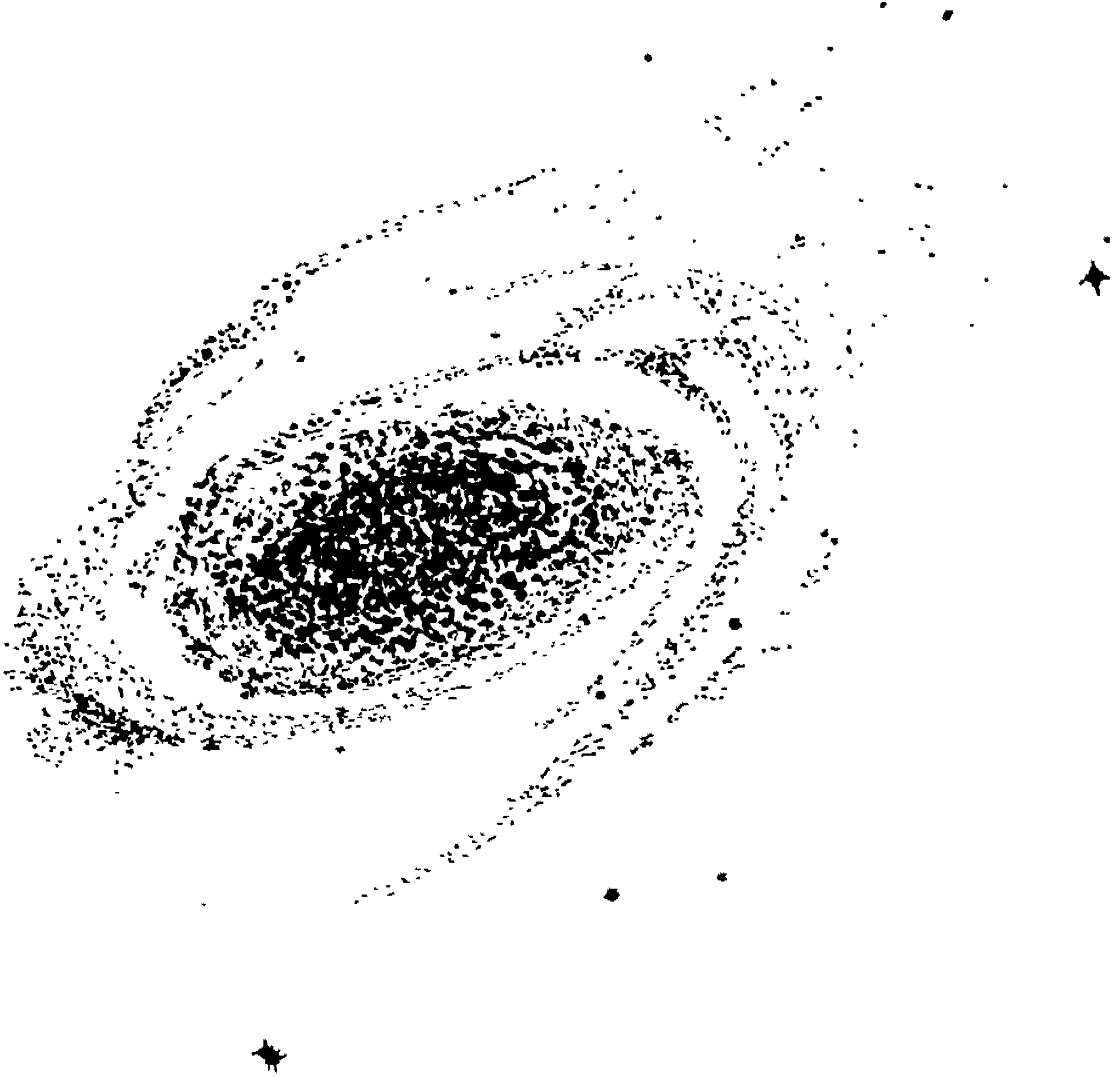
ATLAS:
A COMPUTER PROGRAM FOR CALCULATING MODEL STELLAR ATMOSPHERES

R. L. KURUCZ



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ABSTRACT

The computer program ATLAS calculates model stellar atmospheres in radiative and convective equilibrium for the complete range of stellar temperatures. The approximations used limit the program to plane-parallel, horizontally homogeneous, steady-state, nonmoving atmospheres with energy and abundances constant with depth. The program has been written to allow detailed statistical equilibrium calculations, but only hydrogen continua and H^- are coded at present. Most of the published continuous opacities and hydrogen lines have been included, and provision is made for adding others easily. There is also provision for treating line opacity as line-absorption distribution functions.

In Sections 2 through 7, we discuss all aspects of model atmosphere calculations in considerable detail. These include the radiation field, statistical equilibrium, thermodynamic properties, opacity, convection, and the temperature correction. In Sections 8 and 9, we discuss the computer program itself, by going first through a sample calculation and second through a technical discussion of the program coding and operation.

The program was written in FORTRAN IV and is essentially machine independent. A listing is available on magnetic tape.

RÉSUMÉ

Le programme ATLAS pour ordinateur calcule les modèles des atmosphères stellaires dans un équilibre radiatif et convectif pour toute l'étendue des températures stellaires. Les approximations utilisées limitent le programme à des atmosphères en plans parallèles, homogènes horizontalement, en état stable, immobiles, et ayant une énergie et des abondances constantes avec la profondeur. Le programme a été écrit pour permettre des calculs détaillés de l'équilibre statistique, mais seulement les spectres continus de l'hydrogène et de H^- sont programmés pour l'instant. La plupart des opacités du spectre continu qui ont été publiées et la plupart des raies de l'hydrogène ont été incluses et on peut en ajouter d'autres facilement. On peut aussi traiter l'opacité des raies comme fonctions de distribution des raies d'absorption.

Dans les Sections de 2 à 7 nous discutons de tous les aspects des calculs des modèles d'atmosphères avec beaucoup de détails. Ceux-ci comprennent le champ de radiation, l'équilibre statistique, les propriétés thermodynamiques, l'opacité, les convexions et la correction de températures. Dans les Sections 8 et 9 nous discutons du programme lui-même, en faisant d'abord un calcul simple puis une discussion technique de la séquence d'instructions du programme et de la marche de ce dernier.

Le programme a été écrit en FORTRAN IV et est essentiellement indépendent de l'ordinateur. Un listage sur bande magnétique peut en être obtenu.

КОНСПЕКТ

Программа АТЛАС для электронной счетно-решающей машины вычисляет модельные звездные атмосферы в излучающем и конвективном равновесии для полного диапазона звездных температур. Употребляемые приближения ограничивают программу в рамках плоско-параллельных, горизонтально-однородных, установившегося состояния, недвижущихся атмосфер с энергией и распространенностями постоянными с глубиной. Программа была составлена чтобы позволить подробные вычисления статистического равновесия, но только водородные непрерывные спектры и H^- кодированы в настоящее время. Было включено большинство опубликованных непрерывных непрозрачностей и водородных линий, и предусматрения были сделаны для добавления других. Имеется также предусматрение для рассматривания непрозрачности линий как функций распределения поглощения линий.

В отделах 2 до 7 мы обсуждаем значительно детально все виды вычисления модельной атмосферы. Эти включают поле излучения, статистическое равновесие, термодинамические свойства, непрозрачность, конвекцию и температурную поправку. В отделах 8 и 9 мы обсуждаем саму программу для электронной счетно-решающей машины сперва рассматривая простые вычисления а затем производя техническое обсуждение кодирования и действия программы.

Программа была написана по ФОРТРАН'у IV и является по существу независимой от машины. Имеется список на магнитной ленте.

MAGNETIC TAPE LISTING

The programs listed in this report can be obtained on magnetic tape by sending a tape at least 600 feet long to

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The tape will be written in BCD card images at 800 bpi.

WARNING

There is no way to guarantee that ATLAS5 does not contain errors. In fact, it is almost certain that it does, since the code is so long. There also may be truncation or underflow problems on computers like an IBM 360, even though all those known at present have been allowed for. We also point out that the computation of a model atmosphere should be considered a physical experiment. The program may not be able to calculate a model for conditions that do not occur in real stars or for conditions that violate the initial assumptions on which the program is based.

PREFACE AND ACKNOWLEDGMENTS

The programing described here was started in 1966 as the first step in a project with Dr. Stephen E. Strom for calculating realistic line-blanketed model atmospheres for the whole range of stellar spectral types. Although ATLAS can now calculate models by using distribution functions for the line opacities, I have not yet completed work on the distribution functions themselves. As of now, I have written a program to calculate the distribution functions given a list of lines, but I have atomic data for only about two-thirds of the lines (36, 000) in stars that do not have strong molecular bands. I expect to complete collecting and calculating atomic line data (and molecular data for the sun) in the near future, after which I will publish the line distribution functions for early and middle spectral types in a form that can easily be used in ATLAS.

Almost all the people with whom I have had contact over the last 5 years have contributed to this effort. Dr. Strom, Karen M. Strom, Dr. Owen J. Gingerich, and Dr. David W. Latham taught me programing. I had the benefit of learning about stellar atmospheres through working with programs written by the Stroms. Dr. Wolfgang Kalkofen suggested the use of integration matrices for the radiation field. Thomas Swithenbank took part in the early efforts with partition functions and Saha equations. Conversations and work with Judith G. Cohen are indirectly responsible for the way I have treated molecular equilibrium. Ruth C. Peterson has helped me on several occasions by pointing out errors in my algebra. I. Gene Campbell has often helped me with programing problems. Duane F. Carbon has listened to my ideas and helped me with a number of problems, especially those concerning molecules. Dr. Theodore Simon has worked with the program and suggested many improvements. Over the years, Dr. Deane Peterson has been most helpful. He has worked with the program and made several improvements himself; many of the details of the program have arisen from long arguments (and discussions) with him. Drs. Eric Peytremann, Eugene H. Avrett, and Peterson have kindly read the manuscript and suggested improvements.

ATLAS:
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Robert L. Kurucz

1. INTRODUCTION

The calculation of a model atmosphere is a straightforward process once several assumptions and approximations have been made to simplify the problem physically and computationally. We simplify the problem as follows:

A. The atmosphere is in a steady state.

B. The flux of energy is constant with depth in the atmosphere since the energy source for the star lies far below the atmosphere and since no energy comes into the atmosphere from above. The flux is usually specified by an effective temperature such that flux = $\sigma T_{\mathrm{eff}}^4$, σ = 5.6697E-5.

C. The atmosphere is homogeneous except in the normal direction. We ignore granules, spicules, cells, spots, magnetic fields, etc.

D. The atmosphere is thin relative to the radius of the star, so we can consider plane layers instead of concentric shells.

E. There is no relative motion of the layers in the normal direction and no net acceleration of the atmosphere, so the pressure balances the gravitational attraction,

$$\rho \frac{d^2r}{dt^2} = -\rho g + \frac{dP}{dr} = 0 \quad . \tag{1.1}$$

Here ρ is the density and g is the gravitational acceleration, which is approximately constant because the atmosphere is thin,

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This work was supported in part by the Smithsonian Research Foundation.

$$g = \frac{GM_*}{R_*^2} \quad ,$$

with M_* and R_* the mass and radius of the star.

F. The atomic abundances are specified and constant throughout the atmosphere.

Given these assumptions, we go through an iteration process to find the parameters that describe the model atmosphere. We guess the temperature at a set of depth points in the atmosphere and calculate the pressure, number densities, and opacity at each point. From these quantities we determine the radiation field and convective flux at each point. The total flux does not, in general, equal the prescribed constant flux, so we change the temperature at each point according to a "temperature correction" scheme. We repeat the whole process with successive temperature distributions until the total flux is constant to within a small error.

Since the number densities and pressure also depend on the radiation field, we must carry several quantities from iteration to iteration. However, the radiation field often has only a negligible effect on these quantities, in which case only the temperature need be carried from iteration to iteration.

We describe this iteration process in considerable detail as follows: Section 2 is concerned with the radiative energy-transport equations and the computation techniques required to find the radiation field, given the atomic number densities. In Section 3 we consider the effects of the radiation field on the number densities and the means for carrying this information from iteration to iteration. We discuss the computation of the various thermodynamic properties of the gas in Section 4. Section 5 contains expressions for each of the opacity sources included in ATLAS. We consider convective energy transport and the temperature correction scheme in Sections 6 and 7, respectively. In Section 8 we describe the calculation of a model atmosphere by examining sample input and output; programing details of ATLAS, including the listing, are given. In the last section, we describe and list various utility programs.

2. RADIATIVE ENERGY TRANSPORT

2.1 The Transfer Equation

Our approach will be to follow a beam of photons of frequency ν as it passes through the atmosphere. The number density of photons per unit solid angle and frequency $N_\nu(\omega)$ will change with time owing to the presence of absorbing, emitting, and scattering atoms. (By "atom" we actually mean any atomic system, such as an atom, molecule, electron, negative ion, or ion plus electron.) In the absorption process an atom subtracts a photon of energy $h\nu$ from the beam or adds one to the beam in proportion to the number of photons in the beam. The "adding" process, when considered separately, is called negative absorption or stimulated emission. In the emitting process an atom adds a photon of energy $h\nu$ to the beam independent of the number of photons in the beam. In the scattering process an atom takes a photon from the beam and immediately gives up another, generally of slightly different energy and in a different direction.

If we consider all such atomic processes occurring at frequency ν and let ℓ and u denote lower and upper energy levels of any transition, we can add the absorption, emission, and scattering rates to obtain a differential equation of the form

$$\begin{aligned}\frac{dN_\nu(\omega)}{dt} = {} & -N_\nu(\omega)\,\Sigma\,[\text{absorption coefficient } (\ell \rightarrow u)]\;\; n(\ell) \\ & + N_\nu(\omega)\,\Sigma\,[\text{absorption coefficient } (u \rightarrow \ell)]\;\; n(u) \\ & - N_\nu(\omega)\,\Sigma\,[\text{scattering coefficient } (\ell \rightarrow u)]\;\; n(\ell) \\ & + \Sigma\,[\text{emission coefficient } (u \rightarrow \ell)]\;\; n(u) \\ & + \Sigma\,[\text{scattering emission coefficient } (u \rightarrow \ell)]\;\; n(u) \quad . \qquad (2.1)\end{aligned}$$

While $n(\ell)$ and $n(u)$ are number densities of atoms in the lower and upper levels, we note that if a level is not bound, $n(u)$ or $n(\ell)$ refers to the number density in an energy interval dE corresponding to the frequency interval $h\,d\nu$.

Since we are actually concerned with the structure of the atmosphere instead of with photon beams, we convert from coordinates moving with the photons to coordinates fixed in the atmosphere,

$$\frac{d}{dt} = \vec{v} \cdot \vec{\nabla} + \frac{\partial}{\partial t} \quad , \tag{2.2}$$

which reduces to

$$\frac{d}{dt} = c \frac{d}{dz} \quad , \tag{2.3}$$

because the atmosphere is time independent (Section 1). Also, the number density $N_\nu(\omega)$ corresponds to the intensity (energy area^{-1} sec^{-1} ster^{-1} Hz^{-1})

$$I_\nu(\omega) = c\, h\nu\, N_\nu(\omega) \quad , \tag{2.4}$$

where the photon-velocity factor c converts number density to number flux and the factor $h\nu$ converts to energy intensity. Substituting equations (2.3) and (2.4) into (2.1), we obtain

$$\begin{aligned} \frac{dI_\nu}{dz} = &- I_\nu \frac{\Sigma[\text{absorption coefficient } (\ell \rightarrow u)]}{c}\, n(\ell) \\ &+ I_\nu \frac{\Sigma[\text{absorption coefficient } (u \rightarrow \ell)]}{c}\, n(u) \\ &- I_\nu \frac{\Sigma[\text{scattering coefficient } (\ell \rightarrow u)]}{c}\, n(\ell) \\ &+ \Sigma[\text{emission coefficient } (u \rightarrow \ell)]\, n(u) \\ &+ \Sigma[\text{scattering emission coefficient } (u \rightarrow \ell)]\, n(u) \quad . \end{aligned} \tag{2.5}$$

In model stellar atmospheres it is customary (for simplicity) to assume that the scattering emission is isotropic – i.e., that photons are scattered with equal probability in all directions. Consequently in this approximation,

$$\int \Sigma[\text{scattering emission coefficient } (u \rightarrow \ell)]\ n(u)\ d\omega$$
$$= 4\pi\ \Sigma[\text{scattering emission coefficient } (u \rightarrow \ell)]\ n(u) \quad . \tag{2.6}$$

Furthermore, we assume that the scattering rates are slowly varying functions of frequency, as is the case for electron scattering or for Rayleigh scattering at frequencies away from lines. Then, if we integrate over all solid angles, we find that approximately as many photons are scattered into a frequency interval as are scattered out to other frequencies. Thus, the scattering and scattering emission rates are equal,

$$\int I_\nu \frac{\Sigma[\text{scattering coefficient } (\ell \rightarrow u)]}{c}\ n(\ell)\ d\omega$$
$$= \int \Sigma[\text{scattering emission coefficient } (u \rightarrow \ell)]\ n(u)\ d\omega \quad . \tag{2.7}$$

Combining both scattering approximations (2.6) and (2.7), we obtain

$$\frac{\Sigma[\text{scattering coefficient } (\ell \rightarrow u)]}{c}\ n(\ell) \int I_\nu \frac{d\omega}{4\pi}$$
$$= \Sigma[\text{scattering emission coefficient } (u \rightarrow \ell)]\ n(u) \quad , \tag{2.8}$$

which we can use to simplify equation (2.1).

We adopt a notation for the various coefficients – α for absorption, s for scattering, and ϵ for emission – to obtain the transfer equation

$$\frac{dI_\nu}{dz} = \left[-\Sigma\ n(\ell)\ \alpha_\nu\ (\ell \rightarrow u) + \Sigma\ n(u)\ \alpha_\nu\ (u \rightarrow \ell) - \Sigma\ n(\ell)\ s_\nu\ (\ell \rightarrow u)\right] I_\nu$$
$$+ \left[\Sigma\ n(u)\ \epsilon_\nu\ (u \rightarrow \ell) + \Sigma\ n(\ell)\ s_\nu\ (\ell \rightarrow u) \int I_\nu \frac{d\omega}{4\pi}\right] \quad . \tag{2.9}$$

2.2 The Source Function

We introduce the source function S_ν to simplify the equations describing the radiation field by adopting a notation for the emission process similar to that for the absorption process. We define

$$S_\nu = \frac{\Sigma n(u)\,\epsilon_\nu(u \rightarrow \ell) + \Sigma n(\ell)\, s_\nu(\ell \rightarrow u) \int I_\nu (d\omega/4\pi)}{\Sigma\, n(\ell)\,\alpha_\nu(\ell \rightarrow u) - \Sigma\, n(u)\,\alpha_\nu(u \rightarrow \ell) + \Sigma\, n(\ell)\, s_\nu(\ell \rightarrow u)} \quad . \tag{2.10}$$

The equation for the change in intensity (2.9) becomes

$$\frac{dI_\nu}{dz} = \left[\Sigma n(\ell)\,\alpha_\nu(\ell \rightarrow u) - \Sigma n(u)\,\alpha_\nu(u \rightarrow \ell) + \Sigma n(\ell)\, s_\nu(\ell \rightarrow u)\right](-I_\nu + S_\nu) \quad . \tag{2.11}$$

To simplify further, we now proceed to relate $n(\ell)$ to $n(u)$ and $\alpha_\nu(\ell \rightarrow u)$ to $\alpha_\nu(u \rightarrow \ell)$ and to evaluate ϵ_ν. The relation between $\alpha_\nu(\ell \rightarrow u)$ and $\alpha_\nu(u \rightarrow \ell)$ can be seen if we consider the absorption of a photon from the beam by an isolated atom. By time reversal (since in one case N photons become N - 1, while in the other, N - 1 become N), the two coefficients must be equal. A complication arises if the levels are degenerate with statistical weights $g(\ell)$ and $g(u)$. The transition rates must be proportional to the number of final states available, so that

$$\frac{\alpha_\nu(\ell \rightarrow u)}{g(u)} = \frac{\alpha_\nu(u \rightarrow \ell)}{g(\ell)} \quad . \tag{2.12}$$

Further complications may arise when we consider interactions among a large number of atoms and Doppler shifts in the frequency of the transition; however, we will assume that equation (2.12) holds in any case.

Using the relation (2. 12) between the absorption coefficients, the quantity

$$\Sigma n(\ell)\, a_{\nu}(\ell \rightarrow u) - \Sigma n(u)\, a_{\nu}(u \rightarrow \ell)$$

becomes

$$\Sigma n(\ell)\, a_{\nu}(\ell \rightarrow u) - \Sigma n(u) \frac{g(\ell)}{g(u)}\, a_{\nu}(\ell \rightarrow u)$$

or

$$\Sigma n(\ell)\, a_{\nu}(\ell \rightarrow u) \left[1 - \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)} \right] \quad . \tag{2. 13}$$

The transfer equation (2. 11) becomes

$$\frac{dI_{\nu}}{dz} = \left\{ \Sigma n(\ell)\, a_{\nu}(\ell \rightarrow u) \left[1 - \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)} \right] + \Sigma n(\ell)\, s_{\nu}(\ell \rightarrow u) \right\} (- I_{\nu} + S_{\nu}) \quad , \tag{2. 14}$$

and the source function becomes

$$S_{\nu} = \frac{\Sigma n(u)\, \epsilon_{\nu}(u \rightarrow \ell) + \Sigma n(\ell)\, s_{\nu}(\ell \rightarrow u) \int I_{\nu}\, (d\omega/4\pi)}{\Sigma n(\ell)\, a_{\nu}(\ell \rightarrow u) \{ 1 - [n(u)/n(\ell)]\, [g(\ell)/g(u)] \} + \Sigma n(\ell)\, s_{\nu}(\ell \rightarrow u)} \quad . \tag{2. 15}$$

To evaluate ϵ_{ν}, we consider the special case of thermodynamic equilibrium, for which the following conditions apply:

A. The radiation and matter are described by one temperature, T.

B. There is no net energy transfer, so the radiation field is constant over space, implying from equation (2. 14) that $S_{\nu} = I_{\nu}$.

C. The intensity I_{ν} is described by the Planck function,

$$B_{\nu} = \frac{2h\nu^3}{c^2} (e^{h\nu/kT} - 1)^{-1} \quad .$$

D. The photon number density N_ν is $B_\nu/ch\nu = (2\nu^2/c^3)(e^{h\nu/kT} - 1)^{-1}$.

E. Any process

$$A + B + C + \cdots \rightleftharpoons 1 + 2 + 3 + \cdots \quad ,$$

where A, B, C and 1, 2, 3 represent particles or photons, is in equilibrium (detailed balance) such that

$$n(A)\, n(B)\, n(C) \cdots R(ABC \cdots \rightarrow 123 \cdots) = n(1)\, n(2)\, n(3) \cdots R(123 \cdots \rightarrow ABC \cdots) ,$$

where the R's are the rate coefficients.

F. The energy-level populations are related by the Saha equation

$$\frac{n_1\, n_2\, n_3 \cdots}{n_A\, n_B\, n_C \cdots} = \frac{U_1(2\pi M_1 kT/h^2)^{3/2}\, U_2(2\pi M_2 kT/h^2)^{3/2}\, U_3(2\pi M_3 kT/h^2)^{3/2} \cdots e^{-E_{123\cdots}/kT}}{U_A(2\pi M_A kT/h^2)^{3/2}\, U_B(2\pi M_B kT/h^2)^{3/2}\, U_C(2\pi M_C kT/h^2)^{3/2} \cdots e^{-E_{ABC\cdots}/kT}} ,$$

where the U's are partition functions ($U_X = \Sigma g_i\, e^{-E_i/kT}$ for all i in X) or statistical weights. An example is the Boltzmann equation for two levels of the same ion:

$$\frac{n(u)}{n(\ell)} = \frac{g(u)}{g(\ell)}\, \frac{(2\pi M kT/h^2)^{3/2}\, e^{-E_u/kT}}{(2\pi M kT/h^2)^{3/2}\, e^{-E_\ell/kT}} = \frac{g(u)}{g(\ell)}\, e^{-(E_u - E_\ell)/kT} \quad .$$

Further examples are given in Section 4.

We now apply the equilibrium conditions for the process

$$A(\ell) + h\nu \rightleftharpoons A(u) \quad .$$

From the discussion in Section 2.1 and from E above, we know

$$n(\ell)\, \alpha_\nu(\ell \rightarrow u)\, \frac{I_\nu}{ch\nu} = n(u) \left[\alpha_\nu(u \rightarrow \ell)\, \frac{I_\nu}{ch\nu} + \frac{\epsilon_\nu(u \rightarrow \ell)}{ch\nu} \right]$$

or

$$\epsilon_\nu(u \to \ell) = \frac{n(\ell)}{n(u)} \alpha_\nu(\ell \to u) \left[1 - \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)}\right] I_\nu \quad .$$

Since $I_\nu = B_\nu$ and $[n(u)/n(\ell)]\,[g(\ell)/g(u)] = e^{-h\nu/kT}$, we obtain

$$\epsilon_\nu(u \to \ell) = \frac{g(\ell)}{g(u)} e^{h\nu/kT} \alpha_\nu(\ell \to u)(1 - e^{-h\nu/kT}) \frac{2h\nu^3/c^2}{e^{h\nu/kT} - 1} \quad ,$$

or finally

$$\epsilon_\nu(u \to \ell) = \frac{g(\ell)}{g(u)} \frac{2h\nu^3}{c^2} \alpha_\nu(\ell \to u) \quad . \tag{2.16}$$

Returning to the general case, we assume that the ratio (eq. (2.16))

$$\frac{g(u)}{g(\ell)} \frac{\epsilon_\nu(u \to \ell)}{\alpha_\nu(\ell \to u)} = \frac{2h\nu^3}{c^2}$$

is independent of whether or not the gas is in thermal equilibrium. This is plausible, because in thermal equilibrium the ratio in no way depends on the properties of the gas. We note that for a line transition the emission coefficient (2.16) implies that the absorption and emission profiles are identical. This is, in fact, the case in a high-density, nonmoving atmosphere.

We substitute our result for ϵ_ν (eq. (2.16)) into the source function (2.15), first making the transformation

$$\Sigma n(u)\epsilon_\nu(u \to \ell) = \Sigma n(\ell)\alpha_\nu(\ell \to u) \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)} \frac{2h\nu^3}{c^2}$$

$$= \Sigma n(\ell)\alpha_\nu(\ell \to u) \left[1 - \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)}\right] \frac{2h\nu^3}{c^2} \left[\frac{n(\ell)}{n(u)} \frac{g(u)}{g(\ell)} - 1\right]^{-1} \quad ,$$

to obtain

$$S_\nu = \frac{\Sigma n(\ell)\, a_\nu(\ell \rightarrow u) \left[1 - \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)}\right] \frac{2h\nu^3}{c^2} \left[\frac{n(\ell)}{n(u)} \frac{g(u)}{g(\ell)} - 1\right]^{-1} + \Sigma n(\ell)\, s_\nu(\ell \rightarrow u) \int I_\nu \frac{d\omega}{4\pi}}{\Sigma n(\ell)\, a_\nu(\ell \rightarrow u) \left[1 - \frac{n(u)}{n(\ell)} \frac{g(\ell)}{g(u)}\right] + \Sigma n(\ell)\, s_\nu(\ell \rightarrow u)} \quad . \tag{2.17}$$

2.3 Mass Absorption Coefficients, Optical Depth, and the Plane-Parallel Approximation

We wish to change variables and make some simplifying definitions before proceeding. First, we define the following mass absorption coefficients or opacities:

$$\kappa_\nu(\ell \rightarrow u) = n(\ell)\, a_\nu(\ell \rightarrow u) \left\{\frac{1 - [n(u)/n(\ell)]\,[g(\ell)/g(u)]}{\rho}\right\} \quad , \tag{2.18}$$

$$\kappa_\nu = \Sigma \kappa_\nu(\ell \rightarrow u) \quad , \tag{2.19}$$

$$\sigma_\nu(\ell \rightarrow u) = \frac{n(\ell)\, s_\nu(\ell \rightarrow u)}{\rho} \quad , \tag{2.20}$$

$$\sigma_\nu = \Sigma \sigma_\nu(\ell \rightarrow u) \quad . \tag{2.21}$$

We have divided by the mass density ρ in order to remove the rapid variation caused by the change in the number densities as we pass through the atmosphere. In this notation, the transfer equation (2.14) becomes

$$\frac{dI}{\rho\, dz} = (\kappa_\nu + \sigma_\nu)(-I_\nu + S_\nu) \quad , \tag{2.22}$$

and the source function (2.17) becomes

$$S_\nu = \frac{\Sigma \kappa_\nu(\ell \rightarrow u)\, S_\nu(u \rightarrow \ell) + \sigma_\nu \int I_\nu\, (d\omega/4\pi)}{\kappa_\nu + \sigma_\nu} \quad , \tag{2.23}$$

where we have defined a source function for a single transition,

$$S_\nu(u \rightarrow \ell) = \frac{2h\nu^3}{c^2}\left[\frac{n(\ell)}{n(u)}\,\frac{g(u)}{g(\ell)} - 1\right]^{-1} \quad . \tag{2.24}$$

To make the derivative $dI_\nu/\rho\, dz$ in the transfer equation (2.22) of the same physical magnitude as I_ν, we divide it by $\kappa_\nu + \sigma_\nu$ and define the optical depth along the beam such that $d\tau_\nu = (\kappa_\nu + \sigma_\nu)\,\rho|dz|$. We note that in an optical depth τ, the number of original photons left in the beam decreases by $e^{-\tau}$ (from $dI/d\tau = -I$). Therefore, photons do not travel distances greater than a few optical depths. The density in a stellar atmosphere can be large enough so that the distance corresponding to a few optical depths is small compared to the radius of the star. In this case, the radiation field cannot "see" curvature, and we can treat the atmosphere in plane layers where distances and optical depths are measured in terms of the normal distance x. Then, $z = x/\cos\theta = x/\mu$, $dz = dx/\mu$, and the optical depth along x is determined from

$$d\tau_\nu = -(\kappa_\nu + \sigma_\nu)\,\rho\, dx \quad , \quad \tau = 0 \text{ at } x = \infty \quad . \tag{2.25}$$

The transfer equation then can be written in the simple form

$$\mu\,\frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu \quad . \tag{2.26}$$

2.4 Properties of the Radiation Field

If we assume that S_ν is specified, we can integrate equation (2.26) to obtain I_ν. The homogeneous solution is $I_\nu = c(\tau_\nu)\,e^{\tau_\nu/\mu}$. Substituting this solution into the non-homogeneous equation gives the result

$$I_\nu = -e^{\tau_\nu/\mu}\int_c^{\tau_\nu} S_\nu\, e^{-t/\mu}\,\frac{dt}{\mu} \quad ,$$

where c is an arbitrary constant. There are two cases: $\mu < 0$ and $\mu > 0$. For $\mu < 0$, the boundary condition is no incident radiation at the top of the atmosphere ($\tau_\nu = 0$), with the result

$$I_\nu = - \int_0^{\tau_\nu} S_\nu e^{-(t-\tau_\nu)/\mu} \frac{dt}{\mu} \quad , \qquad \mu < 0 \quad . \tag{2.27a}$$

For $\mu > 0$, the boundary condition is that the intensity contribution from infinity is zero because the energy source in a star is finite:

$$I_\nu = \int_{\tau_\nu}^{\infty} S_\nu e^{-(t-\tau_\nu)/\mu} \frac{dt}{\mu} \quad , \qquad \mu > 0 \quad . \tag{2.27b}$$

We are also interested in properties of the radiation field other than the specific intensity I_ν. The radiation field that each atom sees and that governs the level populations is the integrated intensity $\int I_\nu \, d\omega$. Another quantity, the radiative energy that actually passes through the atmosphere in any outward direction per unit area per second, is the flux $\int \mu I_\nu \, d\omega$. The cosine factor μ subtracts the inward-flowing radiation from the outward-flowing radiation to yield the net outward flow. A third property is the radiation pressure $(1/c) \int \mu^2 I_\nu \, d\omega$. Since photons carry momentum $h\nu/c$, they exert a pressure. The pressure in the normal direction per unit frequency, or the rate of momentum transfer per unit area, is the normal component of the energy flow $\mu(\mu I_\nu)$ integrated over all angles and divided by the photon velocity c.

We can formalize this discussion by introducing the intensity moments

$$J_\nu = \int I_\nu \frac{d\omega}{4\pi} \quad , \tag{2.28}$$

$$H_\nu = \int \mu I_\nu \frac{d\omega}{4\pi} \quad , \tag{2.29}$$

and

$$K_\nu = \int \mu^2 I_\nu \frac{d\omega}{4\pi} \quad ; \tag{2.30}$$

J_ν is called the mean intensity, and the integrated intensity is $4\pi J_\nu$. The flux is $4\pi H_\nu$; for confusion, H_ν is also called the flux. The monochromatic radiation pressure is $4\pi K_\nu/c$, but K_ν does not have a common name. Use of the moments keeps all the radiation quantities in the same units. Note that the source function (2.19) can be written in terms of J_ν as

$$S_\nu = \frac{\Sigma\ \kappa_\nu(\ell \rightarrow u)\, S_\nu(u \rightarrow \ell) + \sigma_\nu J_\nu}{\kappa_\nu + \sigma_\nu} \quad . \tag{2.31}$$

We can also take the moments of the transfer equation (2.26)

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

$$\frac{dH_\nu}{d\tau_\nu} = J_\nu - S_\nu \quad , \tag{2.32}$$

$$\frac{dK_\nu}{d\tau_\nu} = H_\nu \quad . \tag{2.33}$$

If we use the relation $d\omega = 2\pi \sin\theta\, d\theta = -2\pi\, d\mu$, the moments become

$$J_\nu = \frac{1}{2} \int_{-1}^{1} I_\nu\, d\mu \quad , \tag{2.34}$$

$$H_\nu = \frac{1}{2} \int_{-1}^{1} \mu\, I_\nu\, d\mu \quad . \tag{2.35}$$

$$K_\nu = \frac{1}{2} \int_{-1}^{1} \mu^2\, I_\nu\, d\mu \quad . \tag{2.36}$$

To evaluate equations (2.34) through (2.36), we substitute the solution for I_ν (eq. (2.27a, b)) to obtain

$$J_\nu = \frac{1}{2} \int_{-1}^{0} \int_{0}^{\tau_\nu} S_\nu e^{-(\tau_\nu - t)/\mu} \frac{dt}{\mu} d\mu + \frac{1}{2} \int_{0}^{1} \int_{\tau_\nu}^{\infty} S_\nu e^{-(t-\tau_\nu)/\mu} \frac{dt}{\mu} d\mu \quad , \tag{2.37}$$

$$H_\nu = -\frac{1}{2} \int_{-1}^{0} \int_{0}^{\tau_\nu} S_\nu \; e^{-(\tau_\nu - t)/\mu} dt\, d\mu + \frac{1}{2} \int_{0}^{1} \int_{\tau_\nu}^{\infty} S_\nu e^{-(t-\tau_\nu)/\mu} dt\, d\mu \quad , \tag{2.38}$$

and

$$K_\nu = \frac{1}{2} \int_{-1}^{0} \int_{0}^{\tau_\nu} S_\nu e^{-(\tau_\nu - t)/\mu} \mu\, dt\, d\mu + \frac{1}{2} \int_{0}^{1} \int_{\tau_\nu}^{\infty} S_\nu e^{-(t-\tau_\nu)/\mu} \mu\, dt\, d\mu \quad . \tag{2.39}$$

The preceding notation can be considerably simplified if we introduce the exponential integral

$$E_n(x) = \int_{1}^{\infty} \frac{e^{-xz}}{z^n} dz = \int_{0}^{1} e^{-x/\mu} \mu^{n-2} d\mu \quad , \tag{2.40}$$

so that

$$J_\nu(\tau_\nu) = \frac{1}{2} \int_{0}^{\tau_\nu} S_\nu E_1(\tau_\nu - t)\, dt + \frac{1}{2} \int_{\tau_\nu}^{\infty} S_\nu E_1(t - \tau_\nu)\, dt \quad , \tag{2.41}$$

$$H_\nu(\tau_\nu) = -\frac{1}{2} \int_{0}^{\tau_\nu} S_\nu E_2(\tau_\nu - t)\, dt + \frac{1}{2} \int_{\tau_\nu}^{\infty} S_\nu E_2(t - \tau_\nu)\, dt \quad , \tag{2.42}$$

and

$$K_\nu(\tau_\nu) = \frac{1}{2}\int_0^{\tau_\nu} S_\nu E_3(\tau_\nu - t)\,dt + \frac{1}{2}\int_{\tau_\nu}^{\infty} S_\nu E_3(t - \tau_\nu)\,dt \quad . \tag{2.43}$$

We see that the mean intensity is an average over τ of S_ν for τ near τ_ν. The flux is the difference between S_ν for τ greater than τ_ν and S_ν for τ less than τ_ν. We must remember that S_ν depends on J_ν (eq. (2.31)), so we actually must solve an integral equation to determine S_ν or J_ν.

2.5 Computing the Optical Depth

We define a mass variable $-\int \rho\,dx$, which we call rhox (pronounced rocks), and use it to label depth points in the atmosphere. In non-FORTRAN equations, we denote rhox by M and the differential $-\rho\,dx$ by dM.

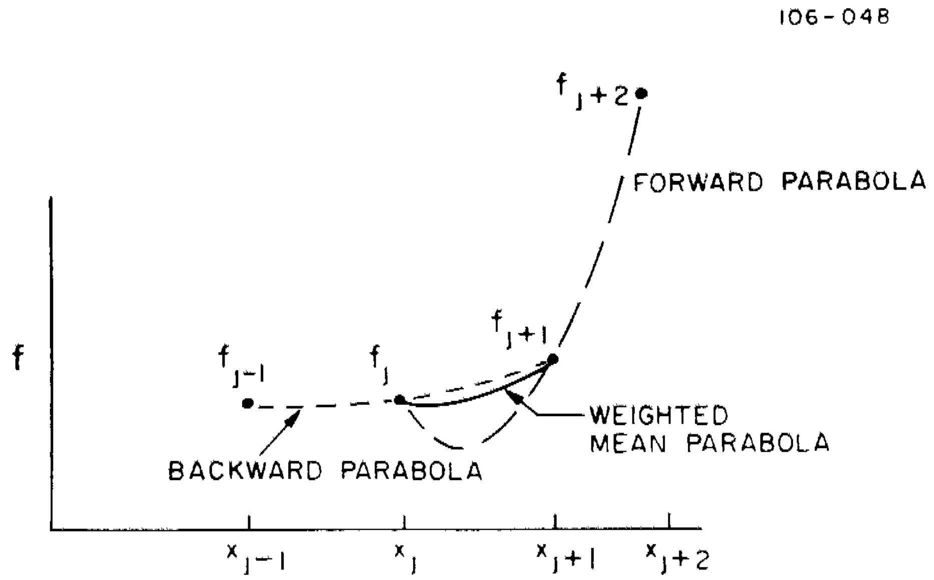
We now consider the numerical calculation of the radiation field, assuming we know the opacity as described in Section 5. We divide the atmosphere into N layers, each labeled by depth M_j. The optical depth is easily found by integrating the opacity,

$$\tau_{\nu j} = \int_0^{M_j} (\kappa_\nu + \sigma_\nu)\,dM \quad . \tag{2.44}$$

Simple integrals like (2.44) are performed by fitting parabolas to the integrand for each depth interval in the atmosphere, as follows:

$$\begin{aligned}\int_0^{x_N} f(x)\,dx &= \sum \int_{x_j}^{x_{j+1}} f(x)\,dx = \sum \int_{x_j}^{x_{j+1}} (a_j + b_j x + c_j x^2)\,dx \\ &= \sum \left[a_j(x_{j+1} - x_j) + \frac{b_j(x_{j+1}^2 - x_j^2)}{2} + \frac{c_j(x_{j+1}^3 - x_j^3)}{3} \right] \\ &= \sum \left[a_j + \frac{b_j(x_{j+1} + x_j)}{2} + \frac{c_j(x_{j+1}^2 + x_{j+1}x_j + x_j^2)}{3} \right] (x_{j+1} - x_j) \quad .\end{aligned} \tag{2.45}$$

In ATLAS, the interpolation coefficients a_j, b_j, and c_j are determined by weighting forward and backward parabolas inversely by their second derivatives, as shown in the following diagram:



This weighting avoids large overshoots, which are a problem with simple parabolic interpolation. The unweighted parabolas are given by the expressions

$$c_j = \frac{f_{j+1}}{(x_{j+1} - x_j)(x_{j+1} - x_{j-1})} - \frac{f_j}{(x_j - x_{j-1})(x_{j+1} - x_j)} + \frac{f_{j-1}}{(x_j - x_{j-1})(x_{j+1} - x_{j-1})} , \tag{2.46c}$$

$$b_j = \frac{f_j - f_{j-1}}{x_j - x_{j-1}} - (x_j + x_{j-1})\, c_j , \tag{2.46b}$$

and

$$a_j = f_{j-1} - x_{j-1} \frac{f_j - f_{j-1}}{x_j - x_{j-1}} + x_j x_{j-1} c_j . \tag{2.46a}$$

The weight is

$$w_j = \frac{|c_{j+1}|}{|c_{j+1}| + |c_j|} , \tag{2.47}$$

so the weighted mean parabola is

$$\bar{a}_j = w_j a_j + (1 - w_j)\, a_{j+1} \quad ,$$

$$\bar{b}_j = w_j b_j + (1 - w_j)\, b_{j+1} \quad ,$$

$$\bar{c}_j = w_j c_j + (1 - w_j)\, c_{j+1} \quad . \tag{2.48}$$

2.6 Computing the Mean Intensity and Flux

The source function, mean intensity, and flux are calculated as described by Kurucz (1969) by using integration matrices.

To derive these matrices, we consider the general moment integral of the specific intensity,

$$M_n(\tau) = \frac{1}{2} \int_0^\infty \text{sign}\,(t - \tau)^{n-1}\, S(t)\, E_n|t - \tau|\, dt \quad . \tag{2.49}$$

Then, from equations (2.41), (2.42), and (2.43),

$$J(\tau) = M_1(\tau) \quad , \quad H(\tau) = M_2(\tau) \quad , \quad \text{and} \quad K(\tau) = M_3(\tau) \quad .$$

We divide the integration range into N subintervals,

$$M_{n\ell} \equiv M_n(\tau_\ell) = \frac{1}{2} \sum_{j=1}^{N} \text{sign}\,(\tau_j - \tau_\ell)^{n-1} \int_{\tau_j}^{\tau_{j+1}} S(t)\, E_n|t - \tau_\ell|\, dt \quad . \tag{2.50}$$

We now assume that S can be represented by a parabola in the interval (τ_j, τ_{j+1}). Thus,

$$S(t) = \sum_{k=1}^{3} t^{k-1} \sum_{i=1}^{N} C_{jki}\, S_i \quad , \tag{2.51}$$

where the C_{jki} are interpolation coefficients. The C_{jki} can be, for example, one-half the sum of the forward-parabolic and the backward-parabolic interpolation coefficients; or they can even be linear if a large number of points is used. In the version of ATLAS described here, however, the interpolation coefficients C_{jki} were found by passing a parabola through S_j and S_{j+1} and by least-squares fitting S_{j-1} and S_{j+2}. These coefficients are listed in Table 1.

Inserting the expression for S(t) (eq. (2.51)) into the jth term of the sum (eq. (2.50)), we find that

$$M_{n\ell j} = \frac{1}{2} \operatorname{sign} (\tau_j - \tau_\ell)^{n-1} \int_{\tau_j}^{\tau_{j+1}} dt\, E_n|t - \tau_\ell| \sum_{k=1}^{3} t^{k-1} \sum_{i=1}^{N} C_{jki} S_i \ . \tag{2.52}$$

This expression can be simplified to

$$M_{n\ell j} = \sum_{k=1}^{3} \eta_{n\ell jk} \sum_{i=1}^{N} C_{jki} S_i \quad , \tag{2.53}$$

where

$$\eta_{n\ell jk} = \frac{1}{2} \operatorname{sign} (\tau_j - \tau_\ell)^{n-1} \int_{\tau_j}^{\tau_{j+1}} t^{k-1} E_n|\tau_\ell - t|\, dt \tag{2.54}$$

is an integral that can be evaluated analytically. To evaluate $\eta_{n\ell jk}$, we use the indefinite integral

$$\int E_n(x)\, dx = -E_{n+1}(x) \tag{2.55}$$

Table 1. Least-squares parabolic interpolation coefficients.

$$D = \tau_{j-1}^2 + \tau_{j+2}^2 - \tau_j \tau_{j-1} - \tau_j \tau_{j+1} - \tau_{j+1} \tau_{j-1} - \tau_{j+1} \tau_{j+2} + 2 \tau_j \tau_{j+1}$$

$$C_{j\,1\,j-1} = \frac{\tau_j \tau_{j+1}}{D}$$

$$C_{j\,1\,j} = \frac{\tau_{j+1}(-\tau_{j-1}^2 - \tau_{j+2}^2 + \tau_{j+1}\tau_{j-1} + \tau_{j+1}\tau_{j+2})}{(\tau_j - \tau_{j+1})\, D}$$

$$C_{j\,1\,j+1} = \frac{\tau_j(\tau_{j-1}^2 + \tau_{j+2}^2 - \tau_j \tau_{j-1} - \tau_j \tau_{j+2})}{(\tau_j - \tau_{j+1})\, D}$$

$$C_{j\,1\,j+2} = \frac{\tau_j \tau_{j+1}}{D}$$

$$C_{j\,2\,j-1} = \frac{-(\tau_j + \tau_{j+1})}{D} \qquad C_{j\,3\,j-1} = \frac{1}{D}$$

$$C_{j\,2\,j} = \frac{\tau_{j-1}^2 - 2\tau_{j+1}^2 + \tau_{j+2}^2}{(\tau_j - \tau_{j+1})\, D} \qquad C_{j\,3\,j} = \frac{-\tau_{j-1} + 2\tau_{j+1} - \tau_{j+2}}{(\tau_j - \tau_{j+1})\, D}$$

$$C_{j\,2\,j+1} = \frac{-\tau_{j-1}^2 + 2\tau_j^2 - \tau_{j+2}^2}{(\tau_j - \tau_{j+1})\, D} \qquad C_{j\,3\,j+1} = \frac{\tau_{j-1} - 2\tau_j + \tau_{j+2}}{(\tau_j - \tau_{j+1})\, D}$$

$$C_{j\,2\,j+2} = \frac{-(\tau_j + \tau_{j+1})}{D} \qquad C_{j\,3\,j+2} = \frac{1}{D}$$

and integrate by parts, obtaining

$$\eta_{n\ell jk} = \frac{1}{2}\,\mathrm{sign}\,(\tau_j - \tau_\ell)^{n-1}\;\Bigg|\;\left(\tau_j^{k-1}\,E_{n+1}|\tau_\ell - \tau_j| - \tau_{j+1}^{k-1}\,E_{n+1}|\tau_\ell - \tau_{j+1}|\right)$$

$$+ (k-1)\,\mathrm{sign}\,(\tau_j - \tau_\ell)\left(\tau_j^{k-2}\,E_{n+2}|\tau_\ell - \tau_j| - \tau_{j+1}^{k-2}\,E_{n+2}|\tau_\ell - \tau_{j+1}|\right)$$

$$+ (k-1)(k-2)\left(\tau_j^{k-3}\,E_{n+3}|\tau_\ell - \tau_j| - \tau_{j+1}^{k-3}\,E_{n+3}|\tau_\ell - \tau_{j+1}|\right)\Bigg| \quad . \tag{2.56}$$

We must evaluate $\eta_{n\ell jk}$ carefully when the τ's are small because of two cases of numerical cancellation. First, for $|\tau_\ell - \tau_j|$ small, we write out the expression for $\eta_{n\ell jk}$ explicitly using the power-series expansion for the exponential integrals and grouping terms in such a way that no loss of accuracy occurs The power series is

$$E_n(x) = \frac{(-x)^{n-1}}{(n-1)!}\left(-\log x - \gamma + \sum_{m=1}^{n-1} \frac{1}{m}\right) - \sum_{\substack{m=0 \\ m\neq n-1}}^{\infty} \frac{(-x)^m}{(m-n+1)\; m!} \;, \tag{2.57}$$

where $\gamma = 0.577215664901533$ is Euler's constant. Second, for τ_j/τ_ℓ small, we use the power-series expansion around τ_ℓ and evaluate only those terms that do not cancel analytically. The expansion is

$$E_n(x-y) = E_n(x) + y\,E_{n-1}(x) + \frac{1}{2}\,y^2\,E_{n-2}(x) + \cdots + \frac{y^{n-2}}{(n-2)!}\,E_2(x)$$

$$+ \frac{y^{n-1}}{(n-1)!}\,E_1(x) + e^{-x}\sum_{m=0}^{\infty}\frac{y^{m+n}}{(m+n)!}\left[1 + \frac{m}{x} + \frac{m(m-1)}{x^2} + \cdots + \frac{m!}{x^{m-1}} + \frac{m!}{x^m}\right] \quad . \tag{2.58}$$

Detailed expressions for $\eta_{n\ell jk}$ can be extracted from program PRETAB listed in Section 9.2.

We now collect terms to achieve the form of a matrix operator on S,

$$M_{n\ell} = \sum_{j=1}^{N} \sum_{k=1}^{3} \eta_{n\ell jk} \sum_{i=1}^{N} C_{jki} S_i = \sum_{j=1}^{N} \sum_{k=1}^{3} \sum_{i=1}^{N} \eta_{n\ell jk} C_{jki} S_i$$

$$= \sum_{j=1}^{N} \sum_{k=1}^{3} \sum_{i=1}^{N} \eta_{n\ell ik} C_{ikj} S_j = \sum_{j=1}^{N} \Xi_{n\ell j} S_j \quad , \tag{2.59}$$

where

$$\Xi_{n\ell j} = \sum_{k=1}^{3} \sum_{i=1}^{N} \eta_{n\ell ik} C_{ikj} \quad . \tag{2.60}$$

The matrix Ξ_n is the desired matrix operator

$$M_n = \Xi_n S \quad . \tag{2.61}$$

To calculate the flux or mean intensity, we simply matrix multiply

$$J = \Lambda S \tag{2.62}$$

and

$$H = \Phi S \quad , \tag{2.63}$$

where we have defined the matrices

$$\Lambda \equiv \Xi_1 \quad \text{and} \quad \Phi \equiv \Xi_2 \quad .$$

2.7 Computing the Source Function

We recall equation (2.31) for the source function

$$S_\nu = \frac{\Sigma\, \kappa_\nu(\ell \rightarrow u)\, S_\nu\, (u \rightarrow \ell) + \sigma_\nu\, J_\nu}{\kappa_\nu + \sigma_\nu}$$

and rewrite it as

$$S_\nu = (1 - a_\nu)\, \overline{S}_\nu + a_\nu\, J_\nu \quad , \tag{2.64}$$

where

$$\overline{S}_\nu \equiv \frac{\Sigma\, \kappa_\nu\, (\ell \rightarrow u)\, S_\nu\, (u \rightarrow \ell)}{\kappa_\nu} \tag{2.65}$$

and

$$a_\nu \equiv \frac{\sigma_\nu}{\kappa_\nu + \sigma_\nu} \quad . \tag{2.66}$$

Equation (2.64) is an integral equation for S_ν since J_ν depends on S_ν. In matrix notation, the integral equation becomes

$$S = (I - a)\, \overline{S} + a\, \Lambda S$$

or

$$(I - a\, \Lambda)\, S = (I - a)\, \overline{S} \quad , \tag{2.67}$$

where I is the identity matrix, a is now a diagonal matrix, and S and $\overline{S}$ are now column vectors. The solution to this system of equations can be rapidly obtained by Gauss-Seidel iteration since the matrix is almost diagonal. The iteration proceeds as follows: An initial guess is made for S, such as $S = \overline{S}$. This vector is multiplied by the matrix $(I - a\, \Lambda)$ to give a vector that differs by Δ from the required result $(I - a)\, \overline{S}$,

$$\Delta = (I - a\, \Lambda)\, S - (I - a)\, \overline{S} \quad . \tag{2.68}$$

We wish to find a correction ΔS so that

$$(I - \alpha \Lambda)(S + \Delta S) = (I - \alpha)\, \overline{S} \quad . \tag{2.69}$$

The solution of equation (2.69) is

$$\Delta S = (I - \alpha \Lambda)^{-1}\left[(I - \alpha)\, \overline{S} - (I - \alpha \Lambda)\, S\right] = -\,(I - \alpha \Lambda)^{-1}\, \Delta \quad . \tag{2.70}$$

Since $(I - \alpha \Lambda)$ is almost diagonal,

$$(I - \alpha \Lambda)^{-1} \simeq \frac{1}{1 - \alpha_i \Lambda_{ii}} \quad , \tag{2.71}$$

so that

$$\Delta S \simeq -\, \frac{\Delta}{1 - \alpha_i \Lambda_{ii}} \quad . \tag{2.72}$$

We iterate on the equation

$$S^{\text{new}} = S^{\text{old}} + \Delta S \tag{2.73}$$

until $\Delta S/S$ is less than some prescribed value, currently 1.E-5.

Equation (2.67) for the source function can be rewritten in a form that avoids the quantity $(1 - \alpha)$, which may lead to numerical difficulties. We have

$$\left(I - \frac{\sigma}{\kappa + \sigma}\, \Lambda\right) S = \left(I - \frac{\sigma}{\kappa + \sigma}\right) \overline{S} \tag{2.74}$$

or

$$\left(\frac{\kappa + \sigma - \sigma \Lambda}{\kappa + \sigma}\right) S = \frac{\kappa}{\kappa + \sigma}\, \overline{S} \quad ,$$

and finally

$$\left(I + \frac{\sigma}{\kappa} - \frac{\sigma}{\kappa}\Lambda\right) S = \overline{S} \quad . \tag{2.75}$$

2.8 Pretabulation of the Matrices and Treatment of Large Depths

Since the integration matrices are rather complicated to evaluate, they have been pretabulated for a fixed τ set, where the values of τ have been chosen to give accurate integrations. The program that does this, PRETAB, is listed in Section 9.2. The 43 points currently used are the following:

1	0	12	0.01	23	0.63	34	3.65
2	0.000032	13	0.016	24	0.78	35	4.15
3	0.000056	14	0.025	25	0.95	36	4.9
4	0.0001	15	0.042	26	1.15	37	6.1
5	0.00018	16	0.065	27	1.35	38	7.7
6	0.00032	17	0.096	28	1.6	39	10.
7	0.00056	18	0.139	29	1.85	40	12.5
8	0.001	19	0.196	30	2.15	41	15.
9	0.0018	20	0.273	31	2.45	42	17.5
10	0.0032	21	0.375	32	2.75	43	20.
11	0.0056	22	0.5	33	3.15		

Note that since there are few points near the surface, integrals at monochromatic optical depths of 10^{-4} and less cannot be very reliable if the source function varies there. The abundance of points at large depths allows better treatment of these regions.

To evaluate S_ν, J_ν, and H_ν, we interpolate α_ν and $\overline{S}_\nu$ from the τ_ν set onto the fixed τ set. Then we solve for S_ν and use it to integrate for J_ν and H_ν. Finally, we interpolate S_ν, J_ν, and H_ν back onto the τ_ν set. For the interpolations we use the method described in Section 2.5.

Optical depths larger than the last value of the fixed τ set ($\tau = 20$) must be treated separately by using the asymptotic forms for the Λ and Φ operators, namely,

$$J_\nu = S_\nu + \frac{1}{3}\frac{d^2S_\nu}{d\tau_\nu^2} \quad \text{and} \quad H_\nu = \frac{1}{3}\frac{dS_\nu}{d\tau_\nu} \quad . \tag{2.76}$$

These asymptotic relations can be derived by evaluating K_ν at large depths and then using the moment equations (2.32) and (2.33) to find J_ν and H_ν by differentiation. From equation (2.43), we have

$$K_\nu(\tau_\nu) = \frac{1}{2}\int_0^\infty S_\nu(t)\, E_3|t - \tau_\nu|\, dt \quad . \tag{2.77}$$

We expand S(t) around τ_ν,

$$S(t) = S(\tau_\nu) + (\tau_\nu - t)\left(\frac{dS_\nu}{dt}\right)_{\tau_\nu} + \frac{1}{2}(\tau_\nu - t)^2\left(\frac{d^2S_\nu}{dt^2}\right)_{\tau_\nu} + \cdots \quad ,$$

and insert the expansion into the integral (2.77),

$$\begin{aligned} K_\nu(\tau_\nu) = {} & \left[S(\tau_\nu) + \tau_\nu\left(\frac{dS}{dt}\right)_{\tau_\nu} + \frac{\tau_\nu^2}{2}\left(\frac{d^2S_\nu}{dt^2}\right)_{\tau_\nu}\right]\left[\frac{1}{2}\int_0^{\tau_\nu} E_3(\tau_\nu - t)\, dt + \frac{1}{2}\int_{\tau_\nu}^\infty E_3(t - \tau_\nu)\, dt\right] \\ & + \left[-\left(\frac{dS}{dt}\right)_{\tau_\nu} - \tau_\nu\left(\frac{d^2S}{dt^2}\right)_{\tau_\nu}\right]\left[\frac{1}{2}\int_0^{\tau_\nu} t\, E_3(\tau_\nu - t)\, dt + \frac{1}{2}\int_{\tau_\nu}^\infty t\, E_3(t - \tau_\nu)\, dt\right] \\ & + \left[\frac{1}{2}\left(\frac{d^2S}{dt^2}\right)_{\tau_\nu}\right]\left[\frac{1}{2}\int_0^{\tau_\nu} t^2\, E_3(\tau_\nu - t)\, dt + \frac{1}{2}\int_{\tau_\nu}^\infty t^2\, E_3(t - \tau_\nu)\, dt\right] \quad . \end{aligned}$$

From equations (2.54) and (2.56), we find

$$K_\nu(\tau_\nu) = \left[S(\tau_\nu) + \tau_\nu \left(\frac{dS}{dt}\right)_{\tau_\nu} + \frac{\tau_\nu^2}{2}\left(\frac{d^2S_\nu}{dt^2}\right)_{\tau_\nu}\right]\left[\frac{1}{3} - \frac{1}{2}E_4(\tau_\nu)\right]$$

$$+ \left[-\left(\frac{dS}{dt}\right)_{\tau_\nu} - \tau_\nu\left(\frac{d^2S}{dt^2}\right)_{\tau_\nu}\right]\left[\frac{1}{3}\tau_\nu + \frac{1}{2}E_5(\tau_\nu)\right]$$

$$+ \left[\frac{1}{2}\left(\frac{d^2S}{dt^2}\right)_{\tau_\nu}\right]\left[\frac{2}{5} + \frac{1}{3}\tau_\nu^2 - E_6(\tau_\nu)\right] \quad .$$

The asymptotic form for the exponential integral

$$E_n(x) \sim \frac{e^{-x}}{x}\left[1 - \frac{n}{x} + \frac{n(n+1)}{x^2} - \cdots\right] \tag{2.78}$$

implies that we can ignore $E_n(\tau_\nu)$ terms for τ_ν large. We find

$$K_\nu(\tau_\nu) \sim \frac{1}{3}S(\tau_\nu) + \frac{1}{5}\left(\frac{d^2S}{dt^2}\right)_{\tau_\nu} \quad , \tag{2.79}$$

so that to second order,

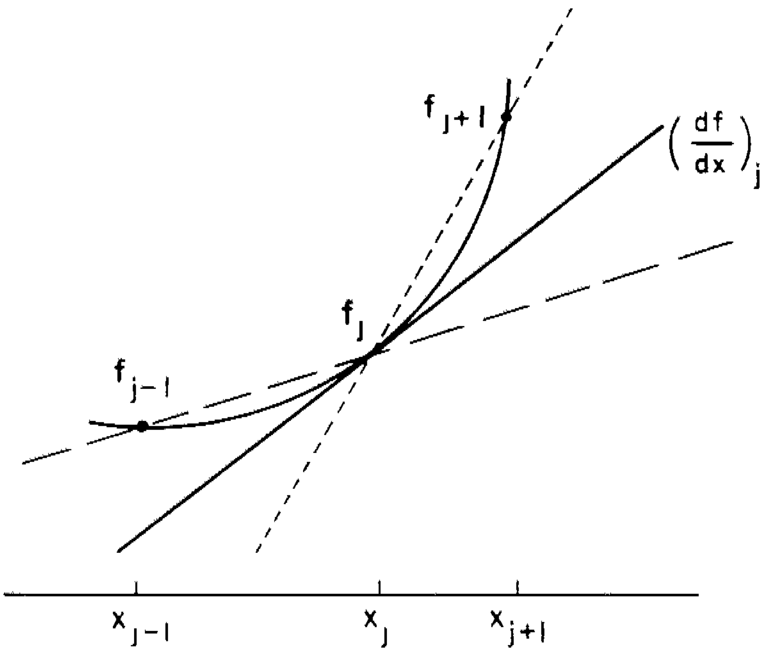
$$H_\nu = \frac{dK_\nu}{d\tau_\nu} = \frac{1}{3}\frac{dS_\nu}{d\tau_\nu}$$

and

$$J_\nu - S_\nu = \frac{dH_\nu}{d\tau_\nu} = \frac{1}{3}\frac{d^2S_\nu}{d\tau_\nu^2} \quad . \tag{2.80}$$

Derivatives are taken by bisecting the angles formed by the extension of the line segments as shown in the following diagram:

106-048



The result is

$$\left(\frac{df}{dx}\right)_j = \frac{S(T_{j+1} + T_j)}{1 - T_{j+1}T_j} \quad ,$$

where

$$T_j = \frac{D_j}{1 + \sqrt{1 + D_j^2}} \quad ,$$

with

$$D_j = \frac{1}{S}\,\frac{f_j - f_{j-1}}{x_j - x_{j-1}} \quad ,$$

and where

$$S = \frac{\max\left(|f_{j-1}|, |f_j|, |f_{j+1}|\right)}{|x_j|} \quad .$$

The scaling factor S converts f and x to the same magnitude

We calculate S_ν by iteration on the numerical derivatives until the relative change in S_ν is less than 1. E-5.

2.9 Computing Specific Intensity

The specific intensity $I_\nu(\mu)$ at the surface for $\cos\theta = \mu$ is often required, especially for solar work,

$$I_\nu(\mu) = \int_0^\infty S_\nu \, e^{-\tau_\nu/\mu} \, \frac{d\tau_\nu}{\mu} \quad . \tag{2.27b$'$}$$

We evaluate this by means of parabolic interpolation coefficients for S_ν, with the following result:

$$I_\nu(\mu) = \sum_{i=1}^{N} \left(e^{-\tau_i/\mu} \left\{ a_i + b_i(\tau_i + \mu) + c_i\left[(\tau_i + \mu)^2 + \mu^2\right] \right\} \right.$$

$$\left. - e^{-\tau_{i+1}/\mu} \left\{ a_i + b_i(\tau_{i+1} + \mu) + c_i\left[(\tau_{i+1} + \mu)^2 + \mu^2\right] \right\} \right) \quad ,$$

or

$$I_\nu(\mu) = \sum_{i=1}^{N} \left\{ e^{-\tau_i/\mu} \left[S_i + (b_i + 2c_i \, \tau_i) \, \mu + 2c_i \, \mu^2 \right] \right.$$

$$\left. - e^{-\tau_{i+1}/\mu} \left[S_{i+1} + (b_i + 2c_i \, \tau_{i+1}) \, \mu + 2c_i \, \mu^2 \right] \right\} \quad . \tag{2.81}$$

At small optical depths, we expand in $\Delta = (\tau_{i+1} - \tau_i)/\mu$ to avoid cancellation problems,

$$I_\nu(\mu) = \sum_{i=1}^{N} e^{-\tau_{i+1}/\mu} \left\{ S_i\Delta + \left[S_i + (b_i + 2c_i\ \tau_i)\ \mu\right] \frac{\Delta^2}{2} \right.$$

$$\left. + \left[S_i + (b_i + 2c_i\ \tau_i)\ \mu + 2c_i\ \mu^2\right] \sum_{n=3}^{\infty} \frac{\Delta^n}{n!} \right\} . \tag{2.82}$$

No allowance is made for the integral from τ_N to infinity, so the last τ_ν/μ must be large.

2.10 Frequency Integrations

Frequency integrals over flux and mean intensity are required for the temperature correction, for radiation pressure, and for photoionization rates. For the integration, we choose as many frequencies as necessary to represent the shapes of the various continua or lines. The integrations are truncated at some maximum frequency, usually an opacity discontinuity, such that inclusion of higher frequency points does not affect the model, except perhaps in the outer surface layers, where some of our assumptions break down in any case, or at such large optical depths as to be unimportant.

The integrals are evaluated by multiplying the various integrands at each frequency f_{ν_i} by a previously determined integration coefficient w_i that is a function only of the frequency spacing. The integration coefficients can be determined in any manner, but in Section 9.1 a program (FRESET) is given that uses the least-squares parabolas defined in Section 2.6.

The integral over all frequencies $f = \int f_\nu\, d\nu$ is the sum $\Sigma\, w_i f_{\nu_i}$. Since the monochromatic quantities are required in ATLAS only as integrands, they need not be saved once they have been added to the integral sums. Consequently, monochromatic quantities can be evaluated for any number of frequencies, one frequency at a time, with a minimum storage requirement.

2.11 Radiation Pressure

The radiation pressure is given by the integral

$$P_{rad} = \frac{4\pi}{c} \int K_\nu \, d\nu \quad ,$$

as discussed in Section 2.4. However, to save computation we do not evaluate K_ν directly but use the moment

$$\frac{dK_\nu}{dM} = (\kappa_\nu + \sigma_\nu) H_\nu \quad .$$

Then,

$$\frac{dP_{rad}}{dM} = \frac{4\pi}{c} \int (\kappa_\nu + \sigma_\nu) H_\nu \, d\nu \quad . \tag{2.83}$$

The quantity on the right side of equation (2.83) is the acceleration the gas experiences when it absorbs photons from below. Once the radiation field is known, P_{rad} is easily evaluated by integrating over M and specifying $P_{rad} = 0$ at $M = 0$. The actual value at the surface could be found by evaluating K_ν (at considerable expense), but there is no current need in ATLAS to know P_{rad} accurately at the surface.

2.12 Rosseland Optical Depth and Opacity

It is sometimes convenient to describe a model atmosphere in terms of a mean optical depth. For example, a good way to get a first guess for a model temperature distribution is to take some existing $T(M)^{old}$, express it as $T(\langle\tau\rangle)^{old}$, then scale the temperature by the ratio of the effective temperatures

$$T(\langle\tau\rangle)^{new} = \frac{T_{eff}^{new}}{T_{eff}^{old}} T(\langle\tau\rangle)^{old} \quad ,$$

and finally convert back to obtain $T(M)^{new}$. The Rosseland optical depth is well suited to this type of scaling, as we will show below.

The Rosseland optical depth τ_{Ross} and the corresponding Rosseland opacity are based on the behavior of the integrated flux at large depths,

$$\int H_\nu \, d\nu = \frac{1}{3} \int \frac{dS_\nu}{d\tau_\nu} \, d\nu \quad . \qquad \text{(from eq. (2.76))}$$

At large (mean) optical depths, S_ν goes to J_ν; and J_ν goes to B_ν because the gas and radiation are almost in thermal equilibrium. Photons created at one temperature are absorbed before they can travel to regions of significantly different temperature, so the mean intensity must reflect the gas temperature The Rosseland depth is defined so that

$$\int H_\nu \, d\nu = \frac{1}{3} \frac{d}{d\tau_{Ross}} \int B_\nu \, d\nu = \frac{1}{3} \int \frac{dB_\nu}{d\tau_\nu} \, d\nu \quad .$$

To find κ_{Ross}, we start with

$$\frac{d}{d\tau_{Ross}} \int B_\nu \, d\nu = \int \frac{dB_\nu}{d\tau_\nu} \, d\nu$$

and substitute $d\tau_{Ross} = \kappa_{Ross} \, dM$ to obtain

$$\frac{1}{\kappa_{Ross}} \frac{d}{dM} \int B_\nu \, d\nu = \int \frac{1}{\kappa_\nu + \sigma_\nu} \frac{dB_\nu}{dM} \, d\nu$$

or

$$\frac{1}{\kappa_{Ross}} = \frac{\int [1/(\kappa_\nu + \sigma_\nu)] \, (dB_\nu/dM) \, d\nu}{\int (dB_\nu/dM) \, d\nu} \quad .$$

We change from dM to dT to make the definition independent of stars,

$$\frac{1}{\kappa_{\mathrm{Ross}}} = \frac{\int [1/(\kappa_\nu + \sigma_\nu)]\,(dB_\nu/dT)\,d\nu}{\int (dB_\nu/dT)\,d\nu} \quad . \tag{2.84}$$

Values of the various derivatives mentioned are

$$\frac{dB_\nu}{dT} = \frac{B_\nu\, h\nu/kT}{T(1 - e^{-h\nu/kT})} \quad , \tag{2.85}$$

$$\int \frac{dB_\nu}{dT}\, d\nu = \frac{4\sigma T^3}{\pi} \quad , \tag{2.86}$$

and

$$\int H_\nu\, d\nu = \frac{1}{3}\,\frac{d}{d\tau_{\mathrm{Ross}}} \int B_\nu\, d\nu = \frac{1}{3}\,\frac{d}{d\tau_{\mathrm{Ross}}}\,\frac{\sigma T^4}{\pi} = \frac{4\sigma T^3}{3\pi}\,\frac{dT}{d\tau_{\mathrm{Ross}}} \quad . \tag{2.87}$$

The scaling properties of $T(\tau_{\mathrm{Ross}})$ follow from equation (2.87) when we substitute the value of the integrated flux

$$\frac{\sigma T_{\mathrm{eff}}^4}{4\pi} = \frac{4\sigma T^3}{3\pi}\,\frac{dT}{d\tau_{\mathrm{Ross}}} \quad .$$

We have a differential equation for $T(\tau_{\mathrm{Ross}})$ at large depths, which has the solution

$$\frac{3}{4}\, T_{\mathrm{eff}}^4\, \tau_{\mathrm{Ross}} + C = T^4 \quad ,$$

or

$$T(\tau_{\mathrm{Ross}}) = T_{\mathrm{eff}} \left(\frac{3}{4}\, \tau_{\mathrm{Ross}} + C \right)^{1/4} \quad .$$

Thus, $T(\tau_{\mathrm{Ross}})$ should scale as T_{eff} for large optical depths in radiative models.

3. STATISTICAL EQUILIBRIUM

3.1 Rates

We turn to the problem of finding the level populations n(k). The rate of change of the population in level k is given by the equation

$$\frac{dn(k)}{dt} = -n(k)\sum_{k'}\left[R(k \rightarrow k') + C(k \rightarrow k')\right] + \sum_{k'} n(k')\left[R(k' \rightarrow k) + C(k' \rightarrow k)\right] \quad , \qquad (3.1)$$

which simply states that the rate of change in population of level k must be the sum of the radiative and collisional rates into level k minus the sum of those rates out of level k. We specify that the level populations be constant (statistical equilibrium), with the result that $dn(k)/dt = 0$.

We assume that electrons are always in thermal equilibrium because the electron density in a stellar atmosphere is sufficient to ensure very frequent electron-electron collisions. We therefore do not need to solve for the electron distribution, and we can simplify the consideration of any transition involving a free electron by integrating out the electron-energy dependence, assuming the Maxwell-Boltzmann distribution. For example, the rate for the recombination of a proton and an electron to a hydrogen atom is expressed in terms of the proton number density times the electron number density, not in terms of the electron density per unit energy. Consequently, we need to solve only for discrete levels.

Also, we can ignore scattering transitions since by definition they cancel from the statistical equilibrium equations.

In considering the radiative and collision rates, it is convenient to treat separately the upward and the downward transitions. We will derive the rates and then summarize the results at the end of this section.

