11) enable us to compute the flux F_k for the given temperature distribution T_k (note that here F_k indicates the TOTAL flux as evaluated at the sampling point k). To compute the new temperature distribution, denoted $T_{new,k}$, we assume that

$$F_k \sim T_k^4 - T_{k-1}^4$$ for $k \geq 2$, and that

$$F_{new,k} = F_k \left(\frac{\mathcal{F}_k}{F_k} \right)$$

where $\mathcal{F}_k$ is the desired flux at the sampling point k. Solving these equations gives expressions for the new temperature structure

$$T^4_{new,1} = T^4_1 \left(\frac{\mathcal{F}_1}{F_1} \right)$$

$$T^4_{new,k} = T^4_{new,k-1} + \left(T^4_k - T^4_{k-1} \right) \frac{\mathcal{F}_k}{F_k} \qquad k \geqslant 2$$

(2.12)

Since we are assuming all energy deposition occurs at the planetary surface, the atmosphere will be in radiative equilibrium (there are no sources or sinks within the atmosphere). In this case, the net outward flux is constant throughout the atmosphere, and will be equal to the black body flux escaping from the surface. Then

$$\mathcal{F}_k = \sigma T^4_{eff} \qquad \text{for all } k \qquad (2.13)$$

The effective temperatures are those given in table 1.

Simple though this method is, it is also only slowly converging (under our conditions) despite claims to the contrary by Pollack and Ohring (1973). These convergence problems led the present author to try to develop an alternative iteration scheme.

Our objective will be to approximate the atmosphere by a system of simultaneous linear equations. This idea is suggested by the linearization technique we used in solving the equation of transfer (section 2.1). Here we will extend the linearization of the Planck function to cover the entire range btween two adjacent sample points k and k+1. The sample points are defined in exactly the same manner as described above. Furthermore, we will remove all frequency dependence by considering only frequency averaged optical depths over the entire frequency band. Then, the averaged Planck function, denoted $\overline{B}_k$, is

$$\overline{B}_k = \sum_i B_i(T_k)$$

where the $B_i(T_k)$ are defined by (2.5). The sum over i indicates the sum over all wavebands i. The averaged optical depths at the sample points k, denoted $\overline{\tau}_k$, will be found in the next Section (2.3).

Consider a specific sample point, labelled ℓ ($k = \ell$). Our objective is to write the flux at ℓ, F_ℓ, as a linear equation in the $\overline{B}_k$'s, namely

$$F_\ell = \sum_{k=1}^{b} C_{\ell k} \overline{B}_k \tag{2.14}$$

where the index b refers to the surface of the planet, and marks the lower boundary sample point (k = b). It is the coefficients, $C_{\ell k}$, which we must now determine.

Each specific sample point ℓ has its own averaged optical depth distribution, $\overline{\tau}'_k$, for sample points k, related to the true distribution $\overline{\tau}_k$ by

$$\overline{\tau}'_k = \overline{\tau}_k - \overline{\tau}_\ell \qquad \text{for } k \geq \ell$$

$$\text{and} \quad \overline{\tau}'_k = \overline{\tau}_\ell - \overline{\tau}_k \qquad \text{for } k < \ell \tag{2.15}$$

where $\bar{\tau}_\ell$ is the value of $\bar{\tau}_k$ at $k = \ell$. It should be noted that $\bar{\tau}'_k$ increases not only for k increasing above ℓ, but for k decreasing below ℓ. Further, $\bar{\tau}'_\ell = 0$ as it must be according to (2.4), the definition of $\tau(z,\bar{z})$ from which the frequency averaged optical depths are calculated.

From (2.7), the flux at ℓ will be given by

$$F_\ell = 2\pi \bar{B}_b E_3(\bar{\tau}'_b) + 2\pi \sum_{k=\ell}^{b-1} \int_{\bar{\tau}'_k}^{\bar{\tau}'_{k+1}} \bar{B} E_2(\bar{\tau}) \cdot d\bar{\tau} - 2\pi \sum_{k=\ell}^{2} \int_{\bar{\tau}'_k}^{\bar{\tau}'_{k-1}} \bar{B} E_2(\bar{\tau}) d\bar{\tau} \qquad (2.16)$$

We have broken up the integrals of (2.7) into sums of integrals between two adjacent sample points. $\bar{\tau}$ is just a dummy variable of integration, while $\bar{B}$ is the frequency averaged Planck function evaluated at $T(\bar{\tau})$.

We can evaluate the integrals of (2.16) using the linearization technique given in the previous section. For k greater than ℓ, we have

$$\int_{\bar{\tau}'_k}^{\bar{\tau}'_{k+1}} \bar{B} E_2(\bar{\tau}) d\bar{\tau} \simeq \left(\frac{\bar{B}_{k+1} + \bar{B}_k}{2}\right)\left[E_3(\bar{\tau}'_k) - E_3(\bar{\tau}'_{k+1})\right] + \left(\bar{B}_{k+1} - \bar{B}_k\right)\left[\frac{E_4(\bar{\tau}'_k) - E_4(\bar{\tau}'_{k+1})}{\bar{\tau}'_{k+1} - \bar{\tau}'_k} - \frac{E_3(\bar{\tau}'_k) + E_3(\bar{\tau}'_{k+1})}{2}\right]$$

It is convenient to make the following identifications

$$x_k^+ = \frac{1}{2}\left[E_3(\bar{\tau}'_k) - E_3(\bar{\tau}'_{k+1})\right]$$

and

$$y_k^+ = \frac{E_4(\bar{\tau}_k') - E_4(\bar{\tau}_{k-1}')}{\bar{\tau}_{k+1}' - \bar{\tau}_k'} - \frac{E_3(\bar{\tau}_k') + E_3(\bar{\tau}_{k+1}')}{2}$$

in which case, the integral above can be rewritten as

$$\int_{\bar{\tau}_k'}^{\bar{\tau}_{k+1}'} \bar{B} E_2(\bar{\tau}) d\bar{\tau} \simeq \bar{B}_k (x_k^+ - y_k^+) + \bar{B}_{k+1} (x_k^+ + y_k^+) \tag{2.17}$$

Similarly, making the identifications

$$x_k^- = \tfrac{1}{2} \left[E_3(\bar{\tau}_k') - E_3(\bar{\tau}_{k-1}') \right]$$

and

$$y_k^- = \frac{E_4(\bar{\tau}_k') - E_4(\bar{\tau}_{k-1}')}{\bar{\tau}_{k-1}' - \bar{\tau}_k'} - \frac{E_3(\bar{\tau}_k') + E_3(\bar{\tau}_{k-1}')}{2}$$

the integral for $k < \ell$ in (2.16) becomes

$$\int_{\bar{\tau}_k'}^{\bar{\tau}_{k-1}'} \bar{B} E_2(\bar{\tau}) d\bar{\tau} \simeq \bar{B}_k (x_k^- - y_k^-) + \bar{B}_{k-1} (x_k^- + y_k^-) \tag{2.18}$$

Remember that in this case, $\tau_{k-1}' > \tau_k'$.

Substituting (2.17) and (2.18) into (2.16), and comparing with (2.14), the expressions for the coefficients C are found to be

$$C_{\ell 1} = -(x_2^- + y_2^-)$$

$$C_{\ell j} = -(x_j^- - y_j^- + x_{j+1}^- + y_{j+1}^-) \quad \text{for } 1 < j < \ell$$

$$C_{\ell\ell} = x_\ell^+ - y_\ell^+ - x_\ell^+ + y_\ell^+$$

$$C_{\ell k} = x_k^+ - y_k^+ + x_{k-1}^+ + y_{k-1}^+$$

$$C_{\ell b} = x_{b-1}^+ + y_{b-1}^+ + E_3(\bar{\tau}_b') \tag{2.19}$$

Two special cases occur when $\ell = 1$, and $\ell = b$. In the former case, there are no layers above, so that the downward flux is zero whence $x_k^- = y_k^- = 0$ for all k. In the latter case, there are no layers below, so that $x_k^+ = y_k^+ = 0$ for all k, and $E_3(\bar{\tau}_b') = 0.5$ (since for $\ell = b$, $\bar{\tau}_b' = 0$).

Naturally, the fluxes computed using these coefficients in (2.14) will not equal the actual fluxes F_ℓ computed by equations (2.7) to (2.11). However, we can scale the coefficients so that the flux from (2.14), denoted F_ℓ', does equal the true flux F_ℓ. This scaling factor, f_ℓ, will be given by

$$f_\ell = \frac{F_\ell}{F_\ell'} \qquad (2.20)$$

whence the system of linear equations (2.14) becomes

$$F_\ell = \sum_{k=1}^{b} f_k C_{\ell k} \bar{B}_k \qquad (2.21)$$

We wish to manipulate the temperature structure T_k so that the new values of $\bar{B}$, denoted $\bar{B}_{new,k}$, satisfy

$$\mathcal{F} = \sum_{k=1}^{b} f_k C_{\ell k} \bar{B}_{new,k} \qquad (2.22)$$

where the desired fluxes $\mathcal{F}$ are given by (2.13).

Unfortunately, the system of simultaneous linear equations (2.22) proves to be ill conditioned, providing answers which oscillate. Because of this effect, (2.22) had to be abandoned as an alternative iteration scheme. However, since (2.22) does approximate the atmosphere by a set of simple linear equations which are very much faster in computing the temperature structure than using the complete equations given in the previous section (2.1), we can use the slowly converging Pollack-Ohring scheme (2.12) by computing the itermediate steps with (2.22) rather than the complete atmosphere equations. It is this method which was adopted herinafter.

2.3 THE INITIAL TEMPERATURE DISTRIBUTION

In order to use any iteration scheme, we must first of all have an initial temperature structure which we can then modify. The grey body approximation is the ideal choice in that the temperature can be found directly from the optical depth distribution, according to

$$T_k^4 = \frac{3}{4} T_{eff}^4 \left(\bar{\tau}_k + \frac{2}{3}\right) \tag{2.23}$$

The optical depth distribution $\bar{\tau}_k$ is frequency averaged so that we can optimize on the frequency dependence of the monochromatic optical depth, and obtain a good initial temperature structure T_k. In addition, $\bar{\tau}_k$ is used in the temperature iteration scheme described in the previous section.

To determine $\bar{\tau}_k$, we note that here we are only attempting to find an approximate optical depth distribution suitable for use in determining an initial temperature structure. It is adequate to use the simple solution of the equation of transfer (obtained by putting the source function equal to zero)

$$I_\nu(k) = I_\nu(0)\, e^{-\tau_\nu}$$

where $I_\nu(k)$ is the specific intensity at the sample point k (with optical depth τ_ν), while $I_\nu(0)$ is the initial specific intensity. Integrating over frequency gives

$$\sum_i \int_{\Delta\nu_i} I_\nu(k)\, d\nu = \sum_i \int_{\Delta\nu_i} I_\nu(0)\, e^{-\tau_\nu} d\nu$$

where we have broken the frequency integral into a sum of integrals over the wavebands i. In our case, the initial specific intensity is the Planck function B_ν which is assumed to be constant over each waveband i. This gives

$$\sum_i \int_{\Delta\nu_i} I_\nu(k)\, d\nu = \sum_i B_\nu \Delta\nu_i \left[\frac{1}{\Delta\nu_i} \int_{\Delta\nu_i} e^{-\tau_\nu} d\nu \right]$$

Using the definitions for B_i (2.5) and τ_i (2.4), we get

$$\sum_i \int_{\Delta\nu_i} I_\nu(k)\, d\nu = \sum_i B_i\, e^{-\tau_i}$$

We wish to define the frequency averaged opacity $\bar{\tau}_k$ such that

$$\sum_i \int_{\Delta\nu_i} I_\nu(k)\, d\nu = \left(\sum_i B_i\right) e^{-\bar{\tau}_k}$$

which leads to

$$e^{-\bar{\tau}_k} = \frac{\sum_i B_i\, e^{-\tau_i}}{\sum_i B_i} \qquad (2.24)$$

Equation (2.24) defines the frequency averaged optical depth scale used in (2.23), and in section 2.2.

2.4 TEST FOR CONVECTION

At present, we do not take the flux carried by convection into account. However, we do at least check for the onset of convection.

A system will be stable against convection if the Schwarzschild criterion holds, namely if

$$\frac{dT}{dz} < \left(1 - \frac{1}{\gamma}\right)\frac{T}{P}\frac{dP}{dz} \tag{2.25}$$

is satisfied.

Here z is measured downwards.

To be able to apply this criterion, we must have a value for the adiabatic index γ of a gas mixture. We consider a number of gas species, labelled j, each of molecular weight M_j, fractional abundance (by number) f_j, specific heat at constant pressure $C_{P,j}$, and specific heat at constant volume $C_{V,j}$. For the gas mixture, we let C_P, and C_V be these two specific heats respectively. If N_j is the actual number of molecules j present in the sample we are considering, then the mass in kilograms of molecule j in the sample is

$$m_j = m_H M_j N_j$$

while the total mass in the sample will be

$$m = m_H \sum_j M_j N_j$$

and m_H is the mass of the amu (atomic mass unit).

The molecular abundance N_j is related to the total number N of molecules in the sample by

$$N_j = f_j N$$

From the definition of specific heat, we have

$$m C_P = \sum_j m_j C_{P,j}$$

and

$$m C_V = \sum_j m_j C_{V,j}$$

Now γ is defined by

$$\gamma = \frac{m C_P}{m C_V}$$

and on substitution of the above variables, we get

$$\gamma = \frac{\sum_j M_j f_j C_{P,j}}{\sum_j M_j f_j C_{V,j}} \qquad (2.26)$$

Using (2.25) and (2.26), we can now find the point of onset of convection for an arbitary gas mixture.

Chapter 3

THE CHARACTERS

3.1 POWER LAW FORMULATION OF THE OPTICAL DEPTH

As it is presently formulated, the average optical depth as defined by (2.4) is of little use. We wish to remove the frequency dependence of (2.4) so that the average optical depth has some meaning. We further wish to reduce (2.4) to an analytic form so that at some given temperature, pressure, and column density, we can readily calculate τ_i without having to deal with the multitudinous values of the monochromatic optical depth τ_ν. In this regard, both Pollack (1969b) and Bartko and Hanel (1968) state that, at least for CO_2 and H_2O, τ_i can be evaluated by a power law. To obtain this power law, we follow Pollack (1969b). For paths at constant pressure P and column density W, we write

$$\tau_i \simeq c_i P^{s_i} W^{r_i}$$

The parameters r_i, s_i, and c_i seem to change only very slowly with large changes in P and W, and thus they can be considered as constants over each of a series of regimes of P and W. In addition, if the various paths, each at a fixed constant temperature T, imply that

$$\tau_i \sim G_i(T)$$

where G_i is some function of T within the waveband i, then the definition for τ_i is

$$\tau_i \simeq c_i W^{r_i} P^{s_i} G_i(T) \tag{3.1}$$

The total column density is defined by equation (1.3).

Equation (3.1) is valid only for paths of constant pressure and temperature (and hence column density), so we must generalize it to the non-constant pressure-temperature paths found in real atmospheres. To do this, we return to basic principles.

The molecular line absorption coefficient α_ℓ can be described by four parameters: the line position ν_ℓ, the line intensity S_ℓ, the line half width $\delta\nu_\ell$, and the line shape function $b(\nu-\nu_\ell, \delta\nu_\ell)$, such that

$$\alpha_\ell(\nu) = S_\ell b(\nu-\nu_\ell, \delta\nu_\ell)$$

for each line ℓ.

Since Doppler broadening is negigible at the low temperatures with with we are dealing, we can use the pressure broadened Lorentz profile for $b(\nu-\nu_\ell, \delta\nu_\ell)$ giving

$$\alpha_\ell(\nu) = \frac{S_\ell}{\pi} \frac{\delta\nu_\ell}{(\nu-\nu_\ell)^2 + \delta\nu_\ell^2}$$

for each line ℓ.

The $\delta\nu_\ell$ behaviour of the Lorentz line shape is such that

$$\frac{\delta\nu_\ell}{(\nu-\nu_\ell)^2 + \delta\nu_\ell^2} \sim \left[\delta\nu_\ell\right]^{-1} \quad \text{for} \quad \nu = \nu_\ell$$

$$\sim \left[\delta\nu_\ell\right]^{+1} \quad \text{for} \quad \nu \neq \nu_\ell$$

which suggests writing the Lorentz profile as a power law in $\delta\nu_\ell$: noting that $P \sim \delta\nu_\ell$ and $G'_\nu(T) \sim S_\ell\,\delta\nu_\ell$ for some function of temperature $G'_\nu(T)$, we write

$$\alpha_\ell(\nu) = K'(\nu)\, G'_\nu(T)\, P^{q'_\nu}$$

where $K'(\nu)$ includes all the constants and frequency dependence outside $P^{q'_\nu}$ and $G'_\nu(T)$, while the exponent q'_ν itself is a function of frequency.

Now, the total line absorption coefficient is the sum of the individual coefficients for each line

$$\alpha(\nu) = \sum_\ell \alpha_\ell(\nu)$$

However, if the lines are sufficiently far apart (that is, there is negligible overlap), then the sum over lines can be replaced by

$$\alpha(\nu) = K(\nu)\, G_\nu(T)\, P^{q_\nu}$$

where now $K(\nu)$, $G_\nu(T)$, and q_ν are functions of the entire spectrum rather than of just one line.

