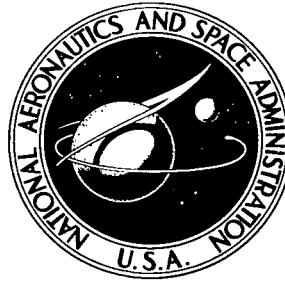


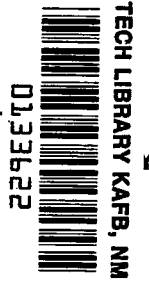
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**A ²⁴COMPUTER PROGRAM FOR CALCULATION
OF SPECTRAL RADIATIVE PROPERTIES
OF GAS MIXTURES**

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A COMPUTER PROGRAM FOR CALCULATION OF SPECTRAL RADIATIVE PROPERTIES OF GAS MIXTURES

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SUMMARY

A computer code is described whereby calculations of radiative properties of gas mixtures may be made. The program is arranged so that distinct radiative processes for each species are computed in individual subroutines. Provision is made for calculating radiative properties in nonequilibrium situations – separate rotational, vibrational, and electronic temperatures may be used. These features should provide a flexibility not currently available in such programs.

The basic equations and the program listing in FORTRAN IV language are presented. Sample calculations are given for high-temperature air and carbon dioxide and are compared to calculations made with previously developed programs.

INTRODUCTION

Radiative properties of gases are of interest for a variety of reasons, and a great number of complex and laborious experiments and calculations have been made on the subject. Basic radiative processes of gas constituents are of prime importance for application to energy-transfer problems such as occur in stellar and planetary atmospheres, combustion reactions, shock layers of reentry vehicles, and high-temperature plasmas.

The program described in this paper has been developed because of a continuing need for a more versatile and general code which can be used to predict the spectral radiative properties of a mixture of gases. Some programs for calculating such properties are in existence (refs. 1 to 5) and have been usefully applied to a number of radiative transfer problems (refs. 6 and 7). For example, the program of reference 1 has been written primarily for application to radiative flow-field problems at the sacrifice of spectral detail. The program of reference 2, on the other hand, provides considerable spectral detail but, because of the large storage requirements, has had more limited application to radiating flow fields. In addition, it was originally developed for radiating species of air, and generalization to arbitrary mixtures is somewhat involved.

This program has been developed in part from earlier programs written by the author for calculating specific radiative processes. A separate smeared-rotational-line band system program has been exercised previously on several occasions (ref. 8) and is included here as a subroutine. Other distinct processes are also handled by individual subroutines. It is felt that such an arrangement adds greatly to the versatility of the program in that it facilitates inclusion of modifications to the various computational procedures.

It is apparent from the literature dealing with gas radiative properties that basic input parameters require updating at frequent intervals. Such input changes should be straightforward and easily accomplished if a radiative-properties program is to retain its applicability. Throughout the development of the program described herein, considerable effort has been directed toward keeping the input simple and well defined. Since the object of the program is to compute radiative properties for a desired gas mixture, the radiative input data for an individual species comprise a completely independent unit containing all parameters required to calculate the radiance for that particular species. This feature greatly facilitates the inclusion or deletion of desired species from case to case and permits the existence of a readily usable punched-card input data file.

SYMBOLS

A	Einstein spontaneous transition probability, sec^{-1}
B	rotational spectroscopic constant, cm^{-1}
B_{λ}^0	Planck blackbody radiation function, $\text{W}/\text{m}^2\text{-}\mu\text{m}\text{-sr}$
c	speed of light, m/sec
E	energy level value, cm^{-1}
e	electronic charge, C
f	oscillator strength, or f-number
g	degeneracy
h	Planck constant, $\text{J}\text{-sec}$

I	ionization energy, cm^{-1}
j	radiative volume emission coefficient, $\text{W}/\text{m}^3\text{-}\mu\text{m}\text{-sr}$
k	Boltzmann constant, J/K
L	path length, m
M	particle molecular weight, kg/kg-mole
m	electron rest mass, kg
N	particle number density, m^{-3}
N_0	Avogadro number, m^{-3}
n	principal quantum number
p	pressure, N/m^2
Q	partition function
q	Franck-Condon factor
R	radiant intensity, $\text{W}/\text{m}^2\text{-}\mu\text{m}\text{-sr}$
R_Y	Rydberg constant
s	parameter in empirical formula (19)
T	temperature, K
v'	upper vibrational quantum number
v''	lower vibrational quantum number
W	integrated spectral radiant intensity, $\text{W}/\text{m}^2\text{-sr}$
w	line half-width, m

Z	degree of ionization
α	polarizability, cm^3
α'	spectroscopic constant for vibration-rotation interaction, cm^{-1}
β	parameter in empirical function (19)
γ	partition function parameter defined by equation (42), cm^{-1}
ϵ_0	permittivity of free space
λ	wavelength, m
μ	absorption coefficient, m^{-1}
ν	frequency, sec^{-1}
$\tilde{\nu}$	wave number, m^{-1}
σ	cross section, m^2
ρ	density, kg/m^3
ρ_0	density of air at standard temperature and pressure, kg/m^3
ω_e	vibrational spectroscopic constant, cm^{-1}
$\omega_e x_e$	vibrational spectroscopic constant, first anharmonic correction, cm^{-1}
$\omega_e y_e$	vibrational spectroscopic constant, second anharmonic correction, cm^{-1}

Subscripts:

A	general particle
D	Doppler broadening
e	electronic

eff	effective value
FB	free-bound process
FF	free-free process
H	hydrogen atom
L	individual atomic line
ℓ	lower energy level
N	general neutral particle
R	resonance broadening
r	rotational
S	Stark broadening
th	threshold value
u	upper energy level
v	vibrational
v'	upper vibrational quantum number
v''	lower vibrational quantum number
0	initial value

COMPUTATIONAL OUTLINE AND GENERAL PROGRAM DESCRIPTION

Basic radiative properties of various substances are well defined in the literature sources treating the subject. There is, however, wide diversity and nonuniversality of nomenclature existing in this field. The important basic properties used in this

paper will all be defined, therefore, and the governing equations used in the calculations will be developed with care.

The spectral intensity of the ultimate radiant emitter-absorber is described by the Planck blackbody function for specific intensity

$$B_{\lambda}^0(T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1} \quad (1)$$

The linear absorption coefficient μ is defined by the Lambert law of exponential attenuation of incident radiation R_0 over path length L

$$R = R_0 e^{-\mu L} \quad (2)$$

For an extended medium of absorption coefficient μ , which also emits radiation with volume emission coefficient j , Kirchhoff's law may be expressed as

$$j = \mu B_{\lambda}^0(T) \quad (3)$$

for media in local thermodynamic equilibrium. At a given condition, this equation may be written for a single radiative process; that is, j and μ for various processes are additive quantities at a given wavelength.

Another basic radiative property is the cross section for absorption, which is simply the absorption coefficient divided by the appropriate contributing particle-number density:

$$\sigma_A = \frac{\mu}{N_A} \quad (4)$$

In this program, μ and σ for the desired processes are computed as functions of wavelength and are used to obtain a value of j . The j 's are then summed for all species included to arrive at the overall spectral emission coefficient for the mixture.

For application to practical problems, the volume emission coefficient of an extended medium must be used in a radiative transfer equation which is integrated over the geometrical dimensions of the medium. The radiative transfer equation is generally difficult to solve, and only one specific case is dealt with here. This is the case of the one-dimensional slab of width L which extends to arbitrarily large dimensions in the other orthogonal directions. It may be shown that the emergent radiant intensity normal to the surface is given by

$$R = B_{\lambda}^0(T) \left(1 - e^{-\mu L}\right) \quad (5)$$

For an optically thin medium, that is, for $\mu L \ll 1$,

$$\frac{R}{L} \approx \mu B_{\lambda}^0 = j \quad (6)$$

To obtain the total energy emergent from a surface of the slab equation (5) is integrated over all wavelengths:

$$W = \int_0^{\infty} B_{\lambda}^0(T) \left(1 - e^{-\mu L}\right) d\lambda \quad (7)$$

This equation has been evaluated for several cases and compared to similar calculations performed with other programs.

The radiative processes for each species (free-free, free-bound, lines, etc.) are also handled separately in the program. Various models for computation of these processes exist, and those chosen for use in this program are described in detail in the text. Empirical formulas may often be employed advantageously because of the computational simplification achieved. Wherever these have been used in the program, the procedure is clearly outlined by which the empirical formulas are obtained from more detailed quantum-mechanical calculations.

Radiative transfer problems often occur in situations for which the various contributing processes take place at different effective temperatures. Examples of such situations are the zone of chemical nonequilibrium in shock layers and plasmas for which the ion and electron temperatures are different. For each of the processes included in the program, an option exists of having a different electron temperature as input. For the molecular band systems, electronic, vibrational, and rotational temperatures may be employed.

An indication of the computational procedure is shown in figure 1, where an abbreviated flow chart is presented. It is seen that the program consists of three sections:

- (1) The main program which handles input data and calls the various subroutines.
- (2) The group of subroutines which computes spectral radiative properties for each process.
- (3) The output section which accumulates and stores the various spectral properties as they are being computed and specifies the form of the final output.

Intermediate output for calculations of the specific radiative processes may also be obtained.

A program listing and detail on the FORTRAN coding is given after a description of the equations used for calculating the various radiative processes occurring in the following subroutines:

FFCON - computes free-free continua for all species

FBCON - computes free-bound continua for atoms and atomic ions

LINES - computes line radiation for atoms and atomic ions

SMEAR - computes molecular band radiation for molecules with smeared-rotational-line model

INFRA - computes infrared vibration-rotation spectra for molecules

RACOM - accumulates, sorts, and adds spectral emission and wavelength points

PUTTY - output section of program

These processes are included in the sample calculations given later. Subroutines for other processes may be easily incorporated once a desirable computational procedure has been determined.

CALCULATION OF FREE-FREE RADIATION

Free-free radiation arises as a result of the process



in which a free electron e^- interacts with the coulomb field of another particle A . The consequent change in energy of the electron results in an emitted photon. The cross section for the process is normally evaluated in units of $(\text{length})^5$ which, when multiplied by the number density product $N_A N_e$, yields the linear absorption coefficient in reciprocal length units. Detailed quantum-mechanical calculations of these cross sections may be reliably made for relatively simple atoms and molecules. An excellent procedural outline on such calculations is given in the text by Armstrong and Nicholls (ref. 9).

The classical expression for the emission cross section of a free electron accelerated in the field of a particle of charge Z was developed by Kramers and may be written (see, for example, ref. 10):

$$\sigma_{\text{FF}} = \frac{16\pi^2}{3\sqrt{3}} \frac{e^6}{hc^4 (2\pi m_e)^{3/2}} \frac{\lambda^3 Z^2}{(kT)^{1/2}} \frac{1}{(4\pi\epsilon_0)^3} \quad (8)$$

The corresponding emission coefficient resulting from the use of equations (1) and (3) is

$$j = \frac{32\pi^2}{3\sqrt{3}} \frac{Z^2 e^6 N_e N_A \exp\left(-\frac{hc}{\lambda kT}\right)}{(4\pi\epsilon_0)^3 c^2 (2\pi m_e)^{3/2} (kT)^{1/2} \lambda^2} \quad (9)$$

with the factor $1 - \exp(-hc/\lambda kT)$ included to account for induced emission. For electrons interacting with ions, this expression appears to give reasonable results (see ref. 11), and has been used in the program in this form.

For electrons interacting with neutral particles, a first approach is to measure or deduce an effective Z^2 for the particle in question and to apply the Kramers equation (eq. (9)). This procedure may be used to give rough order-of-magnitude cross sections for a limited temperature and frequency range. In reference 3 such effective Z^2 parameters have been used over an extensive wavelength and temperature range, but the resultant inaccuracies are minor since free-free radiation from neutral particles is not a significant contributing process in the overall radiance of high-temperature equilibrium gas mixtures.

Detailed calculations of neutral Bremsstrahlung (refs. 12 and 13) indicate that an effective Z^2 must be a function of λ and T . The cross-section calculations of reference 12 have been used here to evaluate an approximate wavelength and temperature dependence of such an effective Z^2 . This variation has then been incorporated into equation (9) with $Z^2 = Z_{\text{eff}}^2$, which has been used in the neutral free-free radiation contributions of the program. The term Z_{eff}^2 is determined from the empirical formula which fits the calculations of references 12 and 13:

$$Z_{\text{eff}}^2 = Z_N^2 \left[3(10)^{-10} \frac{(\lambda T - 20\,000)^2}{\lambda^{5/2}} \right] + T^{5/2} (10)^{-10} \quad (10)$$

where λ is in units of μm and Z_N^2 is now an empirical constant. Since equation (10) only approximates the λ, T dependence of Z_{eff}^2 , Z_N^2 has been evaluated at $T = 10\,000\text{ K}$, $\lambda = 2\ \mu\text{m}$ in order to match cross-section data of references 12 and 13.

Where detailed cross-section calculations are not available, another approach has been utilized. An approximate free-free absorption cross-section formula has been derived in reference 14 for highly polarizable neutral atoms. The polarizability α of a neutral particle has been used to estimate the free-free absorption cross section as

$$\sigma_{\text{FF}} = 1.62(10)^{-31} \sqrt{\alpha} \lambda^3 T \quad (11)$$

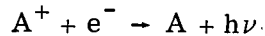
Comparison with equation (8) indicates that Z_{eff}^2 should be given by

$$Z_{\text{eff}}^2 = 11\,900T^{3/2}\sqrt{\alpha} \quad (12)$$

(The constants in eqs. (11) and (12) apply when λ is in μm and α is in cm^3 .) The accuracy of equation (11) is best at high temperatures (above about 10 000 K). Its applicability also decreases as α decreases. However, the values of Z_{eff}^2 determined from equation (10) compare rather favorably with those deduced from equation (12) (at $T = 10\,000\text{ K}$), and use has been made of equation (12) when detailed cross-section calculations have not been available. Table I gives the Z_{N}^2 used for all neutral particles in the illustrative calculations presented later. A comparison of σ_{FF} determined from equations (8) and (10) with the cross sections of reference 12 for the carbon atom is given in table II. The agreement over the range of T and λ is typical for the other species considered thus far.

CALCULATION OF FREE-BOUND RADIATION

As its name implies, free-bound radiation occurs when a free electron combines with an ion and excess energy is emitted as a photon; thus



The absorption cross section (for the inverse process) may be expressed by a relatively simple equation for the hydrogen atom (see, for example, ref. 10):

$$\sigma_{\text{FB,H}} = \frac{64\pi^4}{3\sqrt{3}} \frac{e^{10} m_e Z^4 \lambda^3}{h^6 c^4 n^5 (4\pi\epsilon_0)^5} \quad (13)$$

In order to account for the nonhydrogenic species, several factors should be taken into consideration. For the absorption process, only allowed transitions between the parent atom and its ion should be included. In addition, the hydrogenic formula (13) is inaccurate for transitions involving the lower lying states of the parent atom. It becomes increasingly more applicable for higher levels, or increasing values of n . In the present version of the program equation (13) is used for $n \geq 3$.

As is done in reference 15, an effective Z^2 is defined by

$$Z_{\text{eff,FB}}^2 = n^2 \left(\frac{E_u - E_l}{R_Y} \right) \quad (14)$$

The cross section then becomes

$$\sigma(n) = \frac{64\pi^4 e^{10} m_e Z^4 \lambda^3}{3\sqrt{3} (4\pi\epsilon_0)^5 h^6 c^4 n^5} \quad (15)$$

For the hydrogen-like particle of ionization energy I ,

$$E_\ell = I - \frac{I}{n^2} \quad E_u = I$$

$$\sigma_n = \frac{64\pi^4 e^{10} m_e \lambda^3 I^2}{3\sqrt{3} (4\pi\epsilon_0)^5 h^6 c^4 R_Y^2 n^5} \quad (16)$$

The absorption coefficient is found by summing the product of $\sigma(n)$ and the particle number density in level n :

$$\mu = \frac{2NI^2}{Q} \frac{64\pi^4 e^{10} m_e \lambda^3}{3\sqrt{3} (4\pi\epsilon_0)^5 h^6 c^4 R_Y^2} \sum_n \frac{1}{n^3} \exp \frac{I}{n^2 kT} \quad (17)$$

$$\mu = \sum_n N(n) \sigma(n) = \frac{N}{Q} \sum_n g(n) \sigma(n) \exp \frac{-E_\ell}{kT} \quad (18)$$

where the approximate hydrogenic upper-level degeneracy, $g(n) = 2n^2$ has been used.

As with the free-free processes, detailed quantum-theory calculations for a variety of simple species are available, and for computational convenience some measure of empiricism is desirable. It is particularly important to account for nonclassical effects for the lower lying levels of nonhydrogenic species. The deviation from hydrogenic cross sections is most severe for these levels, and for high-temperature transfer calculations transitions involving these levels are among the most important contributors. A relatively large number of such free-bound cross sections are reported in the literature and have been calculated in various degrees of detail. Due to the importance of N and O atoms in atmospheric photochemical processes and shock layers of reentry vehicles, their free-bound behavior has been studied rather extensively, both experimentally and theoretically (see refs. 16, 17, and 18). More recently, the determination that Mars and Venus have atmospheres composed primarily of CO₂ has led to increased study of the radiative properties of carbon (see refs. 18, 19, and 20).

A large number of ground-state connected free-bound cross sections are reported in reference 21. Each of the cross sections is represented by an empirical formula:

$$\sigma_{\text{FB}} = \sigma_{\text{th}} \left[\beta \left(\frac{\lambda}{\lambda_{\text{th}}} \right)^s + (1 - \beta) \left(\frac{\lambda}{\lambda_{\text{th}}} \right)^{s+1} \right] \quad \lambda \leq \lambda_{\text{th}} \quad (19)$$

The parameters s and β have been determined so that a close fit between equation (19) and a detailed wave-function calculation is obtained. The function (19) is used in the present version of the program, and values of parameters s and β as given in reference 21 for C, N, and O atoms are used as input. Calculations of σ_{FB} for these atoms using equations (15) and (19) in combination are given in table III.

CALCULATION OF LINE RADIATION

The radiation emitted when electronically excited atoms undergo transitions to lower levels gives rise to line radiation of wavelength $\lambda_{\ell u}$, in which the photon energy of such a transition is

$$\frac{hc}{\lambda_{\ell u}} = E_u - E_\ell \quad (20)$$

The radiant intensity of the line is given by

$$I_{u\ell} = \frac{1}{4\pi} N_u A_{u\ell} \frac{hc}{\lambda_{\ell u}} \quad (21)$$

where $A_{u\ell}$ is the Einstein coefficient or spontaneous transition probability. The relationship between the spontaneous transition probability and the absorption oscillator strength, or f-number, is (see, for example, ref. 22):

$$A_{u\ell} = \frac{g_\ell}{g_u} \frac{8\pi^2 e^2 f_{\ell u}}{m_e c \lambda^2 4\pi\epsilon_0} \quad (22)$$

Since

$$\frac{N_u}{N_\ell} = \frac{g_u}{g_\ell} \exp \frac{-hc}{\lambda_{\ell u} kT} \quad (23)$$

and

$$N_{\ell} = \frac{N}{Q} g_{\ell} \exp \frac{-E_{\ell}}{kT} \quad (24)$$

the volume emission coefficient for an individual atomic line may be written as

$$j_{\mathbf{L}} = \frac{2he^2}{(4\pi\epsilon_0)m_e} \frac{N}{Q} \frac{g_{\ell} f_{\ell u}}{\lambda_{\ell u}^3} \frac{\exp \frac{-(E_{\ell} + hc)}{\lambda_{\ell u}}}{kT} \quad (25)$$

This equation is used in the present calculations for line radiancies. The expression gives only the total power radiated in the transition, with no information about the spectral profile of the line.

Spectral-line profiles are almost entirely dependent on the state of the medium in which the line is emitted (p , T , N_e , etc.). The inclusion of the various line-broadening mechanisms into a prediction of half-widths for polyelectronic atoms is very complicated, usually accompanied with a significant degree of uncertainty. In high-temperature plasmas, however, the energy contained in the wings of the lines is of importance and broadening must be accounted for. Several good state-of-the-art approaches to this problem are described in a number of sources. See, for example, references 9, 10, 22, and 23. These references indicate that a function describing combined Doppler and collision broadening is best for the majority of applications. One such function is commonly referred to as the Voigt profile (ref. 9) and is relatively cumbersome mathematically. For this reason, it is often used for line-shape calculations in one of its asymptotic forms. Even though the Voigt function has not been incorporated into this program, it should be recognized that circumstances occur which warrant its use.

The collision, or Lorentz, profile is used for line calculations presented herein. It is particularly applicable to Stark broadening, which dominates in low-density ionized gases. As the degree of ionization in a gas decreases, the Lorentz profile becomes more conservative; that is, there is generally an overprediction of the radiant energy contained in the line wings.

The spectral emission coefficient for a Lorentz line is given by

$$j(\lambda) = \frac{j_{\mathbf{L}}}{\pi} \frac{w_{\mathbf{L}}}{(\lambda - \lambda_{u\ell})^2 + w_{\mathbf{L}}^2} \quad (26)$$

Using Kirchoff's law, the absorption coefficient may be written as

$$\mu_L(\lambda) = \frac{j_L}{\pi B(\lambda_{ul})} \frac{w_L}{(\lambda - \lambda_{ul})^2 + w_L^2} \quad (27)$$

The half-width of the line for Stark broadening w_{LS} is determined in this paper by the approximate formula described in reference 24:

$$w_{LS} = 5.7(10)^{-22} \frac{N_e n_{\text{eff}}^4 T^{-1/2}}{\lambda^2 (Z + 1)^2} \quad (28)$$

where the proportionality constant is valid for SI units. When the effective quantum number of the lower bound state n_{eff} is defined as

$$n_{\text{eff}}^4 = \frac{(Z + 1)^4 R_Y^2}{(I - E_\ell)^2} \quad (29)$$

the line half-width formula becomes

$$w_{LS} = 5.7(10)^{-22} \frac{(Z + 1)^2 \lambda^2 N_e R_Y^2}{T^{1/2} (I - E_\ell)^2} \quad (30)$$

Doppler broadening may contribute significantly at high temperatures and densities. Pure Doppler broadening results in a line shape with wings decaying exponentially instead of quadratically, as is found for the Lorentz shape. The half-width for Doppler broadening is given by

$$w_{LD} = \lambda \sqrt{\frac{2N_0 kT \log_e 2}{Mc^2}} \quad (31)$$

Resonance broadening is important for strong lines of a species in a mixture where this species has a large number density. Collisions between these identical particles have a much larger effect on line half-width than do collisions between unlike particles. The relationship for line half-width for this mechanism is (ref. 23)

$$w_{LR} = \frac{3\pi}{(4\pi\epsilon_0)} \frac{g_\ell}{g_u} N \frac{f_{\ell u} e^2 \lambda^3}{2\pi m_e c^2} \quad (32)$$

where N is the number density of the particular species involved. The line shape for resonance broadening is Lorentzian.

Equations (25) and (26) have been used to compute line radiation from atoms and ions in all illustrative calculations presented later. The line half-width has been taken to be the sum of the half-widths of the Stark and resonance broadening processes previously described

$$w_L = w_{LS} + w_{LR} + w_{LD} \quad (33)$$

Where Doppler broadening is a significant mechanism, however, equation (33) applied to a Lorentzian profile would be inaccurate. In such circumstances, a Doppler or Voigt profile would be more appropriate. For the calculations presented here, and for a wide range of pressure and temperature, equation (33) provides sufficient accuracy.

All basic input data for atomic and ionic lines have been taken from reference 25. Included in the sample calculations are line contributions from the species C, C⁺, C⁺⁺, N, N⁺, O, and O⁺.

CALCULATION OF DIATOMIC MOLECULAR ELECTRONIC BAND SPECTRA

The radiation resulting from transitions between electronic states in molecules is much more complex than the corresponding atomic process. This complexity is due to the additional degrees of freedom by rotation and vibration of the atoms composing the molecule. Instead of a single line, a many-line spectrum or band system results and is seen in a generally well-defined pattern over an extensive wavelength region. The position of the individual lines of a band system is determined by the vibrational and rotational levels within the two electronic states involved in the transition. The spacing between individual lines arising from adjacent rotational levels is usually very narrow, and a commonly used spectral model has been developed which treats these closely spaced lines as a continuum. This model is usually referred to in the literature as the "smeared-line" model, and detailed derivations may be found in references 26 and 27.