Let us first consider an upward radiative transition, where k and k′ can be in the same or in different ions,

$$A(k) + h\nu \equiv A(\ell) + h\nu \rightarrow A(u) \equiv A(k') \quad ,$$

or

$$A(k) + h\nu \equiv A(\ell) + h\nu \rightarrow A(u) \equiv A^{+}(k') + e \quad .$$

Atoms in level k absorb

$$\int n(\ell) \int \alpha_{\nu}(\ell \rightarrow u)\, I_{\nu}\, d\omega\, d\nu = \int n(\ell)\, \alpha_{\nu}(\ell \rightarrow u)\, 4\pi J_{\nu}\, d\nu \quad \text{ergs/sec} \quad ,$$

which corresponds to absorbing

$$\int n(\ell)\, \alpha_{\nu}(\ell \rightarrow u)\, 4\pi \frac{J_{\nu}}{h\nu}\, d\nu \quad \text{photons/sec} \quad .$$

Since the lower level is bound, $n(\ell) \equiv n(k)$ and the rate is

$$n(k)\, R_{up}(k \rightarrow k') = n(k) \int \alpha_{\nu}(\ell \rightarrow u)\, 4\pi \frac{J_{\nu}}{h\nu}\, d\nu \quad . \tag{3.2}$$

Next we consider the downward transition, where k and k′ are in the same or different ions,

$$A(k) \equiv A(u) \rightarrow A(\ell) + h\nu = A(k') + h\nu \quad ,$$

or

$$A^{+}(k) + e \equiv A(u) \rightarrow A(\ell) + h\nu = A(k') + h\nu \quad .$$

The downward absorption rate is similar to the upward one,

$$\int n(u)\, \alpha_{\nu}(u \rightarrow \ell)\, 4\pi \frac{J_{\nu}}{h\nu}\, d\nu \quad ,$$

but there is also an emission rate,

$$\int n(u) \int \epsilon_{\nu}(u \rightarrow \ell) \frac{d\omega}{h\nu}\, d\nu$$

The total rate is thus

$$n(k)\, R_{down}(k \rightarrow k') = \int n(u) \left[\alpha_{\nu}(u \rightarrow \ell)\, 4\pi \frac{J_{\nu}}{h\nu} + \int \epsilon_{\nu}(u \rightarrow \ell) \frac{d\omega}{h\nu}\right] d\nu \quad .$$

This expression can be simplified by using equations (2.12) and (2.16) to reexpress $\alpha_{\nu}(u \rightarrow \ell)$ and $\epsilon_{\nu}(u \rightarrow \ell)$ in terms of $\alpha_{\nu}(\ell \rightarrow u)$,

$$n(k)\, R_{down}\, (k \rightarrow k') = \int n(u) \frac{g(k')}{g(k)}\, \alpha_{\nu}(\ell \rightarrow u) \left(\frac{4\pi J_{\nu}}{h\nu} + \frac{8\pi\nu^2}{c^2}\right) d\nu \quad .$$

The final step is to evaluate n(u). If k and k′ are in the same ion, the upper level is bound, so $n(u) \equiv n(k)$ and the rate is

$$n(k)\, R_{down}\, (k \rightarrow k') = n(k) \frac{g(k')}{g(k)} \int \alpha_{\nu}(\ell \rightarrow u) \left(\frac{4\pi J_{\nu}}{h\nu} + \frac{8\pi\nu^2}{c^2}\right) d\nu \quad . \qquad (3.3)$$

For k and k′ in different ions, the upper level is a continuum state of energy $E(u) = E(k') + h\nu$. Since the electrons are in thermal equilibrium, we have from the discussion in Section 2.2.F,

$$\frac{n(u)}{n(k)\, n_e} = \frac{(2\pi MkT/h^2)^{3/2}\, g(k)\, e^{-E(u)/kT}}{(2\pi MkT/h^2)^{3/2}\, g(k)\, (2\pi mkT/h^2)^{3/2}\, 2e^{-E(k)/kT}} \quad ,$$

or

$$n(u) = n(k)\, n_e \frac{1}{2} \left(\frac{h^2}{2\pi mkT}\right)^{3/2} e^{[E(k) - E(k')]/kT}\, e^{-h\nu/kT} \quad . \qquad (3.4)$$

Then,

$$R_{\text{down}}(k \rightarrow k') = \frac{n_e}{2} \left(\frac{h^2}{2\pi mkT}\right)^{3/2} \frac{g(k')}{g(k)} e^{[E(k) - E(k')]/kT}$$

$$\times \int a_\nu(\ell \rightarrow u)\, e^{-h\nu/kT} \left(\frac{4\pi J_\nu}{h\nu} + \frac{8\pi \nu^2}{c^2}\right) d\nu \quad . \tag{3.5}$$

For later reference, we define

$$\overline{R}(k \rightarrow k') = \int a_\nu(\ell \rightarrow u)\, e^{-h\nu/kT} \left(\frac{4\pi}{h\nu} J_\nu + \frac{8\pi \nu^2}{c^2}\right) d\nu \quad . \tag{3.6}$$

We note that for k and k′ in the same ion, equation (3.3) becomes

$$R_{\text{down}}(k \rightarrow k') = \frac{g(k')}{g(k)} e^{[E(k) - E(k')]/kT}\, \overline{R}(k \rightarrow k') \quad , \tag{3.7}$$

and for k and k′ in different ions, equation (3.5) becomes

$$R_{\text{down}}(k \rightarrow k') = \frac{n_e}{2} \left(\frac{h^2}{2\pi mkT}\right)^{3/2} \frac{g(k')}{g(k)} e^{[E(k) - E(k')]/kT}\, \overline{R}(k \rightarrow k') \quad . \tag{3.8}$$

In thermal equilibrium, equations (3.7) and (3.8) can be written

$$R_{\text{down}}(k \rightarrow k') = \frac{n(k')}{n(k)}\, \overline{R}(k \rightarrow k') \quad . \tag{3.9}$$

To find the upward collision rate by electrons, we integrate the cross section $Q(\ell \rightarrow u)$ over the Maxwell-Boltzmann distribution,

$$n(k)\, C_{\text{up}}(k \rightarrow k') = n(k)\, n_e \sqrt{\frac{8kT}{\pi m}} \int Q(\ell \rightarrow u)\, e^{-E/kT} \frac{E}{kT} \frac{dE}{kT} \quad . \tag{3.10}$$

The downward collision rate, in analogy to the downward radiative rate, is

$$n(k)\ C_{down}(k \rightarrow k') = n_e \sqrt{\frac{8kT}{\pi m}} \int n(u)\ Q(u \rightarrow \ell)\ e^{-E/kT}\ \frac{E}{kT}\ \frac{dE}{kT} \quad .$$

However, it is convenient to express the rate in terms of $Q(\ell \rightarrow u)$. As was the case for the radiative cross sections, the time-reversal argument dictates that the collision cross sections $Q(\ell \rightarrow u)$ and $Q(u \rightarrow \ell)$ be related by

$$\frac{Q(u \rightarrow \ell)}{g(k)} = \frac{Q(\ell \rightarrow u)}{g(k')} \quad , \tag{3.11}$$

but for collisions the two cross sections refer to different energies. If $Q(\ell \rightarrow u)$ is for energy E, $Q(u \rightarrow \ell)$ is for energy $E - [E(u) - E(k')]$. This energy shift results in the appearance of a Boltzmann factor $e^{[E(u) - E(k')]/kT}$ in the integral when equation (3.11) is substituted,

$$n(k)\ C_{down}(k \rightarrow k') = \frac{g(k')}{g(k)}\ n_e \sqrt{\frac{8kT}{\pi m}} \int n(u)\ e^{[E(u) - E(k')]/kT}\ Q(\ell \rightarrow u)\ e^{-E/kT}\ \frac{E}{kT}\ \frac{dE}{kT} \quad .$$

If k and k′ are in the same ion, then $n(u) \equiv n(k)$, so

$$C_{down}(k \rightarrow k') = \frac{g(k')}{g(k)}\ e^{[E(k) - E(k')]/kT}\ n_e \sqrt{\frac{8kT}{\pi m}} \int Q(\ell \rightarrow u)\ e^{-E/kT}\ \frac{E}{kT}\ \frac{dE}{kT} \quad . \tag{3.12}$$

We thus have a simple relation between C_{up} and C_{down},

$$g(k)\ C_{down}(k \rightarrow k')\ e^{-E(k)/kT} = g(k')\ C_{up}(k' \rightarrow k)\ e^{-E(k')/kT} \quad , \tag{3.13}$$

which we could have found easily by using a detailed balance argument. If k and k′ are in different ions, substituting equation (3.4) for n(u) (or detailed balance) yields the relation

$$g(k)\ C_{down}(k \rightarrow k')\ e^{-E(k)/kT} \left(\frac{2\pi mkT}{h^2}\right)^{3/2} \frac{2}{n_e} = g(k')\ C_{up}(k \rightarrow k')\ e^{-E(k')/kT} \quad . \tag{3.14}$$

Summary:

Upward rates, bound-bound and bound-free,

$$R_{up}(k \rightarrow k') = \int \alpha_\nu(\ell \rightarrow u)\ 4\pi \frac{J_\nu}{h\nu}\, d\nu \quad , \tag{3.2'}$$

$$C_{up}(k \rightarrow k') = n_e \sqrt{\frac{8kT}{\pi m}} \int Q(\ell \rightarrow u)\ e^{-E/kT} \frac{E}{kT} \frac{dE}{kT} \quad . \tag{3.10'}$$

Downward rates, bound-bound

$$R_{down}(k \rightarrow k') = \frac{g(k')}{g(k)} \int \alpha_\nu(\ell \rightarrow u) \left(\frac{4\pi J_\nu}{h\nu} + \frac{8\pi \nu^2}{c^2}\right) d\nu \tag{3.3'}$$

$$= \frac{g(k')}{g(k)}\, e^{[E(k) - E(k')]/kT}\, \overline{R}(k \rightarrow k') \quad , \tag{3.7}$$

$$C_{down}(k \rightarrow k') = \frac{g(k')}{g(k)}\, e^{[E(k) - E(k')]/kT}\, C_{up}(k' \rightarrow k) \quad . \tag{3.13'}$$

Downward rates, free-bound,

$$R_{down}(k \rightarrow k') = \frac{n_e}{2} \left(\frac{h^2}{2\pi mkT}\right)^{3/2} \frac{g(k')}{g(k)}\, e^{[E(k) - E(k')]/kT}$$

$$\times \int \alpha_\nu(\ell \rightarrow u)\ e^{-h\nu/kT} \left(\frac{4\pi J_\nu}{h\nu} + \frac{8\pi \nu^2}{c^2}\right) d\nu \tag{3.5}$$

$$= \frac{n_e}{2} \left(\frac{h^2}{2\pi mkT}\right)^{3/2} \frac{g(k')}{g(k)}\, e^{[E(k) - E(k')]/kT}\, \overline{R}(k \rightarrow k') \quad , \tag{3.8}$$

$$C_{down}(k \rightarrow k') = \frac{n_e}{2} \left(\frac{h^2}{2\pi mkT}\right)^{3/2} \frac{g(k')}{g(k)}\, e^{[E(k) - E(k')]/kT}\, C_{up}(k' \rightarrow k) \quad . \tag{3.14'}$$

3.2 Irrelevant Levels

Assuming we know the rates, we can, in principle, write down the statistical equilibrium equations for all levels. However, not all levels need to be considered explicitly. Closely spaced levels near a continuum have very large collision rates with each other and with the continuum. The collision rates are so high that the radiation field has a negligible effect, and since the electrons are in thermal equilibrium, they must force the levels into thermal equilibrium. Therefore, the collision rates between higher levels cancel from the equations (they are in detailed balance), and the higher level radiative terms drop out because they are negligible. The equations for the remaining levels, together with constraint equations, form a matrix equation that can be solved for the level populations. The first constraint is that the total number density is prescribed by the gas pressure $n_{total} = P_{gas}/kT$. The second is that the total number of atoms and ions of a given element must be a prescribed fraction of the total number of atoms and ions, since the element abundances are assumed to be constant. The third constraint is charge conservation.

We can also eliminate radiative transitions that have extremely high opacity if we are interested in a region where the optical depth is very large at frequencies that contribute significantly to the rate integrals. Because the opacity is very large, the source function given by

$$S_\nu = \frac{\Sigma\ \kappa_\nu(\ell \to u)\ (2h\nu^3/c^2)\ \{[n(\ell)/n(u)][g(u)/g(\ell)] - 1\}^{-1} + \sigma_\nu J_\nu}{\kappa_\nu + \sigma_\nu}$$

becomes

$$S_\nu \cong \frac{2h\nu^3}{c^2} \left[\frac{n(\ell)}{n(u)} \frac{g(u)}{g(\ell)} - 1 \right]^{-1} .$$

Since the optical depth is large, $J_\nu = S_\nu + (1/3)(d^2 S_\nu / d\tau_\nu^2)$ (eq. (2.76)); if it is "very large," $J_\nu \simeq S_\nu$, or

$$J_\nu = \frac{2h\nu^3}{c^2}\left[\frac{n(\ell)}{n(u)}\frac{g(u)}{g(\ell)} - 1\right]^{-1} .$$

The upward rate (eq. (3.1)) is

$$n(\ell)\int a_\nu(\ell\to u)\,\frac{8\pi\nu^2}{c^2}\left[\frac{n(\ell)}{n(u)}\frac{g(u)}{g(\ell)} - 1\right]^{-1} d\nu \quad ,$$

and the downward rate (3.3) can be transformed as follows:

$$\int n(u)\,\frac{g(\ell)}{g(u)}\,a_\nu(\ell\to u)\left\{\frac{8\pi\nu^2}{c^2}\left[\frac{n(\ell)}{n(u)}\frac{g(u)}{g(\ell)} - 1\right]^{-1} + \frac{8\pi\nu^2}{c^2}\right\} d\nu$$

$$= n(\ell)\int a_\nu(\ell\to u)\,\frac{8\pi\nu^2}{c^2}\,\frac{n(u)}{n(\ell)}\,\frac{g(\ell)}{g(u)}\left(\frac{1+\{[n(\ell)/n(u)][g(u)/g(\ell)]-1\}}{[n(\ell)/n(u)][g(u)/g(\ell)] - 1}\right)$$

$$= n(\ell)\int a_\nu(\ell\to u)\,\frac{8\pi\nu^2}{c^2}\left[\frac{n(\ell)}{n(u)}\frac{g(u)}{g(\ell)} - 1\right]^{-1} d\nu \quad .$$

In this case of very high optical depths, the rates are equal, so we can drop the transition from our equations. These radiative cancellations often occur, for example, for the Lyman lines and continuum of hydrogen, and even for the Balmer lines. See Peterson (1969) for a discussion of this and for the definition of "very large" optical depths.

3.3 When Are Detailed Calculations Necessary?

For many models we can calculate the total flux accurately even if we make the approximation that the number densities are given by the Boltzmann equation. At large optical depths for a main-sequence model, the densities are often high enough for collision rates to maintain thermal equilibrium in the level populations. This situation is called local thermodynamic equilibrium, or LTE. At small optical depths, this approximation may not, in fact, be valid. However, the total flux cannot be very much affected by conditions at small optical depths.

If the level populations are given by the Boltzmann equation, we can calculate ionization equilibria using the Saha equation without any knowledge of the radiation field, and since the source function becomes $S_\nu = [\kappa_\nu/(\kappa_\nu + \sigma_\nu)] B_\nu + [\sigma_\nu/(\kappa_\nu + \sigma_\nu)] J_\nu$, the calculation of the radiation field is decoupled from the calculation of the level populations and opacities. Therefore, in ATLAS, when pressures are calculated for a given temperature distribution, the ionization, the level populations, and the opacities are calculated at the same time. Then the radiation field is calculated and the temperature correction made. A number of iterations are performed over the whole process to get a self-consistent model.

Because LTE is usually assumed in model calculations, more elaborate statistical equilibrium calculations are introduced, when necessary, as a modification, not *ab initio*. At the end of each iteration, a statistical equilibrium calculation is made and fudge factors b(k) (called departure coefficients) are determined. These factors can be inserted into the Boltzmann equations, Saha equations, opacities, source functions, and rates in the next iteration of the model, as follows:

The Boltzmann equation becomes

$$\frac{n(k')}{n(k)} = \frac{b(k')}{b(k)} \frac{g(k')}{g(k)} e^{-[E(k') - E(k)]/kT} \quad ; \tag{3.15}$$

the Saha equation for ionization,

$$\frac{n(k')n_e}{n(k)} = \frac{b(k')}{b(k)} \frac{g(k')}{g(k)} \, 2 \left(\frac{2\pi mkT}{h^2}\right)^{3/2} e^{-[E(k') - E(k)]/kT} \quad ; \tag{3.16}$$

the partition function,

$$U = \Sigma \, b(k) \, g(k) \, e^{-E(k)/kT} \quad ; \tag{3.17}$$

the source function,

$$S_\nu(k'\rightarrow k) = \frac{2h\nu^3}{c^2}\left[\frac{b(k)}{b(k')}\, e^{h\nu/kT} - 1\right]^{-1} \quad ; \tag{3.18}$$

and the opacity,

$$\kappa_\nu(k\rightarrow k') = n(k)\, \alpha_\nu(\ell\rightarrow u)\, \frac{1 - [b(k')/b(k)]\, e^{-h\nu/kT}}{\rho} \quad . \tag{3.19}$$

The detailed balance principle from Section 2.2 becomes

$$\frac{n(A)}{b(A)}\frac{n(B)}{b(B)}\frac{n(C)}{b(C)} \cdots R(A\,B\,C \cdots \rightarrow 1\,2\,3 \cdots) = \frac{n(1)}{b(1)}\frac{n(2)}{b(2)}\frac{n(3)}{b(3)} \cdots R(1\,2\,3 \cdots \rightarrow A\,B\,C) \ , \tag{3.20}$$

so that we can express any rate in terms of the opposite rate, for example,

$$C(k\rightarrow k') = \frac{b(k)}{n(k)}\frac{n(k')}{b(k')}\, C(k'\rightarrow k) \quad . \tag{3.21}$$

Also, the downward radiative rate (3.9) becomes

$$R_{\text{down}}(k\rightarrow k') = \frac{b(k)}{n(k)}\frac{n(k')}{b(k')}\, \overline{R}\,(k\rightarrow k') \quad . \tag{3.22}$$

The statistical equilibrium equations for one element can be transformed from the number density form to the "b" form as follows. Starting with

$$n(k)\sum\left[R(k\rightarrow k') + C(k\rightarrow k')\right] = \sum n(k')\left[R(k'\rightarrow k) + C(k'\rightarrow k)\right] \quad ,$$

the equilibrium equations in terms of up and down rates are

$$n(k)\left\{\sum_{k'<k}\left[R_{\mathrm{down}}(k\to k') + C_{\mathrm{down}}(k\to k')\right] + \sum_{k'>k}\left[R_{\mathrm{up}}(k\to k') + C_{\mathrm{up}}(k\to k')\right]\right\}$$

$$= \sum_{k'>k} n(k')\left[R_{\mathrm{down}}(k'\to k) + C_{\mathrm{down}}(k'\to k)\right] + \sum_{k'<k} n(k')\left[R_{\mathrm{up}}(k'\to k) + C_{\mathrm{up}}(k'\to k)\right] \quad .$$

Expressing R_{down} in terms of $\overline{R}$ and C_{down} in terms of C_{up} and dividing through by $n(k)$, we find

$$\sum_{k'<k}\frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\left[\overline{R}(k\to k') + C_{\mathrm{up}}(k'\to k)\right] + \sum_{k'>k}\left[R_{\mathrm{up}}(k\to k') + C_{\mathrm{up}}(k\to k')\right]$$

$$= \sum_{k'>k}\frac{n(k')}{n(k)}\,\frac{b(k')}{b(k)}\,\frac{n(k)}{n(k')}\left[\overline{R}(k'\to k) + C_{\mathrm{up}}(k\to k')\right] + \sum_{k'<k}\frac{n(k')}{n(k)}\left[R_{\mathrm{up}}(k'\to k) + C_{\mathrm{up}}(k'\to k)\right] \quad .$$

Then,

$$\sum_{k'<k}\frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\left[\overline{R}(k\to k') + C_{\mathrm{up}}(k'\to k)\right] + \sum_{k'>k}\left[R_{\mathrm{up}}(k\to k') + C_{\mathrm{up}}(k\to k')\right]$$

$$= \sum_{k'>k}\frac{b(k')}{b(k)}\left[\overline{R}(k'\to k) + C_{\mathrm{up}}(k\to k')\right] + \sum_{k'<k}\frac{b(k')}{b(k)}\,\frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\left[R_{\mathrm{up}}(k'\to k) + C_{\mathrm{up}}(k'\to k)\right] \quad .$$

Finally,

$$b(k)\left\{\sum_{k'<k}\frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\left[\overline{R}(k\to k') + C_{\mathrm{up}}(k'\to k)\right] + \sum_{k'>k}\left[R_{\mathrm{up}}(k\to k') + C_{\mathrm{up}}(k\to k')\right]\right\}$$

$$= \sum_{k'>k} b(k')\left[\overline{R}(k'\to k) + C_{\mathrm{up}}(k\to k')\right] + \sum_{k'<k} b(k')\,\frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\left[R_{\mathrm{up}}(k'\to k) + C_{\mathrm{up}}(k'\to k)\right] \quad , \tag{3.23}$$

where [b(k)/b(k′)] [n(k′)/n(k)] is given by either equation (3.15) or equation (3.16), as appropriate.

The b(k) factors have been defined only by ratios. For normalization we require that the highest energy level have b(k) = 1. For example, the proton is the highest hydrogen energy level, so b(p) = 1.

3.4 Statistical Equilibrium in ATLAS

The subroutine that performs the equilibrium calculations is a considerably modified version of one written by Peterson (1969). It finds the b(k) factors for H and H^- but assumes that the number densities of all other species are independent of the radiation field. Detailed equilibrium calculations for other species cannot significantly affect the flux in regions where H or H^- (or Rayleigh scattering or electron scattering) is the dominant opacity. For stars of spectral types from early B through G, these are the principal opacities at frequencies where most of the flux appears. Therefore, statistical equilibrium for H and H^- should be sufficient to determine the surface flux for a large number of stars. At other frequencies, such as in a strong metal continuum in the far ultraviolet, it may be necessary to perform detailed calculations for the metal if the surface flux must be accurately determined. It is a relatively simple matter to modify ATLAS to do statistical equilibrium for any species.

3.5 Computing Statistical Equilibrium for Hydrogen

The hydrogen calculations leave out all the bound-bound radiative transitions on the assumption that the radiative rates cancel for the stronger lines and that the weaker lines have a negligible effect on the level populations compared to the effect of the collisional transition. The radiative rates for the Lyman continuum are also assumed to cancel. The levels above 6 are assumed to have b(k) = 1, and collision rates to and from bound levels higher than 8 are assumed to be inconsequential.

The assumptions concerning the strong lines are obviously not valid at small optical depths in the atmosphere, where the line cores are formed. The bound-bound rates must be included in the equilibrium equations in order to calculate the line cores.

However, line wings and the continuum are formed at depths in the atmosphere where the optical depths in the line cores are in the thousands, so the approximation is valid for computing the line wing and continuum fluxes.

The statistical equilibrium equations (3.23) for hydrogen take the form

$$b(k)\left[R_{up}(k\rightarrow p) + C_{up}(k\rightarrow p) + \sum_{k'=1}^{k} \frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\,C_{up}(k'\rightarrow k)\right.$$

$$\left. + \sum_{k'=k}^{8} C_{up}(k\rightarrow k')\right] = b(p)\left[\overline{R}(p\rightarrow k) + C_{up}(k\rightarrow p)\right]$$

$$+ \sum_{k'=1}^{k} b(k')\,\frac{b(k)}{b(k')}\,\frac{n(k')}{n(k)}\,C_{up}(k'\rightarrow k) + \sum_{k'=k}^{8} b(k')\,C_{up}(k\rightarrow k') \quad .$$

Setting b(7), b(8), and b(p) = 1 and substituting them into equation (3.15), we obtain

$$b(k)\left[R_{up}(k\rightarrow p) + C_{up}(k\rightarrow p) + \sum_{k'=1}^{k} \frac{g(k')}{g(k)}\,e^{-[E(k') - E(k)]/kT}\,C_{up}(k'\rightarrow k)\right.$$

$$\left. + \sum_{k'=k}^{8} C_{up}(k\rightarrow k')\right] - \sum_{k'=1}^{k} b(k')\,\frac{g(k')}{g(k)}\,e^{-[E(k') - E(k)]/kT}\,C_{up}(k'\rightarrow k)$$

$$- \sum_{k'=k}^{6} b(k')\,C_{up}(k\rightarrow k')$$

$$= \overline{R}(p\rightarrow k) + C_{up}(k\rightarrow p) + C_{up}(k\rightarrow 7) + C_{up}(k\rightarrow 8) \quad . \tag{3.24}$$

This system of six equations is easily solved for the b(k)'s once the rates have been calculated.

We will discuss the hydrogen cross sections a_ν in Section 5. The collision cross sections $Q(k \rightarrow k')$ (from Peterson, 1969) are

$$4 f_{kk'} \gamma_{kk'}^{-2} \left[\frac{\ln E/E_{kk'}}{E/E_{kk'}} + \frac{0.148}{(E/E_{kk'})^6} \right] \pi a_0^2 \ , \qquad k' > k \ , \tag{3.25}$$

where $f_{kk'}$ is the transition probability, $\gamma_{kk'} = k^{-2} - k'^{-2}$, $E_{kk'} = E(p)\,\gamma_{kk'}$, and a_0 is the atomic radius. The collision rate coefficient is

$$C_{up}(k \rightarrow k') = n_e \, \pi a_0^2 \sqrt{\frac{8kT}{\pi m}} \, 4 f_{kk'} \gamma_{kk'}^{-2}$$

$$\times \frac{E_{kk'}}{kT} \left[E_1 \left(\frac{E_{kk'}}{kT} \right) + 0.148 \left(\frac{E_{kk'}}{kT} \right) E_5 \left(\frac{E_{kk'}}{kT} \right) \right] \ , \tag{3.26}$$

and the ionization rate coefficient is

$$C_{up}(k \rightarrow p) = n_e \, \pi a_0^2 \sqrt{\frac{8kT}{\pi m}} \, k^3 \, e^{-[E(p) - E(k)]/kT} \ . \tag{3.27}$$

3.6 The Negative Hydrogen Ion

Up to this point, we have ignored the fact that there are processes affecting the level populations other than electron collisions and radiative transitions. There are various heavy-body reactions, including molecule formation. If we consider hydrogen in a stellar atmosphere at temperatures high enough so that molecules are not important, these processes have negligible effect. But for H^-, these reactions dominate the rates, especially since H^- repels electrons.

We have taken reaction rates from Lambert and Pagel (1968) for electron collisions,

$$n(H^-) \, C(H^- + e \rightarrow H + 2e) = n(H^-) \, n_e \, 10^{-8.7} \left(\frac{5040}{T} \right)^{3/2} \ ,$$

where H refers to the ground state of hydrogen, and for charge cancellation,

$$n(H^-)\ n(p)\ C\left[H^- + p \rightarrow H + H(n>1)\right] = n(H^-)\ n(p)\ 10^{-7}\ 4\left(\frac{5040}{T}\right)^{1/3} ,$$

where $H(n>1)$ refers to some excited state of hydrogen near the continuum, which we assume to be in LTE, so that $n[H(n>1)] = n(p)\ n_e f(T)$. From Browne and Dalgarno (1969), we have taken the associative detachment rate

$$n(H^-)\ n(H)\ C(H^- + H \rightarrow H_2 + e) = n(H^-)\ n(H)\ 10^{-8.7}$$

and ignored atomic collisional detachment, as they recommend We have assumed that the levels of H_2 are populated according to the Boltzmann equation, which implies that $n(H_2)$ is related to $n(H)^2$ by a Saha equation

The statistical equilibrium equation is

$$\begin{aligned}
&n(H^-)\ R(H^- + h\nu \rightarrow H + e) + n(H^-)\ n(H)\ C(H^- + H \rightarrow H_2 + e)\\
&\quad + n(H^-)\ n(p)\ C[H^- + p \rightarrow H + H(n>1)] + n(H^-)\ C(H^- + e \rightarrow H + 2e)\\
&= n(H)\ R(H + e \rightarrow H^- + h\nu) + n(H)^2\ C(H_2 + e \rightarrow H^- + H)\\
&\quad + n(H)\ n[H(n>1)]\ C[H + H(n>1) \rightarrow H^- + p] + n(H)\ C(H + 2e \rightarrow H^- + e) \quad .
\end{aligned}$$

Using the detailed-balance relation (3.20) to express both sides of the equation with the same rate coefficients, we find

$$\begin{aligned}
&n(H^-)\ R(H^- + h\nu \rightarrow H + e) + n(H^-)\ n(H)\ C(H^- + H \rightarrow H_2 + e)\\
&\quad + n(H^-)\ n(p)\ C[H^- + p \rightarrow H + H(n>1)] + n(H^-)\ C(H^- + e \rightarrow H + 2e)\\
&= \frac{b(H)}{b(H^-)}\ n(H^-)\ \bar{R}(H + e \rightarrow H^- + h\nu) + \frac{b(H)}{b(H^-)}\ n(H^-)\ n(H)\ C(H^- + H \rightarrow H_2 + e)\\
&\quad + \frac{b(H)}{b(H^-)}\ n(H^-)\ n(p)\ C[H^- + p \rightarrow H + H(n>1)] + \frac{b(H)}{b(H^-)}\ n(H^-)\ C(H^- + e \rightarrow H + 2e) \quad .
\end{aligned}$$

The solution for $b(H^-)$ is

$$b(H^-) = b(H)\ \{\bar{R}(H + e \rightarrow H^- + h\nu) + n(H)\ C(H^- + H \rightarrow H_2 + e)$$

$$+ n(p)\ C[H^- + p \rightarrow H + H(n > 1)] + C(H^- + e \rightarrow H + 2e)\}\Big/$$

$$\{R(H^- + h\nu \rightarrow H + e) + n(H)\ C(H^- + H \rightarrow H_2 + e)$$

$$+ n(p)\ C[H^- + p \rightarrow H + H(n > 1)] + C(H^- + e \rightarrow H + 2e)\} \quad .$$

Since the b factors for these reactions are defined only by ratios, b(H) is taken as unity, so the Saha equation for H^- becomes

$$\frac{n(H)\, n_e}{n(H^-)} = \frac{g(H)\, g_e}{b(H^-)\, g(H^-)} \left(\frac{2\pi\, mkT}{h^2}\right)^{3/2} e^{-0.7552\ ev/kT} \quad ,$$

where

$$g(H) = 2 \quad , \qquad g_e = 2 \quad , \qquad \text{and} \qquad g(H^-) = 1 \quad .$$

3.7 Computational Note

In the statistical equilibrium calculations for H and H^-, the integrals R, $\bar{R}$, and $d\bar{R}/dT$ are computed assuming that J_ν and α_ν are temperature insensitive. After the temperature correction has been made, $\bar{R}$ is corrected by the factor $d\bar{R}/dT\ \Delta T$. The collision rates are calculated with the new temperature distribution, and the matrix equations are set up and solved for the b's. These b's are used in the next iteration of the model to calculate populations, opacities, and source functions.

4. THERMODYNAMIC QUANTITIES

4.1 Gas and Turbulent Pressures

The motion of an atmospheric mass element is described by the equation

$$\rho \frac{d^2x}{dt^2} = - \frac{dP_{total}}{dx} - \rho g \quad , \tag{4.1}$$

where the surface gravity $g = GM_*/R_*^2$ is presumed to be constant since the atmosphere is thin and contains little mass. We assume that the atmosphere is in steady state and that any motions of the gas are random. We ignore convection when discussing pressure.

Since there is no net acceleration, the pressure-balance, or hydrostatic-equilibrium, equation becomes

$$\frac{dP_{total}}{dx} = - g\rho \tag{4.2}$$

or

$$\frac{dP_{total}}{dM} = g \quad , \tag{4.3}$$

with the boundary condition $P_{total} = P_{rad} = 0$ at $M = 0$. Then,

$$P_{total} = gM \quad . \tag{4.4}$$

We identify three components of the total pressure: the gas pressure P, the radiation pressure P_{rad} discussed in Section 2.11, and a turbulent pressure P_{turb}, which is caused by random motion of small gas elements, if such motions exist. Then,

$$P = P_{total} - P_{rad} - P_{turb} \quad , \tag{4.5}$$

where P_{rad} and P_{turb} are the values found in the previous iteration of the model.

Turbulent pressure is included in ATLAS mainly to give qualitative estimates of turbulent effects, if such effects exist. We define

$$P_{turb} = \frac{1}{2} \rho v_{turb}^2 \quad , \tag{4.6}$$

where v_{turb} is a velocity describing the turbulent elements. Arbitrary velocities can be described in the form

$$v_{turb} = A + B\, v_{sound} + C\, \rho^D \tag{4.7}$$

and are computed once v_{sound} has been found as described in Section 4.6. The corresponding turbulent pressure is carried over to the next iteration.

For most models, turbulent pressure is ignored.

4.2 Calculation of the Pressure When $T(\tau)$ or $T(x)$ is Prescribed

If we have an initial $T(\tau)$, where τ is any monochromatic or mean optical depth, or an initial $T(x)$ but do not know $T(M)$, we must go through considerable calculation to find P_{total} and $T(M) = T(P_{total}/g)$. For example, we might have an initial $T(\tau)$ if we scale a temperature distribution from a previous model, as described in Section 2.12. Or we might have an observational determination of $T(\tau)$ or $T(x)$. In either case, we have to integrate the pressure-balance equation (4.2) numerically:

$$\frac{dP_{total}}{dx} = -g\rho \tag{4.8}$$

or

$$\frac{dP_{\text{total}}}{d\tau} = \frac{g}{\kappa} \quad . \tag{4.9}$$

We describe here an integration scheme for $dP_{\text{total}}/d\tau$ that is implemented in ATLAS. A similar scheme could easily be divised for dP_{total}/dx.

The integration starts by prescribing $T(\tau)$, $P_{\text{rad}}(\tau)$, and $P_{\text{turb}}(\tau)$. If either P_{rad} or P_{turb} is not known, it is ignored. A guess is made for κ at a τ near the surface. The differential equation is solved for P_{total} at that depth, and the corresponding gas pressure determined. From P and T we find a new κ, either by computing number densities and cross sections or by interpolating in a table of opacity as a function of T and P. Iteration continues on P_{total} and κ until they are consistent to some specified maximum error. Then the differential equation is used to extrapolate a guess for the pressure at a point farther into the atmosphere. The whole procedure is repeated until the pressure is known all the way through the atmosphere.

The details of the integration are as follows: Since the P's and τ change by many orders of magnitude in going from the top to the bottom of the atmosphere, it is convenient to convert to the logarithmic derivative,

$$\frac{dP_{\text{total}}}{d\tau} = \frac{P_{\text{total}}}{\tau} \frac{d \ln P_{\text{total}}}{d \ln \tau} = \frac{g}{\kappa}$$

or

$$\frac{d \ln P_{\text{total}}}{d \ln \tau} = \frac{g\tau}{\kappa P_{\text{total}}} \quad . \tag{4.10}$$

We choose τ points at uniform intervals in $\ln \tau$ to maintain simple expressions for integration and extrapolation, and we specify T, P_{rad}, and P_{turb} at each point, by interpolation if necessary.

There are three regions where different forms of integration are used. The first is from $\tau = 0$ to the first τ. We assume that κ is constant in this region and use the simple difference equation

$$P_1^{total} - 0 = (\tau_1 - 0) \frac{g}{\kappa_1} \quad . \tag{4.11}$$

Then,

$$P_1 = P_1^{total} - P_1^{rad} - P_1^{turb}$$

and

$$\kappa_1 = \kappa_1(P_1, T_1) \quad .$$

We continue to iterate on κ until $|\ln P_{total}^{new} - \ln P_{total}^{old}| \leq 0.00005$.

For the next three points, we switch to the logarithmic difference equation

$$\Delta \ln P_{total} = \ln P_j^{total} - \ln P_{j-1}^{total} = \frac{g \tau_j}{\kappa_j P_j^{total}} \Delta \ln \tau \quad . \tag{4.12}$$

Our first guess for the pressure is

$$\ln P_j^{total} = \ln P_{j-1}^{total} + \Delta \ln P_{j-1}^{total} \quad . \tag{4.13}$$

The iteration equations are

$$P_j = P_j^{total} - P_j^{rad} - P_j^{turb} \quad ,$$

$$\kappa_j = \kappa_j(P_j, T_j) \quad ,$$

and

$$\Delta \ln P_j^{total} = \frac{g \tau_j}{\kappa_j P_j^{total}} \Delta \ln \tau \quad .$$

Once we have obtained the first four points, we use a much more sophisticated scheme, called Hamming's predictor-corrector method (Carnahan, Luther, and Wilkes, 1969). If we consider a function in the interval (x_{n-3}, x_{n+1}), we can fit interpolating functions to fourth order. Since we know the value f_n, we can predict f_{n+1},

$$f_{n+1} = f_{n-3} + \frac{4}{3} \Delta x (2f'_n - f'_{n-1} + 2f'_{n-2}) + \frac{14}{45} (\Delta x)^5 f^V \quad , \qquad \text{for } f^V_{in}(x_{n-3}, x_{n+1}) . \quad (4.14)$$

Hamming also fitted f with the function

$$f_{n+1} = \frac{9}{8} f_n - \frac{1}{8} f_{n-2} + \frac{3}{8} \Delta x(f'_{n+1} + 2f'_n - f'_{n-1}) - \frac{1}{40} (\Delta x)^5 f^V \quad , \qquad \text{for } f^V_{in}(x_{n-2}, x_{n+1}) \ , \quad (4.15)$$

which can be computed, after use of the prediction for f_{n+1}, to evaluate f'_{n+1}. If f^V is specified constant in the interval (x_{n-3}, x_{n+1}), we can eliminate f^V by combining the two expressions for f_{n+1} to obtain a still better value for f_{n+1}. The result is

$$f_{n+1} = \frac{126f_n - 14f_{n-2} + 9f_{n-3} + \Delta x (42f'_{n+1} + 108f'_n - 54f'_{n-1} + 24f'_{n-2})}{121} \quad . \quad (4.16)$$

Putting the pressure equation into these formulas yields for the guess,

$$\ln P^{total}_j = \frac{3 \ln P^{total}_{j-4} + 8 \Delta \ln P^{total}_{j-1} - 4 \Delta \ln P^{total}_{j-2} + 8 \Delta \ln P^{total}_{j-3}}{3} \quad , \quad (4.17)$$

and for the iteration equation,

$$\ln P^{total}_j = \Big(126 \ln P^{total}_{j-1} - 14 \ln P^{total}_{j-3} + 9 \ln P^{total}_{j-4} + 42 \Delta \ln P^{total}_j$$

$$+ 108 \Delta \ln P^{total}_{j-1} - 54 \Delta \ln P^{total}_{j-2} + 24 \Delta \ln P^{total}_{j-3}\Big) \Big/ 121 \quad . \quad (4.18)$$

Once the pressure is known, rhox is found from equation (4.4).

4.3 Ionization and Molecular Equilibrium Equations

Although we need explicitly only those number densities that affect opacities, others must be considered because of their indirect effects. If ionization is involved, we have to find the number densities of all species that contribute a significant number of electrons. For molecules, we have to know what other molecules compete for the atoms available.

To calculate the equilibrium number densities, we set up as many equations as there are constraints. The first constraint is abundance – the total number density of atoms of each element must be a prescribed fraction of the total number of atoms, n_A. As an example, for a hydrogen-helium atmosphere with abundances X_H and X_{He}, we might write the equations, including most of the species possible, as

$$n(\mathrm{H\ I}) + n(\mathrm{H\ II}) + 2n(\mathrm{H_2}) + 2n(\mathrm{H_2^+}) + n(\mathrm{H^-}) = X_H n_A \tag{4.19}$$

and

$$n(\mathrm{He\ I}) + n(\mathrm{He\ II}) + n(\mathrm{He\ III}) = X_{He} n_A \quad . \tag{4.20}$$

When other elements are included in the atmosphere, there are also cross terms linking the abundance equations. The hydrogen equation would have n(CH), n(NH), n(OH), etc.; the carbon equation, n(CH); the nitrogen equation, n(NH); the oxygen equation, n(OH), etc.

The second constraint is charge conservation. For the same example of a hydrogen-helium atmosphere, we must have

$$n(\mathrm{H\ II}) + n(\mathrm{H_2^+}) + n(\mathrm{He\ II}) + 2n(\mathrm{He\ III}) - n(\mathrm{H^-}) - n_e = 0 \quad . \tag{4.21}$$

The last constraint is that the total number of particles is $n_{total} = P/kT$,

$$\begin{aligned} n(\mathrm{H\ I}) &+ n(\mathrm{H\ II}) + n(\mathrm{H_2}) + n(\mathrm{H_2^+}) + n(\mathrm{H^-}) + n(\mathrm{He\ I}) + n(\mathrm{He\ II}) \\ &+ n(\mathrm{He\ III}) + n_e = n_{total} \quad . \end{aligned} \tag{4.22}$$

Each term in the equilibrium equations can be written as a function of neutral atom and electron number densities by means of a Saha equation (see Sections 2.2, 3.3, and 4.4). Some examples for the abundance equation for hydrogen follow:

$$n(\mathrm{H_2}) = n(\mathrm{H\ I})\, n(\mathrm{H\ I}) \frac{U(\mathrm{H_2})[2\pi M(\mathrm{H_2})kT/h^2]^{3/2}}{\{U(\mathrm{H\ I})[2\pi M(\mathrm{H\ I})kT/h^2]^{3/2}\}^2}\, e^{-[E(\mathrm{H_2})-E(\mathrm{H\ I})]/kT} , \qquad (4.23)$$

$$n(\mathrm{H\ II}) = \frac{n(\mathrm{H\ I})}{n_e} \frac{U_e(2\pi mkT/h^2)^{3/2}\, U(\mathrm{H\ II})[2\pi M(\mathrm{H\ II})kT/h^2]^{3/2}}{U(\mathrm{H\ I})[2\pi M(\mathrm{H\ I})kT/h^2]^{3/2}}\, e^{-[E(\mathrm{H\ II})-E(\mathrm{H\ I})]/kT} , \qquad (4.24)$$

$$n(\mathrm{H_2^+}) = \frac{n(\mathrm{H\ I})\, n(\mathrm{H\ I})}{n_e} \frac{U_e(2\pi mkT/h^2)^{3/2}\, U(\mathrm{H\ II})[2\pi M(\mathrm{H\ II})kT/h^2]^{3/2}}{\{U(\mathrm{H\ I})[2\pi M(\mathrm{H\ I})kT/h^2]^{3/2}\}^2}\, e^{-[E(\mathrm{H_2^+}-E(\mathrm{H\ I})]/kT} , \qquad (4.25)$$

$$n(\mathrm{H^-}) = n(\mathrm{H\ I})\, n_e \frac{U(\mathrm{H^-})[2\pi M(\mathrm{H^-})kT/h^2]^{3/2}}{U(\mathrm{H\ I})[2\pi M(\mathrm{H\ I})kT/h^2]^{3/2}\;\; U_e(2\pi mkT/h^2)^{3/2}}\, e^{-[E(\mathrm{H^-})-E(\mathrm{H\ I})]/kT} , \qquad (4.26)$$

where $U(\mathrm{H\ II}) = 1$, $U_e = 2$, and $M(\mathrm{H\ I}) \cong M(\mathrm{H\ II}) \cong M(\mathrm{H^-})$, and where $E(\mathrm{H_2}) < E(\mathrm{H^-}) < E(\mathrm{H\ I}) < E(\mathrm{H_2^+}) < E(\mathrm{H\ II})$. The evaluation of such Saha equations will be discussed in Section 4.4. We solve the resulting equilibrium equations for the number densities of neutral atoms, for n_A, and for n_e. Once these values have been obtained, any other number density can be found through use of the appropriate Saha equation.

Since the equilibrium equations are not linear, their solution requires an iteration process. In ATLAS a Newton-Raphson technique is used (Carnahan et al., 1969). We specify which atoms, ions, and molecules are to be considered. Then ATLAS writes the equations in the form

$$
\begin{aligned}
&f_{total}\,(n_A, n_H, n_{He}, \ldots, n_e) = 0 \quad , \\
&f_H\,(n_A, n_H, n_{He}, \ldots, n_e) = 0 \quad , \\
&f_{He}\,(n_A, n_H, n_{He}, \ldots, n_e) = 0 \quad , \\
&\quad \vdots \\
&f_e\,(n_A, n_H, n_{He}, \ldots, n_e) = 0 \quad ,
\end{aligned}
\tag{4.27}
$$

and analytically calculates a matrix in which each element is the derivative of each equation with respect to each variable,

$$
\frac{\partial f_i}{\partial n_j} = \begin{pmatrix}
\frac{\partial f_{total}}{\partial n_A} & \frac{\partial f_{total}}{\partial n_H} & \cdots & \frac{\partial f_{total}}{\partial n_e} \\
\frac{\partial f_H}{\partial n_A} & \frac{\partial f_H}{\partial n_H} & \cdots & \frac{\partial f_H}{\partial n_e} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_e}{\partial n_A} & \frac{\partial f_e}{\partial n_H} & \cdots & \frac{\partial f_e}{\partial n_e}
\end{pmatrix} \quad . \tag{4.28}
$$

After making a first guess for the number densities n_i, ATLAS puts them into the equations and the matrix. In general, the guess will be off, so the equations have nonzero values. A first-order correction is obtained from the first-order matrix equation

$$
\sum_j \frac{\partial f_i}{\partial n_j} \Delta_j = f_i \quad , \tag{4.29}
$$

which is solved by Gauss-Jordan elimination (Carnahan et al., 1969). The new number densities are $n_i - \Delta_i$. Iteration continues until the relative change is below 0.0001.

For two special cases, there are faster ways to solve the equilibrium equations than the matrix method just described. If the molecules to be considered and their approximate number densities can be specified in advance, the equilibrium equations can be ordered and transformed for an iterative solution that treats the equations one at a time. However, such a scheme requires considerable revision when new molecules are added or when physical conditions change, so the initial guess for the number densities is no longer valid. The matrix method described above has no such shortcomings.

The second case is when the temperatures in the models are high enough so that molecules are not important in the equation of state. Then $n_{total} = n_A + n_e$, and there are no cross terms linking the abundance equations, so a simple iterative scheme can be used to find the electron number. Once the electron number is known, any atom or ion number can be found by using the electron number to evaluate each term in the appropriate abundance equation and then solving the abundance equation for each ion.

The iteration proceeds as follows: We guess an electron number n_e and find $n_A = n_{total} - n_e$. We go through the abundance equations (in any order) one element at a time. Each equation has the form

$$n(Q) + n(Q^+) + n(Q^{++}) + \cdots = X_Q n_A \quad . \tag{4.30}$$

We write the Saha equations in terms of n(Q) and the provisional value of n_e,

$$n(Q^+) = \frac{n(Q)}{n_e} \, \mathcal{E} \tag{4.31}$$

and

$$n(Q^{++}) = \frac{n(Q^+)}{n_e} \, \mathcal{E}' = \frac{n(Q)}{n_e} \, \mathcal{E} \, \frac{\mathcal{E}'}{n_e} \quad , \quad \text{etc.,} \tag{4.32}$$

which we substitute into the abundance equation,

$$n(Q) + \frac{n(Q)}{n_e}\,\mathcal{E} + \frac{n(Q)}{n_e}\,\mathcal{E}\,\frac{\mathcal{E}'}{n_e} + \cdots = X_Q n_A \quad . \tag{4.33}$$

We solve for n(Q) and use the Saha equations to find $n(Q^+)$, $n(Q^{++})$, etc. We evaluate the charge-conservation equation as we go by adding

$$1n(Q^+) + 2n(Q^{++}) + 3n(Q^{+++}) + \cdots$$

electrons for each element. Once we have evaluated all the abundance equations, the charge equation yields a new value for n_e, which we use as the basis for the next iteration. Convergence can be speeded by averaging the old and the new values for n_e.

4.4 Evaluating Saha Equations

Several different methods are used to evaluate Saha equations in ATLAS. For the equilibrium equations described in Section 4.3, where every number density is written in terms of neutral atoms and electrons, the Saha equation has the general form

$$n^{k+}_{123\cdots m} = \frac{n_1 n_2 n_3 \cdots n_m}{n_e^k}\,\mathcal{E} \quad , \tag{4.34}$$

where

$$\mathcal{E} = \frac{U(n^{k+}_{123})(2\pi M_{123}kT/h^2)^{3/2}[2(2\pi mkT/h^2)^{3/2}]^k}{U_1(2\pi M_1 kT/h^2)^{3/2}\cdots U_m(2\pi M_m kT/h^2)^{3/2}}\; e^{-[E(n^{k+}_{123})-E_1-E_2\cdots-E_m]/kT} \quad .$$

Here, n^{k+}_{123} has m atoms and k positive charges. In a negative molecule, the electron is counted with the atoms. The examples given in Section 4.3 illustrate the general expression. The function $\mathcal{E}$ is evaluated either by finding each partition function as described later or by approximating all the partition functions by one polynomial, as described next.

If we assume that the partition functions are independent of the gas density and the radiation field and that the dissociation energy is independent of gas density, then $\mathcal{E}$ is a function only of the temperature, so it can be approximated by an expression of the form

$$\mathcal{E}(T) = \exp\left[\frac{a}{kT_{ev}} - b + cT - dT^2 + eT^3 - fT^4 - \frac{3}{2}(m - 1 - k)\ln T\right], \qquad (4.35)$$

where

$$a = -\left[E\left(n^{k+}_{123\cdots m}\right) - E_1 - E_2 \cdots - E_m\right] .$$

Note that a is positive for neutral and negatively charged molecules because they have lower energies than do free atoms. In the following pages, we tabulate coefficients for an initial set of $\mathcal{E}$'s, which we found by least-squares fitting the tables by McBride, Heimel, Ehlers, and Gordon (1963). The fit is accurate to better than 1% for $1000\ \mathrm{K} \lesssim T \lesssim 6000\ \mathrm{K}$ and to 1 or 2% as T approaches 500 K. The accuracy of the equilibrium constant itself may be considerably worse because of a large uncertainty in the dissociation energy. Many of the molecules tabulated do not play a significant role in stellar atmospheres.

The code for identifying atoms and molecules is as follows: The atomic number for each component is treated as a base 100 digit, and the digits are ordered increasing from left to right to form a number. An electron component, as in H^-, is written 00 and ordered as 100. The positive charge is written after the decimal point, for example, 2.02 = He^{++} = He III. An example from the table is 608. = CO.

The alternative method for evaluating the Saha equation is to compute each partition function separately. This has the advantage that the dependence of the partition function on the gas density and on the radiation field can be treated explicitly. For this reason, Saha equations for atoms and ions are normally treated by a separate subroutine that tabulates or computes partition functions for all ions through H II, He III, Li IV to C IV, N V, O VI to S VI, Cl V to Ni V, and Cu III to Es III. This subroutine can also solve the abundance equation for an element in order to find the number density for each ion.

CODE	A	B	C	D	E	F
101.0	4.477	4.6628E+01	1.8031E-03	5.0239E-07	8.1424E-11	5.0501E-15
103.0	2.429	4.4942E+01	2.2453E-03	5.5182E-07	8.0615E-11	4.7616E-15
104.0	2.211	4.3816E+01	1.9892E-03	4.9231E-07	7.3716E-11	4.4348E-15
105.0	3.001	4.6403E+01	1.8826E-03	4.6424E-07	6.9646E-11	4.1526E-15
106.0	3.470	4.5506E+01	1.7112E-03	3.6319E-07	5.0164E-11	2.8716E-15
107.0	3.699	4.5244E+01	1.8435E-03	4.9000E-07	7.7353E-11	4.7639E-15
108.0	4.395	4.5746E+01	1.7004E-03	4.4905E-07	7.0861E-11	4.3648E-15
109.0	5.844	4.6618E+01	1.5382E-03	4.0410E-07	6.4407E-11	3.9816E-15
111.0	2.050	4.4709E+01	2.4163E-03	6.1037E-07	9.0492E-11	5.3705E-15
112.0	1.999	4.3437E+01	2.2153E-03	5.4885E-07	8.1160E-11	4.8026E-15
113.0	2.901	4.5688E+01	1.8402E-03	4.1240E-07	5.7606E-11	3.2768E-15
114.0	3.190	4.4770E+01	1.6858E-03	3.7373E-07	5.0857E-11	2.8282E-15
115.0	3.300	4.4680E+01	1.8959E-03	4.6737E-07	6.8061E-11	4.0256E-15
116.0	3.530	4.5272E+01	1.8600E-03	4.7327E-07	7.1690E-11	4.3041E-15
117.0	4.431	4.5886E+01	1.5637E-03	3.9598E-07	6.2107E-11	3.8283E-15
303.0	1.095	4.4533E+01	2.6336E-03	6.5371E-07	9.4532E-11	5.5650E-15
308.0	3.599	4.6142E+01	2.2259E-03	5.3905E-07	7.6894E-11	4.4727E-15
309.0	5.904	4.6714E+01	2.3070E-03	5.7063E-07	8.2626E-11	4.8369E-15
317.0	4.959	4.6136E+01	2.6086E-03	6.9954E-07	1.0618E-10	6.3774E-15
408.0	4.596	4.6777E+01	1.9489E-03	4.7026E-07	7.2325E-11	4.4196E-15
409.0	6.305	4.5612E+01	2.0201E-03	4.8061E-07	6.8880E-11	4.0195E-15
417.0	4.899	4.5188E+01	2.3767E-03	6.2258E-07	9.3904E-11	5.6190E-15
505.0	2.775	4.7647E+01	2.3946E-03	6.0992E-07	8.9752E-11	5.2339E-15
507.0	4.002	4.6300E+01	2.1331E-03	5.2970E-07	7.7658E-11	4.5615E-15
508.0	8.142	4.8023E+01	1.7285E-03	3.9084E-07	5.4649E-11	3.1075E-15
509.0	8.499	4.8234E+01	1.8910E-03	4.3591E-07	6.1263E-11	3.4901E-15
516.0	5.117	4.7420E+01	1.8949E-03	4.3323E-07	5.9586E-11	3.2733E-15
517.0	5.117	4.7698E+01	2.3363E-03	6.0581E-07	9.0605E-11	5.3453E-15
606.0	6.156	4.9635E+01	3.4811E-03	1.0492E-06	1.6849E-10	1.0370E-14
607.0	8.109	4.7853E+01	1.8656E-03	4.6185E-07	7.1497E-11	4.3750E-15
608.0	11.108	4.9170E+01	1.5802E-03	3.4347E-07	4.6870E-11	2.6563E-15
609.0	4.966	4.7368E+01	2.0173E-03	4.7759E-07	6.7404E-11	3.8474E-15
615.0	6.895	4.7509E+01	2.1172E-03	4.9533E-07	7.2805E-11	4.4007E-15
616.0	7.892	4.8547E+01	1.7379E-03	3.6954E-07	4.7608E-11	2.5585E-15
617.0	3.340	4.7009E+01	2.4592E-03	6.5348E-07	9.8261E-11	5.8172E-15
707.0	9.763	4.8696E+01	1.9224E-03	4.9143E-07	7.4692E-11	4.5399E-15
708.0	6.508	4.7365E+01	1.9840E-03	4.9280E-07	7.2933E-11	4.3354E-15
709.0	2.819	4.6770E+01	2.2411E-03	5.5102E-07	7.9899E-11	4.6459E-15
714.0	4.510	4.7147E+01	1.8720E-03	4.1254E-07	5.3950E-11	2.9053E-15
715.0	7.111	4.7683E+01	2.2458E-03	5.5753E-07	7.9113E-11	4.5753E-15
716.0	4.987	4.6988E+01	2.2584E-03	5.7344E-07	8.3948E-11	4.9197E-15
808.0	5.116	4.8625E+01	1.6321E-03	3.3915E-07	4.6025E-11	2.5839E-15
811.0	3.079	4.6421E+01	2.6221E-03	6.8505E-07	1.0200E-10	6.0540E-15
812.0	3.903	4.6567E+01	2.3003E-03	4.3846E-07	5.3231E-11	2.8469E-15
813.0	4.987	4.7561E+01	2.0103E-03	4.5650E-07	6.2393E-11	3.4674E-15
814.0	8.310	4.8477E+01	1.5511E-03	2.9069E-07	3.2807E-11	1.5486E-15
815.0	6.071	4.7307E+01	2.4172E-03	6.2096E-07	8.9966E-11	5.2500E-15
816.0	5.358	4.7488E+01	1.6987E-03	3.5057E-07	4.4497E-11	2.3647E-15
817.0	2.745	4.6832E+01	2.1078E-03	5.1344E-07	7.4414E-11	4.3173E-15
909.0	1.592	4.8632E+01	2.0165E-03	4.6054E-07	6.4288E-11	3.6296E-15
911.0	4.953	4.6717E+01	2.7566E-03	7.4062E-07	1.1213E-10	6.7066E-15
912.0	3.200	4.5468E+01	2.5089E-03	6.5244E-07	9.7170E-11	5.7561E-15
913.0	6.790	4.7788E+01	2.1362E-03	5.0666E-07	7.1400E-11	4.0530E-15
914.0	5.420	4.6897E+01	2.1060E-03	4.9864E-07	6.8598E-11	3.7971E-15
916.0	3.338	4.6706E+01	1.9206E-03	4.3001E-07	5.8063E-11	3.2077E-15

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    CODE       A        B           C           D           E           F
   917.0   2.616 4.7680E+01 2.1411E-03 5.3239E-07 7.8152E-11 4.5625E-15
  1111.0    .730 4.5152E+01 3.6917E-03 1.0752E-06 1.7017E-10 1.0459E-14
  1117.0   4.222 4.6147F+01 3.0037E-03 8.5128E-07 1.3301E-10 8.0960E-15
  1216.0   2.901 4.6082E+01 2.6137E-03 6.8845E-07 1.0253E-10 6.0759E-15
  1217.0   2.701 4.4998E+01 2.8447E-03 7.9686E-07 1.2369E-10 7.4944E-15
  1313.0   1.604 4.7559E+01 2.9097E-03 7.7812E-07 1.1753E-10 6.9499E-15
  1317.0   5.074 4.7276E+01 2.5438E-03 6.7568E-07 1.0182E-10 6.0055E-15
  1414.0   3.252 4.7179E+01 2.0256E-03 4.5186E-07 5.7418E-11 2.9577E-15
  1416.0   6.418 4.7989E+01 1.7935E-03 3.7532E-07 4.5974E-11 2.3242E-15
  1417.0   4.002 4.6541E+01 2.5534E-03 6.8459E-07 1.0209E-10 5.9733E-15
  1515.0   5.033 4.8223E+01 2.6898E-03 7.0362E-07 1.0075E-10 5.8493E-15
  1516.0   5.637 4.6919E+01 2.7644E-03 7.4350E-07 1.0948E-10 6.4205E-15
  1616.0   4.380 4.7693E+01 1.9029E-03 4.2359E-07 5.5948E-11 3.0438E-15
  1617.0   2.749 4.7565E+01 3.5631E-03 1.0897E-06 1.7573E-10 1.0805E-14
  1717.0   2.476 4.8021E+01 2.4184E-03 6.5374E-07 1.0061E-10 6.0420E-15
 10106.0   8.850 9.3457E+01 2.2374E-03 2.9465E-07 2.7708E-11 1.2186E-15
 10108.0   9.511 9.3163E+01 2.6530E-03 5.6946E-07 8.3927E-11 5.0416E-15
 10116.0   7.514 9.2053E+01 2.7514E-03 5.1218E-07 6.6192E-11 3.6540E-15
 10308.0   8.894 9.2675E+01 3.5194E-03 7.8181E-07 1.0862E-10 6.2491E-15
 10607.0  13.135 9.6088E+01 3.4106E-03 6.7378E-07 8.7666E-11 4.8365E-15
 10608.0  12.311 9.4191E+01 3.0252E-03 5.9689E-07 7.7220E-11 4.2351E-15
 10811.0   8.286 9.2701E+01 4.3703E-03 1.0975E-06 1.6241E-10 9.6222E-15
 10812.0   6.823 9.1448E+01 3.9729E-03 9.4759E-07 1.3688E-10 8.0099E-15
 30308.0   7.366 9.4344E+01 4.5560E-03 1.0617E-06 1.4668E-10 8.3566E-15
 40909.0  13.202 9.7539E+01 3.8763E-03 7.4631E-07 9.0689E-11 4.6897E-15
 40917.0  11.168 9.6687E+01 4.5979E-03 1.0294E-06 1.4006E-10 7.8330E-15
 41717.0   9.449 9.7191E+01 5.3790E-03 1.3389E-06 1.9437E-10 1.1303E-14
 50808.0  14.587 9.9071E+01 4.5233E-03 9.7552E-07 1.2807E-10 6.9373E-15
 50809.0  15.397 9.9301E+01 4.0104E-03 8.2171E-07 1.0551E-10 5.6521E-15
 50817.0  13.416 9.9020E+01 4.6174E-03 1.0596E-06 1.4704E-10 8.2987E-15
 50909.0  13.251 9.6613E+01 4.3092E-03 9.9043E-07 1.3679E-10 7.6726E-15
 50917.0  11.196 9.5496E+01 4.9555E-03 1.2437E-06 1.8095E-10 1.0483E-14
 51717.0   9.141 9.5721E+01 5.5387E-03 1.4807E-06 2.2304E-10 1.3192E-14
 60606.0  13.957 1.0081E+02 3.9913E-03 8.1028E-07 1.0167E-10 5.3621E-15
 60717.0  12.126 9.8836F+01 4.8687E-03 1.1673E-06 1.6627E-10 9.5674E-15
 60808.0  16.561 1.0097E+02 3.3659E-03 5.7770E-07 6.3873E-11 3.0525E-15
 60816.0  14.210 1.0000E+02 3.9763E-03 7.8058E-07 9.5929E-11 4.9686E-15
 60909.0  10.268 9.7787E+01 3.7637E-03 7.7313E-07 9.9261E-11 5.3065E-15
 61616.0  11.881 1.0044E+02 4.5422E-03 9.8359E-07 1.2836E-10 6.9210E-15
 70708.0  11.440 9.9172E+01 3.9917E-03 8.1117E-07 1.0518E-10 5.7309E-15
 70808.0   9.621 9.7617E+01 3.6891E-03 7.5141E-07 9.6734E-11 5.2293E-15
 70909.0   6.056 9.6316E+01 4.4386E-03 1.0275E-06 1.4206E-10 7.9873E-15
 80814.0  13.447 1.0004E+02 3.7484E-03 6.5483E-07 6.8677E-11 3.0007E-15
 80816.0  11.023 9.8405E+01 3.7855E-03 7.7032E-07 9.7481E-11 5.1594E-15
 80817.0   5.244 9.7361E+01 4.3717E-03 9.9792E-07 1.3788E-10 7.7489E-15
 80913.0  12.703 9.9135E+01 5.3486E-03 1.2832E-06 1.8036E-10 1.0208E-14
 80916.0   7.482 9.6508E+01 4.0897E-03 8.9324E-07 1.1798E-10 6.4190E-15
 81313.0  10.615 9.7475E+01 4.5545E-03 1.0557E-06 1.4532E-10 8.1253E-15
 81317.0  11.108 9.8747E+01 5.9340E-03 1.5245E-06 2.2355E-10 1.3000E-14
 81617.0   7.696 9.6006E+01 4.6730E-03 1.1339E-06 1.6109E-10 9.2064E-15
 81717.0   4.226 9.7105E+01 4.9032E-03 1.2343E-06 1.8020E-10 1.0475E-14
 90912.0  10.812 9.8160E+01 5.3328E-03 1.2759E-06 1.7933E-10 1.0193E-14
 90914.0  11.835 9.7467E+01 4.3744E-03 9.9177E-07 1.3304E-10 7.2634E-15
 90916.0   6.674 9.7417E+01 4.4298E-03 1.0205E-06 1.3991E-10 7.8045E-15
121717.0   8.360 9.7591E+01 6.5730E-03 1.7908E-06 2.7180E-10 1.6183E-14
141414.0   7.588 9.9755E+01 5.5188E-03 1.3275E-06 1.8099E-10 9.9184E-15
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CODE	A	B	C	D	E	F
141717.0	8.902	9.6471E+01	5.5820E-03	1.4873E-06	2.2154E-10	1.2977E-14
161717.0	5.545	9.6606E+01	5.6007E-03	1.5018E-06	2.2568E-10	1.3326E-14
1010105.0	11.697	1.4035E+02	3.6309E-03	5.3929E-07	5.8765E-11	2.9271E-15
1010106.0	12.600	1.4032E+02	4.1238E-03	7.2477E-07	8.9409E-11	4.8096E-15
1010107.0	12.004	1.3972E+02	3.5646E-03	5.7053E-07	6.8977E-11	3.7564E-15
1010115.0	9.809	1.3915E+02	4.2856E-03	6.7730E-07	7.1115E-11	3.3400E-15
1010606.0	16.864	1.4492E+02	5.1010E-03	9.2490E-07	1.1306E-10	5.9293E-15
1050808.0	19.005	1.4558E+02	4.7586E-03	8.4752E-07	1.0015E-10	5.1064E-15
4040808.0	16.308	1.4586E+02	6.9613E-03	1.5378E-06	2.0635E-10	1.1460E-14
5050808.0	21.561	1.5114E+02	7.3479E-03	1.6545E-06	2.2582E-10	1.2593E-14
6060707.0	21.323	1.5074E+02	7.5974E-03	1.7755E-06	2.4835E-10	1.4136E-14
6080909.0	18.010	1.4925E+02	5.6538E-03	1.0650E-06	1.2623E-10	6.3361E-15
6080917.0	16.353	1.4834E+02	6.4946E-03	1.3929E-06	1.8326E-10	9.9610E-15
6081717.0	14.698	1.4881E+02	7.3795E-03	1.7419E-06	2.4434E-10	1.3858E-14
6090909.0	14.907	1.4924E+02	5.7370E-03	1.0835E-06	1.2821E-10	6.4057E-15
7070909.0	10.459	1.4820E+02	7.0988E-03	1.6054E-06	2.1898E-10	1.2222E-14
7090909.0	8.498	1.4891E+02	6.9578E-03	1.5265E-06	2.0284E-10	1.1073E-14
8080816.0	14.568	1.5135E+02	6.0103E-03	1.1784E-06	1.4333E-10	7.3393E-15
8081313.0	15.827	1.5047E+02	6.7434E-03	1.4313E-06	1.8513E-10	9.9056E-15
8090916.0	11.166	1.4879E+02	7.0308E-03	1.5561E-06	2.0725E-10	1.1314E-14
8161717.0	10.044	1.4792E+02	8.6715E-03	2.2202E-06	3.2508E-10	1.8894E-14
9090915.0	15.220	1.4917E+02	7.8109E-03	1.8403E-06	2.5421E-10	1.4249E-14
9091111.0	12.416	1.4619E+02	1.1031E-02	3.0793E-06	4.7040E-10	2.8095E-14
9091616.0	9.634	1.4894E+02	8.1079E-03	1.9604E-06	2.7548E-10	1.5572E-14
11111717.0	10.590	1.4537E+02	1.1630E-02	3.3523E-06	5.2149E-10	3.1482E-14
15151515.0	12.320	1.5101E+02	9.8958E-03	2.5896E-06	3.7449E-10	2.1697E-14
15171717.0	10.038	1.4827E+02	1.0007E-02	2.7339E-06	4.1313E-10	2.4484E-14
16161717.0	8.382	1.4800E+02	9.6837E-03	2.6048E-06	3.9044E-10	2.2991E-14
101010106.0	17.019	1.8859E+02	3.7864E-03	2.3978E-07	4.9693E-12	1.3678E-15
101010114.0	13.329	1.8810E+02	5.4222E-03	6.7853E-07	4.8867E-11	1.2069E-15
101040808.0	19.626	1.9304E+02	5.1031E-03	5.8373E-07	3.8644E-11	8.8439E-16
505080808.0	28.019	2.0056E+02	9.3202E-03	2.0406E-06	2.7315E-10	1.5035E-14
609090909.0	19.911	2.0282E+02	8.5497E-03	1.6244E-06	1.9675E-10	1.0002E-14
617171717.0	13.406	2.0244E+02	1.2294E-02	3.1728E-06	4.6716E-10	2.7232E-14
707080808.0	19.793	2.5222E+02	1.2135E-02	2.6460E-06	3.5206E-10	1.9324E-14
808090916.0	18.367	2.0205E+02	8.9550E-03	1.8432E-06	2.3302E-10	1.2254E-14
909090914.0	24.676	2.0238E+02	1.0223E-02	2.3178E-06	3.1296E-10	1.7196E-14
909090916.0	13.344	2.0111E+02	1.0262E-02	2.3219E-06	3.1349E-10	1.7243E-14
1417171717.0	16.323	2.0167E+02	1.3270E-02	3.5481E-06	5.3087E-10	3.1197E-14
10101010606.0	23.067	2.3815E+02	6.0074E-03	6.4283E-07	3.6092E-11	3.6357E-16
10103030808.0	20.465	2.4088E+02	1.1084E-02	2.3946E-06	3.2062E-10	1.7815E-14
10108081111.0	18.921	2.4136E+02	1.3325E-02	3.2511E-06	4.6891E-10	2.7211E-14

The density dependence of the ionization energy and the partition function arises from collisions between atoms or between atoms and ions. Levels with very high quantum numbers are no longer bound, and the ionization energy is reduced. The process is not easy to calculate, so in ATLAS we assume that there is a definite cutoff energy and that the bound levels maintain their original values. As described in Drawin and Felenbok (1965), we assume that the energy difference is inversely proportional to the Debye radius, which is a measure of the distance between charged particles in the gas,

$$\Delta E = 1.44\,\mathrm{E}\text{-}7 \frac{Z_{\mathrm{eff}}}{r_{\mathrm{Debye}}} \quad , \quad \text{in ev} \quad , \tag{4.36}$$

where Z_{eff} is 1 for neutral particles, 2 for those once ionized, etc., and

$$r_{\mathrm{Debye}} = \sqrt{\frac{kT}{4\pi e^2 n_c}} \quad , \tag{4.37}$$

with n_c the square charge density. For singly charged ions and electrons, $n_{ci} = n_i$; for doubly charged, $n_{ci} = 4n_i$, etc. If only single ionizations occur or if hydrogen is by far the dominant ion, $n_c = 2n_e$. If He III is important and if heavier elements are negligible, $n_c = n_e + n_A - (n_e - n_A) + 4(n_e - n_A)$, where the excess number of electrons $(n_e - n_A)$ comes from He III.

The partition function has the form

$$U = \Sigma\, b_i g_i\, e^{-E_i/kT} \quad . \tag{3.17'}$$

If there were no energy cutoff, there would be an infinite number of levels and consequently an infinite partition function. Therefore, some sort of energy cutoff is always necessary. At low temperatures ($T \lesssim 800$ E for E in ev, i.e., 4000 K for E = 5 ev), the upper levels are not populated, so the value of the cutoff has a negligible effect on the sum; but at higher temperatures, the cutoff determines the value of the partition function.

As an example of a partition-function calculation, we consider an atom with hydrogenic upper levels that have b's unity. The partition function is

$$U = \sum_{E=0}^{E=E_1} b_i g_i e^{-E_i/kT} + G \sum_{E=E_1}^{E=E_2} n^2 e^{-E_n/kT}$$

or

$$U = U_0 + U_1 \quad , \tag{4.38}$$

where

$$E_n = E_\infty - \frac{13.595\, Z^2}{n^2} = E_\infty - \frac{c}{n^2} \quad \text{in ev} \quad .$$

We can approximate U_1 by an integral over n,

$$U_1 \simeq G \int_{n_1}^{n_2} n^2\, e^{-[E_\infty - (c/n^2)]/kT}\, dn \quad . \tag{4.39}$$

When the upper levels are populated, $E_\infty/kT \lesssim 10$ to 20; choosing $n_1^2 \gtrsim 20$ implies that $c/n_1^2 kT < 1$. Therefore, we can expand the exponential in a power series,

$$U_1 \simeq G\, e^{-E_\infty/kT} \int_{n_1}^{n_2} n^2 \left[1 + \frac{c}{n^2 kT} + \frac{1}{2!} \left(\frac{c}{n^2 kT} \right)^2 + \frac{1}{3!} \left(\frac{c}{n^2 kT} \right)^3 + \cdots \right] dn$$

$$\simeq G\, e^{-E_\infty/kT} \left\{ n^3 \left[\frac{1}{3} + \left(\frac{c}{n^2 kT} \right) \frac{1}{2} \left(\frac{c}{n^2 kT} \right)^2 \frac{1}{18} \left(\frac{c}{n^2 kT} \right)^3 - \cdots \right] \right\}_{n_1}^{n_2} \quad .$$

We change variables from n to $\Delta E = 13.595\ Z^2/n^2 = c/n^2$, with the result

$$U_1 \simeq G\ e^{-E_\infty/kT} \left\{ \left(\frac{13.595\ Z^2}{\Delta E}\right)^{3/2} \left[\frac{1}{3} + \frac{\Delta E}{kT} - \frac{1}{2}\left(\frac{\Delta E}{kT}\right)^2 - \frac{1}{18}\left(\frac{\Delta E}{kT}\right)^3 - \dots\right] \right\}_{\Delta E_1}^{\Delta E_2} . \tag{4.40}$$

To apply this result to hydrogen, we treat the first six levels explicitly,

$$U_0 = \sum_{n=1}^{6} b_n 2n^2\ e^{-[13.595-(13.595/n^2)]/kT} ,$$

and evaluate U_1 by choosing $n_1 = 6.5$, $\Delta E_1 = 13.595/(6.5)^2$, $\Delta E_2 = \Delta E_{cutoff}$, $G = 2$, and $E_\infty = 13.595$.