The monochromatic optical depth is given by

$$\tau_\nu = \int_0^z \rho \kappa_\nu \, dz$$

where κ_ν, the total mass absorption coefficient, is related to the total line absorption coefficient by

$$\rho \kappa_\nu = n\alpha(\nu)$$

Recalling (1.3)

$$dW = \frac{\rho}{m_H M}\, dz$$

and noting that the relation between mass density and number density is

$$\rho = n m_H M$$

we can write for τ_ν

$$\tau_\nu = \int_{z=0}^{z=Z} K(\nu) P^{q_\nu} G_\nu(T) dW \qquad (3.2)$$

on substituting the expression for $\alpha(\nu)$. Substituting (3.2) into (2.4) and subtracting the integrals within the exponential results in

$$\exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] = \int_{\Delta\nu_i} \exp\left[-\frac{1}{\mu}\int_{z=Z}^{z} K(\nu) P^{q_\nu} G_\nu(T) dW\right] \frac{d\nu}{\Delta\nu_i} \qquad (3.3)$$

We can always find an average value $\bar{q}$ of q_ν and an average value $G_i'(T)$ of $G_\nu(T)$ such that the expression

$$\exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] = \int_{\Delta\nu_i} \exp\left[-\frac{1}{\mu}\int_{z=Z}^{z} K(\nu) P^{\bar{q}} G_i'(T) dW\right] \frac{d\nu}{\Delta\nu_i} \qquad (3.4)$$

is valid over the band $\Delta\nu_i$.

We need to eliminate the frequency integration in (3.4) for the average optical depth to have any use. To do this, we note that we already have an expression for τ_i, at least for constant pressure-temperature paths, namely equation (3.1). Substituting (3.1) into (3.4) yields

$$\exp\left[-\frac{c_i \Delta W^{r_i} P^{s_i} G_i(T)}{\mu}\right] = \int_{\Delta\nu_i} \exp\left[-\frac{K(\nu) P^{\bar{q}} G_i'(T) \Delta W}{\mu}\right] \frac{d\nu}{\Delta\nu_i} \qquad (3.5)$$

where we have put $\Delta W = W(z) - W(\bar{z})$. In this constant pressure-temperature case, both $P^{\bar{q}}$ and $G_i'(T)$ are constants with respect to W ($K(\nu)$ is already a constant with respect to W) and can be taken out of the W integral in (3.4). Neither P, ΔW, or $G_i'(T)$ depend on frequency, but they cannot be taken outside the frequency dependence as they are bound up through the exponential. However, the effect of the frequency integration is to form an r_i power dependence of the frequency integrand. This power dependence is more explicit by writing the left hand side of (3.5) as

$$\exp\left[\Delta W^{r_i} P^{s_i} G_i(T)\right] = \exp\left[\left\{\Delta W P^{s_i/r_i} G_i^{1/r_i}(T)\right\}^{r_i}\right]$$

By identifying s_i/r_i as $\bar{q}$, and G_i^{1/r_i} as G_i', the equation above can be rewritten as

$$\exp\left[\Delta W^{r_i} P^{s_i} G_i(T)\right] = \exp\left[\left\{\Delta W P^{\bar{q}} G_i'(T)\right\}^{r_i}\right]$$

where the similarity of the right hand side to the frequency integrand of (3.5) is quite apparent. The power law effect can be completed by identifying c_i with the rest of the frequency integration (which doesn't depend on pressure or temperature). The angular dependence of (3.5) is apparently unaffected by the frequency integration as $1/\mu$ appears unchanged on both sides of (3.5).

We assume that this power law effect still holds in the non-constant pressure-temperature case, so that the frequency dependent part of (3.4) leads to

$$\exp\left[-\frac{\tau_i(z,Z)}{\mu}\right] = \exp\left[-\frac{c_i}{\mu}\left(\int_{z=Z}^{z} P^{\bar{q}}\, G_i'(T)\, dW\right)^{r_i}\right]$$

Substituting back for $\bar{q}$ and $G_i'(T)$, yields, on taking logarithms

$$\tau_i(z,Z) = c_i\left(\int_{z=Z}^{z} P^{s_i/r_i}\, G_i^{1/r_i}(T)\, dW\right)^{r_i}$$

This equation is only valid for one gas species. However, if there is no interconnection between the lines of the various gas species, or if the opacity from one species is dominant, we can simply write the total optical depth as the sum of the individual ones, thus

$$\tau_i(z,Z) = \sum_{j=1}^{J} c_{ij}\left(\int_{z=Z}^{z} P^{s_{ij}/r_{ij}}\, G_{ij}^{1/r_{ij}}(T)\, dW\right)^{r_{ij}} \tag{3.6}$$

where the index j refers to the particular molecule.

Similarly, when we are moving up through the atmosphere, the optical depth is given by

$$\tau_i(Z,z) = -\tau_i(z,Z) = \sum_{j=1}^{J} c_{ij}\left(\int_{z=0}^{Z} P^{s_{ij}/r_{ij}}\, G_{ij}^{1/r_{ij}}\, dW\right)^{r_{ij}} \tag{3.7}$$

for $z < Z$.

Equations (3.6) and (3.7) give the power law optical depth for all points within the atmosphere with respect to a given point Z. We must now determine the parameters c_{ij}, r_{ij}, s_{ij} and $G_{ij}(T)$ of these equations for the various molecules j under consideration.

3.2 CARBON DIOXIDE, WATER AND NITROGEN

Pollack (1969b) gives the parameters for the three molecules CO_2, H_2O and N_2. While r_{ij}, s_{ij} and $G_{ij}(T)$ are dimensionless, c_{ij} is not for its values depend on the units chosen for P and W. The data of Pollack are applicable for P in atm, while W has the units of atm-cm for CO_2, precipitable cm for H_2O, and 1.11 atm for N_2. For the sake of convenience in computing, and comparison, we will convert c_{ij} to use the SI units of P in kpa and W in kpa-m. The relative conversion factors are listed in Table 5

Table 5

Conversion Factors

CO_2 column density unit:	1 atm-cm	=	1.01325 kpa-m
H_2O column density unit:	1 pr. cm	=	1261.0 kpa-m
N_2 column density unit:	1.11 atm	=	9.79(5) kpa-m
pressure unit :	1 atm	=	101.325 kpa
column density unit :	1 kpa-m	=	2.6517(23) molecules/m

To convert the units of c_{ij}, we must consider the definition of τ_i. We need only look at the constant pressure-temperature case (3.1). Because τ_i is dimensionless, it will be unaffected by the change in units; denoting the new units by a prime, we can put

$$c_i W^{r_i} P^{s_i} = c_i' W'^{r_i} P'^{s_i} \qquad (3.8)$$

$G_i(T)$ is dimensionless, and doesn't enter into (3.8). This equation yields

$$c_i' = c_i \left(\frac{W}{W'}\right)^{r_i} \left(\frac{P}{P'}\right)^{s_i}$$

With this equation, and the conversion factors of table 5, Pollack's data can be reduced to common units; these data are presented in Tables 7, 8, and 9. Table 6 contains the information relevent to the wavebands under study, including the blackbody constants required by equations (2.7) and (2.10). These constants are defined by

$$C_i = \frac{2h\bar{\nu}_i^3}{c^2} \Delta\nu_i$$

$$D_i = \frac{h}{k} \bar{\nu}_i \qquad (3.9)$$

so that the black body flux is simply

$$B_i = B_{\bar{\nu}}[T(\tau_{\bar{\nu}})] \Delta\nu_i = \frac{C_i}{\exp[D_i/T] - 1}$$

The data contained in Tables 7 to 13 include two sets of constants for equations (3.6) and (3.7). The first set is applicable in the regime where the optical depth is small, whereas the second set is applicable for the large optical depth regime. To ensure that the optical depth changes smoothly in crossing between the two regimes, we will use a linear weighting technique. Defining the limits of the changeover regime by τ_{chg} and τ_{rge}, the weighted optical depth is given by

$$\tau_i = (1-x)\tau_i(1) + x\tau_i(2)$$

where

$$x = \frac{\tau_i(1) - \tau_{chg}}{\tau_{rge} - \tau_{chg}}$$

while $\tau_i(1)$ is the optical depth calculated by the first regime constants, and $\tau_i(2)$ is that calculated by the second regime constants. The values for τ_{chg} and τ_{rge} are given in the Tables (7 to 13).

Table 6

Waveband Parameters

BAND	WAVELENGTH INTERVAL (μm)	FREQUENCY INT. (10^{12} Hz)	$\Delta\nu_i$ (10^{12} Hz)	C_i ($Jm^{-2}s^{-1}$)	D_i ($°K^{-1}$)
1	50.00 - 100.00	3.0 - 6.0	3.0	4.031(0)	2.160(2)
2	29.41 - 50.00	6.0 - 10.2	4.2	3.292(1)	3.887(2)
3	17.39 - 29.41	10.2 - 17.2	7.0	2.654(2)	6.575(2)
4	12.90 - 17.39	17.2 - 23.2	6.0	7.292(2)	9.695(2)
5	8.89 - 12.90	23.2 - 33.7	10.5	3.584(3)	1.368(3)
6	7.55 - 8.89	33.7 - 39.7	6.0	4.373(3)	1.761(3)
7	5.63 - 7.55	39.7 - 53.2	13.5	2.001(4)	2.232(3)
8	4.82 - 5.63	53.2 - 62.2	9.0	2.549(4)	2.769(3)
9	3.88 - 4.82	62.2 - 77.3	15.1	7.572(4)	3.350(3)
10	3.42 - 3.88	77.3 - 87.7	10.4	8.611(4)	3.960(3)
11	2.92 - 3.42	87.7 - 102.7	15.0	1.908(5)	4.569(3)
12	2.58 - 2.92	102.7 - 116.2	13.5	2.614(5)	5.255(3)
13	2.09 - 2.58	116.2 - 143.4	27.2	8.771(5)	6.230(3)

A lack of temperature information prevented Pollack from determining the temperature dependence function $G_i(T)$ for

Table 7

CO_2 Parameters for (3.6) and (3.7)

BAND	Low Optical Depth			τ_{chg}	τ_{rge}	High Optical Depth		
	r_i	s_i	c_i			r_i	s_i	c_i
4	.331	.235	1.22 (-1)	2	4	.312	.205	1.83 (-1)
5	.610	.358	5.45 (-4)	*				
6	.856	.863	2.37 (-8)	2	5	.816	.783	7.13 (-8)
7	.737	.769	2.26 (-7)	2	5	.702	.697	6.06 (-7)
8	.584	.330	4.43 (-4)	2	5	.405	.462	1.25 (-3)
9	.331	.322	2.90 (-2)	2	3	.508	.270	1.08 (-2)
10	.561	.570	8.49 (-5)	*				
11	.739	.714	7.98 (-7)	*				
12	.230	.172	1.10 (-1)	2	3	.292	.149	7.76 (-2)
13	.380	.368	3.15 (-4)	2	3	.558	.314	4.12 (-5)

Note (*): Data is not given for the high τ_i range, so we must use the low τ_i constants.

Table 8

H_2O parameters for (3.6) and (3.7)

BAND	Low Optical Depth			τ_{chg}	τ_{rge}	High Optical Depth		
	r_i	s_i	c_i			r_i	s_i	c_i
1	.497	.540	6.87 (-2)	2	3	.576	.450	1.08 (-1)
2	.497	.540	4.36 (-2)	2	6	.576	.450	1.10 (-2)
3	.562	.427	1.17 (-2)	*				
4	.439	.307	1.68 (-2)	*				
5	.859	.859	5.87 (-6)	*				
6	.561	.464	7.80 (-4)	2	3	.572	.453	7.53 (-4)
7	.494	.414	2.51 (-2)	2	10	.352	.447	3.88 (-2)
8	.482	.405	1.08 (-2)	2	6	.424	.427	1.35 (-2)
9	.608	.542	1.41 (-4)	2	3	.667	.500	9.59 (-5)
10	.789	.556	2.19 (-5)	#				
11	.527	.444	3.06 (-3)	2	6	.467	.455	4.46 (-3)
12	.490	.406	3.08 (-4)	2	6	.392	.416	4.42 (-2)
13	.548	.405	9.05 (-4)	#				

Note (*): Data is not given for the high τ_i regime, so low regime data is used.
(#): The difference between the two regimes is negigible.

these molecules. We must assume that it is constant; this constant is included in c_i.

Table 9

N_2 Parameters for (3.6) and (3.7)

BAND	r_i	s_i	c_i
1	.997	.997	4.47 (-9)
2	.974	.974	4.43 (-9)
3	.741	.741	8.49 (-8)
9	.712	.712	2.96 (-8)

3.3 AMMONIA

The mean transmission of NH_3 within a band of frequency width $\Delta\nu$ is given by [Gille and Lee (1969)]

$$\overline{T} = \exp(-\tau_\nu) = \exp\left[-\frac{2\pi y u}{\sqrt{2u+1}}\right] \tag{3.10}$$

where

$$u = \frac{W}{8P_e(300/T)^{5/6}}\left[\frac{\sum s_i(T)}{\sum[s_i(T)\alpha_{oi}(300)]^{1/2}}\right]^2$$

and

$$y = \frac{4P_e(300/T)^{5/6}}{\pi\,\Delta\nu}\;\frac{\left(\sum[s_i(T)\alpha_{oi}(300)]^{1/2}\right)^2}{\sum s_i(T)}$$

In these expressions, the column density W is in atm-cm, while the frequency bandwidth $\Delta\nu$ is in cm^{-1}. P_e is an effective pressure taking into account the line broadening, and is in atm. While the average optical depth will be calculated with these parameters in SI units, it is more convenient to use them in (3.10) with the above dimensions as the parameters $\sum S_i$ and $\sum [S_i \alpha_{oi}]^{1/2}$, given in Gille and Lee (1969), are in these non-SI units. With the presence of hydrogen and helium, P_e can be obtained from

$$P_e = P_{NH_3} + \frac{P_{H_2}}{7.9} + \frac{P_{He}}{11.7} \qquad (3.11)$$

where P_{NH_3}, P_{H_2} and P_{He} are the partial pressures of NH_3, H_2 and He respectively.

The average optical depth, as defined by (2.4), is

$$\exp(-\tau_i) = \frac{1}{\Delta\nu_i} \int_{\Delta\nu_i} e^{-\tau_\nu} d\nu$$

However, the τ_ν as defined in (3.10) are already evaluated over a band of width $\Delta\nu_j$. Denoting these values of τ_ν by τ_j, the definition for τ_i becomes

$$\exp(-\tau_i) = \frac{1}{\Delta\nu_i} \sum_{j=1}^{J} \Delta\nu_j \exp[-\tau_j]$$

where J is the number of sub-bands contained within $\Delta\nu_i$.

For a given temperature, the dependence of u and y is such that

$$u \sim \frac{W}{P_e}$$

and

$$y \sim P_e$$

For optically thick lines, $u \gg 1$, for which the pressure-column density dependence of (3.10) reduces to

$$\tau_i = \frac{2\pi y u}{\sqrt{2u+1}} \simeq 2\pi y\sqrt{u} \sim P_e^{1/2} W^{1/2}$$

This result strengthens the idea of converting the ammonia optical depth into a power law expression in P and W. To obtain these opacity parameters, we need only consider the constant pressure-temperature case given by (3.1)

$$\tau_i = c_i P^{s_i} W^{r_i} G_i(T)$$

We shall also choose a power law function for the temperature dependent part so that

$$G_i(T) = T^{t_i}$$

where t_i is to be determined.

With this temperature dependence, and noting that τ_i is actually proportional to P_e, the optical depth equation becomes

$$\tau_i = c_i P_e^{s_i} W^{r_i} T^{t_i} \tag{3.12}$$

For four pairs of values of P_e and W (Pe_1, W_1; Pe_2, W_2; Pe_3, W_3; and Pe_4, W_4) at some given temperature, we can calculate the optical depths from (3.10) obtaining the values τ_i^1, τ_i^2, τ_i^3, and τ_i^4 repectively for the four pairs. Using these values in (3.12), we get four equations in the unknowns which can be solved yielding

$$s_i = \frac{\ln\left(\frac{W_4}{W_3}\right)\ln\left(\frac{\tau_i^2}{\tau_i^1}\right) - \ln\left(\frac{W_2}{W_1}\right)\ln\left(\frac{\tau_i^4}{\tau_i^3}\right)}{\ln\left(\frac{W_4}{W_3}\right)\ln\left(\frac{Pe_2}{Pe_1}\right) - \ln\left(\frac{W_2}{W_1}\right)\ln\left(\frac{Pe_4}{Pe_3}\right)}$$

and

$$r_i = \frac{\ln\left(\frac{Pe_4}{Pe_3}\right)\ln\left(\frac{\tau_i^2}{\tau_i^1}\right) - \ln\left(\frac{Pe_2}{Pe_1}\right)\ln\left(\frac{\tau_i^4}{\tau_i^3}\right)}{\ln\left(\frac{W_2}{W_1}\right)\ln\left(\frac{Pe_4}{Pe_3}\right) - \ln\left(\frac{W_4}{W_3}\right)\ln\left(\frac{Pe_2}{Pe_1}\right)}$$

Now repeating the above, this time with a particular given value of P_e, and of W, (3.10) gives us two optical depths τ_i^5, and τ_i^6 for two given values of temperature, T_1 and T_2 respectively. Using these new values in (3.12), the resulting equations can be solved, yielding

$$t_i = \frac{\ln\left(\frac{\tau_i^6}{\tau_i^5}\right)}{\ln\left(\frac{T_2}{T_1}\right)}$$

and

$$c_i = \frac{\tau_i^6}{P_e^{s_i} W^{r_i} T_2^{t_i}}$$

With this method, and the above equations, we can now obtain the ammonia power law parameters; the results are listed in Table 10.

Table 10

NH_3 parameters for (3.6) and (3.7)

BAND	Low Optical Depth r_i	s_i	t_i	c_i	τ_{chg}	τ_{rge}	High Optical Depth r_i	s_i	t_i	c_i
1	.526	.472	.186	4.14(- 2)	2	4	.487	.488	.234	4.04(- 2)
2	.442	.386	2.773	7.43(- 9)	1.5	2.5	.420	.188	4.060	7.09(-12)
3	.735	.263	4.290	3.22(-14)	1	2	.784	.105	4.730	3.38(-15)
4	.480	.359	1.870	6.45(- 7)	1	2	.289	.256	1.740	6.03(- 6)
5	.429	.442	-.469	2.41	2	3	.387	.387	-.528	4.02
6	.313	.319	1.330	4.39(- 5)	.7	2	.189	.095	2.070	2.50(- 6)

Note: For band 5, the negative temperature dependence is real for the optical depth decreases with increasing temperature.