The positions of the various band heads of a band system are determined by the vibrational levels of the two electronic states

$$\lambda_{v'v''} = \frac{hc}{(E_u - E_l)} \quad (34)$$

where

$$E_u(v') = E_u(0) + hc \left[\omega_e \left(v' + \frac{1}{2} \right) - \omega_e x_e \left(v' + \frac{1}{2} \right)^2 + \omega_e y_e \left(v' + \frac{1}{2} \right)^3 \right] \quad (35)$$

and

$$E_\ell(v'') = E_\ell(0) + hc \left[\omega_e \left(v'' + \frac{1}{2} \right) - \omega_e x_e \left(v'' + \frac{1}{2} \right)^2 + \omega_e y_e \left(v'' + \frac{1}{2} \right)^3 \right] \quad (36)$$

The spectral absorption coefficient for a molecular band system as derived in references 26 and 27 and modified to include separate electronic, vibrational, and rotational temperatures as has been done in reference 28 is given by

$$\mu(\lambda) = \frac{\pi e^2}{mc^2} N_\ell \frac{\lambda_{00}}{\lambda} f_{\ell u} \frac{B_\ell}{Q_v k T_r} \frac{\phi}{\pi \epsilon_0} \quad (37)$$

Here all energy terms and spectroscopic constants are considered to be in units of reciprocal length. The term λ_{00} refers to the band-head wavelength for $v' = v'' = 0$. The function ϕ gives the spectral variation throughout the band system resulting from the $v'' - v'$ transitions

$$\phi = \sum_{v'} \sum_{v''} \frac{q_{v'v''}}{|B_{v'} - B_{v''}|} \exp \left[-\frac{E_\ell(v'')}{kT_v} + \frac{hcB_{v''} \left(\frac{1}{\lambda} - \frac{1}{\lambda_{v'v''}} \right)}{T_v (B_{v'} - B_{v''})} \right] \quad (38)$$

The summation extends over the range of upper and lower vibrational quantum numbers and is nonzero only for (a) $\lambda > \lambda_{v'v''}$ when the band is red-shaded, and (b) $\lambda < \lambda_{v'v''}$ when the band is violet-shaded. The Franck-Condon factors $q_{v'v''}$ are evaluated from vibrational-state wave functions and a large number of sources exist in which these arrays are tabulated. For the present calculations, values listed in reference 28 have been used when possible. The quantities B_v appearing in equation (38) are found from

$$\left. \begin{aligned} B_{v''} &= B_\ell - \alpha'_\ell \left(v'' + \frac{1}{2} \right) \\ B_{v'} &= B_u - \alpha'_u \left(v' + \frac{1}{2} \right) \end{aligned} \right\} \quad (39)$$

The electronic absorption oscillator strength for the band system $f_{\ell u}$ is defined in reference 10 and is often assumed to be wavelength independent. As is pointed out in

references 29 and 30, such is not the case, and provision for a simple functional variation has been anticipated. Since the calculations appearing here have been carried out for purposes of comparison, however, no λ -dependence of $f_{\ell u}$ has been employed.

In order to evaluate the number density of particles in the absorbing state N_ℓ the partition function formula of reference 31 has been used

$$N_\ell = \frac{N}{\sum_n Q(n)} Q_\ell \quad (40)$$

where

$$Q_\ell = g_\ell \exp \frac{E_\ell(0)}{kT_e} \left(\frac{kT_r}{hcB_\ell} \right) \left(1 + \gamma_\ell \frac{T_v T_r}{T_v + T_r} \right) \left(1 - \exp \frac{hc\omega_{e\ell}}{kT_v} \right)^{-1} \quad (41)$$

and

$$\gamma_\ell = \frac{1}{\omega_{e,\ell}} \left(\frac{2\omega_e x_{e,\ell}}{\omega_{e,\ell}} + \frac{\alpha'_\ell}{B_\ell} + 8 \frac{B_\ell}{\omega_{e,\ell}} \right) \frac{hc}{k} \quad (42)$$

In the preceding equations, the form of the partition function has been slightly modified in order to account for different electronic, vibrational, and rotational temperatures.

The diatomic electronic band systems included in the present calculations are given in table IV with references to the input data for each band system. The data are presented later in a punched-card listing. Many band-system calculations have been made with this subroutine and appear to agree well with similar computations reported in references 26, 28, and 32. An example of the subroutine output plotted for the CO^+ comet tail band system is given in figure 2 where the effects of different rotational and vibrational temperatures are illustrated.

CALCULATION OF RADIANCE FROM INFRARED VIBRATION-ROTATION BANDS OF DIATOMIC MOLECULES

At moderate and low temperatures (below about 5000 K) the infrared emission-absorption properties of gases assume greater importance. In an emitting gas, the fractional portion of the radiant energy contained in the infrared generally increases with decreasing temperature, and molecular gases are less dissociated at lower temperatures.

Infrared vibration-rotation spectra arise as a result of transitions between vibrational levels within a given electronic state. This electronic state is commonly the ground state, since the pertinent temperatures are usually so low that a great majority of the molecules are in this state. In the calculations of this paper, only two diatomic species which are not homopolar are of importance (NO and CO) and results are presented for these. (Homopolar molecules such as N₂, O₂, H₂, etc., have no vibrational spectra due to the absence of a dipole moment.) The equations used should apply equally well for other species if adequate input data are available.

A model based on overlapping lines for these infrared bands has been developed by Breene (ref. 33) and is used in this program. The spectral absorption coefficient is given by

$$\mu_{v',v''}(\lambda) = \frac{\pi e^2}{m_e c^2} \frac{N \exp \frac{-E_{v'}}{kT}}{Q} \frac{\exp \frac{-hc(\Delta\tilde{\nu})^2}{4B_{v'}kT}}{4B_{v'}^2} \exp \frac{-hc(\Delta\tilde{\nu})}{2kT} |\Delta\tilde{\nu}| f_{v',v''} \quad (43)$$

where

$$\Delta\tilde{\nu} = \frac{1}{\lambda} - \frac{1}{\lambda_{v',v''}} \quad (44)$$

Here $f_{v',v''}$ is the oscillator strength for a given $v' - v''$ transition and $\lambda_{v',v''}$ is the corresponding wavelength at the band center. The vibrational energy levels are

$$E_{v''} = \left[\omega_e \left(v'' + \frac{1}{2} \right) - \omega_e x_e \left(v'' + \frac{1}{2} \right)^2 \right] hc \quad (45)$$

and the band-center wavelengths may be found from

$$\lambda_{v',v''} = \frac{hc}{(E_{v'} - E_{v''})} \quad (46)$$

The quantities $B_{v'}$ are computed from equation (39), and the partition function Q is given by

$$Q = \left(\sum_v \exp \frac{-E_v}{T} \right) \frac{kT}{hcB} \quad (47)$$

The individual band oscillator strengths may be computed from vibrational wave functions (refs. 34 and 35) or may be measured under conditions for which only one vibrational transition of the ground state is involved (ref. 10). The relationship between

ground-state vibrational transitions and those involving higher levels may then be used to determine other oscillator strengths. In reference 10, the ratios $f_{v',v''}/f_{10}$ are tabulated for the quantum-mechanical harmonic oscillator. For the present calculations, computed oscillator strengths for CO (ref. 35) and for NO (ref. 34) have been used. Equation (43) has been employed in the computation of the spectral profiles for the fundamental $\Delta v = 1$ and the first and second overtones $\Delta v = 2,3$ for these two species.

In figure 3 one of the NO calculations of Breene (ref. 33) has been essentially repeated. Minor differences appear, probably because fewer total vibrational levels have been included, and slight differences in partition-function calculation may exist. In figure 4 the present-program computation for CO is compared to the more refined calculation of reference 36. The agreement is shown to be good in the region of high absorption.

DESCRIPTION OF INPUT AND PROGRAM LISTING

The principal function of the main program is to define the case to be computed, read the input parameters for each species, and call the subroutines related to each particular radiance contribution. How this is accomplished is most readily seen from the main program listing (appendix A) and the description of the input deck setup and key variables. A schematic of a typical deck setup is shown in figure 5.

The first card to be read contains the following:

Card 1: $\left[\text{NSPEC, TT, ELEC} \right]$ Format (I3, 2E14.6)

NSPEC - total number of radiating species (does not include electrons)

TT - particle translational temperature, K

ELEC - electron number density, cm^{-3}

At this time a counter NSP is defined and is increased by 1 for each species encountered.

The data input which follows is in the form of subdecks, each relating to a particular species. These species decks are independent and may be arranged in any order, with the following exception: the first species should be an atom for which a free-free contribution is computed. The minimum of the wavelength range for this free-free must be the absolute minimum wavelength encountered in the remainder of the calculations. If it is not desired to include atomic species, input for a dummy species which does not contribute may be used to establish the minimum wavelength. Examples of dummy inputs may be found in the species input list (appendix B).

The subdecks relating to atomic or ionic species contain input for the free-free, free-bound, and line contributions, respectively. The first card in a species deck defines

the species and specifies its number density:

Card 1A [SPEC, ISPEC, NRAD, CON Format (A6, 2I3, E14.6)]

SPEC - species identifier (chemical symbol)

ISPEC - code distinguishing molecules from atoms (0 for atoms, 1 for molecules)

NRAD - number of radiative contributions for this species (for example, if only free-free and free-bound are to be calculated, NRAD = 2)

CON - species number density, cm^{-3}

For each contributing radiative process, a label card is read:

Card FF1 [TYRAD Format (7A10)]

TYRAD - describes type of process being computed (for example, CARBON ATOM LINE RADIATION)

For atomic or ionic species, the free-free input is read next:

Card FF2 [NEQ, NW, WMIN, DELW, ZZ Format (I2, I5, 3E14.6)]

NEQ - specifies whether this process is to be computed for a temperature other than the local translational temperature (NEQ = 0 for equilibrium calculations; otherwise its value is 1)

NW - number of wavelength points at which the free-free process is computed

DELW - increment between wavelength points, μm

ZZ - Z_N^2 appearing in equation (10)

At this time subroutine FFCOM is called and the radiance calculation is made. If NEQ = 1, an electron temperature, TTRON, Format (E14.6), is read and used in the calculation. The volume emission coefficient is computed for the specified number of wavelengths NW beginning at wavelength WMIN. In addition to the wavelength and emission coefficient, the cross section, absorption coefficient, blackbody function, and a running integral of the radiance are also included in the output.

If this is the first calculation, the wavelengths are placed in an array WF(L) and the corresponding emission coefficients in F(L). This procedure is carried out in order to establish the radiance versus wavelength function to which the remaining contributions are added as the calculation proceeds. In the remainder of the calculations, the spectral radiance functions for a specific process are defined as G(L) and WG(L). For each subsequent radiative process, G(L) and WG(L) are added to the existing function F(L) and WF(L) to yield a new F, WF array. This addition of each individual contribution to the accumulated spectral distribution is performed in subroutine RACOM.

For an atomic species, the free-bound contribution is computed next. (FORTRAN variables common to the various subroutines which have been previously defined will not be redefined.)

Card FB1 [TYRAD Format (7A10)]

Card FB2 [NEQ, NSTAT, NEDGE, XMIM, DELX Format (3I3, 2E14.6)]

NSTAT - the number of states included in the calculation of partition function

NEDGE - number of edges (thresholds for free-bound contributions)

XMIM - minimum wavelength, μm (must be greater than WMIN in first FBCON input)

DELX - wavelength increment establishing threshold discontinuity, μm (here always taken as 0.0001 μm)

Cards FB3 . . . [GA(I), EA(I), I = 1, NSTAT Format (F4.0, E14.6)]

GA(I) - degeneracy of state used in partition function calculation

EA(I) - energy of state used in partition function (units of equivalent degrees K)

Cards FB4 . . . [GL(I), PQN(I), EL(I), EU(I), I = 1, NEDGE Format (F4.0, 3E14.6)]

GL(I) - degeneracy of initial state

PQN(I) - principal quantum number of initial state

EL(I) - energy of initial state (equivalent K)

EU(I) - energy of final state, K (for the hydrogenic approximation, equation (18), EU(I) is the ionization energy of the particle)

Cards FB5 . . . [ESS(I), AL(I), SIG(I), I = 1, NEDGE Format (3F7.3)]

ESS(I) - parameter s in equation (19)

AL(I) - parameter β in equation (19)

SIG(I) - parameter σ in equation (19)

It is seen that both empirical and hydrogenic inputs are required for each edge. When the transition is to be computed empirically, s , β , and σ have their appropriate values and the corresponding hydrogenic inputs are nonzero arbitrary quantities, except PQN, which is zero. If the transition is to be calculated according to the hydrogenic approximation, cards FB4 have their proper values, while SIG is zero and ESS, AL are arbitrary

Card 7M: [TU, VU, VXU, VYU, BU] Format (5E14.6)]

TU - upper-state energy term

VU - upper-state vibrational energy term

VXU - upper-state vibrational first anharmonic energy term

VYU - upper-state vibrational second anharmonic energy term

BU - upper-state rotational energy term

These variables often appear in the literature as T_e , ω_e , $\omega_e x_e$, $\omega_e y_e$, and B_e , respectively, and are often given in units of cm^{-1} . The input data should be in equivalent K, which are hc/k ($=1.4388$) times the given quantities in cm^{-1} .

Card 8M: [TL, VL, VXL, VYL, BL] Format (5E14.6)]

Variables of card 8M are the corresponding lower-state quantities of card 7M, in the same units.

Cards 9M: [FC(KU, KL), KU = 1, KUM; KL = 1, KLM] Format (7E10.4)]

FC(KU, KL) - band-system Franck-Condon factor array

Card 10M: [WMIN, WMAX] Format (2E14.6)]

WMIN - minimum of wavelength range for which band contributes, μm

WMAX - maximum of wavelength range of band

At this time subroutine SMEAR is called and, as before, if $NEQ = 1$, a nonequilibrium case is indicated. For these band systems, however, three nonequilibrium temperatures are provided for:

TTRON - electronic temperature, K

TROT - rotational temperature, K

TVIBR - vibrational temperature, K

When required, these are read on one card (Format 3E14.6). The diatomic partition function is computed according to equations (40), (41), and (42).

In the smeared-line model, only two wavelength points per band are needed to define the spectral profile of the system. One of these wavelengths is at the band head, and another is located at some other wavelength toward the red or violet, contingent on the band shading. In this program, the second wavelength is located at a small increment ($0.0001 \mu\text{m}$) from the adjacent band head. For each band calculation, the number of wavelength points is twice the number of Franck-Condon factors. At each of these wavelengths the band radiance is then computed from equations (37), (38), (39), and (3), and the

subsequent G and WG arrays are added to the accumulated radiance function in RACOM, as before.

The free-free contribution for the molecule is computed next, and input parameters are identical to those described for the atoms; that is, cards FF1 and FF2.

For molecules having infrared vibration-rotation bands, the input is

Card IR1: [TYRAD Format (7A10)]

Card IR2: [RLAM, V0, V1, BE, ALE Format (5E14.6)]

RLAM - rotational spectroscopic constant, equivalent K

V0 - vibrational energy term, cm^{-1}

V1 - vibrational anharmonic constant, cm^{-1}

BE - rotational constant, cm^{-1}

ALE - vibration-rotation interaction constant, cm^{-1}

Card IR3: [NEQ, NV, NW, WMIN, DW Format (3I4, 2E14.6)]

NV - number of vibrational transitions included

NW - number of wavelength points used

WMIN - maximum wave-number value, cm^{-1} (this corresponds to the shortest wavelength)

DW - wave-number increment, cm^{-1}

Cards IR4: [FNR(I), I = 1, NV Format (7E10.4)]

FNR(I) - vibrational transition oscillator strengths

Subroutine INFRA is entered and, if a nonequilibrium calculation is specified, electronic, rotational, and vibrational temperatures are required as inputs in the same manner as with the electronic band systems. The band frequencies for the fundamental and first two harmonics are computed from equations (45) and (46), and equation (47) is used to compute the partition function. Then, for each of the NW wavelength points, the band spectral radiance is computed from equation (43) and is transferred to RACOM.

After all contributions from all species have been computed and added to the cumulative spectral radiance in RACOM, the output subroutine, PUTTY, is called. Here one card defining the overall spectral range is read:

Card 01: [RMIN, RMAX Format (2E14.6)]

Because of the myriad combinations of units presently in use in radiative transfer calculations, the output section of the program has been placed in this separate subroutine

in order that changes may be made in the form of the output with a minimum of confusion. The final output consists of tabulated intensity versus wavelength and optional plots for the slab configuration, in addition to the intermediate tabular output.

Appendixes A and B contain a listing of the program and the printed input data for all of the species subdecks used in the sample calculations.

SAMPLE CALCULATIONS

Several cases are considered for high-temperature gas mixtures, and comparisons are made with similar calculations obtained from other previously developed computer codes. Thermally heated CO₂ and air have been chosen for these comparisons. They cannot be considered as duplications, since some radiating processes are included in one or another of the programs being compared and are omitted elsewhere. Also, basic radiative property data (for example, f-numbers, Franck-Condon factor arrays, etc.) are not consistently the same for all of the programs used. The primary purpose of the sample calculations is to show that the program of this paper computes its solutions in the desired manner.

The equilibrium conditions behind a shock wave in pure CO₂ are used in the first example. The thermodynamic state of the resultant mixture, along with the contributing radiative processes considered in this program (code name SPRAD), is given in table V. References 1 and 2 were used to generate spectral radiative profiles for this mixture and are compared in figure 6 with the output of the subject program. In this figure, the atomic line contributions of references 1 and 2 are not shown in order to avoid confusion. It should also be mentioned that more spectral points could be used in the continuum spectrum of the program of reference 1, which would result in greater spectral detail than is shown in the figure. Even though the result and spectral integrals (which include line contributions for all calculations) are in good agreement (within 10 percent), it is in some measure coincidental, since there are relatively severe differences in certain spectral regions.

High-temperature equilibrium air at one-amagat density is also used as a representative mixture, and the spectral profiles for a 1-cm slab as computed by program SPRAD are shown in figure 7. Reference 4 provides similar spectral profiles with the exception of line contributions which are not included. However, certain spectral features may be compared; in particular, at the lower temperatures (4000 to 6000 K) the NO infrared contribution should be essentially a duplicate calculation since the basic data of Breene (ref. 33) are used in the present calculation. Reference 4 verifies this conclusion.

Reference 3 has also been used to compare the spectral integrals of these air calculations. Line contributions have been included in reference 3, but effects of self-

absorption in-line overlapping were not accounted for. Spectral profiles are not available from this source. The spectral integrals of this program are compared with those of references 3 and 4 in figure 8. It should be noted that reference 4 has no inclusion of line contributions, and calculations do not extend above 9000 K. The SPRAD results on figure 8 are the integrated values of the profiles of figure 7. Differences as large as factors of 3.5 exist among the various calculations.

CONCLUDING REMARKS

The program described herein provides a means of generating spectral radiative properties of gas mixtures in a versatile and convenient manner. It is versatile in the sense that the various contributing processes are computed in distinct subroutines which lend themselves readily to alterations as required by the advancing state of the art. The convenience of using this program is primarily derived from the input arrangement which allows the user to omit contributions known in advance to be insignificant, thereby eliminating unnecessary computation. The inherent ability to maintain an up-to-date and ready-to-use catalog of punched-card basic data is also advantageous.

Sample calculations illustrate that the program in its present form is functional in the desired manner. While comparison calculations do not exactly duplicate calculations of others because of differences in radiative properties included, results are in general agreement with outputs of other programs.

It is expected that this program will undergo continuous change and expansion, which is completely in accordance with the manner in which it is arranged. Such changes should not alter the basic structure of the program, however, but are anticipated to be in the nature of added subroutines and improvements in computational models within existing subroutines.

Langley Research Center
National Aeronautics and Space Administration
Hampton, Va. 23665
February 5, 1975

APPENDIX A

PROGRAM LISTING

```

PROGRAM SPRAD(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE21)
COMMON TT,CON,ELEC
COMMON/RADPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
COMMON/FRBD/GA(15),EA(15),GL(15),PQN(15),EL(15),EU(15),
LESS(15),AL(15),SIG(15)
COMMON/MOLEC/GM(10),T(10),B(10),V(10),VX(10),ALPH(10),TU,VU,VXU,VY
IU,BU,TL,VL,VXL,VYL,BL,FC(15,15),WMIN,WMAX
COMMON/LINER/WLI(50),FLI(50),FLI(50),IG(50),EION,MION,WMOI,IU(50)
COMMON/INRED/RLAM,VO,V1,BE,ALE,FNR(35)
DIMENSION TYRAD(7)
NSP=J
C   VARIABLES IN COMMON BLOCK PTVAR RELATE TO PLOTTING SUBROUTINE
C   INFUPLT
CALL PSEJDD
READ 1,NSPEC,TT,ELEC
1  FORMAT(13,2E14.6)
   PRINT12,TT
12 FORMAT(4X3HTT=F8.C)
2  IF(NSP.EQ.NSPEC)GO TO 13
   READ 3,SPEC,ISPEC,NRAD,CON
3  FORMAT(A6,2I3,E14.6)
   PRINT 11,SPEC,CON
11 FORMAT(1H1,4X,A6,4X,E14.6,2X6HPER CC///// )
   NSP=NSP+1
   IF(ISPEC.EQ.1)GO TO 30
C   ATOMIC SPECIES INPUT
   N=C
4  READ 5,TYRAD
   PRINT 7,TYRAD
5  FORMAT(7A10)
   N=N+1
   READ 6,NEQ,nw,wmin,DELW,ZZ
6  FORMAT(12,15,3L14.6)
   CALL FFCON(NEQ,nw,wmin,DELW,ZZ,NSP)
   IF(N.EQ.NRAD)GO TO 2
C   ATOMIC FREE BOUND INPUT
   READ 5,TYRAD
   PRINT 7,TYRAD
7  FORMAT(/////7A10//)
   N=N+1
   READ 8,NEQ,NSTAT,NEDGE,XMIM,DELX
8  FORMAT(3I3,2E14.6)
   READ 9,(GA(I),EA(I),I=1,NSTAT)
9  FORMAT(F4.0,E14.6)
   READ 10,(GL(I),PQN(I),EL(I),EU(I),I=1,NEDGE)
10 FORMAT(F4.0,3L14.6)
   READ 113,(ESS(I),AL(I),SIG(I),I=1,NEDGE)
113 FORMAT(3F7.3)
   CALL FBCON(NEQ,NSTAT,NEDGE,XMIM,DELX,QA)
   IF(N.EQ.NRAD)GO TO 2
C   ATOMIC LINES INPUT
   READ 5, TYRAD
   PRINT 7,TYRAD

```

APPENDIX A – Continued

```

N=N+1
READ 35,NEQ,LIMAX,MION,EION,WMOL
35 FORMAT(3I3,2E14.6)
READ 34,(WLI(I),ELI(I),FLI(I),IG(I),IU(I),I=1,LIMAX)
34 FOPMAT(3E14.6,2I3)
CALL LINES(NEQ,LIMAX,QA)
IF(N.EQ.NRAD)GO TO 2
30 N=0
C MOLECULAR SPECIES INPUT
NB=0
READ 14,NEQ,NSTAT,NBD
14 FORMAT(3I3)
READ 15,(GM(I),T(I),I=1,NSTAT)
15 FORMAT(F4.0,E14.6)
READ 16,(V(I),VX(I),B(I),ALPH(I),I=1,NSTAT)
16 FURMAT(4E14.6)
20 READ 5,TYRAD
PRINT 7,TYRAD
N=N+1
READ 17,KUM,KLM,IOU,IDL,JRED,FNQ
NB=NB+1
17 FURMAT(5I3,E14.6)
READ 18,TU,VU,VXU,VYU,BU
READ 18,TL,VL,VXL,VYL,BL
18 FURMAT(5E14.6)
READ 19,((FC(KJ,KL),KU=1,KUM),KL=1,KLM)
19 FORMAT(7E10.4)
READ 21,NMIN,NMAX
21 FURMAT(2E14.6)
CALL S HEAR(NEQ,NSTAT,KUM,KLM,IOU,IDL,JRED,FNQ)
IF(N.EQ.NRAD) GO TO 2
IF(NB.EQ.NBD)22,20
22 CONTINUE
C MOLECULAR FREE FREE INPUT
READ 5,TYRAD
PRINT 7,TYRAD
N=N+1
READ 6,NEQ,NW,WMIN,DELW,ZZ
CALL FFCDN(NEQ,NW,WMIN,DELW,ZZ)
IF(N.EQ.NRAD) GO TO 2
C MOLECULAR INFRARED INPUT
READ 5,TYRAD
PRINT 7,TYRAD
N=N+1
READ 13,RLAM,V0,V1,DE,ALE
READ 4J,NEQ,NV,NW,WMIN,DW
40 FURMAT(3I4,2E14.6)
READ 19,(FNR(I),I=1,NV)
CALL INFRA(NEQ,NV,NW,WMIN,DW)
IF(N.EQ.NRAD) GO TO 2
C FINAL OUTPUT
13 CALL PUTTY
STOP
END

```

APPENDIX A - Continued

```

SUBROUTINE FFCON(NEQ,NW,WMIN,DELW,ZZ,NSP)
COMMON TT,CON,ELEC
COMMON/RADPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
COMMON/PTVAR/IN(2),YM(5),XM(5),NXM,NYM,IEC,XMIN,XMAX,YMIN,YMAX,
IISYM,ITAPE
DATA IN/20H1250 JENHSSD MS419 /
DATA Y1/50H RAD(WATTS/MICRON-CC-SR) /
DATA X1/50H WAVELENGTH(MICRONS) /
NXM=5
NYM=5
IEC=1
XMIN=0.
XMAX=0.
YMIN=0.
YMAX=0.
IISYM=14
ITAPE=5LTAPE21
IF(NEQ.EQ.1)1,2
1 READ 3,TTRON
3 FORMAT(E14.6)
GO TO 11
2 TTRON=TT
11 PRINT 12,TTRON
12 FORMAT(4X5HTEMP=,F8.0,1X1HK)
PRINT 13
13 FORMAT(//3X1HN,5X10HWAVELENGTH,3X13HCROSS SECTION,2X9HABS COEFF,
16X8HRADIANCE,5X9HBLACKBODY,6X8HINTEGRAL)
C CALCULATION OF WAVELENGTHS
DO 4 L=1,NW
WG(L)=WMIN+(L-1)*DELW
4 CONTINUE
L=1
RAD=0.
AREA=0.
DELLA=0.
C CALCULATION OF RADIATION
6 TERM=RAD
RAD=(1.63E-31)*ELEC*CON*ZZ*EXP(-14387.886/(WG(L)*TTRON))/(SQRT
1(TTRON)*WG(L)**2)
IF(ZZ.GT.0.999) GO TO 32
RAD=RAD*(3.E-10*(WG(L)*TTRON-20000.))**2/(WG(L)**2.5)
1+1.E-10*TTRON**2.5)
32 CONTINUE
BBL=(1.1906381E+04)/((WG(L)**5)*(EXP(14387.886/(WG(L)*TTRON))-1.))
ARS=RAD/BBL
SIGFF=ARS/(ELEC*CON)
AREA=AREA+.5*DELLA*(TERM+RAD)
DELLA=WG(L+1)-WG(L)
PRINT 5,L,WG(L),SIGFF,ARS,RAD,BBL,AREA
5 FORMAT(+X18,F14.8,5E14.6)
IF(NSP.EQ.1)15,7
15 F(L)=RAD
WF(L)=WG(L)
L=L+1
IF(L.GE.NW)GO TO 8
GO TO 5
7 G(L)=RAD
L=L+1
IF(L.GE.NW)GO TO 9