For elements that do not have b's calculated, we pretabulate the partition functions at a fixed cutoff $\Delta E = 0.1$ ev and specify a G factor. We find the partition function for $\Delta E = 0.1$ for any temperature by linear interpolation. If the actual ΔE is less than 0.1, we use the interpolated value. If ΔE is greater than 0.1, we add the integral U_1, evaluated with $\Delta E_1 = 0.1$ and $\Delta E_2 = \Delta E_{cutoff}$, to the interpolated value.

The table of partition functions is stored in a compact form in subroutine PFSAHA, described in Section 8.5. Many of the partition functions were taken from Drawin and Felenbok (1965), who give tables of partition functions for many elements for $\Delta E = 0.1$, 0.25, 0.5, 1., 2., and 3. ev. By fitting the expression for U_1 to their tabulated U as a function of ΔE, it was possible to obtain an approximate value for G. We computed partition functions for atoms other than those Drawin and Felenbok tabulated by adding all the known energy levels and tossing in a few more for good measure. The principal source was Moore (1949), but more recent papers were used when available. The computed partition functions are lower limits since many of the higher levels have not been found, and in fact for some elements, very little is known about the spectrum. Because of this uncertainty, no effort was made to include ΔE dependence. Even so, these partition functions should be reliable at low temperatures since most of the lower energy levels are known.

Once we have the partition functions, the Saha equation for ionization takes the form

$$\frac{n^{i+1}}{n^i} = 2.4148\mathrm{E}15\,\frac{T^{3/2}}{n_e}\,\frac{2U(T,\Delta E,b's)^{i+1}}{U(T,\Delta E,b's)^i}\,e^{-(E_\infty-\Delta E)/kT} \quad . \tag{4.41}$$

There is one further complication with Saha equations: Once we have solved the equilibrium equations, we continue the model calculation and find that we need to use Boltzmann equations of the form

$$n(\ell) = n(Q)\,\frac{g(\ell)}{U(Q)}\,e^{-[E(\ell)-E(Q)]/kT} \tag{4.42}$$

in order to evaluate number densities for levels that contribute to the opacity. Thus the quantity actually required is n/U, not n. For atoms, we have just described methods for finding partition functions that can be used to obtain n/U easily. However, if the equilibrium constant $\mathcal{E}(T)$ has been used to find n (eq. (4.35)), we evaluate n/U by rewriting the Saha equation (4.34) in the form

$$\frac{n^{k+}_{1\,2\,3\cdots m}}{U(n^{k+}_{1\,2\,3\cdots m})} = \frac{[n_1/U_1(2\pi M_1kT/h^2)^{3/2}]\cdots[n_m/U_m(2\pi M_mkT/h^2)^{3/2}]}{[n_e/2(2\pi mkT/h^2)^{3/2}]^k\,[1/(2\pi M_{1\,2\,3}kT/h^2)^{3/2}]}$$

$$\times\, e^{-[E(n^{k+}_{1\,2\,3})-E_1\cdots E_m]/kT} \quad . \tag{4.43}$$

Since $n^{k+}_{1\,2\,3}$, n_i, and M_i are known, since U_i can be found as described above, since $M_{1\,2\,3}$ is just the sum of M_i, and since the dissociation energy is tabulated (eq. (4.35)), n/U can be evaluated straightforwardly.

4.5 Mass Density and Height

The mass density ρ is simply the atomic number density n_A, found in Section 4.3, times the average mass of each atom. The average atomic weight is

$$\mu = \Sigma\, X_i M_i \quad , \tag{4.44}$$

so

$$\rho = n_A \mu M_A \quad , \tag{4.45}$$

where M_A = 1.660E-24 is 1 atomic mass unit.

The height x is

$$x = -\int_0^M \frac{dM}{\rho} \quad , \tag{4.46}$$

with x arbitrarily 0 at the first rhox. Only the differences in height are meaningful.

The pressure scale height h from equation (4.2) is

$$h = \frac{P_{total}}{\rho g} \quad . \tag{4.47}$$

4.6 Thermodynamic Derivatives

A number of useful partial derivatives, some of which will be needed in Section 6 to calculate the convective flux, follow:

Specific heats,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_\rho \tag{4.48}$$

and

$$C_P = \left(\frac{\partial E}{\partial T}\right)_{P_{total}} + \left[\frac{\partial}{\partial T}\left(\frac{P_{total}}{\rho}\right)\right]_{P_{total}} = \left(\frac{\partial E}{\partial T}\right)_{P_{total}} - \frac{P_{total}}{\rho^2}\left(\frac{\partial \rho}{\partial T}\right)_{P_{total}} \quad , \tag{4.49}$$

where E is the energy per unit mass,

$$E = \frac{3}{2}\,\frac{n_{\rm total}kT}{\rho} + \frac{3P_{\rm rad}}{\rho} + \sum \frac{n_i[E_i + (d\ln U_i/d\ln T)\,kT]}{\rho} \quad , \tag{4.50}$$

with E_i the ground energy and $(d \ln U_i/d \ln T)\,kT$ the internal energy of atom i; the adiabatic gradient,

$$\left(\frac{\partial \ln T}{\partial \ln P}\right)_S = -\frac{P_{\rm total}}{T\rho C_P}\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_{P_{\rm total}} \quad ; \tag{4.51}$$

and the sound velocity,

$$v^2_{\rm sound} = \frac{C_P}{C_V}\left(\frac{\partial P_{\rm total}}{\partial \rho}\right)_T \quad . \tag{4.52}$$

It is convenient in ATLAS to take derivatives holding P or T constant, not $P_{\rm total}$ nor ρ. In general, if we change variables from u, v to x, y, we have the identities

$$\left(\frac{\partial f}{\partial u}\right)_v = \left(\frac{\partial f}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v \tag{4.53}$$

and

$$\left(\frac{\partial y}{\partial u}\right)_v = -\frac{(\partial v/\partial u)_y}{(\partial v/\partial y)_u} \quad . \tag{4.54}$$

In the special case u, v to u, y, we find

$$\left(\frac{\partial f}{\partial u}\right)_v = \left(\frac{\partial f}{\partial u}\right)_y - \frac{(\partial f/\partial y)_u\,(\partial v/\partial u)_y}{(\partial v/\partial y)_u} \quad . \tag{4.55}$$

We use this identity to reexpress the partial derivatives in a form for calculation:

$$C_V = \left(\frac{\partial E}{\partial T}\right)_P - \frac{(\partial E/\partial P)_T\,(\partial \rho/\partial T)_P}{(\partial \rho/\partial P)_T} \quad , \tag{4.56}$$

$$C_P = \left(\frac{\partial E}{\partial T}\right)_P - \frac{(\partial E/\partial P)_T\,(\partial P_{total}/\partial T)_P}{(\partial P_{total}/\partial P)_T} - \frac{P_{total}}{\rho^2}\left[\left(\frac{\partial \rho}{\partial T}\right)_P - \frac{(\partial \rho/\partial P)_T\,(\partial P_{total}/\partial T)_P}{(\partial P_{total}/\partial P)_T}\right] \quad , \tag{4.57}$$

$$\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_{P_{total}} = \frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{P_{total}} = \frac{T}{\rho}\left[\left(\frac{\partial \rho}{\partial T}\right)_P - \frac{(\partial \rho/\partial P)_T\,(\partial P_{total}/\partial T)_P}{(\partial P_{total}/\partial P)_T}\right] \quad , \tag{4.58}$$

and

$$v^2_{sound} = \frac{C_P}{C_V}\;\frac{(\partial P_{total}/\partial P)_T}{(\partial \rho/\partial P)_T} \quad . \tag{4.59}$$

If we ignore any turbulent pressure and assume that radiation pressure varies as T^4, then

$$\left(\frac{\partial P_{total}}{\partial P}\right)_T = 1 \tag{4.60}$$

and

$$\left(\frac{\partial P_{total}}{\partial T}\right)_P = \frac{4P_{rad}}{T} \quad , \tag{4.61}$$

and we are left with only four derivatives to evaluate – $(\partial E/\partial T)_P$, $(\partial E/\partial P)_T$, $(\partial \rho/\partial T)_P$, and $(\partial \rho/\partial P)_T$.

We calculate these four derivatives numerically as follows: We make up a small set of equilibrium equations, as in Section 4.3, that include only the most abundant elements. At present, these equations include only hydrogen and helium, but others can easily be added. We note that considerable approximation is allowed because our object is to find not the exact energy nor mass density but the derivatives of those quantities. We include H I, H II, H_2, He I, He II, and He III, for which the Saha equations are

$$n(\mathrm{H\ II}) = \frac{n(\mathrm{H\ I})}{n_e}\ 2.4148\mathrm{E}15\ T^{3/2}\ e^{-13.595/kT} \quad , \qquad (\mathrm{cf.}\ 4.24)$$

$$n(\mathrm{H}_2) = n(\mathrm{H\ I})\ n(\mathrm{H\ I})\ \exp\left(\frac{4.477}{kT} - 4.6628\mathrm{E}1 + 1.8031\mathrm{E}{-3}\ T - 5.0739\mathrm{E}{-7}\ T^2 + 8.1424\mathrm{E}{-11}\ T^3 - 5.0501\mathrm{E}{-15}\ T^4 - 1.5 \ln T\right) \quad , \qquad (\mathrm{cf.}\ 4.34,\ 4.35)\ (4.62)$$

$$n(\mathrm{He\ II}) = \frac{n(\mathrm{He\ I})}{n_e}\ 4(2.4148\mathrm{E}15)\ T^{3/2}\ e^{-24.508/kT} \quad , \qquad (\mathrm{cf.}\ 4.34)$$

and

$$n(\mathrm{He\ III}) = \frac{n(\mathrm{He\ I})}{n_e^2}\ 4(2.4148\mathrm{E}15)^2\ T^3\ e^{-78.983/kT} \quad , \qquad (\mathrm{cf.}\ 4.34)$$

where we have assumed U(H I) = 2, U(He I) = 1, and U(He II) = 2. We solve the equations keeping either T or P constant and varying the other by ±0.001. For each solution we find the density

$$\rho = n_A\ \mu\ M_A \qquad (4.45)$$

and the energy per unit mass

$$E = \left\{\left[\frac{3}{2}\ n_{\mathrm{total}} + \frac{13.595}{kT}\ n(\mathrm{H\ II}) + \frac{E(\mathrm{H}_2)}{kT}\ n(\mathrm{H}_2) + \frac{24.580}{kT}\ n(\mathrm{He\ II}) + \frac{78.983}{kT}\ n(\mathrm{He\ III})\right] kT + 3P_{\mathrm{rad}} \left(\frac{T}{T_0}\right)^4\right\} \Big/ \rho \quad , \qquad (\mathrm{cf.}\ 4.50)$$

where

$$\frac{E(\mathrm{H}_2)}{kT} = -\frac{4.476}{kT} + 1(1.8031\mathrm{E}{-3})\ T + 2(-5.0739\mathrm{E}{-7})\ T^2 + 3(8.1424\mathrm{E}{-11})\ T^3 + 4(-5.0501\mathrm{E}{-15})\ T^4 \quad , \qquad (\mathrm{cf.}\ 4.50,\ 4.62)\ (4.63)$$

because for H_2, (d ln U/d ln T) is important. The derivatives are

$$\left(\frac{\partial E}{\partial T}\right)_P = \frac{500}{T_0} [E(1.001\ T_0) - E(0.999\ T_0)] \quad ,$$

$$\left(\frac{\partial E}{\partial P}\right)_T = \frac{500}{P_0} [E(1.001\ P_0) - E(0.999\ P_0)] \quad ,$$

$$\left(\frac{\partial \rho}{\partial T}\right)_P = \frac{500}{T_0} [\rho(1.001\ T_0) - \rho(0.999\ T_0)] \quad ,$$

$$\left(\frac{\partial \rho}{\partial P}\right)_T = \frac{500}{P_0} [\rho(1.001\ P_0) - \rho(0.999\ P_0)] \quad .$$

5. OPACITY

For computational convenience, we divide all possible absorption and scattering transitions into the following 20 groups:

1. H I bound-free and free-free transitions. It is customary for astronomers to apply the name of the bound state to both the bound-free and the free-free transitions, even if there is no bound state. Thus the proton-electron free-free is called neutral hydrogen or H I free-free.

2. H_2^+ bound-free and free-free.

3. H^- bound-free and free-free.

4. H I Rayleigh scattering.

5. He I bound-free and free-free.

6. He II bound-free and free-free

7. He^- free-free. There is no bound state.

8. He I Rayleigh scattering

9. Low-temperature absorbers ($T \lesssim 10000$ K): C I + Mg I + Si I + Al I bound-free and free-free.

10. Intermediate-temperature absorbers ($10000 \text{ K} \lesssim T \lesssim 20000$ K): Si II + Mg II + Ca II + N I + O I bound-free and free-free.

11. High-temperature absorbers: C II-IV + N II-V + O II-VI + Ne I-VI bound-free for frequencies greater than the Lyman limit of hydrogen.

12. Electron scattering.

13. H_2 Rayleigh scattering.

14. H I lines.

15. Line-absorption distribution functions.

16. Line-scattering distribution functions, i.e., line opacity considered as scattering because $S_\nu \simeq J_\nu$.

17. Other or experimental absorption lines.

18. Other or experimental scattering lines, i.e., line opacity considered as scattering because $S_\nu \simeq J$.

19. Other or experimental continuous absorptions.

20. Other or experimental continuous scatterings.

For each group we find a total mass absorption or scattering coefficient and a source function, as discussed in a general way in Section 2. These coefficients are labeled $\kappa_\nu(i)$ and $\sigma_\nu^c(i)$ for continuous absorptions and scatterings and $\ell_\nu(i)$ and $\sigma_\nu^\ell(i)$ for lines. The line and continuous opacities are kept separate, so that in small wavelength intervals the continuous opacity can be kept constant while the line opacity is recalculated at several closely spaced wavelength points. Total-absorption coefficients are obtained by summing over groups,

$$\kappa_\nu = \Sigma\ \kappa_\nu(i) \quad ,$$

$$\ell_\nu = \Sigma\ \ell_\nu(i) \quad ,$$

$$\sigma_\nu^c = \Sigma\ \sigma_\nu^c(i) \quad ,$$

$$\sigma_\nu^\ell = \Sigma\ \sigma_\nu^\ell(i) \quad ,$$

and

$$\kappa_\nu(\text{total}) = \kappa_\nu + \ell_\nu + \sigma_\nu^c + \sigma_\nu^\ell \quad . \qquad (5.1)$$

The total source function is the average over all the groups:

$$S_\nu = \frac{\Sigma\ \kappa_\nu(i)\ S_\nu(i) + \Sigma\ \ell_\nu(i)\ S_\nu(i) + \Sigma\ \sigma_\nu^c(i)\ J_\nu + \Sigma\ \sigma_\nu^\ell(i)\ J_\nu}{\kappa_\nu(\text{total})} \quad . \qquad (5.2)$$

In the following, we describe each group, beginning in considerable detail with hydrogen.

5.1 H I Bound-Free and Free-Free

The bound-free absorption coefficient has the form

$$\kappa_\nu(\text{bound-free}) = \sum_{n=1}^{\infty} \frac{n_n}{\rho}\, \alpha_n \left(1 - \frac{1}{b_n} e^{-h\nu/kT}\right) \quad , \tag{5.3}$$

as discussed in Section 3.5. Here the upper level is the proton, for which b = 1. The number density in each level n_n is found from the Boltzmann equation

$$n_n = b_n\, n(\text{H I}) \frac{g_n}{U(\text{H I})} e^{-E_n/kT} \quad , \tag{5.4}$$

where $g_n = 2n^2$ and $E_n = 13.595 \text{ ev } Z^2[1-(1/n^2)]$, and where n(H I)/U(H I) was found earlier as described in Section 4. The cross sections α_n are given by polynomial approximations (Gingerich, 1969) to the Coulomb cross sections of Karsas and Latter (1961),

$$\alpha_n = \frac{2.815\text{E}29\ Z^2}{n^5 \nu^3} \left[A_n + \left(B_n + C_n \frac{Z^2}{\nu}\right) \frac{Z^2}{\nu}\right] \tag{5.5}$$

for

$$\nu \geq 3.28805\text{E}15 \frac{Z^2}{n^2} \quad ,$$

where

$$2.815\text{E}29 = \frac{64\, \pi^4 e^{10} m}{3\sqrt{3}\, c\, h^6} \quad .$$

Note that since 3.28805E15 is the ionization frequency and 13.595 ev is the ionization energy, (3.28805E15) h/kT = 13.595 ev/kT. The polynomial coefficients are as follows:

n	A_n	B_n	C_n
1	0.9916	2.719E13	-2.268E30
2	1.105	-2.375E14	4.077E28
3	1.101	-9.863E13	1.035E28
4	1.101	-5.765E13	4.593E27
5	1.102	-3.909E13	2.371E27
6	1.0986	-2.704E13	1.229E27
$7 \leq n$	1	0	0

For levels above 8, the summation of levels is treated as an integral over n:

$$\frac{n(H\,I)}{U(H\,I)} \sum_{n=n'=9}^{\infty} 2n^2\, e^{-13.595\, Z^2\, [1-(1/n^2)]/kT}\, \frac{2.815E29\, Z^4}{n^5\, \nu^3}\, (1-e^{-h\nu/kT})$$

$$\simeq \frac{n(H\,I)}{U(H\,I)}\, \frac{2.815E29\, Z^4}{\nu^3}\, (1-e^{-h\nu/kT})\; 2 \int_{n'}^{\infty} e^{-13.595\, Z^2\, [1-(1/n^2)]/kT}\, \frac{dn}{n^3}$$

$$= \frac{n(H\,I)}{U(H\,I)}\, \frac{2.815E29\, Z^4}{\nu^3}\, (1-e^{-h\nu/kT})\; 2$$

$$\times\, \frac{1}{2}\, \frac{kT}{13.595\, Z^2} \left(e^{-13.595\, Z^2\, [1-(1/n'^2)]/kT} - e^{-13.595\, Z^2/kT}\right) . \tag{5.6}$$

If $\nu < 3.28805E15\; Z^2/n'^2$, the lower limit of the integral must be increased, which can be accomplished approximately by replacing $13.595\; Z^2/n'^2\; kT$ by $h\nu/kT$.

The free-free absorption coefficient has the form

$$\kappa_\nu(\text{free-free}) = \frac{n(H\,II)}{\rho}\, n_e \sqrt{\frac{8\,kT}{\pi m}} \int \alpha_\nu(E)\; e^{-E/kT}\, \frac{E}{kT}\, \frac{dE}{kT}\, (1-e^{h\nu/kT}) , \tag{5.7}$$

where the integral is over the Maxwell-Boltzmann distribution for electron energies since we have assumed that electrons are in thermal equilibrium. The opacity can be rewritten as

$$\kappa_\nu(\text{free-free}) = n(\text{H II})\, n_e\, F_\nu(T)\, (1 - e^{-h\nu/kT}) \quad , \tag{5.8}$$

where the function $F_\nu(T)$ is interpolated from a table derived from a graph in Karsas and Latter (1961). The values listed in the table below are to be multiplied by $3.6919E8\ Z^2/\nu^3\ T^{1/2}$, where

$$3.6919E8 = \frac{16\,\pi^2}{3\sqrt{3}}\ \frac{e^6}{c\,h^4}\left(\frac{h^2}{2\pi m k}\right)^{3/2} k \quad .$$

		$\log_{10}\left(3.28805E15\,\frac{Z^2h}{kT}\right)$										
		-3.0	-2.5	-2.0	-1.5	-1.0	-0.5	0.0	0.5	1.0	1.5	2.0
$\log_{10}\left(\frac{h\nu}{kT}\right)$	-4.0	5.53	5.49	5.46	5.43	5.40	5.25	5.00	4.69	4.48	4.16	3.85
	-3.5	4.91	4.87	4.84	4.80	4.77	4.63	4.40	4.13	3.87	3.52	3.27
	-3.0	4.29	4.25	4.22	4.18	4.15	4.02	3.80	3.57	3.27	2.98	2.70
	-2.5	3.64	3.61	3.59	3.56	3.54	3.41	3.22	2.97	2.70	2.45	2.20
	-2.0	3.00	2.98	2.97	2.95	2.94	2.81	2.65	2.44	2.21	2.01	1.81
	-1.5	2.41	2.41	2.41	2.41	2.41	2.32	2.19	2.02	1.84	1.67	1.50
	-1.0	1.87	1.89	1.91	1.93	1.95	1.90	1.80	1.68	1.52	1.41	1.30
	-0.5	1.33	1.39	1.44	1.49	1.55	1.56	1.51	1.42	1.33	1.25	1.17
	0.0	0.90	0.95	1.00	1.08	1.17	1.30	1.32	1.30	1.20	1.15	1.11
	0.5	0.45	0.48	0.52	0.60	0.75	0.91	1.15	1.18	1.15	1.11	1.08
	1.0	0.33	0.36	0.39	0.46	0.59	0.76	0.97	1.09	1.13	1.10	1.08
	1.5	0.19	0.21	0.24	0.28	0.38	0.53	0.76	0.96	1.08	1.09	1.09

The source function is

$$S_\nu = \frac{\sum_{n=1}^{\infty} \kappa_n S_n + \kappa_\nu(\text{free-free})\, B_\nu}{\kappa_\nu(\text{bound-free}) + \kappa_\nu(\text{free-free})} \quad , \tag{5.9}$$

where

$$S_n = \frac{2h\nu^3}{c^2}\left(b_n e^{h\nu/kT} - 1\right)^{-1} \quad .$$

Since b_n is computed for only the first six levels, $S_n = B_\nu$ for $n > 6$. The expression for $\kappa_n S_n$,

$$\kappa_n S_n = \left[\frac{n_n}{\rho}\alpha_n\left(1 - \frac{1}{b_n}e^{-h\nu/kT}\right)\right]\left[\frac{2h\nu^3}{c^2}\left(b_n e^{h\nu/kT} - 1\right)^{-1}\right] \quad ,$$

can be rewritten as

$$\kappa_n S_n = \frac{n_n \alpha_n}{\rho} B_\nu \left(1 - \frac{1}{b_n}e^{-h\nu/kT}\right) \quad .$$

5.2 H_2^+ Bound-Free and Free-Free

Although the H_2^+ opacity could be written in terms of the H_2^+ number density, we use the component number densities instead in order to keep the opacity calculation independent of the equilibrium calculations described in Section 4. Thus, because of its low abundance relative to the sum of H_2, H I, and H II, we can find the H_2^+ opacity even if H_2^+ has not been included in the equation of state. Since the photodissociation of H_2^+ results in a proton and a ground-state hydrogen atom, we actually use the number density

$$n(\text{H I},\ n{=}1) = \frac{2b_1}{U(\text{H I})} N(\text{H I}) \quad .$$

Bates has calculated the opacity for the $1s_\sigma - 2p_\sigma$ transition of H_2^+ in several papers. His results for the sum of bound-free and free-free transitions are summarized in a table by Gingerich (1964). This table was fit with polynomials to yield the opacity

$$\kappa_\nu = \frac{n(\mathrm{H\ I}, n=1)}{\rho}\, n(\mathrm{H\ II})\, F_\nu(T)\, (1-e^{-h\nu/kT}) \quad ,$$

where

$$F_\nu(T) = \exp\Big((-E_S/kT) - 3.0233\mathrm{E}3 + \{3.7797\mathrm{E}2 + [-1.82496\mathrm{E}1 + (3.9207\mathrm{E}{-1} - 3.1672\mathrm{E}{-3} \ln \nu) \ln \nu] \ln \nu\} \ln \nu\Big) \quad ,$$

with

$$E_S = -7.342\mathrm{E}{-3} + \big(-2.409\mathrm{E}{-15} + \{1.028\mathrm{E}{-30} + [-4.230\mathrm{E}{-46} + (1.224\mathrm{E}{-61} - 1.351\mathrm{E}{-77}\ \nu)\ \nu]\ \nu\}\nu\big)\nu \ \mathrm{ev} \quad .$$

The source function is assumed to be the Planck function.

5.3 H^- Bound-Free and Free-Free

The bound-free absorption coefficient is

$$\kappa_\nu(\text{bound-free}) = \frac{n(H^-)}{\rho}\, \alpha_\nu \left[1 - \frac{e^{-h\nu/kT}}{b(H^-)}\right] \quad ,$$

where

$$n(H^-) = b(H^-)\, \frac{n(\mathrm{H\ I}, n=1)}{2}\, \frac{n_e}{2} \left(\frac{h^2}{2\pi m k T}\right)^{3/2} e^{0.7552\ \mathrm{ev}/kT} \quad . \tag{5.10}$$

The cross section is from Gingerich (1964), who fit polynomials to Geltman's (1962) calculations. The polynomials have been reexpressed and simplified as follows:

$$\alpha_\nu = 6.801\mathrm{E}{-20} + \{5.358\mathrm{E}{-3} + [1.481\mathrm{E}13 + (-5.519\mathrm{E}27 + 4.808\mathrm{E}41/\nu)/\nu]/\nu\}\,\nu$$

for $\nu \geq 2.111E14$, and

$$\alpha_\nu = 3.695E{-}16 + (-1.251E{-}1 + 1.052E13/\nu)/\nu$$

for $2.111E14 < \nu \leq 1.8259E14$, where 1.8259E14 is the ionization-limit frequency.

The bound-free source function is

$$S_\nu(\text{bound-free}) = \frac{2h\nu^3}{c^2}\left[b(H^-)\, e^{h\nu/kT} - 1\right]^{-1} = B_\nu \frac{1 - e^{-h\nu/kT}}{b(H^-) - e^{-h\nu/kT}} \quad .$$

The free-free absorption coefficient is

$$\kappa_\nu(\text{free-free}) = \frac{n(\text{H I}, n{=}1)}{\rho}\, n_e\, F_\nu(T) \quad ,$$

where $F_\nu(T)$ is given by

$$F_\nu(T) = [1.3727E{-}25 + (4.3748E{-}10 - 2.5993E{-}7\ T)/\nu]/\nu \quad ,$$

which is a fit to the dipole-length calculations by Stilly and Callaway (1970).

5.4 H I Rayleigh Scattering

The cross section is from Dalgarno (1962),

$$\sigma_\nu = \frac{n(\text{H I}, n{=}1)}{\rho}\left(\frac{5.799E{-}13}{\lambda^4} + \frac{1.422E{-}6}{\lambda^6} + \frac{2.784}{\lambda^8}\right) \quad ,$$

where $\lambda = 2.997925E18/\min(\nu, 2.922E15)$.

5.5 He I Bound-Free and Free-Free

The cross sections for the first 11 levels are listed below in the form of power laws:

	Level	g_i	E_i	ν_i	$\ln \alpha_i$
1	1^1S	1	0.0	5.9447E15	$33.32 - 2.0 \ln \nu$
2	2^3S	3	19.819	1.1526E15	$-390.026 + (21.035 - 0.318 \ln \nu) \ln \nu$
3	2^1S	1	20.615	0.96025E15	$26.83 - 1.91 \ln \nu$
4	2^3P^o	9	20.964	0.87607E15	$61.21 - 2.9 \ln \nu$
5	2^1P^o	3	21.217	0.81465E15	$81.35 - 3.5 \ln \nu$
6	3^3S	3	22.718	0.4519E15	$12.69 - 1.54 \ln \nu$
7	3^1S	1	22.920	0.4031E15	$23.85 - 1.86 \ln \nu$
8	3^3P^o	9	23.006	0.3821E15	$49.30 - 2.60 \ln \nu$
9	3^3D+3^1D	20	23.073	0.3659E15	$85.20 - 3.69 \ln \nu$
11	3^1P^o	3	23.086	0.3628E15	$58.81 - 2.89 \ln \nu$

Data for the n = 1 and n = 2 levels were taken with modifications from Gingerich (1964), and the data for the n = 3 levels, from Hunger and van Blerkom (1967). The higher levels starting with n = 4 are treated hydrogenically with $g_n = 4n^2$, with $E_n = E(\text{He II}) - E(\text{H II})/n^2 = 24.587 - 13.595/n^2$, and with $n' = 4$.

The free-free opacity has been calculated by Peach (1967), but since it is approximately the same as the hydrogen value, we have used the latter.

The source function is the Planck function.

It would be straightforward to include the b factors for helium, as was done for hydrogen.

5.6 He II Bound-Free and Free-Free

The opacity is hydrogenic with Z = 2 and $n' = 10$, but $E_n = 54.403/n^2$, not $4(13.595)/n^2$. The source function is the Planck function. Inserting b factors would be easy.

5.7 He^- Free-Free

Carbon, Gingerich, and Latham (1969) give a polynomial fit to the free-free calculations of John (1968). The opacity is

$$\kappa_\nu = \frac{n(\text{He I}, n=1)}{\rho} n_e F_\nu(T) \quad ,$$

where

$$F_\nu(T) = aT + b + \frac{c}{T}$$

with

$$a = 3.397\text{E-}46 + (-5.216\text{E-}31 + 7.039\text{E-}15/\nu)/\nu \quad ,$$

$$b = -4.116\text{E-}42 + (1.067\text{E-}26 + 8.135\text{E-}11/\nu)/\nu \quad ,$$

and

$$c = 5.081\text{E-}37 + (-8.724\text{E-}23 - 5.659\text{E-}8/\nu)/\nu \quad .$$

5.8 He I Rayleigh Scattering

The cross section is from Dalgarno (1962):

$$\sigma_\nu = \frac{n(\text{He I}, n=1)}{\rho} \frac{5.484\text{E-}14}{\lambda^4} \left[1 + \frac{2.44\text{E}5}{\lambda^2} + \frac{5.94\text{E-}10}{\lambda^2(\lambda^2 - 2.90\text{E}5)}\right]^2 \quad ,$$

where

$$\lambda = \frac{2.997925\text{E}18}{\min(\nu, 5.15\text{E}15)} \quad .$$

The frequency cutoff keeps the expression from blowing up in a region where it is not valid.

5.9 Low-Temperature Absorbers

Opacities are included for C I, Mg I, Al I, and Si I. This is by no means a complete list of opacity sources, but these produce almost all the opacity at temperatures high enough so that molecules are not important, except perhaps for Fe I. A hydrogenic calculation for Fe I was done by Travis and Matsushima (1968), but there are large uncertainties in such an approximation, even for astronomers. For models of stars with "evolved" abundances, other opacity sources such as C^- should be investigated.

The opacity routines unfortunately have not been written in a form amenable to insertion of b's for statistical equilibrium calculations. We have included either only low terms that are strong absorbers or opacity tables that give cross sections per atom in the ground term. To rewrite the subroutines in b form, we should find experimental cross sections or calculate them one level at a time.

The best available opacity tables are the quantum-defect calculations by Peach (1970), which give the sum of bound-free and free-free cross sections per atom in the ground term. These tables are put into ATLAS by choosing temperatures at which the opacities are important and choosing the minimum number of frequencies necessary to represent the form of the opacity. These frequencies are both sides of any significant opacity discontinuity, the lowest and the highest frequency tabulated, and, if needed, extra points in the continuum of the ground state. The compact table that results from this procedure is converted to logarithms. To find the opacity for any T and ν, we linearly interpolate or extrapolate in terms of ln T and ln ν.

The C I cross sections are calculations from Henry (1970), but only the three lowest levels are included. The data for these levels follow:

Level	g_i	E_i	ν_i	α_i
^3P	9	0	2.7254E15	$1.219E-17\left[3.317\left(\frac{\nu_i}{\nu}\right)^2 - 2.317\left(\frac{\nu_i}{\nu}\right)^3\right]$
^1D	5	1.264	2.4196E15	$1.030E-17\left[2.789\left(\frac{\nu_i}{\nu}\right)^{3/2} - 1.789\left(\frac{\nu_i}{\nu}\right)^{5/2}\right]$
^1S	1	2.683	2.0761E15	$9.59E-18\left[3.501\left(\frac{\nu_i}{\nu}\right)^{3/2} - 2.501\left(\frac{\nu_i}{\nu}\right)^{5/2}\right]$

The Mg I opacity is from Peach's tables for 4000 to 10000 K. The levels that appear explicitly as discontinuities are the following:

Level	ν_i	Level	ν_i
3s ^{1}S	1.8488510E15	3d ^{1}D	4.5772110E14
3p ^{3}P	1.1925797E15	4p ^{3}P	4.1440977E14
3p ^{1}P	7.9804046E14	3d ^{3}D	4.1113514E14

Al I is represented only by the ground state for which the cross section at the limit was measured by W. Parkinson and E. Reeves (private communication to O. Gingerich and J. Rich) and for which the frequency dependence was guessed:

Level	g_i	E_i	ν_i	α_i
3p ^{2}P	6	0	1.443E15	$2.1\mathrm{E}{-17}\left(\frac{\nu_i}{\nu}\right)^3$

The levels of Si I opacity, from Peach's tables for 4000 to 12000 K, that appear explicitly as discontinuities are as follows:

Level	ν_i	Level	ν_i
3p^2 ^{3}P	1.9723165E15	4p ^{3}D	5.3295914E14
3p^2 ^{1}D	1.7879689E15	3d ^{3}F	4.7886458E14
3p^2 ^{1}S	1.5152920E15	4p ^{1}D	4.7216422E14
3d ^{1}D	5.5723927E14	3d ^{3}P	4.6185133E14

5.10 Intermediate-Temperature Absorbers

Opacities are included for N I, O I, Mg II, Si II, and Ca II; these should be significant mainly for evolved stars with low hydrogen abundance. Many more opacities could be included.

The N I cross sections are calculated from Henry, but only the three most important levels are included:

Level	g_i	E_i	ν_i	α_i
$^4S - {}^3P$	4	0	3.517915E15	$1.142\text{E-}17\left[4.29\left(\frac{\nu_i}{\nu}\right)^2 - 3.29\left(\frac{\nu_i}{\nu}\right)^3\right]$
$^2D - {}^3P$	10	2.384	2.941534E15	$4.41\text{E-}18\left[3.85\left(\frac{\nu_i}{\nu}\right)^{3/2} - 2.85\left(\frac{\nu_i}{\nu}\right)^{5/2}\right]$
$^2P - {}^3P$	6	3.575	2.653317E15	$4.2\text{E-}18\left[4.34\left(\frac{\nu_i}{\nu}\right)^{3/2} - 3.34\left(\frac{\nu_i}{\nu}\right)^{5/2}\right]$

The O I ground-state cross section is from Henry, but the frequency ν_i is defined equal to the hydrogen value:

Level	g_i	E_i	ν_i	α_i
^3P	9	0	3.28805E15	$2.94\text{E-}18\left[2.66\left(\frac{\nu_i}{\nu}\right) - 1.66\left(\frac{\nu_i}{\nu}\right)^2\right]$

The Mg II cross sections are fits to Peach's tables for the two lowest levels:

Level	g_i	E_i	ν_i	α_i
$3s\ ^2S$	2	0	3.635492E15	$1.40\text{E-}19\left[6.7\left(\frac{\nu_i}{\nu}\right)^4 - 5.7\left(\frac{\nu_i}{\nu}\right)^5\right]$
$3p\ ^2P$	6	4.43	2.564306E15	$5.11\text{E-}19\left(\frac{\nu_i}{\nu}\right)^3$

The Si II opacity is from Peach's tables for 10000 to 20000 K. The levels that appear explicitly as discontinuities are the following:

Level	ν_i	Level	ν_i
$3p\ ^2P$	3.9466738E15	$4d\ ^2D$	9.2378947E14
$3d\ ^2D$	1.5736321E15	$5p\ ^2P$	8.3825004E14
$4p\ ^2P$	1.5171539E15		

The Ca II cross sections are fits to Peach's tables for the lowest levels:

Level	g_i	E_i	ν_i	α_i
$4s\ ^2S$	2	0	2.870454E15	$5.4\text{E-}20\left(\frac{\nu_i}{\nu}\right)^3$
$3d\ ^2D$	10	1.697	2.460127E15	$1.64\text{E-}17\left(\frac{\nu_i}{\nu}\right)^{1/2}$
$4p\ ^2P$	6	3.142	2.110779E15	$4.13\text{E-}18\left[0.69\left(\frac{\nu_i}{\nu}\right)^3 + 0.31\left(\frac{\nu_i}{\nu}\right)^4\right]$

5.11 High-Temperature Absorbers

These are opacities for low-lying levels of C II-IV, N II-V, O II-VI, and Ne I-VI that all fall in the Lyman continuum of hydrogen and consequently are important only at temperatures high enough for the Lyman continuum to be somewhat transparent. The cross sections are from several sources, but mainly from Henry; some were fit to Hildago (1968, 1969), a few were taken from Peach, and one was taken from Flower (1968). All the cross sections are approximated by the expression

$$\alpha_\nu = \alpha_i\left[A_i\left(\frac{\nu_i}{\nu}\right)^{p/2} + (1-A_i)\left(\frac{\nu_i}{\nu}\right)^{1+p/2}\right] .$$

The following page lists the transitions in order of frequency.

5.12 Electron Scattering

We assume that the scattering is independent of angle,

$$\sigma_\nu = 6.653\text{E-}24\,\frac{n_e}{\rho} .$$

5.13 H_2 Rayleigh Scattering

The cross section is from Dalgarno (1962),

$$\sigma_\nu = \frac{n(H_2)}{\rho}\left(\frac{8.14\text{E-}13}{\lambda^4} + \frac{1.28\text{E-}6}{\lambda^6} + \frac{1.61}{\lambda^8}\right) ,$$

Code	Transition	g_i	E_i	ν_i	α_i	A_i	p_i	Reference
6.01	2P-3P	6	13.71	4.149945E+15	6.90E-18	1.000	6	PEACH
6.01	2S-3P	2	11.96	4.574341E+15	2.50E-18	1.000	4	
6.01	2D-3P	10	9.28	5.220770E+15	1.08E-17	1.000	4	
10.00	1S-2P	1	0.00	5.222307E+15	5.35E-18	3.769	2	HENRY
6.01	2P-1S	6	0.00	5.892577E+15	4.60E-18	1.950	6	
6.01	4P-3P	12	5.33	6.177022E+15	3.50E-18	1.000	4	PEACH
7.01	1S-2P	1	4.05	6.181062E+15	6.75E-18	3.101	5	HENRY
7.01	1D-2P	5	1.90	6.701879E+15	6.65E-18	2.789	5	
7.01	3P-2P	9	0.00	7.158382E+15	6.65E-18	2.860	6	
8.01	2P-3P	6	5.02	7.284488E+15	3.43E-18	4.174	5	
8.01	2D-3P	10	3.33	7.693612E+15	3.53E-18	3.808	5	
8.01	2P-1D	6	5.02	7.885955E+15	2.32E-18	3.110	5	
8.01	2D-1D	10	3.33	8.295079E+15	3.97E-18	3.033	5	
8.01	4S-3P	4	0.00	8.497686E+15	7.32E-18	3.837	5	
6.02	1P-2S	3	12.69	8.509966E+15	2.00E-18	1.750	7	HIDALGO
8.01	2P-1S	6	5.02	8.572854E+15	1.68E-18	3.751	5	HENRY
10.01	2P-3P	6	0.00	9.906370E+15	4.16E-18	2.717	3	
6.02	3P-2S	9	6.50	1.000693E+16	2.40E-18	1.750	7	HIDALGO
7.02	2D-3P	10	12.53	1.046078E+16	4.80E-18	1.000	4	
10.01	2P-1D	6	0.00	1.067157E+16	2.71E-18	2.148	3	HENRY
7.02	2P-1S	6	0.00	1.146734E+16	2.06E-18	1.626	6	
10.01	2P-1S	6	0.00	1.156813E+16	5.20E-19	2.126	3	
6.02	1S-2S	1	0.00	1.157840E+16	9.10E-19	4.750	4	HIDALGO
7.02	4P-3P	12	7.10	1.177220E+16	5.30E-18	1.000	4	
8.02	1S-2P	1	5.35	1.198813E+16	3.97E-18	2.780	6	HENRY
8.02	1D-2P	5	2.51	1.267503E+16	3.79E-18	2.777	6	
8.02	3P-2P	9	0.00	1.327649E+16	3.65E-18	2.014	6	
8.02	5S-4P	5	7.48	1.361466E+16	7.00E-18	1.000	2	HIDALGO
6.03	2P-1S	6	8.00	1.365932E+16	9.30E-19	1.500	7	
7.03	1P-2S	3	16.20	1.481487E+16	1.10E-18	1.750	7	
10.02	1S-2P	1	6.91	1.490032E+16	5.49E-18	3.000	5	HENRY
10.02	3P-4S	9	0.00	1.533389E+16	1.80E-18	2.277	4	
6.03	2S-1S	2	0.00	1.559452E+16	8.70E-19	3.000	6	HIDALGO
10.02	1D-2D	5	3.20	1.579688E+16	4.17E-18	2.074	4	HENRY
10.02	1D-2P	5	3.20	1.643205E+16	1.39E-18	2.792	5	
10.02	3P-2D	9	0.00	1.656208E+16	2.50E-18	2.346	5	
7.03	3P-2S	9	8.35	1.671401E+16	1.30E-18	1.750	7	HIDALGO
10.02	3P-2P	9	0.00	1.719725E+16	1.48E-18	2.225	5	HENRY
8.03	2D-3P	10	15.74	1.737839E+16	2.70E-18	1.000	4	HIDALGO
8.03	2P-1S	6	0.00	1.871079E+16	1.27E-18	.831	6	HENRY
7.03	1S-2S	1	0.00	1.873298E+16	9.10E-19	3.000	4	HIDALGO
8.03	4P-3P	12	8.88	1.903597E+16	2.90E-18	1.000	4	
10.03	4P-2S	12	22.84	2.060738E+16	4.60E-18	1.000	3	
7.04	2P-1S	6	9.99	2.125492E+16	5.90E-19	1.000	6	
10.03	2P-3P	6	7.71	2.162610E+16	1.69E-18	1.937	5	HENRY
10.03	2D-3P	10	5.08	2.226127E+16	1.69E-18	1.841	5	
10.03	2P-1D	6	7.71	2.251163E+16	9.30E-19	2.455	6	
8.04	3P-2S	9	10.20	2.278001E+16	7.90E-19	1.000	6	HIDALGO
10.03	2D-1D	10	5.08	2.317678E+16	1.65E-18	2.277	6	HENRY
10.03	4S-3P	4	0.00	2.348946E+16	3.11E-18	1.963	6	
10.03	2P-1S	6	7.71	2.351911E+16	7.30E-19	1.486	5	
7.04	2S-1S	2	0.00	2.366973E+16	5.00E-19	1.000	4	HIDALGO
8.04	1P-2S	3	19.69	2.507544E+16	6.90E-19	1.000	6	
8.04	1S-2S	1	0.00	2.754065E+16	7.60E-19	1.000	2	
10.04	1S-2P	1	7.92	2.864850E+16	1.54E-18	2.104	6	HENRY
10.04	1D-2P	5	3.76	2.965598E+16	1.53E-18	2.021	6	
10.04	3P-2P	9	0.00	3.054151E+16	1.40E-18	1.471	6	
10.04	5S-4P	5	11.01	3.085141E+16	2.80E-18	1.000	4	HIDALGO
8.05	2S-1S	2	0.00	3.339687E+16	3.60E-19	1.000	6	FLOWER
10.05	2P-1S	6	0.00	3.818757E+16	4.90E-19	1.145	6	HENRY

where

$$\lambda = \frac{2.997925E18}{\min(\nu, 2.922E15)}$$

and

$$n(H_2) = [n(H\ I)]^2 \exp\left(\frac{4.477}{kT} - 4.6628E1 + 1.8031E-3\ T - 5.0739E-7\ T^2 + 8.1424E-11\ T^3 - 5.0501E-15\ T^4 - 1.5 \ln T\right) , \qquad (4.62)$$

with $n(H\ I) \simeq [n(H\ I)/U(H\ I)]\ 2b_1$ at low temperatures.

5.14 H I Lines

The Stark-broadened line cross sections for $n < 5$ are calculated by a subroutine based on one by Deane Peterson. The theory comes from Griem (1960, 1967) and is strictly valid only for the wings of high-series members. Since various approximations are used for the line cores, this subroutine should be used only for calculating model atmospheres, where some error in opacity is allowable. It should not be used to calculate detailed line profiles for comparison with observation.

The cross section for each line is given by

$$\alpha_\nu(n \rightarrow m) = \frac{\pi e^2}{mc}\ f_{nm}\ P_\nu(|\nu - \nu_{nm}|)\ d\nu \quad , \qquad (5.11)$$

where f_{nm} is the Stark f value for the transition and P is the profile function normalized (ideally) so that

$$\int_{-\infty}^{\infty} P(|\nu - \nu_{nm}|)\ d\nu = 1 \quad . \qquad (5.12)$$

The Stark f value f_{nm} is tabulated by Underhill and Waddell (1959). It is less than the total f value for a line when n+m is odd because there is a line component that is not affected by electric fields and so is not Stark broadened. This component appears at line center with a Voigt profile, but as one of our approximations we ignore it in treating the line core. For large m, the Stark f value approaches the total f value, so the total f value is used for (m - n) > 10 by scaling from $f_{n, m+10}$ as

$$\left(\frac{m}{m^2 - n^2}\right)^3 \quad ,$$

based on Menzel and Pekeris (1935, eq. (1.31)).

The profile function P for Stark broadening by ions and electrons is given by the approximate expression

$$P\, d\nu = p(\beta) \frac{d\beta}{d\nu} R\, d\nu \quad , \tag{5.13}$$

where β is a variable chosen so that all lines have approximately the same profile p(β) dβ:

$$\beta = \frac{1.E8\ c\ \Delta\nu}{F_0 K_{nm} \nu_{nm}^2} \quad , \tag{5.14}$$

where

$$K_{nm} \simeq 5.5E\text{-}5 \frac{n^4 m^4}{m^2 - n^2} \tag{5.15}$$

(if m is small, there is a correction to K_{nm}), and where F_0 is the mean field produced by heavy ions,

$$F_0 = 1.25E\text{-}9\ n_i^{2/3} \quad , \tag{5.16}$$

assuming $n_i = n_e$. Also, the derivative $d\beta/d\nu$ converts the profile to frequency units, and R is a factor that accounts approximately for broadening by electrons. There are two regions where p and R have different expressions:

$$p(\beta) \simeq \frac{8}{80+\beta^3} \quad ,$$

$$R = Q + I \quad , \qquad \text{for} \quad \beta < 20 \quad ; \tag{5.17}$$

and

$$p(\beta) \simeq 1.5\, \beta^{-5/2} \quad ,$$

$$R = Q(1+D) + I \quad , \qquad \text{for} \quad \beta \geq 20 \quad . \tag{5.18}$$

In the above,

$$Q = 1 + \frac{2}{\sqrt{\pi}} \int_0^{y_1} y^{1/2}\, e^{-y}\, dy \simeq 1.5 + 0.5\, \frac{y_1^2 - 1.384}{y_1^2 + 1.384} \quad , \tag{5.19}$$

with

$$y_1 = m^2 \frac{h\Delta\nu}{2kT} \quad ;$$

$$I = \left(\frac{4}{\pi}\right)^{3/2} y_1^{1/2} \left[0.4\, e^{-y_1} + E_1(y_1) - \frac{1}{2} E_1(y_2)\right] \left(1 - \frac{n^2}{m^2}\right)^{1/2} \quad , \tag{5.20}$$

with

$$y_2 = \frac{\pi\, m_e (\Delta\nu)^2}{2e^2\, n_e}$$

and E_1 the exponential integral; and

$$D = 2\pi a_0^3 n_e \left(2m^2 \frac{3.28805E15}{\Delta\nu}\right)$$

$$\times \left[\left(2m^2 \frac{3.28805E15}{\Delta\nu}\right)^{1/2} (1.3Q + 0.30\,I) - 3.9 \frac{3.28805E15\,h}{kT}\right] \quad . \qquad (5.21)$$

We now discuss overlapping lines. If ν is near one of the first lines in a series, we need to consider the effects of only one or two lines, but as we approach the series limit the lines overlap to such an extent that they form a pseudocontinuum with the continuum cross section. The last observable line has been estimated by Griem (1964, eq. (5.46)):

$$m_s = \frac{1100}{n_e^{2/15}} \quad . \qquad (5.22)$$

To find a lower and an upper m to limit the summation over lines, we proceed as follows: We find n from the relation

$$n = \sqrt{\frac{3.28805E15}{\nu}}$$

and the nearest m (on the low-frequency side) from

$$m* = \sqrt{\frac{3.28805E15}{(3.28805E15/n^2) - \nu}} \quad .$$

Then we take

$$\left.\begin{aligned} m_\ell &= \max(m^*, n+1) \quad , \\ m_u &= m^* + 1 \quad , \end{aligned}\right\} \quad \text{for} \quad m^* \leq 6 \quad ,$$

and

$$m_\ell = m^* - 1 \ , \qquad m_u = m^* + 4 \ , \qquad \text{for } 6 < m^* \le m_s \ ;$$

if $m > m_s$, we use the bound-free cross section at the limit ν_n (as computed in Section 5.1). A complication arises when n=4 and m=8 or 9 because Paschen α also falls in the same region; so Paschen α is added separately.

The absorption coefficient (in a simple case) is finally

$$\kappa_\nu = \frac{n(\mathrm{H\ I})}{\rho} \frac{2n^2 b_n}{U(\mathrm{H\ I})} e^{-E_n/kT} \sum_{m=m_\ell}^{m_u} \alpha_\nu(n \to m) \left[1 - \left(\frac{b_m}{b_n}\right) e^{-(E_m - E_n)/kT}\right] \ ,$$

and the source function is

$$S_\nu = \frac{1}{\kappa_\nu} \sum \kappa_\nu(n \to m) \left[1 - \frac{b_m}{b_n} e^{-(E_m - E_n)/kT}\right] \frac{2h\nu^3/c^2}{(b_n/b_m)\, e^{h\nu/kT} - 1} \ .$$

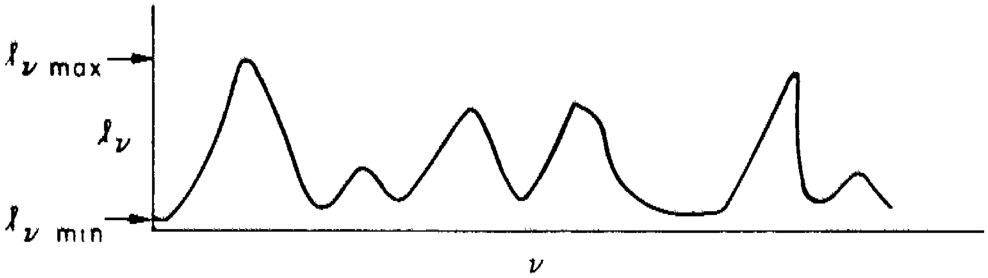
5.15 Line-Absorption Distribution Functions

The remaining opacities are included in ATLAS only as dummy subroutines either because the work has not yet been completed (for distribution functions, helium lines, etc.) or because these opacities are designed to be experimental or to satisfy some objective other than computing a model atmosphere.

We do not need to know the opacity explicitly at every frequency in order to calculate a model atmosphere, because the structure of the atmosphere is determined by integrals that depend not so much on the details of the spectrum but more on its average properties. If only continuum opacities are considered, the integrals can be evaluated accurately by sampling at relatively few frequency points By adopting a line-absorption distribution function, we obtain the same simplification when line opacities are included

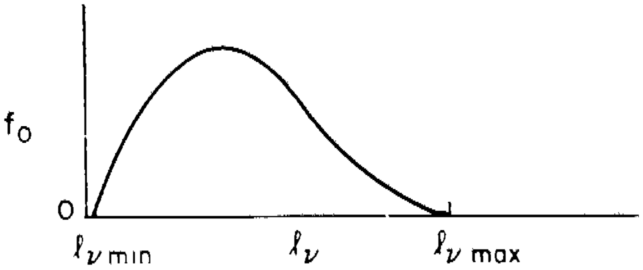
A distribution function can be found and then presented to ATLAS in a subroutine. We choose an interval (not necessarily related to the integration frequencies) for which we want an "average" opacity and compute the line opacity for the whole region as a function of temperature, pressure, electron number, and microturbulence,

106-048



We could take a distribution function f_0 for the fraction of the interval that has ℓ_ν between ℓ_ν and $\ell_\nu + \Delta\ell_\nu$,

106-048



but for our purposes, we take the distribution function in the form where f is the fraction of the interval with opacity ℓ_ν or less,

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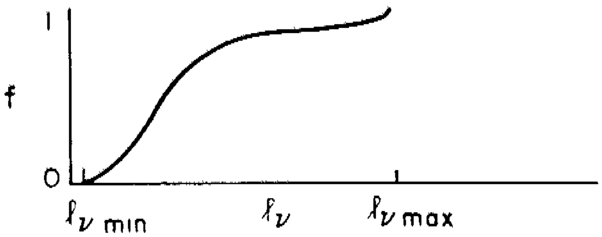

because we can invert this to get something that looks like a line profile:

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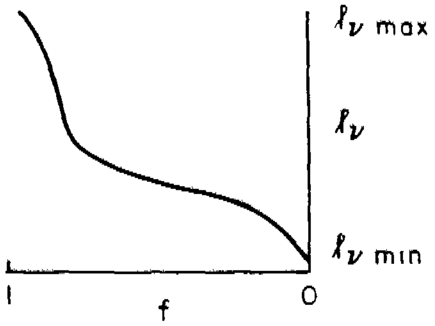


We can describe these last two figures more mathematically. We have

$$f(\ell_\nu) = \int_0^{\ell_\nu} f_0(\ell)\, d\ell \tag{5.23}$$

so that

$$f(0) = f(\ell_{\nu\,\min}) = 0$$

and

$$f(\infty) = f(\ell_{\nu\,\max}) = 1 \quad .$$

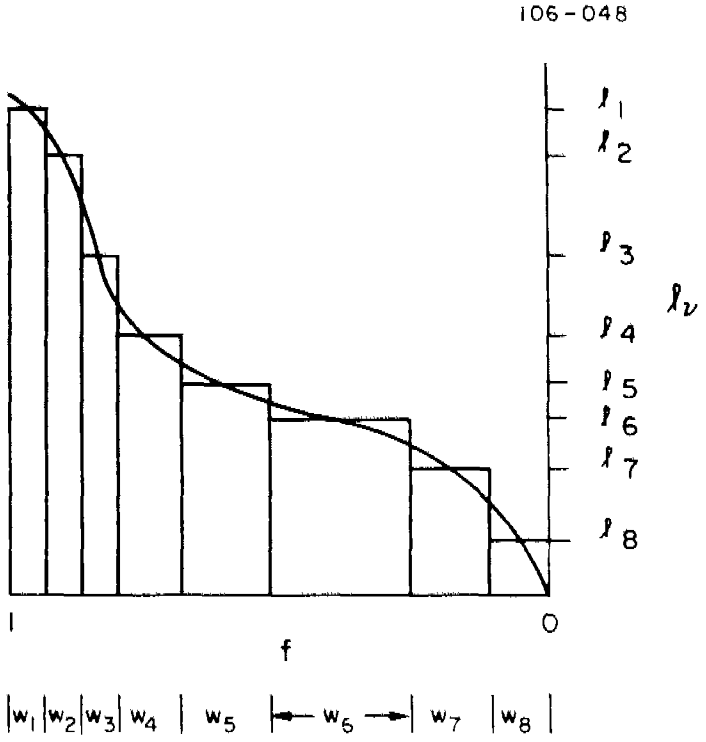
Since the distribution function $f(\ell_\nu)$ is monotonic, the inverse relation $\ell_\nu(f)$ is well defined. The end points are then

$$\ell_\nu(1) = \ell_{\nu\,\max}$$

and

$$\ell_\nu(0) = \ell_{\nu\,\min} \quad .$$

For computation, we represent the distribution function f by n steps, the number and width of which must be empirically determined,

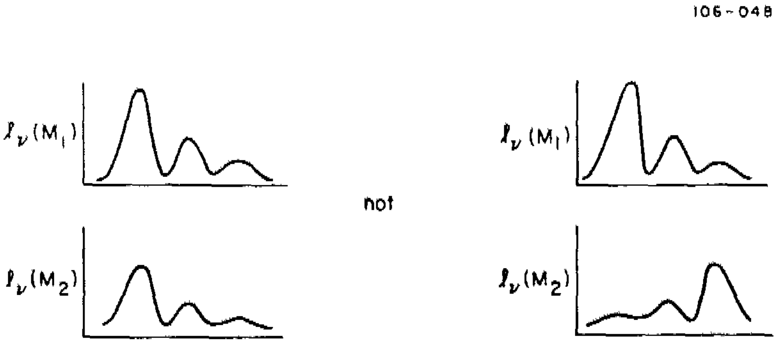


If ATLAS requests line opacity for a frequency in the interval covered by the distribution function, we tell ATLAS the number of steps n and the values of w_i and ℓ_i. Then ATLAS calculates $\tau_\nu(\ell_i)$, $S_\nu(\ell_i)$, $J_\nu(\ell_i)$, and $H_\nu(\ell_i)$ and includes w_i in frequency integrals

$$I = \int \sum_{i=1}^{n} w_i \, I_\nu(\ell_i) \, d\nu \quad , \tag{5.24}$$

assuming the line source function is B_ν. The w_i's must be constant with depth at any given frequency in order for ATLAS to be able to calculate the radiation field.

In representing lines by distribution functions, we make two implicit physical assumptions. The first is that the absorption-coefficient spectrum has the same relative shape at all depths M_j where line opacity is important:

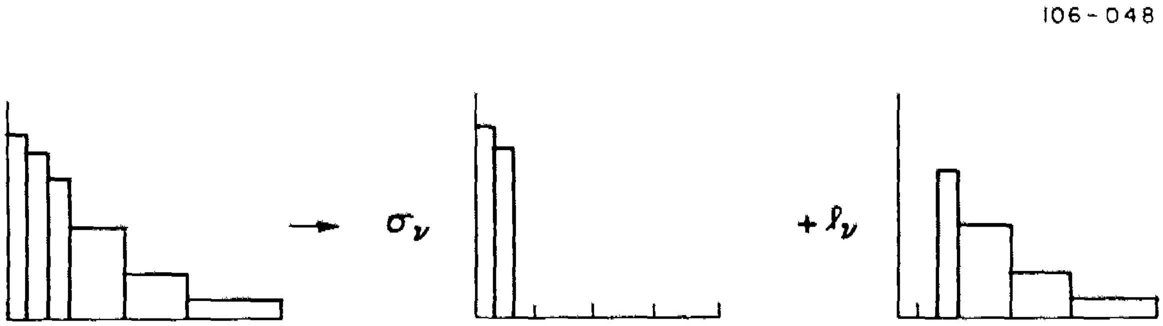


These two cases have identical distribution functions. In the second case, the distribution function predicts the wrong optical depths. The only way to investigate this effect is to compare distribution-function calculations to explicit line calculations.

The second assumption is either that lines of different strengths are uniformly distributed throughout the interval or that the continuum source function and opacity do not vary radically over the frequency interval to which the distribution function applies, so that it makes no difference where in the interval the lines appear. If the interval for the distribution function is chosen such that $\Delta\nu/\nu \lesssim$ 5 to 10%, this assumption should be no problem.

5.16 Line-Scattering Distribution Functions

If we desire that high-opacity regions have $S_\nu \simeq J_\nu$, we can take our previous distribution function and replace the first step or steps ℓ_1 by σ_i:



This approach might be used, for example, to get a qualitative estimate of the effect of detailed line-transfer calculations for strong lines.

5.17 Other or Experimental Absorption Lines

Lines can be calculated explicitly. For example, we can put in several metal lines with Voigt profiles or helium lines with Stark broadening. The source function is arbitrary.

5.18 Other or Experimental Scattering Lines

We might experiment to see what happens if we treat the cores of several strong lines as scattering.

5.19 Other or Experimental Continuous Absorbers

We might want to test the importance of C^-, etc. The source function is arbitrary.

5.20 Other or Experimental Continuous Scatterings

We might want to test the importance of C Rayleigh scattering, etc.

6. CONVECTIVE ENERGY TRANSPORT

Radiation is not the only means available for transporting energy through the atmosphere. If the gradient $(-dT/dx)$ is greater than the adiabatic gradient $(-dT/dx)_A$, the gas is convectively unstable and convection can carry energy by moving hot gas elements into cooler regions. Unfortunately, convection is not well understood, so most researchers resort to an elaborate but essentially dimensional analysis called the mixing-length theory. We present here only a crude dimensional analysis and the relevant results (see Cox and Guili, 1968, for details). The constants are traditional.

The mixing-length theory assumes that the convective elements are rising and falling bubbles. The bubbles, of diameter ℓ, rise a distance ℓ while radiating part of their energy and finally merge into the background. Since ℓ varies through the atmosphere, the ratio ℓ/h is usually specified, where $h = P_{total}/\rho g$ is the pressure scale height (eq. (4.47)). The ratio of mixing length to scale height, ℓ/h, is generally prescribed as a constant such as 1 or 2.

Gradients are usually expressed as logarithmic derivatives $d \ln T/d \ln P \equiv \nabla$ such that

$$-\frac{dT}{dx} = \rho g T \frac{d \ln T}{dP} = \frac{T}{h} \nabla \quad . \tag{6.1}$$

The convective bubbles would follow the adiabatic gradient ∇_A, but radiative losses force a value nearer the average gradient ∇, so

$$\nabla > \nabla_B > \nabla_A \quad . \tag{6.2}$$

The convective flux is obtained through the following argument: In rising a distance ℓ, the bubble (of fixed mass) becomes hotter than its surroundings by an amount ΔT,

$$\Delta T = \left[\left(\frac{-dT}{dx}\right) - \left(\frac{-dT}{dx}\right)_B \right] \ell = (\nabla - \nabla_B)\left(\frac{\ell}{h}\right) T \quad . \tag{6.3}$$

If we multiply by the specific heat at constant pressure, we find the excess energy per unit mass ΔE,

$$\Delta E = \Delta T \, C_P = (\nabla - \nabla_B)\left(\frac{\ell}{h}\right) T \, C_P \quad . \tag{6.4}$$

This energy is converted to a flux by multiplying by ρv_{conv}, where v_{conv} is the bubble velocity,

$$\text{flux} \sim (\nabla - \nabla_B)\left(\frac{\ell}{h}\right) T \, C_P \, \rho v_{conv} \quad .$$

The "exact" expression is

$$4\pi H_{conv} = \frac{1}{2}\left(\frac{\ell}{h}\right) \rho \, C_P \, T \, v_{conv} \, (\nabla - \nabla_B) \quad , \tag{6.5}$$

but we still need to evaluate v_{conv} and $(\nabla - \nabla_B)$.

An expression for the convective velocity is found by considering the force on a bubble when its density is slightly changed. The equation of motion is

$$\frac{d^2x}{dt^2} = -g - \frac{1}{\rho}\frac{dP}{dx} \quad . \tag{4.1'}$$

If there were no density change, d^2x/dt^2 would equal 0, but with $\rho \rightarrow \rho[1 + (\Delta\rho/\rho)]$, the acceleration is

$$\frac{d^2x}{dt^2} = -g - \frac{1}{\rho}\frac{dP}{dx} + \frac{\Delta\rho}{\rho^2}\frac{dP}{dx} = \frac{-\Delta\rho}{\rho} g \quad . \tag{6.6}$$

This acceleration corresponds to a force $-g \, \Delta\rho$ that acts for an average distance ℓ to produce an average kinetic energy for the bubble of $-g\ell \, \Delta\rho$. Then,

$$\rho v_{conv}^2 \sim -g\ell \, \Delta\rho \quad . \tag{6.7}$$

To "evaluate" $\Delta\rho$, we relate it to ΔT and finally to $(\nabla - \nabla_B)$ through equation (6.3),

$$\frac{\Delta\rho}{\rho} = \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P \frac{\Delta T}{T} = \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P (\nabla - \nabla_B)\left(\frac{\ell}{h}\right) . \tag{6.8}$$

Then from equations (6.7) and (6.8),

$$v^2_{\rm conv} \sim -g\ell \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P (\nabla - \nabla_B)\left(\frac{\ell}{h}\right) . \tag{6.9}$$

The "exact" value for the convective velocity is

$$v_{\rm conv} = \sqrt{-\frac{1}{8} gh \left(\frac{\ell}{h}\right)^2 \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P (\nabla - \nabla_B)} . \tag{6.10}$$

An elaborate argument is required to find $(\nabla - \nabla_B)$. We evaluate the ratio of the radiative loss while the bubble rises to the excess bubble energy when the bubble merges. We know that the excess bubble energy is proportional to $(\nabla - \nabla_B)$. If there were no radiative losses, ∇_B would equal ∇_A and the excess energy would be proportional to $(\nabla - \nabla_A)$. Then, $[(\nabla - \nabla_A) - (\nabla - \nabla_B)]/(\nabla - \nabla_B)$ must equal the ratio of radiative loss to excess bubble energy. We can also "calculate" the radiative loss directly. We make the approximation that the bubbles are optically thick. Then from equation (2.87), the radiative flux satisfies the relation

$$4\pi \int H_\nu \, d\nu \simeq 4\pi \frac{4\sigma T^3}{3\pi} \frac{dT}{d\tau_{\rm Ross}} = \frac{16}{3} \frac{\sigma T^3}{\kappa_{\rm Ross}\,\rho} \frac{dT}{dx} .$$

The radiative loss is the flux times the area times the lifetime of each bubble:

$$\sim \frac{16}{3} \frac{\sigma T^3}{\kappa_{\rm Ross}\,\rho} \frac{\Delta T}{\ell/2} A \frac{\ell}{v_{\rm conv}} , \tag{6.11}$$

where $\ell/2$ is the "radius," and A the "area," and $\ell/v_{\rm conv}$ the lifetime of the bubble. The excess bubble energy is the excess energy per unit mass (eq. (6.4)) times the mass of each bubble,

$$(\Delta T\, C_P)(\rho V) , \tag{6.12}$$

where V is the bubble "volume." The ratio of the two energies (6.11) and (6.12) is

$$\frac{(\nabla - \nabla_A) - (\nabla - \nabla_B)}{(\nabla - \nabla_B)} = \frac{[(16\sigma T^3/3)/\kappa_{\text{Ross}}\,\rho]\,(\Delta T/\ell)\,A\,(\ell/v_{\text{conv}})}{\Delta T\,C_P\,\rho V}$$

$$= \frac{16\sigma T^3/3}{\kappa_{\text{Ross}}\,\rho\,C_P\,\rho v_{\text{conv}}}\;\frac{A}{V} \quad .$$

Since $A/V \sim 1/\ell$ and we know v_{conv} from equation (6.10), we find

$$\frac{(\nabla - \nabla_A) - (\nabla - \nabla_B)}{(\nabla - \nabla_B)} = \frac{32\sqrt{2}\,\sigma T^3}{\kappa_{\text{Ross}}\,\rho\ell\,C_P\,\rho\sqrt{-(1/8)\,gh\,(\ell/h)^2(\partial\ln\rho/\partial\ln T)_P(\nabla - \nabla_B)}} \;, \tag{6.13}$$

where we have inserted the "exact" constant $32\sqrt{2}$. To simplify this equation, we define

$$D = \frac{1}{2}\left[\frac{32\sqrt{2}\,\sigma T^3}{\kappa_{\text{Ross}}\,\rho h C_P\,(\ell/h)\,\rho\sqrt{-(1/8)\,gh\,(\ell/h)^2(\partial\ln\rho/\partial\ln T)_P}}\right]^2 \tag{6.14}$$

so that

$$[(\nabla - \nabla_B) - (\nabla - \nabla_A)]^2 = 2D(\nabla - \nabla_B) \quad .$$

The solution is

$$(\nabla - \nabla_B) = D + (\nabla - \nabla_A) - \sqrt{[D + (\nabla - \nabla_A)]^2 - (\nabla - \nabla_A)^2} \tag{6.15}$$

or, expressed as a power series to avoid truncation problems,

$$(\nabla - \nabla_B) = [D + (\nabla - \nabla_A)] \left[\frac{(\nabla - \nabla_A)}{D + (\nabla - \nabla_A)}\right]^2 \left\{ \frac{1}{2} + \frac{1 \cdot 1}{2 \cdot 4} \left[\frac{(\nabla - \nabla_A)}{D + (\nabla - \nabla_A)}\right]^2 + \frac{1 \cdot 1 \cdot 3}{2 \cdot 4 \cdot 6} \left[\frac{(\nabla - \nabla_A)}{D + (\nabla - \nabla_A)}\right]^4 + \cdots \right\} . \qquad (6.16)$$

In summary:

Convective flux,

$$4\pi H_c = \frac{1}{2} \left(\frac{\ell}{h}\right) \rho C_P T v_{conv} (\nabla - \nabla_B) . \qquad (6.5)$$

Convective velocity,

$$v_{conv} = \sqrt{-\frac{1}{8} gh \left(\frac{\ell}{h}\right)^2 \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P (\nabla - \nabla_B)} . \qquad (6.10)$$

Bubble gradient,

$$(\nabla - \nabla_B) = D + (\nabla - \nabla_A) - \sqrt{[D + (\nabla - \nabla_A)]^2 - (\nabla - \nabla_A)^2} , \qquad (6.15)$$

with

$$D = \frac{1}{2} \left[\frac{32\sqrt{2}\, \sigma T^3}{\kappa_{Ross}\, \rho h C_P (\ell/h)\, \rho \sqrt{-(1/8)\, gh (\ell/h)^2 (\partial \ln \rho/\partial \ln T)_P}}\right]^2 . \qquad (6.14)$$

The derivatives C_P, ∇_A, and $(\partial \ln \rho/\partial \ln T)_P$ are discussed in Section 4.6.

7. THE TEMPERATURE CORRECTION

7.1 Introduction

In general, the trial temperature distribution that we have used to calculate the radiation field will not have produced the desired total flux

$$\mathcal{H} = \frac{\sigma T_{\mathrm{eff}}^4}{4\pi} \quad . \tag{7.1}$$

There will be a flux error

$$\Delta H = \mathcal{H} - \int H_\nu \, d\nu - H_{\mathrm{conv}} \tag{7.2}$$

that we must attempt to reduce by modifying the temperature distribution.

We begin by considering the case where there is no convective flux (so the algebra is simple). Since most of the flux we see at the surface comes from the region where the atmosphere is just becoming optically thick, roughly $0.1 \leq \tau \leq 2.0$, the temperature at shallow layers cannot greatly affect the flux. Consequently, it is very difficult to use the flux errors near the surface to derive temperature changes. The flux derivative

$$\frac{dH_\nu}{d\tau_\nu} = J_\nu - S_\nu \tag{2.32}$$

is, however, sensitive to the temperature in the optically thin region and can be used to obtain temperature corrections near the surface by forcing the proper flux derivative up from the optically thick region where the temperature is known. A correction based on the flux derivative is called a Λ correction from the operator used to calculate J_ν.

A temperature correction can be derived by perturbing or expanding a moment of the transfer equation to get a first-order equation. Then a workable temperature correction is found by making some approximation to simplify the first-order equation. The temperature correction need not be very accurate, because successive iterations of the model remove small errors. It should be emphasized that the criterion for judging the effectiveness of a temperature correction is the total amount of computer time needed to calculate a model. Mathematical rigor is irrelevant. Any empirically derived tricks for speeding convergence are completely justified.

In ATLAS we use a flux correction related to one derived by Avrett and Krook (1963) and a Λ correction that is an approximation to an integral-equation temperature correction derived by Böhm-Vitense (1964). We also include a term to smooth out the region where the two operations overlap.