3.4 METHANE

Pollack (1973) gives the methane absorption coefficient in units of cm^5 per $mole^2$; this is readily converted into m^5 per $mole^2$ by

$$A_\nu\,(m^5\ mole^{-2}) = A'_\nu\,(cm^5\ mole^{-2}) \times 10^{-10}$$

A_ν is plotted in Figure 1.

The optical depth is given by

$$\tau_\nu = \left(\frac{n}{A_0}\right)^2 A_\nu\,\Delta z$$

where A_0 is Avogadro's number, and Δz is the thickness of the atmosphere through which we are measuring τ_ν. Recalling from the perfect gas law that

$$P = nkT$$

and by definition

$$\Delta W = n\,\Delta z$$

we can rewrite the above as

$$\tau_\nu = \frac{P}{kT}\,\frac{A_\nu}{A_0}\,\Delta W$$

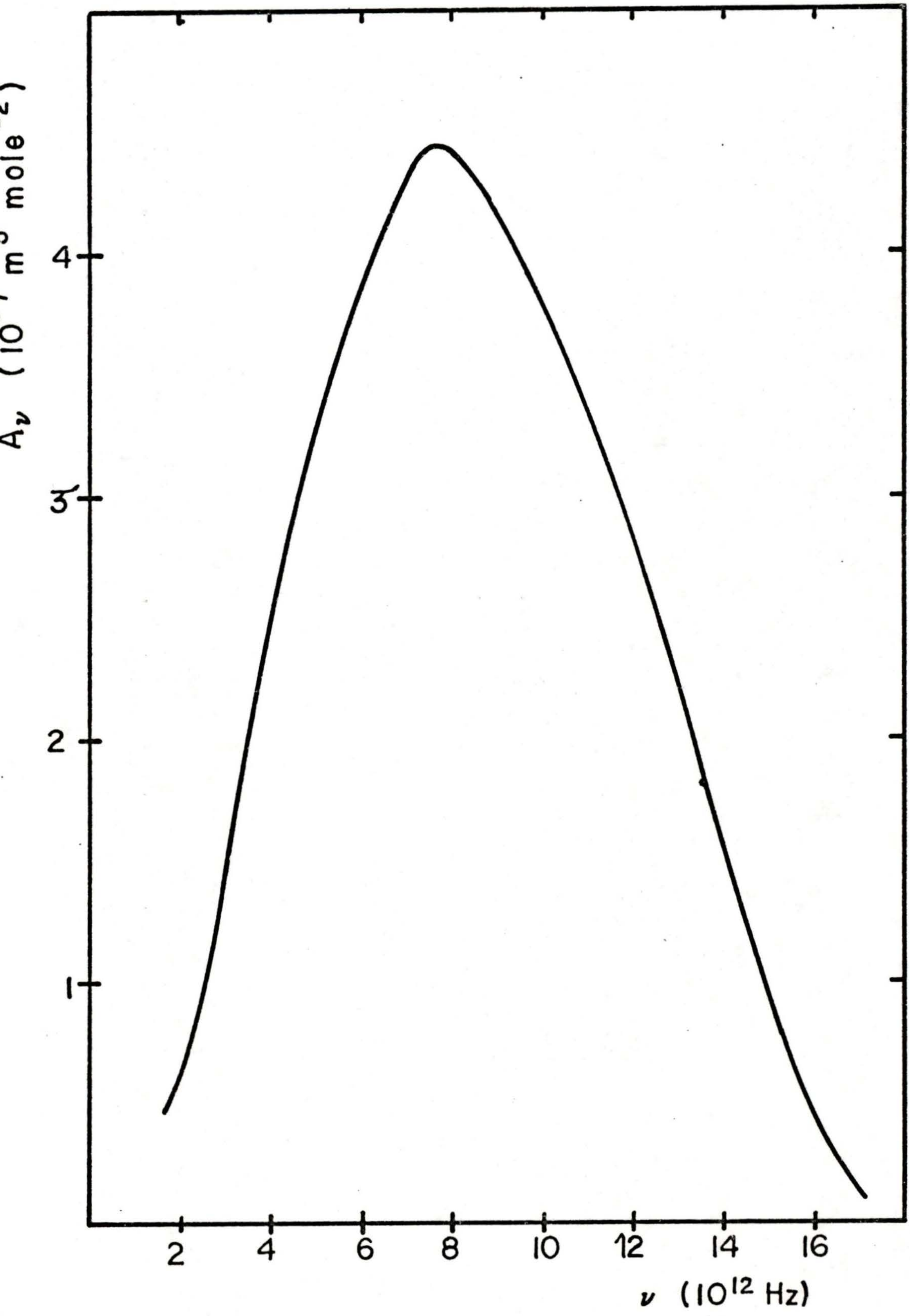
The column density is in the units of molecules per m^2. Using the conversion of ΔW to kpa-m from Table 5, and substituting for A_0 and k, the optical depth equation becomes

$$\tau_\nu = 52.94\,\frac{P}{T}\,A_\nu\,\Delta W$$

for P in kpa and ΔW in kpa-m. A_ν is found from Figure 1.

The CH_4-H_2 pressure induced opacity, according to Pollack (1973), is about 10% of the pure CH_4 opacity. Including

Figure 1: The Methane Absorption Coefficient.
Data from Pollack (1973).



A_ν (10^{-7} m^5 mole^{-2})
1
2
3
4
2
4
6
8
10
12
14
16
ν (10^{12} Hz)

this pressure induced term, the optical depth is finally given by

$$\tau_\nu = 58 \cdot 2 \frac{P}{T} A_\nu \Delta W$$

Substituting for τ_ν in (2.4), the definition of the average depth yields

$$\exp\left[-\tau_i\right] = \frac{1}{\Delta\nu_i} \int_{\Delta\nu_i} \exp\left[-58 \cdot 2 \frac{P}{T} A_\nu \Delta W\right] d\nu \qquad (3.13)$$

The simple dependence of (3.13) on pressure, temperature, and column density suggests setting $r_i = s_i = 1$ and $t_i = -1$ in the power law expression (3.12), leaving only c_i to be determined. We unfortunately do not have enough data to be able to find any dependence of A_ν on pressure and temperature, and thus must assume it to be constant.

Solving (3.13) with A_ν determined from Figure 1 gives us the values for c_i; the final parameters for CH_4 are given in Table 11.

Table 11

CH_4 Parameters for (3.6) and (3.7)

BAND	r_i	s_i	t_i	c_i
1	1	1	-1	1.60 (-5)
2	1	1	-1	2.43 (-5)
3	1	1	-1	9.00 (-6)

3.5 HYDROGEN

The monochromatic optical depth due to hydrogen is given by [Trafton (1967)]

$$\tau_\nu(z_2) - \tau_\nu(z_1) = \frac{1}{c}\int_{z_1}^{z_2} n^2 A_\nu(T)\, dz$$

where $A_\nu(T)$ is the absorption coefficient. Substituting for n using the perfect gas law

$$P = nkT$$

and the definition of the column density

$$dW = n dz$$

the optical depth equation becomes

$$\tau_\nu(z_2) - \tau_\nu(z_1) = \frac{1}{c}\int_{z_1}^{z_2} \frac{1}{k}\frac{P}{T} A_\nu(T)\, dW \qquad (3.14)$$

The simplicity of this equation suggests that we write the average optical depth in the same form, namely

$$\tau_i(z_2, z_1) = \int_{z_1}^{z_2} \frac{P}{T} A_i(T)\, dW \qquad (3.15)$$

Comparing (3.15) with (3.6) immediately enables us to put $r_i = 1$ and $s_i = 1$. Then $A_i(T)$ can be identified with $c_i G_i(T)$. We must now determine A_i.

To do this, we substitute (3.14) into (2.4), the definition of τ_i, obtaining

$$\exp\left[-\tau_i(z_2,z_1)\right] = \frac{1}{\Delta\nu_i}\int_{\Delta\nu_i} \exp\left[-\frac{1}{c}\int_{z_1}^{z_2} \frac{1}{k}\frac{P}{T} A_\nu(T)\,dW\right]d\nu \qquad (3.16)$$

To perform the inner integration, it is preferable to write dW in terms of the pressure change dP between z_1 and z_2. We already have such a relation, namely equation (1.4)

$$dW = 6.1409 \times 10^{28}\ \frac{dP}{M} \qquad (1.4)$$

Noting that the molecular weight of H_2 is 2.016, we substitute for dW in (3.16) obtaining

$$\exp\left[-\tau_i(z_2,z_1)\right] = \frac{1}{\Delta\nu_i}\int_{\Delta\nu_i} \exp\left[-7.3593\times10^{45}\int_{z_1}^{z_2} \frac{P}{T} A_\nu(T)\,dP\right]d\nu$$

We have substituted for the constants c and k, and have converted P to be measured in kpa. For constant temperature paths between P_1 (at z_1) and P_2 (at z_2), the inner integral of the above equation can be evaluated, yielding

$$\exp\left[-\tau_i(z_2,z_1)\right] = \frac{1}{\Delta\nu_i}\int_{\Delta\nu_i} \exp\left[-3.6797\times10^{45}\ \frac{A_\nu(T)}{T}\left(P_2^2 - P_1^2\right)\right]d\nu \qquad (3.17)$$

We can now calculate the average optical depth τ_i for a series of pressures and temperatures, solving the integral of (3.17) with Simpson's Rule. From these τ_i's, (3.15) will then enable us to compute the A_i's, and hence determine $c_i G_i$ for the pressure-temperature series. It is also convenient to substitute for dW in (3.15) and integrate, giving

$$\tau_i(z_2, z_1) = 5.7437 \times 10^4 \frac{A_i(T)}{T} (P_2^2 - P_1^2) \qquad (3.18)$$

The constants were chosen such that P is in kpa while W is in kpa-m.

However, to compute A_i, we must have values for $A_\nu(T)$. This particular parameter is actually composed of three parts, one translational, one rotational-translational (RT), and one vibrational- rotational-translational (VRT). Trafton (1966) graphically gives the translational part for temperatures of 300 K and 600 K as shown in Figure 2, while Linsky (1969) gives the RT part for a temperature of 300 K (Figure 3). For temperatures greater than 600 K, Linsky has given least squares fitted algebraic expressions for the RT and the VRT parts of A_ν. Unfortunately, we do not have any data for the VRT part at 300 K, and hence we must use Linsky's expression in this regime. Doubtless this introduces error, but since the VRT expression is valid over the widest range of temperture, we can tolerate this error. Furthermore, the VRT opacity occurs in the highest frequency bands through which the flux, at atmospheric temperatures, is not particularly dominant. Using these expressions, and the data of Figures 2 and 3, the total absorption coefficient $A_\nu(T)$ for 300 K and for 600 K is shown in Figure 4.

With these A_ν's, we can obtain the A_i's for the two temperatures (300 K and 600 K) using (3.17) and (3.18) as described above. To obtain $A_i(T)$ for temperatues other than these values, we will use linear interpolation

$$A_i(T) = m_i T + b_i$$

The parameters m_i and b_i are given by

$$m_i = \frac{A_i(600\,K) - A_i(300K)}{300}$$

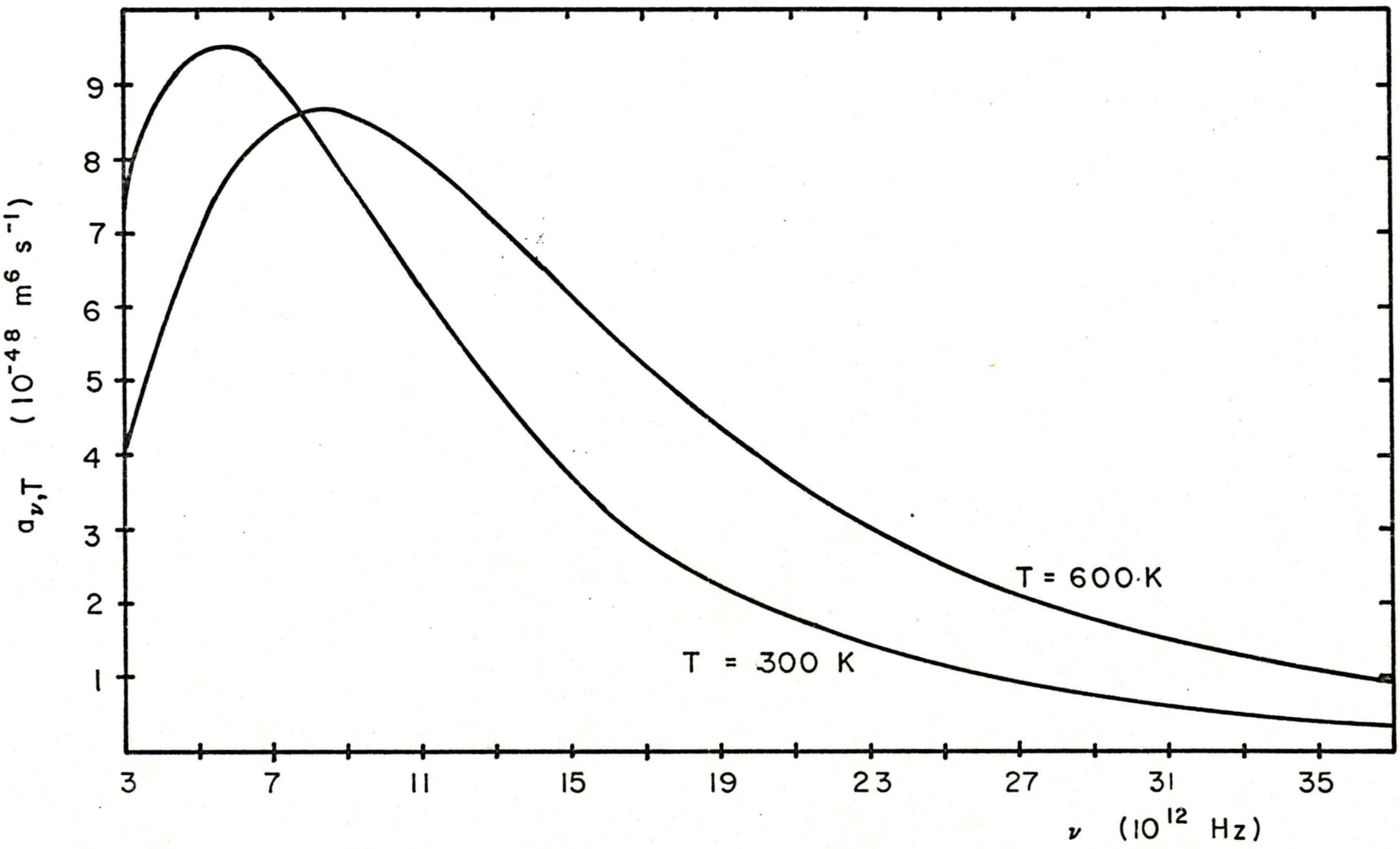
and

$$b_i = A_i(300K) - 300m_i$$

The values for m_i and b_i are given in Table 12.

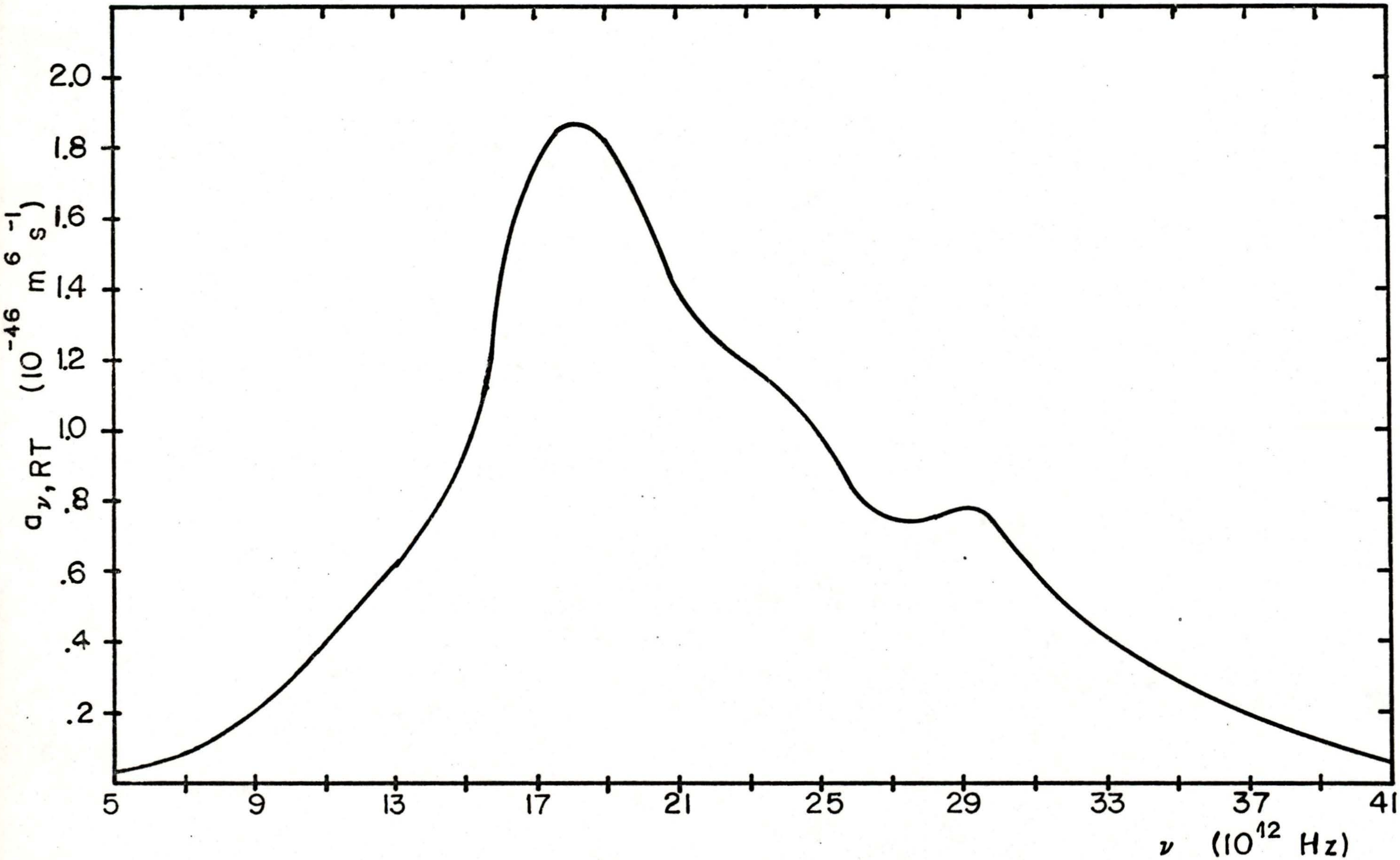
A_i is also a slowly varying function of pressure and column density. We can take some of this pressure dependence into account by dividing the opacity into two regimes as was done before.