```


APPENDIX A - Continued

```
GO TO 6
8 NWD=NW-1
  NFMAX=NWD
  CALL INFDPLT(IEC,NWD,WF,1,F,1,XMIN,XMAX,YMIN,YMAX,0.,NXM,XM,NYM,
1YM,0)
  GO TO 10
9 NWD=NW-1
  NGMAX=NWD
  CALL INFDPLT(IEC,NWD,WG,1,G,1,XMIN,XMAX,YMIN,YMAX,0.,NXM,XM,NYM,
1YM,0)
  CALL RACOM
10 RETURN
  END
```

APPENDIX A – Continued

```

SUBROUTINE FBCON(NEQ,NSTAT,NEGE,XMIM,DELX,QA)
COMMON TT,CON,ELEC
COMMON/FR3D/GA(15),EA(15),GL(15),PQN(15),EL(15),EU(15),
LESS(15),AL(15),SIG(15)
COMMON/RADPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
COMMON/PTVAR/IN(2),YM(5),XM(5),NXM,NYM,IEC,XMIN,XMAX,YMIN,YMAX,
LISYM,ITAPE
DIMENSION ZSQ(15),WEDGE(15),CONC(15)
IF(NEQ.EQ.1)1,2
1 READ 3,TTRON
3 FORMAT(E14.6)
GO TO 11
2 TTRON=TT
11 PRINT 12,TTRON
12 FORMAT(4X5HTEMP=,F8.0,1X1HK)
C CALCULATION OF PARTITION FUNCTION
QA=0.
DO 4 I=1,NSTAT
QA=QA+GA(I)*EXP(-EA(I)/TTRON)
4 CONTINUE
C CALCULATION OF RADIATION
CRACK=-6.33E-06
DO 5 I=1,NEGE
IF(EU(I).LE.EL(I))GO TO 369
ZSQ(I)=-CRACK*PQN(I)**2*(EU(I)-EL(I))
WEDGE(I)=1.4387886E+04/(EU(I)-EL(I))
CONC(I)=(CON/GA)*GL(I)*EXP(-EL(I)/TTRON)
5 CONTINUE
PRINT 5
6 FORMAT(//3X1HN,5X10HWAVELENGTH,3X13HCROSS SECTION,2X9HABS COEFF,
16X8HRADIANCE,5X9HBLACKBODY,6X8HINTEGRAL)
ISIT=1
AREA=0.
DELLA=0.
RX=0.
XPO=0.
DO 10 L=1,NEGE
DO 9 K=1,10
POX=XP
XPO=XMIM+(K-1)*(WEDGE(L)-XMIM)/9.
ABSX=0.
DO 7 I=L,NEGE
ABSX=ABSX+CONC(I)*SIG(I)*1.E-18*(AL(I)*(XPO/WEDGE(I))**ESS(I)+
1(1.-AL(I))*(XPO/WEDGE(I))**2*(ESS(I)+1.))+4.2E-25*XPO**3*EU(I)**2/
1PQN(I)**3*CONC(I)
7 CONTINUE
TERM=RX
BX=(1.1906381E-16)/((XPO**5*1.E-20)*(EXP(1.4387886E+04/(XPO*TTRON)
1)-1.))
RX=ABSX*BX
SIGFB=ABSX/CON
AREA=AREA+.5*DELLA*(TERM+RX)
DELLA=XPO-POX
PRINT 8,ISIT,XPO,SIGFB,ABSX,RX,BX,AREA
8 FORMAT(4X16,F14.8,5E14.6)
WG(ISIT)=XPO
G(ISIT)=RX
NWD=ISIT
ISIT=ISIT+1

```

APPENDIX A - Continued

```
9  CONTINUE
   XMIM=wEDGE(L)+DELX
10  CONTINUE
   NGMAX=NWD
   CALL INFOPLT(IEC,NWD,WG,1,G,1,XMIN,XMAX,YMIN,YMAX,0.,NXM,XM,NYM,
  1YM,0)
   CALL RACOM
369 RETURN
   END
```

APPENDIX A – Continued

```

SUBROUTINE SMEAR(NEQ,NSTAT,KUM,KLM,IDU,IDL,JRED,FNQ)
COMMON TT,CON,ELEC
COMMON/RADPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
COMMON/PTVAR/IN(2),YM(5),XM(5),NXM,NYM,IEC,XMIN,XMAX,YMIN,YMAX,
IISYM,ITAPE
COMMON/MOLEC/GM(10),T(10),B(10),V(10),VX(10),ALPH(10),TU,VU,VXU,VY
IU,BU,TL,VL,VXL,VYL,BL,FC(15,15),WMIN,WMAX
DIMENSION GAM(10),FRACT(10),Q(10)
IF(NEQ.EQ.1)1,2
1 READ 3,TTTRON,TROT,TVIBR
3 FORMAT(3E14.6)
GO TO 4
2 TTTRON=TT
TROT=TT
TVIBR=TT
4 PRINT 5,TTTRON,TROT,TVIBR
5 FORMAT(4X6HTTRON=,F8.0,4X5HTROT=,F8.0,4X5HTVIB=,F8.0)
DELLA=0.
RAD=0.
AREA=0.
C CALCULATION OF PARTITION FUNCTION
QT=0.
DO 9 N=1,NSTAT
GAM(N)=(1./V(N))*(2.*VX(N)+ALPH(N)/B(N)+8.*B(N)/V(N))
Q(N)=GM(N)*EXP(-T(N)/TTTRON)*(TROT/B(N))*(1.+GAM(N)*TVIBR*TROT/(TVI
1BR+TROT))/(1.-EXP(-V(N)/TVIBR))
QT=QT+Q(N)
9 CONTINUE
DO 7 N=1,NSTAT
FRACT(N)=Q(N)/QT
7 CONTINUE
C CALCULATION OF WAVELENGTHS
L=0
DO 10 KU=1,KUM
UKM=KU-.5
ENU=TU+VU*UKM-VXU*UKM**2+VYU*UKM**3
DO 11 KL=1,KLM
BKL=KL-.5
ENL=TL+VL*BKL-VXL*BKL**2+VYL*BKL**3
L=L+1
WG(L)=1.4387386F+04/(ENU-ENL)
KP=L+1
WG(KP)=WG(L)-JRED*.0001
L=L+1
11 CONTINUE
10 CONTINUE
LMAX=KP
C SORT WAVELENGTHS
MLX=KP-1
DO 100 N=1,MLX
J=N+1
DO 100 K=J,LMAX
IF(WG(N)-WG(K))100,100,200
200 DDLT=WG(N)
WG(N)=WG(K)
WG(K)=DDLT
100 CONTINUE
C CALCULATE ABS COEFF CASE CONSTANTS
ZERDL=FL+.5*VL-.25*VXL+.125*VYL

```

APPENDIX A - Continued

```

ZEROU=TJ+.5*VU-.25*VXU+.125*VYU
S00=1.4387886E+04/(ZEROU-ZEROL)
QVL=0.
DO 21 KL=1,50
BKL=KL-.5
TVIB=VL*BKL-VXL*BKL**2+VYL*BKL**3
IF(TVIB.LE.0.) GO TO 21
QVL=QVL+EXP(-TVIB/TVIBR)
21 CONTINUE
BAP=1.2736539E-12*CON*FRACT(IDL)*S00*FNQ*BL/(QVL*TROT)
PRINT 62
62 FORMAT(/5X1HN,5X10HWAVELENGTH,3X13HCROSS SECTION,2X9HABS COEFF,
16X8HRADIANCE,5X9HBLACKBODY,6X8HINTEGRAL)
C CALCULATION OF PHI
L=1
NUB=1
30 PHI=0.
DO 15 KU=1,KUM
BKU=KU-.5
EVU=VU*BKU-VXU*BKU**2+VYU*BKU**3
BVU=BU-ALPH(IDU)*BKU
DO 16 KL=1,KLM
BKL=KL-.5
EVL=VL*BKL-VXL*BKL**2+VYL*BKL**3
BVL=BL-ALPH(IDL)*BKL
X=1.4387886E+04/WG(L)
XVV=TU-TL+EVU-EVL
IF(JREJ.EQ.1) 18,17
17 IF(X.LT.(XVV-.0001)) GO TO 16
GO TO 20
18 IF(X.GT.(XVV+.0001)) GO TO 16
20 CAT=EVL/TVIBR+BVL*(X-XVV)/((BVU-BVL)*TROT)
IF(CAT.LT.0.) GO TO 16
IF(CAT.GT.100.) GO TO 16
DNG=FC(KJ,KL)/ABS(BVU-BVL)
PHI=PHI+DNG*EXP(-CAT)
16 CONTINUE
15 CONTINUE
C CALCULATION OF ABSORPTION COEFFICIENT
ARS=BAP*(1.-EXP(-1.4387886E+04/(WG(L)*TTRON)))*PHI/WG(L)
B5L=1.1906381E-16/((WG(L)**5*1.E-20)*(EXP(1.4387886E+04/
1(WG(L)*TTRON))-1.))
TERM=RAD
RAD=ARS*B5L
SIGMO=ARS/CON
AREA=AREA+.5*DELLA*(TERM+RAD)
DELLA=(WG(L+1)-WG(L))
PRINT 40,L,WG(L),SIGMO,ARS,RAD,B5L,AREA
40 FORMAT(4X18,F14.8,5E14.6)
IF(WG(L).LT.WMIN.OR.WG(L).GT.WMAX) GO TO 94
WG(NUB)=WG(L)
G(NUB)=RAD
NUB=NUB+1
94 L=L+1
IF(L.GE.LMAX)GO TO 95
GO TO 30
95 NWD=NUB-1
CALL 1VFOPLT(IEC,NWD,WG,1,G,1,XMIN,XMAX,YMIN,YMAX,0.,NXM,XM,NYM,
LYM,0)

```

APPENDIX A – Continued

```
NGMAX=NWD  
CALL RACUM  
RETURN  
END
```

APPENDIX A – Continued

```

SUBROUTINE LINES (NEQ, LIMAX, QA)
COMMON TT, CON, ELEC
COMMON/LINER/WLI(50), ELI(50), FLI(50), IG(50), EION, MION, WMOL, IU(50)
COMMON/RADPT/G(650), WG(650), F(8000), WF(8000), NFMAX, NGMAX
COMMON/PTVAR/IN(2), YM(5), XM(5), NXM, NYM, IEC, XMIN, XMAX, YMIN, YMAX,
IISYM, ITAPE
DIMENSION FC(50), HWID(50), FUD(650)
DO 131 I=1, LIMAX
FLI(I)=1.4388*ELI(I)
131 CONTINUE
C
CALCULATION OF RADIATION
PRINT 6
6 FORMAT(/ / 8X1HN, 5X10HWAVELENGTH, 3X13HCROSS SECTION, 2X9HABS COEFF,
16X8HRADIANCE, 5X9HBLACKBODY, 6X8HINTEGRAL)
IF (N.EQ.1) GO TO 85
TTRON=TT
GO TO 87
85 READ 85, TTRON
86 FORMAT(E14.6)
87 CONTINUE
DO 10 N=1, LIMAX
EC(N)=1.045E-12*CON*IG(N)*FLI(N)*EXP(-(ELI(N)+14388/WLI(N))/TTRON)
1/(QA*WLI(N)**3)
DVI=WLI(N)*(MION+1)/(EION-ELI(N))
HWID(N)=7.23E-10*ELEC*DVI**2/SQRT(TTRON)
1+3.581E-07*WLI(N)*SQRT(TTRON/WMOL)
1+4.1353E-22*CON*FLI(N)*WLI(N)**3*SQRT(IG(N)/IU(N))
IF (HWID(N).GT.0.02) HWID(N)=0.02
10 CONTINUE
C
CALCULATION OF WAVELENGTHS
J=0
DO 20 I=1, LIMAX
DO 21 N=1, 6
J=J+1
WG(J)=WLI(I)-HWID(I)*(7-N)**3/12
FUD(J)=1.
IF (N.EQ.1) FUD(J)=0
21 CONTINUE
J=J+1
WG(J)=WLI(I)
FUD(J)=1.
DO 22 N=1, 6
J=J+1
WG(J)=WLI(I)+HWID(I)*N**3/12.
FUD(J)=1.
IF (N.EQ.6) FUD(J)=0.
20 CONTINUE
MMAX=J
MLX=MMAX-1
DO 30 J=1, MLX
I=J+1
DO 30 K=I, MMAX
IF (WG(J).LT.WG(K)) GO TO 30
DOLT=WG(K)
DUMB=1.
WG(K)=WG(J)
FUD(K)=FUD(J)
WG(J)=DOLT
FUD(J)=DUMB

```

APPENDIX A - Continued

```

30 CONTINUE
  DD 40 J=1, MMAX
  RAD=0.
  DD 50 I=1, LIMAX
  QWITN=WLI(I)-18.*HWID(I)
  QWITP=WLI(I)+18.*HWID(I)
  IF(WG(J).LT.QWITN.OR.WG(J).GT.QWITP)GO TO 50
  RAD=RAD+EC(I)*HWID(I)/(3.1416*((WG(J)-WLI(I))**2+HWID(I)**2))
  I*FUD(J)
50 CONTINUE
  G(J)=RAD
40 CONTINUE
  AREA=0.
  DD 90 I=2, MMAX
  RAD=G(I)
  XPO=WG(I)
  BBL=(1.190638E-16)/((XPO**5*1.E-20)*(EXP(1.4387886E+04/(XPO*TTRON)
  I)-1.))
  ARS=RAD/BBL
  SIGL=ARS/CON
  AREA=AREA+RAD*(WG(I)-WG(I-1))
  PRINT 25, I, WG(I), SIGL, ARS, RAD, BBL, AREA
25 FORMAT(4X18, F14.8, 5E14.6)
90 CONTINUE
  NWD=MMAX-1
  CALL INFPLT(IEC, NWD, WG, 1, G, 1, XMIN, XMAX, YMIN, YMAX, 0., NXM, XM, NYM,
  YM, 0)
  NGMAX=NWD
  CALL RACUM
  RETURN
  END

```


APPENDIX A - Continued

```

SUBROUTINE INFRA(NEQ,NV,NW,WMIN,DW)
COMMON TT,CON,ELEC
COMMON/RAOPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
COMMON/PTVAR/IN(2),YM(5),XM(5),NXM,NYM,IEC,XMIN,XMAX,YMIN,YMAX,
IISYM,ITAPE
COMMON/INRLD/RLAM,V0,V1,BE,ALE,FNR(35)
DIMENSION BC(35),BROT(35),ELV(35)
IF(NEQ.EQ.1)100,200
100 READ 300,TTTRON,TROT,TVIBR
300 FORMAT(3E14.6)
GO TO 400
200 TTTRON=TT
TROT=TT
TVIBR=TT
400 PRINT 500,TTTRON,TROT,TVIBR
500 FORMAT(4X5HTTRON=,F8.0,4X5HTROT=,F8.0,4X5HTVIB=,F8.0)
H=1.4338
C CALCULATION OF FUNDAMENTAL BAND FREQUENCIES
I=1
DO 3 KV=1,10
ELV(I)=V0*(KV-0.5)-V1*(KV-0.5)**2
BC(I)=V0*(KV+0.5)-V1*(KV+0.5)**2-ELV(I)
BROT(I)=BE-ALE*(KV-0.5)
I=I+1
3 CONTINUE
DO 4 KV=1,10
ELV(I)=V0*(KV-0.5)-V1*(KV-0.5)**2
BC(I)=V0*(KV+1.5)-V1*(KV+1.5)**2-ELV(I)
BROT(I)=BE-ALE*(KV-0.5)
I=I+1
4 CONTINUE
DO 5 KV=1,10
ELV(I)=V0*(KV-0.5)-V1*(KV-0.5)**2
BC(I)=V0*(KV+2.5)-V1*(KV+2.5)**2-ELV(I)
BROT(I)=BE-ALE*(KV-0.5)
I=I+1
5 CONTINUE
C CALCULATION OF PARTITION FUNCTION
Q=0.
DO 6 I=1,14
Q=Q+EXP((- (I-.5)*V0*H-V1*H*(I-.5)**2)/TVIBR)
60 CONTINUE
Q=Q*TROT/RLAM
A1=8.853E-13*CON/Q
C CALCULATION OF WAVELENGTHS
DO 11 I=1,NW
WG(I)=WMIN-(I-1)*DW
11 CONTINUE
PRINT 62
62 FORMAT(//8X1HN,5X10HWAVELENGTH,3X13HCROSS SECTION,2X9HABS CGEFF,
16X8HRADIANCE,5X9HBLACKBODY,6X9HINTEGRAL)
C CALCULATION OF ABSORPTION COEFFICIENT
DO 8 I=1,NW
AB=0.
DO 7 N=1,NV
DELN=WG(I)-BC(N)
X1=H*ELV(N)/TVIBR
X2=H*DELN**2/(4.*BROT(N)*TROT)
X3=H*DELN/(2.*TVIBR)

```

APPENDIX A - Continued

```

PA=ABS(DFLN)
Z=X1+X2+X3
IF(Z.GT.90.) GO TO 7
AB=A3+EXP(-Z)*FNR(N)*PA/(4.*BROT(N)**2)
7 CONTINUE
G(I)=A3*(1.-EXP(-WG(I)*H/TTRON))*A1
8 CONTINUE
AREA=0.
WS(1)=1.E+04/WG(1)
DO 9 I=2,NW
WG(I)=1.E+04/WG(I)
ARS=G(I)
BPL= (11906.)/((WG(I)**5)*(EXP(14388./(WG(I)*TTRON))-1.))
G(I)=ARS*BPL
SIGMO=ARS/C.DN
AREA=AREA+0.5*(WG(I)-WG(I-1))*(G(I)+G(I-1))
PRINT 40,I,WG(I),SIGMO,ARS,G(I),BBL,AREA
40 FORMAT(4X18,F14.8,5E14.6)
9 CONTINUE
NWD=NW-1
CALL INFDPLT(IEC,NWD,WG,1,G,1,XMIN,XMAX,YMIN,YMAX,0.,NXM,XM,NYM,
LYM,0)
NOMAX=NWD
CALL KACOM
RETURN
END

```

APPENDIX A - Continued

```

SUBROUTINE RACOM
COMMON/RADPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
DIMENSION FF(8000),WW(8000)
I=1
J=1
K=1
3 IF(WF(J).LT.WG(1))1,2
2 IF(WG(I).LE.WF(J))4,5
5 IF(WF(J).LT.WG(I))6,2
1 FF(K)=F(J)
  WW(K)=WF(J)
  IF(J.EQ.NFMAX)GO TO 7
  J=J+1
  K=K+1
  GO TO 3
4 FF(K)=G(I)+F(J)-(WF(J)-WG(I))*(F(J)-F(J-1))/(WF(J)-WF(J-1))
  WW(K)=WG(I)
  IF(I.EQ.NGMAX)GO TO 12
  K=K+1
  I=I+1
  GO TO 2
6 FF(K)=F(J)+G(I)-(WG(I)-WF(J))*(G(I)-G(I-1))/(WG(I)-WG(I-1))
  WW(K)=WF(J)
  IF(J.EQ.NFMAX)GO TO 10
  K=K+1
  J=J+1
  GO TO 5
7 DO 8 I=1,NGMAX
  K=K+1
  FF(K)=G(I)
  WW(K)=WG(I)
8 CONTINUE
  GO TO 9
10 DO 11 II=I,NGMAX
  K=K+1
  FF(K)=G(II)
  WW(K)=WG(II)
11 CONTINUE
  GO TO 9
12 DO 13 JJ=J,NFMAX
  K=K+1
  FF(K)=F(JJ)
  WW(K)=WF(JJ)
13 CONTINUE
  GO TO 9
9 KMAX=K
  DO 14 J=1,KMAX
  F(J)=FF(J)
  WF(J)=WW(J)
14 CONTINUE
  NFMAX=KMAX
  RETURN
END

```

APPENDIX A – Concluded

```

SUBROUTINE PUTTY
COMMON TT,CON,ELEC
COMMON/RADPT/G(650),WG(650),F(8000),WF(8000),NFMAX,NGMAX
COMMON/PTVAR/IN(2),YM(5),XM(5),NXM,NYM,IEC,XMIN,XMAX,YMIN,YMAX,
1 ISYM,ITAPE
PRINT 1
1 FORMAT(1H1,4X13H FINAL OUTPUT////)
PRINT 2
2 FORMAT(8X1HN,5X10HWAVELENGTH,5X8HRADIANCE,5X9HBLACKBODY,6X8HINTEGR
IAL/)
READ 7,RMIN,RMAX
7 FORMAT(2E14.6)
RAD=0.
AREA=0.
DELLA=0.
NPT=0
IPRIN=0
DO 4 I=2,NFMAX
IF(WF(I).LT.RMIN.OR.WF(I).GT.RMAX) GO TO 4
IF(NPT.EQ.0)NFN=I
NPT=NPT+1
BBODY=(1.1906381E-16)/((WF(I)**5*L.E-20)*(EXP(1.4387886E+04/(WF(I)
1*TT))-1.))
ABSCD=F(I)/BBODY
TERM=RAD
RAD=F(I)
DELLA=WF(I)-WF(I-1)
AREA=AREA+.5*DELLA*(TERM+RAD)
F(I)=ALOG10(BBODY*(1.-EXP(-ABSCD*5.00))+1.E-20)
IF(IPRIN.EQ.0) GO TO 4
PRINT 3,I,WF(I),F(I),BBODY,AREA
9 FORMAT(4X18,F14.8,3E14.6)
4 CONTINUE
NWD=NPT
CALL INFOPLT(IEC,NWD,WF(NFN),1,F(NFN),1,XMIN,XMAX,YMIN,YMAX,
10.,NXM,XM,NYM,YM,0)
AREAT=0.
NEWN=NFN+1
F(NFN)=10.**F(NFN)
NOMAD=NFN+NPT-1
DO 5 I=NEWN,NOMAD
F(I)=10.**F(I)
AREAT=AREAT+.5*(WF(I)-WF(I-1))*(F(I)+F(I-1))
5 CONTINUE
PRINT 6,AREAT
6 FORMAT(4X6HFLUX =,E14.6)
DO 8 I=NFN,NOMAD
F(I)=ALOG10(F(I)*0.80657*WF(I)**2)
WF(I)=1.E+04/(WF(I)*8066.)
8 CONTINUE
CALL INFOPLT(IEC,NWD,WF(NFN),1,F(NFN),1,XMIN,XMAX,YMIN,YMAX,
10.,NXM,XM,NYM,YM,0)
RETURN
END

```

APPENDIX B

SAMPLE INPUT DATA: SPECIES RADIATIVE PROPERTIES

```

C 0 3 3.788721E+17
CARBON ATOM FREE-FREE CONTINUUM
0 51 4.990000E-02 5.000000E-02 2.473000E-02
CARBON ATOM FREE-BOUND CONTINUUM (HENRY FORMULA)
0 8 11 5.000000E-02 1.000000E-04
9. 4.263822E+01
5. 1.466731E+04
1. 3.114902E+04
5. 4.854023E+04
9. 8.686884E+04
3. 8.918371E+04
15. 9.221768E+04
3. 9.907702E+04
9. 2.000000E+00 4.263822E+01 1.308226E+05
5. 2.000000E+00 1.466731E+04 1.308226E+05
1. 2.000000E+00 3.114902E+04 1.308226E+05
9. 3.000000E+00 1.162276E+05 1.307560E+05
16. 4.000000E+00 1.225838E+05 1.307560E+05
25. 5.000000E+00 1.255258E+05 1.307560E+05
36. 6.000000E+00 1.271239E+05 1.307560E+05
49. 7.000000E+00 1.280875E+05 1.307560E+05
64. 8.000000E+00 1.287129E+05 1.307560E+05
81. 9.000000E+00 1.291147E+05 1.307560E+05
100. 1.000000E+01 1.294484E+05 1.307560E+05
2.000 3.317 12.190
1.500 2.789 10.300
1.500 3.501 9.590
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
1.000 1.000 0.000
CARBON ATOM LINE RADIATION
0 31 0 1.307560E+05 1.201100E+01
9.454400E-02 3.000000E+01 2.700000E-01 9 3
1.261300E-01 3.000000E+01 2.900000E-02 9 9
1.277500E-01 3.000000E+01 6.300000E-02 9 15
1.280400E-01 3.000000E+01 2.000000E-02 9 9
1.329300E-01 3.000000E+01 3.800000E-02 9 9
1.431900E-01 3.373500E+04 1.300000E-01 5 15
1.463330E-01 1.019400E+04 9.300000E-02 5 7
1.481770E-01 1.019400E+04 1.100000E-02 5 5
1.561000E-01 3.000000E+01 9.100000E-02 9 15
1.657200E-01 3.000000E+01 1.700000E-01 9 9
1.751900E-01 2.164800E+04 1.200000E-01 1 3
1.930930E-01 1.019400E+04 8.200000E-02 5 3
2.478560E-01 2.164800E+04 9.400000E-02 1 3
4.769700E-01 6.037400E+04 5.300000E-03 9 9
4.932000E-01 6.198200E+04 5.500000E-03 3 1