7.2 The Flux Correction

To derive the flux correction, we start with the second moment of the transfer equation

$$\frac{dK_\nu}{d\tau_\nu} = H_\nu \tag{2.33}$$

and rewrite it in terms of rhox

$$\frac{dK_\nu}{dM} = (\kappa_\nu + \sigma_\nu)\, H_\nu \quad . \tag{7.3}$$

Then we perturb with the substitutions

$$K_\nu \rightarrow K_\nu + \Delta K_\nu \quad ,$$

$$M \rightarrow M + \Delta M \quad ,$$

$$(\kappa_\nu + \sigma_\nu) \rightarrow (\kappa_\nu + \sigma_\nu) + \Delta(\kappa_\nu + \sigma_\nu) \quad ,$$

and

$$H_\nu \rightarrow H_\nu + \Delta H_\nu$$

to obtain the first-order equation

$$\frac{d\Delta K_\nu}{dM} = (\kappa_\nu + \sigma_\nu)\, \Delta H_\nu + \Delta(\kappa_\nu + \sigma_\nu)\, H_\nu + (\kappa_\nu + \sigma_\nu)\, H_\nu \,\frac{d\Delta M}{dM} \quad . \tag{7.4}$$

If we can solve equation (7.4) for ΔM, we can find ΔT through

$$\Delta T = - \frac{dT}{dM} \Delta M \quad .$$

We know H_ν, $(\kappa_\nu + \sigma_\nu)$, and $\Delta H = H - \mathcal{H}$, but we do not know ΔH_ν, $\Delta(\kappa_\nu + \sigma_\nu)$, or ΔK_ν, so we must eliminate reference to them. We divide equation (7.4) by $(\kappa_\nu + \sigma_\nu)$ to isolate ΔH_ν, then integrate over frequency to obtain ΔH, and finally assume that

$$\int \frac{1}{(\kappa_\nu + \sigma_\nu)} \frac{d\Delta K_\nu}{dM}\, d\nu = \int \frac{\Delta(\kappa_\nu + \sigma_\nu)}{(\kappa_\nu + \sigma_\nu)} H_\nu \, d\nu \quad . \tag{7.5}$$

We are left with a differential equation for ΔM

$$H \frac{d\Delta M}{dM} = H - \mathcal{H} \quad , \tag{7.6}$$

for which the solution, setting $\Delta M(0) = 0$, is

$$\Delta M = \int_0^M \frac{H(y) - \mathcal{H}(y)}{H(y)}\, dy \quad . \tag{7.7}$$

The final flux correction is

$$\Delta T_{\text{flux}} = - \frac{dT}{dM} \Delta M \quad . \tag{7.8}$$

We now consider the flux correction when convection is included. We rewrite the expressions for the convective flux given in Section 6 so that the dependence on T and ∇ is obvious,

$$H_{\text{conv}} = A\,T \, \frac{(\nabla - \nabla_A)^3}{\left[BT^6 + (\nabla - \nabla_A)\right]^{3/2}} \, \Sigma^{3/2} \quad , \tag{7.9}$$

where

$$A = \frac{1}{4\pi} \, \frac{1}{2} \, \rho \, C_P \, T \left(\frac{\ell}{h}\right) \sqrt{\frac{1}{8} \, gh \left(\frac{\ell}{h}\right)^2 \left(\frac{d \ln \rho}{d \ln T}\right)_P} \quad ,$$

$$B = \frac{D}{T^6} = \frac{1}{2} \left[\frac{32\sqrt{2}\, \sigma}{\kappa_{\text{Ross}} \, \rho \, h \, C_P (\ell/h) \, \rho \sqrt{(1/8)\, gh(\ell/h)^2 \, (d \ln \rho / d \ln T)_P}} \right]^2 \quad ,$$

and

$$\Sigma = \frac{1}{2} + \frac{1 \cdot 1}{2 \cdot 4} \left[\frac{(\nabla - \nabla_A)}{BT^6 + (\nabla - \nabla_A)} \right]^2 + \frac{1 \cdot 1 \cdot 3}{2 \cdot 4 \cdot 6} \left[\frac{(\nabla - \nabla_A)}{BT^6 - (\nabla - \nabla_A)} \right]^4 + \cdots \quad .$$

We obtain a temperature correction by expanding T and ∇ to first order in ΔT and by assuming that the ΔT dependence of Σ is negligible and that all other quantities are independent of ΔT.

The expansion for the flux is

$$\begin{aligned} H_{\text{conv}} + \Delta H_{\text{conv}} &= A\,(T + \Delta T) \left[(\nabla - \nabla_A) + \frac{d\Delta T/T}{d \ln P} \right]^3 \\ &\quad \times \left[B\,T^6 + 6\,BT^5 \, \Delta T + (\nabla - \nabla_A) + \frac{d\Delta T/T}{d \ln P} \right]^{-3/2} \Sigma^{3/2} \quad , \end{aligned} \tag{7.10}$$

where for ∇ we have simplified

$$\nabla = \frac{d \ln T}{d \ln P} \rightarrow \frac{d \ln (T + \Delta T)}{d \ln P} = \frac{d \ln T[1 + (\Delta T/T)]}{d \ln P} = \nabla + \frac{d\Delta T/T}{d \ln P} \quad .$$

Continuing the algebra,

$$H_{conv} + \Delta H_{conv} = A\ T\left(1 + \frac{\Delta T}{T}\right) \frac{(\nabla - \nabla_A)^3}{\left[BT^6 + (\nabla - \nabla_A)\right]^{3/2}} \left(1 + \frac{d\Delta T/T}{d \ln P}\right)$$

$$\times \left\{1 + \frac{(BT^6\ \Delta T/T) + [(d\Delta T/T)/d \ln P]}{BT^6 + (\nabla - \nabla_A)}\right\}^{-3/2} \Sigma^{3/2} \quad ,$$

and to first order,

$$\Delta H_{conv} = H_{conv} \frac{\Delta T}{T} + H_{conv} \left\{\frac{(3/2)[(d\Delta T/T)/d \ln P]}{(\nabla - \nabla_A)} - \frac{(3/2)[(d\Delta T/T)/d \ln P]}{D + (\nabla - \nabla_A)} - \frac{9D\ \Delta T/T}{D + (\nabla - \nabla_A)}\right\} \quad .$$

This differential equation can be written more clearly as

$$\Delta H_{conv} = H_{conv} \frac{\Delta T}{T} \left[1 - \frac{9D}{D + (\nabla - \nabla_A)}\right] + H_{conv} \frac{(3/2)[(d\Delta T/T)/d \ln P]}{(\nabla - \nabla_A)} \left[1 + \frac{D}{D + (\nabla - \nabla_A)}\right] \quad . \tag{7.11}$$

We have found that when H_{conv} is large, the terms containing D can be ignored because $D \ll (\nabla - \nabla_A)$.

To obtain a single expression involving both the radiative and the convective flux, we change the variable from ΔT to ΔM and add ΔH_{conv} to the differential equation for ΔM that we found earlier. We substitute $\Delta T = -dT/dM\ \Delta M$ into the equation for ΔH_{conv}, while noting that

$$\frac{d}{d\ln P}\left(\frac{dT}{dM}\,\frac{\Delta M}{T}\right) = \Delta M\,\frac{d^2\ln T}{d\ln P\,dM} + \frac{d\ln T}{dM}\,\frac{dM}{d\ln P} = \Delta M\,\frac{d\nabla}{dM} + \nabla\,\frac{d\Delta M}{dM} \quad ,$$

to obtain

$$\Delta H_{\mathrm{conv}} = -H_{\mathrm{conv}}\,\frac{dT}{dM}\,\frac{1}{T}\left\{\left[1-\frac{9D}{D+(\nabla-\nabla_A)}\right] + \frac{(3/2)\,(d\nabla/dM)}{(\nabla-\nabla_A)}\left[1+\frac{D}{D+(\nabla-\nabla_A)}\right]\right\}\Delta M$$

$$-\,H_{\mathrm{conv}}\,\frac{(3/2)\nabla}{(\nabla-\nabla_A)}\left[1+\frac{D}{D+(\nabla-\nabla_A)}\right]\frac{d\Delta M}{dM} \quad . \qquad (7.12)$$

The combined differential equation for ΔM is

$$\left\{H_{\mathrm{rad}} + H_{\mathrm{conv}}\,\frac{(3/2)\nabla}{(\nabla-\nabla_A)}\left[1+\frac{D}{D+(\nabla-\nabla_A)}\right]\right\}\frac{d\Delta M}{dM}$$

$$+\,H_{\mathrm{conv}}\left\{\frac{dT}{dM}\,\frac{1}{T}\left[1-\frac{9D}{D+(\nabla-\nabla_A)}\right] + \frac{(3/2)\,(d\nabla/dM)}{(\nabla-\nabla_A)}\left[1+\frac{D}{D+(\nabla-\nabla_A)}\right]\right\}\Delta M$$

$$= H_{\mathrm{rad}} + H_{\mathrm{conv}} - \mathcal{H} \quad . \qquad (7.13)$$

The solution is

$$\Delta M = \int_0^M \frac{g(y)}{g(M)}\,\frac{H_{\mathrm{rad}} + H_{\mathrm{conv}} - \mathcal{H}}{H_{\mathrm{rad}} + H_{\mathrm{conv}}\,[(3/2)\nabla/(\nabla-\nabla_A)]\left(1+\{D/[D+(\nabla-\nabla_A)]\}\right)}\,dy \ , \qquad (7.14)$$

where

$$g(y) = \exp\left(\int_0^y \frac{\text{coef of }\Delta M}{\text{coef of }d\Delta M/dM}\,dy\right) \quad .$$

Since the derivation of ΔM was only to first order, ΔM may not be valid for large flux errors. To prevent difficulties, we establish the limits

$$-\frac{1}{2}\frac{\tau_{\mathrm{Ross}}}{\kappa_{\mathrm{Ross}}} \leq \Delta M \leq \frac{\tau_{\mathrm{Ross}}}{\kappa_{\mathrm{Ross}}} \quad . \tag{7.15}$$

7.3 The Λ Correction

To derive the Λ correction for the case of no convection, we start with the moment equation

$$\frac{dH_\nu}{d\tau_\nu} = J_\nu - S_\nu \quad , \tag{2.32}$$

or

$$\frac{dH_\nu}{dM} = (\kappa_\nu + \sigma_\nu)\,(J_\nu - S_\nu) \quad , \tag{7.16}$$

and express it in the form of an operator equation. Since S_ν is given by the relation

$$S_\nu = (I - \alpha_\nu \Lambda_\nu)^{-1}\,(I - \alpha_\nu)\,B_\nu \quad , \qquad \text{(from 2.67)}$$

we have

$$\frac{dH_\nu}{dM} = (\kappa_\nu + \sigma_\nu)\,(\Lambda_\nu - I)\,(I - \alpha_\nu \Lambda_\nu)^{-1}\,(I - \alpha_\nu)\,B_\nu \quad . \tag{7.17}$$

We expand B_ν in terms of ΔT,

$$B_\nu \rightarrow B_\nu + \frac{dB_\nu}{dT}\,\Delta T \quad , \tag{7.18}$$

but we ignore any ΔT dependence in the functions $(\kappa_\nu + \sigma_\nu)$, Λ_ν, and a_ν. Consequently, we have

$$\frac{d\mathcal{H}_\nu}{dM} = (\kappa_\nu + \sigma_\nu)\,(\Lambda_\nu - I)\,(I - a_\nu \Lambda_\nu)^{-1}\,(I - a_\nu)\left(B_\nu + \frac{dB_\nu}{dT}\,\Delta T\right) ,$$

or for the error in the flux derivative,

$$\frac{d\mathcal{H}_\nu}{dM} - (\kappa_\nu + \sigma_\nu)\,(J_\nu - S_\nu) = (\kappa_\nu + \sigma_\nu)\,(\Lambda_\nu - I_\nu)\,(I - a_\nu\Lambda_\nu)^{-1}\,(I - a_\nu)\,\frac{dB_\nu}{dT}\,\Delta T \quad . \tag{7.19}$$

We integrate equation (7.19) over frequency to remove the frequency dependence of ΔT,

$$\frac{d\mathcal{H}}{dM} - \int (\kappa_\nu + \sigma_\nu)\,(J_\nu - S_\nu)\,d\nu = \int (\kappa_\nu + \sigma_\nu)\,(\Lambda_\nu - I_\nu)\,(I - a_\nu\Lambda_\nu)^{-1}\,(I - a_\nu)\,\frac{dB_\nu}{dT}\,d\nu\,\Delta T \quad . \tag{7.20}$$

This equation can be solved explicitly (cf. Peterson, 1969), but it is extremely time-consuming to evaluate the Λ operator and the inverse operators. Instead, we settle for an approximation – we ignore all but the diagonal matrix elements. This is possible because the off-diagonal elements are small, at least in the upper layers of the atmosphere where the correction is relevant. The inverse $(I - a_\nu\Lambda_\nu)^{-1}$ becomes $(1 - a_\nu \Lambda_{\nu\,\mathrm{diag}})^{-1}$, and the temperature correction becomes

$$\Delta T_\Lambda = \frac{\left(d\mathcal{H}/dM\right) - \int (\kappa_\nu + \sigma_\nu)(J_\nu - S_\nu)\,d\nu}{\int (\kappa_\nu + \sigma_\nu)\left[(\Lambda_{\nu\,\mathrm{diag}} - 1)/(1 - a_\nu\Lambda_{\nu\,\mathrm{diag}})\right](1 - a_\nu)\,(dB_\nu/dT)\,d\nu} \quad . \tag{7.21}$$

If we approximate S_ν by straight-line segments, we can evaluate the diagonal matrix element according to the discussion in Section 2.6 to obtain

```
TEFF 10000.   LOG G  4.00   LTE

TITLE SAMPLE MODEL

XSCALE   1.000   H   .900   HE  .100
LI-11.60 BE -9.60 B  -9.20 C  -3.50 N  -4.12 O  -3.28 F  -6.60 NE -3.50 NA -6.18 MG -4.57
AL -5.65 SI -4.50 P  -6.62 S  -4.84 CL -6.60 AR -5.30 K  -7.00 CA -5.72 SC -9.01 TI -7.55
V  -8.13 CR -6.58 MN -7.17 FE -4.50 CO -8.40 NI -6.97 CU -7.30 ZN -7.63 GA -9.11 GE -8.73
AS -9.70 SE -8.80 BR -9.40 KR -8.80 RB -9.42 SR -9.23 Y  -9.60 ZR -9.60 NB-10.30 MO-10.00
TC-20.00 RU-10.40 RH-11.20 PD-10.70 AG-11.30 CD -9.98 IN-10.34 SN-10.34 SB-10.40 TE-10.00
I -10.60 XE-10.00 CS-10.90 BA-10.15 LA-10.60 CE-10.40 PR-11.20 ND-10.50 PM-20.00 SM-11.00
EU-11.30 GD-10.90 TB-11.60 DY-10.80 HO-11.50 ER-11.10 TM-11.90 YB-10.90 LU-11.70 HF-11.40
TA-11.70 W -10.90 RE-11.40 OS-10.70 IR-10.80 PT-10.40 AU-11.30 HG-11.10 TL-11.50 PB-10.15
BI-11.30 PO-20.00 AT-20.00 RN-20.00 FR-20.00 RA-20.00 AC-20.00 TH-11.70 PA-20.00 U -12.00
NP-20.00 PU-20.00 AM-20.00 CM-20.00 BK-20.00 CF-20.00 ES-20.00

H1 1 H2PLUS 1 HMINUS 1 HRAY 1 HE1 1 HE2 1 HEMINUS 0 HERAY 0 COOL 1 LUKE 0
HOT 0 ELECTRON 1 H2RAY 0 HLINES 0 LINES 0 LINESCAT 0 XLINES 0 XLSCAT 0 XCONT 0 XSCAT 0

IFCORR 1  IFPRES 1  IFSURF 0  IFSCAT 1  IFCONV 0  MIXLTH  1.00  IFMOL 0
IFTURB 0  TRBFDG  0.00  TRBPOW  0.00  TRBSND  0.00  TRBCON  0.00
NUMITS  6  IFPRNT 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2  IFPNCH 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0

FREQID COOL      NJMNU  78   NULO   1   NUHI  78
    1 3.288047E+13 1.644025E+13     21 3.300000E+14 3.781169E+13     41 1.100000E+15 4.989606E+13     61 1.848853E+15 1.206176E+13
    2 3.288053E+13 3.856355E+12     22 3.653385E+14 1.360311E+13     42 1.150000E+15 5.223402E+13     62 1.900000E+15 8.480297E+13
    3 4.059317E+13 3.856355E+12     23 3.653393E+14 1.233977E+13     43 1.192579E+15 1.569611E+13     63 1.972315E+15 2.660077E+13
    4 4.059325E+13 5.391285E+12     24 4.000000E+14 4.607204E+13     44 1.192581E+15 2.172916E+13     64 1.972318E+15 1.424415E+13
    5 5.137573E+13 5.391285E+12     25 4.500000E+14 5.179164E+13     45 1.250000E+15 6.475939E+13     65 2.020000E+15 6.964705E+13
    6 5.137583E+13 7.863640E+12     26 5.000000E+14 4.945765E+13     46 1.300000E+15 4.548211E+13     66 2.076098E+15 1.989230E+13
    7 6.710299E+13 7.863640E+12     27 5.500000E+14 5.000000E+13     47 1.350000E+15 5.000737E+13     67 2.076102E+15 4.743675E+13
    8 6.710313E+13 1.211583E+13     28 6.000000E+14 5.000000E+13     48 1.400000E+15 5.257096E+13     68 2.200000E+15 1.277701E+14
    9 9.133463E+13 1.211583E+13     29 6.500000E+14 4.993776E+13     49 1.442999E+15 1.587131E+13     69 2.300000E+15 1.224355E+14
   10 9.133481E+13 2.009364E+13     30 7.000000E+14 4.846006E+13     50 1.443001E+15 3.614600E+13     70 2.419598E+15 4.585766E+13
   11 1.315219E+14 2.009.64E+13     31 7.500000E+14 5.669134E+13     51 1.515290E+15 3.614600E+13     71 2.419602E+15 3.033106E+13
   12 1.315221E+14 2.5533.8E+13     32 7.980397E+14 1.795130E+13     52 1.515294E+15 1.235998E+13     72 2.500000E+15 8.853588E+13
   13 1.825886E+14 2.553338E+13     33 7.980413E+14 1.198602E+13     53 1.550000E+15 4.714918E+13     73 2.600000E+15 1.397575E+14
   14 1.825890E+14 4.406202E+12     34 8.220117E+14 1.198602E+13     54 1.600000E+15 3.869734E+13     74 2.725397E+15 4.717553E+13
   15 1.950000E+14 1.538290E+13     35 8.220133E+14 9.419266E+12     55 1.650000E+15 8.845605E+13     75 2.725403E+15 2.564418E+13
   16 2.055029E+14 3.125250E+12     36 8.500000E+14 4.114497E+13     56 1.750000E+15 8.185507E+13     76 2.800000E+15 1.005717E+14
   17 2.055033E+14 9.324904E+12     37 9.000000E+14 5.324043E+13     57 1.787967E+15 4.159281E+12     77 3.000000E+15 3.290220E+14
   18 2.300000E+14 2.856851E+13     38 9.500000E+14 4.918284E+13     58 1.787971E+15 1.115443E+13     78 3.288047E+15 1.074121E+14
   19 2.600000E+14 3.681093E+13     39 1.000000E+15 5.000000E+13     59 1.820000E+15 4.069911E+13
   20 3.000000E+14 3.371661E+13     40 1.050000E+15 4.975351E+13     60 1.848849E+15 9.028562E+12
```

7.4 The Surface Correction

The third correction term, which smooths out the region where the first two overlap, is the surface correction. One way to remove a flux error at the surface is simply to reduce or increase the temperature by a constant value all the way through the atmosphere. If we use the fact that the temperature in the region where the surface flux is formed is approximately T_{eff}, we find that $\Delta T \sim 4\, T_{eff}\, H_0/\mathcal{H}$ since $\mathcal{H} = \sigma T_{eff}^4/4\pi$. As a minimum, we take a smaller temperature, $\Delta T \sim 4\, T_0\, H_0/\mathcal{H}$. Part or all of this temperature correction is produced by the flux and the Λ corrections. The average sum of the two corrections in the region forming the surface flux is approximately

$$\Delta T_{av} = \frac{1}{2} \int_{0.1}^{2} (\Delta T_\Lambda + \Delta T_{flux})\, d\tau_{Ross} \quad . \tag{7.26}$$

Then the required surface correction is

$$\Delta T_{surf} = 4\, T_0 \frac{\Delta H_0}{\mathcal{H}} - \Delta T_{av} \quad . \tag{7.27}$$

The limit on this correction is $T_{eff}/25$.

7.5 Other Fudges

The total correction is

$$\Delta T = \Delta T_{flux} + \Delta T_\Lambda + \Delta T_{surf} \quad . \tag{7.28}$$

An empirically derived speeding-up process based on the behavior of ΔT from iteration to iteration is also used when there is no convection. If ΔT changes sign, it is multiplied by 0.5; if it has the same sign, it is multiplied by 1.25.

If the flux errors are large on the first iteration, ATLAS gives up on the old temperature distribution and calculates a new one (although it might eventually get the original one to converge). If there is no convection and the error at the last depth is outside +90% or -50%, the new temperature distribution is

$$T = T_{eff} \left\{ \frac{3}{4} \left[0.710 + \tau_{Ross} - 0.1331 \exp(-3.4488\, \tau_{Ross}) \right] \right\}^{1/4} \quad . \tag{7.29}$$

If convection is included and the error is greater than 1000% at any depth, ATLAS integrates down from the nonconvective surface region using an effective gradient $(d \ln T/d \ln P)_{eff} = (d \ln T/d \ln M)_{eff}$. The gradient is defined as the larger of

$$\left(\frac{d \ln T}{d \ln M} \right)_{eff} = \frac{H_{rad}(d \ln T/d \ln P) + H_{conv}(d \ln T/d \ln P)_A}{H_{rad} + H_{conv}} \tag{7.30a}$$

and

$$\left(\frac{d \ln T}{d \ln M} \right)_{eff} = \frac{(d \ln T/d \ln P) + 1}{3} \quad . \tag{7.30b}$$

8. ATLAS

8.1 A Sample Model Calculation

We will describe the programing twice; first, we will follow a model computation from beginning to end with reference to input and output; the second time, in Sections 8.4 and 8.5, we will discuss the subroutines in order. In Section 8.6, we give a listing of ATLAS5. Numbers in parentheses following subroutine names refer to pages in this listing.

To start a model calculation, ATLAS5, the main program, calls READIN to get instructions. (Look at the first two pages of ATLAS5, then turn to page 19 and glance through READIN and its subroutines up through page 37.) READIN reads the data cards by using subroutines FREEFF, FREEFR, IWORDF, and DUMMYR. If necessary, it calculates a starting temperature distribution by use of TTAUP, filling in any variables for which data have not been read in from BLOCKE and BLOCKR. READIN produces a two-page printout of the data, which it passes to the rest of the program through COMMON blocks. If there are insufficient data or if the data are in the wrong format, READIN complains and quits (calls EXIT).

On the next page, we have a listing of the input deck that produced the sample model that we will discuss. The order of the cards does not matter (much) because each datum or set of data is preceded by a code word and the numbers themselves are read with a free-field format. A number can appear anywhere on the card after the code word and in any format as long as it is followed by a comma or a blank. Input cards will be discussed in detail in Section 8.3.

The input deck requests six iterations on a 10000 K, log g = 4 model, starting from a T (τ_{Ross}) distribution that READIN will determine for 40 τ's, beginning with log $\tau_{\mathrm{Ross}} = -4.5$, in steps of 1/6. Frequency integrals are to be performed using the 78 frequencies listed. The results are to be punched out at the end of the sixth iteration. The card BEGIN indicates the end of the input data and tells ATLAS to begin the model calculation.

```
TEFF 10000 GRAVITY 4
TITLE SAMPLE MODEL
CALCULATE STARTING MODEL 40 -4.5 .1666666666666666666666666666
ITERATIONS 6 PUNCH 0 0 0 0 0 1
READ FREQUENCIES  78   1  78   COOL
     1   3.28804671E+13   1.64402500E+13    2   3.28805329E+13   3.85635500E+12
     3   4.05931694E+13   3.85635500E+12    4   4.05932506E+13   5.39128550E+12
     5   5.13757296E+13   5.39128550E+12    6   5.13758324E+13   7.86364000E+12
     7   6.71029939E+13   7.86364000E+12    8   6.71031281E+13   1.21158305E+13
     9   9.13346307E+13   1.21158305E+13   10   9.13348133E+13   2.00936390E+13
    11   1.31521868E+14   2.00936390E+13   12   1.31522132E+14   2.55333846E+13
    13   1.82588587E+14   2.55333846E+13   14   1.82588952E+14   4.40620250E+12
    15   1.95000000E+14   1.53829037E+13   16   2.05502919E+14   3.12524966E+12
    17   2.05503331E+14   9.32490356E+12   18   2.30000000E+14   2.85685104E+13
    19   2.60000000E+14   3.68109332E+13   20   3.00000000E+14   3.37166143E+13
    21   3.30000000E+14   3.78116947E+13   22   3.65338525E+14   1.36031090E+13
    23   3.65339255E+14   1.23397723E+13   24   4.00000000E+14   4.60720442E+13
    25   4.50000000E+14   5.17916416E+13   26   5.00000000E+14   4.94576518E+13
    27   5.50000000E+14   5.00000000E+13   28   6.00000000E+14   5.00000000E+13
    29   6.50000000E+14   4.99377588E+13   30   7.00000000E+14   4.84600648E+13
    31   7.50000000E+14   5.66913371E+13   32   7.98039662E+14   1.79512994E+13
    33   7.98041258E+14   1.19860200E+13   34   8.22011678E+14   1.19860200E+13
    35   8.22013322E+14   9.41926567E+12   36   8.50000000E+14   4.11449708E+13
    37   9.00000000E+14   5.32404280E+13   38   9.50000000E+14   4.91828356E+13
    39   1.00000000E+15   5.00000000E+13   40   1.05000000E+15   4.97535082E+13
    41   1.10000000E+15   4.98960590E+13   42   1.15000000E+15   5.22340180E+13
    43   1.19257851E+15   1.56961149E+13   44   1.19258089E+15   2.17291574E+13
    45   1.25000000E+15   6.47593919E+13   46   1.30000000E+15   4.54821099E+13
    47   1.35000000E+15   5.00073710E+13   48   1.40000000E+15   5.25709620E+13
    49   1.44299856E+15   1.58713079E+13   50   1.44300144E+15   3.61460000E+13
    51   1.51529048E+15   3.61460000E+13   52   1.51529352E+15   1.23599776E+13
    53   1.55000000E+15   4.71491758E+13   54   1.60000000E+15   3.86973422E+13
    55   1.65000000E+15   8.84560518E+13   56   1.75000000E+15   8.18550714E+13
    57   1.78796711E+15   4.15928130E+12   58   1.78797069E+15   1.11544291E+13
    59   1.82000000E+15   4.06991086E+13   60   1.84884915E+15   9.02856228E+12
    61   1.84885285E+15   1.20617571E+13   62   1.90000000E+15   8.48029699E+13
    63   1.97231453E+15   2.66007730E+13   64   1.97231847E+15   1.42441540E+13
    65   2.02000000E+15   6.96470460E+13   66   2.07609792E+15   1.98923000E+13
    67   2.07610208E+15   4.74367545E+13   68   2.20000000E+15   1.27770122E+14
    69   2.30000000E+15   1.22435459E+14   70   2.41959758E+15   4.58576637E+13
    71   2.41960242E+15   3.03310636E+13   72   2.50000000E+15   8.85358763E+13
    73   2.60000000E+15   1.39757530E+14   74   2.72539727E+15   4.71755303E+13
    75   2.72540273E+15   2.56441836E+13   76   2.80000000E+15   1.00571733E+14
    77   3.00000000E+15   3.29021965E+14   78   3.28804671E+15   1.07412118E+14
BEGIN
END
```

On the first page of the sample printout (p. 121), we find the following information:

Effective temperature.

Log gravity.

A title to label the printout and punchout.

An abundance scaling factor, which varies all the abundances except hydrogen and helium as a group so that, for example, a subdwarf might have a scaling factor 0.01.

The abundances for hydrogen and helium relative to the total number.

The abundances for all the other elements before the scaling factor is applied, in logs relative to the total number.

Twenty opacity switches telling which opacities are to be included (Section 5).

Whether a temperature correction is to be performed (Section 7). If we have a converged model already and, for example, want to find only the surface flux, we would not need a temperature correction.

Whether pressure is to be calculated (Section 4.1).

Whether flux or intensity is to be found only at the surface, as in an emergent spectrum calculation.

Whether scattering is to be included in the source function. In approximate calculations, there is a considerable time savings in setting α to 0 in equation (2.65).

Whether convective flux should be included in the temperature correction (convective flux is always calculated to indicate its importance).

The ratio of mixing length to scale height for convection (Section 6).

Whether molecular-equilibrium equations are to be solved for molecular number densities or only for the electron number through ionization (Section 4.3).

Whether turbulent pressure is to be included (four parameters are given for determining the turbulent velocity) (see Section 4.1).

The number of iterations for the model.

Print and punch switches for each iteration. We will discuss these as we look at the printout and punchout. Zeros mean no output.

The name of the frequency set. Frequency sets are named so that they can be easily distinguished from one another if they differ at only a few points.

The number of frequencies and the limits on the frequency integration. In this case, we are using a frequency set with 78 points, which were chosen to represent the major discontinuities in the cool opacities (Section 5.9). For example, frequencies 74 and 75 mark a C I edge. It might be possible to calculate a model with as few as 50 frequencies (to save computer time) without affecting the values of the frequency integrals, but no effort was made to do this for this sample calculation. The number following each frequency is the frequency integration weight (Section 2.10).

```
TEFF 10000.   LOG G  4.00   LTE

TITLE SAMPLE MODEL

XSCALE    1.000    H    .900    HE  .100
LI-11.60 BE -9.60 B  -9.20 C  -3.50 N  -4.12 O  -3.28 F  -6.60 NE -3.50 NA -6.18 MG -4.57
AL -5.65 SI -4.50 P  -6.62 S  -4.84 CL -6.60 AR -5.30 K  -7.00 CA -5.72 SC -9.01 TI -7.55
V  -8.13 CR -6.58 MN -7.17 FE -4.50 CO -8.40 NI -6.97 CU -7.30 ZN -7.63 GA -9.11 GE -8.73
AS -9.70 SE -8.80 BR -9.40 KR -8.80 RB -9.42 SR -9.23 Y  -9.60 ZR -9.60 NB-10.30 MO-10.00
TC-20.00 RU-10.40 RH-11.20 PD-10.70 AG-11.30 CD -9.98 IN-10.34 SN-10.34 SB-10.40 TE-10.00
I -10.60 XE-10.00 CS-10.90 BA-10.15 LA-10.60 CE-10.40 PR-11.20 ND-10.50 PM-20.00 SM-11.00
EU-11.30 GD-10.90 TB-11.60 DY-10.80 HO-11.50 ER-11.10 TM-11.90 YB-10.90 LU-11.70 HF-11.40
TA-11.70 W -10.90 RE-11.40 OS-10.70 IR-10.80 PT-10.40 AU-11.30 HG-11.10 TL-11.50 PB-10.15
BI-11.30 PO-20.00 AT-20.00 RN-20.00 FR-20.00 RA-20.00 AC-20.00 TH-11.70 PA-20.00 U -12.00
NP-20.00 PU-20.00 AM-20.00 CM-20.00 BK-20.00 CF-20.00 ES-20.00

H1 1 H2PLUS 1 HMINUS 1 HRAY 1 HE1 1 HE2 1 HEMINUS 0 HERAY 0 COOL 1 LUKE 0
HOT 0 ELECTRON 1 H2RAY 0 HLINES 0 LINES 0 LINESCAT 0 XLINES 0 XLSCAT 0 XCONT 0 XSCAT 0

IFCORR 1  IFPRES 1  IFSURF 0  IFSCAT 1  IFCONV 0  MIXLTH  1.00  IFMOL 0
IFTURB 0  TRBFDG  0.00  TRBPOW  0.00  TRBSND  0.00  TRBCON  0.00
NUMITS  6  IFPRNT 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2  IFPNCH 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0

FREQID COOL      NJMNU  78   NULO   1   NUHI  78
    1 3.288047E+13 1.644025E+13    21 3.300000E+14 3.781169E+13    41 1.100000E+15 4.989606E+13    61 1.848853E+15 1.206176E+13
    2 3.288053E+13 3.856355E+12    22 3.653385E+14 1.360311E+13    42 1.150000E+15 5.223402E+13    62 1.900000E+15 8.480297E+13
    3 4.059317E+13 3.856355E+12    23 3.653393E+14 1.233977E+13    43 1.192579E+15 1.569611E+13    63 1.972315E+15 2.660077E+13
    4 4.059325E+13 5.391285E+12    24 4.000000E+14 4.607204E+13    44 1.192581E+15 2.172916E+13    64 1.972318E+15 1.424415E+13
    5 5.137573E+13 5.391285E+12    25 4.500000E+14 5.179164E+13    45 1.250000E+15 6.475939E+13    65 2.020000E+15 6.964705E+13
    6 5.137585E+13 7.863640E+12    26 5.000000E+14 4.945765E+13    46 1.300000E+15 4.548211E+13    66 2.076098E+15 1.989230E+13
    7 6.710299E+13 7.863640E+12    27 5.500000E+14 5.000000E+13    47 1.350000E+15 5.000737E+13    67 2.076102E+15 4.743675E+13
    8 6.710313E+13 1.211583E+13    28 6.000000E+14 5.000000E+13    48 1.400000E+15 5.257096E+13    68 2.200000E+15 1.277701E+14
    9 9.133463E+13 1.211583E+13    29 6.500000E+14 4.993776E+13    49 1.442999E+15 1.587131E+13    69 2.300000E+15 1.224355E+14
   10 9.133481E+13 2.009364E+13    30 7.000000E+14 4.846006E+13    50 1.443001E+15 3.614600E+13    70 2.419598E+15 4.585766E+13
   11 1.315219E+14 2.009.64E+13    31 7.500000E+14 5.669134E+13    51 1.515290E+15 3.614600E+13    71 2.419602E+15 3.033106E+13
   12 1.315221E+14 2.5533.8E+13    32 7.980397E+14 1.795130E+13    52 1.515294E+15 1.235998E+13    72 2.500000E+15 8.853588E+13
   13 1.825886E+14 2.553338E+13    33 7.980413E+14 1.198602E+13    53 1.550000E+15 4.714918E+13    73 2.600000E+15 1.397575E+14
   14 1.825890E+14 4.406202E+12    34 8.220117E+14 1.198602E+13    54 1.600000E+15 3.869734E+13    74 2.725397E+15 4.717553E+13
   15 1.950000E+14 1.538290E+13    35 8.220133E+14 9.419266E+12    55 1.650000E+15 8.845605E+13    75 2.725403E+15 2.564418E+13
   16 2.055029E+14 3.125250E+12    36 8.500000E+14 4.114497E+13    56 1.750000E+15 8.185507E+13    76 2.800000E+15 1.005717E+14
   17 2.055033E+14 9.324904E+12    37 9.000000E+14 5.324043E+13    57 1.787967E+15 4.159281E+12    77 3.000000E+15 3.290220E+14
   18 2.300000E+14 2.856851E+13    38 9.500000E+14 4.918284E+13    58 1.787971E+15 1.115443E+13    78 3.288047E+15 1.074121E+14
   19 2.600000E+14 3.681093E+13    39 1.000000E+15 5.000000E+13    59 1.820000E+15 4.069911E+13
   20 3.000000E+14 3.371661E+13    40 1.050000E+15 4.975351E+13    60 1.848849E+15 9.028562E+12
```

The second page of printout from READIN contains the starting model. Remember that on the input cards we specified 40 Rosseland depths. READIN then takes the gray temperature distribution T(TAUROS)=TEFF*(.75*(.710+TAUROS-.1331*EXP (-3.4488*TAUROS)))**.25 and converts it to T(RHOX) by using subroutine TTAUP for the pressure integration (Section 4.2). TTAUP(34) finds the Rosseland opacity from a table as a function of log T and log P. The results printed out are RHOX, T, P, and ABROSS. Only RHOX and T are used in the model calculation.

We have said nothing about statistical equilibrium calculations, so READIN assumes local thermodynamic equilibrium (LTE) and sets the b's of hydrogen and H^- to unity (Section 3.3).

After READIN returns to the main program, ATLAS5(2) starts DO 100, which is the model iteration. At the beginning of each iteration, ATLAS increments the variable ITEMP, which is stored in COMMON /TEMP/. The subroutines test this variable to see if it changes, and when it does, they recalculate the temperature-dependent parameters.

The first procedure in each iteration is to calculate the pressure in DO 11 (Section 4.1). Then ATLAS5 calls POPS(37) to solve the equilibrium equations for the number densities. The argument CODE identifies atoms and molecules. The atomic number for each component is treated as a base 100 digit, and the digits are ordered increasing from left to right to form a number. An electron component, as in H^-, is written 00 and ordered as 100. The positive charge is written after the decimal point, for example, 2.02 = He^{++} = He III.

If IFMOL were 1, we would go to statement 200 to include molecules. If there is a new temperature distribution (which there is) and if IFPRES is 1 (which it is), POPS will call NMOLEC to solve the equilibrium equations (glance through NMOLEC(50)). NMOLEC stores its results in COMMON array XNMOL, which is available to MOLEC, and in XNE, XNATOM, and RHO. If CODE is any number greater than 0 (as later, when POPS is called by opacity routines), POPS calls MOLEC(48) to retrieve the number density/partition function for the requested atom or molecule. MOLEC and NMOLEC will be discussed in more detail in Section 8.3 because they require special input.

```
       RHOX          T        P        XNE     ABROSS    PRAD      VTURB                      BHYD                      BMIN
 1 8.456913E-05   8110.5 8.457E-01 0.        3.739E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 2 1.225591E-04   8110.6 1.226E+00 0.        4.057E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 3 1.738377E-04   8110.7 1.738E+00 0.        4.414E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 4 2.429862E-04   8110.9 2.430E+00 0.        4.801E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 5 3.361590E-04   8111.1 3.362E+00 0.        5.227E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 6 4.617249E-04   8111.5 4.617E+00 0.        5.692E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 7 6.310274E-04   8112.0 6.310E+00 0.        6.192E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 8 8.596242E-04   8112.7 8.596E+00 0.        6.732E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
 9 1.168668E-03   8113.9 1.169E+01 0.        7.291E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
10 1.588882E-03   8115.5 1.589E+01 0.        7.850E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
11 2.162827E-03   8117.9 2.163E+01 0.        8.428E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
12 2.948143E-03   8121.4 2.948E+01 0.        9.030E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
13 4.024988E-03   8126.5 4.025E+01 0.        9.663E-01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
14 5.501644E-03   8134.0 5.502E+01 0.        1.035E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
15 7.524075E-03   8145.0 7.524E+01 0.        1.110E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
16 1.028345E-02   8160.9 1.028E+02 0.        1.198E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
17 1.401635E-02   8184.0 1.402E+02 0.        1.307E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
18 1.900400E-02   8217.4 1.900E+02 0.        1.447E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
19 2.554869E-02   8265.3 2.555E+02 0.        1.635E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
20 3.392189E-02   8333.3 3.392E+02 0.        1.905E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
21 4.426916E-02   8428.6 4.427E+02 0.        2.305E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
22 5.655042E-02   8559.6 5.655E+02 0.        2.914E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
23 7.046433E-02   8735.9 7.046E+02 0.        3.868E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
24 8.545644E-02   8967.2 8.546E+02 0.        5.402E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
25 1.009172E-01   9262.7 1.009E+03 0.        7.784E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
26 1.165967E-01   9631.3 1.166E+03 0.        1.129E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
27 1.327494E-01  10083.8 1.327E+03 0.        1.558E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
28 1.509153E-01  10635.2 1.509E+03 0.        1.911E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
29 1.742619E-01  11303.9 1.743E+03 0.        2.050E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
30 2.089896E-01  12106.6 2.090E+03 0.        1.864E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
31 2.680793E-01  13054.4 2.681E+03 0.        1.578E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
32 3.704890E-01  14154.2 3.705E+03 0.        1.348E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
33 5.437502E-01  15412.1 5.438E+03 0.        1.182E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
34 8.276808E-01  16835.0 8.277E+03 0.        1.083E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
35 1.272944E+00  18431.5 1.273E+04 0.        1.024E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
36 1.956084E+00  20212.5 1.956E+04 0.        9.937E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
37 2.978449E+00  22191.0 2.978E+04 0.        9.788E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
38 4.482477E+00  24382.6 4.482E+04 0.        9.978E+00 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
39 6.608468E+00  26805.5 6.608E+04 0.        1.042E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
40 9.585259E+00  29480.4 9.585E+04 0.        1.099E+01 0.        0.        1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
```

Going back to the beginning of POPS(37), for the model we are discussing IFMOL = 0, so NELECT(39) finds the electron number XNE, the atom number XNATOM, and the density RHO. It finds these quantities by iterating on the number densities of the more abundant elements through calls to PFSAHA(39). PFSAHA is a general routine for finding partition functions, ionization fractions, ionization fractions/partition functions, or electron contributions. The main body of the routine is a large table of partition functions and ionization potentials followed by a small section (pages 46 and 47) that deciphers the table to find partition functions and then ionization fractions.

The printout from NELECT on the next page (which is printed only on the last iteration of the model in order to save paper) shows how the different elements contribute electrons. The left side gives the fraction of the total electron density contributed by each element. Note that since hydrogen is partially ionized the hydrogen contribution far exceeds all those but for He and C, so the other elements could just as well have not been included. On the right side of the page, we find the number of electrons contributed by each atom. Thus at the first point, H is .146 neutral and .854 ionized, He is all neutral, Na is all ionized, Ca is almost all doubly ionized, etc.

Going back to POPS(37), if CODE is a number greater than 0 but not a molecule, POPS calls PFSAHA to find the ion fraction/partition function. POPS then converts the ion fraction to a number density by multiplying XNATOM and the atomic abundance.

Once the equilibrium equations have been solved, any subsequent call to POPS for the same ITEMP does not have to bother with NELECT or NMOLEC.

Now ATLAS5(2) is ready to calculate opacities and the radiation field. It first calls PUTOUT(4) to initialize page headings. PUTOUT(4) handles all the output from ATLAS5 itself. Next ATLAS5 initializes frequency integrals by calling all the subroutines that do frequency integration: TCORR(8), which does the temperature corrections; STATEQ(11), which does statistical equilibrium; ROSS(13), which calculates Rosseland opacity; and RADIAP(14), which calculates radiation pressure.

```
                                                            ELECTRON CONTRIBUTIONS
       H    HE     C    NA    MG    AL    SI     K    CA    FE     H    HE     C    NA    MG    AL    SI     K    CA    FE
 1  .999  .000  .000  .000  .000  .000  .000  .000  .000  .000  .854  .000  .996 1.000 1.400 1.009 1.031 1.000 1.982 1.097
 2 1.000  .000  .000  .000  .000  .000  .000  .000  .000  .000  .809  .000  .994 1.000 1.319 1.006 1.022 1.000 1.975 1.070
 3  .999  .000  .000  .000  .000  .000  .000  .000  .000  .000  .755  .000  .992 1.000 1.253 1.004 1.016 1.000 1.966 1.052
 4  .999  .000  .000  .000  .000  .000  .000  .000  .000  .000  .701  .000  .990 1.000 1.203 1.003 1.012 1.000 1.955 1.039
 5  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .643  .000  .987 1.000 1.171 1.003 1.010 1.000 1.942 1.032
 6  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .586  .000  .983 1.000 1.139 1.002 1.008 1.000 1.927 1.025
 7  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .528  .000  .979 1.000 1.113 1.002 1.006 1.000 1.908 1.020
 8  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .480  .000  .974 1.000 1.096 1.001 1.005 1.000 1.890 1.017
 9  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .427  .000  .968 1.000 1.079 1.001 1.004 1.000 1.866 1.014
10  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .380  .000  .962 1.000 1.066 1.001 1.003 1.000 1.840 1.011
11  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .338  .000  .954 1.000 1.056 1.001 1.002 1.000 1.825 1.009
12  .998  .000  .001  .000  .000  .000  .000  .000  .000  .000  .300  .000  .945 1.000 1.047 1.001 1.002 1.000 1.798 1.008
13  .998  .000  .001  .000  .000  .000  .000  .000  .000  .000  .267  .000  .936 1.000 1.041 1.000 1.001 1.000 1.769 1.007
14  .998  .000  .001  .000  .000  .000  .000  .000  .000  .000  .238  .000  .925 1.000 1.035 1.000 1.001 1.000 1.739 1.006
15  .998  .000  .002  .000  .000  .000  .000  .000  .000  .000  .214  .000  .914 1.000 1.031 1.000 1.001 1.000 1.708 1.005
16  .998  .000  .002  .000  .000  .000  .000  .000  .000  .000  .195  .000  .903 1.000 1.028 1.000 1.000 1.000 1.680 1.004
17  .998  .000  .002  .000  .000  .000  .000  .000  .000  .000  .177  .000  .890 1.000 1.025 1.000 1.000 1.000 1.650 1.004
18  .997  .000  .002  .000  .000  .000  .000  .000  .000  .000  .166  .000  .880 1.000 1.024 1.000 1.000 1.000 1.627 1.004
19  .997  .000  .002  .000  .000  .000  .000  .000  .000  .000  .159  .000  .871 1.000 1.023 1.000  .999 1.000 1.597 1.004
20  .997  .000  .002  .000  .000  .000  .000  .000  .000  .000  .158  .000  .864 1.000 1.023 1.000  .999 1.000 1.591 1.004
21  .998  .000  .002  .000  .000  .000  .000  .000  .000  .000  .163  .000  .863 1.000 1.025 1.000  .999 1.000 1.597 1.004
22  .998  .000  .002  .000  .000  .000  .000  .000  .000  .000  .177  .000  .867 1.000 1.029 1.000  .999 1.000 1.602 1.005
23  .998  .000  .002  .000  .000  .000  .000  .000  .000  .000  .203  .000  .877 1.000 1.035 1.000 1.000 1.000 1.623 1.006
24  .998  .000  .001  .000  .000  .000  .000  .000  .000  .000  .252  .000  .895 1.000 1.049 1.001 1.001 1.000 1.664 1.010
25  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .330  .000  .917 1.000 1.074 1.003 1.003 1.000 1.720 1.016
26  .999  .000  .001  .000  .000  .000  .000  .000  .000  .000  .441  .000  .939 1.000 1.122 1.006 1.008 1.000 1.812 1.030
27 1.000  .000  .001  .000  .000  .000  .000  .000  .000  .000  .591  .000  .961 1.000 1.218 1.016 1.021 1.000 1.870 1.063
28 1.000  .000  .000  .000  .000  .000  .000  .000  .000  .000  .743  .000  .977 1.000 1.380 1.041 1.050 1.000 1.915 1.135
29 1.000  .000  .000  .000  .000  .000  .000  .000  .000  .000  .861  .000  .987 1.000 1.598 1.109 1.124 1.000 1.949 1.288
30  .999  .000  .000  .000  .000  .000  .000  .000  .000  .000  .931  .002  .994 1.000 1.778 1.265 1.270 1.000 1.971 1.503
31  .998  .001  .000  .000  .000  .000  .000  .000  .000  .000  .965  .008  .997 1.000 1.897 1.520 1.508 1.000 1.984 1.733
32  .995  .004  .000  .000  .000  .000  .000  .000  .000  .000  .981  .036 1.002 1.000 1.953 1.761 1.731 1.000 1.990 1.874
33  .985  .015  .000  .000  .000  .000  .000  .000  .000  .000  .987  .134 1.015 1.000 1.977 1.897 1.867 1.002 1.994 1.942
34  .960  .039  .000  .000  .000  .000  .000  .000  .000  .000  .990  .363 1.057 1.000 1.988 1.961 1.937 1.010 1.995 1.973
35  .931  .069  .000  .000  .000  .000  .000  .000  .000  .000  .992  .659 1.173 1.000 1.993 2.014 1.975 1.051 1.996 1.992
36  .912  .088  .000  .000  .000  .000  .000  .000  .000  .000  .993  .858 1.397 1.000 1.995 2.114 2.014 1.201 1.997 2.020
37  .904  .096  .001  .000  .000  .000  .000  .000  .000  .000  .993  .945 1.656 1.000 1.996 2.322 2.108 1.509 1.997 2.101
38  .901  .099  .001  .000  .000  .000  .000  .000  .000  .000  .993  .979 1.842 1.002 1.997 2.598 2.327 1.796 1.998 2.301
39  .900  .100  .001  .000  .000  .000  .000  .000  .000  .000  .993  .991 1.933 1.016 1.997 2.804 2.621 1.934 2.001 2.588
40  .899  .100  .001  .000  .000  .000  .000  .000  .000  .000  .993  .996 1.987 1.086 1.997 2.911 2.826 2.020 2.017 2.816
```

ATLAS5(3) does a long loop DO 25 over frequencies. There is a special option for doing equally spaced wavelengths instead, which can be brought in with a control card described in Section 8.2. FRESET and RCOSET are the frequencies and integration coefficients described above. ATLAS5 expects the opacity to be in the form of a step representation of the distribution function (Section 5.15), so there is a loop running from statement 24 to the statement IF(N.LT.NSTEPS)GO TO 24, where N is the step number. ATLAS5 does not know how many steps to expect or the weight for each step until the statement CALL KAPP(N, NSTEPS, STEPWT). Normally this option is not used, so both NSTEPS and STEPWT are 1. Backing up a few lines, the statement CALL PUTOUT(2) initializes some sums over the distribution function for surface flux or surface intensity. Then we start into the loop over the steps by calling KAPP to find the opacity.

Now we look at KAPP(55) in detail. The first thing KAPP does is check ITEMP for a new temperature distribution, in which case KAPP calls POPS to get hydrogen and helium number densities over partition functions, XNFPH and XNFPHE, which it stores in COMMON /IONS/ for use by any of the opacity routines. Subroutines that require number densities for other elements call POPS on their own so that they are self-contained for easy modification or deletion. Then KAPP initializes STEPWT and NSTEPS. If N > 1 (not the case in our example), all the continuous opacities have already been calculated for N = 1, so KAPP would skip to the section that treats distribution functions. This section would call LINOP and LINSOP and then adjust the total opacities and source functions for the change in line opacity.

For the normal case when N = 1, KAPP erases the opacity arrays and then calls the opacity subroutines for which the switches are on. The opacities are described in detail in Section 5. The subroutines are as follows:

1. HOP(56) uses COULX(57) for coulomb bound-free cross sections and COULFF(57) for coulomb free-free cross sections.

2. H2PLOP(58).

3. HMINOP(58).

4. HRAYOP(57).

5. HE1OP(59) uses COULFF(57).

6. HE2OP(60) uses COULX(57) and COULFF(57).

7. HEMIOP(60).

8. HERAOP(61).

9. COOLOP(61) uses C1OP(62), SEATON(62), MG2OP(63), AL1OP(62), and SI1OP(64).

10. LUKEOP(65) uses N1OP(65), O1OP(65), MG2OP(66), SI2OP(67), CA2OP(66), and SEATON(62).

11. HOTOP(68).

12. ELECOP(70).

13. H2RAOP(70).

14. HLINOP(71) uses STARK(72).

15. LINOP(73).

16. LINSOP(73).

17. XLINOP(73).

18. XLISOP(73).

19. XCONOP(73).

20. XSOP(73).

Each subroutine returns its opacity through COMMON /OPS/. Five subroutines (HOP, HMINOP, HLINOP, XLINOP, and XCONOP) also return source functions in COMMON /OPS/. The remaining subroutines have source functions BNU or JNU.

KAPP(38) finally constructs from the variables in COMMON /OPS/ the average opacities ACONT, SIGMAC, ALINE, and SIGMAL (Section 5) and the source functions SCONT and SLINE, all of which are stored in COMMON /OPTOT/.

Once the opacity is known, ATLAS5(3) calls JOSH(74) to find the radiation field (Section 2). First JOSH finds the total opacity ABTOT, the scattering fraction ALPHA, and SNUBAR, the part of the source function that is not JNU. Then it finds TAUNU by integrating ABTOT with subroutine INTEG(15). If IFSCAT = 1 (which it is for our example), JOSH solves the integral equation for the source function (Sections 2.7 and 2.8). (See statements with statement numbers in the 30's.) JOSH interpolates ALPHA and SNUBAR to the internal tau set XTAU by use of subroutine MAP1(16) and then solves the integral equation for S on XTAU. The integration matrices for J and H are stored in COMMON /MATX/ as 43 by 43 arrays, which are tabulated in BLOCKJ(77) and BLOCKH(86). The matrix multiplication in the integral equation is written out explicitly to force the compiler to give a fast, efficient code. Once the source function is found, it is interpolated back to TAUNU space.

The matrix solution is good only up to TAUNU = 20, so SNU, JNU, and HNU at large depths are found by taking first and second derivatives of SNU by using subroutine DERIV(14) (Sections 2.7 and 2.8). (See statements with statement numbers in the 40's.)

Next JOSH finds JNU and HNU at depths less than 20 in XTAU and interpolates from the XTAU scale the results to the TAUNU scale.

The special cases of surface flux only or surface intensity only (Section 2.9) come at the end of the routine.

Returning to ATLAS5(3), we now know the monochromatic opacities and the radiation field for step N, so we can compute integrands and add to integrals over frequency. The integration coefficient RCOWT is the frequency weight times the step weight. ATLAS5 calls the four subroutines with integrals, TCORR(8), STATEQ(11), ROSS(13), and RADIAP(14). Then it calls PUTOUT(5) to add to the total for the surface flux at this frequency and to print out the results for the step. Since we are not using distribution functions in this example, we get no results.

ATLAS5(3) continues through the loop over N. When the loop is completed, ATLAS5 calls PUTOUT(5) to print and punch (if IFPRNT or IFPNCH equals 1) the surface flux. The first page of printout is shown on the next page. The wavelength is in nanometers and the magnitudes are -2.5 times the logs. TAUONE is the log RHOX at which TAUNU = 1. TAUNU(NRHOX) is the log optical depth at the last depth. For the flux to be accurate, TAUNU(NRHOX) should be greater than 10 at every frequency. Both these quantities give estimates of the opacity variation with frequency.

The punch has the form

```
     FLUX          3.288047E13          5.9589E-07     .
```

In ATLAS5(3), statement 25 is the end of the loop over frequency. All frequency integrals are determined once this loop is completed, so ATLAS5 can finish the iteration. First it calls ROSS(13) to find ABROSS and TAUROS. Then it calls CONVEC(96) to compute the convective flux. CONVEC first computes the derivatives $(\partial E/\partial T)_P$, $(\partial E/\partial P)_T$, $(\partial \rho/\partial T)_P$, and $(\partial \rho/\partial P)_T$ (Section 4.6), from which it finds C_V, C_P, v_{sound}, $(\partial \ln \rho/\partial \ln T)_P$, $(\partial \ln T/\partial \ln P)_S$, and $d \ln T/d \ln P$. Finally, it computes the convective velocity and flux (Section 6).

Returning to page 3, ATLAS5 calls RADIAP(14) to compute the radiation pressure (Section 2.11).

Next, ATLAS5 calls TCORR(8) to do the temperature correction (Section 7). After statement 30 comes the flux correction; after 40, the Λ correction; and after 43, the surface correction. The total correction is statement 50.

Pages 131 and 132 are samples of what TCORR produces if IFPRNT > 1. The first page is from the first iteration, and the second is from the last, in order to show the improvement. The column CONV/TOTAL is the fraction of convective flux if convection were included in the temperature correction. ERROR is the percentage flux error. DERIV is $100(dH/d\tau_{Ross})/\mathcal{H}$. Note that the starting guess seems good in terms of flux errors. The flux-derivative errors are rather large but should be no problem. Normally, a previously computed starting model would be used as the

```
        WAVE      HLAMBDA      LOG H      MAG       FREQUENCY        HNU        LOG H      MAG        TAUONE TAUNU
 1    9117.647   2.2165E+03   3.34567    -8.364   3.288047E+13   6.1463E-07   -6.21139   15.528      -1.78  5.28    1
 2    9117.629   2.2165E+03   3.34567    -8.364   3.288053E+13   6.1463E-07   -6.21139   15.528      -1.78  5.28    2
 3    7385.294   5.0483E+03   3.70314    -9.258   4.059317E+13   9.1846E-07   -6.03694   15.092      -1.64  5.09    3
 4    7385.279   5.0483E+03   3.70315    -9.258   4.059325E+13   9.1846E-07   -6.03694   15.092      -1.64  5.09    4
 5    5835.294   1.2621E+04   4.10109   -10.253   5.137573E+13   1.4335E-06   -5.84361   14.609      -1.48  4.86    5
 6    5835.283   1.2609E+04   4.10067   -10.252   5.137583E+13   1.4321E-06   -5.84403   14.610      -1.50  4.87    6
 7    4467.647   3.5394E+04   4.54893   -11.372   6.710299E+13   2.3565E-06   -5.62773   14.069      -1.33  4.62    7
 8    4467.638   3.5314E+04   4.54795   -11.370   6.710313E+13   2.3512E-06   -5.62872   14.072      -1.36  4.63    8
 9    3282.353   1.1502E+05   5.06079   -12.652   9.133463E+13   4.1337E-06   -5.38367   13.459      -1.18  4.33    9
10    3282.346   1.1439E+05   5.05840   -12.646   9.133481E+13   4.1110E-06   -5.38606   13.465      -1.22  4.35   10
11    2279.412   4.5345E+05   5.65653   -14.141   1.315219E+14   7.8587E-06   -5.10465   12.762      -1.05  4.00   11
12    2279.407   4.4654E+05   5.64986   -14.125   1.315221E+14   7.7390E-06   -5.11131   12.778      -1.09  4.03   12
13    1641.902   1.5007E+06   6.17630   -15.441   1.825886E+14   1.3495E-05   -4.86982   12.175       -.96  3.72   13
14    1641.898   1.5007E+06   6.17631   -15.441   1.825890E+14   1.3495E-05   -4.86982   12.175       -.96  3.72   14
15    1537.397   1.9075E+06   6.28047   -15.701   1.950000E+14   1.5039E-05   -4.82277   12.057       -.94  3.65   15
16    1458.824   2.3075E+06   6.36315   -15.908   2.055029E+14   1.6381E-05   -4.78566   11.964       -.93  3.60   16
17    1458.821   2.1990E+06   6.34223   -15.856   2.055033E+14   1.5610E-05   -4.80659   12.016       -.99  3.67   17
18    1303.446   3.2775E+06   6.51554   -16.289   2.300000E+14   1.8574E-05   -4.73109   11.828       -.95  3.56   18
19    1153.048   5.0352E+06   6.70201   -16.755   2.600000E+14   2.2330E-05   -4.65111   11.628       -.92  3.44   19
20     999.308   8.2529E+06   6.91661   -17.292   3.000000E+14   2.7491E-05   -4.56081   11.402       -.88  3.30   20
21     908.462   1.1419E+07   7.05765   -17.644   3.300000E+14   3.1437E-05   -4.50256   11.256       -.85  3.20   21
22     820.588   1.6088E+07   7.20649   -18.016   3.653385E+14   3.6135E-05   -4.44208   11.105       -.82  3.10   22
23     820.587   1.3399E+07   7.12707   -17.818   3.653393E+14   3.0095E-05   -4.52150   11.304       -.95  3.25   23
24     749.481   1.7756E+07   7.24934   -18.123   4.000000E+14   3.3269E-05   -4.47796   11.195       -.92  3.18   24
25     666.206   2.5438E+07   7.40548   -18.514   4.500000E+14   3.7659E-05   -4.42413   11.060       -.88  3.06   25
26     599.585   3.4887E+07   7.54266   -18.857   5.000000E+14   4.1835E-05   -4.37846   10.946       -.84  2.95   26
27     545.077   4.6223E+07   7.66485   -19.162   5.500000E+14   4.5809E-05   -4.33905   10.848       -.81  2.85   27
28     499.654   5.9551E+07   7.77489   -19.437   6.000000E+14   4.9592E-05   -4.30459   10.761       -.78  2.76   28
29     461.219   7.4959E+07   7.87482   -19.687   6.500000E+14   5.3188E-05   -4.27418   10.685       -.75  2.67   29
30     428.275   9.2514E+07   7.96621   -19.916   7.000000E+14   5.6602E-05   -4.24717   10.618       -.72  2.59   30
31     399.723   1.1225E+08   8.05019   -20.125   7.500000E+14   5.9826E-05   -4.22311   10.558       -.69  2.52   31
32     375.661   1.3329E+08   8.12479   -20.312   7.980397E+14   6.2743E-05   -4.20244   10.506       -.65  2.45   32
33     375.660   1.3328E+08   8.12478   -20.312   7.980413E+14   6.2741E-05   -4.20245   10.506       -.65  2.45   33
34     364.706   1.4452E+08   8.15993   -20.400   8.220117E+14   6.4120E-05   -4.19301   10.483       -.64  2.43   34
35     364.705   4.6144E+07   7.66411   -19.160   8.220133E+14   2.0473E-05   -4.68883   11.722      -1.14  2.95   35
36     352.697   4.7593E+07   7.67754   -19.194   8.500000E+14   1.9748E-05   -4.70447   11.761      -1.12  2.91   36
37     333.103   4.9955E+07   7.69858   -19.246   9.000000E+14   1.8489E-05   -4.73309   11.833      -1.08  2.88   37
38     315.571   5.2069E+07   7.71658   -19.291   9.500000E+14   1.7296E-05   -4.76205   11.905      -1.05  2.82   38
39     299.792   5.3993E+07   7.73234   -19.331   1.000000E+15   1.6187E-05   -4.79084   11.977      -1.02  2.77   39
40     285.517   5.5786E+07   7.74653   -19.366   1.050000E+15   1.5169E-05   -4.81903   12.048      -1.00  2.71   40
41     272.539   5.7505E+07   7.75970   -19.399   1.100000E+15   1.4248E-05   -4.84626   12.116       -.97  2.66   41
42     260.689   5.9199E+07   7.77231   -19.431   1.150000E+15   1.3419E-05   -4.87226   12.181       -.95  2.61   42
43     251.382   6.0658E+07   7.78289   -19.457   1.192579E+15   1.2786E-05   -4.89327   12.233       -.93  2.57   43
44     251.381   6.0611E+07   7.78255   -19.456   1.192581E+15   1.2776E-05   -4.89360   12.234       -.93  2.57   44
45     239.834   6.2644E+07   7.79688   -19.492   1.250000E+15   1.2019E-05   -4.92012   12.300       -.91  2.51   45
46     230.610   6.4512E+07   7.80964   -19.524   1.300000E+15   1.1444E-05   -4.94143   12.354       -.90  2.47   46
47     222.069   6.6501E+07   7.82283   -19.557   1.350000E+15   1.0939E-05   -4.96102   12.403       -.88  2.43   47
48     214.137   6.8623E+07   7.83647   -19.591   1.400000E+15   1.0496E-05   -4.97896   12.447       -.86  2.38   48
49     207.757   7.0569E+07   7.84861   -19.622   1.442999E+15   1.0160E-05   -4.99310   12.483       -.85  2.35   49
50     207.756   7.0508E+07   7.84824   -19.621   1.443001E+15   1.0151E-05   -4.99348   12.484       -.85  2.35   50
51     197.845   7.4024E+07   7.86937   -19.673   1.515290E+15   9.6650E-06   -5.01480   12.537       -.83  2.29   51
52     197.845   7.3958E+07   7.86898   -19.672   1.515294E+15   9.6563E-06   -5.01519   12.538       -.83  2.29   52
53     193.415   7.5747E+07   7.87936   -19.698   1.550000E+15   9.4520E-06   -5.02448   12.561       -.82  2.26   53
54     187.370   7.8454E+07   7.89462   -19.737   1.600000E+15   9.1875E-06   -5.03680   12.592       -.80  2.23   54
55     181.692   8.1292E+07   7.91005   -19.775   1.650000E+15   8.9516E-06   -5.04810   12.620       -.79  2.19   55
56     171.310   8.7335E+07   7.94119   -19.853   1.750000E+15   8.5493E-06   -5.06807   12.670       -.76  2.12   56
```

```
        RHOX          T      DTLAMB    DTSURF    DTFLUX      TI    CONV/TOTAL      ERROR      DERIV
 1  8.4569E-05    8110.5    -400.0       0.0       0.0    -400.0   0.                -3.106    -15.558
 2  1.2256E-04    8110.6    -400.0       0.0        .0    -400.0   0.                -3.107    -20.148
 3  1.7384E-04    8110.7    -400.0       0.0        .0    -400.0   0.                -3.108    -24.668
 4  2.4299E-04    8110.9    -400.0       0.0        .0    -400.0   0.                -3.108    -30.172
 5  3.3616E-04    8111.1    -400.0       0.0        .0    -400.0   0.                -3.110    -35.603
 6  4.6172E-04    8111.5    -400.0       0.0        .0    -400.0   0.                -3.113    -40.989
 7  6.3103E-04    8112.0    -400.0       0.0        .1    -399.9   0.                -3.117    -46.175
 8  8.5962E-04    8112.7    -400.0       0.0        .1    -399.9   0.                -3.124    -50.930
 9  1.1687E-03    8113.9    -400.0       0.0        .1    -399.9   0.                -3.136    -55.016
10  1.5889E-03    8115.5    -400.0       0.0        .2    -399.8   0.                -3.154    -58.265
11  2.1628E-03    8117.9    -398.0       0.0        .3    -397.7   0.                -3.182    -60.500
12  2.9481E-03    8121.4    -386.1       0.0        .4    -385.6   0.                -3.224    -61.516
13  4.0250E-03    8126.5    -370.7       0.0        .7    -370.1   0.                -3.286    -61.196
14  5.5016E-03    8134.0    -351.2       0.0       1.0    -350.2   0.                -3.376    -59.428
15  7.5241E-03    8145.0    -327.0       0.0       1.4    -325.5   0.                -3.501    -56.160
16  1.0283E-02    8160.9    -297.7       0.0       2.1    -295.6   0.                -3.673    -51.447
17  1.4016E-02    8184.0    -263.5       0.0       3.3    -260.3   0.                -3.899    -45.455
18  1.9004E-02    8217.4    -224.9       0.0       5.0    -219.9   0.                -4.186    -38.468
19  2.5549E-02    8265.3    -182.9       0.0       7.8    -175.1   0.                -4.534    -30.870
20  3.3922E-02    8333.3    -139.5       0.0      12.4    -127.1   0.                -4.931    -23.157
21  4.4269E-02    8428.6     -97.5       0.0      19.8     -77.7   0.                -5.349    -15.902
22  5.6550E-02    8559.6     -60.1       0.0      31.7     -28.5   0.                -5.747     -9.647
23  7.0464E-02    8735.9     -15.3       0.0      50.4      35.2   0.                -6.072     -4.822
24  8.5456E-02    8967.2      -2.7       0.0      79.0      76.3   0.                -6.279     -1.706
25  1.0092E-01    9262.7       -.1       0.0     119.8     119.6   0.                -6.356      -.144
26  1.1660E-01    9631.3        .2       0.0     172.1     172.3   0.                -6.326       .415
27  1.3275E-01   10083.8        .2       0.0     226.6     226.7   0.                -6.191       .728
28  1.5092E-01   10635.2       0.0       0.0     263.5     263.5   0.                -5.878       .893
29  1.7426E-01   11303.9       0.0       0.0     266.8     266.8   0.                -5.366       .816
30  2.0899E-01   12106.6       0.0       0.0     239.1     239.1   0.                -5.195      -.844
31  2.6808E-01   13054.4       0.0       0.0     208.0     208.0   0.                -5.456      -.322
32  3.7049E-01   14154.2       0.0       0.0     188.1     188.1   0.                -4.475       .429
33  5.4375E-01   15412.1       0.0       0.0     167.6     167.6   0.                -2.654       .063
34  8.2768E-01   16835.0       0.0       0.0     140.9     140.9   0.                -1.297      -.104
35  1.2729E+00   18431.5       0.0       0.0     115.3     115.3   0.                 -.763      -.121
36  1.9561E+00   20212.5       0.0       0.0      93.9      93.9   0.                 -.483       .018
37  2.9784E+00   22191.0       0.0       0.0      77.2      77.2   0.                 -.372      -.045
38  4.4825E+00   24382.6       0.0       0.0      67.3      67.3   0.                 -.512      -.026
39  6.6085E+00   26805.5       0.0       0.0      71.9      71.9   0.                -1.231      -.032
40  9.5853E+00   29480.4       0.0       0.0     108.9     108.9   0.                -2.084      -.026
```

```
          RHOX           T      DTLAMB     DTSURF     DTFLUX        T1   CONV/TOTAL        ERROR      DERIV
  1  8.4569E-05     7694.2       4.9        0.0        0.0       4.9   0.                  .789       .186
  2  1.2256E-04     7699.9       5.1        0.0        -.0       5.1   0.                  .789       .246
  3  1.7384E-04     7696.6       4.4        0.0         .0       4.4   0.                  .789       .260
  4  2.4299E-04     7700.8       5.0        0.0        -.1       4.9   0.                  .789       .351
  5  3.3616E-04     7704.6       4.6        0.0        -.1       4.5   0.                  .789       .375
  6  4.6172E-04     7709.0       5.1        0.0        -.1       5.0   0.                  .789       .465
  7  6.3103E-04     7712.6       4.3        0.0        -.2       4.1   0.                  .789       .440
  8  8.5962E-04     7728.6      -1.9        0.0        -.3      -2.2   0.                  .789      -.212
  9  1.1687E-03     7732.7      -1.3        0.0        -.2      -1.5   0.                  .789      -.163
 10  1.5889E-03     7741.8       -.1        0.0        -.3       -.4   0.                  .789      -.015
 11  2.1628E-03     7753.6        .2        0.0        -.3       -.2   0.                  .789       .024
 12  2.9481E-03     7768.5        .2        0.0        -.4       -.2   0.                  .789       .036
 13  4.0250E-03     7786.9        .4        0.0        -.5       -.1   0.                  .789       .058
 14  5.5016E-03     7810.0        .8        0.0        -.6        .1   0.                  .789       .119
 15  7.5241E-03     7838.5        .5        0.0        -.9       -.3   0.                  .789       .081
 16  1.0283E-02     7879.4      -1.7        0.0       -1.0      -2.8   0.                  .789      -.279
 17  1.4016E-02     7917.7       5.1        0.0       -1.2       3.8   0.                  .790       .809
 18  1.9004E-02     7978.8       4.5        0.0       -1.8       2.7   0.                  .793       .720
 19  2.5549E-02     8054.8       3.4        0.0       -2.3       1.0   0.                  .797       .539
 20  3.3922E-02     8152.7       3.4        0.0       -3.2        .2   0.                  .804       .545
 21  4.4269E-02     8280.1       2.6        0.0       -4.5      -1.9   0.                  .811       .411
 22  5.6550E-02     8442.3       4.9        0.0       -6.3      -1.4   0.                  .826       .770
 23  7.0464E-02     8646.1      10.3        0.0       -9.5        .8   0.                  .881      1.606
 24  8.5456E-02     8926.5      -2.4        0.0      -14.4     -16.8   0.                  .913      -.754
 25  1.0092E-01     9272.1      -3.5        0.0      -20.2     -23.7   0.                  .741     -2.163
 26  1.1660E-01     9684.7       -.7        0.0      -26.8     -27.5   0.                  .533      -.851
 27  1.3275E-01    10191.5       -.7        0.0      -31.3     -32.0   0.                  .246     -1.574
 28  1.5092E-01    10769.6       -.1        0.0      -30.6     -30.6   0.                 -.008      -.257
 29  1.7426E-01    11438.9       0.0        0.0      -25.9     -25.9   0.                  .058      -.115
 30  2.0899E-01    12216.1       0.0        0.0      -19.2     -19.2   0.                 -.072      -.824
 31  2.6808E-01    13139.6       0.0        0.0      -12.2     -12.2   0.                 -.163      -.151
 32  3.7049E-01    14227.4       0.0        0.0       -9.0      -9.0   0.                  .332      -.319
 33  5.4375E-01    15463.6       0.0        0.0      -10.2     -10.2   0.                  .438      -.720
 34  8.2768E-01    16859.0       0.0        0.0      -12.9     -12.9   0.                  .499      -.257
 35  1.2729E+00    18435.8       0.0        0.0      -15.3     -15.3   0.                  .360      -.308
 36  1.9561E+00    20202.0       0.0        0.0      -14.4     -14.4   0.                  .054      -.082
 37  2.9784E+00    22163.7       0.0        0.0      -14.7     -14.7   0.                  .400       .014
 38  4.4825E+00    24362.3       0.0        0.0      -19.7     -19.7   0.                  .405      -.017
 39  6.6085E+00    26774.6       0.0        0.0      -19.5     -19.5   0.                 -.034      -.015
 40  9.5853E+00    29472.6       0.0        0.0      -13.1     -13.1   0.                 -.192      -.005
```

first guess for the temperature distribution, in which case the flux error at optical depth unity would be smaller. A much larger flux error at large depths could be handled by TCORR, say +1000% for radiative models or +1000000% for convective models. Large negative flux errors tend to be unstable.