Figure 2: Translational Absorbtion Coefficient for H_2 at 300 K and 600 K.
Data from Trafton (1966).



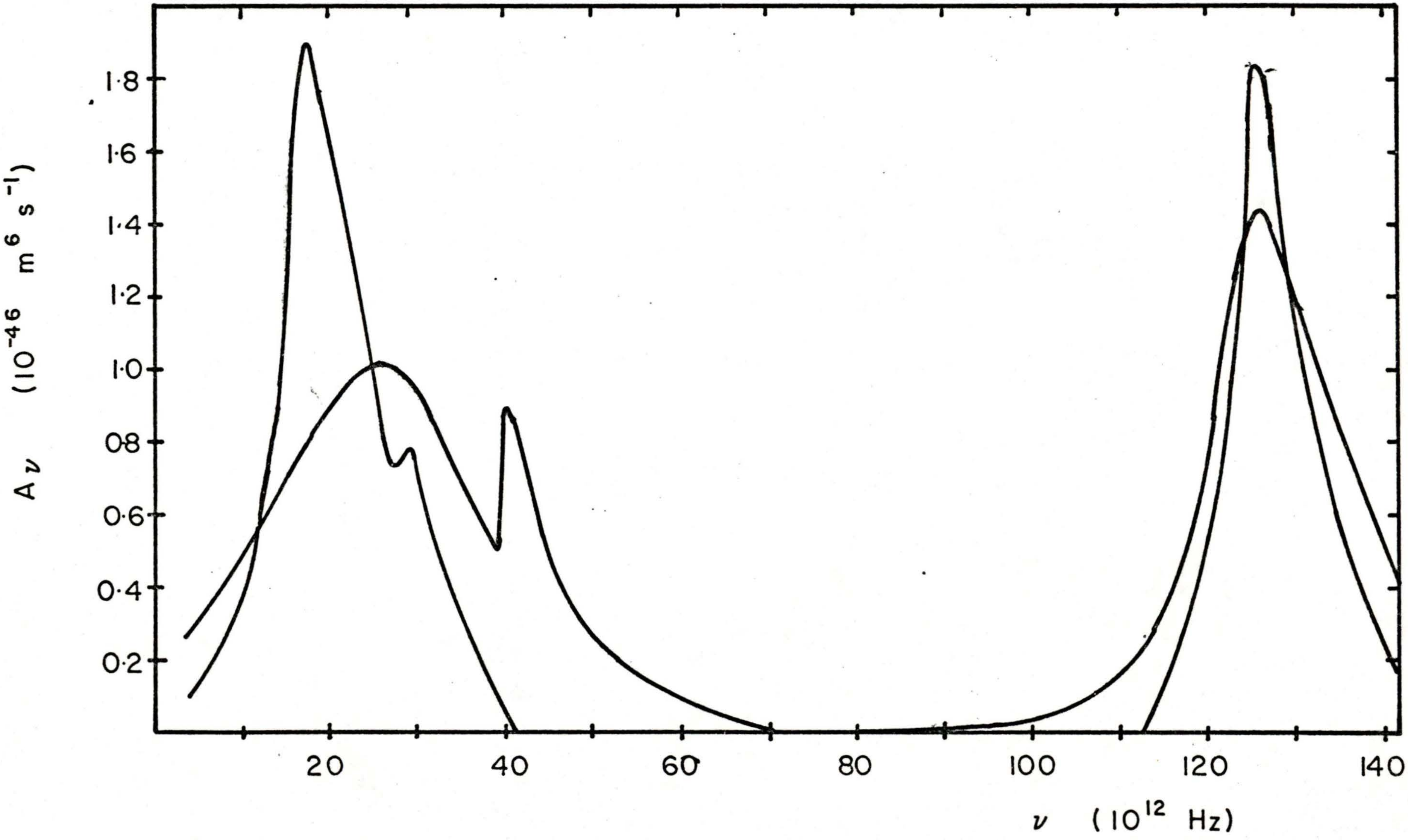
9
8
7
6
5
4
3
2
1
$a_{\nu,T}$ (10^{-48} m^6 s^{-1})
T = 600 K
T = 300 K
3
7
11
15
19
23
27
31
35
ν (10^{12} Hz)

Figure 3: Rotational-Translational Absorbtion Coefficient for H_2 at 300 K.
Data from Linsky (1969).



2.0
1.8
1.6
1.4
1.2
1.0
.8
.6
.4
.2
$a_{\nu,RT}$ $(10^{-46}\ m^6\ s^{-1})$
5
9
13
17
21
25
29
33
37
41
ν $(10^{12}$ Hz)

Figure 4: Total H_2 Absorption Coefficient at 300 K and 600 K.
Obtained from Linsky's and Trafton's data, and Linsky's algebraic expressions.



1·8
1·6
1·4
1·2
1·0
0·8
0·6
0·4
0·2
Aν (10⁻⁴⁶ m⁶ s⁻¹)
20
40
60
80
100
120
140
ν (10¹² Hz)

Table 12

H_2 Parameters for (3.6) and (3.7)

BAND	Low Optical Depth m_i	Low Optical Depth b_i	τ_{chg}	τ_{rge}	High Optical Depth m_i	High Optical Depth b_i
1	2.22(- 9)	3.86(- 8)	2	4	2.16(- 9)	-2.00(- 8)
2	2.92(- 9)	5.40(- 7)	2	4	3.34(- 9)	1.60(- 8)
3	-3.30(- 9)	5.82(- 6)	2	4	1.26(-10)	3.50(- 6)
4	-1.40(- 8)	1.42(- 5)	2	4	-1.19(- 8)	1.28(- 5)
5	5.26(- 9)	2.96(- 6)	2	4	8.30(- 9)	1.07(- 6)
6	9.74(- 9)	-1.60(- 6)	2	5	1.02(- 8)	-2.14(- 6)
7	8.34(- 9)	-2.48(- 6)	2	3	5.02(- 9)	-1.53(- 6)
8	2.08(- 9)	-6.24(- 7)	*			
9	5.06(-10)	-1.57(- 7)	#			
10	1.41(-10)	-4.22(- 8)	#			
11	2.48(-10)	-7.10(- 8)	#			
12	2.08(- 9)	-5.18(- 7)	*			
13	5.68(- 9)	1.82(- 6)	2	7	5.72(- 9)	-3.28(- 8)

Note (*): The difference between the two regimes is negligible.
(#): The band is essentially transparent, with no large optical depth at the conditions we are considering.
Note also: In (3.6) and (3.7), $c_i G_i(T) = m_i T + b_i$ while $r_i = s_i = 1$.

3.6 HYDROGEN - HELIUM INTERACTION

It is convenient to consider the opacity of hydrogen due to the interaction with helium as separate from the pure hydrogen opacity. The resulting optical depth will be given by an expression similar to (3.18) in which the pressure will be the partial pressure of helium, while the A_i's for H_2-He have to be determined. For the VRT contribution to the optical depth (occurring in wavebands 11 to 13) we have simply

$$A_i(H_2 - He) = A_i(H_2)$$

However, for the RT part (which is dominant over the translational part) in wavebands 1 to 10, we have [Linsky (1969)]

$$A_i(H_2-He) = \emptyset.1 \frac{f(H_2)}{f(He)} A_i(H_2)$$

where $f(H_2)$ and $f(He)$ are the fractions by number of H_2 and He respectively. Obviously, $A_i(H_2\text{-}He)$ depends on $f(H_2)$, but in order to use (3.6) and (3.7), we need it to be a function of f(He) only. We can make it so since this interaction opacity is small compared to the pure H_2 opacity. This means that very little error is introduced by assuming a constant value for the ratio $f(H_2)/f(He)$. Based on the abundances of H_2 and He, a good average value for this ratio is 6, so that in bands 1 to 10

$$A_i(H_2-He) = 0.6\, A_i(H_2)$$

In turn this gives

$$m_i(H_2-He) = 0.6\, m_i(H_2)$$

and

$$b_i(H_2-He) = 0.6\, b_i(H_2)$$

in these wavebands.

The relevent interaction parameters are given in Table 13.

Table 13

H_2 - He Parameters for (3.6) and (3.7)

BAND	Low Optical Depth m_i	b_i	τ_{chg}	τ_{rge}	High Optical Depth m_i	b_i
1	1.33(- 9)	2.32(- 8)	2	4	1.30(- 9)	-1.20(- 8)
2	1.75(- 9)	3.24(- 7)	2	4	2.04(- 9)	9.60(- 8)
3	-1.98(- 9)	3.50(- 6)	2	4	7.60(-11)	2.10(- 6)
4	-8.42(- 9)	8.50(- 6)	2	4	-7.12(- 9)	7.66(- 6)
5	3.16(- 9)	1.78(- 6)	2	4	4.98(- 9)	6.42(- 7)
6	5.84(- 9)	-9.58(- 7)	2	5	6.10(- 9)	-1.28(- 6)
7	5.00(- 9)	-1.49(- 6)	2	3	3.12(- 9)	-9.20(- 7)
8	1.25(- 9)	-3.74(- 7)	*			
9	3.04(-10)	-9.12(- 8)	#			
10	8.46(-11)	-2.54(- 8)	#			
11	2.48(-10)	-7.10(- 8)	#			
12	2.08(- 9)	-5.18(- 7)	*			
13	5.68(- 9)	1.82(- 6)	2	7	5.72(- 9)	-3.28(- 8)

Note (*): The differences between the two regimes are negligible.
(#): The band is essentially transparent, with no large optical depths at the conditions we are considering.
Note also: In (3.6) and (3.7), $c_i G_i(T) = m_i T + b_i$ while $r_i = s_i = 1$.

3.7 RELATIVE STRENGTHS

It is illuminating to find the relative strengths of the various opacity sources. To facilitate this comparision, we will compute the optical depth through a column of gas which contains 100 kg of gas. For a column with a surface area of one square metre, the pressure is simply

$$P = mg$$

which for a mass m of 100 kg becomes

$$P = 0.981 \text{ kpa}$$

The column density is given by

$$W = 231583 \frac{P}{M} = \frac{2.27 \times 10^5}{M} \quad \text{kpa-m}$$

where M is the molecular weight.

For a temperature of 300 K, we can compute the optical depth τ_i for each waveband using (3.6). The results are shown in Figure 5. It is obvious that NH_3, H_2O (and CO_2) are the dominant sources of optical depth, but these molecules are present only in small quantities (see Table 4). The hydrogen opacity is some three orders of magnitude lower, but is the dominant molecule in our atmosphere. The scaling effect is best seen by comparing figure 5 with figure 6, the latter being computed with molecular column density in proportion to a hydrogen abundance of 1000 kg, according to Table 4.

Figure 6 shows that NH_3 and H_2O are still the chief opacity sources, although H_2 has now become a significant contibutor to the optical depth.

Figure 5: Relative Optical Depths for 100 kg of each Molecule

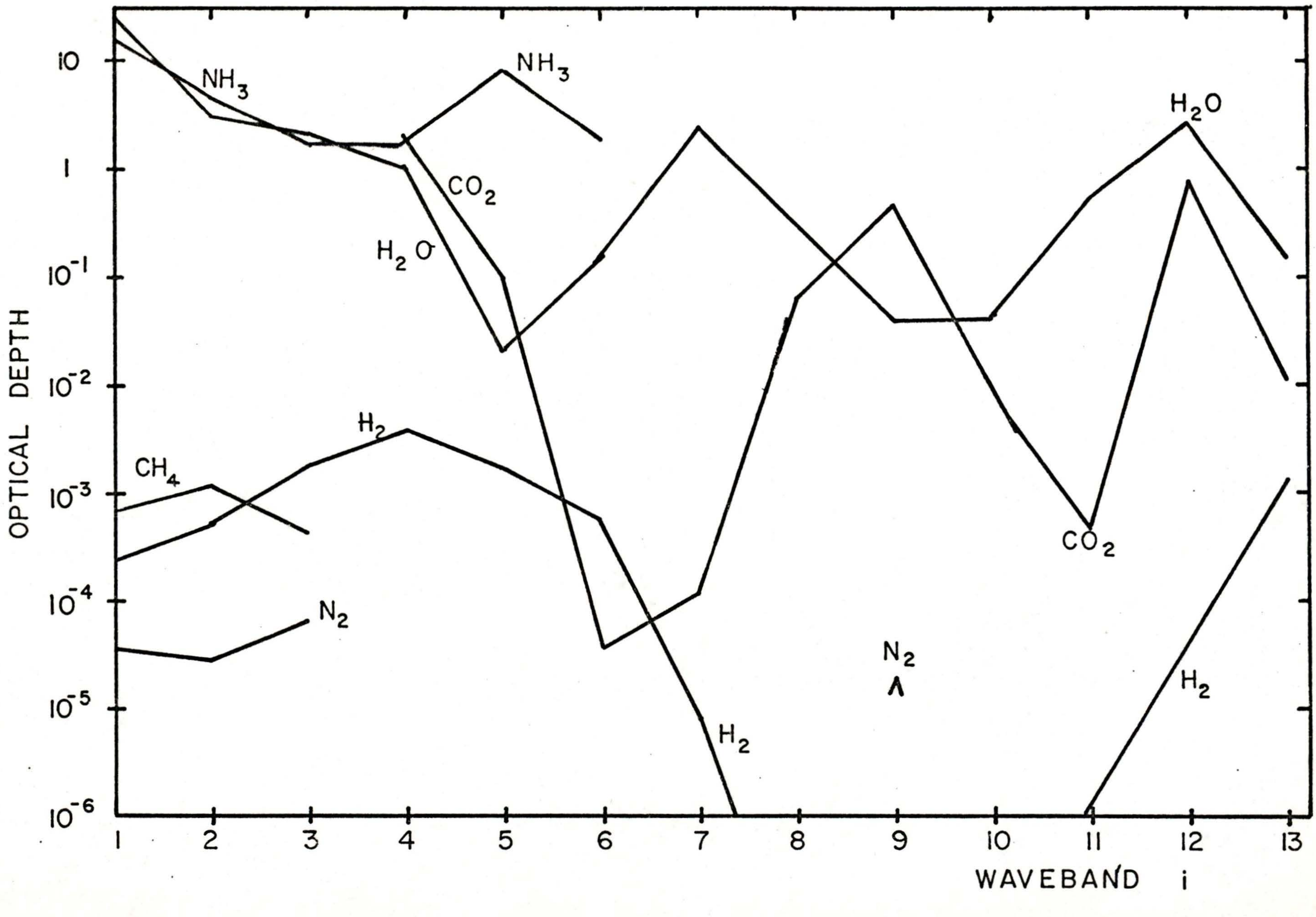
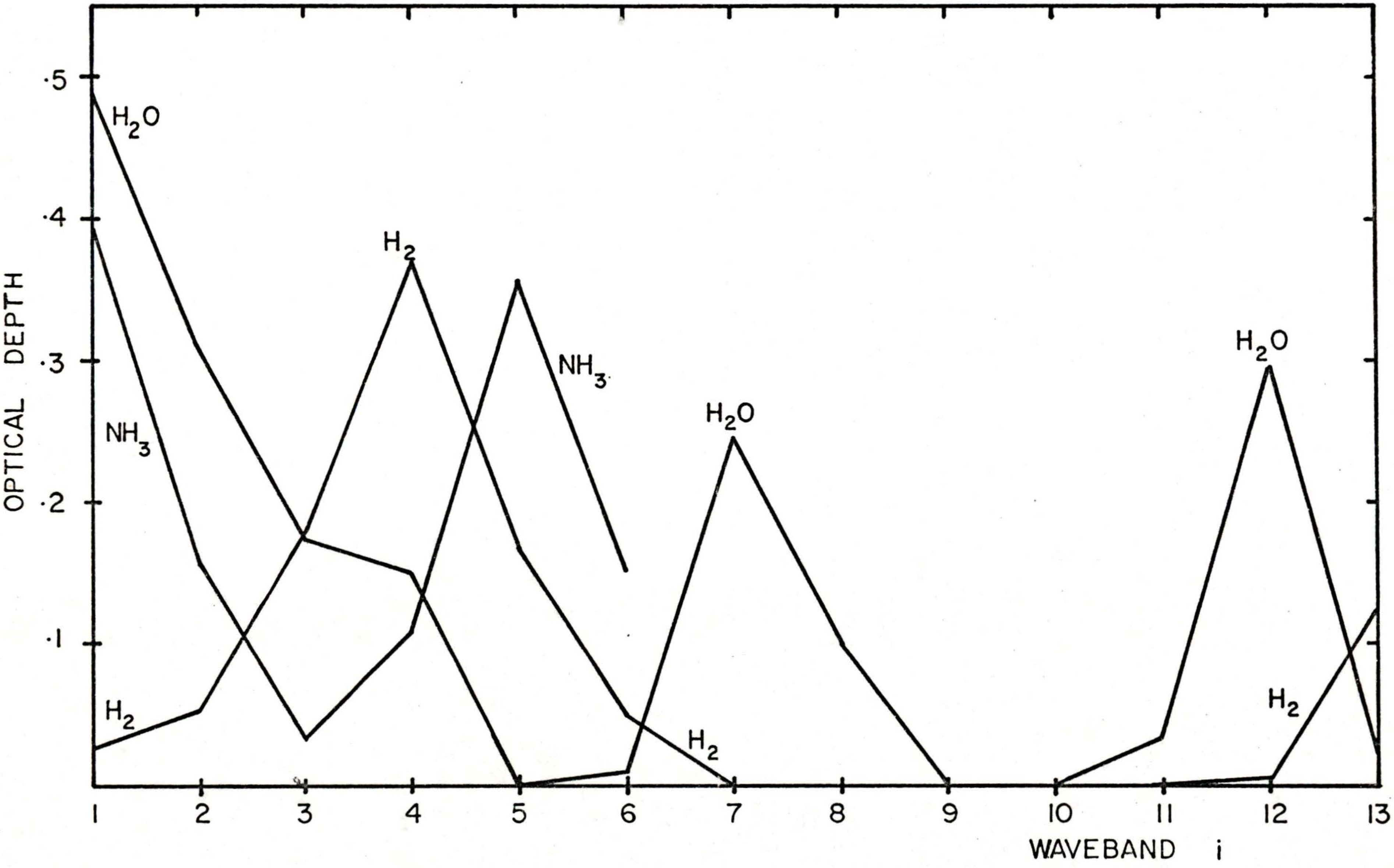

OPTICAL DEPTH
10
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
1
2
3
4
5
6
7
8
9
10
11
12
13
WAVEBAND i
NH_3
NH_3
CO_2
H_2O
H_2O
H_2
CH_4
N_2
H_2
N_2
CO_2
H_2

Figure 6: Relative Optical Depths for a Typical Planetary Composition
Composition is the average abundance from table 2.