```

APPENDIX B – Continued

5.041700E-01	6.037400E+04	2.500000E-03	9	15
5.052120E-01	6.198200E+04	1.100000E-02	3	5
5.380240E-01	6.198200E+04	7.000000E-03	3	3
8.335190E-01	6.198200E+04	1.100000E-01	3	1
9.087600E-01	6.037400E+04	3.100000E-01	9	9
9.640600E-01	6.037400E+04	1.000000E-01	9	3
1.012400E+00	6.885800E+04	2.620000E-01	3	3
1.069500E+00	6.037400E+04	5.000000E-01	9	15
1.133030E+00	6.198200E+04	4.200000E-01	3	5
1.133040E+00	6.885800E+04	6.300000E-01	3	5
1.164100E+00	6.972200E+04	1.320000E-01	15	15
1.166400E+00	7.074400E+04	9.600000E-01	3	9
1.188600E+00	6.972200E+04	1.400000E-01	15	9
1.175500E+00	6.972200E+04	7.000000E-01	15	21
1.259100E+00	7.137500E+04	2.490000E-01	9	9
1.698000E+00	7.261100E+04	7.400000E-01	5	7

C+ 0 3 1.141238E+18
 C+ FREE-FREE CONTINUUM
 0 51 5.010000E-02 5.000000E-02 1.000000E+00
 C+ DUMMY FREE-BOUND (PARTITION FUNCTION DATA)
 0 2 1 5.021000E-02 1.000000E-04
 6. 6.139136E+01
 12. 6.191796E+04
 1. 1.000000E+00 1.000000E+00 0.000000E+00
 1.000 1.000 0.000
 CARBON ION LINE RADIATION
 0 20 1 2.829530E+05 1.201100E+01
 6.872500E-02 4.300000E+01 2.600000E-01 6 10
 8.584100E-02 4.300000E+01 4.600000E-02 6 2
 9.040900E-02 4.300000E+01 5.200000E-01 6 6
 1.010200E-01 4.303300E+04 1.600000E-01 12 4
 1.066000E-01 7.493200E+04 8.300000E-02 10 6
 1.036800E-01 4.300000E+01 5.900000E-02 6 2
 1.323900E-01 7.493200E+04 2.300000E-01 10 10
 1.335300E-01 4.300000E+01 2.700000E-01 6 10
 2.511000E-01 1.106520E+05 1.500000E-01 6 10
 2.837000E-01 9.649400E+04 1.300000E-01 2 6
 2.992600E-01 1.455510E+05 1.690000E-01 10 14
 3.589300E-01 1.817400E+05 1.070000E-01 20 12
 3.920200E-01 1.317320E+05 1.430000E-01 6 2
 4.267200E-01 1.455510E+05 9.400000E-01 10 14
 5.141800E-01 1.670070E+05 3.420000E-01 12 12
 5.653900E-01 1.670070E+05 1.040000E-01 12 4
 6.579700E-01 1.165380E+05 9.300000E-01 2 6
 6.785600E-01 1.670070E+05 4.240000E-01 12 20
 7.234400E-01 1.317320E+05 5.900000E-01 6 10
 1.890200E+00 1.572340E+05 1.180000E+00 2 6

C++ 0 3 3.337000E+15
 CARBON DOUBLE ION FREE-FREE CONTINUUM
 0 51 5.025000E-02 5.000000E-02 2.000000E+00
 C++ DUMMY FREE-BOUND (PARTITION FUNCTION DATA)
 0 2 1 5.021000E-02 1.000000E-04
 1. 0.000000E+00
 9. 7.534564E+04
 1. 1.000000E+00 1.000000E+00 0.000000E+00
 1.000 1.000 0.000

APPENDIX B - Continued

CARBON DOUBLE ION LINE RADIATION

0 15 2 5.556850E+05 1.201100E+01
 9.770260E-02 0.000000E+00 8.100000E-01 1 3
 1.175700E-01 5.241900E+04 2.600000E-01 9 9
 2.296890E-01 1.023510E+05 4.700000E-01 3 5
 3.170160E-01 3.117120E+05 1.470000E-01 1 3
 3.609300E-01 3.177980E+05 3.080000E-01 9 15
 3.887100E-01 3.214350E+05 5.800000E-01 15 21
 4.056060E-01 3.242120E+05 5.000000E-01 5 7
 4.122050E-01 3.224030E+05 4.430000E-01 3 5
 4.325700E-01 3.100050E+05 5.000000E-01 3 5
 4.516500E-01 3.177980E+05 1.690000E-01 9 3
 4.648800E-01 2.382120E+05 7.600000E-01 3 9
 4.662700E-01 3.082830E+05 2.730000E-01 9 9
 5.249600E-01 3.242120E+05 1.280000E-01 5 3
 5.696000E-01 2.589310E+05 4.070000E-01 3 5
 6.740800E-01 3.082830E+05 3.030000E-01 9 15

C2 1 3 1.310000E+13

0 3 2

6. 0.000000E+00

6. 2.777763E+04

6. 5.766724E+04

2.3615557E+03 1.6790663E+01 2.3489663E+00 2.4214812E-02

2.5728705E+03 2.3653685E+01 2.5217648E+00 2.3135721E-02

1.5921059E+03 5.6486840E+01 1.7153238E+00 3.4818684E-02

C2 FOX-HERZBERG BAND SYSTEM

7 7 3 1 1 8.180000E-01

5.766724E+04 1.592106E+03 5.648684E+01 3.100000E+00 1.715324E+00

0.000000E+00 2.361556E+03 1.679066E+01 0.000000E+00 2.348966E+00

2000-02 6000-02 1100-01 1700-01 2300-01 2700-01 3100-01

1400-01 3600-01 5000-02 6700-01 7200-01 7000-01 6500-01

5300-01 9700-01 1060+00 8700-01 5700-01 3000-01 1100-01

1240+00 1410+00 7900-01 2000-01 0000+00 1500-01 4200-01

2020+00 1020+00 3000-02 2900-01 8900-01 0000+00 0000+00

2410+00 1500-01 6800-01 0000+00 0000+00 0000+00 0000+00

2130+00 2900-01 0000+00 0000+00 0000+00 0000+00 0000+00

2.500000E-01 3.300000E-01

C2 SWAN BAND SYSTEM

6 10 2 1 -1 1.500000E-02

2.7777627E+04 2.5728705E+03 2.3653685E+01 -7.2903418E-01 2.5217648E+00

0.0000000E+00 2.3615557E+03 1.6790663E+01 0.0000000E+00 2.3489663E+00

7352+00 2396+00 2445-01 7100-03 0000+00 0000+00 2130+00

3636+00 3614+00 5983-01 2180-02 0000+00 4312-01 2784+00

1620+00 4140+00 9832-01 4300-02 7370-02 9158-01 2706+00

6010-01 4305+00 1274+00 1130-02 2168-01 1293+00 2290+00

1099-01 5615+00 1600-03 4220-02 3872-01 1363+00 8880-01

APPENDIX B - Continued

0000+00 2000-04 6300-03 6390-02 1216-01 0000+00 0000+00
 0000+00 0000+00 3170-02 0000+00 0000+00 0000+00 1000-04
 2710-02 0000+00 0000+00 0000+00 0000+00 3800-03 0000+00
 0000+00 0000+00 0000+00 0000+00

4.000000E-01 6.500000E-01

C2 MOLECULE FREE-FREE RADIATION

0 51 5.030000E-02 5.000000E-02 4.946000E-02

CH 1 3 3.512151E+14

0 4 2

2. 0.000000E+00

2. 3.330822E+04

1. 3.733542E+04

1. 4.578405E+04

4.117270E+03 9.251484E+01 2.080073E+01 7.683192E-01

4.202735E+03 1.300675E+02 2.145539E+01 9.639960E-01

3.658149E+03 5.378234E+02 1.854182E+01 6.978180E-01

4.063315E+03 1.522250E+02 2.104821E+01 1.070467E+00

CH BAND (A-X)

7 7 2 1 -1 5.000000E-03

3.330822E+04 4.202735E+03 1.300675E+02 0.000000E+00 2.145539E+01

0.000000E+00 4.117270E+03 9.251484E+01 0.000000E+00 2.080073E+01

9996+00 2000-03 0000+00 0000+00 0000+00 0000+00 0000+00

2000-03 9986+00 1000-03 0000+00 0000+00 0000+00 0000+00

0000+00 1000-03 9947+00 3200-02 0000+00 0000+00 1000-03

0000+00 0000+00 2800-02 9819+00 1460-01 0000+00 2300-02

0000+00 1000+03 0000+00 1310-01 9253+00 4960-01 1280-01

0000+00 0000+00 0000+00 1600-02 4210-01 8862+00 0000+00

0000+00 0000+00 0000+00 1000-03 0000+00 0000+00 0000+00

3.200000E-01 6.200000E-01

CH BAND (B-X)

7 7 3 1 1 3.000000E-03

3.733542E+04 3.658149E+03 5.378234E+02 0.000000E+00 1.854182E+01

0.000000E+00 4.117270E+03 9.251484E+01 0.000000E+00 2.080073E+01

5937+00 1300-02 1845+00 0000+00 8110-01 7000-03 3830-01

6000-03 2176+00 1660-01 2174+00 1650-01 1610+00 1020-01

1691+00 1670-01 4000-03 1200-02 5760-01 2150-01 8130-01

5250-01 1116+00 1620-01 7450-01 1420-01 1000-02 5130-01

8000-02 1397+00 1800-02 8700-02 3890-01 0000+00 0000+00

5570-01 6800-02 4530-01 9200-02 4900-02 0000+00 0000+00

3310-01 4570-01 2440-01 4280-01 3900-02 0000+00 0000+00

3.000000E-01 7.000000E-01

CH MOLECULE FREE-FREE RADIATION

0 25 5.100000E-02 1.800000E-01 9.956254E-03

CN 1 3 1.000000E+00

0 3 2

1. 0.000000E+00

2. 1.329690E+04

1. 3.705169E+04

2.976453E+03 1.891159E+01 2.733144E+00 2.496318E-02

2.610602E+03 1.853606E+01 2.469700E+00 2.512145E-02

3.113750E+03 2.913570E+01 2.834580E+00 3.186942E-02

CN RED BAND SYSTEM

7 7 2 1 1 7.000000E-03

1.329690E+04 2.610602E+03 1.853606E+01 0.000000E+00 2.469700E+00

0.000000E+00 2.976453E+03 1.891159E+01 0.000000E+00 2.733144E+00

4990+00 3210+00 1260+00 4000-01 1100-01 3000-02 0000+00

APPENDIX B - Continued

3700+00 4600-01 2420+00 1950+00 9400-01 3600-01 0000+00
 1110+00 3480+00 1200-01 1000+00 1840+00 0000+00 0000+00
 1800-01 2230+00 2090+00 8900-01 0000+00 0000+00 0000+00
 2000-02 5500-01 2880+00 0000+00 0000+00 0000+00 0000+00
 0000+00 7000-02 0000+00 0000+00 0000+00 0000+00 0000+00
 0000+00 0000+00 0000+00 0000+00 0000+00 0000+00 0000+00

5.000000E-01 2.500000E+00

CN VIOLET BAND SYSTEM

7 7 3 1 -1 3.500000E-02

3.705169E+04 3.113750E+03 2.913570E+01 0.000000E+00 2.834580E+00

0.000000E+00 2.976453E+03 1.891159E+01 0.000000E+00 2.733144E+00

9200+00 7900+00 1000-02 0000+00 0000+00 0000+00 0000+00

7300-01 7870+00 1370+00 3000-02 0000+00 0000+00 0000+00

5000-02 1210+00 6910+00 1800+00 3000-02 0000+00 0000+00

0000+00 1400-01 1470+00 6250+00 2110+00 3000-02 0000+00

0000+00 0000+00 2400-01 1630+00 5700+00 2080+00 2500-01

0000+00 0000+00 0000+00 2900-01 1710+00 5290+00 2320+00

0000+00 0000+00 0000+00 0000+00 4500-01 2040+00 4900+00

3.400000E-01 4.900000E-01

CN MOLECULE FREE-FREE RADIATION

0 51 5.055000E-02 1.000000E-01 4.270000E-02

CO 1 5 1.000000E+00

0 7 3

1. 0.000000E+00

6. 7.005102E+04

3. 8.042972E+04

6. 8.963567E+04

2. 9.362888E+04

3. 1.205762E+05

1. 1.250998E+05

3.1224734E+03 1.9367533E+01 2.7787324E+00 2.5150025E-02

2.5024131E+03 2.0819271E+01 2.4186036E+00 2.7768620E-02

1.7524445E+03 1.3668492E+01 1.9150276E+00 2.3020618E-02

1.6370393E+03 1.0969324E+01 1.8150318E+00 2.4459406E-02

2.1806424E+03 2.4819823E+01 2.3187517E+00 3.2070598E-02

3.1624573E+03 0.0000000E+00 2.9854863E+00 4.7480024E-02

2.9956586E+03 0.0000000E+00 2.8214644E+00 3.8847292E-02

CO ANGSTROM BAND SYSTEM

7 7 7 5 -1 3.000000E-02

1.250998E+05 2.995659E+03 0.000000E+00 0.000000E+00 2.821464E+00

9.362888E+04 2.180642E+03 2.481982E+01 0.000000E+00 2.318752E+00

8898-01 2505+00 3093+00 2190+00 9767-01 2842-01 5400-02

1816+00 1757+00 8330-02 8323-01 2320+00 2020+00 9010-01

2106+00 3039-01 7102-01 1232+00 1870-02 1052+00 2280+00

1834+00 4200-02 1173+00 2690-02 9680-01 6931-01 1153-01

1340+00 5214-01 5215-01 4339-01 6583-01 1591-01 1123+00

8706-01 9553-01 2650-02 8487-01 2500-03 8492-01 3957-01

6211-01 1066+00 1132-01 5222-01 3376-01 3583-01 6574-01

2.200000E-01 1.000000E+00

CO HOPFIELD-BIRGE (B-X) BAND SYSTEM

2 9 6 1 -1 1.200000E-02

1.205762E+05 3.162457E+03 0.000000E+00 0.000000E+00 2.985486E+00

0.000000E+00 3.122473E+03 1.936753E+01 4.431504E-02 2.778732E+00

6468+00 2836+00 2597+00 1632+00 6832-01 2998+00 1767-01

1552+00 5070-02 6032-01 1580-02 2289-01 5200-03 8930-02

1800-03 3550-02 6000-04 1430-02

1.150000E-01 1.600000E-01

APPENDIX B - Continued

CO FOURTH POSITIVE BAND SYSTEM
14 14 5 1 1 1.500000E-01
9.3628880E+04 2.1806424E+03 2.4819823E+01 0.0000000E+00 2.3187517E+00
0.0000000E+00 3.1224734E+03 1.9367533E+01 4.4314689E-02 2.7787324E+00
1132+00 2161+00 2300+00 1813+00 1188+00 6885-01 3668-01
1843-01 8897-02 4184-02 1937-02 8894-03 4079-03 1877-03
2609+00 1549+00 1218-01 2049-01 8728-01 1230+00 1160+00
8806-01 5837-01 3537-01 2016-01 1102-01 5864-02 3067-02
2848+00 3051-02 9013-01 1170+00 3443-01 3236-03 3211-01
7347-01 9097-01 8453-01 6633-01 4664-01 3045-01 1888-01
1963+00 7644-01 1161+00 6454-03 5763-01 9125-01 4220-01
2234-02 9899-02 4063-01 6476-01 7175-01 6509-01 5204-01
9604-01 1931+00 5083-02 8957-01 6656-01 1384-04 4290-01
7389-01 4462-01 7969-02 1462-02 1948-01 4177-01 5531-01
3554-01 1857+00 5718-01 8416-01 6171-02 8236-01 4226-01
4267-04 3278-01 6081-01 4505-01 1450-01 1714-03 6720-02
1034-01 1083+00 1650+00 4713-03 9803-01 2268-01 2178-01
6988-01 2974-01 3829-04 2418-01 4970-01 4418-01 2100-01
2428-02 4465-01 1668+00 6766-01 5141-01 3155-01 7288-01
2902-02 3061-01 5834-01 2373-01 1103-04 1630-01 3919-01
4686-03 1380-01 9963-01 1588+00 2720-02 9438-01 5930-03
5818-01 4267-01 1669-04 3252-01 4944-01 2159-01 4229-03
7526-04 3374-02 4131-01 1486+00 8911-01 2109-01 6352-01
3750-01 9839-02 5888-01 2374-01 1094-02 3020-01 4288-01
1015-04 6664-03 1283-01 8454-01 1568+00 1802-01 7283-01
1010-01 6822-01 5967-02 2480-01 4991-01 1438-01 1718-02
1157-05 1081-03 3115-02 3372-01 1291+00 1130+00 2433-02
8281-01 6076-02 4350-01 4170-01 5751-05 3144-01 4100-01
1118-06 1458-04 6072-03 1011-01 6761-01 1510+00 4547-01
4048-01 4075-01 4454-01 4708-02 5187-01 2062-01 2127-02
9187-08 1646-05 9671-04 2372-02 2528-01 1078+00 1321+00
2740-02 7797-01 2455-02 6218-01 8492-02 2073-01 4459-01
1.200000E-01 2.400000E-01
CO MOLECULE FREE-FREE CONTINUUM
0 51 5.000000E-02 5.000000E-02 4.000000E-02
CO INFRARED VIBRATION-ROTATION BANDS
2.779000E+00 2.169560E+03 1.345300E+01 1.930240E+00 1.747000E-02
0 30 300 1.000000E+04 2.866666E+01
1090-04 2210-04 3360-04 4560-04 5800-04 7100-04 8450-04
9850-04 1130-03 1270-03 7500-07 2230-06 4370-06 7210-06
1070-05 1500-05 2000-05 2560-05 3180-05 3850-05 2820-09
1250-08 3440-08 7550-08 1450-07 2520-07 4050-07 6110-07
8710-07 1180-06
CO+ 1 3 1.000000E+00
0 3 2
2. 0.000000E+00
4. 2.983160E+04
2. 6.600920E+04
3.4737100E+03 2.1819000E+01 2.8449000E+00 4.3520000E-02
2.2475500E+03 1.9470000E+01 2.2869000E+00 2.7940000E-02
2.4952100E+03 4.0182000E+01 2.5898000E+00 2.7280000E-02
CO+ FIRST NEGATIVE BAND SYSTEM
10 10 3 1 1 1.700000E-02
6.6009200E+04 2.4952100E+03 4.0182000E+01 4.7240000E-01 2.5898000E+00
0.0000000E+00 3.4737100E+03 2.1819000E+01 -1.0072000E-03 2.8449000E+00
5315+00 3125+00 1115+00 3247-01 8761-02 2351-01 6548-03
1938-03 6161-04 2106-04 3394+00 5651-01 2578+00 1984+00

APPENDIX B - Continued

9334-01	3557-01	1242-01	4255-02	1486-02	5412-03	1039+00
3180+00	1763-01	9127-01	1864+00	1445+00	7765-01	3518-01
1478-01	6087-02	2142-01	2170+00	1464+00	1230+00	2037-02
9643-01	1438+00	1134+00	6772-01	3522-01	3383-02	7490-01
2550+00	1728-01	1646+00	3359-01	1413-01	8642-01	1139+00
9377-01	4328-03	1748-01	1471+00	1927+00	1306-01	9965-01
1028+00	7692-02	1929-01	7072-01	4649-04	3087-02	5006-01
2009+00	8076-01	8407-01	1652-01	1102+00	6058-01	2128-02
4280-05	4378-03	1203-01	1011+00	1977+00	5947-02	1233+00
7172-02	4898-01	9238-01	3420-06	5162-04	2228-02	3311-01
1548+00	1306+00	1665-01	8166-01	6065-01	1171-02	2395-07
5168-05	3333-03	7975-02	7009-01	1811+00	4288-01	7613-01
1476-01	8754-01					

1.700000E-01 3.500000E-01
CO+ COMET TAIL BAND SYSTEM

10 10 2 1 1 7.240000E-03
2.9831600E+04 2.2475500E+03 1.9470000E+01 1.8800000E-02 2.2869000E+00
0.0000000E+00 3.4737100E+03 2.1819000E+01-1.0072000E-03 2.8449000E+00

4274-01	1151+00	1698+00	1824+00	1600+00	1219+00	8369-01
5316-01	3182-01	1818-01	1520+00	1932+00	9746-01	1272-01
5796-02	4537-01	8359-01	9854-01	9185-01	7381-01	2429+00
8046-01	3228-02	7483-01	9618-01	4719-01	4973-02	5155-02
3212-01	5927-01	2516+00	5677-03	1083+00	6884-01	5787-03
3336-01	7197-01	5649-01	1880-01	2345-03	1734+00	9166-01
8454-01	4186-02	7785-01	5594-01	2730-02	1681-01	5238-01
5427-01	8654-01	1905+00	3505-03	9742-01	3532-01	9275-02
6355-01	4599-01	4066-02	9005-02	3233-01	1760+00	7225-01
6206-01	1993-01	7857-01	1316-01	1385-01	5420-01	3865-01
9207-02	9992-01	1724+00	1054-02	9837-01	5569-02	4380-01
5538-01	3702-02	1694-01	2018-02	3897-01	1613+00	9145-01
2964-01	5383-01	5073-01	2289-02	5217-01	3607-01	3414-03
1097-01	8830-01	1724+00	1638-01	8163-01	4949-02	6917-01
1343-01	1486-01					

3.000000E-01 8.500000E-01
CO+ FREE-FREE RADIATION

0 51 5.040000E-02 5.000000E-02 1.000000E+00

H 0 3 1.510000E+17

HYDROGEN ATOM FREE-FREE CONTINUUM

0 50 5.250000E-02 1.000000E-01 7.315000E-02

HYDROGEN ATOM FREE-BOUND CONTINUUM

0 6 6 5.100000E-02 1.000000E-04

2.	0.000000E+00		
8.	1.183540E+05		
14.	1.402710E+05		
22.	1.479430E+05		
32.	1.514940E+05		
44.	1.534220E+05		
2.	1.000000E+00	0.000000E+00	1.578060E+05
8.	2.000000E+00	1.183540E+05	1.578060E+05
14.	3.000000E+00	1.402710E+05	1.578060E+05
22.	4.000000E+00	1.479430E+05	1.578060E+05
32.	5.000000E+00	1.514940E+05	1.578060E+05
44.	6.000000E+00	1.534220E+05	1.578060E+05

1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000

APPENDIX B – Continued

HYDROGEN ATOM LINE RADIATION

0 20 0 1.578060E+04 1.008000E+00
 9.378030E-02 0.000000E+00 7.799000E-03 2 12
 9.497430E-02 0.000000E+00 1.394000E-02 2 50
 9.925370E-02 0.000000E+00 2.899000E-02 2 32
 1.025720E-01 0.000000E+00 7.910000E-02 2 18
 1.215670E-01 0.000000E+00 4.162000E-01 2 8
 3.970070E-01 8.225900E+04 1.270000E-02 8 98
 4.101730E-01 8.225900E+04 2.209000E-02 8 72
 4.340360E-01 8.225900E+04 4.467000E-02 8 50
 4.861320E-01 8.225900E+04 1.193000E-01 8 32
 6.562800E-01 8.225900E+04 6.407000E-01 8 18
 9.545980E-01 9.749200E+04 1.604000E-02 18128
 1.004940E+00 9.749200E+04 2.768000E-02 18 98
 1.093810E+00 9.749200E+04 5.584000E-02 18 72
 1.281810E+00 9.749200E+04 1.506000E-01 18 50
 1.817410E+00 1.028240E+05 1.870000E-02 32162
 1.875100E+00 9.749200E+04 8.421000E-01 18 32
 1.944560E+00 1.028240E+05 3.230000E-02 32128
 2.165500E+00 1.028240E+05 6.549000E-02 32 98
 2.625200E+00 1.028240E+05 1.793000E-01 32 72
 4.051200E+00 1.028240E+05 1.038000E+00 32 50