On the second sample page, that is, the sixth iteration of our example, the flux error is down to 1%, the flux derivative error is down to 2%, and the temperature correction is on the order of 30 K. A few more iterations can be made to bring the errors as close to 0 as required.

In TCORR, the remainder of the subroutine is made up of various fudges for salvaging bad starting guesses or for speeding convergence. Finally, the temperatures are changed to their new values.

After TCORR, ATLAS5(3) would call STATEQ(11, 12) if we were doing statistical equilibrium. STATEQ would first compute the collisional rates for H^- and combine them with the previously calculated radiative rates to find $b(H^-)$. Then STATEQ would do the same for hydrogen.

Next, ATLAS5(3) calls HIGH(99) and TURB(99) to find geometric HEIGHT, VTURB, and PTURB.

At the end of each iteration, ATLAS5 calls PUTOUT(6) to spew out the results for the iteration. If IFPRNT > 1, PUTOUT prints all the variables that it has lying about in labeled COMMON blocks and that are not to be printed in the summary table (see the next two pages). Finally, if IFPRNT > 0, PUTOUT prints the summary shown on page 136. Note that the temperatures on the summary table are the corrected values, so the data in the table are not consistent with the temperatures until the model converges.

Also if IFPNCH > 0, PUTOUT punches the results in a form that can be read in again, as shown on pages 137 and 138, either to continue the calculation if the model has not converged or to accomplish whatever purpose the model was calculated for.

```
        RHOX       PTOTAL      PTURB          GRDADB     DLTDLP      VELSND     DLRDLT      HEATCP      HSCALE      VCONV        FLXCNV
  1  8.457E-05  8.457E-01  0.            1.098E-01  2.082E-05  1.046E+06 -1.516E+00  1.598E+09  9.390E+07  0.           0.
  2  1.226E-04  1.226E+00  0.            9.495E-02  3.149E-05  1.033E+06 -1.705E+00  2.057E+09  9.294E+07  0.           0.
  3  1.738E-04  1.738E+00  0.            8.439E-02  4.859E-05  1.021E+06 -1.927E+00  2.584E+09  9.175E+07  0.           0.
  4  2.430E-04  2.430E+00  0.            7.683E-02  7.395E-05  1.009E+06 -2.180E+00  3.158E+09  9.029E+07  0.           0.
  5  3.362E-04  3.362E+00  0.            7.141E-02  1.114E-04  9.967E+05 -2.451E+00  3.748E+09  8.856E+07  0.           0.
  6  4.617E-04  4.617E+00  0.            6.755E-02  1.666E-04  9.835E+05 -2.727E+00  4.308E+09  8.656E+07  0.           0.
  7  6.310E-04  6.310E+00  0.            6.483E-02  2.476E-04  9.694E+05 -2.987E+00  4.789E+09  8.432E+07  0.           0.
  8  8.596E-04  8.596E+00  0.            6.297E-02  3.662E-04  9.544E+05 -3.212E+00  5.149E+09  8.189E+07  0.           0.
  9  1.169E-03  1.169E+01  0.            6.179E-02  5.384E-04  9.388E+05 -3.384E+00  5.356E+09  7.933E+07  0.           0.
 10  1.589E-03  1.589E+01  0.            6.113E-02  7.874E-04  9.229E+05 -3.492E+00  5.401E+09  7.672E+07  0.           0.
 11  2.163E-03  2.163E+01  0.            6.091E-02  1.149E-03  9.071E+05 -3.532E+00  5.296E+09  7.413E+07  0.           0.
 12  2.948E-03  2.948E+01  0.            6.108E-02  1.674E-03  8.919E+05 -3.508E+00  5.066E+09  7.164E+07  0.           0.
 13  4.025E-03  4.025E+01  0.            6.159E-02  2.437E-03  8.776E+05 -3.428E+00  4.748E+09  6.932E+07  0.           0.
 14  5.502E-03  5.502E+01  0.            6.243E-02  3.548E-03  8.646E+05 -3.309E+00  4.381E+09  6.723E+07  0.           0.
 15  7.524E-03  7.524E+01  0.            6.356E-02  5.169E-03  8.532E+05 -3.165E+00  3.998E+09  6.540E+07  0.           0.
 16  1.028E-02  1.028E+02  0.            6.496E-02  7.546E-03  8.437E+05 -3.011E+00  3.627E+09  6.386E+07  0.           0.
 17  1.402E-02  1.402E+02  0.            6.656E-02  1.104E-02  8.364E+05 -2.862E+00  3.291E+09  6.265E+07  0.           0.
 18  1.900E-02  1.900E+02  0.            6.828E-02  1.621E-02  8.314E+05 -2.728E+00  3.005E+09  6.179E+07  0.           0.
 19  2.555E-02  2.555E+02  0.            6.999E-02  2.386E-02  8.292E+05 -2.621E+00  2.779E+09  6.134E+07  0.           0.
 20  3.392E-02  3.392E+02  0.            7.150E-02  3.526E-02  8.300E+05 -2.548E+00  2.624E+09  6.136E+07  0.           0.
 21  4.427E-02  4.427E+02  0.            7.261E-02  5.218E-02  8.347E+05 -2.520E+00  2.551E+09  6.196E+07  0.           0.
 22  5.655E-02  5.655E+02  0.            7.317E-02  7.710E-02  8.441E+05 -2.543E+00  2.570E+09  6.329E+07  5.263E-01  5.667E-10
 23  7.046E-02  7.046E+02  0.            7.317E-02  1.133E-01  8.597E+05 -2.628E+00  2.697E+09  6.561E+07  1.132E+01  6.779E-06
 24  8.546E-02  8.546E+02  0.            7.283E-02  1.645E-01  8.837E+05 -2.775E+00  2.944E+09  6.928E+07  5.649E+01  9.721E-04
 25  1.009E-01  1.009E+03  0.            7.264E-02  2.321E-01  9.191E+05 -2.963E+00  3.296E+09  7.484E+07  2.142E+02  5.807E-02
 26  1.166E-01  1.166E+03  0.            7.346E-02  3.117E-01  9.692E+05 -3.117E+00  3.657E+09  8.301E+07  6.442E+02  1.627E+00
 27  1.327E-01  1.327E+03  0.            7.660E-02  3.841E-01  1.036E+06 -3.076E+00  3.758E+09  9.435E+07  1.322E+03  1.352E+01
 28  1.509E-01  1.509E+03  0.            8.467E-02  4.185E-01  1.117E+06 -2.679E+00  3.229E+09  1.086E+08  1.470E+03  1.661E+01
 29  1.743E-01  1.743E+03  0.            1.037E-01  3.984E-01  1.207E+06 -2.038E+00  2.152E+09  1.238E+08  7.722E+02  1.989E+00
 30  2.090E-01  2.090E+03  0.            1.444E-01  3.370E-01  1.304E+06 -1.505E+00  1.191E+09  1.383E+08  2.201E+02  3.553E-02
 31  2.681E-01  2.681E+03  0.            2.070E-01  2.743E-01  1.416E+06 -1.225E+00  6.903E+08  1.522E+08  4.044E+01  1.790E-04
 32  3.705E-01  3.705E+03  0.            2.444E-01  2.352E-01  1.511E+06 -1.128E+00  5.437E+08  1.667E+08  0.           0.
 33  5.438E-01  5.438E+03  0.            2.097E-01  2.162E-01  1.548E+06 -1.158E+00  6.555E+08  1.830E+08  6.459E+00  1.216E-06
 34  8.277E-01  8.277E+03  0.            1.740E-01  2.111E-01  1.597E+06 -1.243E+00  8.601E+08  2.026E+08  8.485E+01  4.564E-03
 35  1.273E+00  1.273E+04  0.            1.921E-01  2.136E-01  1.704E+06 -1.213E+00  7.725E+08  2.255E+08  7.427E+01  3.833E-03
 36  1.956E+00  1.956E+04  0.            2.590E-01  2.196E-01  1.866E+06 -1.106E+00  5.279E+08  2.499E+08  0.           0.
 37  2.978E+00  2.978E+04  0.            3.308E-01  2.275E-01  2.050E+06 -1.040E+00  3.907E+08  2.757E+08  0.           0.
 38  4.482E+00  4.482E+04  0.            3.716E-01  2.385E-01  2.209E+06 -1.014E+00  3.397E+08  3.035E+08  0.           0.
 39  6.608E+00  6.608E+04  0.            3.881E-01  2.511E-01  2.343E+06 -1.004E+00  3.223E+08  3.338E+08  0.           0.
 40  9.585E+00  9.585E+04  0.            3.926E-01  2.922E-01  2.464E+06 -1.001E+00  3.177E+08  3.673E+08  0.           0.

                                                                                                                     FLUX  4.5118E+10
```

```
      XNATOM      ACCRAD      PRAD        XNFPH1      XNFPH2      XNFPHE1     XNFPHE2     XNFPHE3
 1  4.075E+11   6.811E+00   5.065E-04   9.609E+09   3.476E+11   4.075E+10   2.197E+05   3.483E-19
 2  5.967E+11   7.549E+00   7.792E-04   1.969E+10   4.977E+11   5.967E+10   2.248E+05   2.492E-19
 3  8.574E+11   8.474E+00   1.190E-03   3.838E+10   6.949E+11   8.574E+10   2.314E+05   1.839E-19
 4  1.218E+12   9.607E+00   1.816E-03   7.200E+10   9.519E+11   1.218E+11   2.401E+05   1.396E-19
 5  1.718E+12   1.096E+01   2.776E-03   1.309E+11   1.284E+12   1.718E+11   2.514E+05   1.086E-19
 6  2.414E+12   1.253E+01   4.253E-03   2.316E+11   1.709E+12   2.414E+11   2.658E+05   8.659E-20
 7  3.386E+12   1.431E+01   6.531E-03   4.001E+11   2.247E+12   3.386E+11   2.843E+05   7.078E-20
 8  4.750E+12   1.627E+01   1.003E-02   6.757E+11   2.924E+12   4.750E+11   3.076E+05   5.932E-20
 9  6.666E+12   1.836E+01   1.540E-02   1.117E+12   3.765E+12   6.666E+11   3.369E+05   5.102E-20
10  9.372E+12   2.054E+01   2.359E-02   1.814E+12   4.807E+12   9.372E+11   3.738E+05   4.504E-20
11  1.320E+13   2.277E+01   3.605E-02   2.895E+12   6.092E+12   1.320E+12   4.200E+05   4.089E-20
12  1.862E+13   2.502E+01   5.486E-02   4.545E+12   7.669E+12   1.862E+12   4.781E+05   3.828E-20
13  2.627E+13   2.726E+01   8.306E-02   7.024E+12   9.597E+12   2.627E+12   5.517E+05   3.711E-20
14  3.703E+13   2.951E+01   1.251E-01   1.069E+13   1.195E+13   3.703E+12   6.458E+05   3.753E-20
15  5.206E+13   3.181E+01   1.872E-01   1.601E+13   1.483E+13   5.206E+12   7.683E+05   4.001E-20
16  7.287E+13   3.424E+01   2.784E-01   2.360E+13   1.838E+13   7.287E+12   9.320E+05   4.571E-20
17  1.012E+14   3.698E+01   4.114E-01   3.417E+13   2.278E+13   1.012E+13   1.158E+06   5.731E-20
18  1.392E+14   4.026E+01   6.041E-01   4.847E+13   2.830E+13   1.392E+13   1.486E+06   8.148E-20
19  1.885E+14   4.449E+01   8.814E-01   6.712E+13   3.537E+13   1.885E+13   1.987E+06   1.373E-19
20  2.502E+14   5.031E+01   1.278E+00   9.026E+13   4.461E+13   2.502E+13   2.805E+06   2.904E-19
21  3.233E+14   5.872E+01   1.841E+00   1.170E+14   5.702E+13   3.233E+13   4.249E+06   8.245E-19
22  4.043E+14   7.133E+01   2.636E+00   1.449E+14   7.410E+13   4.043E+13   7.028E+06   3.383E-18
23  4.860E+14   9.068E+01   3.755E+00   1.697E+14   9.809E+13   4.860E+13   1.290E+07   2.146E-17
24  5.581E+14   1.205E+02   5.325E+00   1.852E+14   1.320E+14   5.581E+13   2.661E+07   2.210E-16
25  6.101E+14   1.651E+02   7.513E+00   1.847E+14   1.788E+14   6.101E+13   6.222E+07   3.788E-15
26  6.356E+14   2.275E+02   1.057E+01   1.648E+14   2.411E+14   6.356E+13   1.658E+08   1.079E-13
27  6.366E+14   3.017E+02   1.485E+01   1.272E+14   3.167E+14   6.366E+13   5.119E+08   5.152E-12
28  6.291E+14   3.628E+02   2.093E+01   8.262E+13   3.986E+14   6.291E+13   1.888E+09   4.204E-10
29  6.369E+14   3.792E+02   2.968E+01   4.538E+13   4.796E+14   6.367E+13   8.507E+09   5.780E-08
30  6.835E+14   3.456E+02   4.226E+01   2.265E+13   5.666E+14   6.826E+13   4.559E+10   1.179E-05
31  7.969E+14   2.921E+02   6.107E+01   1.165E+13   6.898E+14   7.915E+13   2.688E+11   2.815E-03
32  1.006E+15   2.474E+02   8.844E+01   6.686E+12   8.867E+14   9.742E+13   1.583E+12   6.224E-01
33  1.344E+15   2.155E+02   1.282E+02   4.341E+12   1.194E+15   1.179E+14   8.286E+12   1.037E+02
34  1.848E+15   1.952E+02   1.862E+02   3.122E+12   1.647E+15   1.198E+14   3.250E+13   1.048E+04
35  2.555E+15   1.814E+02   2.697E+02   2.394E+12   2.280E+15   8.844E+13   8.348E+13   5.558E+05
36  3.541E+15   1.686E+02   3.889E+02   1.927E+12   3.164E+15   5.069E+13   1.517E+14   1.675E+07
37  4.889E+15   1.574E+02   5.551E+02   1.607E+12   4.369E+15   2.657E+13   2.310E+14   3.412E+08
38  6.684E+15   1.490E+02   7.850E+02   1.382E+12   5.975E+15   1.411E+13   3.270E+14   5.231E+09
39  8.957E+15   1.418E+02   1.093E+03   1.201E+12   8.008E+15   7.739E+12   4.437E+14   6.332E+10
40  1.181E+16   1.405E+02   1.511E+03   1.062E+12   1.056E+16   4.464E+12   5.876E+14   6.212E+11
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```
TEFF  10000.   LOG G  4.000          SAMPLE MODEL                                                                   ITERATION  1

                                    ELECTRON               ROSSELAND     HEIGHT    ROSSELAND    FRACTION                           PER CENT FLUX
       RHOX       TEMP    PRESSURE   NUMBER     DENSITY      MEAN         (KM)       DEPTH     CONV FLUX     VTURB                  ERROR   DERIV
  1 8.457E-05    7710.5  8.457E-01  3.478E+11  9.007E-13  3.740E-01  1.270E+03  0.          0.           0.                      -3.106 -15.558
  2 1.226E-04    7710.6  1.226E+00  4.979E+11  1.319E-12  4.052E-01  1.625E+03  4.775E-05  0.           0.                      -3.107 -20.148
  3 1.738E-04    7710.7  1.738E+00  6.951E+11  1.895E-12  4.406E-01  1.949E+03  6.943E-05  0.           0.                      -3.108 -24.668
  4 2.430E-04    7710.9  2.430E+00  9.523E+11  2.691E-12  4.802E-01  2.254E+03  1.013E-04  0.           0.                      -3.108 -30.172
  5 3.362E-04    7711.1  3.362E+00  1.285E+12  3.796E-12  5.240E-01  2.545E+03  1.482E-04  0.           0.                      -3.110 -35.603
  6 4.617E-04    7711.5  4.617E+00  1.710E+12  5.334E-12  5.715E-01  2.824E+03  2.170E-04  0.           0.                      -3.113 -40.989
  7 6.310E-04    7712.1  6.310E+00  2.249E+12  7.483E-12  6.222E-01  3.091E+03  3.183E-04  0.           0.                      -3.117 -46.175
  8 8.596E-04    7712.8  8.596E+00  2.925E+12  1.050E-11  6.754E-01  3.348E+03  4.668E-04  0.           0.                      -3.124 -50.930
  9 1.169E-03    7714.0  1.169E+01  3.767E+12  1.473E-11  7.305E-01  3.596E+03  6.844E-04  0.           0.                      -3.136 -55.016
 10 1.589E-03    7715.7  1.589E+01  4.810E+12  2.071E-11  7.871E-01  3.837E+03  1.004E-03  0.           0.                      -3.154 -58.265
 11 2.163E-03    7720.2  2.163E+01  6.096E+12  2.918E-11  8.453E-01  4.070E+03  1.473E-03  0.           0.                      -3.182 -60.500
 12 2.948E-03    7735.7  2.948E+01  7.674E+12  4.115E-11  9.053E-01  4.296E+03  2.161E-03  0.           0.                      -3.224 -61.516
 13 4.025E-03    7756.5  4.025E+01  9.605E+12  5.806E-11  9.682E-01  4.515E+03  3.172E-03  0.           0.                      -3.286 -61.196
 14 5.502E-03    7783.8  5.502E+01  1.196E+13  8.184E-11  1.036E+00  4.729E+03  4.653E-03  0.           0.                      -3.376 -59.428
 15 7.524E-03    7819.4  7.524E+01  1.485E+13  1.151E-10  1.111E+00  4.937E+03  6.826E-03  0.           0.                      -3.501 -56.160
 16 1.028E-02    7865.3  1.028E+02  1.841E+13  1.610E-10  1.200E+00  5.139E+03  1.002E-02  0.           0.                      -3.673 -51.447
 17 1.402E-02    7923.7  1.402E+02  2.282E+13  2.237E-10  1.308E+00  5.335E+03  1.470E-02  0.           0.                      -3.899 -45.455
 18 1.900E-02    7997.5  1.900E+02  2.836E+13  3.075E-10  1.449E+00  5.525E+03  2.157E-02  0.           0.                      -4.186 -38.468
 19 2.555E-02    8090.2  2.555E+02  3.544E+13  4.165E-10  1.639E+00  5.707E+03  3.167E-02  0.           0.                      -4.534 -30.870
 20 3.392E-02    8206.2  3.392E+02  4.471E+13  5.528E-10  1.909E+00  5.881E+03  4.650E-02  0.           0.                      -4.931 -23.157
 21 4.427E-02    8350.9  4.427E+02  5.714E+13  7.145E-10  2.308E+00  6.045E+03  6.825E-02  0.           0.                      -5.349 -15.902
 22 5.655E-02    8531.1  5.655E+02  7.424E+13  8.935E-10  2.917E+00  6.199E+03  1.001E-01  1.333E-20   0.                      -5.747  -9.647
 23 7.046E-02    8771.1  7.046E+02  9.827E+13  1.074E-09  3.875E+00  6.340E+03  1.470E-01  1.600E-16   0.                      -6.072  -4.822
 24 8.546E-02    9043.5  8.546E+02  1.322E+14  1.233E-09  5.404E+00  6.470E+03  2.158E-01  2.299E-14   0.                      -6.279  -1.706
 25 1.009E-01    9382.4  1.009E+03  1.791E+14  1.348E-09  7.790E+00  6.589E+03  3.166E-01  1.374E-12   0.                      -6.356   -.144
 26 1.166E-01    9803.6  1.166E+03  2.413E+14  1.405E-09  1.131E+01  6.703E+03  4.652E-01  3.850E-11   0.                      -6.326    .415
 27 1.327E-01   10310.5  1.327E+03  3.170E+14  1.407E-09  1.571E+01  6.818E+03  6.834E-01  3.193E-10   0.                      -6.191    .728
 28 1.509E-01   10898.7  1.509E+03  3.988E+14  1.390E-09  1.951E+01  6.947E+03  1.006E+00  3.912E-10   0.                      -5.878    .893
 29 1.743E-01   11570.7  1.743E+03  4.798E+14  1.408E-09  2.063E+01  7.115E+03  1.479E+00  4.659E-11   0.                      -5.366    .816
 30 2.090E-01   12345.7  2.090E+03  5.669E+14  1.511E-09  1.881E+01  7.353E+03  2.164E+00  8.306E-13   0.                      -5.195   -.844
 31 2.681E-01   13262.4  2.681E+03  6.906E+14  1.761E-09  1.596E+01  7.717E+03  3.189E+00  4.197E-15   0.                      -5.456   -.322
 32 3.705E-01   14342.3  3.705E+03  8.902E+14  2.223E-09  1.348E+01  8.234E+03  4.683E+00  0.           0.                      -4.475    .429
 33 5.438E-01   15579.7  5.438E+03  1.211E+15  2.971E-09  1.176E+01  8.906E+03  6.850E+00  2.768E-17   0.                      -2.654    .063
 34 8.277E-01   16975.9  8.277E+03  1.713E+15  4.085E-09  1.080E+01  9.718E+03  1.003E+01  1.025E-13   0.                      -1.297   -.104
 35 1.273E+00   18546.8  1.273E+04  2.448E+15  5.645E-09  1.030E+01  1.064E+04  1.472E+01  8.560E-14   0.                       -.763   -.121
 36 1.956E+00   20306.4  1.956E+04  3.469E+15  7.827E-09  9.953E+00  1.167E+04  2.162E+01  0.           0.                       -.483    .018
 37 2.978E+00   22268.2  2.978E+04  4.833E+15  1.080E-08  9.808E+00  1.277E+04  3.170E+01  0.           0.                       -.372   -.045
 38 4.482E+00   24449.9  4.482E+04  6.632E+15  1.477E-08  1.000E+01  1.396E+04  4.657E+01  0.           0.                       -.512   -.026
 39 6.608E+00   26877.4  6.608E+04  8.901E+15  1.980E-08  1.051E+01  1.520E+04  6.835E+01  0.           0.                      -1.231   -.032
 40 9.585E+00   29589.3  9.585E+04  1.174E+16  2.610E-08  1.138E+01  1.648E+04  1.009E+02  0.           0.                      -2.084   -.026
```

```
TEFF  10000. GRAVITY 4.000 LTE
TITLE SAMPLE MODEL
 OPACITY IFOP 1 1 1 1 1 1 0 0 1 0 0 1 0 0 0 0 0 0 0 0
 CONVECTION OFF  1.00 TURBULENCE OFF  0.00  0.00  0.00  0.00
ABUNDANCE SCALE   1.000 ABUNDANCE CHANGE 1  .900 2  .100
  ABUNDANCE CHANGE  3 -11.60  4  -9.60  5  -9.20  6  -3.50  7  -4.12  8  -3.28
  ABUNDANCE CHANGE  9  -6.60 10  -3.50 11  -6.18 12  -4.57 13  -5.65 14  -4.50
  ABUNDANCE CHANGE 15  -6.62 16  -4.84 17  -6.60 18  -5.30 19  -7.00 20  -5.72
  ABUNDANCE CHANGE 21  -9.01 22  -7.55 23  -8.13 24  -6.58 25  -7.17 26  -4.50
  ABUNDANCE CHANGE 27  -8.40 28  -6.97 29  -7.30 30  -7.63 31  -9.11 32  -8.73
  ABUNDANCE CHANGE 33  -9.70 34  -8.80 35  -9.40 36  -8.80 37  -9.42 38  -9.23
  ABUNDANCE CHANGE 39  -9.60 40  -9.60 41 -10.30 42 -10.00 43 -20.00 44 -10.40
  ABUNDANCE CHANGE 45 -11.20 46 -10.70 47 -11.30 48  -9.98 49 -10.34 50 -10.34
  ABUNDANCE CHANGE 51 -10.40 52 -10.00 53 -10.60 54 -10.00 55 -10.90 56 -10.15
  ABUNDANCE CHANGE 57 -10.60 58 -10.40 59 -11.20 60 -10.50 61 -20.00 62 -11.00
  ABUNDANCE CHANGE 63 -11.30 64 -10.90 65 -11.60 66 -10.80 67 -11.50 68 -11.10
  ABUNDANCE CHANGE 69 -11.90 70 -10.90 71 -11.70 72 -11.40 73 -11.70 74 -10.90
  ABUNDANCE CHANGE 75 -11.40 76 -10.70 77 -10.80 78 -10.40 79 -11.30 80 -11.10
  ABUNDANCE CHANGE 81 -11.50 82 -10.15 83 -11.30 84 -20.00 85 -20.00 86 -20.00
  ABUNDANCE CHANGE 87 -20.00 88 -20.00 89 -20.00 90 -11.70 91 -20.00 92 -12.00
  ABUNDANCE CHANGE 93 -20.00 94 -20.00 95 -20.00 96 -20.00 97 -20.00 98 -20.00
  ABUNDANCE CHANGE 99 -20.00
READ DECK 40 RHOX,T,P,XNE,ABROSS,PRAD,VTURB
  8.45691298E-05    7700.3 8.452E-01 3.460E+11 3.578E-01 5.312E-04 0.
  1.22559051E-04    7706.2 1.225E+00 4.857E+11 3.760E-01 8.074E-04 0.
  1.73837744E-04    7702.1 1.737E+00 6.618E+11 3.921E-01 1.214E-03 0.
  2.42986209E-04    7707.0 2.428E+00 8.835E+11 4.087E-01 1.812E-03 0.
  3.36158983E-04    7710.3 3.359E+00 1.158E+12 4.243E-01 2.692E-03 0.
  4.61724880E-04    7715.2 4.613E+00 1.497E+12 4.395E-01 3.983E-03 0.
  6.31027399E-04    7717.7 6.304E+00 1.909E+12 4.536E-01 5.872E-03 0.
  8.59624197E-04    7727.5 8.588E+00 2.428E+12 4.744E-01 8.646E-03 0.
  1.16866788E-03    7730.8 1.167E+01 3.038E+12 4.890E-01 1.270E-02 0.
  1.58888214E-03    7741.3 1.587E+01 3.788E+12 5.077E-01 1.863E-02 0.
  2.16282711E-03    7753.4 2.160E+01 4.709E+12 5.299E-01 2.734E-02 0.
  2.94814345E-03    7768.2 2.944E+01 5.844E+12 5.570E-01 4.015E-02 0.
  4.02498758E-03    7786.7 4.019E+01 7.249E+12 5.906E-01 5.909E-02 0.
  5.50164396E-03    7810.0 5.493E+01 9.005E+12 6.334E-01 8.718E-02 0.
  7.52407493E-03    7838.1 7.511E+01 1.121E+13 6.880E-01 1.290E-01 0.
  1.02834532E-02    7876.0 1.026E+02 1.410E+13 7.661E-01 1.919E-01 0.
  1.40163540E-02    7922.4 1.399E+02 1.761E+13 8.516E-01 2.859E-01 0.
  1.90040002E-02    7982.2 1.896E+02 2.242E+13 9.862E-01 4.271E-01 0.
  2.55486879E-02    8056.1 2.548E+02 2.879E+13 1.171E+00 6.404E-01 0.
  3.39218929E-02    8153.0 3.383E+02 3.748E+13 1.439E+00 9.621E-01 0.
  4.42691601E-02    8279.2 4.412E+02 4.960E+13 1.842E+00 1.446E+00 0.
  5.65504204E-02    8440.6 5.633E+02 6.670E+13 2.460E+00 2.171E+00 0.
  7.04643319E-02    8646.5 7.014E+02 9.097E+13 3.429E+00 3.245E+00 0.
  8.54564361E-02    8905.5 8.496E+02 1.278E+14 5.137E+00 4.839E+00 0.
  1.00917247E-01    9242.4 1.002E+03 1.792E+14 7.849E+00 7.192E+00 0.
  1.16596651E-01    9650.4 1.155E+03 2.457E+14 1.174E+01 1.060E+01 0.
  1.32749420E-01   10151.5 1.312E+03 3.240E+14 1.633E+01 1.536E+01 0.
  1.50915325E-01   10731.3 1.487E+03 4.009E+14 1.947E+01 2.198E+01 0.
  1.74261950E-01   11406.5 1.711E+03 4.733E+14 1.972E+01 3.103E+01 0.
  2.08989640E-01   12192.0 2.046E+03 5.532E+14 1.770E+01 4.366E+01 0.
  2.68079327E-01   13133.4 2.618E+03 6.716E+14 1.505E+01 6.235E+01 0.
  3.70489029E-01   14222.9 3.615E+03 8.651E+14 1.278E+01 8.970E+01 0.
  5.43750161E-01   15458.5 5.309E+03 1.180E+15 1.129E+01 1.291E+02 0.
  8.27680811E-01   16852.6 8.091E+03 1.673E+15 1.051E+01 1.862E+02 0.
  1.27294426E+00   18428.2 1.246E+04 2.397E+15 1.009E+01 2.686E+02 0.
  1.95608422E+00   20194.8 1.917E+04 3.402E+15 9.794E+00 3.864E+02 0.
```

```
 2.97844858E+00  22145.3 2.923E+04 4.750E+15 9.688E+00 5.509E+02 0.
 4.48247664E+00  24337.7 4.405E+04 6.523E+15 9.872E+00 7.790E+02 0.
 6.60846847E+00  26750.2 6.500E+04 8.765E+15 1.038E+01 1.086E+03 0.
 9.58525890E+00  29456.2 9.435E+04 1.156E+16 1.122E+01 1.506E+03 0.
READ FREQUENCIES  78   1  78   COOL
    1   3.28804671E+13   1.64402500E+13    2   3.28805329E+13   3.85635500E+12
    3   4.05931694E+13   3.85635500E+12    4   4.05932506E+13   5.39128550E+12
    5   5.13757296E+13   5.39128550E+12    6   5.13758324F+13   7.86364000E+12
    7   6.71029939E+13   7.86364000E+12    8   6.71031281E+13   1.21158305E+13
    9   9.13346307E+13   1.21158305E+13   10   9.13348133E+13   2.00936390E+13
   11   1.31521868E+14   2.00936390E+13   12   1.31522132E+14   2.55333846E+13
   13   1.82588587E+14   2.55333846E+13   14   1.82588952E+14   4.40620250E+12
   15   1.95000000E+14   1.53829037E+13   16   2.05502919E+14   3.12524966E+12
   17   2.05503331E+14   9.32490356E+12   18   2.30000000E+14   2.85685104E+13
   19   2.60000000E+14   3.68109332E+13   20   3.00000000E+14   3.37166143E+13
   21   3.30000000E+14   3.78116947E+13   22   3.65338525E+14   1.36031090E+13
   23   3.65339255E+14   1.23397723E+13   24   4.00000000E+14   4.60720442E+13
   25   4.50000000E+14   5.17916416E+13   26   5.00000000E+14   4.94576518E+13
   27   5.50000000E+14   5.00000000E+13   28   6.00000000E+14   5.00000000E+13
   29   6.50000000E+14   4.99377588E+13   30   7.00000000E+14   4.84600648E+13
   31   7.50000000E+14   5.66913371E+13   32   7.98039662E+14   1.79512994E+13
   33   7.98041258E+14   1.19860200E+13   34   8.22011678E+14   1.19860200E+13
   35   8.22013322E+14   9.41926567E+12   36   8.50000000E+14   4.11449708E+13
   37   9.00000000E+14   5.32404280E+13   38   9.50000000E+14   4.91828356E+13
   39   1.00000000E+15   5.00000000E+13   40   1.05000000E+15   4.97535082E+13
   41   1.10000000E+15   4.98960590E+13   42   1.15000000E+15   5.22340180E+13
   43   1.19257851E+15   1.56961149E+13   44   1.19258089E+15   2.17291574E+13
   45   1.25000000E+15   6.47593919E+13   46   1.30000000E+15   4.54821099E+13
   47   1.35000000E+15   5.00073710E+13   48   1.40000000E+15   5.25709620E+13
   49   1.44299856E+15   1.58713079E+13   50   1.44300144E+15   3.61460000E+13
   51   1.51529048E+15   3.61460000E+13   52   1.51529352E+15   1.23599776E+13
   53   1.55000000E+15   4.71491758E+13   54   1.60000000E+15   3.86973422E+13
   55   1.65000000E+15   8.84560518E+13   56   1.75000000E+15   8.18550714E+13
   57   1.78796711E+15   4.15928130E+12   58   1.78797069E+15   1.11544291E+13
   59   1.82000000E+15   4.06991086E+13   60   1.84884915E+15   9.02856228E+12
   61   1.84885285E+15   1.20617571E+13   62   1.90000000E+15   8.48029699E+13
   63   1.97231453F+15   2.66007730E+13   64   1.97231847E+15   1.42441540E+13
   65   2.02000000E+15   6.96470460E+13   66   2.07609792E+15   1.98923000E+13
   67   2.07610208E+15   4.74367545E+13   68   2.20000000E+15   1.27770122E+14
   69   2.30000000E+15   1.22435459E+14   70   2.41959758E+15   4.58576637E+13
   71   2.41960242E+15   3.03310636E+13   72   2.50000000E+15   8.85358763E+13
   73   2.60000000E+15   1.39757530E+14   74   2.72539727E+15   4.71755303E+13
   75   2.72540273E+15   2.56441836E+13   76   2.80000000E+15   1.00571733E+14
   77   3.00000000E+15   3.29021965E+14   78   3.28804671E+15   1.07412118E+14
BEGIN                        ITERATION   6 COMPLETED
```

ATLAS5(3) continues to iterate on the model for NUMITS iterations. Once the model is completed, ATLAS5 calls READIN for more instructions. If READIN finds an END card, it calls EXIT.

8.2 Control Cards for ATLAS5

The control cards for ATLAS were designed to be simple and straightforward. The easiest way to avoid error is to consider whether all the information needed to calculate a model atmosphere is being supplied to READIN. First, the physical parameters: effective temperature, surface gravity, and abundances. Second, the physical processes: opacities, statistical equilibrium, convection, and turbulence. Third, the operational procedure: the starting model, the frequency set, and the number of iterations. Fourth, the type and form of output.

The data and instructions are either presented as code words or preceded by identifying code words. This allows each set of data identified by a code word to appear in any order, with several to a card. READIN reads with a free-field format in which the end of a field is signified by a blank or a comma (a code word can also be ended with an equal sign). Numbers can be written in any I, E, or F format, and words can be any length but only the first six letters are read. The following are examples of equivalent input cards:

```
            TEFF=1.E4
                          TEFF      1.E 4
TEFF           10000
TEFF=10000
TEFF, 1.E+4,
```

For several models to be calculated in succession, only those data that change need be specified. If no new data are specified, the calculation continues from the last iteration of the previous model.

We list here sample input cards with brief descriptions as necessary. The letters and numbers actually read are underlined. Cards that require special input or produce special output will be discussed further in Section 8.3.

TEFF=10000

Effective temperature, TEFF.

GRAVITY=4 or GRAVITY=1.E4

Gravity, GRAV. The log is assumed if the number is less than 10.

OPACITY ON HLINES, HOT

OPACITY OFF HLINES, HOT

OPACITY IFOP 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

The 20 code words and their defaults are as follows:

1.	H1	ON	11.	HOT	OFF
2.	H2PLUS	ON	12.	ELECTRON	ON
3.	HMINUS	ON	13.	H2RAY	OFF
4.	HRAY	ON	14.	HLINES	OFF
5.	HE1	ON	15.	LINES	OFF
6.	HE2	ON	16.	LINESCAT	OFF
7.	HEMINUS	ON	17.	XLINES	OFF
8.	HERAY	ON	18.	XLSCAT	OFF
9.	COOL	ON	19.	XCONT	OFF
10.	LUKE	OFF	20.	XSCAT	OFF

IFOP is a list of all 20 switches.

ITERATIONS 6

Number of iterations, NUMITS. Maximum is 15.

MOLECULES ON

MOLECULES OFF

Molecules in equilibrium equations. If ON, special data are read in separately as described in Section 8.3. Defaults OFF.

CALCULATE STARTING MODEL 40 DEPTHS STARTING AT -3.5 SPACING .125

Used only after TEFF and GRAV are defined. The 40 optical depths are in TAUROS, Rosseland tau, against which READIN defines a temperature distribution,
T = TEFF*(.75*(.710+TAUROS-.1331*EXP(-3.4488*TAUROS)))**.25.
Then READIN uses subroutine TTAUP to find T(RHOX). The maximum value for NRHOX, the number of depths, is 40

ABUNDANCE SCALE 1.

ABUNDANCE CHANGE 1 .5, 2 .5, 6 -3

The default abundances (number fractions) are listed in subroutine BLOCKE(32) and stored in array ABUND in COMMON /ELEM/. The actual abundances used are stored in array XABUND in COMMON /XABUND/. The abundances in array ABUND can be changed with an ABUNDANCE CHANGE card by specifying the atomic number and the new abundance. Negative numbers are assumed to be logarithms. The array XABUND is filled by taking the abundances in ABUND and multiplying them, except for H and He, by a scaling factor XSCALE, which defaults 1. Thus we might get abundances for a subdwarf by setting XSCALE to 0.01.

PRINT 1 1 1 1 2

PUNCH 0 0 0 0 1

Requires one integer for each iteration, so the number of iterations must be specified before these cards are read. The print options are (IFPRNT=)

0 no print,
1 print only summary table,
2 print temperature correction, surface fluxes, etc.,
3 print 2 and TAUNU, SNU, JNU, etc., at each frequency,
4 print 2 and all opacities at each frequency.

Defaults 2. See Section 8.3 for examples of 3 and 4.

The punch options are (IFPNCH=)

0 no punch,
1 punch model,
2 punch 1 and surface fluxes or intensities,
5 punch 2 and molecular number densities over partition functions.

Defaults 0, except 1 on the last iteration. See Section 8.3 for examples of 5.

READ FREQUENCIES 65 FREQS. INTEGRATE FROM 1 to 50. TEST1 IS THE ID.

Starting with the next card, reads 65 triplets of subscript, frequency, and integration coefficient in any order on as many cards as necessary. Each card may contain any number of complete triplets. If there are extremely large opacity edges, the model calculation may be left unchanged by simply ignoring regions of high opacity. In this example, integration runs from frequency 1 to frequency 50. TEST1 is simply a name used to identify the frequency set to avoid confusion when several different sets are available.

READ DEPARTURE COEFFICIENTS 40

Starting with the next card, reads a previously calculated set of b's for 40 depths on 40 cards. READIN expects to find RHOX, BHYD for n = 1 to 6, and BMIN on each card. The RHOX on these cards is a dummy for identification only. Defaults all b's unity.

READ STARTING T-TAU FOR 40 TAUS

Starting with the next card, reads TAUROS and T for a starting model. TAUROS may be in logarithms. READIN proceeds as for a CALCULATE card

READ DECK 40 RHOX

Starting with the next card, reads 40 cards each with RHOX, T, P, XNE, ABROSS, PRAD, and VTURB. If this deck is to be used as a starting model, the calculation will depend only on RHOX, T, PRAD, and VTURB and can get by with only RHOX and T if PRAD or VTURB is not critical. Once RHOX and T have been read, READIN will supply zeros to fill out the list if the card is left blank after any variable.

LTE

NLTE

NLTE stands for non-LTE, which is a negative way of saying statistical equilibrium calculations are requested. Defaults LTE with all b's unity.

BEGIN MODEL

Marks the end of data for READIN and the return to ATLAS to begin the model calculation.

SCATTERING ON

SCATTERING OFF

Compute the source function exactly with scattering or approximately without. Defaults ON.

END

In ATLAS5 this calls EXIT.

TITLE=TEST OF NEW OPACITY ROUTINES

Columns 7 to 80 are printed as a title on the summary table at the end of each iteration.

CONVECTION ON   MIXLTH=1.5

CONVECTION OFF

If ON, the total flux that enters the temperature correction includes convective flux as well as radiative flux. MIXLTH, the ratio of mixing length to scale height, is 1.5. Defaults OFF with MIXLTH 1. The convective flux is always calculated to indicate its possible importance, as long as IFPRES is 1 and MIXLTH > 0.

TURBULENCE ON TRBFDG=0, TRBPOW=0, TRBSND=0, TRBCON=5.

TURBULENCE OFF

If ON, pressure computation includes turbulent pressure. The turbulent velocity in kilometers per second is

VTURB = TRBFDG*RHO**TRBPOW + TRBSND*VELSND/1.E5 + TRBCON ,

where the sound velocity is in centimeters per second. Defaults OFF.

CHANGE RHOX 35 1.E-5, 1.57E-5, etc.

Reads 35 new rhoxes on as many cards as necessary. This card is used, only after a model has been defined, to change point spacing or to extrapolate to greater or smaller depths. In changing RHOX, READIN interpolates T, P, XNE, ABROSS, VTURB, PRAD, BHYD, and BMIN and sets NRHOX to 35.

SURFACE FLUX

SURFACE INTENSITY FOR 5 ANGLES=1., .8, .6, .4, .3

SURFACE OFF

Calculate flux (IFSURF=1) or intensity (IFSURF=2) only at the surface, as in a spectrum calculation. There is a maximum of 20 angles. Defaults OFF.

PRESSURE ON

PRESSURE OFF

Compute pressure and number densities. Defaults ON.

CORRECTION ON

CORRECTION OFF

Do temperature corrections. Defaults ON.

WAVELENGTH 500. BY .001 TO 501.

Instead of frequencies, uses equally spaced wavelengths. The units are nanometers.

SCALE MODEL 40 -4.5 .1666666666 TEFF=5000 GRAVITY=3

This card must come after a model has been defined and TEFF and GRAV have been specified. This instruction scales models with gravity and effective temperature. The numbers define TAUROS, as on a CALCULATE card, and the TEFF and GRAV for the new model. READIN computes TAUROS for the existing model by integrating ABROSS. It then interpolates all the existing variables, as with a CHANGE RHOX card, to the new TAUROS. READIN then makes the scalings

$$T^{new} = T^{old}(TEFF^{new}/TEFF^{old})$$

and

$$PRAD^{new} = PRAD^{old}(TEFF^{new}/TEFF^{old})^4(GRAV^{new}/GRAV^{old}) \quad .$$

Then READIN calls TTAUP to find RHOX for the new model. If the new TEFF and GRAV are the same as the old, the result is just an interpolation of the old model onto a log TAUROS scale.

CALL DUMMYR

This allows additional data to be read in by using DUMMYR without having to modify READIN.

8.3 Options

We will go through the control cards again pointing out the results of using special options.

MOLECULES ON

There are two cases. When IFPRES = 1 (PRESSURE ON), NMOLEC(50) solves the molecular equilibrium equations. In the loop DO 20, NMOLEC reads a card for every species to be considered in the molecular equilibrium equations. The data are read by NMOLEC instead of READIN, so NMOLEC can be deleted to save central memory space without leaving a big array behind in READIN. (This can be changed if memory space is no object.) Since NMOLEC reads after READIN has finished, the data cards must come after the BEGIN card. On each card, NMOLEC expects the molecule code and six constants that go into the polynomial form of the Saha equation (Section 4.4) in the format (F18.2, F7.3, 5E11.4). For atoms, these constants can be left blank, in which case NMOLEC uses PFSAHA to do the Saha equation. The cards are printed out as they are read in as shown on the following two pages. The end of the data is denoted by a 0 card or a blank card. Since NMOLEC reads only once each time ATLAS5 is executed, all models run at the same time must include the same molecules.

```
MOLECULES INPUT
   1           1.00  -0.000-0.        -0.        -0.        -0.        -0.
   2           1.01  -0.000-0.        -0.        -0.        -0.        -0.
   3           2.00  -0.000-0.        -0.        -0.        -0.        -0.
   4           2.01  -0.000-0.        -0.        -0.        -0.        -0.
   5           2.02  -0.000-0.        -0.        -0.        -0.        -0.
   6           6.00  -0.000-0.        -0.        -0.        -0.        -0.
   7           6.01  -0.000-0.        -0.        -0.        -0.        -0.
   8           7.00  -0.000-0.        -0.        -0.        -0.        -0.
   9           7.01  -0.000-0.        -0.        -0.        -0.        -0.
  10           8.00  -0.000-0.        -0.        -0.        -0.        -0.
  11           8.01  -0.000-0.        -0.        -0.        -0.        -0.
  12           9.00  -0.000-0.        -0.        -0.        -0.        -0.
  13          11.00  -0.000-0.        -0.        -0.        -0.        -0.
  14          11.01  -0.000-0.        -0.        -0.        -0.        -0.
  15          12.00  -0.000-0.        -0.        -0.        -0.        -0.
  16          12.01  -0.000-0.        -0.        -0.        -0.        -0.
  17          13.00  -0.000-0.        -0.        -0.        -0.        -0.
  18          13.01  -0.000-0.        -0.        -0.        -0.        -0.
  19          14.00  -0.000-0.        -0.        -0.        -0.        -0.
  20          14.01  -0.000-0.        -0.        -0.        -0.        -0.
  21          15.00  -0.000-0.        -0.        -0.        -0.        -0.
  22          16.00  -0.000-0.        -0.        -0.        -0.        -0.
  23          17.00  -0.000-0.        -0.        -0.        -0.        -0.
  24          19.00  -0.000-0.        -0.        -0.        -0.        -0.
  25          19.01  -0.000-0.        -0.        -0.        -0.        -0.
  26          20.00  -0.000-0.        -0.        -0.        -0.        -0.
  27          20.01  -0.000-0.        -0.        -0.        -0.        -0.
  28          20.02  -0.000-0.        -0.        -0.        -0.        -0.
  29         101.00   4.477 4.6628E+01 1.8031E-03 5.0239E-07 8.1424E-11 5.0501E-15
  30         106.00   3.470 4.5506E+01 1.7112E-03 3.6319E-07 5.0164E-11 2.8716E-15
  31         107.00   3.699 4.5244E+01 1.8435E-03 4.9000E-07 7.7353E-11 4.7639E-15
  32         108.00   4.395 4.5746E+01 1.7004E-03 4.4905E-07 7.0861E-11 4.3648E-15
  33         109.00   5.844 4.6618E+01 1.5382E-03 4.0410E-07 6.4407E-11 3.9816E-15
  34         111.00   2.050 4.4709E+01 2.4163E-03 6.1037E-07 9.0492E-11 5.3705E-15
  35         112.00   1.999 4.3437E+01 2.2153E-03 5.4885E-07 8.1160E-11 4.8026E-15
  36         113.00   2.901 4.5688E+01 1.8402E-03 4.1240E-07 5.7606E-11 3.2768E-15
  37         114.00   3.190 4.4770E+01 1.6858E-03 3.7373E-07 5.0857E-11 2.8282E-15
  38         115.00   3.300 4.4680E+01 1.8959E-03 4.6737E-07 6.8061E-11 4.0256E-15
  39         116.00   3.530 4.5272E+01 1.8600E-03 4.7327E-07 7.1690E-11 4.3041E-15
  40         117.00   4.431 4.5886E+01 1.5637E-03 3.9598E-07 6.2107E-11 3.8283E-15
  41         606.00   6.156 4.9635E+01 3.4811E-03 1.0492E-06 1.6849E-10 1.0370E-14
  42         607.00   8.109 4.7853E+01 1.8656E-03 4.6185E-07 7.1497E-11 4.3750E-15
  43         608.00  11.108 4.9170E+01 1.5802E-03 3.4347E-07 4.6870E-11 2.6563E-15
  44         609.00   4.966 4.7368E+01 2.0173E-03 4.7759E-07 6.7404E-11 3.8474E-15
  45         615.00   6.895 4.7509E+01 2.1172E-03 4.9533E-07 7.2805E-11 4.4007E-15
  46         616.00   7.892 4.8547E+01 1.7379E-03 3.6954E-07 4.7608E-11 2.5585E-15
  47         617.00   3.340 4.7009E+01 2.4592E-03 6.5348E-07 9.8261E-11 5.8172E-15
  48         707.00   9.763 4.8696E+01 1.9224E-03 4.9143E-07 7.4692E-11 4.5399E-15
  49         708.00   6.508 4.7365E+01 1.9840E-03 4.9280E-07 7.2933E-11 4.3354E-15
  50         709.00   2.819 4.6770E+01 2.2411E-03 5.5102E-07 7.9899E-11 4.6459E-15
  51         714.00   4.510 4.7147E+01 1.8720E-03 4.1254E-07 5.3950E-11 2.9053E-15
  52         715.00   7.111 4.7683E+01 2.2458E-03 5.5753E-07 7.9113E-11 4.5753E-15
  53         716.00   4.987 4.6988E+01 2.2584E-03 5.7344E-07 8.3948E-11 4.9197E-15
  54         808.00   5.116 4.8625E+01 1.6321E-03 3.3915E-07 4.6025E-11 2.5839E-15
  55         811.00   3.079 4.6421E+01 2.6221E-03 6.8505E-07 1.0200E-10 6.0540E-15
  56         812.00   3.903 4.6567E+01 2.3003E-03 4.3846E-07 5.3231E-11 2.8469E-15
  57         813.00   4.987 4.7561E+01 2.0103E-03 4.5650E-07 6.2393E-11 3.4674E-15
  58         814.00   8.310 4.8477E+01 1.5511E-03 2.9069E-07 3.2807E-11 1.5486E-15
  59         815.00   6.071 4.7307E+01 2.4172E-03 6.2096E-07 8.9966E-11 5.2500E-15
  60         816.00   5.358 4.7488E+01 1.6987E-03 3.5057E-07 4.4497E-11 2.3647E-15
  61         817.00   2.745 4.6832E+01 2.1078E-03 5.1344E-07 7.4414E-11 4.3173E-15
```

```
 62            909.00  1.592 4.8632E+01 2.0165E-03 4.6054E-07 6.4288E-11 3.6296E-15
 63            911.00  4.953 4.6717E+01 2.7566E-03 7.4062E-07 1.1213E-10 6.7066E-15
 64            912.00  3.200 4.5468E+01 2.5089E-03 6.5244E-07 9.7170E-11 5.7561E-15
 65            913.00  6.790 4.7788E+01 2.1362E-03 5.0666E-07 7.1400E-11 4.0530E-15
 66            914.00  5.420 4.6897E+01 2.1060E-03 4.9864E-07 6.8598E-11 3.7971E-15
 67            916.00  3.338 4.6706E+01 1.9206E-03 4.3001E-07 5.8062E-11 3.2077E-15
 68            917.00  2.616 4.7680E+01 2.1411E-03 5.3239E-07 7.8152E-11 4.5625E-15
 69           1111.00   .730 4.5152E+01 3.6917E-03 1.0752E-06 1.7017E-10 1.0459E-14
 70           1117.00  4.222 4.6147E+01 3.0037E-03 8.5128E-07 1.3301E-10 8.0960E-15
 71           1216.00  2.901 4.6082E+01 2.6137E-03 6.8845E-07 1.0253E-10 6.0759E-15
 72           1217.00  2.701 4.4998E+01 2.8447E-03 7.9686E-07 1.2369E-10 7.4944E-15
 73           1313.00  1.604 4.7559E+01 2.9097E-03 7.7812E-07 1.1753E-10 6.9499E-15
 74           1317.00  5.074 4.7276E+01 2.5438E-03 6.7568E-07 1.0182E-10 6.0055E-15
 75           1414.00  3.252 4.7179E+01 2.0256E-03 4.5186E-07 5.7418E-11 2.9577E-15
 76           1416.00  6.418 4.7989E+01 1.7935E-03 3.7532E-07 4.5974E-11 2.3242E-15
 77           1417.00  4.002 4.6541E+01 2.5534E-03 6.8459E-07 1.0209E-10 5.9733E-15
 78           1515.00  5.033 4.8223E+01 2.6898E-03 7.0362E-07 1.0075E-10 5.8493E-15
 79           1516.00  5.637 4.6919E+01 2.7644E-03 7.4350E-07 1.0948E-10 6.4205E-15
 80           1616.00  4.380 4.7693E+01 1.9029E-03 4.2359E-07 5.5948E-11 3.0438E-15
 81           1617.00  2.749 4.7565E+01 3.5631E-03 1.0897E-06 1.7573E-10 1.0805E-14
 82           1717.00  2.476 4.8021E+01 2.4184E-03 6.5374E-07 1.0061E-10 6.0420E-15
 83          10106.00  8.850 9.3457E+01 2.2374E-03 2.9465E-07 2.7708E-11 1.2186E-15
 84          10108.00  9.511 9.3163E+01 2.6530E-03 5.6946E-07 8.3927E-11 5.0416E-15
 85          10116.00  7.514 9.2053E+01 2.7514E-03 5.1218E-07 6.6192E-11 3.6540E-15
 86          10607.00 13.135 9.6088E+01 3.4106E-03 6.7378E-07 8.7666E-11 4.8365E-15
 87          10608.00 12.311 9.4191E+01 3.0252E-03 5.9689E-07 7.7220E-11 4.2351E-15
 88          10811.00  8.286 9.2701E+01 4.3703E-03 1.0975E-06 1.6241E-10 9.6222E-15
 89          10812.00  6.823 9.1448E+01 3.9729E-03 9.4759E-07 1.3688E-10 8.0099E-15
 90          60606.00 13.957 1.0081E+02 3.9913E-03 8.1028E-07 1.0167E-10 5.3621E-15
 91          60717.00 12.126 9.8836E+01 4.8667E-03 1.1673E-06 1.6627E-10 9.5674E-15
 92          60808.00 16.561 1.0097E+02 3.3659E-03 5.7770E-07 6.3873E-11 3.0525E-15
 93          60816.00 14.210 1.0000E+02 3.9763E-03 7.8058E-07 9.5929E-11 4.9686E-15
 94          60909.00 10.268 9.7787E+01 3.7637E-03 7.7313E-07 9.9261E-11 5.3065E-15
 95          61616.00 11.881 1.0044E+02 4.5422E-03 9.8359E-07 1.2836E-10 6.9210E-15
 96          70708.00 11.440 9.9172E+01 3.9917E-03 8.1117E-07 1.0518E-10 5.7309E-15
 97          70808.00  9.621 9.7617E+01 3.6891E-03 7.5141E-07 9.6734E-11 5.2293E-15
 98          70909.00  6.056 9.6316E+01 4.4386E-03 1.0275E-06 1.4206E-10 7.9873E-15
 99          80814.00 13.447 1.0004E+02 3.7484E-03 6.5483E-07 6.8677E-11 3.0007E-15
100          80816.00 11.023 9.8405E+01 3.7855E-03 7.7032E-07 9.7481E-11 5.1594E-15
```

For this sample run we have put in 100 species, the maximum allowed by the dimensions, to find out which molecules are important in the sun (assuming complete ignorance). The constants are taken from the table in Section 4. 4. Once we know which molecules are important, if any, we can restrict the input list to those. There is also a maximum of 25 different elements.

NMOLEC continues to process input data up through statement 28. On any subsequent call to NMOLEC, the data are already in a usable form, so NMOLEC skips directly to statement 30 to make a guess for the number densities at the first depth. Then NMOLEC sets up and differentiates the equilibrium equations to get a set of linear equations for the correction to the number densities (through statement 99) (Section 4. 3). NMOLEC calls SOLVIT(17) to solve the equations. The number densities are corrected, and iteration continues until the number densities converge. NMOLEC repeats this process for every depth, then prints out (only on the last iteration, to save paper) the results as shown on the following three pages.

Once NMOLEC has found the number densities, it goes through the list to find number densities/partition functions (in ATLAS5). These are stored in array XNMOL in COMMON. Using blank COMMON saves core on CDC machines, but if space is no object, this could be converted to COMMON /MOLS/. The same COMMON must occur in MOLEC.

Finally, if IFPNCH = 5, NMOLEC prints and punches XNMOL, XNATOM, and RHO, as shown on pages 152 and 153.

XNMOL is used by MOLEC(48) as its source of data. If a molecule is requested that is not in XNMOL, MOLEC quits; if an atom is requested that is not in XNMOL, MOLEC calls PFSAHA. The only way to find a molecular number that is not in XNMOL is to request the neutral-atom number densities for the components and to use a Saha equation to construct the molecular number density completely independently of the molecule routines.

```
        RHOX         T          P          XNE        XNATOM       RHO
 1   2.471E-03  5.300E+03  6.806E+01  1.018E+11  9.282E+13  2.051E-10
 2   4.916E-03  5.040E+03  1.354E+02  7.118E+10  1.943E+14  4.295E-10
 3   9.407E-03  4.790E+03  2.591E+02  5.386E+10  3.914E+14  8.649E-10
 4   1.637E-02  4.530E+03  4.509E+02  5.219E+10  7.202E+14  1.592E-09
 5   2.465E-02  4.280E+03  6.789E+02  6.482E+10  1.148E+15  2.537E-09
 6   3.422E-02  4.170E+03  9.425E+02  8.055E+10  1.636E+15  3.615E-09
 7   4.622E-02  4.190E+03  1.273E+03  1.051E+11  2.199E+15  4.860E-09
 8   6.154E-02  4.225E+03  1.695E+03  1.370E+11  2.904E+15  6.418E-09
 9   8.118E-02  4.280E+03  2.236E+03  1.798E+11  3.782E+15  8.357E-09
10   1.065E-01  4.330E+03  2.933E+03  2.338E+11  4.904E+15  1.084E-08
11   1.390E-01  4.380E+03  3.828E+03  3.025E+11  6.328E+15  1.398E-08
12   1.810E-01  4.430E+03  4.985E+03  3.903E+11  8.147E+15  1.800E-08
13   2.351E-01  4.490E+03  6.475E+03  5.060E+11  1.044E+16  2.307E-08
14   3.050E-01  4.550E+03  8.400E+03  6.548E+11  1.337E+16  2.954E-08
15   3.950E-01  4.600E+03  1.088E+04  8.398E+11  1.712E+16  3.785E-08
16   5.116E-01  4.660E+03  1.409E+04  1.084E+12  2.190E+16  4.839E-08
17   6.612E-01  4.720E+03  1.821E+04  1.397E+12  2.794E+16  6.175E-08
18   8.547E-01  4.790E+03  2.354E+04  1.812E+12  3.559E+16  7.865E-08
19   1.103E+00  4.895E+03  3.038E+04  2.410E+12  4.494E+16  9.933E-08
20   1.422E+00  5.010E+03  3.917E+04  3.236E+12  5.661E+16  1.251E-07
21   1.828E+00  5.160E+03  5.035E+04  4.509E+12  7.065E+16  1.561E-07
22   2.334E+00  5.330E+03  6.428E+04  6.528E+12  8.733E+16  1.930E-07
23   2.937E+00  5.540E+03  8.089E+04  1.023E+13  1.057E+17  2.336E-07
24   3.617E+00  5.765E+03  9.962E+04  1.690E+13  1.251E+17  2.764E-07
25   4.335E+00  6.035E+03  1.194E+05  3.051E+13  1.432E+17  3.164E-07
26   5.021E+00  6.390E+03  1.383E+05  6.320E+13  1.566E+17  3.460E-07
27   5.330E+00  6.610E+03  1.468E+05  9.622E+13  1.606E+17  3.550E-07
28   5.602E+00  6.860E+03  1.543E+05  1.506E+14  1.626E+17  3.594E-07
29   5.842E+00  7.140E+03  1.609E+05  2.404E+14  1.628E+17  3.599E-07
30   6.053E+00  7.440E+03  1.667E+05  3.822E+14  1.618E+17  3.575E-07
31   6.230E+00  7.750E+03  1.716E+05  5.947E+14  1.596E+17  3.528E-07
32   6.394E+00  8.030E+03  1.761E+05  8.629E+14  1.578E+17  3.488E-07
33   6.543E+00  8.290E+03  1.802E+05  1.193E+15  1.561E+17  3.450E-07
34   6.688E+00  8.520E+03  1.842E+05  1.565E+15  1.549E+17  3.423E-07
35   6.833E+00  8.710E+03  1.882E+05  1.941E+15  1.544E+17  3.413E-07
36   6.986E+00  8.880E+03  1.924E+05  2.339E+15  1.545E+17  3.414E-07
37   7.145E+00  9.050E+03  1.968E+05  2.799E+15  1.546E+17  3.416E-07
38   7.316E+00  9.220E+03  2.015E+05  3.330E+15  1.548E+17  3.422E-07
39   7.494E+00  9.390E+03  2.064E+05  3.937E+15  1.551E+17  3.428E-07
40   7.683E+00  9.560E+03  2.116E+05  4.629E+15  1.555E+17  3.438E-07
```

```
                                                          MOLECULAR NUMBER DENSITIES
          1.00        1.01        2.00        2.01        2.02        6.00        6.01        7.00        7.01        8.00
  1  8.345E+13   9.034E+10   9.282E+12   1.436E+00   4.891E-34   2.381E+10   5.541E+09   7.037E+09   4.226E+06   4.867E+10
  2  1.748E+14   5.398E+10   1.943E+13   2.479E-01   1.120E-34   5.652E+10   4.906E+09   1.474E+10   2.270E+06   1.019E+11
  3  3.522E+14   2.599E+10   3.914E+13   3.187E-02   1.762E-35   1.200E+11   3.307E+09   2.968E+10   9.762E+05   2.049E+11
  4  6.481E+14   6.854E+09   7.202E+13   1.825E-03   9.574E-37   2.189E+11   1.202E+09   5.459E+10   2.259E+05   3.703E+11
  5  1.033E+15   1.056E+09   1.148E+14   5.434E-05   2.109E-38   2.880E+11   2.176E+08   8.664E+10   3.013E+04   5.276E+11
  6  1.472E+15   4.405E+08   1.636E+14   1.033E-05   3.102E-39   3.041E+11   7.964E+07   1.224E+11   1.165E+04   6.452E+11
  7  1.978E+15   5.473E+08   2.199E+14   1.485E-05   3.442E-39   3.877E+11   9.095E+07   1.641E+11   1.462E+04   8.462E+11
  8  2.612E+15   7.672E+08   2.904E+14   2.679E-05   4.824E-39   5.073E+11   1.197E+08   2.164E+11   2.092E+04   1.113E+12
  9  3.401E+15   1.254E+09   3.782E+14   6.455E-05   9.031E-39   6.915E+11   1.885E+08   2.822E+11   3.539E+04   1.480E+12
 10  4.411E+15   1.948E+09   4.904E+14   1.414E-04   1.549E-38   9.239E+11   2.801E+08   3.662E+11   5.664E+04   1.946E+12
 11  5.690E+15   2.996E+09   6.328E+14   3.044E-04   2.621E-38   1.226E+12   4.121E+08   4.727E+11   8.970E+04   2.544E+12
 12  7.326E+15   4.566E+09   8.147E+14   6.444E-04   4.373E-38   1.618E+12   6.000E+08   6.089E+11   1.407E+05   3.315E+12
 13  9.388E+15   7.413E+09   1.044E+15   1.537E-03   8.211E-38   2.163E+12   9.355E+08   7.813E+11   2.363E+05   4.338E+12
 14  1.202E+16   1.189E+10   1.337E+15   3.586E-03   1.510E-37   2.872E+12   1.436E+09   1.001E+12   3.917E+05   5.657E+12
 15  1.539E+16   1.760E+10   1.712E+15   7.198E-03   2.402E-37   3.738E+12   2.023E+09   1.283E+12   5.952E+05   7.306E+12
 16  1.968E+16   2.764E+10   2.190E+15   1.615E-02   4.257E-37   4.921E+12   3.030E+09   1.641E+12   9.643E+05   9.482E+12
 17  2.511E+16   4.291E+10   2.794E+15   3.552E-02   7.407E-37   6.443E+12   4.480E+09   2.095E+12   1.543E+06   1.226E+13
 18  3.198E+16   7.019E+10   3.559E+15   8.623E-02   1.417E-36   8.499E+12   6.971E+09   2.672E+12   2.614E+06   1.591E+13
 19  4.038E+16   1.396E+11   4.494E+15   3.035E-01   3.875E-36   1.146E+13   1.310E+10   3.381E+12   5.471E+06   2.082E+13
 20  5.086E+16   2.842E+11   5.661E+15   1.123E+00   1.106E-35   1.528E+13   2.479E+10   4.267E+12   1.174E+07   2.707E+13
 21  6.349E+16   6.648E+11   7.065E+15   5.507E+00   4.067E-35   2.018E+13   5.232E+10   5.336E+12   2.931E+07   3.493E+13
 22  7.848E+16   1.581E+12   8.733E+15   2.878E+01   1.541E-34   2.594E+13   1.091E+11   6.604E+12   7.463E+07   4.422E+13
 23  9.502E+16   3.974E+12   1.057E+16   1.792E+02   6.488E-34   3.223E+13   2.312E+11   8.003E+12   2.030E+08   5.446E+13
 24  1.125E+17   9.190E+12   1.251E+16   1.017E+03   2.366E-33   3.855E+13   4.443E+11   9.476E+12   5.070E+08   6.503E+13
 25  1.287E+17   2.124E+13   1.432E+16   6.321E+03   8.725E-33   4.417E+13   8.288E+11   1.085E+13   1.276E+09   7.481E+13
 26  1.408E+17   5.226E+13   1.566E+16   5.029E+04   1.221E-31   4.785E+13   1.563E+12   1.187E+13   3.470E+09   8.202E+13
 27  1.444E+17   8.436E+13   1.606E+16   1.577E+05   7.109E-30   4.858E+13   2.161E+12   1.218E+13   5.929E+09   8.419E+13
 28  1.462E+17   1.377E+14   1.626E+16   5.202E+05   5.153E-28   4.842E+13   2.978E+12   1.232E+13   1.023E+10   8.524E+13
 29  1.463E+17   2.263E+14   1.628E+16   1.772E+06   4.323E-26   4.740E+13   4.078E+12   1.233E+13   1.778E+10   8.533E+13
 30  1.452E+17   3.666E+14   1.618E+16   5.905E+06   3.415E-24   4.568E+13   5.473E+12   1.224E+13   3.046E+10   8.471E+13
 31  1.431E+17   5.774E+14   1.596E+16   1.848E+07   2.183E-22   4.334E+13   7.132E+12   1.206E+13   5.055E+10   8.348E+13
 32  1.412E+17   8.438E+14   1.578E+16   4.803E+07   7.086E-21   4.110E+13   8.815E+12   1.190E+13   7.714E+10   8.241E+13
 33  1.393E+17   1.172E+15   1.561E+16   1.100E+08   1.455E-19   3.886E+13   1.050E+13   1.173E+13   1.112E+11   8.134E+13
 34  1.379E+17   1.542E+15   1.549E+16   2.199E+08   1.811E-18   3.689E+13   1.209E+13   1.160E+13   1.509E+11   8.050E+13
 35  1.371E+17   1.917E+15   1.544E+16   3.798E+08   1.317E-17   3.537E+13   1.346E+13   1.152E+13   1.920E+11   8.006E+13
 36  1.367E+17   2.313E+15   1.545E+16   6.083E+08   7.237E-17   3.409E+13   1.475E+13   1.148E+13   2.363E+11   7.988E+13
 37  1.363E+17   2.772E+15   1.546E+16   9.580E+08   3.735E-16   3.282E+13   1.606E+13   1.144E+13   2.886E+11   7.969E+13
 38  1.360E+17   3.301E+15   1.548E+16   1.485E+09   1.816E-15   3.157E+13   1.739E+13   1.139E+13   3.499E+11   7.955E+13
 39  1.357E+17   3.906E+15   1.551E+16   2.268E+09   8.346E-15   3.033E+13   1.873E+13   1.135E+13   4.201E+11   7.939E+13
 40  1.354E+17   4.597E+15   1.555E+16   3.414E+09   3.639E-14   2.912E+13   2.007E+13   1.130E+13   5.007E+11   7.925E+13
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                                                 MOLECULAR NUMBER DENSITIES
        107.00      108.00      109.00      111.00      112.00      113.00      114.00      115.00      116.00      117.00
  1   4.843E+03   7.179E+04   2.659E+02   5.315E-05   3.093E-01   3.728E-03   5.536E+00   1.258E+01   6.699E+02   2.887E+01
  2   3.181E+04   5.127E+05   2.237E+03   3.806E-04   2.938E+00   3.285E-02   6.439E+01   8.003E+01   4.327E+03   2.066E+02
  3   1.981E+05   3.482E+06   1.815E+04   2.885E-03   2.991E+01   3.085E-01   8.073E+02   4.806E+02   2.647E+04   1.410E+03
  4   1.102E+06   2.111E+07   1.372E+05   2.687E-02   3.930E+02   3.685E+00   1.304E+04   2.561E+03   1.444E+05   8.735E+03
  5   4.777E+06   9.167E+07   8.287E+05   2.602E-01   5.432E+03   4.650E+01   1.956E+05   1.060E+04   6.140E+05   4.262E+04
  6   1.245E+07   2.181E+08   2.543E+06   1.122E+00   2.721E+04   2.270E+02   8.754E+05   2.717E+04   1.596E+06   1.184E+05
  7   2.139E+07   3.628E+08   4.246E+06   2.395E+00   5.572E+04   4.728E+02   1.653E+06   4.702E+04   2.755E+06   2.018E+05
  8   3.429E+07   5.700E+08   6.470E+06   4.581E+00   1.002E+05   8.675E+02   2.781E+06   7.605E+04   4.437E+06   3.181E+05
  9   5.124E+07   8.467E+08   8.930E+06   7.825E+00   1.568E+05   1.391E+03   4.149E+06   1.149E+05   6.659E+06   4.622E+05
 10   7.700E+07   1.260E+09   1.251E+07   1.353E+01   2.506E+05   2.274E+03   6.299E+06   1.745E+05   1.005E+07   6.777E+05
 11   1.149E+08   1.862E+09   1.742E+07   2.317E+01   3.974E+05   3.685E+03   9.496E+06   2.628E+05   1.506E+07   9.870E+05
 12   1.711E+08   2.743E+09   2.425E+07   3.961E+01   6.300E+05   5.969E+03   1.431E+07   3.952E+05   2.251E+07   1.436E+06
 13   2.480E+08   3.953E+09   3.250E+07   6.485E+01   9.469E+05   9.179E+03   2.057E+07   5.790E+05   3.278E+07   2.024E+06
 14   3.600E+08   5.695E+09   4.370E+07   1.065E+02   1.430E+06   1.418E+04   2.970E+07   8.491E+05   4.778E+07   2.860E+06
 15   5.350E+08   8.356E+09   6.100E+07   1.820E+02   2.278E+06   2.305E+04   4.492E+07   1.273E+06   7.129E+07   4.160E+06
 16   7.790E+08   1.205E+10   8.257E+07   3.011E+02   3.476E+06   3.594E+04   6.539E+07   1.872E+06   1.042E+08   5.904E+06
 17   1.133E+09   1.735E+10   1.119E+08   4.979E+02   5.314E+06   5.613E+04   9.532E+07   2.748E+06   1.523E+08   8.377E+06
 18   1.619E+09   2.455E+10   1.474E+08   8.002E+02   7.824E+06   8.456E+04   1.343E+08   3.966E+06   2.184E+08   1.163E+07
 19   2.149E+09   3.245E+10   1.743E+08   1.148E+03   9.944E+06   1.106E+05   1.647E+08   5.339E+06   2.916E+08   1.481E+07
 20   2.814E+09   4.204E+10   2.024E+08   1.624E+03   1.240E+07   1.421E+05   1.967E+08   7.091E+06   3.842E+08   1.856E+07
 21   3.455E+09   5.065E+10   2.143E+08   2.123E+03   1.386E+07   1.648E+05   2.082E+08   8.858E+06   4.754E+08   2.161E+07
 22   4.090E+09   5.816E+10   2.169E+08   2.748E+03   1.506E+07   1.867E+05   2.103E+08   1.068E+07   5.679E+08   2.419E+07
 23   4.456E+09   6.059E+10   1.976E+08   3.393E+03   1.517E+07   1.981E+05   1.918E+08   1.189E+07   6.257E+08   2.474E+07
 24   4.627E+09   5.974E+10   1.720E+08   4.213E+03   1.538E+07   2.121E+05   1.737E+08   1.261E+07   6.575E+08   2.417E+07
 25   4.313E+09   5.241E+10   1.323E+08   4.956E+03   1.447E+07   2.132E+05   1.436E+08   1.203E+07   6.222E+08   2.113E+07
 26   3.354E+09   3.787E+10   8.232E+07   5.332E+03   1.174E+07   1.885E+05   9.979E+07   9.646E+06   4.943E+08   1.531E+07
 27   2.709E+09   2.938E+10   5.884E+07   5.211E+03   9.855E+06   1.663E+05   7.678E+07   7.948E+06   4.053E+08   1.193E+07
 28   2.044E+09   2.128E+10   3.918E+07   4.817E+03   7.776E+06   1.396E+05   5.587E+07   6.147E+06   3.119E+08   8.712E+06
 29   1.433E+09   1.435E+10   2.431E+07   4.232E+03   5.729E+06   1.115E+05   3.852E+07   4.449E+06   2.243E+08   5.954E+06
 30   9.373E+08   9.067E+09   1.423E+07   3.508E+03   3.949E+06   8.548E+04   2.551E+07   3.030E+06   1.516E+08   3.840E+06
 31   5.704E+08   5.377E+09   7.903E+06   2.657E+03   2.561E+06   6.244E+04   1.633E+07   1.943E+06   9.626E+07   2.343E+06
 32   3.467E+08   3.220E+09   4.513E+06   1.954E+03   1.678E+06   4.575E+04   1.079E+07   1.251E+06   6.129E+07   1.451E+06
 33   2.066E+08   1.908E+09   2.586E+06   1.397E+03   1.072E+06   3.333E+04   7.228E+06   7.962E+05   3.846E+07   8.935E+05
 34   1.247E+08   1.153E+09   1.530E+06   9.742E+02   6.889E+05   2.464E+04   5.005E+06   5.144E+05   2.448E+07   5.627E+05
 35   7.932E+07   7.387E+08   9.695E+05   6.923E+02   4.629E+05   1.882E+04   3.662E+06   3.494E+05   1.638E+07   3.750E+05
 36   5.140E+07   4.836E+08   6.317E+05   4.922E+02   3.157E+05   1.457E+04   2.748E+06   2.418E+05   1.116E+07   2.555E+05
 37   3.214E+07   3.067E+08   4.007E+05   3.423E+02   2.085E+05   1.104E+04   2.031E+06   1.626E+05   7.380E+06   1.695E+05
 38   1.935E+07   1.882E+08   2.472E+05   2.272E+02   1.359E+05   8.182E+03   1.478E+06   1.062E+05   4.726E+06   1.093E+05
 39   1.117E+07   1.113E+08   1.476E+05   1.432E+02   8.484E+04   5.954E+03   1.055E+06   6.709E+04   2.919E+06   6.827E+04
 40   6.169E+06   6.320E+07   8.523E+04   8.561E+01   5.068E+04   4.222E+03   7.378E+05   4.091E+04   1.736E+06   4.122E+04
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                         NUMBER DENSITIES / PARTITION FUNCTIONS
 100 MOLECULES
                 1.00
4.172E+13 8.742E+13 1.761E+14 3.241E+14 5.165E+14 7.359E+14 9.892E+14 1.306E+15
1.701E+15 2.205E+15 2.845E+15 3.663E+15 4.694E+15 6.009E+15 7.697E+15 9.839E+15
1.255E+16 1.599E+16 2.019E+16 2.543E+16 3.174E+16 3.924E+16 4.751E+16 5.623E+16
6.437E+16 7.040E+16 7.222E+16 7.309E+16 7.315E+16 7.261E+16 7.154E+16 7.060E+16
6.966E+16 6.893E+16 6.853E+16 6.835E+16 6.815E+16 6.800E+16 6.783E+16 6.767E+16
                 1.01
9.034E+10 5.398E+10 2.599E+10 6.854E+09 1.056E+09 4.405E+08 5.473E+08 7.672E+08
1.254E+09 1.948E+09 2.996E+09 4.566E+09 7.413E+09 1.189E+10 1.760E+10 2.764E+10
4.291E+10 7.019E+10 1.396E+11 2.842E+11 6.648E+11 1.581E+12 3.974E+12 9.190E+12
2.124E+13 5.226E+13 8.436E+13 1.377E+14 2.263E+14 3.666E+14 5.774E+14 8.438E+14
1.172E+15 1.542E+15 1.917E+15 2.313E+15 2.772E+15 3.301E+15 3.906E+15 4.597E+15
                 2.00
9.282E+12 1.943E+13 3.914E+13 7.202E+13 1.148E+14 1.636E+14 2.199E+14 2.904E+14
3.782E+14 4.904E+14 6.328E+14 8.147E+14 1.044E+15 1.337E+15 1.712E+15 2.190E+15
2.794E+15 3.559E+15 4.494E+15 5.661E+15 7.065E+15 8.733E+15 1.057E+16 1.251E+16
1.432E+16 1.566E+16 1.606E+16 1.626E+16 1.628E+16 1.618E+16 1.596E+16 1.578E+16
1.561E+16 1.549E+16 1.544E+16 1.545E+16 1.546E+16 1.548E+16 1.551E+16 1.555E+16
                 2.01
7.182E-01 1.240E-01 1.594E-02 9.123E-04 2.717E-05 5.165E-06 7.427E-06 1.340E-05
3.227E-05 7.072E-05 1.522E-04 3.222E-04 7.686E-04 1.793E-03 3.599E-03 8.076E-03
1.776E-02 4.312E-02 1.518E-01 5.617E-01 2.753E+00 1.439E+01 8.960E+01 5.085E+02
3.161E+03 2.514E+04 7.886E+04 2.601E+05 8.860E+05 2.952E+06 9.241E+06 2.401E+07
5.501E+07 1.099E+08 1.899E+08 3.042E+08 4.790E+08 7.425E+08 1.134E+09 1.707E+09
                 2.02
4.891E-34 1.120E-34 1.762E-35 9.574E-37 2.109E-38 3.102E-39 3.442E-39 4.824E-39
9.031E-39 1.549E-38 2.621E-38 4.373E-38 8.211E-38 1.510E-37 2.402E-37 4.257E-37
7.407E-37 1.417E-36 3.875E-36 1.106E-35 4.067E-35 1.541E-34 6.488E-34 2.366E-33
8.725E-33 1.221E-31 7.109E-30 5.153E-28 4.323E-26 3.415E-24 2.183E-22 7.086E-21
1.455E-19 1.811E-18 1.317E-17 7.237E-17 3.735E-16 1.816E-15 8.346E-15 3.639E-14
                 6.00
2.571E+09 6.132E+09 1.307E+10 2.394E+10 3.162E+10 3.345E+10 4.263E+10 5.576E+10
7.594E+10 1.014E+11 1.344E+11 1.772E+11 2.367E+11 3.141E+11 4.085E+11 5.372E+11
7.027E+11 9.258E+11 1.247E+12 1.658E+12 2.185E+12 2.800E+12 3.463E+12 4.123E+12
4.700E+12 5.055E+12 5.110E+12 5.068E+12 4.935E+12 4.724E+12 4.453E+12 4.197E+12
3.947E+12 3.728E+12 3.560E+12 3.419E+12 3.279E+12 3.143E+12 3.008E+12 2.876E+12
                 6.01
9.349E+08 8.283E+08 5.588E+08 2.032E+08 3.683E+07 1.348E+07 1.539E+07 2.026E+07
3.189E+07 4.740E+07 6.971E+07 1.015E+08 1.582E+08 2.429E+08 3.421E+08 5.122E+08
7.571E+08 1.178E+09 2.212E+09 4.186E+09 8.831E+09 1.840E+10 3.897E+10 7.487E+10
1.395E+11 2.630E+11 3.632E+11 5.002E+11 6.845E+11 9.178E+11 1.195E+12 1.476E+12
1.757E+12 2.020E+12 2.250E+12 2.463E+12 2.681E+12 2.902E+12 3.123E+12 3.346E+12
                 7.00
1.713E+09 3.600E+09 7.277E+09 1.343E+10 2.139E+10 3.026E+10 4.057E+10 5.349E+10
6.969E+10 9.036E+10 1.166E+11 1.500E+11 1.923E+11 2.463E+11 3.153E+11 4.031E+11
5.142E+11 6.550E+11 8.277E+11 1.043E+12 1.301E+12 1.607E+12 1.941E+12 2.291E+12
2.614E+12 2.845E+12 2.909E+12 2.919E+12 2.893E+12 2.842E+12 2.771E+12 2.708E+12
2.648E+12 2.598E+12 2.565E+12 2.542E+12 2.518E+12 2.495E+12 2.465E+12 2.435E+12
                 7.01
4.797E+05 2.588E+05 1.117E+05 2.596E+04 3.477E+03 1.346E+03 1.689E+03 2.416E+03
4.084E+03 6.531E+03 1.034E+04 1.619E+04 2.717E+04 4.500E+04 6.833E+04 1.106E+05
1.769E+05 2.992E+05 6.251E+05 1.339E+06 3.335E+06 8.468E+06 2.295E+07 5.713E+07
1.431E+08 3.872E+08 6.593E+08 1.133E+09 1.961E+09 3.344E+09 5.522E+09 8.392E+09
1.205E+10 1.629E+10 2.067E+10 2.538E+10 3.092E+10 3.739E+10 4.477E+10 5.322E+10
                 8.00
5.475E+09 1.150E+10 2.317E+10 4.198E+10 5.996E+10 7.342E+10 9.627E+10 1.265E+11
1.682E+11 2.211E+11 2.889E+11 3.763E+11 4.920E+11 6.413E+11 8.277E+11 1.074E+12
1.387E+12 1.799E+12 2.352E+12 3.055E+12 3.935E+12 4.973E+12 6.112E+12 7.282E+12
8.354E+12 9.121E+12 9.337E+12 9.424E+12 9.401E+12 9.299E+12 9.129E+12 8.981E+12
8.836E+12 8.721E+12 8.653E+12 8.612E+12 8.571E+12 8.536E+12 8.498E+12 8.463E+12
```

```
1.104E-18 1.182E-18 1.126E-18 1.014E-18 8.680E-19 7.159E-19 5.735E-19 4.692E-19
3.876E-19 3.283E-19 2.888E-19 2.595E-19 2.331E-19 2.099E-19 1.888E-19 1.701E-19
          60909.00
9.899E-33 1.207E-31 1.218E-30 8.948E-30 3.554E-29 8.211E-29 1.858E-28 4.122E-28
9.142E-28 1.978E-27 4.208E-27 8.872E-27 1.866E-26 3.892E-26 8.016E-26 1.654E-25
3.382E-25 6.905E-25 1.391E-24 2.741E-24 5.163E-24 9.194E-24 1.488E-23 2.205E-23
2.873E-23 3.112E-23 2.989E-23 2.713E-23 2.345E-23 1.953E-23 1.581E-23 1.307E-23
1.091E-23 9.338E-24 8.287E-24 7.509E-24 6.806E-24 6.185E-24 5.620E-24 5.116E-24
          61616.00
5.332E-30 6.589E-29 6.738E-28 5.029E-27 2.036E-26 4.764E-26 1.080E-25 2.396E-25
5.303E-25 1.146E-24 2.434E-24 5.125E-24 1.075E-23 2.238E-23 4.606E-23 9.486E-23
1.936E-22 3.943E-22 7.882E-22 1.540E-21 2.867E-21 5.039E-21 8.031E-21 1.172E-20
1.501E-20 1.593E-20 1.512E-20 1.356E-20 1.157E-20 9.505E-21 7.591E-21 6.196E-21
5.111E-21 4.326E-21 3.805E-21 3.421E-21 3.076E-21 2.774E-21 2.501E-21 2.259E-21
          70708.00
5.083E-27 5.486E-26 5.261E-25 3.841E-24 1.651E-23 4.373E-23 1.016E-22 2.264E-22
4.912E-22 1.048E-21 2.203E-21 4.594E-21 9.481E-21 1.946E-20 3.985E-20 8.125E-20
1.645E-19 3.310E-19 6.475E-19 1.245E-18 2.285E-18 3.995E-18 6.382E-18 9.400E-18
1.223E-17 1.333E-17 1.289E-17 1.171E-17 1.018E-17 8.589E-18 7.090E-18 5.990E-18
5.120E-18 4.482E-18 4.056E-18 3.741E-18 3.452E-18 3.193E-18 2.938E-18 2.703E-18
          70808.00
1.422E-26 1.533E-25 1.466E-24 1.051E-23 4.049E-23 9.284E-23 2.109E-22 4.687E-22
1.038E-21 2.245E-21 4.778E-21 1.008E-20 2.123E-20 4.436E-20 9.156E-20 1.894E-19
3.884E-19 7.956E-19 1.611E-18 3.191E-18 6.047E-18 1.082E-17 1.759E-17 2.615E-17
3.422E-17 3.740E-17 3.620E-17 3.310E-17 2.896E-17 2.460E-17 2.045E-17 1.739E-17
1.496E-17 1.317E-17 1.198E-17 1.110E-17 1.029E-17 9.560E-18 8.864E-18 8.224E-18
          70909.00
5.547E-33 5.959E-32 5.704E-31 4.222E-30 2.022E-29 6.247E-29 1.487E-28 3.326E-28
7.055E-28 1.483E-27 3.070E-27 6.317E-27 1.275E-26 2.567E-26 5.205E-26 1.044E-25
2.081E-25 4.108E-25 7.766E-25 1.450E-24 2.586E-24 4.438E-24 7.017E-24 1.031E-23
1.344E-23 1.473E-23 1.431E-23 1.315E-23 1.156E-23 9.884E-24 8.277E-24 7.096E-24
6.160E-24 5.475E-24 5.024E-24 4.697E-24 4.397E-24 4.131E-24 3.876E-24 3.644E-24
          80814.00
6.884E-30 1.398E-28 2.871E-27 6.432E-26 9.291E-25 3.803E-24 9.432E-24 2.172E-23
4.711E-23 1.012E-22 2.142E-22 4.501E-22 9.223E-22 1.882E-21 3.896E-21 7.919E-21
1.600E-20 3.171E-20 5.768E-20 1.012E-19 1.595E-19 2.340E-19 3.038E-19 3.745E-19
4.085E-19 3.649E-19 3.162E-19 2.585E-19 2.013E-19 1.523E-19 1.132E-19 8.779E-20
6.966E-20 5.739E-20 4.964E-20 4.412E-20 3.932E-20 3.522E-20 3.162E-20 2.848E-20
          80816.00
5.907E-28 6.393E-27 6.138E-26 4.424E-25 1.721E-24 3.990E-24 9.082E-24 2.019E-23
4.459E-23 9.630E-23 2.046E-22 4.312E-22 9.057E-22 1.889E-21 3.894E-21 8.039E-21
1.646E-20 3.364E-20 6.783E-20 1.339E-19 2.526E-19 4.502E-19 7.283E-19 1.078E-18
1.405E-18 1.526E-18 1.473E-18 1.350E-18 1.184E-18 1.009E-18 8.418E-19 7.189E-19
6.213E-19 5.498E-19 5.025E-19 4.679E-19 4.362E-19 4.080E-19 3.820E-19 3.583E-19
XNATOM.RHO
9.282E+13 2.051E-10 1.943E+14 4.295E-10 3.914E+14 8.649E-10 7.202E+14 1.592E-09
1.148E+15 2.537E-09 1.636E+15 3.615E-09 2.199E+15 4.860E-09 2.904E+15 6.418E-09
3.782E+15 8.357E-09 4.904E+15 1.084E-08 6.328E+15 1.398E-08 8.147E+15 1.800E-08
1.044E+16 2.307E-08 1.337E+16 2.954E-08 1.712E+16 3.785E-08 2.190E+16 4.839E-08
2.794E+16 6.175E-08 3.559E+16 7.865E-08 4.494E+16 9.933E-08 5.661E+16 1.251E-07
7.065E+16 1.561E-07 8.733E+16 1.930E-07 1.057E+17 2.336E-07 1.251E+17 2.764E-07
1.432E+17 3.164E-07 1.566E+17 3.460E-07 1.606E+17 3.550E-07 1.626E+17 3.594E-07
1.628E+17 3.599E-07 1.618E+17 3.575E-07 1.596E+17 3.528E-07 1.578E+17 3.488E-07
1.561E+17 3.450E-07 1.549E+17 3.423E-07 1.544E+17 3.413E-07 1.545E+17 3.414E-07
1.546E+17 3.416E-07 1.548E+17 3.422E-07 1.551E+17 3.428E-07 1.555E+17 3.438E-07
```