OPTICAL DEPTH
·5
·4
·3
·2
·1
H_2O
NH_3
H_2
H_2
NH_3
H_2O
H_2
H_2O
H_2
1
2
3
4
5
6
7
8
9
10
11
12
13
WAVEBAND i

Chapter 4

THE PLOT

4.1 RESULTS AND CONCLUSIONS

Now that we have obtained the solution to the equation of transfer (chapter 2), and have obtained expressions for the molecular optical depth (chapter 3), we can write a computer program which will generate the temperature structure given an effective temperature with an atmosphere. This program appears in the Appendix. Our desired effective temperatures are given in table 1, while the desired compositions are given in table 4. The resulting temperature structures are shown in figures 8 to 10, while the corresponding surface temperatures are given in tables 15 and 16. We have assumed a fully mixed atmosphere, a necessary assumption for this approximate model with which we are dealing. We also include our results computed from data given in Hart (1978), and in Pollack and Ohring (1973), for comparison with their respective results. Table 14 compares our models with those of Hart (1978), while figure 7 compares a pure hydrogen model computed with the present model with that of Pollack and Ohring (1973). As can be seen, the present results agree with the previous models to within 5%, indicating that our model computes the true temperature structure as accurately as the approximations allow.

Table 14

The Hart (1978) Models

Surface Pressure (kpa)	Abundance by Number (percent) N_2	CO_2	CH_4	NH_3	H_2O	T_{eff}	T_{Hart}	$T_{Present}$
127	9.17	18.06	71.96	0.001	0.79	217	305	311
140	2.79	4.59	91.30	0.003	1.31	219	317	304
111	9.62	1.74	87.99	0.003	0.65	221	304	284
63	55.22	1.69	41.69	0.004	0.75	238	294	284

Note: Temperatures are given in degrees Kelvin.

Table 15

Surface Temperatures

T_{eff}	Composition (table 4) 10 times	100 times
91	147	243
205	302	448
225	327	475
295	399	585
320	423	619
400	504	744
600	708	1110

Note: Temperatures are given in degrees Kelvin.

Table 16

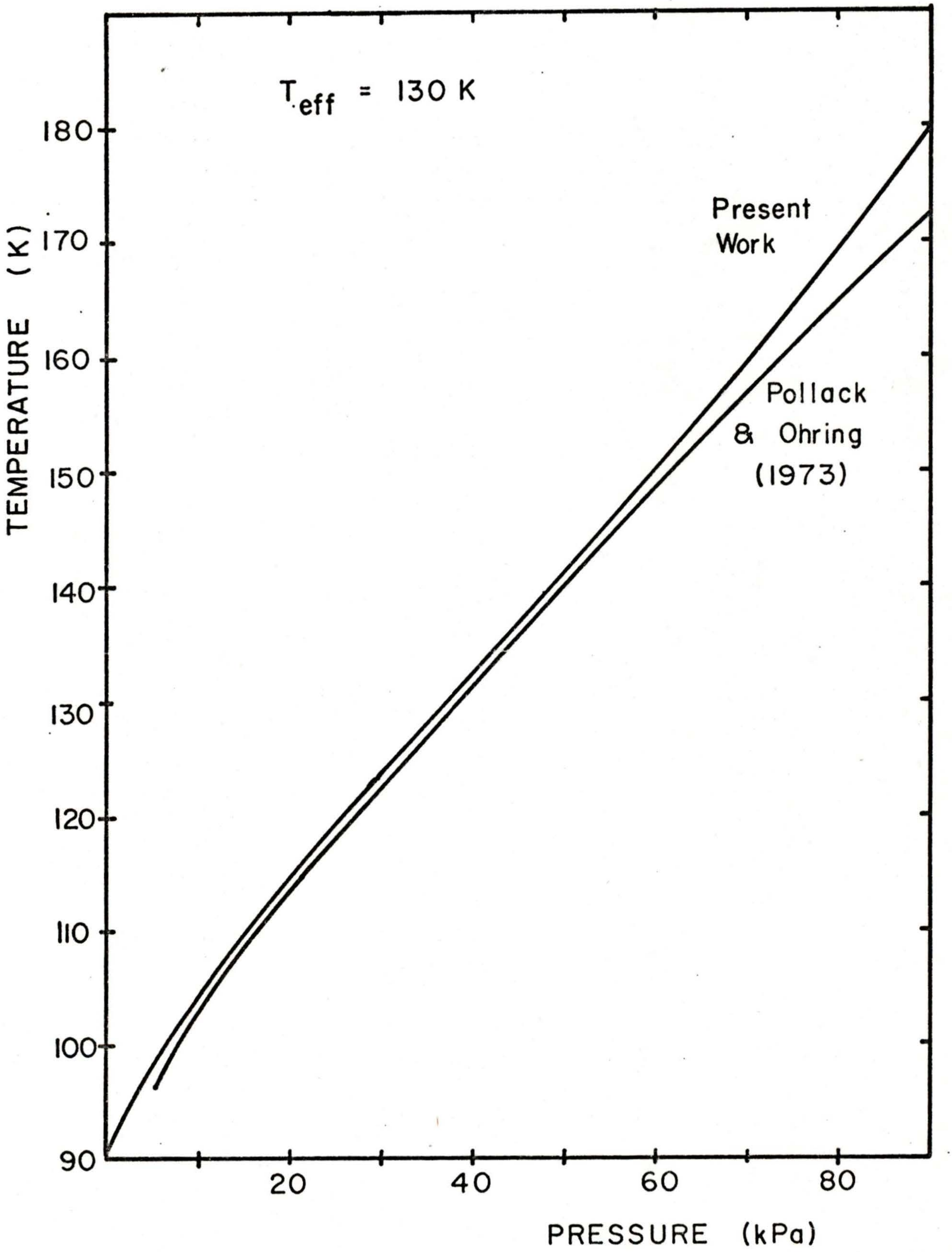
Surface Temperatures for Varying H_2 Composition

Size	Fraction of Hydrogen 100%	80%	60%	40%	20%	0%
10 times	708	701	689	678	674	667
100 times	1110					740

Note: Temperatures are in degrees Kelvin

These temperature structures can be used in the chemical reaction schemes computing the activity of the preboitic molecules, the objective we set out to accomplish initially.

Figure 7: Comparison of Present Results with Pollack and Ohring (1973)
Both curves are for a pure hydrogen atmosphere.



T_eff = 130 K
Present Work
Pollack & Ohring (1973)
TEMPERATURE (K)
180
170
160
150
140
130
120
110
100
90
20
40
60
80
PRESSURE (kPa)

While these reaction schemes are beyond the scope of this work, we can make a few comments about our results.

Probably the prime ingredient for life as we know it to exist is a temperature range which enables water to be a liquid (at one atmosphere of pressure). Some answers, albeit first order ones, to our problem outlined in section (1.1), namely whether the prebiotic molecules of the interstellar medium could have found a comfortable home on the primordial Earth, can be obtained by seeing if any of our molecules have this life zone of temperatures.

Figure 8 and table 15 give the results for the case where the atmospheric size is ten times that of the present Earth. The 205 K and the 225 K effective temperature curves are ideal, if slightly on the warm side at the surface! The 91 K curve has too low a surface temperature however, while the higher effective temperature curves are too hot. In these latter cases, there is a region within the atmosphere itself which has the right temperature range, but here we run the risk that any downdraft will circulate the primative biological material through the furnace below, probably destroying it. The evaporation of the hydrogen makes little difference to the surface temperature, as is shown in figures 9 and table 16, computed from the remaining compositions of table 1. The temperature drops from 708 K to 667 K, which is quite hot enough to destroy biological life.

Figure 8: Results for an atmosphere of ten times the present atmosphere.
(by number)

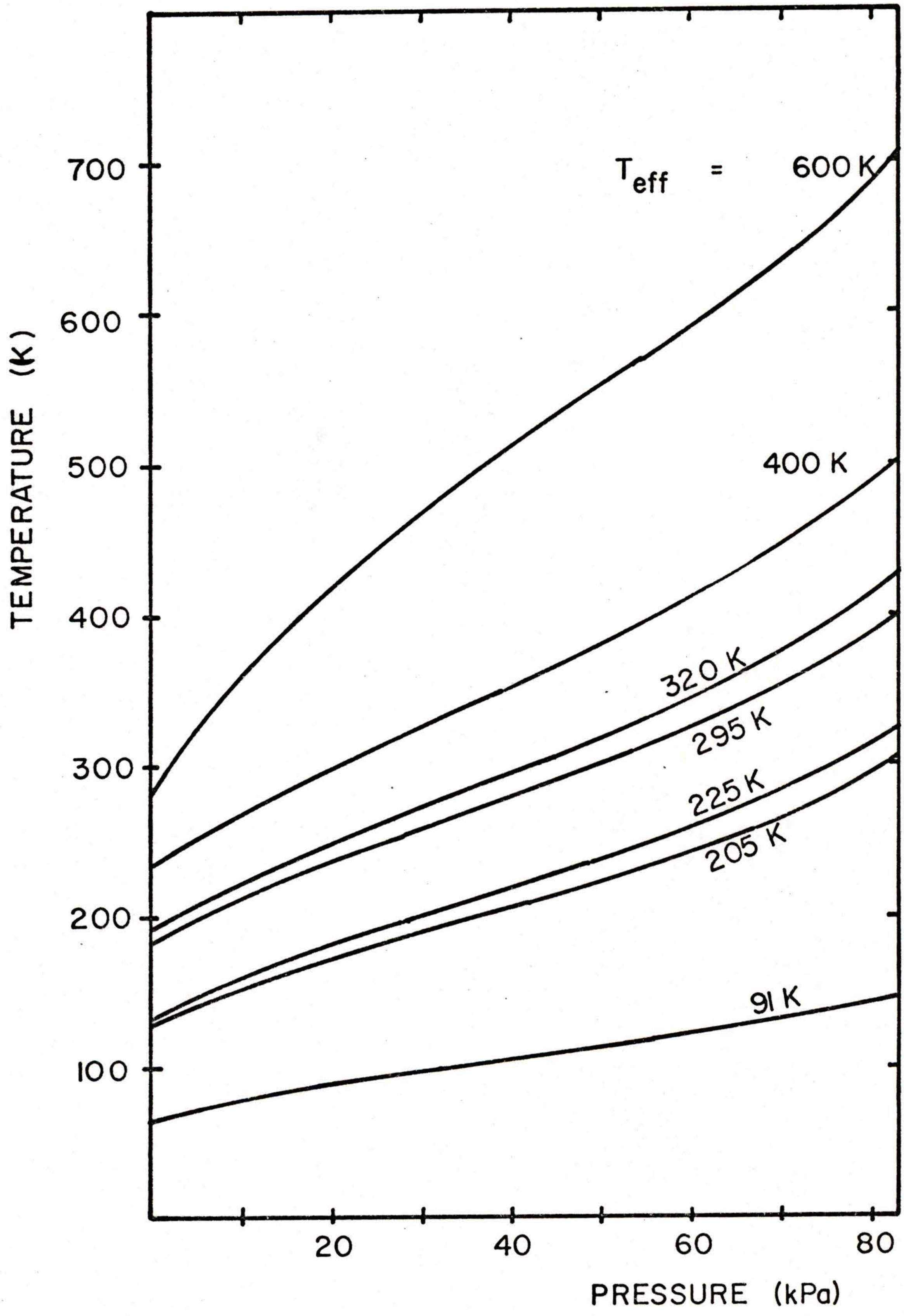
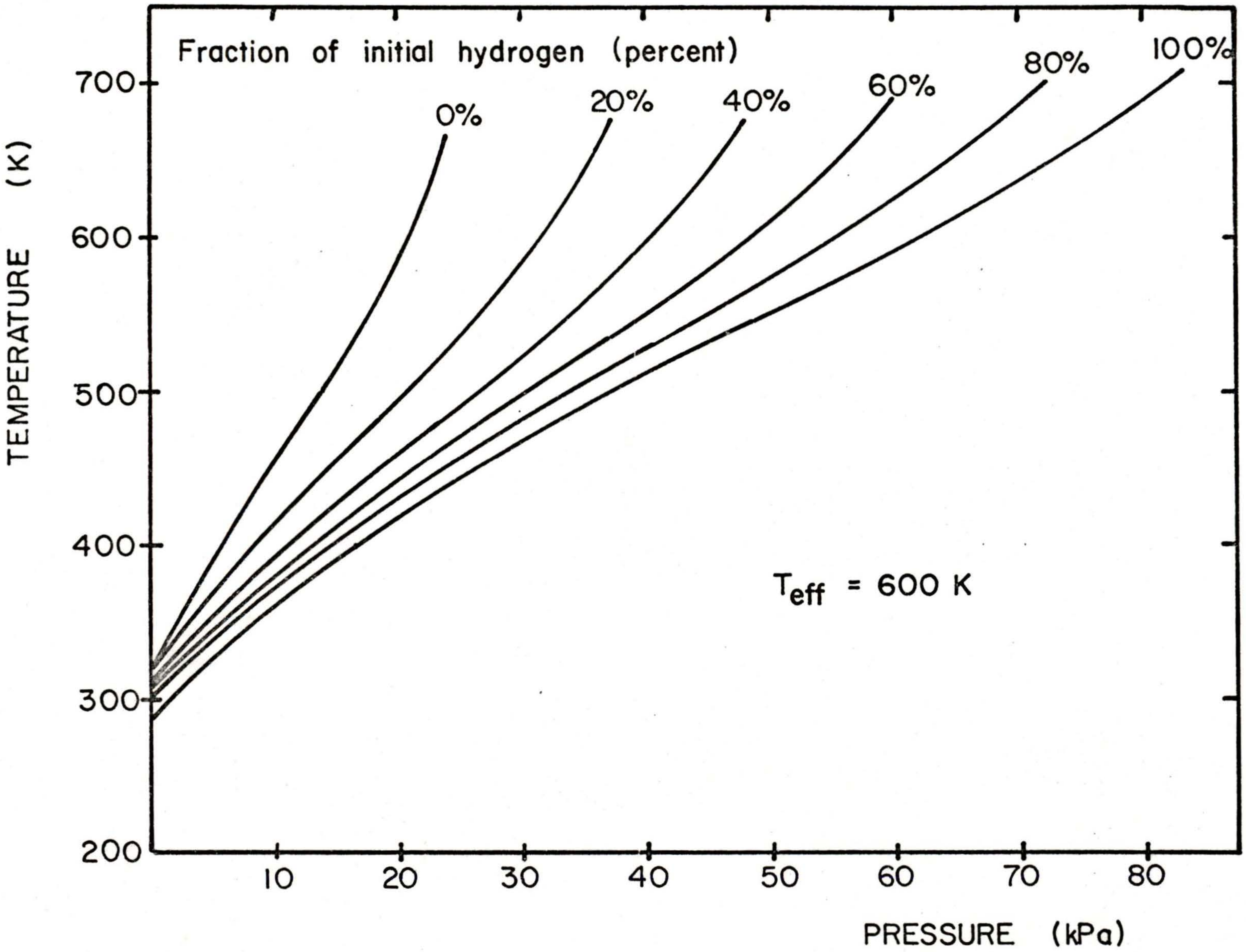

TEMPERATURE (K)
100
200
300
400
500
600
700
PRESSURE (kPa)
20
40
60
80
T eff = 600 K
400 K
320 K
295 K
225 K
205 K
91 K

Figure 9: Results allowing for the escape of hydrogen. Ten times atmosphere at 600 K.