H+ 0 1 5.260000E+16

HYDROGEN ION FREE-FREE CONTINUUM

0 48 5.150000E-02 1.000000E-01 1.000000E+00

H2 1 3 2.357000E+12

0 3 2

1. 0.000000E+00

1. 1.319220E+05

2. 1.439420E+05

6.323800E+03 1.696300E+02 8.748000E+01 4.306000E+00

1.952300E+03 2.867800E+01 2.880000E+01 1.716900E+00

3.514600E+03 9.644300E+01 4.509200E+01 2.339500E+00

H2 LYMAN BAND SYSTEM

4 14 2 1 1 5.000000E-01

1.319220E+05 1.952300E+03 2.867800E+01 5.797000E-01 2.880000E+01

0.000000E+00 6.323800E+03 1.696300E+02 4.173000E-01 8.748000E+01

7240-02 3214-01 7476-01 1211+00 3630-01 1004+00 1318+00

1013+00 9947-01 1500+00 8068-01 7843-02 1816+00 1056+00

1740-02 3713-01 2353+00 1467-01 5008-01 7850-01 2186+00

2471-01 1055+00 7121-02 1423+00 1510+00 2582-01 4748-01

6144-01 2208+00 3014-01 8990-01 1579-01 1485+00 1960+00

5371-03 1927-02 4679-01 2177+00 1410+00 5652-04 5213-02

7925-01 2655+00 4436-06 4187-04 6404-02 9883-01 4491-07

8971-05 2222-04 3255-02 1060-07 9728-07 1667-04 4856-03

8.000000E-02 1.900000E-01

H2 WERNER BAND SYSTEM

4 14 3 1 1 3.900000E-01

1.439420E+05 3.345400E+03 9.644300E+01 0.000000E+00 4.509200E+01

0.000000E+00 6.323800E+03 1.696300E+02 4.173000E-01 8.748000E+01

1221+00 1868+00 1790+00 1403+00 3364+00 1434+00 1266-01

6821-02 3592+00 3669-02 1163+00 1066+00 1901+00 2324+00

8277-01 3844-02 5246-01 3315+00 4172-01 1445+00 7144-02

1564+00 3223+00 4631-02 3872-03 2941-01 2723+00 2157+00

3554-05 1793-02 6903-01 3628+00 5523-07 8195-05 4344-02

1210+00 2138-09 8631-06 8292-06 6826-02 1009-09 2946-08

APPENDIX B - Continued

4428-06 4679-04 9523-11 1353-08 2403-06 6928-05 4728-11
 5313-09 1579-08 2207-05 5023-11 1265-09 1136-08 3221-06
 8.000000E-02 2.000000E-01
 HYDROGEN MOLECULE FREE-FREE CONTINUUM
 0 48 5.075000E-02 1.000000E-01 1.070000E-02

HE 0 3 1.890000E+19
 HELIUM ATOM FREE-FREE CONTINUUM
 0 50 5.000000E-02 1.000000E-01 2.256345E-02
 HELIUM ATOM FREE-BOUND CONTINUUM
 0 3 2 5.500000E-02 1.000000E-04

1. 0.000000E+00
 3. 2.299920E+05
 1. 2.392320E+05
 3. 2.000000E+00 2.299920E+05 2.853210E+05
 1. 2.000000E+00 2.392320E+05 2.853210E+05
 1.000 1.000 0.000
 1.000 1.000 0.000

HELIUM ATOM LINE RADIATION
 0 41 0 2.853210E+04 4.003000E+00

5.370300E-02 0.000000E+00 7.340000E-02 1 3
 5.843340E-02 0.000000E+00 2.762000E-01 1 3
 3.447590E-01 1.662780E+05 1.280000E-02 1 3
 3.613640E-01 1.662780E+05 2.210000E-02 1 3
 3.964730E-01 1.662780E+05 5.070000E-02 1 3
 4.437550E-01 1.711350E+05 3.080000E-03 3 1
 4.471500E-01 1.690870E+05 1.250000E-01 9 15
 4.921930E-01 1.711350E+05 1.220000E-01 3 5
 5.015680E-01 1.662780E+05 1.514000E-01 1 3
 5.047740E-01 1.711350E+05 8.340000E-03 3 1
 5.875700E-01 1.690870E+05 6.090000E-01 9 15
 6.678150E-01 1.711350E+05 7.110000E-01 3 5
 7.065300E-01 1.690870E+05 6.930000E-02 9 3
 7.281350E-01 1.711350E+05 4.800000E-02 3 1
 1.083000E+00 1.598560E+05 5.391000E-01 3 9
 1.101310E+00 1.848650E+05 5.210000E-02 1 3
 1.196910E+00 1.855650E+05 1.230000E-01 9 15
 1.278500E+00 1.861020E+05 1.580000E-01 15 21
 1.279030E+00 1.861050E+05 1.580000E-01 5 7
 1.296840E+00 1.862100E+05 1.390000E-01 3 5
 1.508370E+00 1.848650E+05 1.400000E-01 1 3
 1.700200E+00 1.855650E+05 4.820000E-01 9 15
 1.868600E+00 1.861020E+05 1.020000E+00 15 21
 1.869690E+00 1.861050E+05 1.010000E+00 5 7
 1.908940E+00 1.862100E+05 6.470000E-01 3 5
 2.058130E+00 1.662780E+05 3.764000E-01 1 3
 2.112000E+00 1.855650E+05 1.450000E-01 9 3
 2.113200E+00 1.862100E+05 1.030000E-01 3 1
 2.161700E+00 1.914470E+05 7.190000E-02 5 7
 2.472700E+00 1.912170E+05 1.210000E-01 9 15
 2.618500E+00 1.914450E+05 1.870000E-01 15 21
 2.619800E+00 1.914470E+05 1.870000E-01 5 7
 2.653100E+00 1.914930E+05 1.520000E-01 3 5
 3.329900E+00 1.909400E+05 1.510000E-01 1 3
 3.702600E+00 1.912170E+05 4.420000E-01 9 15
 4.036500E+00 1.914450E+05 8.880000E-01 15 21
 4.039600E+00 1.914470E+05 8.870000E-01 5 7
 4.121600E+00 1.914930E+05 6.490000E-01 3 5

APPENDIX B - Continued

4.294700E+00 1.832370E+05 8.960000E-01 3 9
 4.605300E+00 1.914930E+05 1.590000E-01 3 1
 4.693600E+00 1.912170E+05 2.230000E-01 9 3

HE+ 0 1 1.390000E+18

HELIUM ION FREE-FREE RADIATION

0 48 5.150000E-02 1.000000E-01 1.000000E+00

HG 0 3 6.440700E+12

HG F-F

0 51 1.990000E-01 1.000000E-02 2.000000E-02

HG F-B

0 5 5 2.000000E-01 1.000000E-04

1. 0.000000E+00

9. 6.012500E+04

2. 7.779400E+04

2. 8.970900E+04

1. 9.198000E+04

9. 6.000000E+00 6.012500E+04 1.211240E+05

3. 6.000000E+00 7.779400E+04 1.211240E+05

3. 7.000000E+00 8.970900E+04 1.211240E+05

1. 7.000000E+00 9.198000E+04 1.211240E+05

128. 8.000000E+00 1.192310E+05 1.211240E+05

1.000 1.000 0.000

1.000 1.000 0.000

1.000 1.000 0.000

1.000 1.000 0.000

1.000 1.000 0.000

HG LINES

0 19 0 1.211240E+05 2.006100E+02

2.536520E-01 0.000000E+00 3.400000E-01 1 3

2.752780E-01 3.764500E+04 1.200000E-01 1 3

2.893600E-01 3.941200E+04 7.666667E-02 3 3

2.967280E-01 3.764500E+04 2.900000E+00 1 3

3.021500E-01 4.404300E+04 1.080000E-01 5 7

3.125660E-01 3.941200E+04 3.666667E-02 3 5

3.131550E-01 3.941200E+04 3.066667E-01 3 3

3.131830E-01 3.941200E+04 3.080000E-01 3 5

3.341480E-01 4.404300E+04 4.040000E-02 5 3

3.650150E-01 4.404300E+04 2.600000E+00 5 7

3.654830E-01 4.404300E+04 7.000000E-01 5 5

3.662880E-01 4.404300E+04 7.400000E-02 5 3

3.663280E-01 4.404300E+04 2.020000E-01 5 5

4.046560E-01 3.764500E+04 8.800000E+00 1 3

4.077810E-01 3.941200E+04 2.133333E-01 3 1

4.358350E-01 3.941200E+04 8.000000E-01 3 3

5.460740E-01 4.404300E+04 7.600000E+00 5 3

5.769590E-01 5.406900E+04 1.433333E+00 3 5

5.790650E-01 5.406900E+04 1.700000E+00 3 5

N 0 3 1.892000E+19

NITROGEN ATOM FREE-FREE RADIATION

0 51 4.990000E-02 1.000000E-01 1.796849E-02

3 NITROGEN ATOM FREE-BOUND RADIATION

0 3 14 5.000000E-02 1.000000E-04

4. 0.000000E+00

10. 2.766265E+04

6. 4.149500E+04

APPENDIX B – Continued

6.	2.000000E+00	4.149500E+04	2.156775E+05
4.	2.000000E+00	0.000000E+00	1.687760E+05
10.	2.000000E+00	2.766200E+04	1.906835E+05
6.	2.000000E+00	4.149500E+04	1.906835E+05
10.	2.000000E+00	2.766200E+04	1.687760E+05
6.	2.000000E+00	4.149500E+04	1.687760E+05
9.	3.000000E+00	1.499089E+05	1.686475E+05
16.	4.000000E+00	1.581070E+05	1.686475E+05
25.	5.000000E+00	1.619016E+05	1.686475E+05
36.	6.000000E+00	1.639629E+05	1.686475E+05
49.	7.000000E+00	1.652057E+05	1.686475E+05
64.	8.000000E+00	1.660124E+05	1.686475E+05
81.	9.000000E+00	1.665654E+05	1.686475E+05
100.	1.000000E+01	1.669610E+05	1.686475E+05

2.000	4.727	2.030
2.000	4.287	11.420
2.000	4.826	5.020
2.000	5.112	2.870
1.500	3.847	4.410
1.500	4.337	4.200
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000
1.000	1.000	0.000

NITROGEN ATOM LINE RADIATION

0	26	0	1.686470E+05	1.400800E+01		
1.134600E-01		0.000000E+00		1.300000E-01	4	12
1.167900E-01		1.922800E+04		3.400000E-02	10	14
1.176900E-01		1.922800E+04		1.400000E-02	10	6
1.199900E-01		0.000000E+00		3.500000E-01	4	12
1.243300E-01		1.922800E+04		1.100000E-01	10	10
1.310700E-01		2.884000E+04		5.600000E-02	6	10
1.319500E-01		2.884000E+04		3.400000E-02	6	6
1.411940E-01		2.884000E+04		2.600000E-02	6	10
1.493300E-01		1.922800E+04		1.100000E-01	10	6
1.743600E-01		2.884000E+04		9.100000E-02	6	6
8.211800E-01		8.333700E+04		2.310000E-02	12	12
8.617500E-01		8.619300E+04		3.180000E-01	6	6
8.691600E-01		8.333700E+04		3.580000E-02	12	20
9.047600E-01		9.966300E+04		4.670000E-01	10	14
9.050400E-01		9.358200E+04		9.450000E-01	2	6
9.395300E-01		8.619300E+04		4.780000E-01	6	10
9.829200E-01		9.483900E+04		1.440000E-01	20	20
1.011700E+00		9.483900E+04		8.020000E-01	20	28
1.052500E+00		9.551100E+04		6.880000E-01	12	20
1.059500E+00		1.107130E+05		7.310000E-01	14	18
1.070800E+00		9.551100E+04		2.160000E-01	12	12
1.129000E+00		9.483900E+04		1.680000E-01	20	12
1.204300E+00		9.683400E+04		1.300000E-01	10	10
1.221700E+00		9.551100E+04		1.710000E-01	12	12
1.235000E+00		9.675200E+04		8.500000E-01	4	12
1.246900E+00		9.683400E+04		7.100000E-01	10	14

APPENDIX B – Continued

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N+ 0 3 2.806000E+15
NITROGEN ION FREE-FREE RADIATION
0 51 5.020000E-02 1.000000E-01 1.000000E+00
NITROGEN ION DUMMY F-B
0 3 1 5.021000E-02 1.000000E-04
9. 1.285000E+02
5. 2.203600E+04
1. 4.703000E+04
0. 0.000000E+00 0.000000E+00 0.000000E+00
0.000 0.000 0.000
NITROGEN ION LINE RADIATION
0 39 1 3.435151E+05 1.400800E+01
9.163400E-02 8.930000E+01 2.200000E-01 9 9
1.085100E-01 8.930000E+01 1.700000E-01 9 15
3.328300E-01 1.666160E+05 1.110000E-01 15 9
3.437160E-01 1.491890E+05 1.420000E-01 3 1
3.601300E-01 1.688930E+05 1.340000E-01 3 9
3.842700E-01 1.706370E+05 1.530000E-01 9 9
3.919010E-01 1.646120E+05 2.310000E-01 3 3
3.995000E-01 1.491890E+05 6.300000E-01 3 5
4.026080E-01 1.865720E+05 2.800000E-01 7 9
4.040900E-01 1.865930E+05 8.300000E-01 21 27
4.137400E-01 2.056770E+05 1.170000E-01 15 5
4.176160E-01 1.870920E+05 8.000000E-01 5 7
4.227750E-01 1.742130E+05 1.710000E-01 5 3
4.239400E-01 1.874720E+05 8.100000E-01 15 21
4.434600E-01 1.888840E+05 9.100000E-01 9 15
4.447030E-01 1.646120E+05 6.420000E-01 3 5
4.530400E-01 1.893360E+05 6.700000E-01 7 9
4.552540E-01 1.893360E+05 3.050000E-01 7 9
4.623200E-01 1.490130E+05 3.370000E-01 9 9
4.677930E-01 1.901210E+05 9.000000E-01 3 5
4.793500E-01 1.666160E+05 1.230000E-01 15 15
5.000800E-01 1.688930E+05 8.400000E-01 3 9
5.004000E-01 1.666160E+05 6.390000E-01 15 21
5.006900E-01 2.056770E+05 2.910000E-01 15 15
5.028800E-01 1.490130E+05 9.700000E-02 9 3
5.104450E-01 1.782740E+05 2.220000E-01 1 3
5.175900E-01 2.256440E+05 5.600000E-01 15 25
5.177800E-01 2.237310E+05 5.700000E-01 25 35
5.335800E-01 2.256440E+05 1.780000E-01 15 15
5.478800E-01 1.706370E+05 1.800000E-01 9 9
5.537400E-01 2.056770E+05 4.320000E-01 15 25
5.679400E-01 1.490130E+05 4.520000E-01 9 15
5.938500E-01 1.706370E+05 4.980000E-01 9 15
6.168100E-01 1.865930E+05 1.480000E-01 21 15
6.242520E-01 1.893360E+05 1.420000E-01 7 5
6.345800E-01 1.874720E+05 1.110000E-01 15 9
6.482070E-01 1.491890E+05 2.300000E-01 3 3
6.610580E-01 1.742130E+05 5.400000E-01 5 7
6.629800E-01 1.870920E+05 1.120000E-01 5 3

N2 1 4 1.000000E+00
0 6 3
1. 0.000000E+00
1. 7.223639E+04
2. 8.578989E+04
2. 9.969445E+04
2. 1.282647E+05

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APPENDIX B - Continued

1. 1.503260E+05
3.395007E+03 2.079929E+01 2.891988E+00 2.690556E-02
2.101180E+03 1.998637E+01 2.071782E+00 1.870440E-02
2.495037E+03 2.081944E+01 2.356754E+00 2.647392E-02
2.434464E+03 1.840369E+01 2.355316E+00 3.165360E-02
2.928102E+03 2.457470E+01 2.627105E+00 2.834436E-02
1.081460E+03 6.935016E+00 1.660375E+00 6.906240E-03
N2 FIRST POSITIVE BAND SYSTEM
14 14 3 2 -1 3.000000E-03
8.578989E+04 2.495037E+03 2.081944E+01 0.000000E+00 2.356754E+00
7.223639E+04 2.101180E+03 1.998637E+01 -3.597000E-02 2.071782E+00
3382+00 4064+00 1975+00 5014-01 7190-02 5871-03 2616-04
5698-06 4722-08 6508-11 2780-14 8114-15 2515-15 5962-16
3248+00 2310-02 2120+00 2987+00 1318+00 2729-01 2925-02
1613-03 4174-05 3963-07 6055-10 3322-13 5035-15 1662-15
1900+00 1032+00 1132+00 3868-01 2738+00 2106+00 6148-01
8462-02 5675-03 1719-04 1848-06 3035-09 2138-12 4334-15
8857-01 1782+00 1205-02 1623+00 1806-02 1808+00 2605+00
1065+00 1857-01 1495-02 5241-04 6322-06 1101-08 1051-11
3649-01 1450+00 7724-01 3227-01 1139+00 4780-01 8305-01
2706+00 1561+00 3420-01 3274-02 1318-03 1769-05 3236-08
1399-01 8647-01 1275+00 9050-02 8823-01 4262-01 1040+00
1916-02 2438+00 2029+00 5569-01 6298-02 2890-03 4290-05
5146-02 4367-01 1127+00 6910-01 5227-02 1057+00 3171-02
1290+00 2766-04 1918+00 2402+00 8265-01 1099-01 5717-03
1351-02 2000-01 7496-01 1009+00 1798-01 3829-01 8078-01
6748-02 1159+00 1694-01 1299+00 2530+00 1140+00 1777-01
6595-03 8626-02 4247-01 9079-01 6361-01 1230-05 6967-01
3946-01 3633-01 7862-01 5219-01 7206-01 2688+00 1480+00
2348-03 3589-02 2182-01 5406-01 8349-01 2454-01 1289-01
7733-01 8360-02 5773-01 3764-01 3779-01 2857-01 2675+00
8403-04 1463-02 1053-01 3917-01 7511-01 5820-01 2460-02
3833-01 6077-01 3194-03 8370-01 9012-02 1109-01 4687-02
3038-04 5907-03 4884-02 2187-01 5510-01 7056-01 2810-01
2738-02 5721-01 3305-01 1307-01 7897-01 2617-04 1156+00
1114-04 2380-03 2212-02 1151-01 3567-01 6338-01 5261-01
6400-02 1852-01 5945-01 9576-02 3527-01 5846-01 9342-02
4147-05 9627-04 9884-03 5824-02 2128-01 4795-01 6039-01
2912-01 8677-04 3729-01 4603-01 6687-04 5423-01 3235-01
4.800000E-01 2.000000E+00
N2 SECOND POSITIVE BAND SYSTEM
7 7 5 3 -1 6.000000E-02
1.282647E+05 2.928102E+03 2.457470E+01 -3.093420E+00 2.627105E+00
8.578989E+04 2.495037E+03 2.081944E+01 0.000000E+00 2.356754E+00
4493+00 3899+00 1349+00 2363-01 2190-02 0000+00 0000+00
3287+00 1868-01 3223+00 2515+00 6957-01 0000+00 0000+00
1469+00 2038+00 3299-01 1630+00 3034+00 0000+00 0000+00
5226-01 2003+00 5957-01 1181+00 4752-01 0000+00 0000+00
1634-01 1124+00 1614+00 1841-02 1570+00 0000+00 0000+00
4726-02 4839-01 1427-01 8891-01 1416-01 0000+00 0000+00
1300-02 1790-01 8303-01 1345+00 2939-01 0000+00 0000+00
2.600000E-01 5.500000E-01
N2 BIRGE-HOPFIELD BAND SYSTEM NO. 2
14 14 6 1 1 4.300000E-01
1.503260E+05 1.081460E+03 6.935016E+00 0.000000E+00 1.660375E+00
0.000000E+00 3.395007E+03 2.079929E+01 -2.876600E-02 2.891988E+00
2030-06 2673-05 1800-04 8201-04 8162-03 8162-03 1975-02
4176-02 7869-02 1343-01 2100-01 3040-01 4107-01 5211-01
2878-05 3336-04 1961-03 7784-03 5708-02 5708-02 1168-01

APPENDIX B - Continued

2062-01	3197-01	4407-01	5445-01	6053-01	6050-01	5404-01
2113-04	2141-03	1091-02	3720-02	1942-01	1942-01	3272-01
4651-01	5638-01	5832-01	5085-01	3613-01	1919-01	5814-02
1063-03	9324-03	4070-02	1173-01	4130-01	4130-01	5475-01
5846-01	4940-01	3110-01	1209-01	1074-02	1929-02	1196-01
4098-03	3076-02	1132-01	2695-01	5878-01	5878-01	5620-01
3822-01	1533-01	1250-02	2797-02	1551-01	2806-01	3106-01
1284-02	8129-02	2468-01	4702-01	5468-01	5468-01	3050-01
6758-02	4457-03	1221-01	2752-01	3141-01	2129-01	6910-02
3396-02	1779-01	4332-01	6286-01	2809-01	2809-01	3394-02
3245-02	2080-01	3262-01	2576-01	9103-02	6593-04	5677-02
7757-02	3287-01	6166-01	6290-01	3065-02	3065-02	5377-02
2616-01	3340-01	1858-01	2114-02	2807-02	1620-01	2439-01
1657-01	5180-01	7053-01	4333-01	4927-02	4927-02	2847-01
3350-01	1376-01	6984-04	9006-02	2344-01	2239-01	8604-02
2782-01	6982-01	6261-01	1557-01	2758-01	2758-01	3513-01
1227-01	1776-03	1439-01	2641-01	1694-01	2066-02	2643-02
4466-01	8004-01	3936-01	2292-04	3852-01	3852-01	1459-01
2976-03	1745-01	2734-01	1223-01	3466-04	8758-02	2074-01
6484-01	7664-01	1304-01	9250-02	2196-01	2196-01	5961-06
1773-01	2839-01	9869-02	4287-03	1434-01	2229-01	1069-01
8563-01	5880-01	1031-03	3278-01	1637-02	1637-02	1441-01
3046-01	1026-01	1053-02	1801-01	2177-01	5835-02	9240-03
1033+00	3266-01	9064-02	4681-01	6908-02	6908-02	3231-01
1414-01	7642-03	1971-01	2150-01	3233-02	3700-02	1801-01
9.000000E-02 1.600000E-01						
N2 MOLECULE FREE-FREE RADIATION						
0	51	5.045000E-02	1.000000E-01	3.593699E-02		
N2+ 1 3 2.027000E+14						
0	4	2				
1.	0.000000E+00					
2.	1.295200E+04					
1.	3.663400E+04					
1.	9.297800E+04					
3.175700E+03	2.321650E+01	2.779800E+00	2.877600E-02			
2.736600E+03	2.145250E+01	2.503500E+00	0.000000E+00			
3.481670E+03	3.336580E+01	2.997000E+00	2.806000E-02			
2.949540E+03	0.000000E+00	2.374000E+00	7.194000E-02			
N2+ MEINEL BAND SYSTEM						
7	7	2	1	1	1.200000E-02	
1.295200E+04	2.736600E+03	2.145250E+01	0.000000E+00	2.503500E+00		
0.000000E+00	3.175700E+03	2.321650E+01	-5.755200E-02	2.779800E+00		
4751+00	3255+00	1360+00	4526-01	1329-01	3624-02	0000+00
3798+00	3115-01	2245+00	1990+00	1032+00	4145-01	0000+00
1226+00	3358+00	2137-01	7974-01	1745+00	1395+00	0000+00
2055-01	2368+00	1851+00	1048+00	7195-02	1078+00	0000+00
1914-02	6236-01	2946+00	6274-01	1553+00	6918-02	0000+00
9822-04	7946-02	1171+00	2929+00	5808-02	1509+00	0000+00
2573-05	5163-03	1972-01	1738+00	2479+00	5609-02	0000+00
5.000000E-01 5.000000E+00						
N2+ FIRST NEGATIVE BAND SYSTEM						
14	14	3	1	-1	3.500000E-02	
3.663400E+04	3.481670E+03	3.336580E+01	-7.733550E-01	2.997000E+00		
0.000000E+00	3.175700E+03	2.321650E+01	-5.755200E-02	2.779800E+00		
6509+00	3014+00	4537-01	2248-03	1452-04	4634-06	9482-08
6438-09	4200-12	1275-11	3949-13	2877-15	5259-15	7421-19
2588+00	2226+00	4060+00	1056+00	6935-02	3986-04	3088-05