The second case for MOLECULES ON is IFPRES = 0 (PRESSURE OFF), where NMOLEC is not called but MOLEC reads XNMOL as a punch deck, which must come after the BEGIN card. MOLEC prints the data as they are read in.

PRINT 3 and PRINT 4

Samples of the printout for these two options appear on the next two pages.

NLTE

If IFPRNT > 0, STATEQ(11) prints out H^- and H rates and b's, as shown on the third, fourth, and fifth pages following. If IFPNCH > 0, PUTOUT(7) punches the deck listed on the sixth page following.

SURFACE INTENSITY

PUTOUT prints and punches surface intensities instead of surface fluxes, as follows:

Print:

```
 WAVE     FREQUENCY      TAUONE    TAUNU     MU      INTENSITY
109.999   2.725403E+15    -2.04     1.83    1.000    1.732E-08    etc.
```

Punch:

```
FREQUENCY   2.725403E+15   1.000   1.732E-08  etc.
```

```
WAVELENGTH  109.999   FREQUENCY 2.725403E+15

       RHOX       TAUNU        ABTOT      ALPHA        BNU         SNU         JNJ        JMINS        HNU
 1  8.457E-05  0.           7.261E+00  4.224E-02  1.253E-08  1.233E-08  7.767E-09 -4.559E-09  4.052E-09
 2  1.226E-04  1.053E-03  9.927E+00  3.199E-02  1.269E-08  1.252E-08  7.819E-09 -4.704E-09  4.047E-09
 3  1.738E-04  1.655E-03  1.352E+01  2.447E-02  1.258E-08  1.249E-08  7.844E-09 -4.647E-09  4.044E-09
 4  2.430E-04  2.737E-03  1.771E+01  1.944E-02  1.271E-08  1.259E-08  7.886E-09 -4.708E-09  4.039E-09
 5  3.362E-04  4.631E-03  2.287E+01  1.567E-02  1.280E-08  1.273E-08  7.955E-09 -4.780E-09  4.030E-09
 6  4.617E-04  7.896E-03  2.902E+01  1.284E-02  1.295E-08  1.286E-08  8.061E-09 -4.795E-09  4.014E-09
 7  6.310E-04  1.346E-02  3.654E+01  1.060E-02  1.302E-08  1.299E-08  8.222E-09 -4.768E-09  3.988E-09
 8  8.596E-04  2.281E-02  4.508E+01  8.906E-03  1.330E-08  1.322E-08  8.465E-09 -4.751E-09  3.943E-09
 9  1.169E-03  3.839E-02  5.553E+01  7.472E-03  1.339E-08  1.338E-08  8.817E-09 -4.560E-09  3.871E-09
10  1.589E-03  6.420E-02  6.699E+01  6.362E-03  1.371E-08  1.368E-08  9.327E-09 -4.351E-09  3.756E-09
11  2.163E-03  1.066E-01  8.022E+01  5.444E-03  1.407E-08  1.405E-08  1.003E-08 -4.021E-09  3.579E-09
12  2.948E-03  1.756E-01  9.517E+01  4.688E-03  1.453E-08  1.451E-08  1.097E-08 -3.545E-09  3.318E-09
13  4.025E-03  2.874E-01  1.118E+02  4.064E-03  1.512E-08  1.511E-08  1.218E-08 -2.931E-09  2.958E-09
14  5.502E-03  4.664E-01  1.300E+02  3.550E-03  1.590E-08  1.589E-08  1.368E-08 -2.210E-09  2.501E-09
15  7.524E-03  7.501E-01  1.498E+02  3.123E-03  1.689E-08  1.688E-08  1.544E-08 -1.437E-09  1.993E-09
16  1.028E-02  1.193E+00  1.703E+02  2.778E-03  1.830E-08  1.829E-08  1.748E-08 -8.057E-10  1.513E-09
17  1.402E-02  1.866E+00  1.891E+02  2.517E-03  2.017E-08  2.017E-08  1.983E-08 -3.351E-10  1.153E-09
18  1.900E-02  2.858E+00  2.079E+02  2.304E-03  2.282E-08  2.282E-08  2.272E-08 -9.601E-11  9.632E-10
19  2.555E-02  4.277E+00  2.244E+02  2.144E-03  2.653E-08  2.653E-08  2.657E-08  4.046E-11  9.319E-10
20  3.392E-02  6.208E+00  2.352E+02  2.047E-03  3.217E-08  3.217E-08  3.227E-08  9.586E-11  1.073E-09
21  4.427E-02  8.666E+00  2.383E+02  2.016E-03  4.108E-08  4.106E-08  4.120E-08  1.434E-10  1.389E-09
22  5.655E-02  1.156E+01  2.318E+02  2.058E-03  5.557E-08  5.555E-08  5.583E-08  2.746E-10  2.057E-09
23  7.046E-02  1.467E+01  2.142E+02  2.195E-03  8.038E-08  8.027E-08  8.085E-08  5.820E-10  3.530E-09
24  8.546E-02  1.771E+01  1.897E+02  2.436E-03  1.248E-07  1.257E-07  1.283E-07  2.685E-09  7.908E-09
25  1.009E-01  2.036E+01  1.524E+02  2.915E-03  2.132E-07  2.132E-07  2.188E-07  5.647E-09  1.624E-08
26  1.166E-01  2.244E+01  1.122E+02  3.715E-03  3.877E-07  3.878E-07  4.089E-07  2.105E-08  4.252E-08
27  1.327E-01  2.393E+01  7.411E+01  5.113E-03  7.570E-07  7.575E-07  8.449E-07  8.739E-08  1.233E-07
28  1.509E-01  2.499E+01  4.498E+01  7.504E-03  1.519E-06  1.521E-06  1.862E-06  3.406E-07  3.548E-07
29  1.743E-01  2.580E+01  2.576E+01  1.183E-02  3.125E-06  3.138E-06  4.252E-06  1.114E-06  9.660E-07
30  2.090E-01  2.647E+01  1.473E+01  1.939E-02  6.541E-06  6.595E-06  9.295E-06  2.700E-06  2.353E-06
31  2.681E-01  2.714E+01  8.870E+00  3.122E-02  1.411E-05  1.426E-05  1.886E-05  4.601E-06  5.010E-06
32  3.705E-01  2.789E+01  6.040E+00  4.533E-02  3.027E-05  3.053E-05  3.596E-05  5.434E-06  9.083E-06
33  5.438E-01  2.880E+01  4.751E+00  5.789E-02  6.314E-05  6.342E-05  6.796E-05  4.543E-06  1.401E-05
34  8.277E-01  3.006E+01  4.237E+00  6.634E-02  1.272E-04  1.274E-04  1.304E-04  3.006E-06  1.897E-05
35  1.273E+00  3.191E+01  4.084E+00  7.089E-02  2.470E-04  2.471E-04  2.488E-04  1.664E-06  2.344E-05
36  1.956E+00  3.469E+01  4.061E+00  7.272E-02  4.599E-04  4.600E-04  4.608E-04  8.447E-07  2.684E-05
37  2.978E+00  3.887E+01  4.129E+00  7.205E-02  8.146E-04  8.146E-04  8.151E-04  4.085E-07  2.928E-05
38  4.482E+00  4.518E+01  4.263E+00  7.000E-02  1.390E-03  1.390E-03  1.390E-03  1.796E-07  3.092E-05
39  6.608E+00  5.442E+01  4.425E+00  6.752E-02  2.263E-03  2.263E-03  2.263E-03  6.511E-08  3.187E-05
40  9.585E+00  6.784E+01  4.578E+00  6.534E-02  3.561E-03  3.561E-03  3.561E-03  2.821E-08  3.225E-05
```

```
       AHYD  AH2P AHMIN  SIGH  AHE1 AHE2 AHEMIN SIGHE ACOOL ALUKE AHOT SIGEL SIGH2 AHLINEALINESSIGLINAXLINE SIGXLAXCONT  SIGX
  1   -1.65 -4.69 -4.41 -1.13 -8.05-31.90  0.00  0.00   .84  0.00  0.00  -.63  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   1
  2   -1.52 -4.43 -4.15 -1.01 -8.04-32.01  0.00  0.00   .98  0.00  0.00  -.66  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   2
  3   -1.42 -4.19 -3.91  -.90 -8.05-32.17  0.00  0.00  1.12  0.00  0.00  -.69  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   3
  4   -1.33 -3.97 -3.69  -.81 -8.04-32.26  0.00  0.00  1.24  0.00  0.00  -.72  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   4
  5   -1.25 -3.78 -3.50  -.74 -8.03-32.36  0.00  0.00  1.35  0.00  0.00  -.76  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   5
  6   -1.18 -3.60 -3.32  -.67 -8.03-32.44  0.00  0.00  1.46  0.00  0.00  -.80  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   6
  7   -1.12 -3.44 -3.16  -.61 -8.02-32.53  0.00  0.00  1.56  0.00  0.00  -.84  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   7
  8   -1.06 -3.30 -3.01  -.57 -8.00-32.57  0.00  0.00  1.65  0.00  0.00  -.89  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   8
  9   -1.02 -3.16 -2.87  -.52 -8.00-32.65  0.00  0.00  1.74  0.00  0.00  -.94  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00   9
 10    -.98 -3.03 -2.75  -.49 -7.98-32.68  0.00  0.00  1.82  0.00  0.00  -.99  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  10
 11    -.94 -2.91 -2.62  -.46 -7.96-32.70  0.00  0.00  1.90  0.00  0.00 -1.04  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  11
 12    -.90 -2.79 -2.51  -.44 -7.93-32.70  0.00  0.00  1.98  0.00  0.00 -1.09  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  12
 13    -.86 -2.69 -2.40  -.42 -7.90-32.68  0.00  0.00  2.05  0.00  0.00 -1.14  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  13
 14    -.83 -2.58 -2.29  -.40 -7.86-32.63  0.00  0.00  2.11  0.00  0.00 -1.19  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  14
 15    -.79 -2.48 -2.18  -.39 -7.81-32.56  0.00  0.00  2.17  0.00  0.00 -1.24  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  15
 16    -.75 -2.38 -2.08  -.38 -7.75-32.43  0.00  0.00  2.23  0.00  0.00 -1.28  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  16
 17    -.70 -2.28 -1.98  -.37 -7.67-32.25  0.00  0.00  2.28  0.00  0.00 -1.32  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  17
 18    -.65 -2.18 -1.88  -.36 -7.57-32.00  0.00  0.00  2.32  0.00  0.00 -1.35  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  18
 19    -.58 -2.09 -1.77  -.36 -7.45-31.68  0.00  0.00  2.35  0.00  0.00 -1.36  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  19
 20    -.51 -1.99 -1.67  -.36 -7.30-31.24  0.00  0.00  2.37  0.00  0.00 -1.37  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  20
 21    -.41 -1.90 -1.57  -.36 -7.10-30.67  0.00  0.00  2.38  0.00  0.00 -1.35  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  21
 22    -.30 -1.81 -1.47  -.37 -6.86-29.93  0.00  0.00  2.36  0.00  0.00 -1.32  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  22
 23    -.17 -1.73 -1.37  -.38 -6.56-29.01  0.00  0.00  2.33  0.00  0.00 -1.26  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  23
 24    -.02 -1.67 -1.28  -.40 -6.21-27.90  0.00  0.00  2.27  0.00  0.00 -1.17  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  24
 25     .15 -1.62 -1.21  -.45 -5.78-26.52  0.00  0.00  2.18  0.00  0.00 -1.05  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  25
 26     .31 -1.62 -1.19  -.53 -5.29-24.95  0.00  0.00  2.04  0.00  0.00  -.92  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  26
 27     .45 -1.70 -1.25  -.66 -4.76-23.15  0.00  0.00  1.85  0.00  0.00  -.80  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  27
 28     .52 -1.88 -1.41  -.86 -4.19-21.25  0.00  0.00  1.62  0.00  0.00  -.70  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  28
 29     .53 -2.16 -1.67 -1.14 -3.61-19.25  0.00  0.00  1.34  0.00  0.00  -.63  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  29
 30     .50 -2.50 -1.99 -1.47 -3.01-17.20  0.00  0.00  1.05  0.00  0.00  -.60  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  30
 31     .46 -2.85 -2.31 -1.82 -2.39-15.07  0.00  0.00   .76  0.00  0.00  -.58  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  31
 32     .43 -3.16 -2.60 -2.15 -1.79-12.99  0.00  0.00   .49  0.00  0.00  -.57  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  32
 33     .42 -3.41 -2.82 -2.45 -1.23-11.04  0.00  0.00   .24  0.00  0.00  -.57  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  33
 34     .44 -3.61 -3.00 -2.72  -.80 -9.30  0.00  0.00   .02  0.00  0.00  -.55  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  34
 35     .46 -3.79 -3.15 -2.97  -.52 -7.79  0.00  0.00  -.23  0.00  0.00  -.54  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  35
 36     .49 -3.95 -3.28 -3.21  -.40 -6.51  0.00  0.00  -.55  0.00  0.00  -.53  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  36
 37     .51 -4.08 -3.40 -3.42  -.34 -5.39  0.00  0.00  -.97  0.00  0.00  -.53  0.00  0.00  0.00  0.00  0.00  0.00  0.01  0.00  37
 38     .54 -4.20 -3.51 -3.62  -.31 -4.37  0.00  0.00 -1.47  0.00  0.00  -.53  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  38
 39     .56 -4.32 -3.61 -3.81  -.30 -3.45  0.00  0.00 -1.99  0.00  0.00  -.52  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  39
 40     .58 -4.42 -3.71 -3.99  -.29 -2.59  0.00  0.00 -2.51  0.00  0.00  -.52  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  40
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                                       HMINUS STATISTICAL EQUILIBRIUM
        RHOX        QELECT       QASSOC       QCHARG       QRDKHM       QRDHMK        FMIN
 1   8.457E-05   3.655E+02   7.304E+01   1.196E+04   6.328E+06   6.006E+06     1.0536
 2   1.226E-04   5.126E+02   1.417E+02   1.681E+04   6.342E+06   6.007E+06     1.0556
 3   1.738E-04   6.990E+02   2.663E+02   2.292E+04   6.332E+06   6.008E+06     1.0538
 4   2.430E-04   9.322E+02   4.686E+02   3.063E+04   6.344E+06   6.009E+06     1.0555
 5   3.362E-04   1.222E+03   7.986E+02   4.019E+04   6.352E+06   6.010E+06     1.0565
 6   4.617E-04   1.577E+03   1.316E+03   5.199E+04   6.365E+06   6.012E+06     1.0581
 7   6.310E-04   2.010E+03   2.126E+03   6.628E+04   6.371E+06   6.015E+06     1.0585
 8   8.596E-04   2.552E+03   3.319E+03   8.365E+04   6.395E+06   6.019E+06     1.0616
 9   1.169E-03   3.191E+03   5.140E+03   1.045E+05   6.403E+06   6.024E+06     1.0619
10   1.589E-03   3.971E+03   7.772E+03   1.305E+05   6.430E+06   6.031E+06     1.0646
11   2.163E-03   4.925E+03   1.161E+04   1.622E+05   6.460E+06   6.041E+06     1.0674
12   2.948E-03   6.094E+03   1.714E+04   2.010E+05   6.497E+06   6.054E+06     1.0705
13   4.025E-03   7.532E+03   2.504E+04   2.492E+05   6.544E+06   6.074E+06     1.0740
14   5.502E-03   9.314E+03   3.620E+04   3.093E+05   6.604E+06   6.101E+06     1.0779
15   7.524E-03   1.154E+04   5.187E+04   3.842E+05   6.677E+06   6.139E+06     1.0816
16   1.028E-02   1.440E+04   7.340E+04   4.792E+05   6.776E+06   6.193E+06     1.0861
17   1.402E-02   1.783E+04   1.026E+05   6.075E+05   6.899E+06   6.271E+06     1.0898
18   1.900E-02   2.244E+04   1.412E+05   7.691E+05   7.060E+06   6.380E+06     1.0930
19   2.555E-02   2.843E+04   1.908E+05   9.804E+05   7.264E+06   6.536E+06     1.0941
20   3.392E-02   3.635E+04   2.510E+05   1.268E+06   7.538E+06   6.758E+06     1.0938
21   4.427E-02   4.701E+04   3.190E+05   1.666E+06   7.904E+06   7.073E+06     1.0912
22   5.655E-02   6.141E+04   3.887E+05   2.224E+06   8.389E+06   7.518E+06     1.0855
23   7.046E-02   8.077E+04   4.483E+05   3.021E+06   9.034E+06   8.139E+06     1.0765
24   8.546E-02   1.086E+05   4.825E+05   4.073E+06   9.886E+06   9.001E+06     1.0648
25   1.009E-01   1.440E+05   4.680E+05   5.617E+06   1.106E+07   1.019E+07     1.0530
26   1.166E-01   1.850E+05   4.026E+05   7.632E+06   1.257E+07   1.179E+07     1.0391
27   1.327E-01   2.262E+05   2.922E+05   9.989E+06   1.457E+07   1.389E+07     1.0279
28   1.509E-01   2.575E+05   1.800E+05   1.229E+07   1.707E+07   1.653E+07     1.0183
29   1.743E-01   2.773E+05   9.667E+04   1.433E+07   2.021E+07   1.981E+07     1.0116
30   2.090E-01   2.934E+05   4.916E+04   1.643E+07   2.418E+07   2.390E+07     1.0070
31   2.681E-01   3.185E+05   2.558E+04   1.942E+07   2.940E+07   2.922E+07     1.0037
32   3.705E-01   3.641E+05   1.496E+04   2.428E+07   3.605E+07   3.596E+07     1.0015
33   5.438E-01   4.382E+05   1.000E+04   3.185E+07   4.438E+07   4.434E+07     1.0005
34   8.277E-01   5.460E+05   7.413E+03   4.282E+07   5.476E+07   5.474E+07     1.0001
35   1.273E+00   6.840E+05   5.788E+03   5.770E+07   6.770E+07   6.769E+07     1.0000
36   1.956E+00   8.463E+05   4.708E+03   7.782E+07   8.368E+07   8.368E+07     1.0000
37   2.978E+00   1.029E+06   3.984E+03   1.045E+08   1.030E+08   1.030E+08     1.0000
38   4.482E+00   1.226E+06   3.421E+03   1.387E+08   1.268E+08   1.268E+08     1.0000
39   6.608E+00   1.430E+06   2.983E+03   1.803E+08   1.553E+08   1.553E+08     1.0000
40   9.585E+00   1.633E+06   2.610E+03   2.300E+08   1.899E+08   1.899E+08     1.0000
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                               STATISTICAL EQUILIBRIUM RATES     RATE=SIGN(ALOG10(AMAX1(ABS(RATE*1.E20),1.)),RATE)

RAD     1-K    K-1    2-K    K-2    3-K    K-3    4-K    K-4    5-K    K-5    6-K    K-6   COLL    1-K    2-K    3-K    4-K    5-K    6-K    5-8    6-8
COLL    1-2    1-3    1-4    1-5    1-6    1-7    2-3    2-4    2-5    2-6    2-7    3-4    3-5    3-6    3-7    4-5    4-6    4-7    5-6    5-7    6-7

   1   0.00   0.00  25.36  25.34  26.00  26.03  25.96  26.07  25.84  25.97  25.70  25.84         14.33  21.90  23.67  24.48  24.97  25.31  25.37  26.44
      17.45  15.40  14.51  13.98  13.61  13.33  24.08  22.72  22.02  21.57  21.24  25.74  24.52  23.87  23.44  26.59  25.42  24.79  27.16  26.01  27.59

   2   0.00   0.00  25.36  25.35  26.00  26.03  25.96  26.07  25.84  25.97  25.70  25.84         14.48  22.05  23.82  24.62  25.11  25.46  25.52  26.59
      17.60  15.56  14.66  14.13  13.76  13.48  24.23  22.87  22.17  21.72  21.39  25.88  24.67  24.02  23.59  26.74  25.57  24.93  27.31  26.16  27.73

   3   0.00   0.00  25.36  25.34  26.00  26.03  25.96  26.07  25.84  25.97  25.70  25.84         14.61  22.19  23.95  24.76  25.25  25.59  25.66  26.72
      17.73  15.69  14.79  14.26  13.89  13.61  24.36  23.00  22.30  21.85  21.52  26.02  24.80  24.15  23.72  26.87  25.70  25.07  27.44  26.29  27.87

   4   0.00   0.00  25.36  25.35  26.00  26.03  25.96  26.07  25.84  25.97  25.70  25.84         14.74  22.31  24.08  24.88  25.37  25.72  25.78  26.85
      17.86  15.82  14.92  14.39  14.02  13.75  24.49  23.13  22.43  21.98  21.65  26.14  24.93  24.28  23.85  27.00  25.83  25.19  27.56  26.42  27.99

   5   0.00   0.00  25.37  25.35  26.00  26.03  25.96  26.07  25.84  25.97  25.70  25.84         14.86  22.43  24.19  25.00  25.49  25.84  25.90  26.97
      17.98  15.94  15.04  14.51  14.15  13.87  24.61  23.25  22.55  22.09  21.77  26.26  25.05  24.40  23.97  27.11  25.95  25.31  27.68  26.53  28.11

   6   0.00   0.00  25.37  25.35  26.00  26.03  25.96  26.07  25.84  25.98  25.70  25.84         14.98  22.55  24.31  25.11  25.60  25.95  26.01  27.08
      18.09  16.05  15.16  14.63  14.26  13.98  24.72  23.36  22.66  22.21  21.88  26.37  25.16  24.51  24.08  27.23  26.06  25.42  27.79  26.64  28.22

   7   0.00   0.00  25.37  25.35  26.00  26.03  25.96  26.07  25.84  25.98  25.70  25.84         15.09  22.65  24.41  25.22  25.71  26.06  26.12  27.18
      18.20  16.16  15.27  14.74  14.37  14.09  24.83  23.46  22.76  22.31  21.99  26.48  25.26  24.61  24.18  27.33  26.16  25.53  27.90  26.75  28.33

   8   0.00   0.00  25.37  25.35  26.00  26.03  25.96  26.07  25.84  25.98  25.70  25.84         15.21  22.76  24.52  25.32  25.81  26.16  26.22  27.29
      18.31  16.28  15.38  14.85  14.49  14.21  24.93  23.57  22.87  22.42  22.09  26.58  25.37  24.72  24.29  27.44  26.27  25.63  28.00  26.85  28.43

   9   0.00   0.00  25.37  25.35  26.00  26.04  25.96  26.07  25.84  25.98  25.70  25.84         15.31  22.86  24.62  25.42  25.91  26.26  26.32  27.38
      18.41  16.38  15.48  14.95  14.59  14.31  25.03  23.67  22.97  22.52  22.19  26.68  25.47  24.82  24.39  27.53  26.37  25.73  28.10  26.95  28.53

  10   0.00   0.00  25.37  25.36  26.00  26.04  25.96  26.07  25.84  25.98  25.71  25.84         15.42  22.96  24.71  25.52  26.01  26.35  26.42  27.48
      18.52  16.48  15.59  15.06  14.69  14.42  25.13  23.77  23.07  22.62  22.29  26.78  25.56  24.91  24.48  27.63  26.46  25.83  28.20  27.05  28.62

  11   0.00   0.00  25.37  25.36  26.00  26.04  25.96  26.08  25.84  25.98  25.71  25.84         15.52  23.05  24.81  25.61  26.10  26.45  26.51  27.58
      18.62  16.59  15.70  15.17  14.80  14.52  25.22  23.86  23.16  22.71  22.39  26.87  25.66  25.01  24.58  27.72  26.56  25.92  28.29  27.14  28.72

  12   0.00   0.00  25.37  25.37  26.00  26.04  25.96  26.08  25.85  25.98  25.71  25.85         15.64  23.15  24.91  25.71  26.20  26.54  26.60  27.67
      18.73  16.70  15.81  15.28  14.91  14.63  25.32  23.96  23.26  22.81  22.49  26.97  25.76  25.11  24.68  27.82  26.65  26.02  28.39  27.24  28.81

  13   0.00   0.00  25.38  25.37  26.00  26.04  25.96  26.08  25.85  25.98  25.72  25.85         15.75  23.25  25.00  25.81  26.29  26.64  26.70  27.76
      18.84  16.81  15.92  15.39  15.03  14.75  25.42  24.06  23.36  22.91  22.58  27.06  25.85  25.20  24.77  27.91  26.75  26.11  28.48  27.33  28.91

  14   0.00   0.00  25.38  25.38  26.00  26.05  25.97  26.08  25.85  25.99  25.72  25.85         15.87  23.35  25.10  25.90  26.39  26.73  26.79  27.86
      18.95  16.93  16.04  15.51  15.14  14.87  25.52  24.16  23.46  23.01  22.68  27.16  25.95  25.30  24.87  28.01  26.84  26.21  28.57  27.43  29.00

  15   0.00   0.00  25.39  25.39  26.01  26.05  25.97  26.09  25.86  25.99  25.73  25.86         16.00  23.46  25.20  26.00  26.49  26.83  26.89  27.95
      19.07  17.05  16.16  15.64  15.27  14.99  25.62  24.26  23.56  23.11  22.79  27.26  26.04  25.40  24.97  28.10  26.94  26.30  28.67  27.52  29.10

  16   0.00   0.00  25.40  25.40  26.01  26.06  25.97  26.09  25.86  25.99  25.74  25.86         16.14  23.57  25.31  26.10  26.59  26.93  26.99  28.05
      19.20  17.19  16.30  15.77  15.41  15.13  25.72  24.37  23.67  23.22  22.90  27.36  26.15  25.50  25.07  28.20  27.04  26.41  28.77  27.62  29.20

  17   0.00   0.00  25.42  25.42  26.02  26.07  25.98  26.10  25.87  26.00  25.75  25.87         16.29  23.68  25.41  26.20  26.69  27.03  27.09  28.15
      19.34  17.33  16.44  15.92  15.55  15.28  25.82  24.47  23.78  23.33  23.00  27.46  26.25  25.60  25.17  28.30  27.14  26.50  28.87  27.72  29.29

  18   0.00   0.00  25.43  25.44  26.02  26.08  25.99  26.10  25.89  26.01  25.77  25.88         16.46  23.80  25.52  26.31  26.80  27.14  27.20  28.26
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                      STATISTICAL EQUILIBRIUM FOR HYDROGEN
      RHOX          B1       B2       B3       B4       B5       B6
 1 8.4569E-05     .9613    .9601   1.0720   1.0783   1.0362   1.0122
 2 1.2256E-04     .9665    .9655   1.0649   1.0617   1.0276   1.0091
 3 1.7384E-04     .9650    .9640   1.0548   1.0482   1.0211   1.0069
 4 2.4299E-04     .9697    .9688   1.0475   1.0385   1.0165   1.0054
 5 3.3616E-04     .9729    .9722   1.0404   1.0308   1.0130   1.0042
 6 4.6172E-04     .9770    .9764   1.0344   1.0249   1.0104   1.0033
 7 6.3103E-04     .9790    .9785   1.0287   1.0201   1.0083   1.0027
 8 8.5962E-04     .9850    .9845   1.0248   1.0164   1.0067   1.0021
 9 1.1687E-03     .9862    .9858   1.0206   1.0134   1.0054   1.0017
10 1.5889E-03     .9905    .9902   1.0178   1.0111   1.0045   1.0014
11 2.1628E-03     .9942    .9940   1.0154   1.0092   1.0037   1.0012
12 2.9481E-03     .9976    .9974   1.0135   1.0077   1.0030   1.0009
13 4.0250E-03    1.0005   1.0004   1.0118   1.0064   1.0025   1.0008
14 5.5016E-03    1.0029   1.0029   1.0104   1.0054   1.0021   1.0006
15 7.5241E-03    1.0043   1.0043   1.0090   1.0045   1.0017   1.0005
16 1.0283E-02    1.0056   1.0056   1.0079   1.0037   1.0014   1.0004
17 1.4016E-02    1.0057   1.0057   1.0068   1.0031   1.0011   1.0003
18 1.9004E-02    1.0052   1.0052   1.0057   1.0025   1.0009   1.0003
19 2.5549E-02    1.0038   1.0038   1.0045   1.0019   1.0007   1.0002
20 3.3922E-02    1.0024   1.0024   1.0035   1.0015   1.0005   1.0002
21 4.4269E-02    1.0012   1.0011   1.0026   1.0011   1.0004   1.0001
22 5.6550E-02    1.0001   1.0001   1.0018   1.0007   1.0003   1.0001
23 7.0464E-02     .9994    .9993   1.0012   1.0005   1.0002   1.0000
24 8.5456E-02     .9990    .9989   1.0007   1.0003   1.0001   1.0000
25 1.0092E-01     .9992    .9992   1.0005   1.0002   1.0001   1.0000
26 1.1660E-01     .9993    .9993   1.0002   1.0001   1.0000   1.0000
27 1.3275E-01     .9996    .9996   1.0002   1.0001   1.0000   1.0000
28 1.5092E-01     .9997    .9997   1.0001   1.0000   1.0000   1.0000
29 1.7426E-01     .9998    .9998   1.0000   1.0000   1.0000   1.0000
30 2.0899E-01     .9999    .9999   1.0000   1.0000   1.0000   1.0000
31 2.6808E-01    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
32 3.7049E-01    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
33 5.4375E-01    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
34 8.2768E-01    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
35 1.2729E+00    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
36 1.9561E+00    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
37 2.9784E+00    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
38 4.4825E+00    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
39 6.6085E+00    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
40 9.5853E+00    1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
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READ DEPARTURE COEFFICIENTS 40 RHOX  BHYD 1-6  BMIN
 8.4569E-05    .9613    .9601   1.0720   1.0783   1.0362   1.0122   1.0536
 1.2256E-04    .9665    .9655   1.0649   1.0617   1.0276   1.0091   1.0556
 1.7384E-04    .9650    .9640   1.0548   1.0482   1.0211   1.0069   1.0538
 2.4299E-04    .9697    .9688   1.0475   1.0385   1.0165   1.0054   1.0555
 3.3616E-04    .9729    .9722   1.0404   1.0308   1.0130   1.0042   1.0565
 4.6172E-04    .9770    .9764   1.0344   1.0249   1.0104   1.0033   1.0581
 6.3103E-04    .9790    .9785   1.0287   1.0201   1.0083   1.0027   1.0585
 8.5962E-04    .9850    .9845   1.0248   1.0164   1.0067   1.0021   1.0616
 1.1687E-03    .9862    .9858   1.0206   1.0134   1.0054   1.0017   1.0619
 1.5889E-03    .9905    .9902   1.0178   1.0111   1.0045   1.0014   1.0646
 2.1628E-03    .9942    .9940   1.0154   1.0092   1.0037   1.0012   1.0674
 2.9481E-03    .9976    .9974   1.0135   1.0077   1.0030   1.0009   1.0705
 4.0250E-03   1.0005   1.0004   1.0118   1.0064   1.0025   1.0008   1.0740
 5.5016E-03   1.0029   1.0029   1.0104   1.0054   1.0021   1.0006   1.0779
 7.5241E-03   1.0043   1.0043   1.0090   1.0045   1.0017   1.0005   1.0816
 1.0283E-02   1.0056   1.0056   1.0079   1.0037   1.0014   1.0004   1.0861
 1.4016E-02   1.0057   1.0057   1.0068   1.0031   1.0011   1.0003   1.0898
 1.9004E-02   1.0052   1.0052   1.0057   1.0025   1.0009   1.0003   1.0930
 2.5549E-02   1.0038   1.0038   1.0045   1.0019   1.0007   1.0002   1.0941
 3.3922E-02   1.0024   1.0024   1.0035   1.0015   1.0005   1.0002   1.0938
 4.4269E-02   1.0012   1.0011   1.0026   1.0011   1.0004   1.0001   1.0912
 5.6550E-02   1.0001   1.0001   1.0018   1.0007   1.0003   1.0001   1.0855
 7.0464E-02    .9994    .9993   1.0012   1.0005   1.0002   1.0000   1.0765
 8.5456E-02    .9990    .9989   1.0007   1.0003   1.0001   1.0000   1.0648
 1.0092E-01    .9992    .9992   1.0005   1.0002   1.0001   1.0000   1.0530
 1.1660E-01    .9993    .9993   1.0002   1.0001   1.0000   1.0000   1.0391
 1.3275E-01    .9996    .9996   1.0002   1.0001   1.0000   1.0000   1.0279
 1.5092E-01    .9997    .9997   1.0001   1.0000   1.0000   1.0000   1.0183
 1.7426E-01    .9998    .9998   1.0000   1.0000   1.0000   1.0000   1.0116
 2.0899E-01    .9999    .9999   1.0000   1.0000   1.0000   1.0000   1.0070
 2.6808E-01   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0037
 3.7049E-01   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0015
 5.4375E-01   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0005
 8.2768E-01   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0001
 1.2729E+00   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
 1.9561E+00   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
 2.9784E+00   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
 4.4825E+00   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
 6.6085E+00   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
 9.5853E+00   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000   1.0000
```

8.4 Programing Details of ATLAS5

ATLAS5 is programed in essentially machine-independent FORTRAN IV. The whole program can be logically divided into six blocks of subroutines:

MAIN	READIN	POPS	KAPP		JOSH	CONVEC
ATLAS5	READIN	POPS	KAPP	HOP	JOSH	CONVEC
PUTOUT	DUMMYR	NELECT	COULX	COULFF	BLOCKJ	HIGH
TCORR	FREEFR	PFSAHA	H2PLOP	HMINOP	BLOCKH	TURB
STATEQ	FREEFF	MOLEC	HRAYOP	HE1OP		
ROSS	IWORDF	NMOLEC	HE2OP	HEMIOP		
RADIAP	TTAUP		HERAOP	COOLOP		
DERIV	BLOCKE		C1OP	SEATON		
INTEG	BLOCKR		MG1OP	AL1OP		
PARCOE			SI1OP	LUKEOP		
MAP1			N1OP	O1OP		
SOLVIT			MG2OP	SI2OP		
EXPI			CA2OP	HOTOP		
W			ELECOP	H2RAOP		
			HLINOP	STARK		
			LINOP	LINSOP		
			XLINOP	XLISOP		
			XCONOP	XSOP		

As presented in this report, the blocks are not distinguished but are loaded together. This requires slightly less than 120000 octal locations on a CDC 6400. If the molecule routines were completely integrated without use of blank COMMON, the requirement would be about 130000. However, it is more often necessary to cut down on field length, in which case subroutines that are not used can be replaced by dummies or the blocks can be treated as overlays.

Some possible deletions are as follows:

if no statistical equilibrium, STATEQ;

if no molecules, MOLEC and NMOLEC;

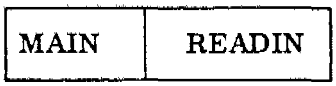
if opacity not needed, LUKEOP and its functions or HOTOP, etc.;

if no convection, CONVEC.

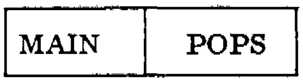
Some modification is required to set up overlays because of calls to block POPS from several points in block KAPP. The opacity routines call POPS individually so that they are completely self-contained for easy deletion or change. The calls to POPS can be removed from the subroutines and put into ATLAS5, and the data can be transmitted to the subroutines through additional common blocks.

The overlay layout would be as follows:

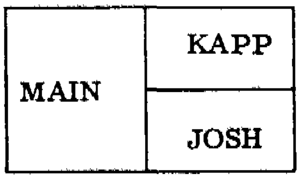
Start model



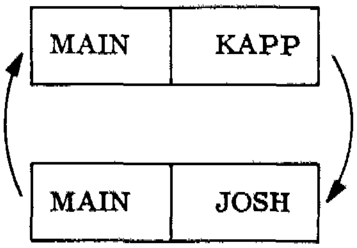
Start iteration



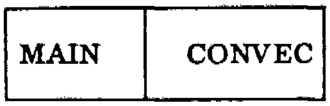
Start frequency integration



or



Finish iteration



The second alternative for KAPP and JOSH would require changing overlays at every frequency.

8.5 Subroutines

ATLAS5(1)	We discussed ATLAS5 fully in Section 8.1.
PUTOUT(4)	Output (see Section 8.1). The only thing to mention here is that there are alternate formats for different p scaling on different computers.
TCORR(8)	Temperature correction (see Sections 7 and 8.1).
STATEQ(11)	Statistical equilibrium (see Sections 3.5, 3.6, 8.1, and 8.3).
ROSS(13)	Rosseland opacity and optical depth (see Section 2.12).
RADIAP(14)	Radiation pressure (see Section 2.11).
DERIV(14)	Derivatives (see Section 2.8). A scaling factor is included to avoid truncation problems.
INTEG(15)	Integrals (see Section 2.5). Uses PARCOE.
PARCOE(15)	Parabolic interpolation coefficients (see Section 2.5).
MAP1(16)	Parabolic interpolation. (Maps one vector at a time.) Uses same formulas as PARCOE but is faster. MAP1 is set equal to the number of points required for the inverse interpolation, as in JOSH.
SOLVIT(17)	Solves linear equations using Gauss-Jordan elimination.
EXPI(18)	Exponential integrals.

W(18)	Writes debugging aids. For example, CALL W(6HOPACIT, AHYD, 1000) would produce an opacity table 1000 words long, and CALL W (6HI , FLOAT(I), 1) would print a subscript.
READIN(19)	Reads input (see Sections 8.1 and 8.2). This routine is very long, but the logic is easy to follow once FREEFR, FREEFF, and IWORDF are understood. Data not read in are filled in from BLOCKE and BLOCKR. The printout is produced in the section with statement numbers in the 1500's.
DUMMYR(28)	Dummy routine for modifying READIN.
FREEFF(29)	Free-field function for reading numbers. FREEFF is called once for every number required from array CARD. CARD is an array of LAST Hollerith characters, the last one of which must be a blank. The most convenient way to read cards is to dimension an array CARD for 80, equivalence a blank to CARD(81), and set LAST to 81. In general, there is no restriction on the length of CARD, nor does LAST have to be the last member of CARD (but simply the last member to be searched). To find a number, FREEFF sets IFFAIL to 0 and starts searching through CARD, starting at CARD(NUMCOL), for any field in an E, F, or I format that is followed by either a comma or a blank and with an exponent less than MAXPOW. If FREEFF does not find a number, it calls EXIT when MORE = 0, or it returns with a 0. and IFFAIL = 1 when MORE = 1. When FREEFF returns, NUMCOL is set at the blank or the comma marking the end of the number. All numbers are returned floating point, so an integer is produced with a statement like M=FREEFF(CARD).
FREEFR(30)	Free-field routine for reading numbers from cards. FREEFR calls FREEFF with MORE = 1. If FREEFF does not find a number, FREEFR reads another card and calls FREEFF again.

IWORDF(31)	Free-field function for reading words as integers. Any method for reading words in a machine-independent fashion turns out to be rather cumbersome. The approach here is based on converting each letter or digit to an integer, then combining the integers into one large integer. The maximum word length is set by the computer with the smallest integer size, $2^{31}-1$ for an IBM 360. This allows 6-digit base-37 numbers, so that words of up to six characters can be converted uniquely. Words longer than six characters are truncated after the first six. The processing logic for IWORDF is similar to that for FREEFF except that LETCOL marks the starting place. Words can be made up of any number of letters and decimal digits as long as the word starts with a letter. Ends of words are marked by blanks, commas, or equal signs. IWORDF also stores the characters it reads in array WORD.
TTAUP(34)	Solves the pressure-balance equation for a $T(\tau)$ distribution (see Section 4.2). TTAUP uses an opacity table, which is produced by a special version of ATLAS5, listed in Section 9. TTAUP is currently set up for Rosseland depths and Rosseland opacity for $3100 < T < 28000$ and $0.01 < P < 10^6$. The table would have to be recalculated for significantly higher or lower temperatures or pressures or for radically nonstandard abundances. Opacities other than Rosseland can also be used.
BLOCKE(32)	This is actually a BLOCK DATA for COMMON /ELEM/.
BLOCKR(33)	This is actually a BLOCK DATA for many of the COMMON's that appear in READIN.
POPS(37)	Populations (see Section 8.1). The argument MODE can take the values 1 or 11 for the number density/partition function of the atom or molecule CODE;

2 or 12 for the number density of the atom or molecule CODE. If IFMOL = 1, calls to POPS must be all 1's and 11's or 2's and 12's.

11 and 12 are the same as 1 and 2 except that if CODE is an atom, POPS returns all ionization stages through CODE.

NELECT(38) Finds the electron number (see Sections 4.3, 4.4, and 8.1). The only point we have not already discussed is that the iteration is speeded up by dropping elements from the calculation if they contribute less than 10^{-5} of the electrons.

PFSAHA(39) Partition functions, Saha equations for ionization fractions (see Sections 4.4 and 8.1). Since the partition-function table is complicated, the easiest way to explain it is to decode an example. For 2.01 the table reads

200020001, 200020071, 208524971, 382669341, 128222452, 5440302, D+F

The code letters at the end of the row refer to the source, Drawin and Felenbok. Others refer to the ground state only, summed energy levels, and fake sources for the partition function. The number 5440302 decodes into the ionization potential, 54.403, and the scaling factor G, 2. The other numbers decode into the partition function at 10 temperatures, as follows:

T	U
54.403* 2000/22 * 3 = 14837	2.000
5 = 24728	2.000
7 = 34620	2.000
9 = 44511	2.007
11 = 54403	2.085
13 = 64294	2.497
15 = 74186	3.826
17 = 84077	6.934
19 = 93969	12.82
21 = 103860	22.45

For any given T, the partition function is found by linear interpolation or extrapolation in this table. PFSAHA finds the ionization fractions by first computing n^{i+1}/n^i for the ions considered, then solving the equation

$$\frac{n^1}{n} + \frac{n^1}{n}\frac{n^2}{n^1} + \frac{n^1}{n}\frac{n^2}{n^1}\frac{n^3}{n^2} + \dots = 1$$

for n^1/n, and finally constructing each ionization fraction n^i/n.

MOLEC(48)	Molecular and atomic number densities/partition functions (see Sections 8.1 and 8.3).
NMOLEC(50)	Solves molecular equilibrium equations (see Sections 4.3, 4.4, 8.1, and 8.3). We have described the general features, but the details are too complicated to explain without going through every statement. In ATLAS5, NMOLEC is called with a MODE 1 or 11 to get number densities/partition functions, but for other applications it can be called with a MODE 2 or 12 to get number densities.
KAPP(55)	See Sections 5 and 8.1.
HOP(56)	Uses COULX and COULFF (see Section 5.1).
COULX(57)	See Section 5.1.
COULFF(57)	See Section 5.1.
H2PLOP(58)	See Section 5.2.
HMINOP(58)	See Section 5.3.
HRAYOP(57)	See Section 5.4.
HE1OP(59)	Uses COULFF (see Section 5.5).

HE2OP(60)	Uses COULX and COULFF (see Section 5.6).
HEMIOP(60)	See Section 5.7.
HERAOP(61)	See Section 5.8.
COOLOP(61)	Uses C1OP, MG1OP, AL1OP, and SI1OP (see Section 5.9).
C1OP(62)	Uses SEATON (see Section 5.9).
SEATON(62)	Seaton's cross-section formula, $\alpha_\nu = \alpha_0 \left[A \left(\frac{\nu_0}{\nu}\right)^p + (1 - A) \left(\frac{\nu_0}{\nu}\right)^{p+1} \right]$.
MG1OP(63)	See Section 5.9.
AL1OP(62)	See Section 5.9.
SI1OP(64)	See Section 5.9.
LUKEOP(65)	Uses N1OP, O1OP, MG2OP, SI2OP, and CA2OP (see Section 5.10).
N1OP(65)	Uses SEATON (see Section 5.10).
O1OP(65)	Uses SEATON (see Section 5.10).
MG2OP(66)	Uses SEATON (see Section 5.10).
SI2OP(67)	See Section 5.10.
CA2OP(66)	Uses SEATON (see Section 5.10).

HOTOP(68)	See Section 5. 11. The last column in the table is a subscript for identifying ions in XNFP. In DO 10, those cross sections that do not contribute a significant amount of opacity are passed over.
ELECOP(70)	See Section 5. 12.
H2RAOP(70)	See Section 5. 13.
HLINOP(71)	Uses STARK (see Section 5. 14).
STARK(72)	See Section 5. 14.
LINOP(73)	See Section 5. 15.
LINSOP(73)	See Section 5. 16.
XLINOP(73)	See Section 5. 17.
XLISOP(73)	See Section 5. 18.
XCONOP(73)	See Section 5. 19.
XSOP(73)	See Section 5. 20.
JOSH(74)	Finds J and S and H (and I) (see Sections 2. 7, 2. 8, 2. 9, 5, and 8. 1).
BLOCKJ(77)	This is actually a BLOCK DATA for COMMON /MATX/. The data are computed by program PRETAB, listed in Section 9. 2.
BLOCKH(86)	This is actually a BLOCK DATA for COMMON /MATX/. The data are computed by PRETAB.

CONVEC(96)	Calculates thermodynamic derivatives and convective flux (see Sections 4.6 and 6).
HIGH(99)	Geometric height in kilometers (see Section 4.5).
TURB(99)	Turbulent velocity and pressure (see Section 4.1).