Fraction of initial hydrogen (percent)
0%
20%
40%
60%
80%
100%
T_{eff} = 600 K
TEMPERATURE (K)
700
600
500
400
300
200
10
20
30
40
50
60
70
80
PRESSURE (kPa)

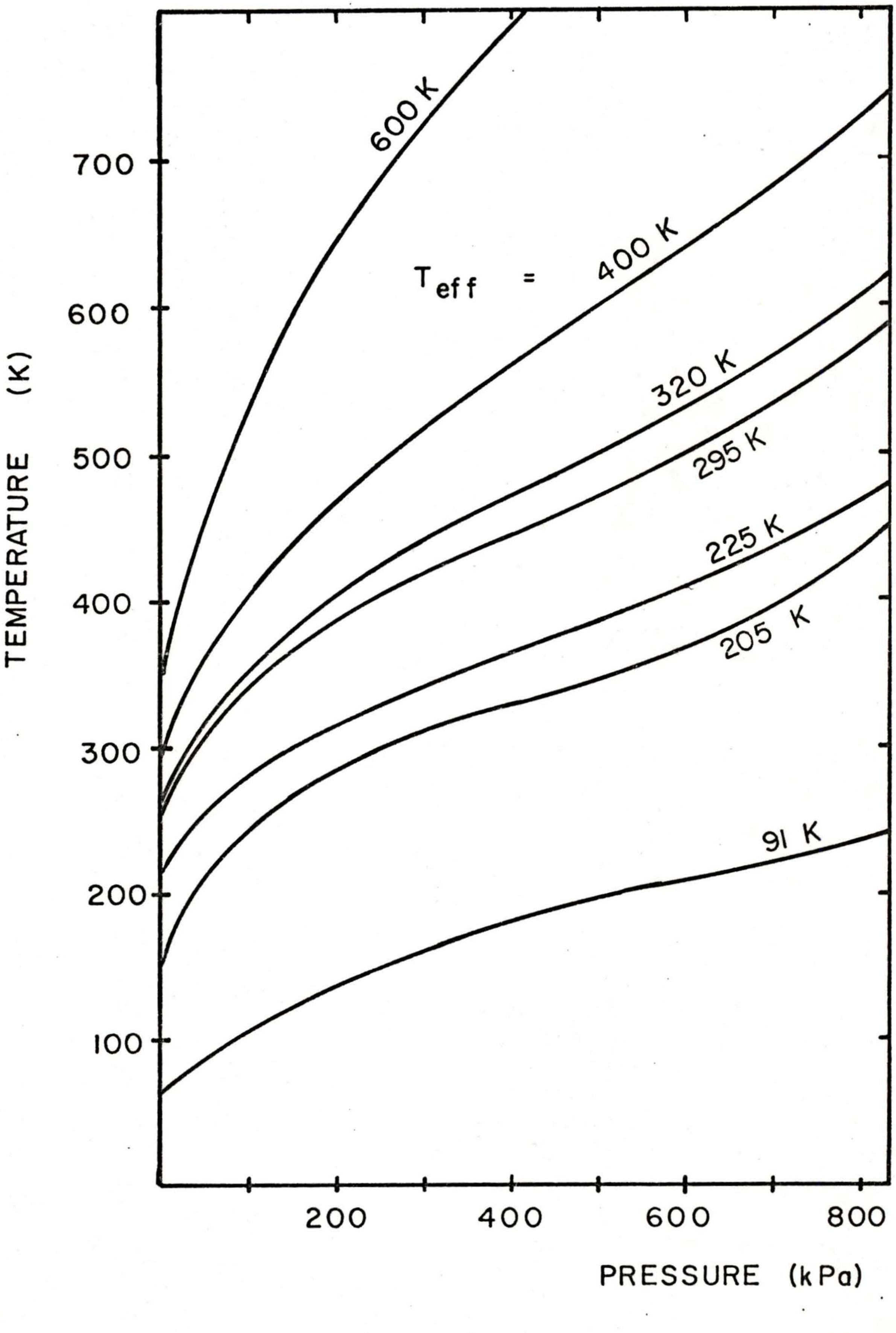
The temperature structures for models containing a hundred times as much gas as the present atmosphere (by number) are shown in figure 10, with surface temperatures given in table 15. It can be seen that all effective temperature curves, except the 91 K case, have surface temperatures well above the life zones. The 91 K case is still below the freezing point of water, but only by a small margin.

Even allowing for the approximate nature of the present model, we have an upper temperature limit determined by the opacity data. These data are strictly valid for temperatures of a few hundred degrees Kelvin, especially in the case of ammonia as this is one of the chief opacity sources. Temperatures above a few hundred degrees Kelvin become unreliable, but for completeness of results, we have extended the upper temperature limit to around 750 K. It is not worthwhile to compute models with surface temperatures above this limit, not only because they will be too unreliable, but because they are definitely quite hostile to our premise.

This is especially the case for the 600 K curve, which rapidly exceeds the temperature limit. Even allowing for the evaporation of hydrogen, the surface temperature is 740 K, and thus it again is not worthwhile to compute the temperature structures for the remaining compositions of table 4.

In conclusion, a few words about convection are in order. Convection forces the temperature to increase more slowly

Figure 10: Results for an atmosphere of a hundred times the present atmosphere.
(by number)



700
600
500
400
300
200
100
TEMPERATURE (K)
200
400
600
800
PRESSURE (kPa)
T_{eff} = 400 K
600 K
320 K
295 K
225 K
205 K
91 K

with incresing pressure than it would in the purely radiative case, resulting in lower surface temperatures than those we have obtained here. Therefore, the reliability of our results is in question if convection proves to be important. It turns out that it is important, beginning about halfway down through our various atmospheres, and continuing to the planetary surface. This means that our surface temperatures are not accurate, but they are a good zeroth order approximation to a far more complex problem, and do indicate which conditions are worth investigating further with more complete models, and which can be neglected.

4.2 FURTHER WORK

We have made a number of approximations in this work, all of which should be removed, or at least improved. While the formal solution to the equation of transfer (equations 2.1) is completely general for the plane parallel case, the method we used to evaluate the solution is not. In our case, we ignored scattering so that the source function would equal the Planck function. Scattering may be important at the temperatures and wavelenths being considered here, and should be investigated.

Convection is another important method of energy transfer, and should be included. As we have seen, convection forces the temperature to increase more slowly with increasing pressure than it would in the purely radiative case, resulting in lower surface temperatures than we have obtained. Convection is also the main agent which mixes the atmosphere, something we have tacitly assumed to occur even though we have ignored convection per se.

Diffusion also complicates the issue by causing some mixing even in regions where the convection is absent. Further complications result from the uneven heating of the planetary surface (the equator is hotter than the poles) and from planetary rotation. The problem is rapidly becoming a meteorologist's nightmare!

In addition, we haven't allowed for the vapour pressure curves of our molecular species. The condensing out of the major opacity sources (such as water and ammonia) significantly alters the temperature structure of the atmosphere by substantially changing the opacity. Further complications in this regard are caused by the interactions between the atmospheric constituents (such as ammonia readily dissolving in liquid water). The changing composition not only affects the temperature structure by altering the opacity, but also affects the onset of convection by changing the adiabatic index γ used in the Schwarzschild criterion (2.25).

Another area which has room for improvement is the power law function for the optical depth, and its associated constants. While the power dependence of the optical depth on pressure and column density is reasonable, much more data are needed to get a good temperature dependence function

$G_i(T)$ which covers the entire desired range in temperature. Data covering a larger range of frequencies would also improve the optical depth averaging technique used in this work.

While it can be seen that there is much room for improvements in our model atmosphere, it does give an order of magnitude temperature structure, suiting the present knowledge (or lack of it!) of the conditions of the primordial Earth.

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Appendix

THE COMPUTER PROGRAM

We give in this appendix the computer program used to construct the temperature structure, described herein, from equations (2.7) to (2.11) and the data of chapter 3. A few notes on the method are in order.

Equation (2.8) requires increasing steps in the optical depth, something we cannot perform readily due to the power law nature of the optical depth. Instead, we stepwise increase the pressure, computing the optical depth for each frequency point, as required for (2.8). The initial pressure steps are chosen so that the total number of steps throughout the atmosphere is twice the number of sample points. If the optical depth step corresponding to each pressure step is greater than some arbitary value (set at $\Delta\tau = 0.4$), the pressure step is reduced so that $\Delta\tau = 0.4$. In addition, if the change in the optical depth is less than another predetermined value (equal to the total range in divided by twice the number of sample points) the pressure step is doubled. For each new pressure, the temperature associated with it is found by linear interpolation of the known temperatures at each sample point. With these pressures and temperatures, the optical depth is calculated with the FUNCTION OPACTY.

The flux at each sample point is then computed with (2.7) to (2.11). We need expressions for E to do this [expressions for the higher order exponential integrals are given by the recursion relation given in section (2.1)]. One approximation is due to Mewe (1972):

$$E_1(\tau) = e^{-\tau}\left[\ln\left(\frac{\tau+1}{\tau}\right) - \frac{0.4}{(\tau+1)^2}\right]$$

while a more accurate expression is given by Abramowitz and Stegun (1964):

$$E_1(\tau) = -\ln\tau - 0.57721566 + 0.99999193\,\tau - 0.24991055\,\tau^2 + 0.05519968\,\tau^3 - 0.00976004\,\tau^4 + 0.00107857\,\tau^5 \quad \text{for } \tau \le 1$$

and

$$E_1(\tau) = \frac{1}{\tau e^{\tau}}\;\frac{\tau^4 + a_1\tau^3 + a_2\tau^2 + a_3\tau + a_4}{\tau^4 + b_1\tau^3 + b_2\tau^2 + b_3\tau + b_4} \quad \text{for } \tau > 1$$

where

a_1 = 8.5733287401, b_1 = 9.5733223454

a_2 = 18.0590169730, b_2 = 25.6329561486

a_3 = 8.6347608925, b_3 = 21.0996530827

a_4 = 0.2677737343, b_4 = 3.9584969228

FUNCTION E2 evaluates this more accurate expression.

With these fluxes, the new temperature structure was computed using the techniques outlined in section 2.3. SUBROUTINE COEFFT calculates the coefficients required by equations (2.21) and (2.22). The total frequency averaged optical depths required by the correction scheme, and by the initial temperature structure (2.23), are computed in SUBROUTINE TAUGRY with equation (2.24).

Finally SUBROUTINE PARAM evaluated the Schwarzschild criterion (2.25), with the derivative being calculated using Lagrangian three point interpolation (FUNCTION DLG3PT)