APPENDIX B – Continued

3417-07	5755-08	3877-11	1028-10	7000-12	2491-14	9910-15
7016-01	2860+00	5065-01	4137+00	1660+00	1340-01	5729-04
1132-04	4951-07	2659-07	1710-09	3877-10	5560-11	1009-12
1600-01	1324+00	2290+00	2100-02	3792+00	2205+00	2069-01
4930-04	3006-04	1742-07	8356-07	1676-08	7849-10	2755-10
3297-02	4273-01	1654+00	1557+00	6726-02	3310+00	2673+00
2789-01	1807-04	6420-04	3295-07	1969-06	9184-08	5702-10
6342-03	1140-01	7113-01	1706+00	9290-01	2925-01	2830+00
3068+00	3419-01	1067-05	1161-03	6715-06	3593-06	3519-07
1155-03	2700-02	2362-01	9451-01	1569+00	4815-01	5331-01
2414+00	3401+00	3890-01	8094-04	1823-03	3522-05	4993-06
2000-04	5861-03	6691-02	3801-01	1096+00	1333+00	2044-01
7236-01	2083+00	3686+00	4153-01	3872-03	2509-03	1172-04
3280-05	1185-03	1695-02	1261-01	5236-01	1161+00	1065+00
5939-02	8469-01	1837+00	3933+00	4170-01	1087-02	3010-03
5034-06	2239-04	3934-03	3668-02	2003-01	6488-01	1150+00
8084-01	4743-03	9065-01	1672+00	4149+00	3928-01	2361-02
7027-07	3931-05	8445-04	9639-03	6598-02	2826-01	7442-01
1084+00	5865-01	5552-03	9141-01	1579+00	4338+00	3432-01
8419-08	6286-06	1675-04	2324-03	1942-02	1043-01	3652-01
8051-01	9821-01	4075-01	3604-02	8818-01	1554+00	4496+00
7471-09	8755-07	3030-05	5156-04	5207-03	3406-02	1496-01
4411-01	8319-01	8628-01	2710-01	7896-02	8204-01	1593+00
2725-10	9533-08	4831-06	1044-04	1281-03	1007-02	5378-02
1991-01	5053-01	8288-01	7393-01	1720-01	1238-01	7384-01
2.500000E-01	6.500000E-01					
N2+ MOLECULAR ION FREE-FREE RADIATION						
0	51	5.030000E-02	1.000000E-01	1.000000E+00		
NO 1 4 2.694000E+16						
0	3	2				
2.	8.640000E+01					
1.	6.325785E+04					
2.	6.608747E+04					
2.739270E+03	2.010000E+01	2.452580E+00	2.561060E-02			
3.411830E+03	2.083380E+01	2.870690E+00	2.359630E-02			
1.493020E+03	1.093920E+01	1.620810E+00	2.194170E-02			
NO GAMMA BAND SYSTEM						
7	7	2	1	-1	2.500000E-02	
6.325785E+04	3.411830E+03	2.083380E+01	-4.028640E-01	2.870690E+00		
8.640000E+01	2.739270E+03	2.010000E+01	-1.726560E-03	2.452580E+00		
1653+00	3291+00	2906+00	1504+00	5080-01	1160-01	3200-02
2636+00	1050+00	1460-01	1904+00	2370+00	1588+00	3520-01
2377+00	8000-03	1545+00	5000-01	3660-01	1077+00	0000+00
1606+00	7210-01	7530-01	3090-01	1526+00	0000+00	0000+00
9080-01	1349+00	6000-03	2950-01	0000+00	0000+00	0000+00
4560-01	1340+00	3420-01	0000+00	0000+00	0000+00	0000+00
2110-01	9870-01	8840-01	0000+00	0000+00	0000+00	0000+00
1.900000E-01	3.500000E-01					
NO BETA BAND SYSTEM						
7	7	3	1	1	1.000000E-02	
6.608747E+04	1.493020E+03	1.093920E+01	1.391320E-01	1.620810E+00		
8.640000E+01	2.739270E+03	2.010000E+01	-1.726560E-03	2.452580E+00		
2264-04	1851-03	7921-03	2364-02	5530-02	1080-01	1834-01
3110-03	2089-02	7278-02	1749-01	3249-01	4959-01	6444-01
2046-02	1093-01	2975-01	5445-01	7450-01	7975-01	6747-01
8569-02	3487-01	6959-01	8817-01	7569-01	4184-01	1072-01

APPENDIX B - Continued

2560-01 7461-01 9835-01 7012-01 2192-01 3716-04 1382-01
 5799-01 1103+00 7784-01 1483-01 3280-02 3385-01 4922-01
 1033+00 1097+00 2228-01 5985-02 4703-01 4824-01 1336-01
 2.100000E-01 5.000000E-01

NITRIC OXIDE FREE-FREE RADIATION

0 51 5.050000E-02 1.000000E-01 3.065373E-02

NO INFRARED VIBRATION-ROTATION BANDS

2.450000E+00 1.903850E+03 1.397000E+01 1.704600E+00 1.780000E-02
 0 30 300 6.000000E+03 1.666666E+01
 2942-05 5969-05 9081-05 1230-04 1565-04 1915-04 2280-04
 2657-04 3041-04 3425-04 1138-06 3388-06 6636-06 1092-05
 1628-05 2275-05 3028-05 3884-05 4826-05 5840-05 6820-09
 2834-08 8956-08 2510-07 6278-07 1392-06 2743-06 4844-06
 7771-06 1147-05

0 0 3 8.692000E+18

OXYGEN ATOM FREE-FREE CONTINUUM

0 51 5.020000E-02 5.000000E-02 1.268524E-02

OXYGEN ATOM FREE-BOUND CONTINUUM (HENRY FORMULA)

0 3 14 5.010000E-02 1.000000E-04
 9. 1.122311E+02
 5. 2.283140E+04
 1. 4.862253E+04
 9. 2.000000E+00 1.122311E+02 2.162665E+05
 9. 2.000000E+00 1.122311E+02 1.966252E+05
 5. 2.000000E+00 2.283140E+04 2.162665E+05
 5. 2.000000E+00 2.283140E+04 1.966252E+05
 1. 2.000000E+00 4.862253E+04 2.162665E+05
 9. 2.000000E+00 1.122311E+02 1.580396E+05
 9. 3.000000E+00 1.404738E+05 1.580330E+05
 16. 4.000000E+00 1.481559E+05 1.580330E+05
 25. 5.000000E+00 1.517117E+05 1.580330E+05
 36. 6.000000E+00 1.536432E+05 1.580330E+05
 49. 7.000000E+00 1.548078E+05 1.580330E+05
 64. 8.000000E+00 1.555637E+05 1.580330E+05
 81. 9.000000E+00 1.560820E+05 1.580330E+05
 100. 1.000000E+01 1.564527E+05 1.580330E+05
 1.500 4.311 2.260
 1.500 4.378 3.850
 1.500 4.800 1.950
 1.500 6.829 4.640
 1.500 5.124 7.650
 1.000 2.661 2.940
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000
 1.000 1.000 0.000

OXYGEN ATOM LINE RADIATION

0 25 0 1.580330E+05 1.600000E+01
 8.113700E-02 7.800000E+01 7.700000E-03 9 9
 8.784500E-02 7.800000E+01 3.700000E-02 9 9
 9.360110E-02 1.586800E+04 1.500000E-02 5 7
 9.894600E-02 7.800000E+01 5.600000E-02 9 15
 9.994940E-02 1.586800E+04 3.500000E-02 5 3

APPENDIX B - Continued

1.026600E-01	7.800000E+01	1.000000E-02	9	15
1.152160E-01	1.586800E+04	9.000000E-02	5	5
1.217640E-01	3.379200E+04	1.300000E-01	1	3
1.303500E-01	7.800000E+01	3.100000E-02	9	3
6.157300E-01	8.662900E+04	6.640000E-02	15	25
6.653780E-01	1.159180E+05	1.330000E-01	3	1
7.156800E-01	1.026620E+05	3.630000E-01	5	5
7.477300E-01	1.139160E+05	5.700000E-01	9	15
7.773400E-01	7.376800E+04	9.220000E-01	5	15
7.886310E-01	1.159180E+05	5.750000E-01	3	5
7.949300E-01	1.011430E+05	4.950000E-01	15	21
7.989900E-01	8.863100E+04	4.600000E-01	9	15
8.226800E-01	1.011430E+05	3.270000E-01	15	15
8.446500E-01	7.679500E+04	8.980000E-01	3	9
8.508630E-01	1.159180E+05	3.140000E-01	3	3
8.820450E-01	1.026620E+05	4.260000E-01	5	7
9.263900E-01	8.662900E+04	9.000000E-01	15	25
1.128700E+00	8.863100E+04	7.500000E-01	9	15
1.129900E+00	8.662900E+04	1.730000E-01	15	5
1.316400E+00	8.863100E+04	1.630000E-01	9	3
O+ 0 3 1.621000E+16				
O+ FREE-FREE CONTINUUM				
0	51	5.010000E-02	5.050000E-02	1.000000E+00
O+ DUMMY FREE-BOUND (PARTITION FUNCTION DATA)				
0	3	1	5.020000E-02	1.000000E-04
4.	0.000000E+00			
10.	3.858401E+04			
6.	5.822450E+04			
1.	1.000000E+00	1.000000E+00	0.000000E+00	
1.000	1.000	0.000		
OXYGEN ION LINE RADIATION				
0	50	1	4.075310E+05	1.600000E+01
5.181300E-02	4.046700E+04	4.500000E-02	6	6
5.155500E-02	4.046700E+04	9.700000E-01	6	10
5.393700E-02	0.000000E+00	1.100000E-01	4	12
5.550800E-02	2.681700E+04	6.700000E-02	10	10
6.005850E-02	4.046700E+04	3.900000E-02	6	10
6.441480E-02	4.046700E+04	1.500000E-01	6	2
6.732200E-02	4.046700E+04	6.300000E-02	6	6
7.185400E-02	2.681700E+04	2.500000E-01	10	10
7.966610E-02	4.046700E+04	7.000000E-02	6	10
8.338000E-02	0.000000E+00	4.300000E-01	4	12
2.738000E-01	2.039420E+05	1.200000E-01	2	6
3.133900E-01	2.068950E+05	1.350000E-01	20	12
3.272400E-01	2.287370E+05	1.370000E-01	14	10
3.292400E-01	2.084310E+05	1.380000E-01	12	12
3.385900E-01	2.039420E+05	9.600000E-01	2	6
3.408400E-01	2.299560E+05	1.400000E-01	10	10
3.469100E-01	2.116360E+05	1.350000E-01	10	6
3.733900E-01	2.325130E+05	1.450000E-01	6	10
3.735900E-01	1.854020E+05	1.230000E-01	12	4
3.753700E-01	2.121620E+05	1.680000E-01	4	12
3.809300E-01	2.142100E+05	1.420000E-01	6	6
3.867200E-01	2.068950E+05	1.300000E-01	20	20
3.914400E-01	2.069720E+05	1.930000E-01	10	6
3.966900E-01	1.890080E+05	3.430000E-01	6	6
4.074800E-01	2.068950E+05	6.900000E-01	20	28
4.093700E-01	2.314290E+05	8.400000E-01	28	36

APPENDIX B - Continued

4.111400E-01	2.084310E+05	6.300000E-01	12	20
4.151700E-01	2.084310E+05	2.610000E-01	12	12
4.187900E-01	2.287370E+05	8.500000E-01	14	18
4.272300E-01	2.268510E+05	8.900000E-01	2	6
4.278000E-01	2.327460E+05	8.100000E-01	20	28
4.293800E-01	2.325110E+05	9.100000E-01	12	20
4.314300E-01	1.854020E+05	2.970000E-01	12	12
4.314700E-01	2.328890E+05	8.400000E-01	14	18
4.325700E-01	2.325110E+05	1.700000E-01	6	2
4.349700E-01	2.069720E+05	2.960000E-01	10	10
4.385300E-01	2.116360E+05	1.240000E-01	10	10
4.418100E-01	1.890080E+05	5.500000E-01	6	10
4.446100E-01	2.287370E+05	1.760000E-01	14	14
4.467200E-01	2.453960E+05	8.300000E-01	6	18
4.593200E-01	2.069720E+05	4.900000E-01	10	14
4.651500E-01	1.854020E+05	5.500000E-01	12	20
4.698000E-01	2.325110E+05	3.470000E-01	6	6
4.700800E-01	2.299550E+05	4.100000E-01	10	14
4.703900E-01	2.116360E+05	6.400000E-01	10	14
4.868100E-01	2.325110E+05	2.590000E-01	6	10
4.913000E-01	2.121620E+05	7.300000E-01	4	12
4.943200E-01	2.142100E+05	6.500000E-01	6	10
5.191100E-01	2.142100E+05	2.130000E-01	6	6
6.897500E-01	2.314290E+05	1.700000E-01	28	20

02 1 2 3.536000E+13
0 5 1

3. 0.000000E+00
2. 1.139247E+04
1. 1.898513E+04
3. 5.193451E+04
3. 7.165469E+04

2.273805E+03	1.737049E+01	2.079999E+00	2.271847E-02
2.171132E+03	1.726546E+01	2.052288E+00	2.460328E-02
2.061334E+03	2.007110E+01	2.014894E+00	2.614279E-02
1.178368E+03	3.237274E+01	1.510728E+00	0.000000E+00
1.007670E+03	1.151319E+01	1.178368E+00	1.582667E-02

02 SCHUMANN-RUNGE BAND SYSTEM
14 14 5 1 1 4.000000E-02

7.165469E+04	1.007670E+03	1.151319E+01	-5.399774E-01	1.178368E+00		
0.000000E+00	2.273805E+03	1.737049E+01	7.855786E-02	2.079999E+00		
1418-08	1338-07	6657-07	2325-06	6399-06	1477-05	2972-05
5352-05	8786-05	1333-04	1888-04	2516-04	3172-04	3799-04
4680-07	4065-06	1868-05	6046-05	1546-04	3328-04	6264-04
1059-03	1637-03	2347-03	3152-03	3999-03	4817-03	5533-03
7335-06	5809-05	2442-04	7247-04	1705-03	3387-03	5903-03
9269-03	1336-02	1792-02	2261-02	2703-02	3082-02	3365-02
7269-05	5189-04	1971-03	5299-03	1133-02	2049-02	3262-02
4692-02	6214-02	7686-02	8973-02	9968-02	1060-01	1085-01
5117-04	3247-03	1098-02	2632-02	5025-02	8131-02	1160-01
1497-01	1783-01	1988-01	2097-01	2111-01	2043-01	1909-01
2725-03	1511-02	4464-02	9348-02	1557-01	2195-01	2724-01
3054-01	3152-01	3037-01	2762-01	2391-01	1984-01	1587-01
1142-02	5416-02	1364-01	2423-01	3402-01	4010-01	4115-01
3762-01	3108-01	2338-01	1605-01	1000-01	5574-02	2688-02
3865-02	1527-01	3170-01	4576-01	5118-01	4669-01	3551-01
2245-01	1134-01	4049-02	6138-03	6403-04	1146-02	2790-02
1077-01	3419-01	5571-01	6090-01	4862-01	2844-01	1098-01

APPENDIX B -- Concluded

1650-02	2457-03	3576-02	8194-02	1182-01	1356-01	1351-01
2507-01	6087-01	7208-01	5200-01	2204-01	3195-02	7186-03
8008-02	1631-01	2053-01	1990-01	1609-01	1120-01	6783-02
4921-01	8522-01	6377-01	2094-01	4144-03	6729-02	2086-01
2744-01	2383-01	1505-01	6688-02	1620-02	1202-04	6704-03
8217-01	9095-01	3108-01	1193-03	1397-01	3223-01	3134-01
1743-01	4693-02	2771-04	2165-02	6786-02	1049-01	1195-01
1174-00	6854-01	2393-02	1685-01	4101-01	3129-01	9194-02
1109-04	5175-02	1389-01	1812-01	1656-01	1179-01	6697-02
1442-00	2905-01	9461-02	4830-01	3394-01	4514-02	2764-02
1697-01	2421-01	1930-01	9601-02	2400-02	1062-04	1101-02
1.700000E-01	3.800000E-01					
OXYGEN MOLECULE FREE-FREE CONTINUUM						
0	51	5.010000E-02	5.000000E-02	2.540000E-02		

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TABLE I.- PARAMETERS FOR CALCULATION OF NEUTRAL BREMSSTRAHLUNG

[Z_N^2 obtained from eq. (12) for species H_2 , CO, C_2 , NO, and CN, using polarizability tables in ref. 37, p. 950. All other values of Z_N^2 obtained from eq. (10) and calculations of refs. 12 and 13]

Species	Z_N^2 used in program
C	0.02473
O	.01269
H	.07315
H _e	.02256
H ₂	.0107
CO	.0167
O ₂	.0174
C ₂	.01535
N	.018
NO	.020
N ₂	.0361
CN	.0167

TABLE II.- NEUTRAL BREMSSTRAHLUNG CROSS SECTIONS (CARBON ATOM)

[Values in parentheses are taken from ref. 12. Values not in parentheses are computed from eqs. (8) and (10) for $Z_N^2 = 0.02473$]

$\lambda, \mu\text{m}$	$\sigma_{FF} \times 10^{40}, \text{cm}^5$			
	T = 2000 K	T = 5000 K	T = 10 000 K	T = 15 000 K
0.5	5.97 (2.48)	4.16 (4.45)	5.52 (7.10)	8.91 (9.67)
1	8.71 (5.29)	11.04 (12.3)	26.61 (26.1)	47.14 (42.4)
2	18.54 (16.8)	53.23 (51.9)	139.0 (139)	232.7 (254)
5	133.1 (129)	463.6 (539)	1064 (1720)	1673 (3380)

TABLE III.- PHOTOIONIZATION CROSS SECTIONS

[The power-of-ten multiplier appears as a signed integer at the right of each entry
(for example, 7.014 - 18 = 7.014×10^{-18})]

(a) Carbon

$\lambda, \mu\text{m}$	$\sigma_{\text{FB}}, \text{cm}^2$		
	T = 5000 K	T = 8000 K	T = 12 000 K
0.0567	7.014-18	6.932-18	6.875-18
.0700	9.364-18	9.208-18	9.117-18
.0833	1.139-17	1.117-17	1.105-17
.0967	1.281-17	1.256-17	1.243-17
.1100	1.333-17	1.311-17	1.299-17
.1101	3.367-19	1.355-18	1.682-18
.1132	3.408-19	1.372-18	1.702-18
.1162	3.442-19	1.386-18	1.720-18
.1193	3.471-19	1.397-18	1.734-18
.1223	3.493-19	1.406-18	1.746-18
.1239	3.501-19	1.410-18	1.750-18
.1240	2.580-21	5.239-20	8.463-20
.1285	2.609-21	5.297-20	8.558-20
.1330	2.628-21	5.336-20	8.622-20
.1376	2.638-21	5.356-20	8.655-20
.1421	2.638-21	5.357-20	8.657-20
.1444	2.634-21	5.349-20	8.645-20
.1445	9.312-29	1.402-23	1.024-22
.3324	1.135-27	1.709-22	1.249-21
.5204	4.354-27	6.555-22	4.790-21
.7084	1.098-26	1.653-21	1.208-20
.8963	2.225-26	3.349-21	2.448-20
.9903	3.001-26	4.517-21	3.301-20
.9904	9.705-27	2.476-21	1.941-20
1.1616	1.566-26	3.995-21	3.130-20
1.3327	2.365-26	6.033-21	4.728-20
1.5039	3.398-26	8.669-21	6.793-20
1.6750	4.695-26	1.198-20	9.387-20
1.7606	5.452-26	1.391-20	1.090-19

TABLE III.- PHOTOIONIZATION CROSS SECTIONS - Continued

(b) Nitrogen

$\lambda, \mu\text{m}$	$\sigma_{\text{FB}}, \text{cm}^2$		
	T = 5000 K	T = 8000 K	T = 12 000 K
0.0838	1.253-17	1.246-17	1.241-17
.0844	1.246-17	1.240-17	1.236-17
.0850	1.238-17	1.234-17	1.231-17
.0852	1.235-17	1.231-17	1.228-17
.0853	1.247-19	1.853-18	2.755-18
.0860	1.246-19	1.853-18	2.754-18
.0866	1.245-19	1.852-18	2.753-18
.0873	1.244-19	1.850-18	2.751-18
.0879	1.242-19	1.848-18	2.748-18
.0883	1.241-19	1.846-18	2.746-18
.0884	6.208-20	1.004-18	1.529-18
.0902	6.241-20	1.009-18	1.538-18
.0920	6.267-20	1.014-18	1.545-18
.0937	6.285-20	1.017-18	1.550-18
.0955	6.296-20	1.019-18	1.553-18
.0964	6.298-20	1.020-18	1.554-18
.0965	6.129-20	9.278-19	1.387-18
.0977	6.130-20	9.282-19	1.388-18
.0989	6.127-20	9.282-19	1.388-18
.1002	6.120-20	9.276-19	1.387-18
.1014	6.111-20	9.265-19	1.386-18
.1020	6.105-20	9.257-19	1.385-18
.1021	2.349-21	1.274-19	2.318-19
.1045	2.357-21	1.278-19	2.325-19
.1069	2.360-21	1.280-19	2.328-19
.1094	2.359-21	1.280-19	2.327-19
.1118	2.354-21	1.277-19	2.322-19
.1130	2.349-21	1.274-19	2.317-19
.1131	1.750-31	7.233-25	8.885-24
.2586	2.091-30	8.639-24	1.061-22
.4041	7.976-30	3.296-23	4.049-22
.5496	2.006-29	8.291-23	1.018-21
.6951	4.058-29	1.677-22	2.060-21

TABLE III.- PHOTOIONIZATION CROSS SECTIONS – Concluded

(c) Oxygen

$\lambda, \mu\text{m}$	$\sigma_{\text{FB}}, \text{cm}^2$		
	T = 5000 K	T = 8000 K	T = 12 000 K
0.0710	8.391-18	8.494-18	8.544-18
.0725	8.338-18	8.436-18	8.484-18
.0732	8.306-18	8.402-18	8.449-18
.0733	3.689-18	4.012-18	4.169-18
.0736	3.693-18	4.015-18	4.171-18
.0738	3.698-18	4.018-18	4.174-18
.0740	3.703-18	4.021-18	4.176-18
.0743	3.707-18	4.023-18	4.178-18
.0744	3.709-18	4.025-18	4.178-18
.0745	3.694-18	3.866-18	3.951-18
.0763	3.728-18	3.887-18	3.966-18
.0782	3.761-18	3.904-18	3.976-18
.0800	3.791-18	3.918-18	3.982-18
.0819	3.819-18	3.929-18	3.984-18
.0828	3.832-18	3.932-18	3.983-18
.0829	3.800-18	3.620-18	3.538-18
.0835	3.810-18	3.629-18	3.547-18
.0842	3.819-18	3.639-18	3.556-18
.0848	3.829-18	3.647-18	3.564-18
.0855	3.838-18	3.656-18	3.573-18
.0858	3.843-18	3.660-18	3.577-18
.0859	3.844-18	3.654-18	3.562-18
.0871	3.859-18	3.669-18	3.576-18
.0882	3.874-18	3.683-18	3.590-18
.0894	3.888-18	3.696-18	3.603-18
.0905	3.902-18	3.709-18	3.615-18
.0911	3.908-18	3.715-18	3.622-18
.0912	2.507-31	4.451-25	4.978-24
.2530	5.353-30	9.505-24	1.063-22
.4148	2.359-29	4.189-23	4.685-22
.5767	6.337-29	1.125-22	1.258-21
.7385	1.331-28	2.363-22	2.643-21

TABLE IV.- MOLECULAR BAND SYSTEMS USED IN PROGRAM SPRAD

Species	Band	λ_{00} , μm	f_{el}	Ref. no.	Franck-Condon factor (Ref. no.)
H ₂	Lyman	0.1103	0.2	1	38
	Werner	.1006	.4	1	39
O ₂	Schumann-Runge	.2026	.04	26	28
N ₂ ⁺	Meinel	1.1091	.012	28	28
	First negative	.3914	.035	28	28
N ₂	First positive	1.0510	.003	28	28
	Second positive	.3371	.06	28	28
	Birge-Hopfield No. 2	.0964	.43	28	28
NO	Gamma	.2263	.025	28	28
	Beta	.2199	.01	28	28
CO	Angstrom	.4511	.003	40	26
	Hopfield-Birge (B-X)	.1150	.012	41	26
	Fourth positive	.1544	.15	42	41
C ₂	Fox-Herzberg	.2512	.818	43	26
	Swan	.5165	.013	44	26
CO ⁺	First negative	.2190	.017	40	41
	Comet-tail	.4910	.0022	41	41

TABLE V.- THERMODYNAMIC STATE AND RADIATIVE CONTRIBUTORS
IN SHOCKED CO₂

[Shock speed; 10.97 km/sec (36 000 ft/sec);
initial pressure, 0.0133 N/cm² (1 torr);
initial temperature, 300 K;
mixture temperature, 11 168 K;
mixture pressure, 26.64 N/cm² (2.63 atm)]

Species	Concentration	Contributing radiation
e ⁻	1.209E+17	
CO	2.241E+15	(4+), Angstrom (B-A), Hopfield-Birge (B-X), free-free
O ₂	3.536E+13	Schumann-Runge, free-free
C	4.329E+17	Free-free, free-bound, lines
O	1.055E+18	Free-free, free-bound, lines
C ⁺	9.794E+16	Free-free, lines
O ⁺	1.621E+16	Free-free, lines
C ⁺⁺	3.337E+15	Free-free, lines
C ₂	3.873E+13	Swan, Fox-Herzberg (B-X), free-free
CO ⁺	1.192E+14	Comet-tail, (1-), free-free