8.6 Listing of ATLAS5

```
      PROGRAM ATLAS5(INPUT=513,OUTPUT=513,PUNCH=513,TAPE5=INPUT,
     1TAPE6=OUTPUT,TAPE7=PUNCH)
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1             GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2             IFCONV
      REAL MIXLTH
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /FRESET/FRESET(500),RCOSET(500),NULO,NUHI,NUMNU
      COMMON /HEIGHT/HEIGHT(40)
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /IFOP/IFOP(20)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /JUNK/TITLE(74),FREQID(6),WLTE,XSCALE
      COMMON /MUS/ANGLE(20),SURFI(20),NMU
      COMMON /OPS/AHYD(40),AH2P(40),AHMIN(40),SIGH(40),AHE1(40),
     1       AHE2(40),AHEMIN(40),SIGHE(40),ACOOL(40),ALUKE(40),AHOT(40),
     2            SIGEL(40),SIGH2(40),AHLINE(40),ALINES(40),SIGLIN(40),
     3            AXLINE(40),SIGXL(40),AXCONT(40),SIGX(40),SHYD(40),
     4            SHMIN(40),SHLINE(40),SXLINE(40),SXCONT(40)
      COMMON /OPTOT/ACONT(40),SCONT(40),ALINE(40),SLINE(40),SIGMAC(40),
     1              SIGMAL(40)
      COMMON /PTOTAL/PTOTAL(40)
      COMMON /PUT/PUT,IPUT
      COMMON /RAD/ ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNJ,JMINS
      COMMON /TEFF/TEFF,GRAV,GLOG
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1               IFTURB
      COMMON /WAVEY/WBEGIN,DELTAW,IFWAVE
      COMMON /XABUND/XABUND(99),WTMOLE
C     K=1.38054E-16
C     H=6.6256E-27
C     C=2.997925E10
C     E=1.60210E-19
C     ATMASS=1.660E-24
C
C
C     INPUT SECTION
C     PREFIX P  PRESSURE
C     PREFIX T  TEMPERATURE
C     PREFIX X  ABUNDANCE FRACTION
C     PREFIX F  IONIZATION FRACTION
C     PREFIX R  FREQUENCY INTEGRAL OR INTEGRATION COEFFICIENT
C     PREFIX A OR AB  MASS ABSORPTION COEFFICIENT
C     PREFIX XNFP  NUMBER DENSITY OVER PARTITION FUNCTION
C     ALPHA IS THE FRACTION OF OPACITY CAUSED BY SCATTERING
C     NLTEON=0 LTE
C     NLTEON=1 NLTE
C     BHYD  STATISTICAL EQUILIBRIUM FACTOR FOR HYDROGEN
C     BMIN  STATISTICAL EQUILIBRIUM FACTOR FOR HMINUS
```

```
C     ABUND CONTAINS THE NORMALLY ASSUMED ABUNDANCES
C     ELEM CONTAINS THE LETTER CODES FOR ELEMENTS
C     RCOSET HAS INTEGRATION COEFFICIENTS FOR THE FREQUENCIES IN FRESET
C     NUMNU  NUMBER OF FREQUENCIES IN THE FREQUENCY SET
C     NULO  NUMBER OF THE FREQUENCY AT WHICH INTEGRATION STARTS
C     NUHI  NUMBER OF THE FREQUENCY AT WHICH INTEGRATION STOPS
C     IFCORR  TEMPERATURE CORRECTION ON OR OFF
C     IFPRES PRESSURE INTEGRATION ON OR OFF
C     IFSURF=0  CALCULATE FLUX FOR EVERY DEPTH
C     IFSURF=1  CALCULATE FLUX AT SURFACE ONLY
C     IFSURF=2  CALCULATE INTENSITY AT SURFACE
C     IFSCAT=0 NO SCATTERING IN SOURCE FUNCTION  SNU=BNU
C     IFSCAT=1 SCATTERING IN SOURCE FUNCTION  SOLVE MATRIX EQUATION
C     IFMOL=1 SET UP EQUILIBRIUM EQUATIONS FOR NUMBER DENSITIES
C     IFMOL=0  ASSUME NO MOLECULES AND ITERATE FOR NUMBER DENSITIES
C     NUMITS  NUMBER OF ITERATIONS
C     FREQID IS A LABEL FOR THE FREQUENCY SET
C     XSCALE IS A SCALING FACTOR FOR METAL ABUNDANCES
C     IFPRNT(I)=0 DO NOT PRINT ANYTHING FOR ITERATION I
C     IFPRNT(I)=1 PRINT MINIMAL SUMMARY TABLE AT END OF ITERATION
C     IFPRNT(I)=2 PRINT ALL FREQUENCY INDEPENDENT DATA
C     IFPRNT(I)=3 PRINT SNU,TAUNU,JNU,ETC.
C     IFPRNT(I)=4 PRINT OPACITIES
C     IFPNCH(I)=0 DO NOT PUNCH FOR ITERATION I
C     IFPNCH(I)=1 PUNCH STRUCTURE
C     IFPNCH(I)=2 PUNCH STRUCTURE AND SURFACE FLUX OR INTENSITY
C     IFPNCH(I)=5 PUNCH 2 AND MOLECULAR NUMBER DENSITIES/PART FNS
C     FOR IFSURF=2 HAVE NMU ANGLES
C     IFWAVE=1 STEP NUMNU WAVELENGTHS STARTING AT WBEGIN BY WSTEP
C     XABUND ARE THE ABUNDANCES USED IN THE MODEL
      EXP10(X)=EXP(X*2.30258509299405E0)
      ITEMP=0
    1 CALL READIN(1)
C
C     ITERATION SECTION
      DO 100 ITERAT=1,NUMITS
      ITER=ITERAT
C     CHANGING ITEMP TELLS THE SUBROUTINES THEY HAVE A NEW TEMPERATURE
      ITEMP=ITEMP+ITER
C
      IF(IFPRES.EQ.0)GO TO 12
C     INTEGRATE EQUATION OF HYDROSTATIC EQUILIBRIUM
      DO 11 J=1,NRHOX
      PTOTAL(J)=GRAV*RHOX(J)
   11 P(J)=PTOTAL(J)-PRAD(J)-PTURB(J)
      IF(RHOX(1).EQ.0.)P(1)=P(2)/2.
      IF(RHOX(1).EQ.0.)PTOTAL(1)=PTOTAL(2)/2.
      CALL POPS(0.,1,XNE)
   12 CONTINUE
      CALL PUTOUT(1)
C
C     ERASE FREQUENCY INTEGRALS
      IF(IFCORR.EQ.1)CALL TCORR(1,0)
      CALL ROSS(1,0)
      CALL RADIAP(1,0)
      IF(NLTEON.EQ.1)CALL STATEQ(1,0)
C
C     FREQUENCY INTEGRATION SECTION
      DO 25 NU=NULO,NUHI
      IF(IFWAVE.EQ.0)GO TO 21
```

```
      WAVE=WBEGIN+FLOAT(NU-NULO)*DELTAW
      FREQ=2.997925E17/WAVE
      RCO=ABS(DELTAW/WAVE*FREQ)
      GO TO 22
   21 FREQ=FRESET(NU)
      RCO=RCOSET(NU)
   22 FREQLG=ALOG(FREQ)
      DO 20 J=1,NRHOX
      EHVKT(J)=EXP(-FREQ*HKT(J))
      STIM(J)=1.-EHVKT(J)
   20 BNU(J)=1.47439E-47*FREQ**3*EHVKT(J)/STIM(J)
      CALL PUTOUT(2)
      N=0
   24 N=N+1
      CALL KAPP(N,NSTEPS,STEPWT)
      CALL JOSH(IFSCAT,IFSURF)
      RCOWT=RCO*STEPWT
C
      IF(IFSURF.GT.0)GO TO 23
      IF(IFCORR.EQ.1)CALL TCORR(2,RCOWT)
      CALL RADIAP(2,RCOWT)
      CALL ROSS(2,RCOWT)
      IF(NLTEON.EQ.1)CALL STATEQ(2,RCOWT)
C     THIS PASSES VALUE OF STEPWT TO PUTOUT
   23 PUT=STEPWT
      IPUT=NSTEPS
      CALL PUTOUT(3)
      IF(N.LT.NSTEPS)GO TO 24
      CALL PUTOUT(4)
   25 CONTINUE
      IF(IFSURF.GT.0)GO TO 1
C
C     FINISH ITERATION
      CALL ROSS(3,0)
      IF(IFPRES.EQ.1)CALL CONVEC
      CALL RADIAP(3,0)
      IF(IFCORR.EQ.1)CALL TCORR(3,0)
      IF(NLTEON.EQ.1)CALL STATEQ(3,0)
      CALL HIGH
      IF(IFTURB.EQ.1)CALL TURB
      CALL PUTOUT(5)
C
  100 CONTINUE
      GO TO 1
      END
```

```
      SUBROUTINE PUTOUT(MODE)
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1              GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2              IFCONV
      REAL MIXLTH
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /FRESET/FRESET(500),RCOSET(500),NULO,NUHI,NUMNU
      COMMON /HEIGHT/HEIGHT(40)
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /IFOP/IFOP(20)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /JUNK/TITLE(74),FREQID(6),WLTE,XSCALE
      COMMON /MUS/ANGLE(20),SURFI(20),NMU
      COMMON /OPS/AHYD(40),AH2P(40),AHMIN(40),SIGH(40),AHE1(40),
     1       AHE2(40),AHEMIN(40),SIGHE(40),ACOOL(40),ALUKE(40),AHOT(40),
     2            SIGEL(40),SIGH2(40),AHLINE(40),ALINES(40),SIGLIN(40),
     3            AXLINE(40),SIGXL(40),AXCONT(40),SIGX(40),SHYD(40),
     4            SHMIN(40),SHLINE(40),SXLINE(40),SXCONT(40)
      COMMON /OPTOT/ACONT(40),SCONT(40),ALINE(40),SLINE(40),SIGMAC(40),
     1              SIGMAL(40)
      COMMON /PTOTAL/PTOTAL(40)
      COMMON /PUT/PUT,IPUT
      COMMON /RAD/ ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNU,JMINS
      COMMON /TEFF/TEFF,GRAV,GLOG
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1              IFTURB
      COMMON /WAVEY/WBEGIN,DELTAW,IFWAVE
      COMMON /XABUND/XABUND(99),WTMOLE
      DIMENSION SURFIN(20),F(20),DUMMY(40,25),ABLOG(20)
      EQUIVALENCE (DUMMY(1),AHYD(1)),(F(1),STIM(1))
      DATA ON,OFF/3HON ,3HOFF/
      EXP10(X)=EXP(X*2.30258509299405E0)
C
      GO TO(100,200,300,400,500),MODE
C
C     HEADINGS
  100 IF(IFPRNT(ITER).EQ.0)RETURN
      IFHEAD=0
      NU=NULO-1
      RETURN
C
C     INITIALIZE SUMS OVER STEPS
  200 HSURF=0.
      HNU(1)=0.
      WAVE=2.997925E17/FREQ
      NU=NU+1
      DO 201 MU=1,NMU
  201 SURFIN(MU)=0.
      N=0
```

```
      RETURN
C
C     SUM OVER STEPS AND STEP DEPENDENT QUANTITIES
  300 N=N+1
      NSTEPS=IPUT
      STEPWT=PUT
      HSURF=HSURF+HNU(1)*STEPWT
      DO 301 MU=1,NMU
  301 SURFIN(MU)=SURFIN(MU)+SURFI(MU)*STEPWT
      IF(IFPRNT(ITER).EQ.0)RETURN
      IF(NSTEPS.EQ.1)GO TO 310
      IF(IFHEAD.EQ.0)WRITE(6,101)
      IFHEAD=1
      IF(N.EQ.1)WRITE(6,303)
  303 FORMAT(1H0)
      HNULG=ALOG10(HNU(1))
      IDUM=MAP1(TAUNU,RHOX,NRHOX,1.,RHOX1,1)
      RHOX1=ALOG10(RHOX1)
      TAUEND=ALOG10(TAUNU(NRHOX))
      WRITE(6,305)STEPWT,HNU(1),HNULG,RHOX1,TAUEND
  305 FORMAT(61X,F10.8,1PE13.4,0PF12.5,19X,2F6.2)
C 305 FORMAT(61X,F10.8,0PE13.4,0PF12.5,19X,2F6.2)
  310 IF(IFPRNT(ITER).EQ.4)GO TO 320
      IF(IFPRNT(ITER).NE.3)RETURN
      WRITE(6,312)WAVE,FREQ,(J,RHOX(J),TAUNU(J),ABTOT(J),
     1ALPHA(J),BNU(J),SNU(J),JNU(J),JMINS(J),HNU(J),J=1,NRHOX)
C 312 FORMAT(1H1//6X10HWAVELENGTHF9.3,3X9HFREQUENCY0PE13.6/
  312 FORMAT(1H1//6X10HWAVELENGTHF9.3,3X9HFREQUENCY1PE13.6/
     1/12X4HRHOX,7X5HTAUNU,6X5HABTOT,5X5HALPHA,8X3HBNU,8X3HSNU,
     28X3HJNU,7X5HJMINS,7X3HHNU/(6XI2,1P9E11.3))
C    28X3HJNU,7X5HJMINS,7X3HHNU/(6XI2,0P9E11.3))
      RETURN
  320 WRITE(6,321)
  321 FORMAT( 126H1        AHYD  AH2P AHMIN  SIGH  AHE1 AHE2 AHEMIN SIGHE
     1 ACOOL ALUKE AHOT SIGEL SIGH2 AHLINEALINESSIGLINAXLINE SIGXLAXCONT
     2  SIGX)
      DO 325 J=1,NRHOX
      DO 322 I=1,20
      ABLOG(I)=0.
      IF(DUMMY(J,I).GT.0.)ABLOG(I)=ALOG10(DUMMY(J,I))
  322 CONTINUE
  325 WRITE(6,326)J,ABLOG,J
  326 FORMAT(I4,2X20F6.2,1XI3)
      RETURN
C
C     PRINT SUMS OVER STEPS
  400 IF(IFPRNT(ITER).EQ.0)RETURN
      IDUM=MAP1(TAUNU,RHOX,NRHOX,1.,RHOX1,1)
      RHOX1=ALOG10(RHOX1)
      TAUEND=ALOG10(TAUNU(NRHOX))
      IF(NSTEPS.GT.1)RHOX1=0.
      IF(NSTEPS.GT.1)TAUEND=0.
      IF(IFSURF.NE.0.AND.IFSURF.NE.1)GO TO 405
      IF(IFHEAD.EQ.0)WRITE(6,101)
  101 FORMAT(1H1/////10X4HWAVE,7X7HHLAMBDA,7X5HLOG H,7X3HMAG,
     110X9HFREQUENCY,8X3HHNU,10X5HLOG H,7X3HMAG,10X6HTAUONE,6H TAUNU)
      IFHEAD=1
      IF(HSURF.LE.0.)HSURF=1.E-30
      HLAM=HSURF*FREQ/WAVE
      HNULG=ALOG10(HSURF)
```

```
      HLAMLG=ALOG10(HLAM)
      HLAMMG=-2.5*HLAMLG
      HNUMG=-2.5*HNULG
      WRITE (6,401)NU,WAVE,HLAM,HLAMLG,HLAMMG,FREQ,HSURF,HNULG,HNUMG,
     1RHOX1,TAUEND,NU
C 401 FORMAT(I5,F11.3,0PE13.4,0PF12.5,F10.3,0PE20.6,E13.4,0PF12.5,F10.3,
  401 FORMAT(I5,F11.3,1PE13.4,0PF12.5,F10.3,1PE20.6,E13.4,0PF12.5,F10.3,
     1 9X2F6.2,I5)
  405 IF(IFSURF.NE.2)GO TO 410
      IF(IFHEAD.EQ.0)WRITE(6,102)
  102 FORMAT(1H1/////10X4HWAVE,5X9HFREQUENCY,3X12HTAUONE TAUNU,
     15(17H    MU  INTENSITY ))
      IFHEAD=1
      WRITE(6,406)NU,WAVE,FREQ,RHOX1,TAUEND,
     1(ANGLE(MU),SURFIN(MU),MU=1,NMU)
  406 FORMAT(I5,F10.3,1PE15.6,0P2F6.2,(5(0PF6.3,1PE11.3)))
C 406 FORMAT(I5,F10.3,0PE15.6,0P2F6.2,(5(0PF6.3,0PE11.3)))
  410 IF(IFPNCH(ITER).LT.2)RETURN
      IF(IFSURF.GT.2)RETURN
      IF(IFSURF.EQ.2)GO TO 415
      WRITE(7,411)FREQ,HSURF
  411 FORMAT(4HFLUX,1PE20.6,E13.4)
C 411 FORMAT(4HFLUX,0PE20.6,E13.4)
      RETURN
  415 WRITE(7,416)FREQ,(ANGLE(MU),SURFIN(MU),MU=1,NMU)
  416 FORMAT(9HINTENSITY,1PE15.6,3(0PF5.2,1PE11.4)/(5(0PF5.2,1PE11.4)))
C 416 FORMAT(9HINTENSITY,0PE15.6,3(0PF5.2,0PE11.4)/(5(0PF5.2,0PE11.4)))
      RETURN
C
C     SUMMARIES
  500 IF(IFPRNT(ITER).EQ.0)GO TO 550
      IF(IFPRNT(ITER).EQ.1)GO TO 540
      WRITE(6,501)(J,RHOX(J),PTOTAL(J),PTURB(J),GRDADB(J),DLTDLP(J),
     1VELSND(J),DLRDLT(J),HEATCP(J),HSCALE(J),VCONV(J),FLXCNV(J),
     2J=1,NRHOX)
  501 FORMAT(1H1/////132H        RHOX          PTOTAL        PTURB         GRDADB
     1     DLTDLP      VELSND       DLRDLT       HEATCP        HSCALE        VCONV
     2     FLXCNV               /(I3,1P11E11.3))
C    2     FLXCNV               /(I3,0P11E11.3))
      WRITE(6,502)FLUX
  502 FORMAT(1H0108X4HFLUX1PE12.4)
C 502 FORMAT(1H0108X4HFLUX0PE12.4)
      WRITE(6,503)(J,XNATOM(J),ACCRAD(J),PRAD(J),XNFPH(J,1),XNFPH(J,2),
     1XNFPHE(J,1),XNFPHE(J,2),XNFPHE(J,3),J=1,NRHOX)
  503 FORMAT(1H1/////132H       XNATOM        ACCRAD          PRAD         XNFPH1
     1    XNFPH2      XNFPHE1     XNFPHE2     XNFPHE3
     2                          /(I3,1P8E11.3))
C    2                          /(I3,0P8E11.3))
      DO 539 J=1,NRHOX
      IF(IFCORR.EQ.0)FLXRAD(J)=FLUX-FLXCNV(J)
  539 FLXCNV(J)=FLXCNV(J)/(FLXCNV(J)+FLXRAD(J))
  540 WRITE(6,541) TEFF,GLOG,TITLE,ITER
  541 FORMAT(1H1//////5H TEFF,F8.0,8H   LOG G,F7.3,10X74A1,2X,
     19HITERATION,I3)
      WRITE(6,542)(J,RHOX(J),T(J),P(J),XNE(J),RHO(J),ABROSS(J),
     1HEIGHT(J),TAUROS(J),FLXCNV(J),VTURB(J),FLXERR(J),FLXDRV(J),
     2J=1,NRHOX)
  542 FORMAT(132H0                                                ELECTRON
     1  ROSSELAND    HEIGHT   ROSSELAND   FRACTION                          PE
     2R CENT FLUX/132H          RHOX         TEMP     PRESSURE     NUMBER    DEN
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     4SITY        MEAN         (KM)        DEPTH     CONV FLUX     VTURB
     5   ERROR   DERIV/(I3,1PE10.3,0PF9.1,1P8E11.3,0PF14.3,F8.3))
C    5   ERROR   DERIV/(I3,0PE10.3,0PF9.1,0P8E11.3,0PF14.3,F8.3))
  550 IF(IFPNCH(ITER).EQ.0)RETURN
C
C      PUNCHOUT
       A=OFF
       IF(IFCONV.EQ.1)A=ON
       B=OFF
       IF(IFTURB.EQ.1)B=ON
       WRITE(7,552) TEFF,GLOG,WLTE,TITLE,IFOP,A,MIXLTH,B,TRBFDG,
     1TRBPOW,TRBSND,TRBCON,XSCALE,(IZ,ABUND(IZ),IZ=1,99)
  552 FORMAT(5HTEFF F7.0,9H GRAVITY F5.3,1XA4/6HTITLE 74A1
     1/13H OPACITY IFOP20I2/12H CONVECTION A3,F6.2,12H TURBULENCE A3,
     24F6.2/16HABUNDANCE SCALE F7.3,17H ABUNDANCE CHANGE2(I2,F6.3)/
     3(17H ABUNDANCE CHANGE6(I3,F7.2)))
       WRITE(7,554)NRHOX,(RHOX(J),T(J),P(J),XNE(J),ABROSS(J),PRAD(J),
     1VTURB(J),J=1,NRHOX)
  554 FORMAT(9HREAD DECKI3,31H RHOX,T,P,XNE,ABROSS,PRAD,VTURB/
     1(1PE15.8,0PF9.1,1P5E10.3))
C    1(0PE15.8,0PF9.1,0P5E10.3))
       IF(NLTEON.EQ.0)GO TO 560
       WRITE(7,556)NRHOX,(RHOX(J),(BHYD(J,I),I=1,6),BMIN(J),J=1,NRHOX)
  556 FORMAT(27HREAD DEPARTURE COEFFICIENTSI3,21H RHOX  BHYD 1-6  BMIN/
     1(1PE11.4,0P7F9.4))
C    1(0PE11.4,0P7F9.4))
  560 IF(IFWAVE.EQ.1)GO TO 570
       WRITE(7,562)NUMNU,NULO,NUHI,FREQID,(NJ,FRESET(NU),RCOSET(NU),
     1NU=1,NUMNU)
  562 FORMAT(16HREAD FREQUENCIES3I4,3X6A1/(I5,1P2E17.8,I5,2E17.8))
C 562 FORMAT(16HREAD FREQUENCIES3I4,3X6A1/(I5,0P2E17.8,I5,2E17.8))
  570 WRITE(7,571)ITER
  571 FORMAT(5HBEGIN,20X10HITERATION I3,10H COMPLETED )
      RETURN
      END
```

```
      SUBROUTINE TCORR(MODE,RCOWT)
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1             GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2             IFCONV
      REAL MIXLTH
      COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /PTOTAL/PTOTAL(40)
      COMMON /RAD/ ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNU,JMINS
      COMMON /TEFF/TEFF,GRAV,GLOG
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1                IFTURB
      DIMENSION RJMINS(40),RDABH(40),RDIAGJ(40),OLDT1(40)
      DIMENSION DABTOT(40),DTDRHX(40),HRATIO(40),CODRHX(40),G(40),
     1GFLUX(40),DDLT(40),DRHOX(40),DTFLUX(40),DTLAMB(40),DUM(40),
     2TINTEG(40),DTSURF(40),T1(40),CNVFLX(40),GRDEFF(40),RHOXL(40)
      EQUIVALENCE (HKT(1),G(1),DUM(1),DTSURF(1))
      EQUIVALENCE (TKEV(1),CNVFLX(1),RHOXL(1))
      EQUIVALENCE (TLOG(1),DTDRHX(1),DTFLUX(1)),(TK(1),T1(1))
      EQUIVALENCE (FLXERR(1),DABTOT(1),DRHOX(1)),(TAUNU(1),DDLT(1))
      EQUIVALENCE (RDABH(1),CODRHX(1),GFLUX(1),TINTEG(1),HRATIO(1))
      EQUIVALENCE (RDIAGJ(1),DTLAMB(1),GRDEFF(1))
      GO TO (10,20,30),MODE
C     ERASE FREQUENCY INTEGRALS
   10 DO 11 J=1,NRHOX
      RJMINS(J)=0.
      RDABH(J)=0.
      RDIAGJ(J)=0.
   11 FLXRAD(J)=0.
      RETURN
C
C     FREQUENCY INTEGRATION
   20 DO 21 J=1,NRHOX
      RJMINS(J)=RJMINS(J)+ABTOT(J)*JMINS(J)*RCOWT
   21 FLXRAD(J)=FLXRAD(J)+HNU(J)*RCOWT
      TERM2=0.
      DO 24 J=1,NRHOX
      TERM1=TERM2
      IF(J.NE.NRHOX)D=TAUNU(J+1)-TAUNU(J)
      IF(D.LE..01)GO TO 23
      EX=0.
      IF(D.LT.10.)EX=EXPI(3,D)
      TERM2=.5*(D+EX-.5)/D
      GO TO 22
   23 TERM2=(.922784335098467-ALOG(D))*D*(.25+D*(8.33333333333333E-2+D*
     1(1.04166666666667E-2+D*1.38888888888889E-3)))
   22 DIAGJ=TERM1+TERM2
      DBDT=BNJ(J)*FREQ*HKT(J)/T(J)/STIM(J)
   24 RDIAGJ(J)=RDIAGJ(J)+ABTOT(J)*(DIAGJ-1.)/(1.-ALPHA(J)*DIAGJ)*
     1(1.-ALPHA(J))*DBDT*RCOWT
      RETURN
C
```

```
C     AVRETT-KROOK TAU CORRECTION MODIFIED FOR CONVECTION
   30 CALL DERIV(RHOX,T,DTDRHX,NRHOX)
      CALL DERIV(RHOX,DLTDLP,DDLT,NRHOX)
      DO 31 J=1,NRHOX
      CNVFLX(J)=0.
      DEL=1.
      D=0.
      IF(IFCONV.EQ.1)CNVFLX(J)=FLXCNV(J)
      IF(CNVFLX(J).GT.0.)DEL=DLTDLP(J)-GRDADB(J)
      VCO=.5*MIXLTH*SQRT(-.5*PTOTAL(J)/RHO(J)*DLRDLT(J))
      FLUXCO=.5*RHO(J)*HEATCP(J)*T(J)*MIXLTH/12.5664
      IF(MIXLTH.GT.0.)D=8.*5.6697E-5*T(J)**4/
     1(ABROSS(J)*HSCALE(J)*RHO(J))/(FLUXCO*12.5664)/VCO
      D=D**2/2.
   31 CODRHX(J)=(RDABH(J)+CNVFLX(J)*(DTDRHX(J)/T(J)*(1.-9.*D/(D+DEL))+
     1 1.5*DDLT(J)/DEL*(1.+D/(D+DEL))))/(FLXRAD(J)+CNVFLX(J)*
     2 1.5*DLTDLP(J)/DEL*(1.+D/(D+DEL)))
      CALL INTEG(RHOX,CODRHX,G,NRHOX)
      DO 32 J=1,NRHOX
      G(J)=EXP(G(J))
   32 GFLUX(J)=G(J)*(FLXRAD(J)+CNVFLX(J)-FLUX)/(FLXRAD(J)+CNVFLX(J)*
     1 1.5*DLTDLP(J)/DEL*(1.+D/(D+DEL)))
      CALL INTEG(RHOX,GFLUX,DRHOX,NRHOX)
      DO 33 J=1,NRHOX
      DRHOX(J)=DRHOX(J)/G(J)
      DRHOX(J)=AMAX1(-TAUROS(J)/ABROSS(J)/2.,AMIN1(TAUROS(J)/ABROSS(J),
     1DRHOX(J)))
   33 DTFLUX(J)=-DRHOX(J)*DTDRHX(J)
      DTFLUX(1)=0.
C
      DO 41 J=1,NRHOX
   41 FLXERR(J)=(FLXRAD(J)+CNVFLX(J)-FLUX)/FLUX*100.
      CALL DERIV(TAUROS,FLXERR,FLXDRV,NRHOX)
      TEFF25=TEFF/25.
      DO 43 J=1,NRHOX
      IF(CNVFLX(J)/FLXRAD(J).LT.1.E-5)FLXDRV(J)=RJMINS(J)/ABROSS(J)/
     1FLUX*100.
      DTLAMB(J)=-FLXDRV(J)*FLUX/100./RDIAGJ(J)*ABROSS(J)
      IF(CNVFLX(J)/FLXRAD(J).LT.1.E-5.AND.TAUROS(J).LT.1.)GO TO 42
      DTLAMB(J)=0.
      DTLAMB(J-1)=DTLAMB(J-1)/2.
      DTLAMB(J-2)=DTLAMB(J-2)/2.
      DTLAMB(J-3)=DTLAMB(J-3)/2.
      DTLAMB(J-4)=DTLAMB(J-4)/2.
      DTLAMB(J-5)=DTLAMB(J-5)/2.
C     FUDGE TO AVOID VERY LARGE TEMPERATURE CORRECTIONS
   42 DTLAMB(J)=AMAX1(-TEFF25,AMIN1(TEFF25,DTLAMB(J)))
   43 CONTINUE
C
      DTSUR=(FLUX-FLXRAD(1))/FLUX*.25*T(1)
      DTSUR=AMAX1(-TEFF25,AMIN1(TEFF25,DTSUR))
      DO 45 J=1,NRHOX
   45 DUM(J)=DTFLUX(J)+DTLAMB(J)
      CALL INTEG(TAUROS,DUM,TINTEG,NRHOX)
      IDUM=MAP1(TAUROS,TINTEG,NRHOX,.1,TONE,1)
      IDUM=MAP1(TAUROS,TINTEG,NRHOX,2.,TTWO,1)
      TAV=(TTWO-TONE)/2.
      IF(DTSUR*TAV.LE.0.)TAV=0.
      IF(ABS(TAV).GT.ABS(DTSUR))TAV=DTSUR
      DTSUR=DTSUR-TAV
```

```
      DO 49 J=1,NRHOX
   49 DTSURF(J)=DTSUR
C
      DO 50 J=1,NRHOX
      HRATIO(J)=CNVFLX(J)/(CNVFLX(J)+FLXRAD(J))
   50 T1(J)=DTFLUX(J)+DTLAMB(J)+DTSURF(J)
      IF(IFPRNT(ITER).LE.1)GO TO 60
      WRITE(6,100)  (J,RHOX(J),T(J),DTLAMB(J),DTSURF(J),DTFLUX(J),T1(J),
     1HRATIO(J),FLXERR(J),FLXDRV(J),J=1,NRHOX)
  100 FORMAT(1H1///94H0           RHOX          T       DTLAMB    DTSURF    DTFL
     1UX        T1    CONV/TOTAL         ERROR      DERIV/
     2(I3,1PE12.4,0PF10.1,4F9.1,1X1PE11.3,1X0P2F10.3))
C    2(I3,0PE12.4,0PF10.1,4F9.1,1X0PE11.3,1X0P2F10.3))
C
   60 DO 61 J=1,NRHOX
      IF(IFCONV.EQ.1)GO TO 62
      IF(ITER.EQ.1)GO TO 62
      IF(OLDT1(J)*T1(J).GT.0.)T1(J)=T1(J)*1.25
      IF(OLDT1(J)*T1(J).LT.0.)T1(J)=T1(J)*.5
   62 OLDT1(J)=T1(J)
   61 T(J)=T(J)+T1(J)
C
C     FUDGES TO MAKE UP FOR BAD STARTING GUESSES
      IF(IFCONV.EQ.1)GO TO 71
      IF(ITER.GT.1)GO TO 80
      IF(FLXERR(NRHOX).LT.90..AND.FLXERR(NRHOX).GT.-50.)GO TO 80
      DO 70 J=1,NRHOX
   70 T(J)=TEFF*(.75*(.710+TAUROS(J)-.1331*EXP(-3.4488*TAUROS(J))))**.25
      GO TO 80
   71 DO 72 J=1,NRHOX
      IF(FLXERR(J).GT.1000.)GO TO 73
   72 CONTINUE
      GO TO 80
   73 DO 74 J=1,NRHOX
      GRDEFF(J)=(FLXRAD(J)*DLTDLP(J)+FLXCNV(J)*GRDADB(J))/(FLXRAD(J)+
     1FLXCNV(J))
      IF(FLXCNV(J).GT.0.)GRDEFF(J)=AMAX1(GRDEFF(J),(1.+DLTDLP(J))/3.)
   74 RHOXL(J)=ALOG(RHOX(J))
      CALL INTEG(RHOXL,GRDEFF,TLOG,NRHOX)
      DO 75 JSTART=1,NRHOX
      IF(FLXCNV(JSTART).GT.0.)GO TO 76
   75 CONTINUE
      GO TO 80
   76 DO 77 J=JSTART,NRHOX
   77 T(J)=T(J-1)*EXP(TLOG(J)-TLOG(J-1))
   80 DO 81 J=1,NRHOX
      TK(J)=1.38054E-16*T(J)
      HKT(J)=6.6256E-27/TK(J)
      TKEV(J)=8.6171E-5*T(J)
   81 TLOG(J)=ALOG(T(J))
      RETURN
      END
```

```
      SUBROUTINE STATEQ(MODE,RCOWT)
C     THE BOUND-BOUND COLLISION RATES WERE DERIVED FROM AN ANALYTIC FIT
C     TO THE CROSS SECTION CALCULATIONS OF BURKE,ORMONDE AND WHITAKER,
C     PROC. PHYS. SOC., 1968, VOL 92, 319
C
C     THE CROSS SECTION USED (IN UNITS OF PI*A0**2) IS
C
C     QIJ = 4*FIJ*(EH/E0)**2*(LOG(E/E0)/(E/E0)+.148 /(E/E0)**6)
C
C     FIJ = OSCILLATOR STRENGTH
C     EH = GROUND STATE BINDING ENERGY
C     E0 = THRESHOLD ENERGY
C                                                 D M PETERSON MAY 1968
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNU,JMINS
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION QRADIK(40,6),QRADKI(40,6),QRDHMK(40),QRDKHM(40)
      DIMENSION DQRAD(40,6),DQRD(40),TOLD(40)
      DIMENSION HCONT(6),DUMMY(6)
      DIMENSION A(6,6),RIGHT(6),QCOLL(8,8)
      EQUIVALENCE (A(1),TAUNU(1)),(QCOLL(1),HNU(1)),(HCONT(1),DUMMY(1))
      DIMENSION F(8,8)
      DATA F/8*0.,.4162,7*0.,.07910,.6408,6*0.,.02899,.1193,.8420,5*0.,
     1.01394,.04467,.1506,1.038,4*0.,.007800,.02209,.05585,.1794,1.231,
     23*0.,.004814,.01271,.02768,.06551,.2070,1.425,2*0.,.003184,.008037
     3,.01604,.03229,.07455,.2340,1.615,0./
      GO TO(10,20,30),MODE
C     ERASE FREQUENCY INTEGRALS
   10 DO 11 I=1,6
      DO 11 J=1,NRHOX
      TOLD(J)=T(J)
      QRDHMK(J)=0.
      QRDKHM(J)=0.
      DQRD(J)=0.
      DQRAD(J,I)=0.
      QRADKI(J,I)=0.
   11 QRADIK(J,I)=0.
      RETURN
C     FREQUENCY INTEGRALS
   20 RFRWT=12.5664/6.6256E-27*RCOWT/FREQ
      HVC=2.*6.6256E-27*FREQ*(FREQ/2.997925E10)**2
      DO 21 N=2,6
   21 HCONT(N)=COULX(N,FREQ,1.)
      HMINBF=0.
      IF(FREQ.GT.1.8259E14.AND.FREQ.LT.2.111E14)HMINBF=
     1 3.695E-16+(-1.251E-1+1.052E13/FREQ)/FREQ
      IF(FREQ.GE.2.111E14)HMINBF=6.801E-20+(5.358E-3+(1.481E13+
     1(-5.519E27+4.808E41/FREQ)/FREQ)/FREQ)/FREQ
      DO 25 J=1,NRHOX
      RJ=RFRWT*JNU(J)
      RJE=RFRWT*EHVKT(J)*(JNU(J)+HVC)
      RJEDT=RJE*HKT(J)*FREQ/T(J)
      DO 26 I=2,6
      QRADIK(J,I)=QRADIK(J,I)+HCONT(I)*RJ
```

```
      DQRAD(J,I)=DQRAD(J,I)+HCONT(I)*RJEDT
   26 QRADKI(J,I)=QRADKI(J,I)+HCONT(I)*RJE
      QRDHMK(J)=QPDHMK(J)+HMINBF*RJ
      DQRD(J)=DQRD(J)+HMINBF*RJEDT
   25 QRDKHM(J)=QRDKHM(J)+HMINBF*RJE
      RETURN
C
   30 IF(IFPRNT(ITER).GT.0)WRITE(6,201)
  201 FORMAT(1H1/////36X30HHMINUS STATISTICAL EQUILIBRIUM/10X4HRHOX,
     1 7X6HQELECT,6X6HQASSOC,6X6HQCHARG,6X6HQRDKHM,6X6HQRDHMK,7X4HBMIN)
      DO 210 J=1,NRHOX
      DT=T(J)-TOLD(J)
      THETA=5040./T(J)
      QELECT=10.**(-8.7)*THETA**(1.5)*XNE(J)
      QASSOC=10.**(-8.7)*2.*BHYD(J,1)*XNFPH(J,1)
      QCHARG=10.**(-7.4)*THETA**.333333*XNFPH(J,2)
      QRDKHM(J)=QRDKHM(J)+DQRD(J)*DT
      BMIN(J)=(QRDKHM(J)+QELECT+QASSOC+QCHARG)/
     1(QRDHMK(J)+QELECT+QASSOC+QCHARG)
  210 WRITE(6,211)J,RHOX(J),QELECT,QASSOC,QCHARG,QRDKHM(J),
     1QRDHMK(J),BMIN(J)
  211 FORMAT(I5,1P6E12.3,0PF10.4)
C 211 FORMAT(I5,0P6E12.3,0PF10.4)
C
      IF(IFPRNT(ITER).GT.0)WRITE(6,31)
   31 FORMAT(1H1/////30X83HSTATISTICAL EQUILIBRIJM RATES    RATE=SIGN(AL
     1OG10(AMAX1(ABS(RATE*1.E20),1.)),RATE) /
     2132H0 RAD    1-K     K-1     2-K     K-2     3-K     K-3     4-K     K-4     5-K
     3K-5    6-K     K-6     COLL    1-K     2-K     3-K     4-K     5-K     6-K     5-8
     46-8   /
     5132H  COLL   1-2     1-3     1-4     1-5     1-6     1-7     2-3     2-4     2-5
     62-6    2-7     3-4     3-5     3-6     3-7     4-5     4-6     4-7     5-6     5-7
     76-7   )
C
      DO 120 J=1,NRHOX
      DT=T(J)-TOLD(J)
      TH=13.595/TKEV(J)
      DO 50 I=1,8
      Y=I
      QCOLL(I,I)=2.2E-8*Y**3/SQRT(TH)*EXP(-TH/Y**2)*XNE(J)
C     QCOLL(I,I) IS THE BOUND FREE RATE
      IF (I.EQ.8) GO TO 50
      I1=I+1
      DO 40 K=I1,8
      Z=K
      GIK=1./Y**2-1./Z**2
      X0=TH*GIK
      Q=2.186E-10*F(I,K)/GIK**2*X0*SQRT(T(J))*(EXPI(1,X0)+.148*X0*
     2EXPI(5,X0))
      QCOLL(I,K)=Q*XNE(J)
      QCOLL(K,I)=QCOLL(I,K)*(Y/Z)**2*EXP(X0)
   40 CONTINUE
   50 CONTINUE
      DO 65 I=1,6
      A(I,I)=QRADIK(J,I)
      QRADKI(J,I)=QRADKI(J,I)+DQRAD(J,I)*DT
      RIGHT(I)=QRADKI(J,I)+QCOLL(I,I)+QCOLL(I,7)+QCOLL(I,8)
      DO 55 K=1,8
   55 A(I,I)=A(I,I)+QCOLL(I,K)
```

```
      IF (I.EQ.6) GO TO 65
      I1=I+1
      DO 60 K=I1,6
      A(I,K)=-QCOLL(I,K)
   60 A(K,I)=-QCOLL(K,I)
   65 CONTINUE
C
      CALL SOLVIT(A,6,RIGHT,DUMMY)
      DO 80 L=1,6
   80 BHYD(J,L)=RIGHT(L)
      IF (IFPRNT(ITER).LE.1) GO TO 120
      DO 90 I=1,6
      QRADKI(J,I)=SIGN(ALOG10(AMAX1(ABS(QRADKI(J,I)*1.E20),1.)),
     1QRADKI(J,I))
   90 QRADIK(J,I)=SIGN(ALOG10(AMAX1(ABS(QRADIK(J,I)*1.E20),1.)),
     1QRADIK(J,I))
      DO 95 I=1,8
      DO 95 K=1,8
   95 QCOLL(I,K)=SIGN(ALOG10(AMAX1(ABS(QCOLL(I,K)*1.E20),1.)),
     1QCOLL(I,K))
      WRITE (6,100) J,(QRADIK(J,I),QRADKI(J,I),I=1,6),
     1(QCOLL(I,I),I=1,6),QCOLL(5,8),QCOLL(6,8)
  100 FORMAT (1H0I5,12F6.2,6X8F6.2)
      WRITE (6,110)    (QCOLL(1,K),K=2,7),(QCOLL(2,K),K=3,7),(QCOLL(3,K),
     1K=4,7),(QCOLL(4,K),K=5,7),(QCOLL(5,K),K=6,7),QCOLL(6,7)
  110 FORMAT (6X21F6.2)
  120 CONTINUE
C
  160 WRITE (6,170)(J,RHOX(J),(BHYD(J,I),I=1,6),J=1,NRHOX)
  170 FORMAT(1H1/////30X36HSTATISTICAL EQUILIBRIUM FOR HYDROGEN/
     1 15X4HRHOX,10X2HB1,8X2HB2,8X2HB3,8X2HB4,8X2HB5,8X2HB6/
     2(8XI2,1PE11.4,1X0P6F10.4))
C    2(8XI2,0PE11.4,1X0P6F10.4))
C
      RETURN
      END


      SUBROUTINE ROSS(MODE,RCOWT)
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      GO TO(10,20,30),MODE
   10 DO 11 J=1,NRHOX
   11 ABROSS(J)=0.
      RETURN
   20 DO 21 J=1,NRHOX
      DBDT=BNJ(J)*FREQ*HKT(J)/T(J)/STIM(J)
   21 ABROSS(J)=ABROSS(J)+DBDT/ABTOT(J)*RCOWT
      RETURN
   30 DO 31 J=1,NRHOX
   31 ABROSS(J)=(4.*5.6697E-5/3.14159)*T(J)**3/ABROSS(J)
      RHOX0=RHOX(1)
      RHOX(1)=0.
      CALL INTEG(RHOX,ABROSS,TAUROS,NRHOX)
      RHOX(1)=RHOX0
      RETURN
      END
```

```
      SUBROUTINE RADIAP(MODE,RCOWT)
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
      COMMON /RAD/ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNU,JMINS
      DIMENSION DUM(40),H(40)
      EQUIVALENCE (DUM(1),ABTOT(1))
      GO TO (10,20,30),MODE
   10 DO 11 J=1,NRHOX
      H(J)=0.
   11 ACCRAD(J)=0.
      RETURN
   20 DO 21 J=1,NRHOX
      H(J)=H(J)+HNU(J)*RCOWT
   21 ACCRAD(J)=ACCRAD(J)+ABTOT(J)*HNU(J)*RCOWT
      RETURN
   30 DO 31 J=1,NRHOX
      ACCRAD(J)=ACCRAD(J)*12.5664/2.997925E10
C     FUDGE TO KEEP MODEL FROM BLOWING UP WITH LARGE FLUX ERRORS
      IF(H(J)/FLUX.GT.1.)ACCRAD(J)=ACCRAD(J)*FLUX/H(J)
   31 CONTINUE
      CALL INTEG(RHOX,ACCRAD,PRAD,NRHOX)
      RETURN
      END
```

```
      SUBROUTINE DERIV(X,F,DFDX,N)
C     ASSUMES THAT ANY ZERO IN X OCCURS AT A ENDPOINT
      DIMENSION X(1),F(1),DFDX(1)
      DFDX(1)=(F(2)-F(1))/(X(2)-X(1))
      N1=N-1
      DFDX(N)=(F(N)-F(N1))/(X(N)-X(N1))
      IF(N.EQ.2)RETURN
      S=ABS(X(2)-X(1))/(X(2)-X(1))
      DO 1 J=2,N1
      SCALE=AMAX1(ABS(F(J-1)),ABS(F(J)),ABS(F(J+1)))/ABS(X(J))
      IF(SCALE.EQ.0.)SCALE=1.
      D1=(F(J+1)-F(J))/(X(J+1)-X(J))/SCALE
      D=(F(J)-F(J-1))/(X(J)-X(J-1))/SCALE
      TAN1=D1/(S*SQRT(1.+D1**2)+1.)
      TAN=D/(S*SQRT(1.+D**2)+1.)
    1 DFDX(J)=(TAN1+TAN)/(1.-TAN1*TAN)*SCALE
      RETURN
      END
```

```
      SUBROUTINE INTEG(X,F,FINT,N)
      DIMENSION X(1),F(1),FINT(1)
      DIMENSION A(40),B(40),C(40)
      CALL PARCOE(F,X,A,B,C,N)
      FINT(1)=(A(1)+(B(1)/2.+C(1)/3.*X(1))*X(1))*X(1)
      FINT(2)=(A(1)+(B(1)/2.+C(1)/3.*X(2))*X(2))*X(2)
      IF(N.EQ.2)RETURN
      N1=N-1
      DO 10 I=2,N1
   10 FINT(I+1)=FINT(I)+(A(I)+B(I)/2.*(X(I+1)+X(I))+
     1C(I)/3.*((X(I+1)+X(I))*X(I+1)+X(I)*X(I)))*(X(I+1)-X(I))
      RETURN
      END


      SUBROUTINE PARCOE(F,X,A,B,C,N)
      DIMENSION F(1),X(1),A(1),B(1),C(1)
      C(1)=0.
      B(1)=(F(2)-F(1))/(X(2)-X(1))
      A(1)=F(1)-X(1)*B(1)
      N1=N-1
      C(N)=0.
      B(N)=(F(N)-F(N1))/(X(N)-X(N1))
      A(N)=F(N)-X(N)*B(N)
      IF(N.EQ.2)RETURN
      DO 1 J=2,N1
      J1=J-1
      D=(F(J)-F(J1))/(X(J)-X(J1))
      C(J)=F(J+1)/((X(J+1)-X(J))*(X(J+1)-X(J1)))-F(J)/((X(J)-X(J1))*
     1(X(J+1)-X(J)))+F(J1)/((X(J)-X(J1))*(X(J+1)-X(J1)))
      B(J)=D-(X(J)+X(J1))*C(J)
    1 A(J)=F(J1)-X(J1)*D+X(J)*X(J1)*C(J)
      N1=N1-1
      DO 2 J=2,N1
      IF(C(J).EQ.0.)GO TO 2
      J1=J+1
      WT=ABS(C(J1))/(ABS(C(J1))+ABS(C(J)))
      A(J)=A(J1)+WT*(A(J)-A(J1))
      B(J)=B(J1)+WT*(B(J)-B(J1))
      C(J)=C(J1)+WT*(C(J)-C(J1))
    2 CONTINUE
      RETURN
      END
```

```
      FUNCTION MAP1(XOLD,FOLD,NOLD,XNEW,FNEW,NNEW)
      DIMENSION XOLD(1),FOLD(1),XNEW(1),FNEW(1)
      L=2
      LL=0
      DO 50 K=1,NNEW
   10 IF(XNEW(K).LT.XOLD(L))GO TO 20
      L=L+1
      IF(L.GT.NOLD)GO TO 30
      GO TO 10
   20 IF(L.EQ.LL)GO TO 50
      IF(L.EQ.2)GO TO 30
      L1=L-1
      IF(L.GT.LL+1.OR.L.EQ.3)GO TO 21
      CBAC=CFOR
      BBAC=BFOR
      ABAC=AFOR
      IF(L.EQ.NOLD)GO TO 22
      GO TO 25
   21 L2=L-2
      D=(FOLD(L1)-FOLD(L2))/(XOLD(L1)-XOLD(L2))
      CBAC=FOLD(L)/((XOLD(L)-XOLD(L1))*(XOLD(L)-XOLD(L2)))+
     1(FOLD(L2)/(XOLD(L)-XOLD(L2))-FOLD(L1)/(XOLD(L)-XOLD(L1)))/
     2(XOLD(L1)-XOLD(L2))
      BBAC=D-(XOLD(L1)+XOLD(L2))*CBAC
      ABAC=FOLD(L2)-XOLD(L2)*D+XOLD(L1)*XOLD(L2)*CBAC
      IF(L.LT.NOLD)GO TO 25
   22 C=CBAC
      B=BBAC
      A=ABAC
      LL=L
      GO TO 50
   25 D=(FOLD(L)-FOLD(L1))/(XOLD(L)-XOLD(L1))
      CFOR=FOLD(L+1)/((XOLD(L+1)-XOLD(L))*(XOLD(L+1)-XOLD(L1)))+
     1(FOLD(L1)/(XOLD(L+1)-XOLD(L1))-FOLD(L)/(XOLD(L+1)-XOLD(L)))/
     2(XOLD(L)-XOLD(L1))
      BFOR=D-(XOLD(L)+XOLD(L1))*CFOR
      AFOR=FOLD(L1)-XOLD(L1)*D+XOLD(L)*XOLD(L1)*CFOR
      WT=0.
      IF(ABS(CFOR).NE.0.)WT=ABS(CFOR)/(ABS(CFOR)+ABS(CBAC))
      A=AFOR+WT*(ABAC-AFOR)
      B=BFOR+WT*(BBAC-BFOR)
      C=CFOR+WT*(CBAC-CFOR)
      LL=L
      GO TO 50
   30 IF(L.EQ.LL)GO TO 50
      L=AMIN0(NOLD,L)
      C=0.
      B=(FOLD(L)-FOLD(L-1))/(XOLD(L)-XOLD(L-1))
      A=FOLD(L)-XOLD(L)*B
      LL=L
   50 FNEW(K)=A+(B+C*XNEW(K))*XNEW(K)
      MAP1=LL-1
      RETURN
      END
```

```
      SUBROUTINE SOLVIT(A.N.B.IPIVOT)
C     SOLVES LINEAR EQUATIONS
C     A IS A COMPLETELY FILLED N BY N ARRAY WHICH IS DESTROYED.
C     B IS THE RIGHT SIDE VECTOR OF LENGTH N AND RETURNS AS THE SOLUTION
C     IPIVOT IS A SCRATCH AREA OF LENGTH N.
      DIMENSION A(1).B(1).IPIVOT(1)
      EQUIVALENCE(AMAX.SWAP.PIVOT.T)
      DO 20 J=1.N
   20 IPIVOT(J)=0
      DO 550 I=1.N
      AMAX=0.
      DO 105 J=1.N
      IF(IPIVOT(J).EQ.1)GO TO 105
      JK=J-N
      DO 100 K=1.N
      JK=JK+N
      IF(IPIVOT(K).EQ.1)GO TO 100
      AA=ABS(A(JK))
      IF(AMAX.GE.AA)GO TO 100
      IROW=J
      ICOLUM=K
      AMAX=AA
  100 CONTINUE
  105 CONTINUE
      IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
      IF(IROW.EQ.ICOLUM)GO TO 260
      IRL=IROW-N
      ICL=ICOLUM-N
      DO 200 L=1.N
      IRL=IRL+N
      SWAP=A(IRL)
      ICL=ICL+N
      A(IRL)=A(ICL)
  200 A(ICL)=SWAP
      SWAP=B(IROW)
      B(IROW)=B(ICOLUM)
      B(ICOLUM)=SWAP
  260 ICIC=ICOLUM*N+ICOLUM-N
      PIVOT=A(ICIC)
      A(ICIC)=1.
      ICL=ICOLUM-N
      DO 350 L=1.N
      ICL=ICL+N
  350 A(ICL)=A(ICL)/PIVOT
      B(ICOLUM)=B(ICOLUM)/PIVOT
      L1IC=ICOLUM*N-N
      DO 550 L1=1.N
      L1IC=L1IC+1
      IF(L1.EQ.ICOLUM)GO TO 550
      T=A(L1IC)
      A(L1IC)=0.
      L1L=L1-N
      ICL=ICOLUM-N
      DO 450 L=1.N
      L1L=L1L+N
      ICL=ICL+N
  450 A(L1L)=A(L1L)-A(ICL)*T
      B(L1)=B(L1)-B(ICOLUM)*T
  550 CONTINUE
      RETURN
      END
```

```
      FUNCTION EXPI(N,X)
C     EXPONENTIAL INTEGRAL FOR POSITIVE ARGUMENTS AFTER CODY AND
C     THACHER, MATH. OF COMP.,22,641(1968)
      DATA X1/-1.E20/
      DATA A0,A1,A2,A3,A4,A5,B0,B1,B2,B3,B4/
     1-44178.5471728217,57721.7247139444,9938.31388962037,
     2 1842.11088668000,101.093806161906,5.03416184097568,
     3 76537.3323337614,32597.1881290275,6106.10794245759,
     4 635.419418378382,37.2298352833327/
      DATA C0,C1,C2,C3,C4,C5,C6,D1,D2,D3,D4,D5,D6/
     1 4.65627107975096E-7,
     2 .999979577051595,9.04161556946329,24.3784088791317,
     3 23.0192559391333,6.90522522784444,.430967839469389,
     4 10.0411643829054,32.4264210695138,41.2807841891424,
     5 20.4494785013794,3.31909213593302,.103400130404874/
      DATA E0,E1,E2,E3,E4,E5,E6,F1,F2,F3,F4,F5,F6/
     1-.999999999998447,-26.6271060431811,-241.055827097015,
     2-895.927957772937,-1298.85688746484,-545.374158883133,
     3-5.66575206533869, 28.6271060422192, 292.310039388533,
     4 1332.78537748257, 2777.61949509163, 2404.01713225909,
     5 631.657483280800/
      IF(X.EQ.X1)GO TO 40
      EX=EXP(-X)
      X1=X
      IF(X.GT.4.)GO TO 10
      IF(X.GT.1.)GO TO 20
      IF(X.GT.0.)GO TO 30
      EX1=0.
      GO TO 40
   10 EX1=(EX+EX*(E0+(E1+(E2+(E3+(E4+(E5+E6/X)/X)/X)/X)/X)/X)/
     1          (X+ F1+(F2+(F3+(F4+(F5+F6/X)/X)/X)/X)/X))/X
      GO TO 40
   20 EX1=EX*(C6+(C5+(C4+(C3+(C2+(C1+C0*X)*X)*X)*X)*X)*X)/
     1      (D6+(D5+(D4+(D3+(D2+(D1+X)*X)*X)*X)*X)*X)
      GO TO 40
   30 EX1=(A0+(A1+(A2+(A3+(A4+A5*X)*X)*X)*X)*X)/
     1    (B0+(B1+(B2+(B3+(B4+X)*X)*X)*X)*X)-ALOG(X)
   40 EXPI=EX1
      IF(N.EQ.1)RETURN
      N1=N-1
      DO 41 I=1,N1
   41 EXPI=(EX-X*EXPI)/FLOAT(I)
      RETURN
      END


      SUBROUTINE W(A,B,N)
      DIMENSION B(1)
      WRITE(6,100)A,(B(I),I=1,N)
C 100 FORMAT(1H0,A6,0P10E12.4/(7X,10E12.4))
  100 FORMAT(1H0,A6,1P10E12.4/(7X,10E12.4))
      RETURN
      END
```

```
      SUBROUTINE READIN(MODE)
C     MODE=1 COMPUTE A MODEL
C     MODE=2 READ A PREVIOUSLY CALCULATED MODEL FOR SOME APPLICATION
C     MODE=20 SAME AS 2 BUT ON ENCOUNTERING END RETURN WITH NRHOX=0
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1               GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2               IFCONV
      REAL MIXLTH
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
      COMMON /FREE/WORD(6),NUMCOL,LETCOL,LAST,MORE,IFFAIL,MAXPOW
      COMMON /FRESET/FRESET(500),RCOSET(500),NULO,NUHI,NUMNU
      COMMON /HEIGHT/HEIGHT(40)
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /IFOP/IFOP(20)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /JUNK/TITLE(74),FREQID(6),WLTE,XSCALE
      COMMON /MUS/ANGLE(20),SURFI(20),NMU
      COMMON /PTOTAL/PTOTAL(40)
      COMMON /RAD/ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEFF/TEFF,GRAV,GLOG
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1                 IFTURB
      COMMON /WAVEY/WBEGIN,DELTAW,IFWAVE
      COMMON /XABUND/XABUND(99),WTMOLE
      DIMENSION CARD(80)
      EQUIVALENCE (CARD(1),XABUND(1)),(CARD81,XABUND(81))
      DIMENSION RHOXA(40),DUM1(40),DUM2(40),DUM3(40),DUM4(40),DUM5(40)
      DIMENSION DUM6(40),DUM7(40),DUM8(40),TAUSTD(40)
      EQUIVALENCE (DUM1(1),DLTDLP(1)),(DUM2(1),HEATCP(1))
      EQUIVALENCE (DUM3(1),DLRDLT(1)),(DUM4(1),VELSND(1))
      EQUIVALENCE (DUM5(1),GRDADB(1)),(DUM6(1),HSCALE(1))
      EQUIVALENCE (DUM7(1),FLXCNV(1)),(RHOXA(1),VCONV(1),DUM8(1))
      EQUIVALENCE (TAUSTD(1),XNATOM(1))
      DIMENSION IFOP1(20)
C     H1,H2PLUS,HMINUS,HRAY,HE1,HE2,HEMINUS,HERAY,COOL,LUKE,
C     HOT,ELECTRON,H2RAY,HLINES,LINES,LINESCAT,XLINES,XLSCAT,XCONT,XSCAT
      DATA IFOP1/324,609929997,579591588,429928,11165,11166,564793810,
     1 15271257,173061,636997,11527,369467847,16486929,577716835,
     2 22965179,849711626,1687220147,1687711471,45152896,45946435/
      DATA WWLTE,WWNLTE/4HLTE ,4HNLTE/
      DATA BLANK/1H /
      EXP10(X)=EXP(X*2.30258509299405E0)
      CARD81=BLANK
      LAST=81
      MAXPOW=38
   98 MORE=0
      LETCOL=1
   99 READ(5,1) CARD
    1 FORMAT(80A1)
C     (M)ACHINE (I)NDEPENDENT (A)LPHAMERIC (C)ODE
C     BASE 37    A=1, Z=26, 0=27, 9=36
      MIAC=IWORDF(CARD)
      NUMCOL=LETCOL
C     TEFF
```

```
    3 IF(MIAC.EQ.1020133)GO TO 100
C     GRAVITY
      IF(MIAC.EQ.519223721)GO TO 200
C     OPACITY
      IF(MIAC.EQ.1070201044)GO TO 300
C     KAPPA
      IF(MIAC.EQ.20688921)GO TO 400
C     ITERATIONS
      IF(MIAC.EQ.661856797)GO TO 500
C     MOLECULES
      IF(MIAC.EQ.930198669)GO TO 600
C     CALCULATE
      IF(MIAC.EQ.210518764)GO TO 700
C     ABUNDANCE
      IF(MIAC.EQ.74175307)GO TO 800
C     PRINT
      IF(MIAC.EQ.30911189)GO TO 900
C     PUNCH
      IF(MIAC.EQ.31069574)GO TO 1000
C     READ
      IF(MIAC.EQ.918640)GO TO 1100
C     LTE
      IF(MIAC.EQ.17173)GO TO 1200
C     NLTE
      IF(MIAC.EQ.726315)GO TO 1300
C     BEGIN
      IF(MIAC.EQ.4011517)GO TO 1500
C     SCATTERING
      IF(MIAC.EQ.1323236444)GO TO 1600
C     END
      IF(MIAC.EQ.7367)GO TO 1700
C     TITLE
      IF(MIAC.EQ.37966926)GO TO 1800
C     CONVECTION
      IF(MIAC.EQ.236883734)GO TO 1900
C     TURBULENCE
      IF(MIAC.EQ.1427151802)GO TO 2000
C     CHANGE RHOX
      IF(MIAC.EQ.223095242)GO TO 2100
C     FREQUENCIES
C     IF(MIAC.EQ.450075960)GO TO 2200
C     SURFACE
      IF(MIAC.EQ.1357812572)GO TO 2300
C     PRESSURE
      IF(MIAC.EQ.1143518210)GO TO 2400
C     CORRECTION
      IF(MIAC.EQ.237080870)GO TO 2500
C     WAVELENGTH
      IF(MIAC.EQ.1597906832)GO TO 2600
C     SCALE MODEL
      IF(MIAC.EQ.35762836)GO TO 2700
C     CALL
      IF(MIAC.EQ.153784)GO TO 2800
C
 9000 WRITE(6,2) CARD
    2 FORMAT(21H I DO NOT UNDERSTAND 80A1)
      CALL EXIT
   97 LETCOL=MAX0(LETCOL,NUMCOL)
      MORE=1
      MIAC=IWORDF(CARD)
```

```
      IF(IFFAIL.EQ.1)GO TO 98
      MORE=0
      GO TO 3
C************
  100 TEFF=FREEFF(CARD)
      FLUX=5.6697E-5/12.5664*TEFF**4
      GO TO 97
C************
  200 GRAV=FREEFF(CARD)
      IF(GRAV.LT.10.)GRAV=EXP10(GRAV)
      GLOG=ALOG10(GRAV)
      GO TO 97
C************
  300 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 380
C     OFF
      IF(MIAC.EQ.20763)GO TO 390
C     IFOP
      IF(MIAC.EQ.464662)GO TO 370
      GO TO 9000
  370 NUMCOL=LETCOL
      DO 371 I=1,20
  371 IFOP(I)=FREEFF(CARD)
      GO TO 98
C     ON
  380 ISWCH=1
      GO TO 391
C     OFF
  390 ISWCH=0
  391 MORE=1
  395 MIAC=IWORDF(CARD)
      IF(IFFAIL.EQ.1)GO TO 97
      DO 392 I=1,20
      II=I
      IF(MIAC.EQ.IFOP1(I))GO TO 393
  392 CONTINUE
      GO TO 9000
  393 IFOP(II)=ISWCH
      GO TO 395
C************
  400 GO TO 9000
C************
  500 NUMITS=FREEFF(CARD)
      DO 501 I=1,15
  501 IFPNCH(I)=0
      IFPNCH(NUMITS)=1
      GO TO 97
C************
  600 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 610
C     OFF
      IF(MIAC.EQ.20763)GO TO 620
      GO TO 9000
  610 IFMOL=1
      GO TO 97
  620 IFMOL=0
      GO TO 97
C************
```

```
  700 NRHOX=FREEFF(CARD)
      TAU1LG=FREEFF(CARD)
      STEPLG=FREEFF(CARD)
      DO 701 J=1,NRHOX
      XNE(J)=0.
      PRAD(J)=0.
      VTURB(J)=0.
      PTURB(J)=0.
      TAUROS(J)=EXP10(TAU1LG+FLOAT(J-1)*STEPLG)
  701 T(J)=TEFF*(.75*(.710+TAUROS(J)-.1331*EXP(-3.4488*TAUROS(J))))**.25
      CALL TTAUP(T,TAUROS,ABROSS,PTOTAL,P,PRAD,PTURB,GRAV,NRHOX)
      DO 702 J=1,NRHOX
  702 RHOX(J)=PTOTAL(J)/GRAV
      GO TO 97
C************
  800 MIAC=IWORDF(CARD)
C     SCALE
      IF(MIAC.EQ.35762836)GO TO 810
C     CHANGE
      IF(MIAC.EQ.223095242)GO TO 820
      GO TO 9000
  810 NUMCOL=LETCOL
      XSCALE=FREEFF(CARD)
      GO TO 97
  820 MORE=1
  821 IZ=FREEFF(CARD)
      IF(IFFAIL.EQ.1)GO TO 98
      ABUND(IZ)=FREEFF(CARD)
      GO TO 821
C************
  900 DO 901 I=1,NUMITS
  901 IFPRNT(I)=FREEFF(CARD)
      GO TO 97
C************
 1000 DO 1001 I=1,NUMITS
 1001 IFPNCH(I)=FREEFF(CARD)
      GO TO 97
C************
 1100 MIAC=IWORDF(CARD)
      NUMCOL=LETCOL
C     FREQUENCIES
      IF(MIAC.EQ.450075960)GO TO 1110
C     DEPARTURE COEFFICIENTS
      IF(MIAC.EQ.287559136)GO TO 1120
C     STARTING T-TAU
      IF(MIAC.EQ.1355094447)GO TO 1130
C     DECK
      IF(MIAC.EQ.209579)GO TO 1140
      GO TO 9000
C     FREQUENCIES
 1110 NUM=FREEFF(CARD)
      NULO=FREEFF(CARD)
      NUHI=FREEFF(CARD)
      NUMNU=NUM
      LETCOL=NUMCOL
      NDUMMY=IWORDF(CARD)
      DO 1111 I=1,6
 1111 FREQID(I)=WORD(I)
      NUMCOL=LETCOL
      DO 1112 I=1,NUMNU
```

```
      NU=FREEFR(CARD)
      FRESET(NU)=FREEFF(CARD)
C     PROVISION FOR READING WAVELENGTHS
      IF(FRESET(NU).LT.1.E7)FRESET(NU)=2.997925E17/FRESET(NU)
 1112 RCOSET(NU)=FREEFF(CARD)
      GO TO 98
C     DEPARTURE COEFFICIENTS
 1120 NRHOX=FREEFF(CARD)
      DO 1122 J=1,NRHOX
      NUMCOL=1
      READ(5,1)CARD
      DUMMY=FREEFF(CARD)
      DO 1121 I=1,6
 1121 BHYD(J,I)=FREEFF(CARD)
 1122 BMIN(J)=FREEFF(CARD)
      WLTE=WWNLTE
      NLTEON=1
      GO TO 98
 1130 NRHOX=FREEFF(CARD)
      DO 1131 J=1,NRHOX
      NUMCOL=1
      READ(5,1)CARD
      TAUROS(J)=FREEFF(CARD)
      T(J)=FREEFF(CARD)
      PRAD(J)=0.
      XNE(J)=0.
      VTURB(J)=0.
 1131 PTURB(J)=0.
      IF(TAUROS(1).GT.0.)GO TO 1135
      DO 1132 J=1,NRHOX
 1132 TAUROS(J)=EXP10(TAUROS(J))
 1135 CALL TTAUP(T,TAUROS,ABROSS,PTOTAL,P,PRAD,PTURB,GRAV,NRHOX)
      DO 1136 J=1,NRHOX
 1136 RHOX(J)=PTOTAL(J)/GRAV
      GO TO 98
 1140 NRHOX=FREEFF(CARD)
      DO 1141 J=1,NRHOX
      NUMCOL=1
      READ(5,1)CARD
      RHOX(J)=FREEFF(CARD)
      T(J)=FREEFF(CARD)
      MORE=1
      P(J)=FREEFF(CARD)
      XNE(J)=FREEFF(CARD)
      ABROSS(J)=FREEFF(CARD)
      PRAD(J)=FREEFF(CARD)
      VTURB(J)=FREEFF(CARD)
 1141 MORE=0
      IF(RHOX(1).GE.0.)GO TO 98
      DO 1142 J=1,NRHOX
 1142 RHOX(J)=EXP10(RHOX(J))
      GO TO 98
C************
 1200 NLTEON=0
      WLTE=WWLTE
      DO 1202 J=1,40
      DO 1201 I=1,6
 1201 BHYD(J,I)=1.
 1202 BMIN(J)=1.
      GO TO 97
```

```
C************
 1300 NLTEON=1
      WLTE=WWNLTE
      GO TO 97
C************
 1500 IF(MODE.NE.1)GO TO 1510
      IF(NUMITS.EQ.0)WRITE(6,1501)
      IF(NRHOX.EQ.0)WRITE(6,1502)
      IF(NUMNJ.EQ.0)WRITE(6,1503)
      IF(TEFF.EQ.0.)WRITE(6,1504)
      IF(GRAV.EQ.0.)WRITE(6,1505)
 1501 FORMAT(20H HOW MANY ITERATIONS)
 1502 FORMAT(14H HOW MANY RHOX)
 1503 FORMAT(21H HOW MANY FREQUENCIES)
 1504 FORMAT(10H WHAT TEFF)
 1505 FORMAT(13H WHAT GRAVITY)
      IF(NUMITS.EQ.0)CALL EXIT
      IF(NRHOX.EQ.0)CALL EXIT
      IF(NUMNJ.EQ.0)CALL EXIT
      IF(TEFF.EQ.0.)CALL EXIT
      IF(GRAV.EQ.0.)CALL EXIT
 1510 CONTINUE
      IF(ABUND(1).LT.0.)ABUND(1)=EXP10(ABUND(1))
      IF(ABUND(2).LT.0.)ABUND(2)=EXP10(ABUND(2))
      DO 1511 IZ=3,99
      IF(ABUND(IZ).GT.0.)ABUND(IZ)=ALOG10(ABUND(IZ))
 1511 CONTINUE
      WRITE(6,1512)TEFF,GLOG,WLTE,TITLE,XSCALE,
     1(ELEM(IZ),ABUND(IZ),IZ=1,99)
 1512 FORMAT(1H1/////5H TEFFF7.0,8H   LOG GF6.2,3XA4/
     17HOTITLE ,74A1/7HOXSCALEF8.3,2(3X,A2,F6.3)/(10(1XA2,F6.2)))
      DO 1513 IZ=3,99
 1513 XABUND(IZ)=EXP10(ABUND(IZ))*XSCALE
      XABUND(1)=ABUND(1)
      XABUND(2)=ABUND(2)
      WTMOLE=0.
      DO 1514 IZ=1,99
 1514 WTMOLE=WTMOLE+XABUND(IZ)*ATMASS(IZ)
      DO 1516 J=1,NRHOX
      TK(J)=1.38054E-16*T(J)
      HKT(J)=6.6256E-27/TK(J)
      TKEV(J)=8.6171E-5*T(J)
      TLOG(J)=ALOG(T(J))
      XNATOM(J)=P(J)/TK(J)-XNE(J)
      RHO(J)=XNATOM(J)*WTMOLE*1.660E-24
 1516 PTURB(J)=.5*RHO(J)*VTURB(J)**2
      WRITE(6,1517)IFOP
 1517 FORMAT(3HOH1I2,7H H2PLUSI2,7H HMINUSI2,5H HRAYI2,4H HE1I2,
     1 4H HE2I2,8H HEMINUSI2,6H HERAYI2,5H COOLI2,5H LUKEI2/
     2 4H HOTI2,9H ELECTRONI2,6H H2RAYI2,7H HLINESI2,6H LINESI2,
     3 9H LINESCATI2,7H XLINESI2,7H XLSCATI2,6H XCONTI2,6H XSCATI2)
      WRITE(6,1518)IFCORR,IFPRES,IFSURF,IFSCAT,IFCONV,MIXLTH,IFMOL,
     1IFTURB,TRBFDG,TRBPOW,TRBSND,TRBCON
 1518 FORMAT(7HOIFCORRI2,8H  IFPRESI2,8H  IFSURFI2,8H  IFSCATI2,
     1 8H  IFCONVI2,8H  MIXLTHF6.2,7H  IFMOLI2/7H IFTURBI2,
     2 8H  TRBFDGF6.2,8H  TRBPOWF6.2,8H  TRBSNDF6.2,8H  TRBCONF6.2)
      IF(MODE.NE.1)GO TO 1575
      WRITE(6,1521)NUMITS,IFPRNT,IFPNCH
 1521 FORMAT(7H NUMITSI3,8H  IFPRNT15I2,8H  IFPNCH15I2)
      IF(IFWAVE.EQ.0)GO TO 1560
```

```
      WRITE(6,1536)WBEGIN,DELTAW,NUMNU
 1536 FORMAT(7H0WBEGINF11.4,9H   DELTAWF7.4,8H   NUMNUI5)
      GO TO 1575
 1560 WRITE(6,1561)FREQID,NUMNU,NULO,NUHI
 1561 FORMAT(8H0FREQID 6A1,8H   NUMNUI4,7H   NULOI4,7H   NUHII4)
      NN=(NUMNU+3)/4
      NNN=NUMNU-NN*3
      IF(NNN.LT.1)NN=1
      IF(NNN.LT.1)NNN=1
      WRITE(6,1563)((NU,FRESET(NU),RCOSET(NU),NU=I,NUMNU,NN),I=1,NNN)
 1563 FORMAT((4(3XI3,1P2E13.6)))
C1563 FORMAT((4(3XI3,0P2E13.6)))
      IF(NN.EQ.NNN)GO TO 1575
      NNN=NNN+1
      WRITE(6,1564)((NU,FRESET(NU),RCOSET(NU),NU=I,NUMNU,NN),I=NNN,NN)
 1564 FORMAT((3(3XI3,1P2E13.6)))
C1564 FORMAT((3(3XI3,0P2E13.6)))
C
 1575 CONTINUE
      WRITE(6,1576)(J,RHOX(J),T(J),P(J),XNE(J),ABROSS(J),PRAD(J),
     1VTURB(J),(BHYD(J,I),I=1,6),BMIN(J),J=1,NRHOX)
 1576 FORMAT(1H1/////8X4HRHOX,9X1HT,8X1HP,8X3HXNE,6X6HABROSS,5X4HPRAD,
     1 6X5HVTURB,24X4HBHYD,25X4HBMIN/
     2(I3,1PE13.6,0PF9.1,1P5E10.3,1X0P7F8.4))
C    2(I3,0PE13.6,0PF9.1,0P5E10.3,1X0P7F8.4))
C
      RETURN
C************
 1600 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 1610
C     OFF
      IF(MIAC.EQ.20763)GO TO 1620
      GO TO 9000
 1610 IFSCAT=1
      GO TO 97
 1620 IFSCAT=0
      GO TO 97
C************
 1700 IF(MODE.NE.20)CALL EXIT
      NRHOX=0
      RETURN
C************
 1800 DO 1801 I=1,74
 1801 TITLE(I)=CARD(I+6)
      GO TO 98
C************
 1900 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 1910
C     OFF
      IF(MIAC.EQ.20763)GO TO 1920
      GO TO 9000
 1910 IFCONV=1
      NUMCOL=LETCOL
      MIXLTH=FREEFF(CARD)
      GO TO 97
 1920 IFCONV=0
      MIXLTH=1.
      DO 1921 J=1,NRHOX
```

```
      DLTDLP(J)=0.
      HEATCP(J)=0.
      DLRDLT(J)=0.
      VELSND(J)=0.
      GRDADB(J)=0.
      HSCALE(J)=0.
      FLXCNV(J)=0.
 1921 VCONV(J)=0.
      GO TO 97
C************
 2000 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 2010
C     OFF
      IF(MIAC.EQ.20763)GO TO 2020
      GO TO 9000
 2010 IFTURB=1
      NUMCOL=LETCOL
      TRBFDG=FREEFF(CARD)
      TRBPOW=FREEFF(CARD)
      TRBSND=FREEFF(CARD)
      TRBCON=FREEFF(CARD)
      GO TO 97
 2020 IFTURB=0
      TRBFDG=0.
      TRBPOW=0.
      TRBSND=0.
      TRBCON=0.
      GO TO 97
C************
 2100 NNEW=FREEFF(CARD)
      DO 2101 J=1,NNEW
 2101 RHOXA(J)=FREEFR(CARD)
      IDUM=MAP1(RHOX,T,NRHOX,RHOXA,DUM1,NNEW)
      IDUM=MAP1(RHOX,P,NRHOX,RHOXA,DUM2,NNEW)
      IDUM=MAP1(RHOX,XNE,NRHOX,RHOXA,DUM3,NNEW)
      IDUM=MAP1(RHOX,ABROSS,NRHOX,RHOXA,DUM4,NNEW)
      IDUM=MAP1(RHOX,VTURB,NRHOX,RHOXA,DUM5,NNEW)
      IDUM=MAP1(RHOX,PRAD,NRHOX,RHOXA,DUM6,NNEW)
      IDUM=MAP1(RHOX,BMIN,NRHOX,RHOXA,DUM7,NNEW)
      DO 2102 J=1,NNEW
      T(J)=DUM1(J)
      P(J)=DUM2(J)
      XNE(J)=DUM3(J)
      ABROSS(J)=DUM4(J)
      VTURB(J)=DUM5(J)
      PRAD(J)=DUM6(J)
 2102 BMIN(J)=DUM7(J)
      DO 2105 I=1,6
      IDUM=MAP1(RHOX,BHYD(1,I),NRHOX,RHOXA,DUM1,NNEW)
      DO 2104 J=1,NNEW
 2104 BHYD(J,I)=DUM1(J)
 2105 CONTINUE
      NRHOX=NNEW
      DO 2106 J=1,NRHOX
 2106 RHOX(J)=RHOXA(J)
      GO TO 97
C************
 2300 MIAC=IWORDF(CARD)
C     INTENSITY
```

```
      IF(MIAC.EQ.651354309)GO TO 2310
C     FLUX
      IF(MIAC.EQ.321147)GO TO 2320
C     OFF
      IF(MIAC.EQ.20763)GO TO 2330
      GO TO 9000
 2310 NMU=FREEFF(CARD)
      DO 2311 MU=1,NMU
 2311 ANGLE(MU)=FREEFF(CARD)
      IFSURF=2
      GO TO 97
 2320 IFSURF=1
      GO TO 97
 2330 IFSURF=0
      GO TO 97
C************
 2400 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 2410
C     OFF
      IF(MIAC.EQ.20763)GO TO 2420
      GO TO 9000
 2410 IFPRES=1
      GO TO 97
 2420 IFPRES=0
      GO TO 97
C************
 2500 MIAC=IWORDF(CARD)
C     ON
      IF(MIAC.EQ.569)GO TO 2510
C     OFF
      IF(MIAC.EQ.20763)GO TO 2520
      GO TO 9000
 2510 IFCORR=1
      GO TO 97
 2520 IFCORR=0
      DO 2521 J=1,40
      FLXERR(J)=0.
 2521 FLXDRV(J)=0.
      GO TO 97
C************
 2600 WBEGIN=FREEFF(CARD)
      DELTAW=FREEFF(CARD)
      WEND=FREEFF(CARD)
      IFWAVE=1
      NULO=1
      NUHI=IFIX((WEND-WBEGIN)/DELTAW+.5)+1
      NUMNU=NUHI
      GO TO 97
C************
C     SCALING MODELS OR CHANGING RHOX SPACING TO BE UNIFORM IN TAUROS
 2700 NRHOX=FREEFF(CARD)
      TAU1LG=FREEFF(CARD)
      STEPLG=FREEFF(CARD)
      MORE=1
      TEFF1=FREEFF(CARD)
      GNEW=FREEFF(CARD)
      IF(GNEW.LT.10.)GNEW=EXP10(GNEW)
      MORE=0
      DO 2701 J=1,NRHOX
```

```
 2701 TAUSTD(J)=EXP10(TAU1LG+FLOAT(J-1)*STEPLG)
      RHOX0=RHOX(1)
      RHOX(1)=0.
      CALL INTEG(RHOX,ABROSS,TAUROS,NRHOX)
      RHOX(1)=RHOX0
      IDUM=MAP1(TAUROS,RHOX,NRHOX,TAUSTD,DUM1,NRHOX)
      IDUM=MAP1(TAUROS,T,NRHOX,TAUSTD,DUM2,NRHOX)
      IDUM=MAP1(TAUROS,P,NRHOX,TAUSTD,DUM3,NRHOX)
      IDUM=MAP1(TAUROS,XNE,NRHOX,TAUSTD,DUM4,NRHOX)
      IDUM=MAP1(TAUROS,ABROSS,NRHOX,TAUSTD,DUM5,NRHOX)
      IDUM=MAP1(TAUROS,PRAD,NRHOX,TAUSTD,DUM6,NRHOX)
      IDUM=MAP1(TAUROS,VTURB,NRHOX,TAUSTD,DUM7,NRHOX)
      IDUM=MAP1(TAUROS,BMIN,NRHOX,TAUSTD,DUM8,NRHOX)
      DO 2702 J=1,NRHOX
      RHOX(J)=DUM1(J)
      T(J)=DUM2(J)
      P(J)=DUM3(J)
      XNE(J)=DUM4(J)
      ABROSS(J)=DUM5(J)
      PRAD(J)=DUM6(J)
      VTURB(J)=DUM7(J)
 2702 BMIN(J)=DUM8(J)
      DO 2704 I=1,6
      IDUM=MAP1(TAUROS,BHYD(1,I),NRHOX,TAUSTD,DUM1,NRHOX)
      DO 2703 J=1,NRHOX
 2703 BHYD(J,I)=DUM1(J)
 2704 CONTINUE
      IF(TEFF1.EQ.0.)GO TO 97
      IF(TEFF1.EQ.TEFF.AND.GNEW.EQ.GRAV)GO TO 97
      DO 2710 J=1,NRHOX
      TAUROS(J)=TAUSTD(J)
      T(J)=T(J)*TEFF1/TEFF
C     FOR DETAILED WORK WITH RADIATION PRESSURE OR TURBULENT PRESSURE
C        BETTER METHODS FOR SCALING THOSE QUANTITIES SHOULD BE INSERTED
      PTURB(J)=0.
 2710 PRAD(J)=PRAD(J)*(TEFF1/TEFF)**4*(GNEW/GRAV)
      TEFF=TEFF1
      FLUX=5.6697E-5/12.5664*TEFF**4
      GRAV=GNEW
      GLOG=ALOG10(GRAV)
      CALL TTAUP(T,TAUROS,ABROSS,PTOTAL,P,PRAD,PTURB,GRAV,NRHOX)
      DO 2711 J=1,NRHOX
 2711 RHOX(J)=PTOTAL(J)/GRAV
      GO TO 97
C************
 2800 CALL DUMMYR
      GO TO 97
C************
      END


      SUBROUTINE DUMMYR
C     DUMMY INPUT ROUTINE FOR MODIFYING READIN
      RETURN
      END
```

```
    FUNCTION FREEFF(CARD)
    COMMON /FREE/WORD(6),NUMCOL,LETCOL,LAST,MORE,IFFAIL,MAXPOW
    DIMENSION CARD(1)
    DIMENSION A(10)
    DATA A/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/
    DATA QPT/1H./,QCM/1H,/,QMI/1H-/,QE/1HE/,QPL/1H+/,QBL/1H /
    IFFAIL=0
    IF(NUMCOL.GT.LAST)GO TO 3002
    ANSWER=0.
    ASIGN=1.
    ISIGN=1
    NPT=0
    IFO=0
    N=0
    ASSIGN 100 TO NSWCH
    DO 1000 NCOL=NUMCOL,LAST
    C=CARD(NCOL)
    GO TO NSWCH,(100,200,300,400)
100 IF(C.EQ.QBL)GO TO 104
    DO 101 I=1,10
    IF(C.EQ.A(I))GO TO 102
101 CONTINUE
    IF(C.EQ.QPT)GO TO 103
    IF(C.EQ.QCM)GO TO 104
    IF(C.EQ.QMI)GO TO 105
999 ASIGN=1.
    ANSWER=0.
    NPT=0
    IFO=0
    N=0
    ASSIGN 100 TO NSWCH
    GO TO 1000
102 N=N+1
    ANSWER=10.*ANSWER+FLOAT(I-1)
    GO TO 1000
103 ASSIGN 200 TO NSWCH
    GO TO 1000
104 IF(N.EQ.0)GO TO 999
    FREEFF=ANSWER*ASIGN
998 NUMCOL=NCOL+1
    RETURN
105 IF(N.EQ.0)GO TO 106
    GO TO 999
106 ASIGN=-1.
    GO TO 1000
200 DO 201 I=1,10
    IF(C.EQ.A(I))GO TO 202
201 CONTINUE
    IF(C.EQ.QE )GO TO 203
    IF(C.EQ.QBL)GO TO 204
    IF(C.EQ.QCM)GO TO 204
    GO TO 999
202 N=N+1
    NPT=NPT+1
    ANSWER=10.*ANSWER+FLOAT(I-1)
    GO TO 1000