$$\frac{dy}{dx} = X_1 y_1 + X_2 y_2 + X_3 y_3$$

where

$$X_1 = \frac{(x - x_2) + (x - x_3)}{(x_1 - x_2)(x_1 - x_3)}$$

$$X_2 = \frac{(x - x_1) + (x - x_3)}{(x_2 - x_1)(x_2 - x_3)}$$

$$X_3 = \frac{(x - x_1) + (x - x_2)}{(x_3 - x_1)(x_3 - x_2)}$$

This subroutine also calculates the relative physical parameters characterizing the atmosphere (height, density, and total column density) using (1.3) and the equations for hydrostatic equilibrium and for a perfect gas (see 1.2.2). The program itself now follows.

```
C:- NONGREY ATMOSPHERE
C:- MULTIPLE OPACITY SOURCE
      DIMENSION TEMP(15),ATM(15),PTAB(15),DFREQ(15),SPEC(5),
     1          THICK(15),DENSE(15),FLUX(15,2),PEVAL(15),
     2          R(15,5,2),S(15,5,2),TI(15,5,2),C(15,5,2),
     3          REGIME(15,5,2),IRGIME(5),B1(15),B2(15),XLAG(3),
     4          TOTFLX(15),STABLE(15),K4(5,2),LABEL(2,2),CP(5),
     5          CV(5),NAME(5), CORFLX(15),TAUPT(15),DELTA(15),
     6          TYPE(5),FP(5),F1(5,2),F2(5,2),INTGRL(5,2),
     7          RANGE(15,5,2),B(15),COEFF(15,15),FACTOR(15),
     8          MWT(5),IRGE(15,5),TCOEFF(15,16),T4(15),T4N(15)
      REAL MOLWT,MWT,K1,K2,K3,K4,K5,K6,LTFLUX,INTGRL,M
      INTEGER FREQPT,FLUXPT,STOP,SKIP,TYPE
      DOUBLE PRECISION TCOEFF
      COMMON /ALL/ FLUXPT,FREQPT,PTAB,TEMP,K1,K2,K3
      COMMON /OPAC/ IRGIME,INTGRL,F1,F2,K4
      COMMON /INT/ B1,B2,FP,TEFF,SPEC,MWT,DFREQ
      COMMON /INTTAU/ R,S,TI,C,REGIME,TYPE,MOLS,RANGE,IRGE
      COMMON /RST/ DENSE,THICK,ATM,PEVAL,CONV,STABLE,MOLWT
      DATA LABEL/'T','M','C','B'/
    1 FORMAT (3I3,F5.0)
    2 FORMAT (A4,I2,3F7.3)
    3 FORMAT (10F7.3)
   19 FORMAT (2(2F5.3,2E8.3,2F4.1))
    4 FORMAT ('1FINAL ITERATION     (EMITTED FLUX: ',F6.0,')'
     1,//,'   ALTITUDE  TOTAL AMT    DENSITY   PRESSURE',
     2 4X,'TEMP   FLUX',5X,'STABLE',/,5X,
     3'(KM)    (EARTH ATM)   (KG/M3)      (KPA)       (K)',
     4 '   (W/M2)',4X,'IF +VE',/)
    5 FORMAT (3X,F7.3,14X,1PE9.2,2X,E9.2,2X,0PF6.1,1X,F6.0)
    6 FORMAT (3X,0PF7.3,3X,1PE9.2,2X,E9.2,2X,E9.2,2X,0PF6.1,
     1  1X,F6.0,3X, E9.2)
    7 FORMAT(' ITERATION ',I1,4X,'PRESSURE    TEMP      FLUX',
     1    7X,'TAU',/)
    8 FORMAT (15X,1PE9.2,3X,0PF5.0,2X,1PE9.2,2X,E9.2)
    9 FORMAT ('1')
   10 FORMAT ('0',/,'0')
   17 FORMAT ('1EFFECTIVE TEMP: ',F4.0,'    FLUX: ',F6.1,//,
     1  ' FREQPT   DFREQ        B1',9X,'B2',/)
   18 FORMAT (5X,I2,2X,F6.2,2X,1PE10.3,2X,E10.3)
   11 FORMAT ('-',8X,'MOL ',I1,' - ',A4,': AMOUNT:',F7.3,'%',
     1  '        P FACTOR:',F8.6)
   12 FORMAT (9X,'(TYPE ',I1,')',6X,'WEIGHT: ',F6.3,2X)
   14 FORMAT (23X,'S.H.-P: ',F6.1,9X)
   15 FORMAT (23X,'S.H.-V: ',F6.1,9X,/)
   16 FORMAT ('0FREQPT ',2(4X,'R',6X,'S',7X,A1,10X,A1,7X,
     1  'CNG    RGE'))
   13 FORMAT (5X,I2,2(2X,F5.3,2X,F5.3,2X,1PE9.2,2X,E9.2,2X,
     1  0PF4.0,2X,F4.0))
      PI = 3.141592654
      PI2 = 2.*PI
   20 FORMAT (3I2,F5.0)
      WRITE (7,26)
   26 FORMAT ('ENTER ITLMT,LPLMT,INITT: (I2); & TEFF (F5.0)')
```

```
      READ (4,20) ITLMT, LPLMT, INITT, TEFF
C   FREQPT: NUMBER OF WAVEBANDS
C   FLUXPT: NUMBER OF SAMPLE POINTS
C   B1     : PLANCK FUNCTION CONST (J/M2S)
C   B2     : PLANCK FUNCTION CONST (K-1)
C   MOLS   : NUMBER OF MOLECULES
C   TEFF   : EFFECTIVE TEMPERATURE
C   NAME   : MOLECULE NAME
C   TYPE   : TYPE OF OPACITY (=1  T FOLLOWS POWER LAW C*(T**TI)
C                            (=2  T IS LINEAR TI + C/T
C   MWT    : MOLECULAR WEIGHT OF MOLECULE
C   CP     : SPECIFIC HEAT AT CONSTANT PRESSURE
C   CV     : SPECIFIC HEAT AT CONSTANT VOLUME
C   SPEC   : FRACTION OF GAS PRESENT
C   FP     : PRESSURE SCALING FACTOR  = PARTIAL P/TOTAL P
C                          EXCEPT NH3   = PE/TOTAL P
C   R,S,TI,C: OPACITY CONSTANTS
C   REGIME: LOWER TAU LIMIT FOR CHANGEOVER REGIME
C   RANGE : UPPER TAU LIMIT FOR CHANGEOVER REGIME
C   PTAB   : TABULATED PRESSURE VALES DEFINING THE SAMPLE POINTS
C   TEMP   : TABULATED TEMPERATURE VALES AT EACH SAMPLE POINT
C   G      : ACCELERATION DUE TO GRAVITY
C
C   READ BLOCK FOR INPUT PARAMETERS
C
      READ (5, 1) FREQPT,FLUXPT,MOLS
      READ (5, 3) G
      READ (5, 3) (DFREQ(IR),IR = 1,FREQPT)
      READ (5, 3) (B1(IR),IR = 1,FREQPT)
      READ (5, 3) (B2(IR),IR = 1,FREQPT)
      DO 100 IS = 1,MOLS
      READ (5, 2) NAME(IS), TYPE(IS), MWT(IS), CP(IS), CV(IS)
      READ (5, 3) SPEC(IS),FP(IS)
      DO 100 IR = 1,FREQPT
  100 READ (5,19) (R(IR,IS,IP),S(IR,IS,IP),TI(IR,IS,IP),
     1             C(IR,IS,IP),REGIME(IR,IS,IP),RANGE(IR,IS,IP),
     2             IP = 1,2)
      READ (5, 3) (PTAB(IR),IR=1,FLUXPT)
      TFLUX = 5.6703E-8*TEFF**4
      WRITE (6, 17) TEFF, TFLUX
      WRITE (7, 17) TEFF, TFLUX
      DO 110 I = 1,FREQPT
  110 WRITE (6, 18) I, DFREQ(I), B1(I), B2(I)
      DO 120 IS = 1,MOLS
      SPECPC = 100.*SPEC(IS)
      WRITE (6, 11) IS,NAME(IS),SPECPC, FP(IS)
      WRITE (6, 12) (TYPE(IS),MWT(IS))
      WRITE (6, 14) (CP(IS))
      WRITE (6, 15) (CV(IS))
      IT = TYPE(IS)
      WRITE (6, 16) LABEL(IT,1),LABEL(IT,2),LABEL(IT,1),
     1 LABEL(IT,2)
      DO 120 I = 1,FREQPT
      IRGE(I,IS) = 1
```

```
      IF (REGIME(I,IS,1).LT.35..AND.C(I,IS,1).GT.-0.5)
     1   IRGE(I,IS) = 2
      IW1 = IRGE(I,IS)
      WRITE (6, 13) I,(R(I,IS,IW),S(I,IS,IW),TI(I,IS,IW),
     1              C(I,IS,IW),REGIME(I,IS,IW),RANGE(I,IS,IW),
     2              IW = 1,IW1)
  120 CONTINUE
      WRITE (6, 9)
      PTOP = PTAB(1)
      PBTM = PTAB(FLUXPT)
C
C  COMPUTES (1. - 1/GAMMA) FOR THE GAS MIXTURE
C
      MOLWT = 0.
      CPT = 0.
      CVT = 0.
      DO 130 IS = 1,MOLS
      SM = SPEC(IS)*MWT(IS)
      MOLWT = MOLWT + SM
      CPT = CPT + SM*CP(IS)
  130 CVT = CVT + SM*CV(IS)
      CONV = (1. - CVT/CPT)
C
C  K1: CONSTANT FOR DW = (K1)DP/MWT
C  K2: DENSITY CONSTANT (AMU/K)*AVERAGE MWT
C  K3: HEIGHT CONSTANT DW = (K1)DP/MWT = NDZ
C
      K1 = 2.270966E6/G
      K2 = 0.120274*MOLWT
      K3 = 8314.34/(G*MOLWT)
      IF (INITT.EQ.1) GO TO 143
      DO 133 IK = 1,FLUXPT
C
C  COMPUTES THE INITIAL TEMPERATURE DISTRIBUTION
C   LOOPS THREE TIMES CORRECTING THE PREVIOUS STRUCTURE
C
  133 TEMP(IK) = 300.
      DO 138 LOOP = 1,3
      CALL TAUGRY(TAUPT,B)
      DO 136 IK = 1,FLUXPT
  136 TEMP(IK) = 0.9306*TEFF*SQRT(SQRT(TAUPT(IK) + 0.26667))
      WRITE(6,22) LOOP
  138 WRITE (6,23) (TEMP(IW),IW = 1,FLUXPT)
   22 FORMAT ('0INITILIZATION LOOP ',I1)
   23 FORMAT ('0',15F6.1)
      WRITE (6,9)
      GO TO 148
  143 WRITE (7, 27)
   27 FORMAT (' ENTER T(K) [F5.0]')
      READ (7,28) (TEMP(IR), IR = 1,FLUXPT)
   28 FORMAT (15F5.0)
      CALL TAUGRY (TAUPT,B)
  148 CONTINUE
      DO 140 IK = 1,FLUXPT
```

```
  140 T4(IK) = TEMP(IK)**4
C
C  ITERATION LOOP
C
      DO 650 ITER = 1,ITLMT
C
C SAMPLE POINT LOOP
C
      DO 520 IK = 1,FLUXPT
      FLUX(IK,1) = 0.
      FLUX(IK,2) = 0.
C
C  FREQUENCY BAND LOOP
C
      DO 510 I = 1,FREQPT
C
C  CONTRIBUTION DOWN FROM LAYERS ABOVE
C
      P = PTAB(IK)
      T = TEMP(IK)
C
C  INITIAL CONSTANTS FOR THE OPTICAL DEPTH
C   (OPTICAL DEPTH IS CALCULATED WITH A TRAPEZIODAL RULE;
C    THE PREVIOUS FUNCTION VALUES BEING STORED IN  F1
C    AND THE NEW VALUES IN  F2)
C
      DO 150 IS = 1,MOLS
      IF (C(I,IS,1).LE.(-0.5)) GO TO 150
      IPLL = IRGE(I,IS)
      DO 150 IP = 1,IPLL
      F1(IS,IP) = 0.
      K4(IS,IP)=(0.5*K1*SPEC(IS)/MWT(IS))**R(I,IS,IP)*FP(IS)
     1  **S(I,IS,IP)
      IF (TYPE(IS).EQ.2) GO TO 147
      F1(IS,IP) = (P**S(I,IS,IP)*C(I,IS,IP)*T**TI(I,IS,IP))
     1    **(1./R(I,IS,IP))
      GO TO 150
  147 CG = TI(I,IS,IP) + C(I,IS,IP)/T
      IF (CG.GT.0.) F1(IS,IP) = P*CG
  150 CONTINUE
      BK1 = B1(I)
      BK2 = B2(I)
      BSTART = 0.
      EXPON = BK2/T
      IF (EXPON.LE.30.) BSTART = BK1/(EXP(EXPON) - 1.)
      IF (IK.EQ.1) GO TO 320
      FLUXI = 0.
      BOLD = BSTART
      STOP = 0
      TAUOLD = 0.
      E2OLD = 1.
      E3OLD = 0.5
      E4OLD = 0.3333333
C
```

```
C  COMPUTES APPROX. OPTICAL DEPTH RANGE OF THE ATMOSPHERE
C
      TAURGE = 0.
      DO 160 IS = 1,MOLS
      IF (C(I,IS,1).LE.(-0.5)) GO TO 160
      IF (TYPE(IS).EQ.2) GO TO 155
      F2(IS,1) = (C(I,IS,1)*PTOP**S(I,IS,1)*TEMP(1)**TI(I,IS,1))
     1     **(1./R(I,IS,1))
      TAURGE = TAURGE + K4(IS,1)*((F1(IS,1) + F2(IS,1))*(P -
     1   PTOP))**R(I,IS,1)
      GO TO 160
  155 CG = TI(I,IS,1) + C(I,IS,1)/TEMP(1)
      IF (CG.LE.0.) GO TO 160
      F2(IS,1) = CG*PTOP
      TAURGE = TAURGE + K4(IS,1)*(F1(IS,1) + F2(IS,1))*(P
     1   - PTOP)
  160 CONTINUE
C
C  COMPUTES THE PRESSURE STEP
C
      DFLUX = 0.
      DIV = 2*(IK - 1)
      DTAULT = TAURGE/(2.*DIV)
      IF (DTAULT.GT.0.3) DTAULT = 0.3
      TAUCHG = 2.5*TAURGE
      IF (TAUCHG.GT.DIV) DIV = TAUCHG
      DELTAP = (P - PTOP)/DIV
      DO 180 IC = 1,3
      DO 165 IS = 1,MOLS
      IRGIME(IS) = 1
      DO 165 IP = 1,2
  165 INTGRL(IS,IP) = 0.
      P = PTAB(IK) - DELTAP
      ISTART = IK
C
C  LINEAR INTERPOLATION OF NEW  T  AT NEW  P
C
      DO 200 LAG = 2,IK
      ISTART = IK - LAG + 1
      IF (P.GT.PTAB(ISTART)) GO TO 210
  200 CONTINUE
  210 M = (TEMP(ISTART+1)-TEMP(ISTART))/(PTAB(ISTART+1)-
     1   PTAB(ISTART))
      T = M*(P - PTAB(ISTART)) + TEMP(ISTART)
      TAU = OPACTY(I,T,P,DELTAP)
      IF (TAU.LE.0.4.OR.IC.EQ.3) GO TO 190
      DELTAP = 0.04*DELTAP/(TAU*TAU)
      IF (DELTAP.GE.(1.E-6*P)) GO TO 180
      DELTAP = 1.E-6*P
      GO TO 190
  180 CONTINUE
  190 DTAU2 = TAU
C
C  COMPUTES THE EXPONENTIAL AND PLANCK FUNCTIONS
```

```
C
  250 EXPON = BK2/T
      IF (TAU.LE.0.) GO TO 310
      IF (EXPON.GT.30.) GO TO 310
      BNEW = BK1/(EXP(EXPON) - 1.)
      E2NEW = E2(TAU)
      EXPT = EXP(-TAU)
      E3NEW = (EXPT - TAU*E2NEW)/2.
      E4NEW = (EXPT - TAU*E3NEW)/3.
C
C  INTEGRATION OF (2.8)
C
      DE3 = E3OLD - E3NEW
      DE4DT2 = 0.
      IF (DTAU2.GT.0.) DE4DT2 = 2.*(E4OLD - E4NEW)/DTAU2
      DFLUX = PI*((BNEW + BOLD)*DE3 + (BNEW - BOLD)*(DE4DT2
     1   - E3OLD - E3NEW))
      FLUXI = FLUXI + DFLUX
      FLUX(IK,1) = FLUX(IK,1) + DFLUX
      IF (DFLUX.LE.(1.E-6*FLUX(IK,1)).OR.STOP.EQ.1.OR.TAU.GT.
     1   20.) GO TO 310
      E2OLD = E2NEW
      E3OLD = E3NEW
      E4OLD = E4NEW
      BOLD = BNEW
      TAUOLD = TAU
      DFLUX = 0.
      POLD = P
      P = P - DELTAP
      IF (P.GT.PTOP) GO TO 260
C
C  AT TOP OF ATMOSPHERE
C
      STOP = 1
      T = TEMP(1)
      DO 255 IS = 1,MOLS
      DO 255 IPL = 1,2
  255 F1(IS,IPL) = F2(IS,IPL)
      TAU = OPACTY(I,T,PTOP,POLD - PTOP)
      DTAU2 = TAU - TAUOLD
      P = PTOP
      GO TO 250
C
C  SETS NEW  P, AND FINDS NEW  T  AND OPTICAL DEPTH
C
  260 IF (P.GT.PTAB(ISTART )) GO TO 290
  270 ISTART = ISTART - 1
      IF (P.LE.PTAB(ISTART)) GO TO 270
      M = (TEMP(ISTART+1)-TEMP(ISTART))/(PTAB(ISTART+1)-
     1 PTAB(ISTART))
  290 T = M*(P - PTAB(ISTART)) + TEMP(ISTART)
      DO 300 IS = 1,MOLS
      DO 300 IPL = 1,2
  300 F1(IS,IPL) = F2(IS,IPL)
```

```
      TAU = OPACTY(I,T,P,DELTAP)
      DTAU2 = TAU - TAUOLD
      IF (DTAU2.LE.DTAULT) DELTAP = 2.*DELTAP
      GO TO 250
C
C  CONTRIBUTION UP FROM LAYERS BELOW
C
  310 IF (IK.LT.FLUXPT) GO TO 320
      BFLUX = PI*BK1/(EXP(BK2/TEMP(FLUXPT)) - 1.)
      GO TO 500
  320 P = PTAB(IK)
      T = TEMP(IK)
C
C  INITIAL CONSTANTS FOR OPTICAL DEPTH
C
      DO 322 IS = 1,MOLS
      IF (C(I,IS,1).LE.(-0.5)) GO TO 322
      IPLL = IRGE(I,IS)
      DO 322 IP = 1,IPLL
      F1(IS,IPL) = 0.
      IF (TYPE(IS).EQ.2) GO TO 321
      F1(IS,IP) = (P**S(I,IS,IP)*C(I,IS,IP)*T**TI(I,IS,IP))
     1   **(1./R(I,IS,IP))
      GO TO 322
  321 CG = TI(I,IS,IP) + C(I,IS,IP)/T
      IF (CG.GT.0.) F1(IS,IP) = P*CG
  322 CONTINUE
      STOP = 0
      BOLD = BSTART
      TAUOLD = 0.
      FLUXO = 0.
      E2OLD = 1.
      E3OLD = 0.5
      E4OLD = 0.3333333
      E3NEW = 0.5
C
C  COMPUTES APPROX. OPTICAL DEPTH
C
      TAURGE = 0.
      DO 330 IS = 1,MOLS
      IF (C(I,IS,1).LE.(-0.5)) GO TO 330
      IF (TYPE(IS).EQ.2) GO TO 325
      F2(IS,1) = (C(I,IS,1)*PBTM**S(I,IS,1)*TEMP(FLUXPT)
     1      **TI(I,IS,1))**(1./R(I,IS,1))
      TAURGE = TAURGE + K4(IS,1)*((F1(IS,1) + F2(IS,1))*(PBTM
     1   - P))**R(I,IS,1)
      GO TO 330
  325 CG = TI(I,IS,1) + C(I,IS,1)/TEMP(FLUXPT)
      IF (CG.LE.0.) GO TO 330
      F2(IS,1) = CG*PBTM
      TAURGE = TAURGE + K4(IS,1)*(F1(IS,1) + F2(IS,1))*(PBTM
     1 - P)
  330 CONTINUE
C
```

```
C  COMPUTES THE PRESSURE STEP
C
      OLDFLX = 0.
      DFLUX = 0.
      DIV = 2*(FLUXPT - IK)
      DTAULT = TAURGE/(2.*DIV)
      IF (DTAULT.GT.0.3) DTAULT = 0.3
      TAUCHG = 2.5*TAURGE
      IF (TAUCHG.GT.DIV) DIV = TAUCHG
      DELTAP = (PBTM - P)/DIV
      DO 350 IC = 1,3
      DO 335 IS = 1,MOLS
      IRGIME(IS) = 1
      DO 335 IP = 1,2
  335 INTGRL(IS,IP) = 0.
      P = PTAB(IK) + DELTAP
C
C  LINEAR INTERPOLATION OF NEW  T  AT NEW  P
C
      LAG1 = FLUXPT - 1
      DO 370 LAG = IK,LAG1
      IF (P.LT.PTAB(LAG)) GO TO 380
  370 CONTINUE
      LAG = FLUXPT
  380 ISTART = LAG - 1
      M = (TEMP(ISTART+1)-TEMP(ISTART))/(PTAB(ISTART+1)
     1   - PTAB(ISTART))
      T = M*(P - PTAB(ISTART)) + TEMP(ISTART)
      TAU = OPACTY(I,T,P,DELTAP)
      IF (TAU.LE.0.4.OR.IC.EQ.3) GO TO 360
      DELTAP = 0.04*DELTAP/(TAU*TAU)
      IF (DELTAP.GE.(1.E-6*P)) GO TO 350
      DELTAP = 1.E-6*P
      GO TO 360
  350 CONTINUE
  360 DTAU2 = TAU
C