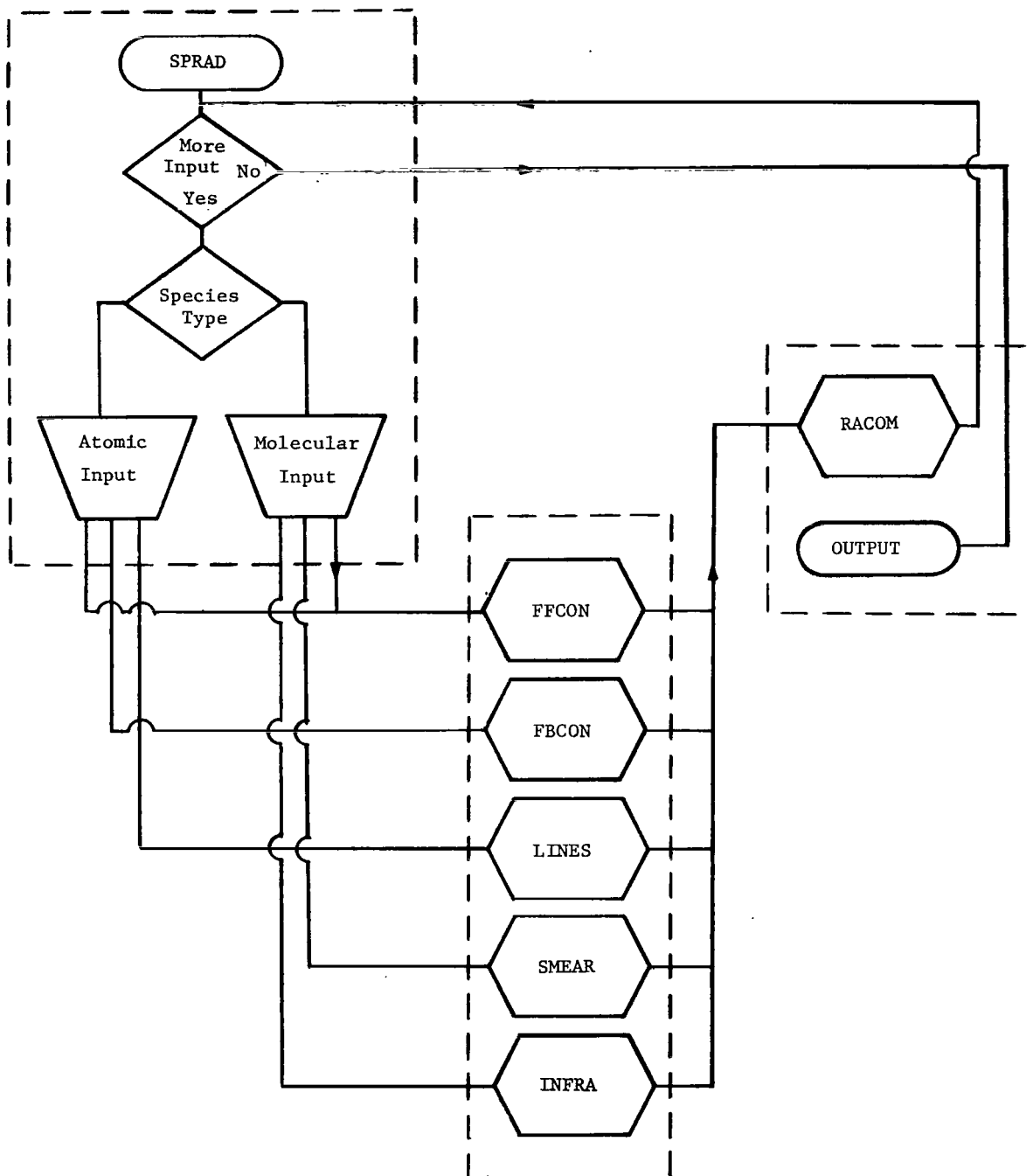
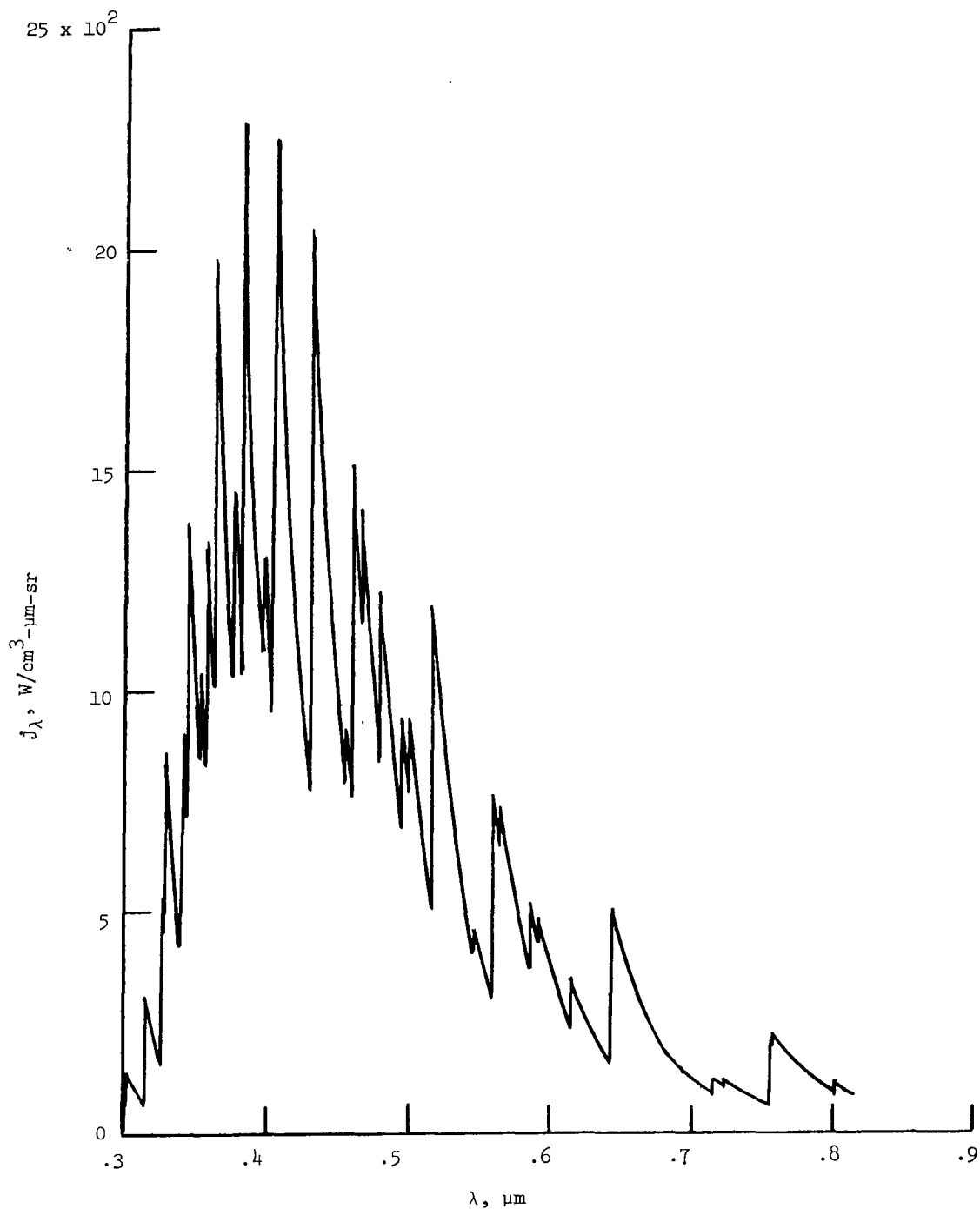
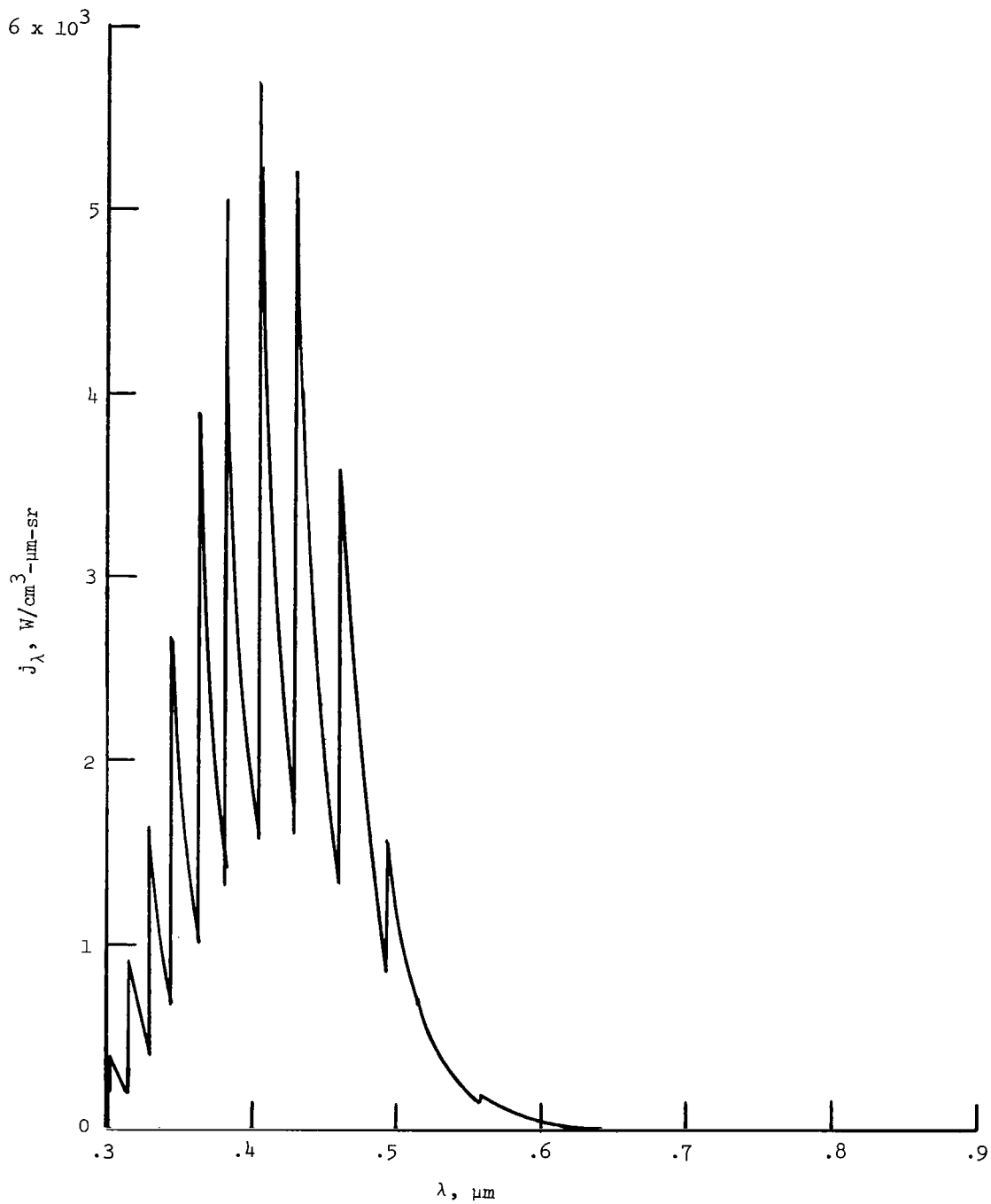


Figure 1.- Brief flow chart of spectral properties program SPRAD.



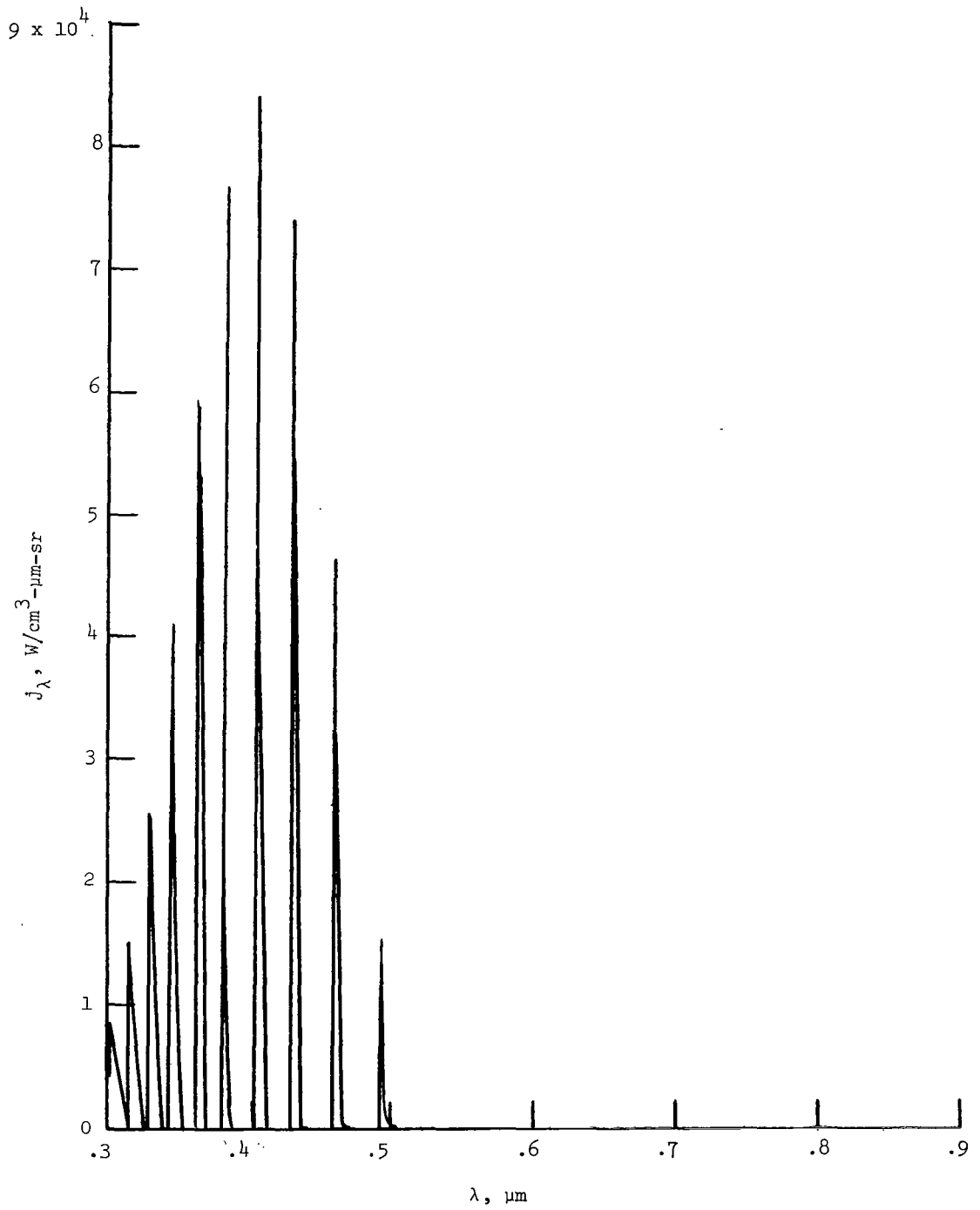
(a) $T_e = T_v = T_r = 8000 \text{ K.}$

Figure 2.- Radiance of CO⁺ comet tail band system. ($N_{\text{CO}^+} = 10^{18} \text{ cm}^{-3}$.)



(b) $T_e = T_r = 8000 \text{ K}$, $T_v = 800 \text{ K}$.

Figure 2.- Continued.



(c) $T_e = 8000 \text{ K}$, $T_v = T_r = 400 \text{ K}$.

Figure 2.- Concluded.

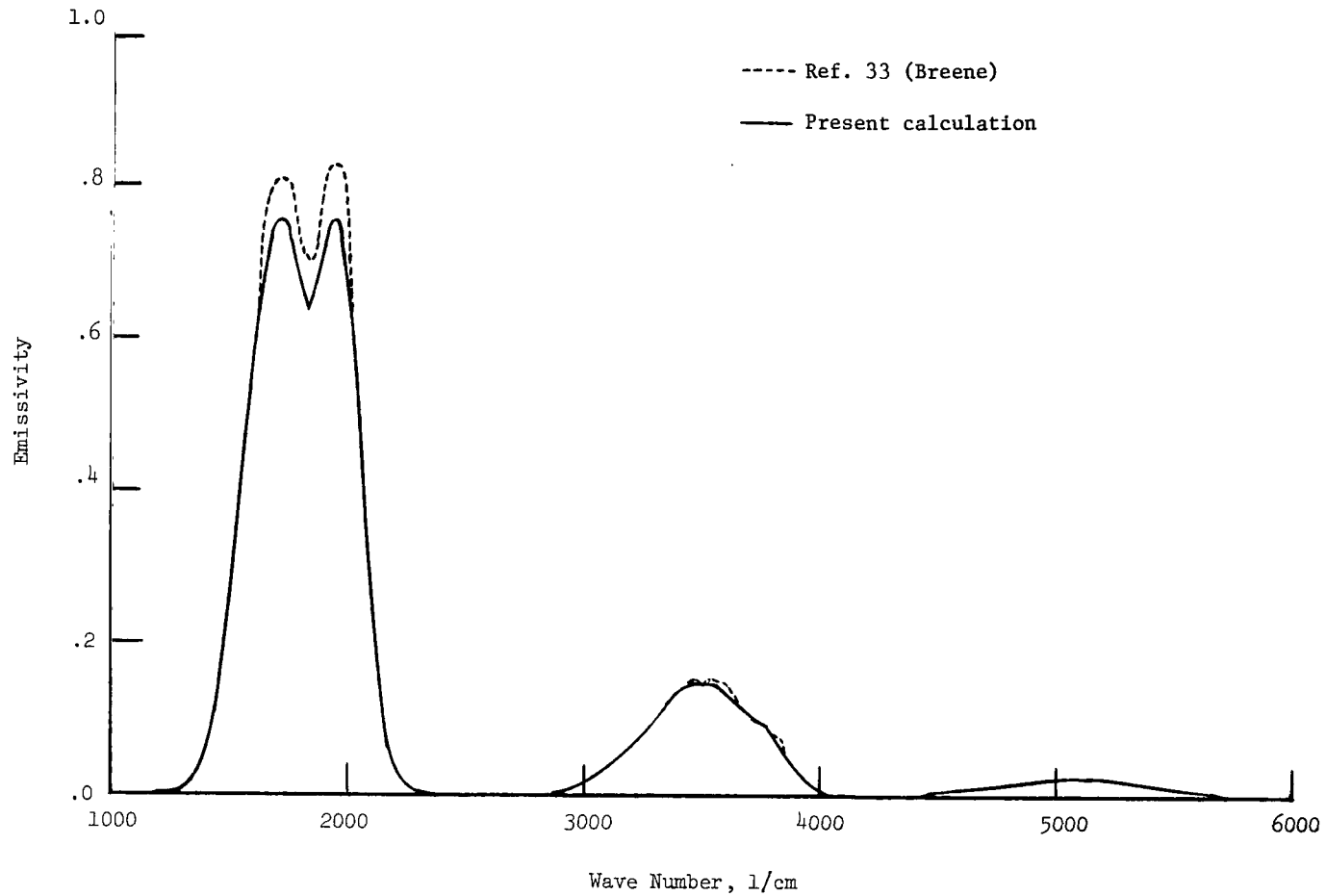
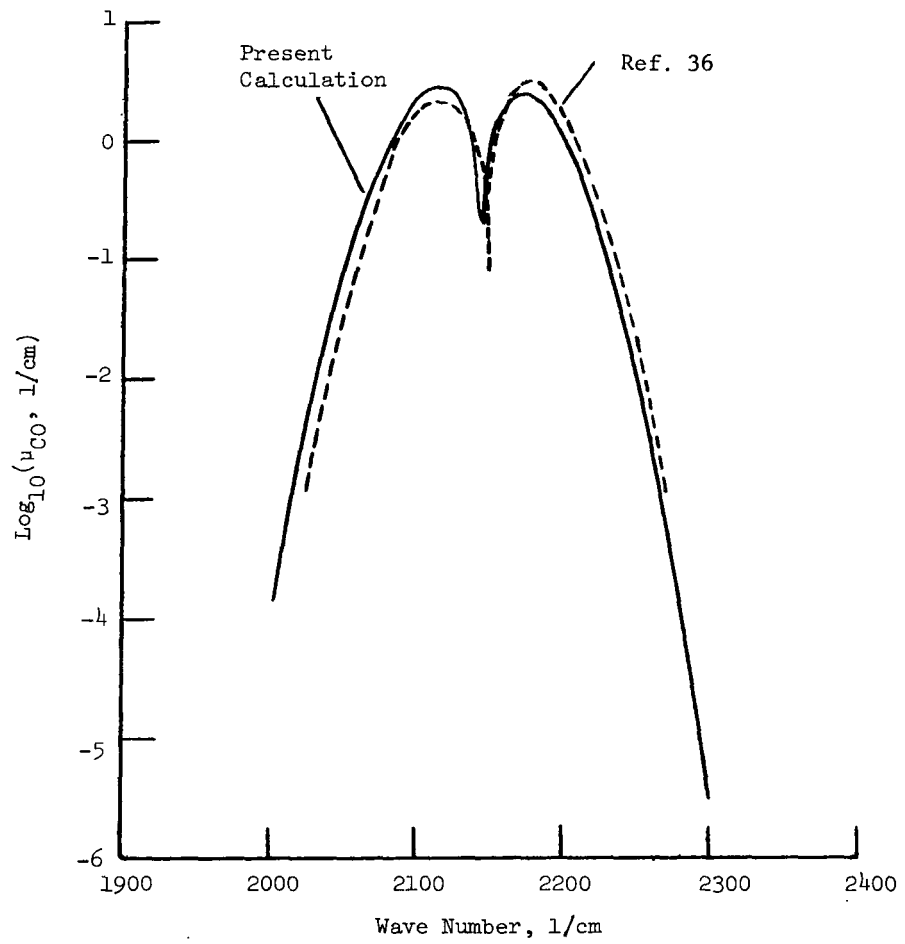
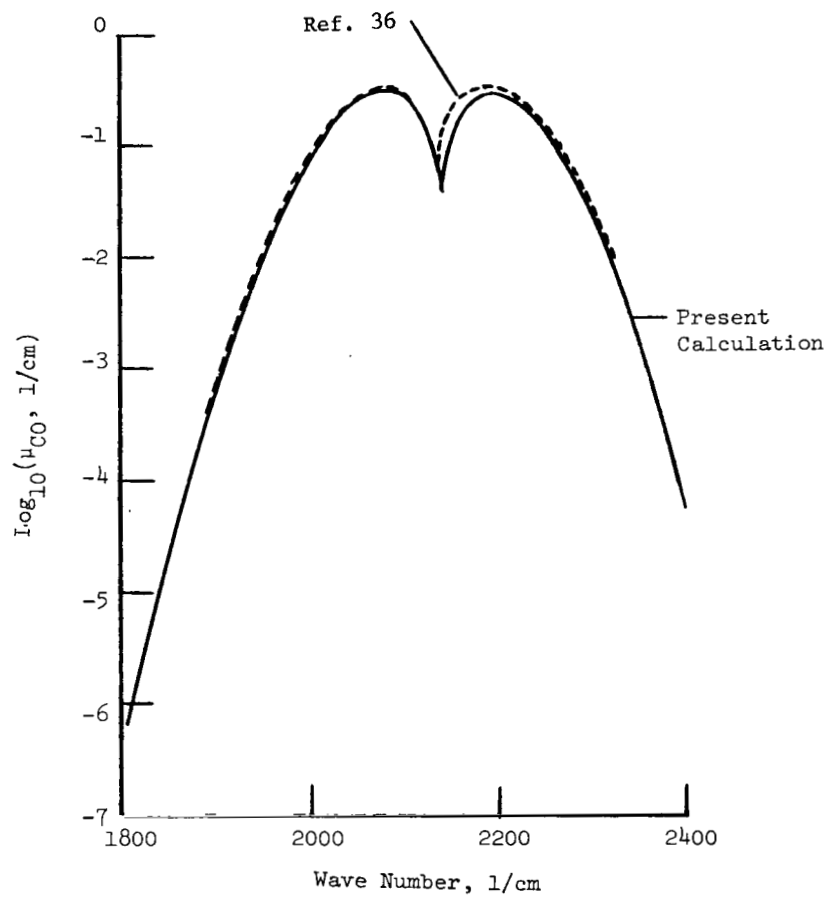


Figure 3.- Emissivity of nitric oxide NO computed from smeared-line model of reference 41.
 ($N_{NO} = 3.215(10)^{19}$, $T = 5000$ K, $L = 5$ cm.)



(a) $N_{\text{CO}} = 2.447(10)^{19}$, $T = 300 \text{ K}$.

Figure 4.- Comparison of infrared absorption-coefficient calculations for CO.



(b) $N_{\text{CO}} = 6.12(10)^{18}$, $T = 1200 \text{ K}$.

Figure 4.- Concluded.

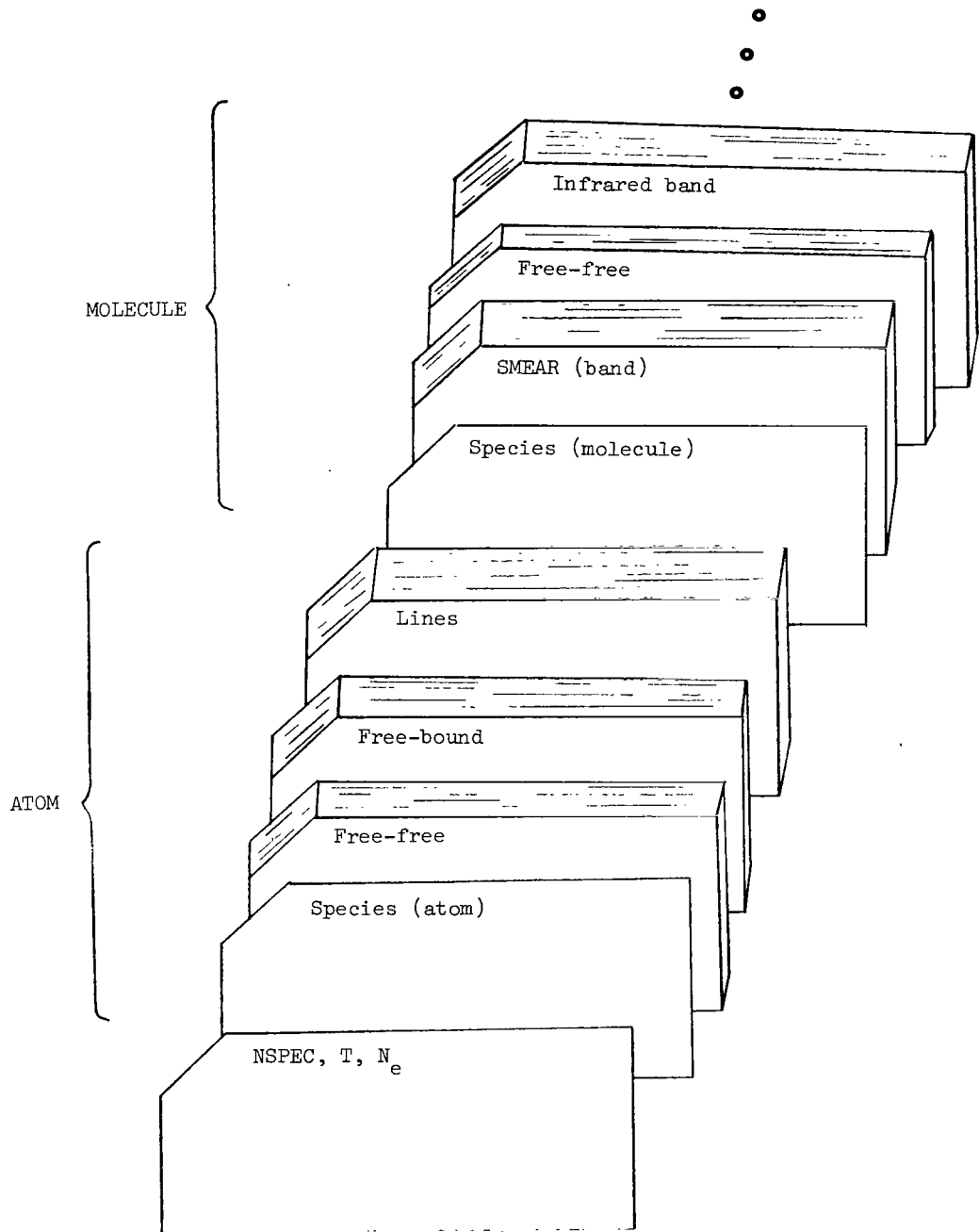


Figure 5.- Sample input deck sequence for radiative properties program SPRAD.