C  COMPUTES THE EXPONENTIAL AND PLANCK FUNCTIONS
C
  410 EXPON = BK2/T
      IF (TAU.LE.0.) GO TO 423
      IF (EXPON.GT.30.) GO TO 510
      BNEW = BK1/(EXP(EXPON) - 1.)
      E2NEW = E2(TAU)
      EXPT = EXP(-TAU)
      E3NEW = (EXPT - TAU*E2NEW)/2.
      E4NEW = (EXPT - TAU*E3NEW)/3.
C
C  INTEGRATION OF (2.8)
C
      DE3 = E3OLD - E3NEW
      DE4DT2 = 0.
      IF (DTAU2.GT.0.) DE4DT2 = 2.*(E4OLD - E4NEW)/DTAU2
      DFLUX = PI*((BNEW + BOLD)*DE3 + (BNEW - BOLD)*(DE4DT2
```

```
     1    - E3OLD - E3NEW))
      FLUXO = FLUXO + DFLUX
      FLUX(IK,2) = FLUX(IK,2) + DFLUX
      IF (STOP.EQ.1) GO TO 490
      IF (TAU.GT.20.) GO TO 510
  420 OLDFLX = DFLUX
      E2OLD = E2NEW
      E3OLD = E3NEW
      E4OLD = E4NEW
      BOLD = BNEW
      TAUOLD = TAU
      DFLUX = 0.
  423 POLD = P
      P = P + DELTAP
      IF (P.LT.PBTM) GO TO 430
C
C  BOTTOM OF ATMOSPHERE
C
      IF (STOP.EQ.1) GO TO 490
      STOP = 1
      T = TEMP(FLUXPT)
      DO 425 IS = 1,MOLS
      DO 425 IPL = 1,2
  425 F1(IS,IPL) = F2(IS,IPL)
      TAU = OPACTY(I,T,PBTM,PBTM - POLD)
      DTAU2 = TAU - TAUOLD
      P = PBTM
      GO TO 410
C
C  SETS UP NEW  P AND FINDS NEW  T  AND OPTICAL DEPTH


C
  430 IF (P.LT.PTAB(ISTART + 1)) GO TO 460
  440 ISTART = ISTART + 1
      IF (P.GE.PTAB(ISTART + 1)) GO TO 440
      M = (TEMP(ISTART+1)-TEMP(ISTART))/(PTAB(ISTART+1)-
     1   PTAB(ISTART))
  460 T = M*(P - PTAB(ISTART)) + TEMP(ISTART)
      DO 470 IS = 1,MOLS
      DO 470 IPL = 1,2
  470 F1(IS,IPL) = F2(IS,IPL)
      TAU = OPACTY(I,T,P,DELTAP)
      DTAU2 = TAU - TAUOLD
      IF (DTAU2.LE.DTAULT) DELTAP = 2.*DELTAP
      GO TO 410
  490 BFLUX = 2.*PI*E3NEW*BK1/(EXP(BK2/TEMP(FLUXPT)) - 1.)
  500 FLUX(IK,2) = FLUX(IK,2) + BFLUX
  510 CONTINUE
C
C  EVALUATES THE TOTAL FLUX AT EACH SAMPLE POINT
C
      TOTFLX(IK) = FLUX(IK,2) - FLUX(IK,1)
  520 CONTINUE
      IF (ITER.GE.ITLMT) GO TO 660
      WRITE (6, 7) ITER
```

```
      WRITE (7,7) ITER
      WRITE (6, 8)(PTAB(IP),TEMP(IP),TOTFLX(IP),TAUPT(IP),
     1   IP = 1,FLUXPT)
      WRITE (7, 8)(PTAB(IP),TEMP(IP),TOTFLX(IP),TAUPT(IP),
     1   IP = 1,FLUXPT)
      WRITE (6, 10)
      TSTFLX = 0.05*TFLUX
      DO 530 IK = 1,FLUXPT
      IF (ABS(TOTFLX(IK) - TFLUX).GT.TSTFLX) GO TO 540
  530 CONTINUE
      GO TO 660
  540 CALL COEFFT(FLUXPT,TAUPT,COEFF)
  877 CONTINUE
C
C  TEMPERATURE ITERATION ROUTINE
C
      DO 895 IAPROX = 1,LPLMT
      DO 850 IK = 1,FLUXPT
      SUM = 0.
      DO 840 ISUM = 1,FLUXPT
  840 SUM = SUM + COEFF(IK,ISUM)*B(ISUM)
      FACTOR(IK) = SUM/TOTFLX(IK)
  850 CONTINUE
      RATIO = (TFLUX/TOTFLX(1))**1.333
      IF (RATIO.GT.5.) RATIO = 5.
      IF (RATIO.LT.0.2) RATIO = 0.2
      T4N(1) = T4(1)*RATIO
      DO 630 IK = 2,FLUXPT
      RATIO = (TFLUX/TOTFLX(IK))**1.333
      IF (RATIO.GT.5.) RATIO = 5.
      IF (RATIO.LT.0.2) RATIO = 0.2
  630 T4N(IK) = T4N(IK-1) + (T4(IK) - T4(IK-1))*RATIO
  635 DO 640 IK = 1,FLUXPT
      T4(IK) = T4N(IK)
  640 TEMP(IK) = SQRT(SQRT(T4(IK)))
      CALL TAUGRY(TAUPT,B)
      CALL COEFFT (FLUXPT,TAUPT,COEFF)
      DO 570 IK = 1,FLUXPT
      TOTFLX(IK) = 0.
      DO 890 J = 1,FLUXPT
  890 TOTFLX(IK) = TOTFLX(IK) + COEFF(IK,J)*B(J)
  570 TOTFLX(IK) = TOTFLX(IK)/FACTOR(IK)
      WRITE (6,21) IAPROX
      WRITE (7,21) IAPROX
   21 FORMAT (6X,'LOOP ',I1,4X,'PRESSURE    TEMP      FLUX',
     1   7X,'TAU',/)
      WRITE (6,8) (PTAB(IP),TEMP(IP),TOTFLX(IP),TAUPT(IP),
     1   IP = 1,FLUXPT)
      WRITE (7,8) (PTAB(IP),TEMP(IP),TOTFLX(IP),TAUPT(IP),
     1   IP = 1,FLUXPT)
      WRITE(6,10)
  895 CONTINUE
  650 CONTINUE
  660 CONTINUE
```

```
      IF (ITLMT.NE.1) CALL PARAM
      NPT = 6
      IF (ITLMT.EQ.1) NPT = 7
      WRITE (NPT, 4) TFLUX
      WRITE (NPT, 5) THICK(1),DENSE(1),PEVAL(1),TEMP(1),
     1   TOTFLX(1)
      WRITE (NPT, 6)(THICK(IP),ATM(IP),DENSE(IP),PEVAL(IP),
     1  TEMP(IP),TOTFLX(IP),STABLE(IP), IP = 2,FLUXPT)
      STOP
      END

      SUBROUTINE COEFFT(FLUXPT,TAUPT,COEFF)
C
C  COMPUTES COEFFICIENTS NEEDED BY (2.21) AND (2.22)
C
      DIMENSION TAUPT(15),COEFF(15,15),XUP(15),YUP(15),
     1          XDN(15),YDN(15)
      INTEGER FLUXPT
      E2APRX(TAU) = EXP(-TAU)*(1.-TAU*(ALOG((TAU+1.)/TAU) -
     1  0.4/(TAU + 1.)**2))
      PI2 = 6.2831853
      DO 820 IK = 1,FLUXPT
      E3BDRY = 0.5
      IF (IK.EQ.FLUXPT) GO TO 740
      E2OLD = 1.
      E3OLD = 0.5
      E4OLD = 0.3333333
      IKCU = FLUXPT - 1
      DO 730 IKC = IK,IKCU
      TAUUP = TAUPT(IKC+1) - TAUPT(IK)
      E2NEW = E2APRX(TAUUP)
      E3NEW = 0.5*(EXP(-TAUUP) - TAUUP*E2NEW)
      E4NEW = (EXP(-TAUUP) - TAUUP*E3NEW)/3.
      XUP(IKC) = 0.5*(E3OLD - E3NEW)
      YUP(IKC) = (E4OLD - E4NEW)/(TAUPT(IKC+1)-TAUPT(IKC))
     1  - (E3OLD + E3NEW)/2.
      E2OLD = E2NEW
      E3OLD = E3NEW
  730 E4OLD = E4NEW
      E3BDRY = E3NEW
      XDN(1) = 0.
      YDN(1) = 0.
      IF (IK.EQ.1) GO TO 780
  740 E2OLD = 1.
      E3OLD = 0.5
      E4OLD = 0.3333333
      DO 750 IKC = 2,IK
      IKR = IK + 1 - IKC
      TAUDN = TAUPT(IK) - TAUPT(IKR)
      E2NEW = E2APRX(TAUDN)
      E3NEW = 0.5*(EXP(-TAUDN) - TAUDN*E2NEW)
      E4NEW = (EXP(-TAUDN) - TAUDN*E3NEW)/3.
      XDN(IKR+1) = 0.5*(E3OLD - E3NEW)
      YDN(IKR+1)  = (E4OLD - E4NEW)/(TAUPT(IKR+1) - TAUPT(IKR))
```

```
     1    - (E3OLD + E3NEW)/2.
      E2OLD = E2NEW
      E3OLD = E3NEW
  750 E4OLD = E4NEW
      IKCU = IK - 1
      DO 770 J = 1,IKCU
  770 COEFF(IK,J) = - (XDN(J+1) + YDN(J+1) + XDN(J) - YDN(J))
     1    *PI2
      XUP(FLUXPT) = 0.
      YUP(FLUXPT) = 0.
      IF (IK.EQ.FLUXPT) GO TO 800
  780 IKCL = IK + 1
      DO 790 J = IKCL,FLUXPT
  790 COEFF(IK,J) = (XUP(J) - YUP(J) + XUP(J-1) + YUP(J-1))*PI2
  800 COEFF(IK,IK) = (XUP(IK)-XDN(IK)-YUP(IK)+YDN(IK))*PI2
      COEFF(IK,FLUXPT) = COEFF(IK,FLUXPT) + E3BDRY*PI2
  820 CONTINUE
      RETURN
      END

      SUBROUTINE PARAM
C
C  COMPUTES THE ONSET OF CONVECTION & OTHER PARAMETERS
C
      DIMENSION TEMP(15),ATM(15),PTAB(15),THICK(15),DENSE(15),
     1           PEVAL(15),XLAG(3),YLAG(3),STABLE(15)
      REAL MOLWT,K1,K2,K3,M
      INTEGER FREQPT,FLUXPT
      COMMON /ALL/ FLUXPT,FREQPT,PTAB,TEMP,K1,K2,K3
      COMMON /RST/ DENSE,THICK,ATM,PEVAL,CONV,STABLE,MOLWT
      P1 = PTAB(1)
      DP = 0.2*(PTAB(2) - PTAB(1))
      PEVAL(1) = PTAB(1)
      T = TEMP(1)
      DENSE(1) = K2*P1/T
      THICK(1) = 0.
      DEPTH = 0.
      DO 100 IT = 1,3
      XLAG(IT) = PTAB(IT)
  100 YLAG(IT) = TEMP(IT)
      M = (TEMP(2) - TEMP(1))/(PTAB(2) - PTAB(1))
      IK = 2
      TSTLP = PTAB(IK)
      DO 150 K = 1,2000
C
C  CALCULATES THE PHYSICAL DEPTH
C
      P2 = P1 + DP
      TOLD = T
      T = M*(P2 - PTAB(IK-1)) + TEMP(IK-1)
      AVE = (T + TOLD)/(P2 + P1)
      Z = K3*DP*AVE
      DEPTH = DEPTH + Z
  110 IF (P2.LT.(0.999*TSTLP)) GO TO 140
```

```
      DENSE(IK) = K2/AVE
      THICK(IK) = DEPTH/1000.
      ATM(IK) = 0.285*P2/MOLWT
C
C  TEST FOR SCHWARZSCHILD CRITERION
C
      CALL DLG3PT(P2,XLAG,YLAG,DTDP)
      STABLE(IK) = CONV*AVE - DTDP
      PEVAL(IK) = P2
      IF (IK.GE.FLUXPT) GO TO 160
      ISTART = IK
      IF (ISTART.GT.(FLUXPT-2)) ISTART = FLUXPT - 2
      DO 130 LAG = 1,3
      XLAG(LAG) = PTAB(ISTART + LAG - 1)
  130 YLAG(LAG) = TEMP(ISTART + LAG - 1)
      IK = IK + 1
      M = (TEMP(IK) - TEMP(IK-1))/(PTAB(IK) - PTAB(IK-1))
      TSTLP = PTAB(IK)
      PDIFF = TSTLP - PTAB(IK-1)
      NDIV = 0.2*PDIFF
      DIV = NDIV
      IF (DIV.LT.5.) DIV = 5.
      DP = PDIFF/DIV
  140 P1 = P2
  150 CONTINUE
  160 ALTUDE = THICK(FLUXPT)
      DO 170 IK = 1,FLUXPT
  170 THICK(IK) = ALTUDE - THICK(IK)
      RETURN
      END

      FUNCTION OPACTY (I,T,P,DELTAP)
C
C  COMPUTES OPACITY USING (3.6) AND (3.7)
C
      DIMENSION R(15,5,2),S(15,5,2),TI(15,5,2),C(15,5,2),
     1          REGIME(15,5,2),IRGIME(5),TYPE(5),INTGRL(5,2),
     2          F1(5,2),F2(5,2),K4(5,2),RANGE(15,5,2),
     3          IRGE(15,5)
      INTEGER TYPE
      REAL K4,INTGRL
      COMMON /OPAC/ IRGIME,INTGRL,F1,F2,K4
      COMMON /INTTAU/ R,S,TI,C,REGIME,TYPE,MOLS,RANGE,IRGE
      OPACTY = 0.
      DO 500 IS = 1,MOLS
      IF (C(I,IS,1).LE.(-0.5)) GO TO 500
      JP = IRGIME(IS)
      IPLL = IRGE(I,IS)
      IF (TYPE(IS).EQ.2) GO TO 200
      DO 100 IPL = JP,IPLL
      F2(IS,IPL) = (C(I,IS,IPL)*P**S(I,IS,IPL)*T**TI(I,IS,IPL))
     1   **(1./R(I,IS,IPL))
  100 INTGRL(IS,IPL) = INTGRL(IS,IPL) + (F1(IS,IPL) +
     1      F2(IS,IPL))*DELTAP
```

```
      TAU = K4(IS,JP)*INTGRL(IS,JP)**R(I,IS,JP)
      IF (TAU.LT.REGIME(I,IS,JP)) GO TO 400
      TAU2 = K4(IS,2)*INTGRL(IS,2)**R(I,IS,2)
      IF (TAU.GT.RANGE(I,IS,JP)) GO TO 350
      TAUNEW = (TAU*(RANGE(I,IS,1) - TAU) + TAU2*(TAU -
     1  REGIME(I,IS,1)))/(RANGE(I,IS,1) - REGIME(I,IS,1))
      TAU = TAUNEW
      GO TO 400
  200 DO 300 IPL = JP,IPLL
      CG = TI(I,IS,IPL) + C(I,IS,IPL)/T
      IF (CG.LE.0.) GO TO 500
      F2(IS,IPL) = CG*P
  300 INTGRL(IS,IPL) = INTGRL(IS,IPL) + (F1(IS,IPL) +
     1  F2(IS,IPL))*DELTAP
      TAU = K4(IS,JP)*INTGRL(IS,JP)
      IF (TAU.LT.REGIME(I,IS,JP)) GO TO 400
      TAU2 = K4(IS,2)*INTGRL(IS,2)
      IF (TAU.GT.RANGE(I,IS,JP)) GO TO 350
      TAUNEW = (TAU*(RANGE(I,IS,1) - TAU) + TAU2*(TAU -
     1  REGIME(I,IS,1)))/(RANGE(I,IS,1) - REGIME(I,IS,1))
      TAU = TAUNEW
      GO TO 400
  350 TAU = TAU2
      IRGIME(IS) = 2
  400 OPACTY = OPACTY + TAU
  500 CONTINUE
      RETURN
      END

      SUBROUTINE DLG3PT (X,A,YA,Y)
C
C  DERIVATIVE USING LAGRANGIAN THREE POINT INTERPOLATION
C
C    A  IS THE ARRAY OF  X0,X1,X2
C    YA  IS THE ARRAY OF  Y0,Y1,Y2
      DIMENSION A(3),B(3),D(3),YA(3)
      DO 1 I = 1,3
    1 D(I) = X - A(I)
      X12 = A(1) - A(2)
      X13 = A(1) - A(3)
      X23 = A(2) - A(3)
      B(1) = (D(2) + D(3))/(X12*X13)
      B(2) = -(D(1) + D(3))/(X12*X23)
      B(3) = (D(1) + D(2))/(X13*X23)
      Y = B(1)*YA(1) + B(2)*YA(2) + B(3)*YA(3)
      RETURN
      END

      FUNCTION E2(XX)
C
C  COMPUTES THE SECOND EXPONENTIAL INTEGRAL
C
      DOUBLE PRECISION X,DLOG,DEXP
      X = DBLE(XX)
```

```
      IF (X.LE.1.D0) E2 = DEXP(-X) - X*(-DLOG(X) -
     1        0.57721566D0 + X*(0.99999193D0 - X*(
     2        0.24991055D0 - X*(0.05519968D0 - X*(
     3        0.00976004D0 - X*0.00107857D0)))))
      IF (X.GT.1.D0) E2 = DEXP(-X)*(1.D0 - (0.2677737343D0 +
     1        X*(8.6347608925D0 + X*(18.059016973D0 + X*(
     2        8.573328401D0 + X))))/(3.9584969228D0 + X*(
     3        21.099653027D0 + X*(25.6329561486D0 + X*(
     4        9.5733223454D0 + X)))))
      RETURN
      END

      SUBROUTINE TAUGRY(TAUPT,B)
C
C  COMPUTES THE AVERAGE OPTICAL DEPTH
C
      DIMENSION TEMP(15),PTAB(15),DFREQ(15),S(15,5,2),R(15,5,2),
     1          C(15,5,2),TI(15,5,2),SPEC(5),MWT(5),B1(15),
     2          B2(15),B(15),TYPE(5),FP(5),TAUPT(15),INTGRL(2),
     3          F1(15,5,2),F2(15,5,2),REGIME(15,5,2),
     4          IRGE(15,5),TAU(15,5),TAUJ(2),IRGIME(15,5),
     5          RANGE(15,5,2)
      REAL K1,K2,K3,K4,K5,MWT,INTGRL
      INTEGER FLUXPT,FREQPT, TYPE
      COMMON /ALL/ FLUXPT,FREQPT,PTAB,TEMP,K1,K2,K3
      COMMON /INT/ B1,B2,FP,TEFF,SPEC,MWT,DFREQ
      COMMON /INTTAU/ R,S,TI,C,REGIME,TYPE,MOLS,RANGE,IRGE
      TAUPT(1) = 0.
      DO 100 I = 1,FREQPT
      FREQT = FREQT + DFREQ(I)
      DO 100 IS = 1,MOLS
      TAU(I,IS) = 0.
      DO 100 JP = 1,2
  100 IRGIME(I,IS) = 1
      DO 150 IK = 1,FLUXPT
      P = PTAB(IK)
      T = TEMP(IK)
      SUM = 0.
      B(IK) = 0.
      DO 110 I = 1,FREQPT
      DO 110 IS = 1,MOLS
      IPLL = IRGE(I,IS)
      DO 110 JP = 1,IPLL
      F2(I,IS,JP) = 0.
      IF (C(I,IS,1).LE.(-0.5)) GO TO 110
      IF (TYPE(IS).EQ.2) GO TO 107
      F2(I,IS,JP) = (C(I,IS,JP)*P**S(I,IS,JP)*T**TI(I,IS,JP))
     1     **(1./R(I,IS,JP))
      GO TO 110
  107 CG = TI(I,IS,JP) + C(I,IS,JP)/T
      IF (CG.LE.0.) GO TO 110
      F2(I,IS,JP) = CG*P
  110 CONTINUE
      IF (IK.EQ.1) GO TO 140
```

```
      DELTAP = P - POLD
      DO 130 I = 1,FREQPT
      TAUSUM = 0.
      DO 125 IS = 1,MOLS
      IF (C(I,IS,1).LE.(-0.5)) GO TO 125
      IPL = IRGIME(I,IS)
      IPLL = IRGE(I,IS)
      DO 113 JP = IPL,IPLL
      INTGRL(JP) = 0.5*(F1(I,IS,JP) + F2(I,IS,JP))*DELTAP
      TAUJ(JP) = (SPEC(IS)*K1*INTGRL(JP)/MWT(IS))**R(I,IS,JP)
     1   *FP(IS)**S(I,IS,JP)
  113 CONTINUE
      TAUTST = TAU(I,IS) + TAUJ(IPL)
      IF (TAUTST.LT.REGIME(I,IS,IPL)) GO TO 120
      IF (TAUTST.GT.RANGE(I,IS,IPL)) GO TO 115
      TAUTS2 = TAU(I,IS) + TAUJ(2)
      TAUNEW = (TAUTST*(RANGE(I,IS,1)-TAUTST)+TAUTS2*(TAUTST-
     1   REGIME(I,IS,1))) /(RANGE(I,IS,1) - REGIME(I,IS,1))
      TAUSUM = TAUSUM + TAUNEW - TAU(I,IS)
      TAU(I,IS) = TAUNEW
      GO TO 125
  115 TAUTST = TAU(I,IS) + TAUJ(2)
      IRGIME(I,IS) = IRGE(I,IS)
      IPL = IRGE(I,IS)
  120 TAU(I,IS) = TAUTST
      TAUSUM = TAUSUM + TAUJ(IPL)
  125 CONTINUE
      BB = B1(I)/(EXP(B2(I)/T) - 1.)
      IF (TAUSUM.LE.60.) SUM = SUM + BB*EXP(-TAUSUM)
      B(IK) = B(IK) + BB
  130 CONTINUE
      TAUPT(IK) = TAUPT(IK-1) - ALOG(SUM/B(IK))
  140 POLD = P
      DO 150 I = 1,FREQPT
      DO 150 IS = 1,MOLS
      DO 150 JP = 1,2
      F1(I,IS,JP) = F2(I,IS,JP)
  150 CONTINUE
      DO 160 I = 1,FREQPT
  160 B(1) = B(1) + B1(I)/(EXP(B2(I)/TEMP(1)) - 1.)
      RETURN
      END
```

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