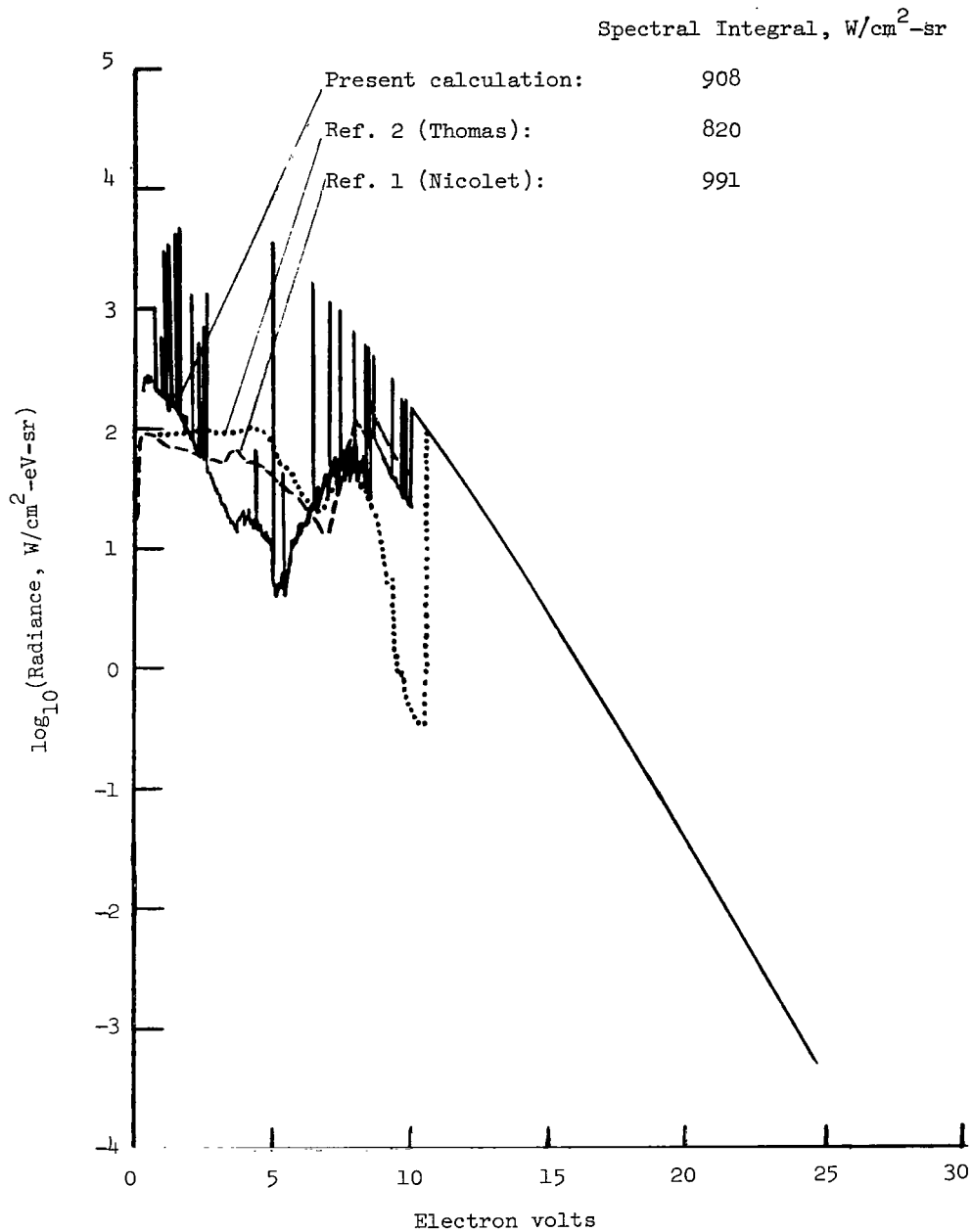
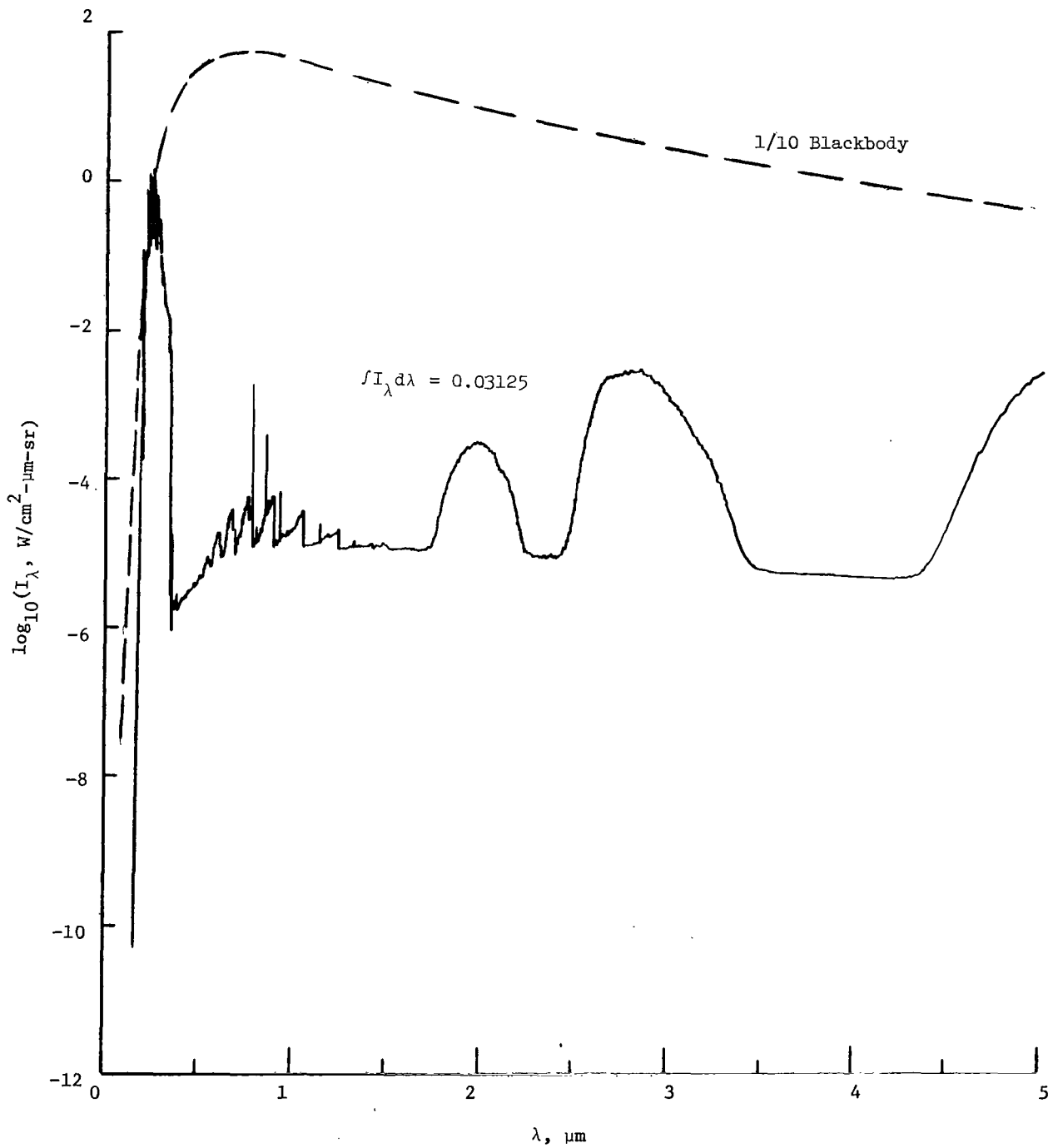
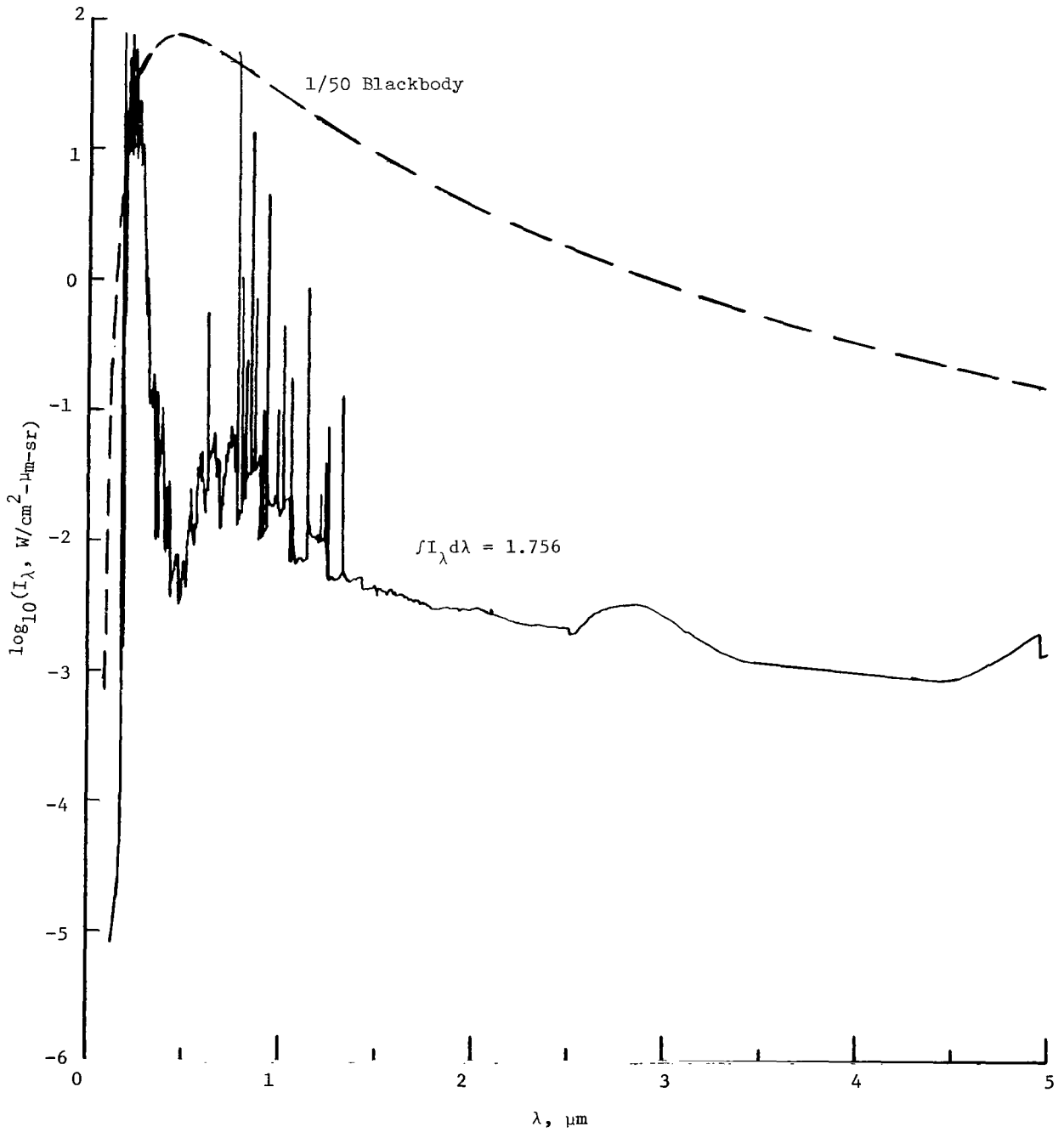


Figure 6.- Computed spectral radiation profiles in heated CO₂ for T = 11 168 K, p = 26.64 N/cm², L = 5 cm. (Atomic line contribution not shown in plot for curves of refs. 1 and 2 but included in values of the integral.)



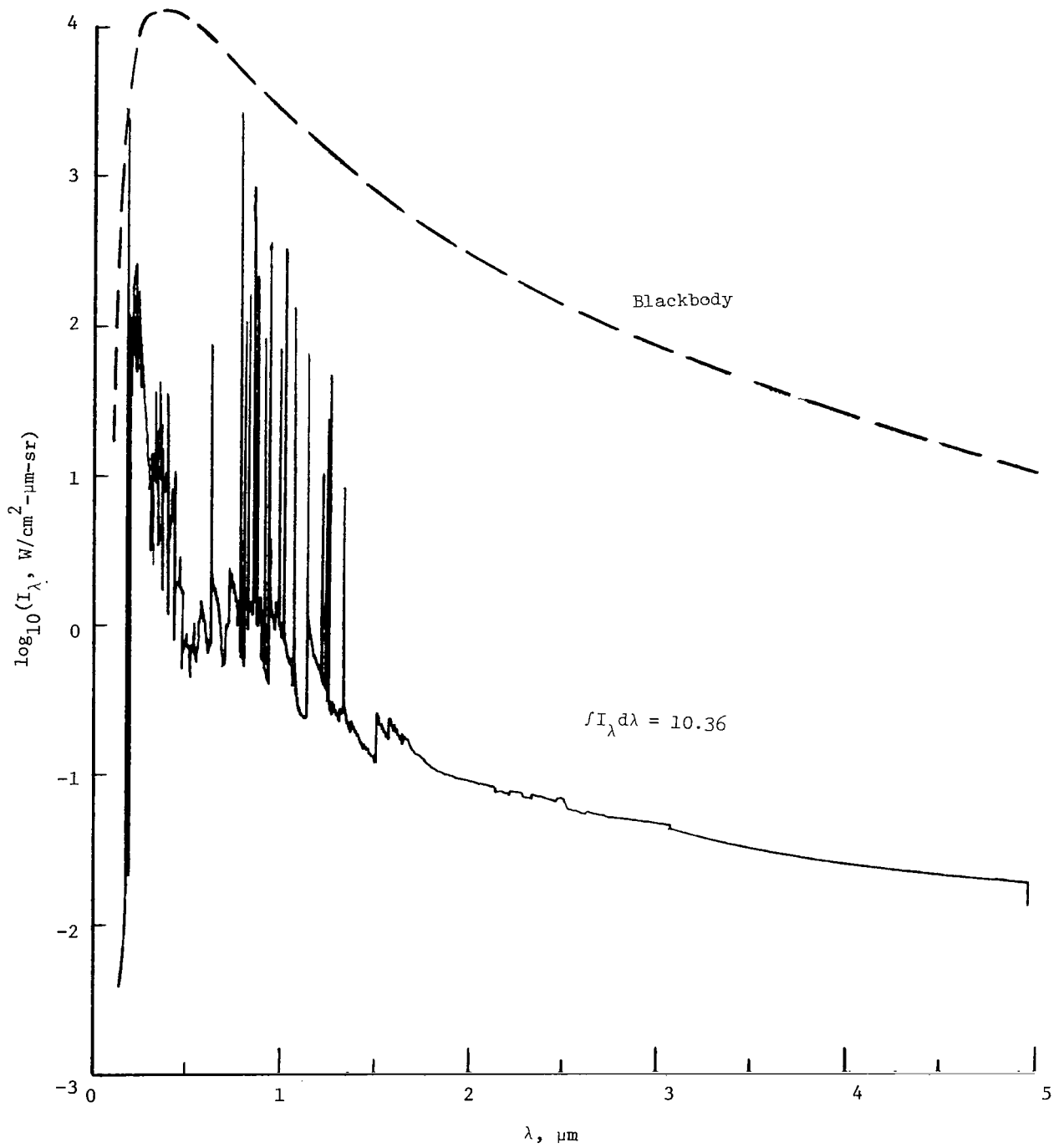
(a) $T = 4000 \text{ K}$, $\rho/\rho_0 = 0.1$, $L = 1 \text{ cm}$.

Figure 7.- Spectral radiance of equilibrium air.



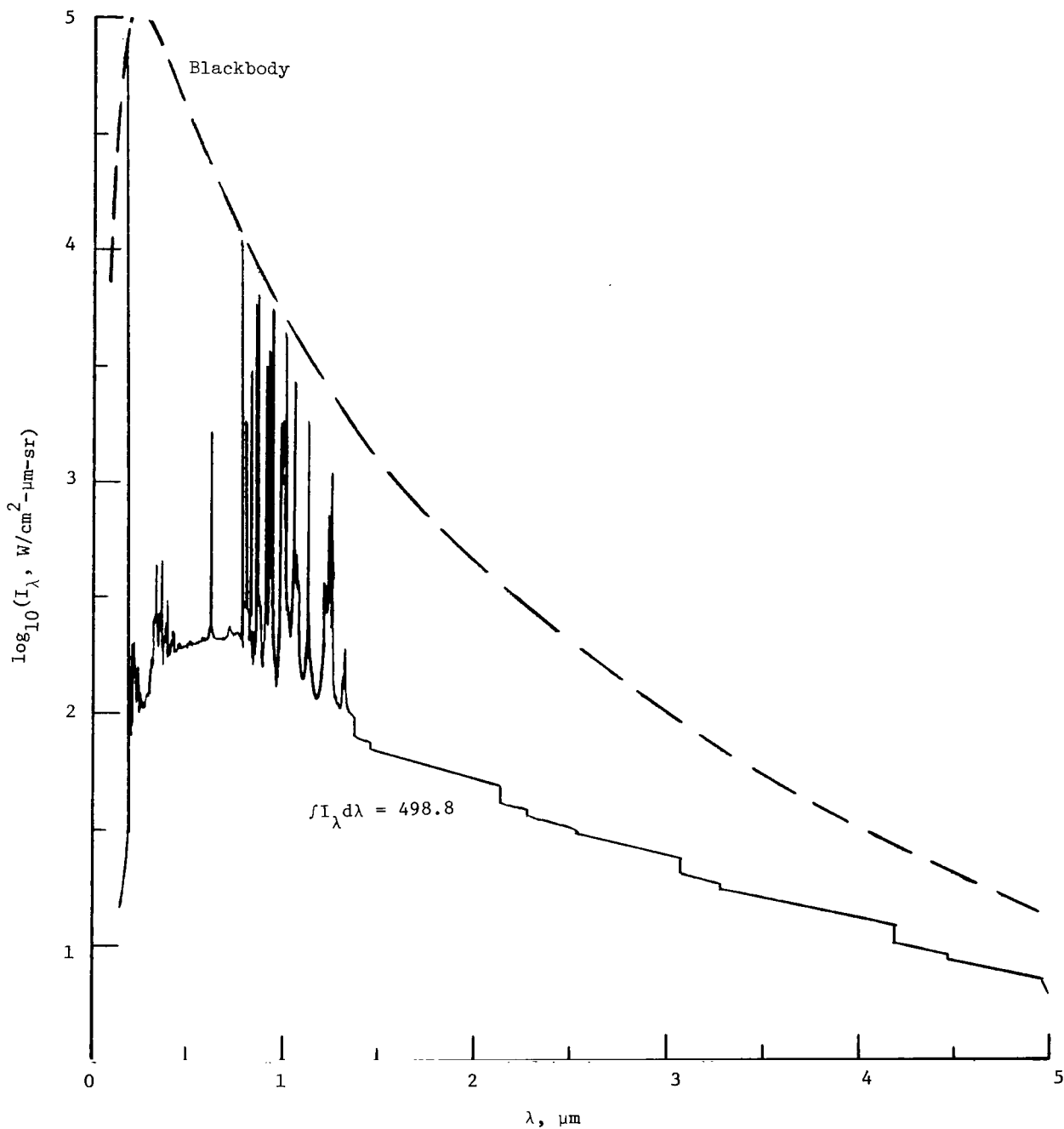
(b) $T = 6000 \text{ K}, \rho/\rho_0 = 0.1, L = 1 \text{ cm}.$

Figure 7.- Continued.



(c) $T = 8000 \text{ K}$, $\rho/\rho_0 = 0.1$, $L = 1 \text{ cm}$.

Figure 7.- Continued.



(d) $T = 12\,000\text{ K}$, $\rho/\rho_0 = 0.1$, $L = 1\text{ cm}$.

Figure 7.- Concluded.

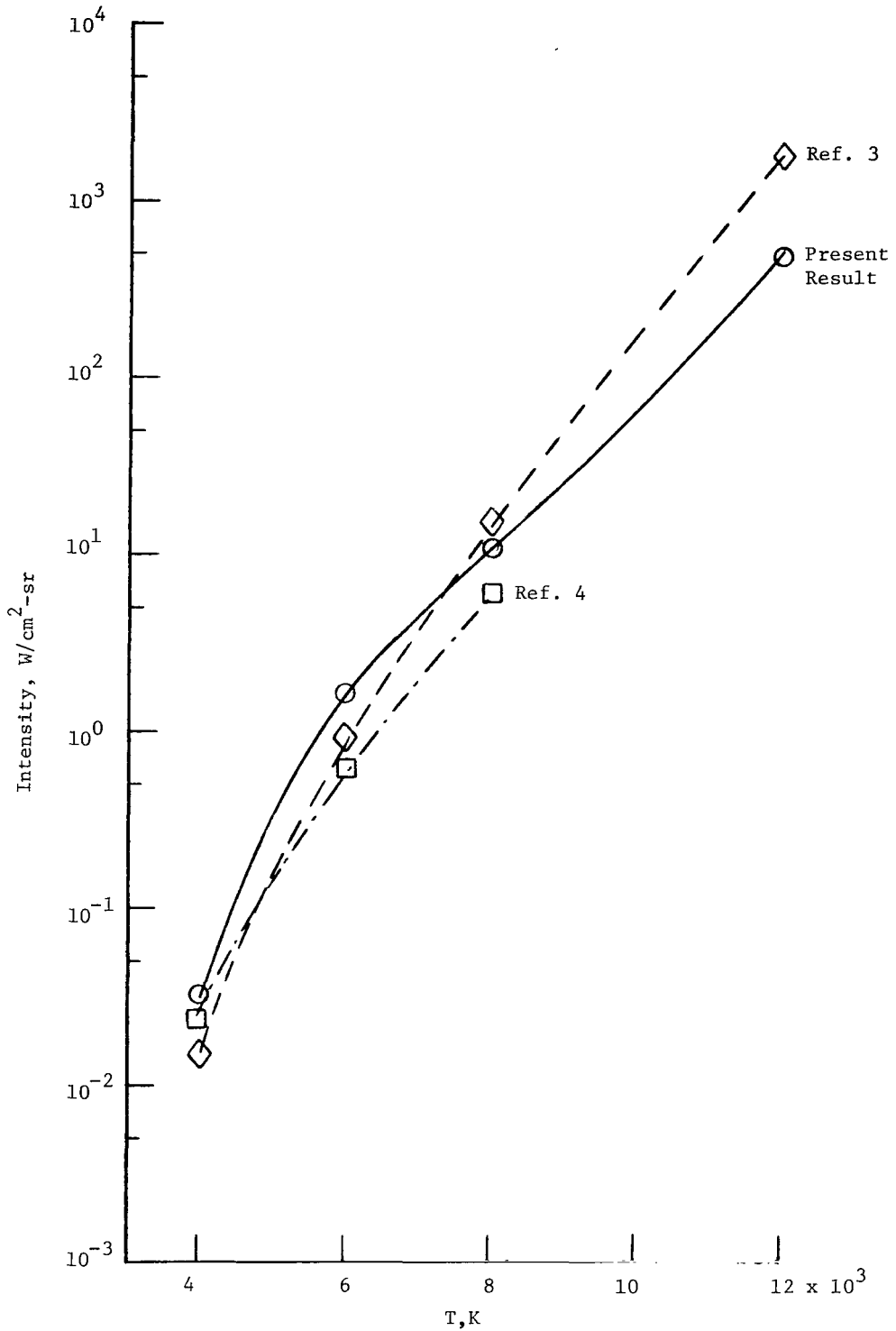


Figure 8.- Comparison of spectrally integrated intensity of equilibrium air.
 ($\rho/\rho_0 = 0.1$, $L = 1$ cm.)



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