203 ASSIGN 300 TO NSWCH
    GO TO 1000
204 IF(N.EQ.0)GO TO 999
    FREEFF=ANSWER*ASIGN/10.**NPT
```

```
      GO TO 998
  300 DO 301 I=1,10
      IF(C.EQ.A(I))GO TO 302
  301 CONTINUE
      IF(C.EQ.QBL)GO TO 303
      IF(C.EQ.QMI)GO TO 304
      IF(C.EQ.QPL)GO TO 303
      GO TO 999
  302 NPOWER=I-1
      IFO=1
  310 ASSIGN 400 TO NSWCH
      GO TO 1000
  303 NPOWER=0
      GO TO 310
  304 ISIGN=-1
      NPOWER=0
      GO TO 310
  400 DO 401 I=1,10
      IF(C.EQ.A(I))GO TO 402
  401 CONTINUE
      IF(C.EQ.QCM)GO TO 403
      IF(C.EQ.QBL)GO TO 403
      GO TO 999
  402 NPOWER=10*NPOWER+I-1
      IFO=1
      IF(NPOWER.GE.MAXPOW)GO TO 999
      GO TO 1000
  403 IF(IFO.EQ.0)GO TO 999
      FREEFF=ANSWER*ASIGN*10.**(ISIGN*NPOWER-NPT)
      GO TO 998
 1000 CONTINUE
      NUMCOL=LAST+1
 3002 IFFAIL=1
      IF(MORE.GT.0)GO TO 3000
      WRITE(6,3001)(CARD(I),I=1,LAST)
 3001 FORMAT(28H1FREEFF HAS READ OFF THE END/(1X80A1))
      CALL EXIT
 3000 FREEFF=0.
      RETURN
      END


      FUNCTION FREEFR(CARD)
      COMMON /FREE/WORD(6),NUMCOL,LETCOL,LAST,MORE,IFFAIL,MAXPOW
      DIMENSION CARD(1)
      MORE=1
      FREEFR=FREEFF(CARD)
      IF(IFFAIL.EQ.0)RETURN
      L=LAST-1
      READ(5,1)(CARD(I),I=1,L)
    1 FORMAT(80A1)
      NUMCOL=1
      FREEFR=FREEFF(CARD)
      RETURN
      END
```

```
      FUNCTION IWORDF(CARD)
      COMMON /FREE/WORD(6),NUMCOL,LETCOL,LAST,MORE,IFFAIL,MAXPOW
      DIMENSION CARD(1)
      DIMENSION A(36)
      EQUIVALENCE (QE,A(5))
      DATA A/1HA,1HB,1HC,1HD,1HE,1HF,1HG,1HH,1HI,1HJ,1HK,1HL,1HM,1HN,
     11HO,1HP,1HQ,1HR,1HS,1HT,1HU,1HV,1HW,1HX,1HY,1HZ,1H0,1H1,1H2,1H3,
     21H4,1H5,1H6,1H7,1H8,1H9/
      DATA QPT/1H./,QCM/1H,/,QEQ/1H=/,QBL/1H /
      DO 1 I=1,6
    1 WORD(I)=QBL
      IFFAIL=0
      IF(LETCOL.GT.LAST)GO TO 4002
      N=0
C     (M)ACHINE (I)NDEPENDENT (A)LPHAMERIC (C)ODE
      MIAC=0
      ASSIGN 500 TO NSWCH
      DO 2000 NCOL=LETCOL,LAST
      C=CARD(NCOL)
      GO TO NSWCH,(500,600)
  500 IF(C.EQ.QBL)GO TO 1999
      DO 501 II=1,26
      IF(C.EQ.A(II))GO TO 502
  501 CONTINUE
 1999 MIAC=0
      N=0
      ASSIGN 500 TO NSWCH
      GO TO 2000
  502 IF(C.NE.QE )GO TO 506
      IF(NCOL.EQ.1)GO TO 506
      C=CARD(NCOL-1)
      DO 503 I=27,36
      IF(C.EQ.A(I))GO TO 504
  503 CONTINUE
      IF(C.NE.QPT)GO TO 506
  504 C=CARD(NCOL+1)
      DO 505 I=27,36
      IF(C.EQ.A(I))GO TO 1999
  505 CONTINUE
      IF(C.EQ.QBL)GO TO 1999
  506 N=N+1
      MIAC=II
      WORD(1)=A(II)
      ASSIGN 600 TO NSWCH
      GO TO 2000
  600 IF(C.EQ.QBL)GO TO 603
      IF(C.EQ.QEQ)GO TO 603
      IF(C.EQ.QCM)GO TO 603
      DO 601 II=1,36
      IF(C.EQ.A(II))GO TO 602
  601 CONTINUE
      GO TO 1999
  602 N=N+1
      IF(N.GT.6)GO TO 604
      MIAC=37*MIAC+II
      WORD(N)=A(II)
  604 GO TO 2000
  603 IWORDF=MIAC
      LETCOL=NCOL+1
      RETURN
```

```
 2000 CONTINJE
      LETCOL=LAST+1
 4002 IFFAIL=1
      IF(MORE.GT.0)GO TO 4000
      WRITE(6,4001)(CARD(I),I=1,LAST)
 4001 FORMAT(28H1IWORDF HAS READ OFF THE END/(1X80A1))
      CALL EXIT
 4000 IWORDF=0
      RETJRN
      END


      SUBROJTINE BLOCKE
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
C                    1H     2HE
      DATA ABJND/     .9,    .1,
C       3LI    4BE    5B     6C     7N     8O     9F     10NE   11NA   12MG
     1-11.6, -9.6, -9.2,-3.50,-4.12,-3.28, -6.6, -3.5,-6.18,-4.57,
C       13AL   14SI   15P    16S    17CL   18AR   19K    20CA   21SC   22TI
     2-5.65,-4.50,-6.62,-4.84, -6.6, -5.3,-7.00,-5.72,-9.01,-7.55,
C       23V    24CR   25MN   26FE   27CO   28NI   29CU   30ZN   31GA   33GE
     3-8.13,-6.58,-7.17,-4.5 , -8.4,-6.97, -7.3,-7.63,-9.11,-8.73,
C       33AS   34SE   35BR   36KR   37RB   38SR   39Y    40ZR   41NB   42MO
     4 -9.7, -8.8, -9.4, -8.8,-9.42,-9.23, -9.6, -9.6,-10.3,-10.0,
C       43TC   44RU   45RH   46PD   47AG   48CD   49IN   50SN   51SB   52TE
     5-20.0,-10.4,-11.2,-10.7,-11.3,-9.98,-10.34,-10.34,-10.4,-10.0,
C       53I    54XE   55CS   56BA   57LA   58CE   59PR   60ND   61PM   62SM
     6-10.6,-10.0,-10.9,-10.15,-10.6,-10.4,-11.2,-10.5,-20.0,-11.0,
C       63EU   64GD   65TB   66DY   67HO   68ER   69TM   70YB   71LJ   72HF
     7-11.3,-10.9,-11.6,-10.8,-11.5,-11.1,-11.9,-10.9,-11.7,-11.4,
C       73TA   74W    75RE   76OS   77IR   78PT   79AU   80HG   81TL   82PB
     8-11.7,-10.9,-11.4,-10.7,-10.8,-10.4,-11.3,-11.1,-11.5,-10.15,
C       83BI   84PO   85AT   86RN   87FR   88RA   89AC   90TH   91PA   92J
     9-11.3,-20.0,-20.0,-20.0,-20.0,-20.0,-20.0,-11.7,-20.0,-12.0,
C       93NP   94PU   95AM   96CM   97BK   98CF   99ES
     T-20.0,-20.0,-20.0,-20.0,-20.0,-20.0,-20.0/
      DATA ATMASS/ 1.008,4.003,
     1 6.939,9.013,10.81,12.01,14.01,16.00,19.00,20.18,22.99,24.31,
     2 26.98,28.09,30.98,32.07,35.45,39.95,39.10,40.08,44.96,47.90,
     3 50.94,52.00,54.94,55.85,58.94,58.71,63.55,65.37,69.72,72.60,
     4 74.92,78.96,79.91,83.80,85.48,87.63,88.91,91.22,92.91,95.95,
     5 99.00,101.1,102.9,106.4,107.9,112.4,114.8,118.7,121.8,127.6,
     6 126.9,131.3,132.9,137.4,138.9,140.1,140.9,144.3,147.0,150.4,
     7 152.0,157.3,158.9,162.5,164.9,167.3,168.9,173.0,175.0,178.5,
     8 181.0,183.9,186.3,190.2,192.2,195.1,197.0,200.6,204.4,207.2,
     9 209.0,210.0,211.0,222.0,223.0,226.1,227.1,232.0,231.0,238.0,
     T 237.0,244.0,243.0,247.0,247.0,251.0,254.0/
      DATA ELEM/    2HH , 2HHE,
     1 2HLI, 2HBE, 2HB , 2HC , 2HN , 2HO , 2HF , 2HNE, 2HNA, 2HMG,
     2 2HAL, 2HSI, 2HP , 2HS , 2HCL, 2HAR, 2HK , 2HCA, 2HSC, 2HTI,
     3 2HV , 2HCR, 2HMN, 2HFE, 2HCO, 2HNI, 2HCU, 2HZN, 2HGA, 2HGE,
     4 2HAS, 2HSE, 2HBR, 2HKR, 2HRB, 2HSR, 2HY , 2HZR, 2HNB, 2HMO,
     5 2HTC, 2HRU, 2HRH, 2HPD, 2HAG, 2HCD, 2HIN, 2HSN, 2HSB, 2HTE,
     6 2HI , 2HXE, 2HCS, 2HBA, 2HLA, 2HCE, 2HPR, 2HND, 2HPM, 2HSM,
     7 2HEU, 2HGD, 2HTB, 2HDY, 2HHO, 2HER, 2HTM, 2HYB, 2HLU, 2HHF,
     8 2HTA, 2HW , 2HRE, 2HOS, 2HIR, 2HPT, 2HAU, 2HHG, 2HTL, 2HPB,
     9 2HBI, 2HPO, 2HAT, 2HRN, 2HFR, 2HRA, 2HAC, 2HTH, 2HPA, 2HJ ,
     T 2HNP, 2HPU, 2HAM, 2HCM, 2HBK, 2HCF, 2HES/
      END
```

```
 SUBROUTINE BLOCKR
 COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
1            GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
2            IFCONV
 REAL MIXLTH
 COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
 COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
 COMMON /FRESET/FRESET(500),RCOSET(500),NULO,NUHI,NUMNU
 COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
 COMMON /IFOP/IFOP(20)
 COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
 COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
 COMMON /JUNK/TITLE(74),FREQID(6),WLTE,XSCALE
 COMMON /MUS/ANGLE(20),SURFI(20),NMU
 COMMON /RAD/ACCRAD(40),PRAD(40)
 COMMON /RHOX/RHOX(40),NRHOX
 COMMON /TEFF/TEFF,GRAV,GLOG
 COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
1              IFTURB
 COMMON /WAVEY/WBEGIN,DELTAW,IFWAVE
 DATA DLTDLP,HEATCP,DLRDLT,VELSND,GRDADB,HSCALE,FLXCNV,VCONV/
1 40*0.,40*0.,40*0.,40*0.,40*0.,40*0.,40*0.,40*0./
 DATA IFCONV,MIXLTH/0,1./
 DATA BHYD,BMIN/40*1.,40*1.,40*1.,40*1.,40*1.,40*1.,40*1./
 DATA NLTEON/0/
 DATA FLUX/0./
 DATA FLXERR,FLXDRV/40*0.,40*0./
 DATA NUMNU/0/
 DATA IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL/1,1,0,1,0/
 DATA IFOP/1,1,1,1,1,1,0,0,1,0,0,1,0,0,0,0,0,0,0,0/
 DATA XNFPH,XNFPHE/40*0.,40*0.,40*0.,40*0.,40*0./
 DATA IFPRNT/2,2,2,2,2,2,2,2,2,2,2,2,2,2,2/
 DATA IFPNCH/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
 DATA NUMITS/0/
 DATA TITLE/74*1H /
 DATA WLTE/4HLTE /
 DATA XSCALE/1./
 DATA SURFI/20*0./,NMU/1/
 DATA ACCRAD/40*0./,PRAD/40*0./
 DATA NRHOX/0/
 DATA TEFF/0./
 DATA GRAV/0./
 DATA VTURB/40*0./
 DATA PTURB/40*0./
 DATA IFTURB,TRBFDG,TRBPOW,TRBSND,TRBCON/0,0.,0.,0.,0./
 DATA IFWAVE/0/
 END
```

```
      SUBROUTINE TTAUP(T,TAU,ABSTD,PTOTAL,P,PRAD,PTURB,GRAV,NUMTAU)
C     ROSSELAND OPACITY, NORMAL ABUNDANCES, T=3100 TO 28000, P=-2 TO +6
C     TAUS MUST HAVE LOG SPACING
      DIMENSION T(1),TAU(1),ABSTD(1),PTOTAL(1),P(1),PRAD(1),PTURB(1)
      DIMENSION TABT(30),TABP(30)
      DIMENSION TABKAP(30,30),KTAB(30,30),PKAP(30)
      EQUIVALENCE (TABKAP(1),KTAB(1))
      DIMENSION KTAB01(30),KTAB02(30),KTAB03(30),KTAB04(30)
      DIMENSION KTAB05(30),KTAB06(30),KTAB07(30),KTAB08(30)
      DIMENSION KTAB09(30),KTAB10(30),KTAB11(30),KTAB12(30)
      DIMENSION KTAB13(30),KTAB14(30),KTAB15(30),KTAB16(30)
      DIMENSION KTAB17(30),KTAB18(30),KTAB19(30),KTAB20(30)
      DIMENSION KTAB21(30),KTAB22(30),KTAB23(30),KTAB24(30)
      DIMENSION KTAB25(30),KTAB26(30),KTAB27(30),KTAB28(30)
      DIMENSION KTAB29(30),KTAB30(30)
      EQUIVALENCE (KTAB(001),KTAB01(1)),(KTAB(031),KTAB02(1))
      EQUIVALENCE (KTAB(061),KTAB03(1)),(KTAB(091),KTAB04(1))
      EQUIVALENCE (KTAB(121),KTAB05(1)),(KTAB(151),KTAB06(1))
      EQUIVALENCE (KTAB(181),KTAB07(1)),(KTAB(211),KTAB08(1))
      EQUIVALENCE (KTAB(241),KTAB09(1)),(KTAB(271),KTAB10(1))
      EQUIVALENCE (KTAB(301),KTAB11(1)),(KTAB(331),KTAB12(1))
      EQUIVALENCE (KTAB(361),KTAB13(1)),(KTAB(391),KTAB14(1))
      EQUIVALENCE (KTAB(421),KTAB15(1)),(KTAB(451),KTAB16(1))
      EQUIVALENCE (KTAB(481),KTAB17(1)),(KTAB(511),KTAB18(1))
      EQUIVALENCE (KTAB(541),KTAB19(1)),(KTAB(571),KTAB20(1))
      EQUIVALENCE (KTAB(601),KTAB21(1)),(KTAB(631),KTAB22(1))
      EQUIVALENCE (KTAB(661),KTAB23(1)),(KTAB(691),KTAB24(1))
      EQUIVALENCE (KTAB(721),KTAB25(1)),(KTAB(751),KTAB26(1))
      EQUIVALENCE (KTAB(781),KTAB27(1)),(KTAB(811),KTAB28(1))
      EQUIVALENCE (KTAB(841),KTAB29(1)),(KTAB(871),KTAB30(1))
      DATA NT,NP/30,30/
      DATA TABT/     3.500, 3.525, 3.550, 3.575, 3.600, 3.625, 3.650,
     1 3.675, 3.700, 3.725, 3.750, 3.775, 3.800, 3.825, 3.850, 3.875,
     2 3.900, 3.925, 3.950, 3.975, 4.000, 4.050, 4.100, 4.150, 4.200,
     3 4.250, 4.300, 4.350, 4.400, 4.450/
      DATA TABP/    -2.000,-1.500,-1.000, -.500, 0.000,  .500, 1.000,
     1 1.250, 1.500, 1.750, 2.000, 2.250, 2.500, 2.750, 3.000, 3.200,
     2 3.400, 3.600, 3.800, 4.000, 4.200, 4.400, 4.600, 4.800, 5.000,
     3 5.200, 5.400, 5.600, 5.800, 6.000/
 DATA KTAB01/                                                   -2.000
1-4282,-4245,-4166,-3949,-3612,-3220,-2804,-2383,-1967,-1564,   -2.000
2-1187, -865, -661, -585, -566, -563, -563, -564, -563, -558,   -2.000
3 -541, -521, -519, -519, -520, -520, -518, -490, -480, -479/   -2.000
 DATA KTAB02/                                                   -1.500
1-4287,-4248,-4198,-4055,-3772,-3410,-3015,-2608,-2200,-1799,   -1.500
2-1414,-1060, -776, -618, -566, -556, -557, -559, -560, -560,   -1.500
3 -551, -522, -518, -518, -518, -519, -519, -500, -481, -479/   -1.500
 DATA KTAB03/                                                   -1.000
1-4298,-4246,-4206,-4122,-3906,-3583,-3212,-2821,-2424,-2029,   -1.000
2-1641,-1271, -938, -691, -571, -539, -538, -544, -549, -553,   -1.000
3 -553, -526, -517, -515, -515, -517, -518, -510, -483, -479/   -1.000
 DATA KTAB04/                                                    -.500
1-4310,-4235,-4195,-4145,-4003,-3731,-3389,-3018,-2635,-2247,    -.500
2-1860,-1481,-1121, -809, -597, -508, -494, -504, -518, -530,    -.500
3 -538, -528, -513, -512, -511, -512, -514, -513, -489, -479/    -.500
 DATA KTAB05/                                                    0.000
1-4309,-4205,-4154,-4120,-4041,-3836,-3531,-3185,-2820,-2444,    0.000
2-2060,-1676,-1300, -948, -656, -476, -415, -418, -442, -469,    0.000
3 -492, -513, -502, -504, -504, -503, -506, -509, -496, -479/    0.000
 DATA KTAB06/                                                     .500
1-4276,-4136,-4061,-4031,-3995,-3867,-3613,-3296,-2953,-2594,     .500
```

```
2-2221,-1839,-1454,-1078, -733, -462, -311, -275, -298, -340,       .500
3 -384, -451, -469, -482, -490, -491, -491, -496, -496, -477/       .500
 DATA KTAB07/                                                      1.000
1-4202,-4018,-3905,-3857,-3842,-3784,-3598,-3317,-2999,-2662,      1.000
2-2308,-1937,-1555,-1169, -795, -462, -213,  -90,  -78, -122,      1.000
3 -185, -309, -386, -424, -455, -468, -469, -472, -479, -470/      1.000
 DATA KTAB08/                                                      1.250
1-4146,-3940,-3804,-3739,-3723,-3691,-3546,-3287,-2981,-2656,      1.250
2-2313,-1952,-1577,-1193, -813, -460, -173,    2,   52,   18,      1.250
3  -48, -200, -313, -373, -422, -447, -454, -456, -463, -460/      1.250
 DATA KTAB09/                                                      1.500
1-4074,-3849,-3691,-3605,-3579,-3564,-3461,-3230,-2938,-2623,      1.500
2-2291,-1942,-1576,-1198, -818, -453, -137,   87,  186,  176,      1.500
3  111,  -63, -214, -303, -374, -416, -433, -437, -442, -444/      1.500
 DATA KTAB10/                                                      1.750
1-3986,-3746,-3565,-3458,-3417,-3409,-3344,-3147,-2872,-2567,      1.750
2-2245,-1907,-1553,-1185, -809, -440, -103,  161,  313,  341,      1.750
3  290,  101,  -86, -211, -306, -371, -403, -412, -417, -422/      1.750
 DATA KTAB11/                                                      2.000
1-3881,-3631,-3430,-3301,-3242,-3232,-3197,-3040,-2785,-2491,      2.000
2-2178,-1851,-1510,-1153, -786, -418,  -70,  224,  426,  503,      2.000
3  478,  288,   69,  -94, -217, -308, -359, -381, -388, -393/      2.000
 DATA KTAB12/                                                      2.250
1-3761,-3505,-3288,-3139,-3060,-3040,-3025,-2911,-2681,-2399,      2.250
2-2096,-1778,-1449,-1105, -749, -387,  -36,  279,  520,  650,      2.250
3  664,  492,  251,   47, -104, -225, -300, -337, -352, -358/      2.250
 DATA KTAB13/                                                      2.500
1-3627,-3372,-3142,-2973,-2875,-2841,-2835,-2760,-2562,-2296,      2.500
2-2001,-1693,-1374,-1043, -700, -347,    1,  327,  598,  776,      2.500
3  839,  706,  453,  215,   32, -118, -220, -279, -305, -315/      2.500
 DATA KTAB14/                                                      2.750
1-3481,-3231,-2993,-2807,-2691,-2639,-2632,-2591,-2430,-2182,      2.750
2-1897,-1597,-1288, -970, -639, -299,   43,  372,  663,  880,      2.750
3  994,  922,  671,  406,  194,   13, -119, -201, -245, -263/      2.750
 DATA KTAB15/                                                      3.000
1-3324,-3085,-2844,-2644,-2508,-2439,-2424,-2405,-2285,-2060,      3.000
2-1787,-1496,-1196, -888, -570, -242,   90,  417,  718,  964,      3.000
3 1123, 1132,  897,  616,  377,  170,    7, -102, -167, -199/      3.000
 DATA KTAB16/                                                      3.200
1-3192,-2964,-2724,-2515,-2366,-2282,-2256,-2247,-2158,-1956,      3.200
2-1695,-1410,-1117, -818, -509, -192,  132,  454,  758, 1019,      3.200
3 1209, 1290, 1080,  793,  536,  314,  127,   -4,  -88, -134/      3.200
 DATA KTAB17/                                                      3.400
1-3055,-2839,-2603,-2389,-2226,-2128,-2090,-2084,-2023,-1847,      3.400
2-1599,-1323,-1036, -744, -445, -137,  177,  493,  797, 1067,      3.400
3 1281, 1434, 1262,  977,  704,  471,  264,  110,    6,  -56/      3.400
 DATA KTAB18/                                                      3.600
1-2916,-2710,-2481,-2264,-2090,-1978,-1927,-1917,-1878,-1732,      3.600
2-1499,-1232, -953, -667, -376,  -78,  226,  534,  835, 1111,      3.600
3 1341, 1563, 1440, 1164,  880,  638,  416,  242,  118,   37/      3.600
 DATA KTAB19/                                                      3.800
1-2774,-2578,-2358,-2140,-1957,-1831,-1767,-1749,-1726,-1609,      3.800
2-1396,-1139, -867, -589, -305,  -16,  279,  578,  874, 1151,      3.800
3 1392, 1674, 1610, 1351, 1062,  812,  581,  390,  247,  148/      3.800
 DATA KTAB20/                                                      4.000
1-2632,-2443,-2233,-2017,-1827,-1689,-1610,-1583,-1568,-1480,      4.000
2-1289,-1044, -779, -508, -232,   48,  335,  625,  914, 1190,      4.000
3 1438, 1768, 1770, 1538, 1248,  991,  757,  552,  393,  277/      4.000
 DATA KTAB21/                                                      4.200
1-2489,-2306,-2105,-1894,-1700,-1551,-1458,-1419,-1405,-1342,      4.200
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2-1176, -945, -690, -425, -157,  115,  393,  675,  957, 1229,        4.200
3 1460, 1846, 1916, 1720, 1436, 1173,  938,  725,  554,  423/        4.200
 DATA KTAB22/                                                        4.400
1-2347,-2167,-1976,-1771,-1575,-1416,-1311,-1259,-1241,-1198,        4.400
2-1058, -844, -598, -341,  -79,  185,  455,  728, 1002, 1269,        4.400
3 1519, 1912, 2046, 1897, 1625, 1357, 1124,  906,  725,  583/        4.400
 DATA KTAB23/                                                        4.600
1-2206,-2027,-1844,-1646,-1452,-1286,-1168,-1103,-1078,-1047,        4.600
2 -934, -738, -503, -254,    0,  258,  519,  784, 1049, 1310,        4.600
3 1558, 1968, 2158, 2065, 1812, 1543, 1311, 1093,  906,  755/        4.600
 DATA KTAB24/                                                        4.800
1-2067,-1887,-1710,-1520,-1329,-1158,-1029, -951, -917, -892,        4.800
2 -804, -629, -406, -165,   81,  332,  586,  842, 1099, 1353,        4.800
3 1597, 2016, 2253, 2220, 1996, 1730, 1498, 1283, 1092,  935/        4.800
 DATA KTAB25/                                                        5.000
1-1929,-1747,-1574,-1393,-1206,-1033, -895, -804, -759, -735,        5.000
2 -667, -515, -306,  -74,  165,  409,  655,  903, 1152, 1399,        5.000
3 1637, 2060, 2332, 2361, 2175, 1917, 1684, 1475, 1282, 1121/        5.000
 DATA KTAB26/                                                        5.200
1-1794,-1608,-1437,-1264,-1082, -909, -765, -662, -605, -577,        5.200
2 -525, -396, -203,   18,  251,  487,  726,  967, 1208, 1447,        5.200
3 1680, 2101, 2399, 2484, 2345, 2103, 1870, 1666, 1475, 1312/        5.200
 DATA KTAB27/                                                        5.400
1-1660,-1470,-1300,-1133, -958, -787, -637, -525, -456, -421,        5.400
2 -379, -272,  -96,  114,  339,  568,  800, 1033, 1266, 1498,        5.400
3 1724, 2140, 2457, 2591, 2504, 2285, 2055, 1855, 1669, 1504/        5.400
 DATA KTAB28/                                                        5.600
1-1528,-1335,-1163,-1000, -833, -665, -513, -392, -312, -268,        5.600
2 -230, -142,   14,  213,  430,  652,  876, 1102, 1328, 1552,        5.600
3 1771, 2180, 2507, 2682, 2649, 2462, 2239, 2043, 1862, 1699/        5.600
 DATA KTAB29/                                                        5.800
1-1397,-1201,-1027, -867, -706, -543, -390, -263, -172, -119,        5.800
2  -80,   -8,  129,  315,  523,  738,  955, 1174, 1392, 1609,        5.800
3 1821, 2221, 2553, 2759, 2779, 2631, 2421, 2228, 2054, 1693/        5.800
 DATA KTAB30/                                                        6.000
1-1268,-1069, -892, -733, -578, -420, -268, -137,  -37,   25,        6.000
2   67,  128,  248,  420,  619,  826, 1037, 1248, 1460, 1669,        6.000
3 1874, 2263, 2596, 2825, 2892, 2789, 2600, 2411, 2244, 2088/        6.000
         DATA ISTART/0/
         EXP10(X)=EXP(X*2.30258509299405E0)
         IF(ISTART.EQ.1)GO TO 19
         ISTART=1
         DO 13 IP=1,NP
         DO 13 IT=1,NT
      13 TABKAP(IT,IP)=FLOAT(KTAB(IT,IP))/1000.
      19 DLGTAU=ALOG(TAU(2)/TAU(1))
         PLOG3=0.
         PLOG2=0.
         PLOG1=0.
         DPLOG2=0.
         DPLOG1=0.
   C     ASSUME CONSTANT OPACITY NEAR SURFACE.  FIRST GUESS=.1
         ABSTD(1)=.1
         DO 22 J=1,NUMTAU
         DO 24 IP=1,NP
         IDUM=MAP1(TABT,TABKAP(1,IP),NT,ALOG10(T(J)),PKAP(IP),1)
      24 CONTINUE
         IF(J.EQ.1)PLOG=ALOG(GRAV/ABSTD(1)*TAU(1))
         IF(J.GT.1.AND.J.LE.4)PLOG=PLOG1+DPLOG1
         IF(J.GT.4)PLOG=(3.*PLOG4+8.*DPLOG1-4.*DPLOG2+8.*DPLOG3)/3.
         ERROR=1.
```

```
      GO TO 21
   20 IF(J.EQ.1)PNEW=ALOG(GRAV/ABSTD(1)*TAU(1))
      IF(J.GT.1.AND.J.LE.4)PNEW=(PLOG+2.*PLOG1+DPLOG+DPLOG1)/3.
      IF(J.GT.4)PNEW=(126.*PLOG1-14.*PLOG3+9.*PLOG4+42.*DPLOG+
     1 108.*DPLOG1-54.*DPLOG2+24.*DPLOG3)/121.
      ERROR=ABS(PNEW-PLOG)
      PLOG=PNEW
   21 PTOTAL(J)=EXP(PLOG)
      P(J)=PTOTAL(J)-PRAD(J)-PTURB(J)
      IDUM=MAP1(TAUP,PKAP,NP,ALOG10(P(J)),ABSTD(J),1)
      ABSTD(J)=EXP10(ABSTD(J))
      DPLOG=GRAV/ABSTD(J)*TAU(J)/PTOTAL(J)*DLGTAU
      IF(ERROR.GT..00005)GO TO 20
      PLOG4=PLOG3
      PLOG3=PLOG2
      PLOG2=PLOG1
      PLOG1=PLOG
      DPLOG3=DPLOG2
      DPLOG2=DPLOG1
      DPLOG1=DPLOG
   22 CONTINUE
      RETURN
      END



      SUBROUTINE POPS(CODE,MODE,NUMBER)
      DIMENSION NUMBER(40,1)
      REAL NUMBER
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /XABUND/XABUND(99),WTMOLE
      DATA ITEMP1/0/
      IF(IFMOL.EQ.1)GO TO 200
      IF(IFPRES.EQ.1.AND.ITEMP.NE.ITEMP1)CALL NELECT
      ITEMP1=ITEMP
      IF(CODE.EQ.0)RETURN
      IF(CODE.LT.100.)GO TO 110
      WRITE(6,106)
  106 FORMAT(14H1MOLECULES OFF)
      CALL EXIT
  110 IZ=CODE
      NION=(CODE-FLOAT(IZ))*100.+1.5
      DO 115 J=1,NRHOX
      CALL PFSAHA(J,IZ,NION,MODE,NUMBER)
C     PFSAHA RETURNS IONIZATION FRACTIONS OR IONIZATION FRACTIONS/
C        PARTITION FUNCTIONS SO CONVERT TO NUMBER DENSITIES
      NNNN=NION
      IF(MODE.LT.10)NNNN=1
      DO 115 ION=1,NNNN
  115 NUMBER(J,ION)=NUMBER(J,ION)*XNATOM(J)*XABUND(IZ)
      RETURN
  200 IF(IFPRES.EQ.1.AND.ITEMP.NE.ITEMP1)CALL NMOLEC(MODE)
      ITEMP1=ITEMP
      IF(CODE.EQ.0)RETURN
      CALL MOLEC(CODE,MODE,NUMBER)
      RETURN
      END
```

```
      SUBROUTINE NELECT
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /XABUND/XABUND(99),WTMOLE
      DIMENSION ELEC(40),E(10),X(10),MASK(10),NELEMZ(10),NIONZ(10)
      DATA NELEMZ/1,2,6,11,12,13,14,19,20,26/
      DATA NIONZ/1,2,2,2,2,2,2,2,2,2/,NZ/10/
      IF(ITER.LT.NUMITS)GO TO 406
      DO 401 I=1,NZ
      NELEM=NELEMZ(I)
  401 E(I)=ELEM(NELEM)
      WRITE(6,402)(E(I),I=1,NZ),(E(I),I=1,NZ)
  402 FORMAT(1H1////50X22HELECTRON CONTRIBUTIONS/2X,20(4X,A2))
  406 XNE(1)=P(1)/TK(1)/2.
      DO 500 J=1,NRHOX
      IF(J.GT.1)XNE(J)=XNE(J-1)*P(J)/P(J-1)
      XNTOT=P(J)/TK(J)
      XNATOM(J)=XNTOT-XNE(J)
      DO 1 I=1,NZ
    1 MASK(I)=1
      DO 20 L=1,200
      XNENEW=0.
      DO 11 I=1,NZ
      IF(MASK(I).EQ.0)GO TO 11
      IZ=NELEMZ(I)
      NION=NIONZ(I)
      CALL PFSAHA(J,IZ,NION,4,ELEC)
      E(I)=ELEC(J)
      X(I)=ELEC(J)*XNATOM(J)*XABUND(IZ)
      XNENEW=XNENEW+X(I)
   11 CONTINUE
      XNENEW=(XNENEW+XNE(J))/2.
      ERROR=ABS((XNE(J)-XNENEW)/XNENEW)
      XNE(J)=XNENEW
      XNATOM(J)=XNTOT-XNE(J)
      IF(ERROR.LT..0005)GO TO 400
      IF(J.EQ.1)GO TO 20
      X1=.00001*XNE(J)
      IF(ERROR.LT..05)X1=X1*10.
      DO 12 I=1,NZ
      IF(X(I).LT.X1)MASK(I)=0
   12 CONTINUE
   20 CONTINUE
      WRITE(6,250)
  250 FORMAT(22H XNE DOES NOT CONVERGE)
      CALL EXIT
  400 RHO(J)=XNATOM(J)*WTMOLE*1.660E-24
      IF(ITER.LT.NUMITS)GO TO 500
      DO 403 I=1,NZ
  403 X(I)=X(I)/XNE(J)
      WRITE(6,404)J,(X(I),I=1,NZ),(E(I),I=1,NZ)
  404 FORMAT(I3,20F6.3)
  500 CONTINUE
      RETURN
      END
```

```
             SUBROUTINE PFSAHA(J,IZ,NION,MODE,ANSWER)
        C    MODE 1 RETURNS IONIZATION FRACTION /PARTITION FUNCTION
        C    MODE 2 RETURNS IONIZATION FRACTION
        C    MODE 3 RETURNS PARTITION FUNCTION
        C    MODE 4 RETURNS NUMBER OF ELECTRONS PRODUCED
        C    MODE + 10 RETURN ALL IONS TO NION.   MODE ALONE RETURN NION ONLY.
             COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
             COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
             COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
             DIMENSION ANSWER(40,6),F(6),IP(6),PART(6),POTLO(6),LOCZ(29)
             REAL IP
             DIMENSION SCALE(4)
             DIMENSION NNN(6,353)
             DIMENSION NNN01(54),NNN02(54),NNN03(54),NNN04(54),NNN05(54)
             DIMENSION NNN06(54),NNN07(54),NNN08(54),NNN09(54),NNN10(54)
             DIMENSION NNN11(54),NNN12(54),NNN13(54),NNN14(54),NNN15(54)
             DIMENSION NNN16(54),NNN17(54),NNN18(54),NNN19(54),NNN20(54)
             DIMENSION NNN21(54),NNN22(54),NNN23(54),NNN24(54),NNN25(54)
             DIMENSION NNN26(54),NNN27(54),NNN28(54),NNN29(54),NNN30(54)
             DIMENSION NNN31(54),NNN32(54),NNN33(54),NNN34(54),NNN35(54)
             DIMENSION NNN36(54),NNN37(54),NNN38(54),NNN39(54),NNN40(12)
             EQUIVALENCE (NNN(   1),NNN01(1)),(NNN(  55),NNN02(1))
             EQUIVALENCE (NNN( 109),NNN03(1)),(NNN( 163),NNN04(1))
             EQUIVALENCE (NNN( 217),NNN05(1)),(NNN( 271),NNN06(1))
             EQUIVALENCE (NNN( 325),NNN07(1)),(NNN( 379),NNN08(1))
             EQUIVALENCE (NNN( 433),NNN09(1)),(NNN( 487),NNN10(1))
             EQUIVALENCE (NNN( 541),NNN11(1)),(NNN( 595),NNN12(1))
             EQUIVALENCE (NNN( 649),NNN13(1)),(NNN( 703),NNN14(1))
             EQUIVALENCE (NNN( 757),NNN15(1)),(NNN( 811),NNN16(1))
             EQUIVALENCE (NNN( 865),NNN17(1)),(NNN( 919),NNN18(1))
             EQUIVALENCE (NNN( 973),NNN19(1)),(NNN(1027),NNN20(1))
             EQUIVALENCE (NNN(1081),NNN21(1)),(NNN(1135),NNN22(1))
             EQUIVALENCE (NNN(1189),NNN23(1)),(NNN(1243),NNN24(1))
             EQUIVALENCE (NNN(1297),NNN25(1)),(NNN(1351),NNN26(1))
             EQUIVALENCE (NNN(1405),NNN27(1)),(NNN(1459),NNN28(1))
             EQUIVALENCE (NNN(1513),NNN29(1)),(NNN(1567),NNN30(1))
             EQUIVALENCE (NNN(1621),NNN31(1)),(NNN(1675),NNN32(1))
             EQUIVALENCE (NNN(1729),NNN33(1)),(NNN(1783),NNN34(1))
             EQUIVALENCE (NNN(1837),NNN35(1)),(NNN(1891),NNN36(1))
             EQUIVALENCE (NNN(1945),NNN37(1)),(NNN(1999),NNN38(1))
             EQUIVALENCE (NNN(2053),NNN39(1)),(NNN(2107),NNN40(1))
C      ( 1)( 2)   ( 3)( 4)   ( 5)( 6)   ( 7)( 8)   ( 9)(10)   ( IP ) G  REF
             DATA NNN01/
     1 200020001, 200020011, 201620881, 231228281, 378953411,  1359502, D+F 1.00
     2 100010001, 100010001, 100010001, 100010001, 100010001,  1359500, G   1.01
     3 100010001, 100010011, 102111241, 145022061, 363059451,  2458104, D+F 2.00
     4 200020001, 200020071, 208524971, 382669341, 128222452,  5440302, D+F 2.01
     5 100010001, 100010001, 100010001, 100010001, 100010001,  5440300, G   2.02
     6 200020011, 201220481, 212922881, 258731081, 394251691,   538901, D+F 3.00
     7 100010001, 100010201, 126225521,  67216512, 351165562,  7561907, D+F 3.01
     8 200020001, 200020211, 227936571,  69610342, 137217102, 12241800, D+F 3.02
     9 100010001, 100010001, 100010001, 100010001, 100010001, 12241800/ G   3.03
             DATA NNN02/
     1 100010051, 104311441, 131615641, 190623681, 298037691,   931900, AEL 4.00
     2 200120231, 211422771, 249627631, 309034911, 398545051,  1820600, AEL 4.01
     3 100010001, 100010201, 126225521,  67216512, 351165562, 15385000, AEL 4.02
     4 200020001, 200020011, 201220661, 223426161, 332644691, 21765700, AEL 4.03
     5 600060001, 600560281, 608761991, 637466191, 693973361,   829500, AEL 5.00
     6 100310831, 132016901, 214226411, 315736741, 419147071,  2514900, AEL 5.01
     7 200721061, 233526401, 297533311, 369040481, 440747651,  3792000, AEL 5.02
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8 100010001, 100010001, 100010001, 100010001, 100010001, 25929800, G   5.03
9 893292271,  96110042, 105311262, 126315202, 196126432,  1125508/ D+F 6.00
        DATA NNN03/
1 595060251, 620865751, 713280191,  95712292, 167623542,  2437501, D+F 6.01
2 105513201, 180324851, 341851341,  68416332, 296550722,  4787101, D+F 6.02
3 204922771, 262630421, 350941931, 494556971, 644872001,  6447600, D+F 6.03
4 403141851, 457051681, 594071181,  92913362, 203331152,  1452915, D+F 7.00
5 919899541, 107211512, 124914302, 182526232, 403762662,  2959202, D+F 7.01
6 596862721, 684177081,  88110342, 128317062, 239334312,  4742501, D+F 7.02
7 112816481, 240733751, 462068491, 116419932, 283736822,  7744900, D+F 7.03
8 210124681, 293634211, 391145791, 539862151, 703178471,  9786200, D+F 7.04
9 874789691, 924795711,  99410492, 115213492, 169022242,  1361307/ D+F 8.00
        DATA NNN04/
1 424151091, 622874781,  91312832, 221842502,  79914013,  3510711, D+F 8.01
2  95610702, 118113032, 149619922, 329761642, 101914173,  5488500, D+F 8.02
3 603567171, 775391141, 106612482, 143716252, 181420032,  7739300, D+F 8.03
4 124420321, 306943181, 606281181, 101712232, 142916342, 11387300, D+F 8.04
5 215026541, 323137551, 421546491, 508255151, 594863811, 13807900, AEL 8.05
6 575958511, 589859231, 595860671, 636470031, 815199581,  1741802, D+F 9.00
7 900296401, 102610802, 113912542, 152921152, 318348952,  3498003, D+F 9.01
8 469162651, 791295541, 121419552, 402686872, 154822203,  6264500, D+F 9.02
9  99511422, 129214572, 170523002, 320140922, 498458762,  8713900/ D+F 9.03
        DATA NNN05/
1 615472711,  87710602, 127215002, 172919582, 218624152, 11421300, D+F 9.04
2 135324181, 377252001, 661580261,  94410852, 122613672, 15711700, AEL 9.05
3 100010001, 100010051, 105313051, 210239461,  74013022,  2155808, D+F10.00
4 580158751, 591759741, 642687101, 159332652,  64111533,  4106907, D+F10.01
5  93510272, 110411662, 127116062, 257647882,  75110223,  6350000, D+F10.02
6 529774371,  94611322, 135816202, 188221442, 240626682,  9701900, D+F10.03
7 103312152, 140616092, 181320182, 222224262, 263128352, 12630000, AEL10.04
8 629178711,  98311802, 136715512, 173619202, 210422892, 15790900, AEL10.05
9 200020001, 200320211, 207322131, 253031421, 417657451,   513802/ D+F11.00
        DATA NNN06/
1 100010001, 100010161, 119621261,  50711872, 246445382,  4728901, D+F11.01
2 580158751, 591860351,  71813142, 321968812, 106014333,  7165000, D+F11.02
3  96910772, 116012242, 130714232, 153916552, 177118872,  9888000, D+F11.03
4 601386081, 108812932, 148916832, 187820722, 226624612, 13836900, AEL11.04
5 105712442, 144616652, 189221182, 234425702, 279630222, 17209000, AEL11.05
6 100010011, 101410621, 118414581, 204831781, 509479731,   764404, D+F12.00
7 200120051, 202921001, 226926901, 368457091,  92814872,  1503101, D+F12.01
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1 156718872, 279244452, 678196342, 128316243, 197823443,   1205000, AEL69.01
2  93517192, 364666132, 103414613, 192624193, 293334613,   2370000, AEL69.02
3 100010011, 101310651, 118613951, 169120661, 250629971,    625000, AEL70.00
4 200120901, 270345231,  81714042, 223533112, 461959862,   1217000, AEL70.01
5 100312561, 250851931,  91914182, 198626022, 323638692,   2000000, AEL70.02
6 514664441, 759086851,  99211442, 133315612, 182721252,    609900, AEL71.00
7 125924831, 438667801,  98714112, 199727872, 380850742,   1389900, AEL71.01
8 323948621, 661297271, 158626482, 426865032,  93712843,   1900000, AEL71.02
9 659294081, 128016962, 222528952, 372047062, 585171462,    700000/ AEL72.00
        DATA NNN31/
1  99117882, 274638812, 520867322,  84410313, 123314453,   1489900, AEL72.01
2 187427702, 343739872, 448049452, 539358282, 625266642,   2329900, AEL72.02
3  65210892, 171325762, 373552252, 705192012, 116414343,    787900, AEL73.00
4 192837842, 600784802, 111113823, 165419233, 218524383,   1620000, AEL73.01
5  99117872, 274638812, 520867312,  84410313, 123314453,   2400000, FAK73.02
6 398981651, 130019172, 273438022, 516168382,  88411163,    797900, AEL74.00
7 131429482, 523279952, 111414623, 183422233, 262130233,   1770000, AEL74.01
8 192837842, 600784792, 111113823, 165419233, 218524383,   2500000, FAK74.02
9 600963001,  75910412, 150121572, 301940972, 539168952,    787000/ AEL75.00
        DATA NNN32/
1  73710852, 190731262, 464964142,  83810503, 127315053,   1660000, AEL75.01
2 131429482, 523279952, 111414623, 183422233, 262130233,   2600000, FAK75.02
3 110815502, 216829732, 398752322, 672484682, 104612673,    850000, AEL76.00
4 168225972, 362046562, 566766422, 757484612,  93010103,   1700000, AEL76.01
5  73710852, 190731262, 464964142,  83810503, 127315053,   2700000, FAK76.02
6 129117892, 239430882, 388748292, 596173252,  89510843,    910000, AEL77.00
7 110815502, 216829732, 398752322, 672484682, 104612673,   2000000, FAK77.01
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                                                                  PAGE 45
8 168225972, 362046562, 566766422, 757484612,  93010103,  2800000, FAK77.02
9 158918512, 207523002, 254328242, 316335762, 407246582,   900000/ AEL78.00
        DATA NNN33/
1  98115462, 224930742, 401150612, 623475412,  89910583,  1855900, AEL78.01
2 110815502, 216829732, 398752322, 672484682, 104612673,  2900000, FAK78.02
3 203222611, 265731251, 364042301, 494958601, 702084731,   922000, AEL79.00
4 120521331, 357753801,  75310062, 130516572, 206925452,  2050000, AEL79.01
5 651780821, 108814772, 195925252, 316338622, 460853882,  3000000, AEL79.02
6 100010001, 100110111, 105211851, 152122101, 341552811,  1043002, D+F80.00
7 200320211, 210023021, 268834231, 480472341, 111416912,  1875000, D+F80.01
8 104012871, 186129471, 458664151,  82410072, 119013732,  3420000, D+F80.02
9 200420711, 222424271, 265429161, 325637371, 442853911,   610500/ AEL81.00
        DATA NNN34/
1 100010021, 101910801, 121414641, 189525811, 358949721,  2041900, AEL81.01
2 200020311, 216624611, 296337451, 489064791,  85711212,  2979900, AEL81.02
3 103411711, 147819101, 244331781, 434862751,  93113762,   741404, D+F82.00
4 204122231, 248227841, 311535621, 429153941, 651976431,  1502800, D+F82.01
5 100210131, 106812201, 154522671, 381665951,  95512512,  3192900, D+F82.02
6 400140351, 416944121, 474851591, 564362181, 690477231,   728700, AEL83.00
7 106814451, 204427341, 350744811, 586879131, 108314772,  1667900, AEL83.01
8 205523051, 264830231, 345439921, 469156001, 675281671,  2555900, AEL83.02
9 500950661, 518153561, 559058941, 628968071, 748483501,   843000/ AEL84.00
        DATA NNN35/
1 443756241, 696282451,  95411012, 128615262, 182922012,  1900000, FAK84.01
2 336953201, 682481011,  93810882, 127915272, 184622442,  2700000, FAK84.02
3 402841621, 431544771, 463148311, 520059491, 734896851,   930000, FAK85.00
4 576168741, 788387631,  96910642, 116012552, 135014462,  2000000, FAK85.01
5 490265341, 812797201, 116614322, 179622692, 285035302,  2900000, FAK85.02
6 100010001, 100010031, 102311051, 133018071, 264539391,  1074500, AEL86.00
7 402841621, 431544771, 463148311, 520059491, 734996851,  2000000, FAK86.01
8 576168741, 788387631,  96910642, 116012552, 135014462,  3000000, FAK86.02
9 200020011, 201220591, 218124481, 296538611, 488859141,   400000/ FAK87.00
        DATA NNN36/
1 100010001, 100010031, 102311051, 133018071, 264539401,  2200000, FAK87.01
2 421645151, 477449611, 511852711, 542455761, 572958821,  3300000, FAK87.02
3 100010041, 105212131, 153220271, 270435641, 460258111,   527600, AEL88.00
4 201221791, 258131471, 381645781, 546365131, 777592781,  1014400, AEL88.01
5 100010001, 100010031, 102311051, 133018071, 264539391,  3400000, FAK88.02
6 510064491,  82710872, 142718412, 232328712, 348341572,   690000, AEL89.00
7 228951571,  88513232, 183324132, 305537492, 448152402,  1210000, AEL89.01
8 723989131, 103511752, 130814352, 155416652, 177018682,  2000000, AEL89.02
9 620099241, 162725772, 391457072,  80110833, 141818023,   600000/ AEL90.00
        DATA NNN37/
1 620099241, 162725772, 391457072,  80110833, 141818023,  1200000, FAK90.01
2 620099251, 162725772, 391457072,  80110833, 141818023,  2000000, FAK90.02
3 347877992, 129318323, 240730533, 380546863, 570368573,   600000, AEL91.00
4 347877992, 129318323, 240730533, 380546863, 570368573,  1200000, FAK91.01
5 347777992, 129318323, 240730533, 380546863, 570368573,  2000000, FAK91.02
6 209530092, 450866762,  96613623, 186524763, 318839893,   600000, AEL92.00
7 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK92.01
8 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK92.02
9 209530092, 450866762,  96613623, 186524763, 318839893,   600000/ FAK93.00
        DATA NNN38/
1 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK93.01
2 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK93.02
3 209530092, 450866762,  96613623, 186524763, 318839893,   600000, FAK94.00
4 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK94.01
5 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK94.02
6 209530092, 450866762,  96613623, 186524763, 318839893,   600000, FAK95.00
7 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK95.01
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8 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK95.02
9 209530092, 450866762,  96613623, 186524763, 318839893,   600000/ FAK96.00
        DATA NNN39/
1 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK96.01
2 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK96.02
3 209530092, 450866762,  96613623, 186524763, 318839893,   600000, FAK97.00
4 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK97.01
5 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK97.02
6 209530092, 450866762,  96613623, 186524763, 318839893,   600000, FAK98.00
7 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK98.01
8 209530092, 450866762,  96613623, 186524763, 318839893,  2000000, FAK98.02
9 209530092, 450866762,  96613623, 186524763, 318839893,   600000/ FAK99.00
        DATA NNN40/
1 209530092, 450866762,  96613623, 186524763, 318839893,  1200000, FAK99.01
2 209530092, 450866762,  96613623, 186524763, 318839893,  2000000/ FAK99.02
        DATA LOCZ/1,3,6,10,14,18,22,27,33,39,45,51,57,63,69,75,81,86,91,
       196,101,106,111,116,121,126,131,136,141/
        DATA SCALE/.001,.01,.1,1./
  C
        MODE1=MODE
        IF(MODE1.GT.10)MODE1=MODE1-10
  C     LOWERING OF THE IONIZATION POTENTIAL IN VOLTS FOR UNIT ZEFF
        CHARGE=XNE(J)*2.
        EXCESS=2.*XNE(J)-P(J)/TK(J)
  C     ALLOWANCE FOR DOUBLY IONIZED HELIUM
        IF(EXCESS.GT.0.)CHARGE=CHARGE-EXCESS+(2.*EXCESS)*4.
        DEBYE=SQRT(TK(J)/2.8965E-18/CHARGE)
  C     DEBYE=SQRT(TK(J)/12.5664/4.801E-10**2/CHARGE)
        POTLOW=AMIN1(1.,1.44E-7/DEBYE)
        TV=TKEV(J)
        IF(IZ.LE.28)N=LOCZ(IZ)
        IF(IZ.GT.28)N=3*IZ+54
        IF(IZ.LE.28)NIONS=LOCZ(IZ+1)-N
        IF(IZ.GT.28)NIONS=3
        NION2=MIN0(NION+2,NIONS)
        N=N-1
  C
        DO 18 ION=1,NION2
        Z=ION
        POTLO(ION)=POTLOW*Z
        N=N+1
        NNN100=NNN(6,N)/100
        IP(ION)=FLOAT(NNN100)/1000.
        G=NNN(6,N)-NNN100*100
        IF(N.EQ.1)GO TO 16
        T2000=IP(ION)*2000./11.
        IT=MAX0(1,MIN0(9,IFIX(T(J)/T2000-.5)))
        DT=T(J)/T2000-FLOAT(IT)-.5
        PMIN=1.
        I=(IT+1)/2
        K1=NNN(I,N)/100000
        K2=NNN(I,N)-K1*100000
        K3=K2/10
        KSCALE=K2-K3*10
        IF(MOD(IT,2).EQ.0)GO TO 12
        P1=FLOAT(K1)*SCALE(KSCALE)
        P2=FLOAT(K3)*SCALE(KSCALE)
        IF(DT.GE.0.)GO TO 13
        IF(KSCALE.GT.1)GO TO 13
        KP1=P1
```

```
      IF(KP1.NE.IFIX(P2+.5))GO TO 13
      PMIN=KP1
      GO TO 13
   12 P1=FLOAT(K3)*SCALE(KSCALE)
      K1=NNN(I+1,N)/100000
      KSCALE=MOD(NNN(I+1,N),10)
      P2=FLOAT(K1)*SCALE(KSCALE)
   13 PART(ION)=AMAX1(PMIN,P1+(P2-P1)*DT)
      IF(G.EQ.0..OR.POTLO(ION).LT..1.OR.T(J).LT.T2000*4.)GO TO 18
      IF(T(J).GT.(T2000*11.))TV=(T2000*11.)*8.6171E-5
      D1=.1/TV
   14 D2=POTLO(ION)/TV
      PART(ION)=PART(ION)+G*EXP(-IP(ION)/TV)*(SQRT(13.595*Z*Z/TV/D2)**3*
     1(1./3.+(1.-(.5+(1./18.+D2/120.)*D2)*D2)*D2)-
     2SQRT(13.595*Z*Z/TV/D1)**3*
     3(1./3.+(1.-(.5+(1./18.+D1/120.)*D1)*D1)*D1))
      TV=TKEV(J)
      GO TO 18
   16 PART(1)=2.*BHYD(J,1)
      IF(T(J).LT.9000.)GO TO 18
      PART(1)=PART(1)+8.*BHYD(J,2)*EXP(-10.196/TV)+18.*BHYD(J,3)*
     1EXP(-12.084/TV)+32.*BHYD(J,4)*EXP(-12.745/TV)+50.*BHYD(J,5)*
     2EXP(-13.051/TV)+72.*BHYD(J,6)*EXP(-13.217/TV)
      D1=13.595/6.5/6.5/TV
      D2=POTLO(1)/TV
      GO TO 14
   18 CONTINUE
C
   19 IF(MODE1.EQ.3)GO TO 35
C
      N=N-NION2
      CF=2.*2.4148E15*T(J)*SQRT(T(J))/XNE(J)
      DO 20 ION=2,NION2
      N=N+1
C     THE AMIN IS FOR ANY UNFORTUNATE WHO HAS A 360
   20 F(ION)=CF*PART(ION)/PART(ION-1)*
     1EXP(-AMIN1((IP(ION-1)-POTLO(ION-1))/TV,100.))
      F(1)=1.
      L=NION2+1
      DO 21 ION=2,NION2
      L=L-1
   21 F(1)=1.+F(L)*F(1)
      F(1)=1./F(1)
      DO 22 ION=2,NION2
   22 F(ION)=F(ION-1)*F(ION)
C
   35 IF(MODE.LT.10)GO TO 40
      GO TO(23,25,27,29),MODE1
   23 DO 24 ION=1,NION
   24 ANSWER(J,ION)=F(ION)/PART(ION)
      RETURN
   25 DO 26 ION=1,NION
   26 ANSWER(J,ION)=F(ION)
      RETURN
   27 DO 28 ION=1,NION
   28 ANSWER(J,ION)=PART(ION)
      RETURN
   29 ANSWER(J,1)=0.
      DO 30 ION=2,NION2
   30 ANSWER(J,1)=ANSWER(J,1)+F(ION)*FLOAT(ION-1)
```

```
      RETURN
   40 GO TO(41,42,43,29),MODE1
   41 ANSWER(J,1)=F(NION)/PART(NION)
      RETURN
   42 ANSWER(J,1)=F(NION)
      RETURN
   43 ANSWER(J,1)=PART(NION)
      RETURN
      END


      SUBROUTINE MOLEC(CODOUT,MODE,NUMBER)
      DIMENSION NUMBER(40,1)
      REAL NUMBER
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /XABUND/XABUND(99),WTMOLE
      COMMON NUMMOL,CODE(100),XNMOL(40,100)
      DATA IREAD/0/
      IF(IREAD.EQ.1)GO TO 200
      IF(IFPRES.EQ.1)GO TO 200
      READ(5,151)NUMMOL
  151 FORMAT(I5)
      DO 155 JMOL=1,NUMMOL
      READ(5,152)CODE(JMOL)
  152 FORMAT(F20.2)
      READ(5,153)(XNMOL(J,JMOL),J=1,NRHOX)
  153 FORMAT(1P8E10.3)
C 153 FORMAT(0P8E10.3)
      WRITE(6,154)CODE(JMOL),(XNMOL(J,JMOL),J=1,NRHOX)
  154 FORMAT(F20.2/(1P8E10.3))
C 154 FORMAT(F20.2/(0P8E10.3))
  155 CONTINUE
      READ(5,158)
      READ(5,158)(XNATOM(J),RHO(J),J=1,NRHOX)
      WRITE(6,158)(XNATOM(J),RHO(J),J=1,NRHOX)
  158 FORMAT(1P8E10.3)
C 158 FORMAT(0P8E10.3)
      IREAD=1
  200 IF(CODOUT.LT.100.)GO TO 300
      DO 201 JMOL=1,NUMMOL
      IF(CODE(JMOL).EQ.CODOUT)GO TO 203
  201 CONTINUE
      WRITE(6,202)CODOUT
  202 FORMAT(22H1BETTER LUCK NEXT TIMEF20.2)
      CALL EXIT
  203 DO 204 J=1,NRHOX
  204 NUMBER(J,ION)=XNMOL(J,JMOL)
      RETURN
  300 C=CODOUT
      NN=1
      IF(MODE.EQ.11)NN=(C-FLOAT(IFIX(C)))*100.+1.5
      DO 321 I=1,NN
      DO 301 JMOL=1,NUMMOL
      ION=NN-I+1
```

```
      IF(CODE(JMOL)+.001.GT.C.AND.CODE(JMOL)-.001.LT.C)GO TO 303
  301 CONTINUE
      GO TO 305
  303 DO 304 J=1,NRHOX
  304 NUMBER(J,ION)=XNMOL(J,JMOL)
      GO TO 321
  305 ID=CODOUT
      DO 311 JMOL=1,NUMMOL
      IF(IFIX(CODE(JMOL)).EQ.ID)GO TO 313
  311 CONTINUE
      GO TO 400
  313 DO 314 J=1,NRHOX
  314 NUMBER(J,ION)=0.
  321 C=C-.01
      RETURN
  400 ION=(CODOUT-FLOAT(ID))*100.+1.5
      NN=ION
      IF(MODE.EQ.1)NN=1
      DO 401 J=1,NRHOX
      CALL PFSAHA(J,ID,ION,MODE,NUMBER)
      DO 401 I=1,NN
  401 NUMBER(J,I)=NUMBER(J,I)*XNATOM(J)*XABUND(ID)
      RETURN
      END
```

```
      SUBROUTINE NMOLEC(MODE)
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /XABUND/XABUND(99),WTMOLE
      DIMENSION EQUILJ(100),LOCJ(101),KCOMPS(300)
      DIMENSION XNZ(40,25)
      DIMENSION IFEQUA(101)
      DIMENSION EQUIL(6,100)
      DIMENSION EQ(25),XN(25),XAB(25),DTERM(25),DEQ(625)
      DIMENSION FRAC(40,6)
      EQUIVALENCE (FRAC(1),DEQ(1))
      DIMENSION EQOLD(25)
      DIMENSION IDEQUA(25)
      DIMENSION XCODE(8)
      COMMON NUMMOL,CODE(100),XNMOL(40,100)
      DATA XCODE/1.E14,1.E12,1.E10,1.E8,1.E6,1.E4,1.E2,1.E0/
      DATA IREAD/0/
C     MAKE TABLE OF ALL COMPONENTS OF ALL MOLECULES
C     SAMPLE CODES FOR ATOMS AND MOLECULES
C                     EXTERNAL CODE     INTERNAL COMPONENTS
C     CARBON DIOXIDE    60808.           6,8,8
C     HMINUS            100.             1,100
C     NEUTRAL IRON      26.              26
C     H2PLUS            101.01           1,1,101
C     HYDROGEN ION      1.01             1,101
C     SILICON 3+        14.03            14,101,101,101
      IF(IREAD.EQ.1)GO TO 30
      IREAD=1
      DO 1 JMOL=1,100
      CODE(JMOL)=0.
      DO 1 J=1,NRHOX
    1 XNMOL(J,JMOL)=0.
      WRITE(6,10)
   10 FORMAT(16H1MOLECULES INPUT)
      DO 11 I=1,101
   11 IFEQUA(I)=0
C     IF IFEQUA=1 AN EQUATION MUST BE SET UP FOR ELEMENT I
      KLOC=1
      LOCJ(1)=1
      DO 20 JMOL=1,101
      IF(KLOC.EQ.301)WRITE(6,199)
      READ(5,13)C,E1,E2,E3,E4,E5,E6
   13 FORMAT(F18.2,F7.3,5E11.4)
      IF(C.EQ.0.)GO TO 23
      WRITE(6,14)JMOL,C,E1,E2,E3,E4,E5,E6
   14 FORMAT(I5,F18.2,F7.3,1P5E11.4)
C  14 FORMAT(I5,F18.2,F7.3,0P5E11.4)
      DO 15 II=1,8
      IF(C.GE.XCODE(II))GO TO 16
   15 CONTINUE
      CALL EXIT
   16 X=C
      DO 17 I=II,8
      ID=X/XCODE(I)
      X=X-FLOAT(ID)*XCODE(I)
      IF(ID.EQ.0)ID=100
      IFEQUA(ID)=1
```

```
      KCOMPS(KLOC)=ID
   17 KLOC=KLOC+1
      ION=X*100.+.5
      IF(ION.LT.1)GO TO 19
      IFEQUA(100)=1
      IFEQUA(101)=1
      DO 18 I=1,ION
      KCOMPS(KLOC)=101
   18 KLOC=KLOC+1
   19 LOCJ(JMOL+1)=KLOC
      CODE(JMOL)=C
      EQUIL(1,JMOL)=E1
      EQUIL(2,JMOL)=E2
      EQUIL(3,JMOL)=E3
      EQUIL(4,JMOL)=E4
      EQUIL(5,JMOL)=E5
   20 EQUIL(6,JMOL)=E6
      WRITE(6,199)
  199 FORMAT(19H1TOO MANY MOLECULES)
   23 NUMMOL=JMOL-1
      NLOC=KLOC-1
C     ASSIGN AN EQUATION NUMBER TO EACH COMPONENT
C     THE FIRST EQUATION IS FOR THE TOTAL NUMBER OF PARTICLES
C     THE FIRST VARIABLE IS XNATOM
C     IF ANY COMPONENT IS 100 OR 101 VARIABLE NEQUA IS XNE
C          AND EQUATION NEQUA IS CHARGE CONSERVATION
C     FOR PROGRAMMING CONVENIENCE VARIABLE NEQUA1 IS INVERSE XNE
C     DIMENSIONS ARE SET FOR A MAXIMUM 25 EQUATIONS
      IEQUA=1
      DO 25 I=1,100
      IF(IFEQUA(I).EQ.0)GO TO 25
      IEQUA=IEQUA+1
      IFEQUA(I)=IEQUA
      IDEQUA(IEQUA)=I
   25 CONTINUE
      NEQUA=IEQUA
      NEQUA1=NEQUA+1
      IFEQUA(101)=NEQUA1
      NEQNEQ=NEQUA**2
      DO 28 KLOC=1,NLOC
      ID=KCOMPS(KLOC)
   28 KCOMPS(KLOC)=IFEQUA(ID)
   30 DO 31 K=2,NEQUA
      ID=IDEQUA(K)
      IF(ID.LT.100)XAB(K)=AMAX1(XABUND(ID),1.E-20)
   31 CONTINUE
      IF(ID.EQ.100)XAB(NEQUA)=0.
      XNTOT=P(1)/TK(1)
      XN(1)=XNTOT/2.
      X=XN(1)/10.
      DO 32 K=2,NEQUA
   32 XN(K)=X*XAB(K)
      IF(ID.EQ.100)XN(NEQUA)=X
      XNE(1)=X
      DO 110 J=1,NRHOX
      XNTOT=P(J)/TK(J)
      IF(J.EQ.1)GO TO 34
      RATIO=P(J)/P(J-1)
      XNE(J)=XNE(J-1)*RATIO
      DO 33 K=1,NEQUA
   33 XN(K)=XN(K)*RATIO
```

```
   34 DO 37 JMOL=1,NUMMOL
      NCOMP=LOCJ(JMOL+1)-LOCJ(JMOL)
      IF(EQUIL(1,JMOL).EQ.0.)GO TO 35
      ION=(CODE(JMOL)-FLOAT(IFIX(CODE(JMOL))))*100.+.5
      EQUILJ(JMOL)=EXP(EQUIL(1,JMOL)/TKEV(J)-EQUIL(2,JMOL)+
     1(EQUIL(3,JMOL)+(-EQUIL(4,JMOL)+(EQUIL(5,JMOL)-EQUIL(6,JMOL)*
     2T(J))*T(J))*T(J))*T(J)-1.5*(FLOAT(NCOMP-ION-ION-1))*TLOG(J))
      GO TO 37
   35 IF(NCOMP.GT.1)GO TO 36
      EQUILJ(JMOL)=1.
      GO TO 37
   36 ID=CODE(JMOL)
      ION=NCOMP-1
      CALL PFSAHA(J,ID,NCOMP,12,FRAC)
      EQUILJ(JMOL)=FRAC(J,NCOMP)/FRAC(J,1)*XNE(J)**ION
   37 CONTINUE
      DO 48 K=1,NEQUA
   48 EQOLD(K)=0.
C
C     SET UP 1ST ORDER EQUATIONS FOR THE CHANGE IN NUMBER DENSITY OF
C        EACH ELEMENT.
   50 DO 60 KL=1,NEQNEQ
   60 DEQ(KL)=0.
      EQ(1)=-XNTOT
      K1=1
      KK=1
      DO 61 K=2,NEQUA
      EQ(1)=EQ(1)+XN(K)
      K1=K1+NEQUA
C     K1 IS ACTUALLY 1K
      DEQ(K1)=1.
      EQ(K)=XN(K)-XAB(K)*XN(1)
      KK=KK+NEQUA1
      DEQ(KK)=1.
   61 DEQ(K)=-XAB(K)
      IF(IDEQUA(NEQUA).LT.100)GO TO 62
      EQ(NEQUA)=-XN(NEQUA)
      DEQ(NEQNEQ)=-1.
   62 CONTINUE
      DO 99 JMOL=1,NUMMOL
      NCOMP=LOCJ(JMOL+1)-LOCJ(JMOL)
      IF(NCOMP.EQ.1)GO TO 99
      TERM=EQUILJ(JMOL)
      LOCJ1=LOCJ(JMOL)
      LOCJ2=LOCJ(JMOL+1)-1
      DO 80 LOCK=LOCJ1,LOCJ2
      K=KCOMPS(LOCK)
      IF(K.EQ.NEQUA1)GO TO 79
      TERM=TERM*XN(K)
      GO TO 80
   79 TERM=TERM/XN(NEQUA)
   80 CONTINUE
      EQ(1)=EQ(1)+TERM
      DO 85 LOCK=LOCJ1,LOCJ2
      K=KCOMPS(LOCK)
      IF(K.LT.NEQUA1)GO TO 81
      K=NEQUA
      D=-TERM/XN(K)
      GO TO 82
   81 D=TERM/XN(K)
   82 EQ(K)=EQ(K)+TERM
```

```
      NEQUAK=NEQUA*K-NEQUA
      K1=NEQUAK+1
      DEQ(K1)=DEQ(K1)+D
      DO 83 LOCM=LOCJ1,LOCJ2
      M=KCOMPS(LOCM)
      IF(M.EQ.NEQUA1)M=NEQUA
      MK=M+NEQUAK
   83 DEQ(MK)=DEQ(MK)+D
   85 CONTINUE
   99 CONTINUE
C
      CALL SOLVIT(DEQ,NEQUA,EQ,DTERM)
      IFERR=0
      SCALE=100.
      DO 105 K=1,NEQUA
      RATIO=ABS(EQ(K)/XN(K))
      IF(RATIO.GT..001)IFERR=1
      IF(EQOLD(K)*EQ(K).LT.0.)EQ(K)=EQ(K)*.69
      XNEQ=XN(K)-EQ(K)
      XN100=XN(K)/100.
      IF(XNEQ.LT.XN100)GO TO 101
      XN100=XN(K)*100.
C     IF(XNEQ.GT.XN100)GO TO 102
      XN(K)=XNEQ
      GO TO 105
  101 XN(K)=XN(K)/SCALE
      IF(EQOLD(K)*EQ(K).LT.0.)SCALE=SQRT(SCALE)
      GO TO 105
  102 XN(K)=XN100
  105 EQOLD(K)=EQ(K)
      IF(IFERR.EQ.1)GO TO 50
C
      DO 107 K=1,NEQUA
  107 XNZ(J,K)=XN(K)
      XNATOM(J)=XN(1)
      RHO(J)=XNATOM(J)*WTMOLE*1.660E-24
      IF(IDEQUA(NEQUA).EQ.100)XNE(J)=XN(NEQUA)
      DO 109 JMOL=1,NUMMOL
      NCOMP=LOCJ(JMOL+1)-LOCJ(JMOL)
      XNMOL(J,JMOL)=EQUILJ(JMOL)
      LOCJ1=LOCJ(JMOL)
      LOCJ2=LOCJ(JMOL+1)-1
      DO 109 LOCK=LOCJ1,LOCJ2
      K=KCOMPS(LOCK)
      IF(K.EQ.NEQUA1)GO TO 108
      XNMOL(J,JMOL)=XNMOL(J,JMOL)*XN(K)
      GO TO 109
  108 XNMOL(J,JMOL)=XNMOL(J,JMOL)/XN(NEQUA)
  109 CONTINUE
  110 CONTINUE
      IF(ITER.LT.NUMITS)GO TO 120
      WRITE(6,112)(J,RHOX(J),T(J),P(J),XNE(J),XNATOM(J),RHO(J),
     1J=1,NRHOX)
  112 FORMAT(1H1////11X4HRHOX,9X1HT,11X1HP,10X3HXNE,8X6HXNATOM,8X3HRHO/
     1(I5,1P6E12.3))
C    1(I5,0P6E12.3))
      NN=(NUMMOL/10)*10
      IF(NN.LT.NUMMOL)NN=NN+10
      DO 111 JMOL1=1,NN,10
      JMOL10=JMOL1+9
  111 WRITE(6,113)(CODE(JMOL),JMOL=JMOL1,JMOL10),(J,(XNMOL(J,JMOL),
```

```
     1JMOL=JMOL1,JMOL10),J=1,NRHOX)
  113 FORMAT(1H1////50X26HMOLECULAR NUMBER DENSITIES/5X10F12.2/
     1(I5,1P10E12.3))
C    1(I5,0P10E12.3))
  120 IF(MODE.EQ.2.OR.MODE.EQ.12)GO TO 149
      DO 125 K=2,NEQUA
      ID=IDEQUA(K)
      IF(ID.EQ.100)GO TO 122
      DO 121 J=1,NRHOX
C     CALCULATE PARTITION FUNCTIONS
      CALL PFSAHA(J,ID,1,3,FRAC)
  121 XNZ(J,K)=XNZ(J,K)/FRAC(J,1)/1.8786E20/SQRT((ATMASS(ID)*T(J))**3)
      GO TO 125
  122 DO 123 J=1,NRHOX
  123 XNZ(J,K)=XNZ(J,K)/2./2.4148E15/T(J)/SQRT(T(J))
  125 CONTINUE
      DO 140 JMOL=1,NUMMOL
      NCOMP=LOCJ(JMOL+1)-LOCJ(JMOL)
      IF(EQUIL(1,JMOL).EQ.0.)GO TO 135
      DO 126 J=1,NRHOX
  126 XNMOL(J,JMOL)=EXP(EQUIL(1,JMOL)/T(J))
      AMASS=0.
      LOCJ1=LOCJ(JMOL)
      LOCJ2=LOCJ(JMOL+1)-1
      DO 130 LOCK=LOCJ1,LOCJ2
      K=KCOMPS(LOCK)
      IF(K.EQ.NEQUA1)GO TO 128
      ID=IDEQUA(K)
      IF(ID.LT.100)AMASS=AMASS+ATMASS(ID)
      DO 127 J=1,NRHOX
  127 XNMOL(J,JMOL)=XNMOL(J,JMOL)*XNZ(J,K)
      GO TO 130
  128 DO 129 J=1,NRHOX
  129 XNMOL(J,JMOL)=XNMOL(J,JMOL)/XNZ(J,NEQUA)
  130 CONTINUE
      DO 131 J=1,NRHOX
  131 XNMOL(J,JMOL)=XNMOL(J,JMOL)*1.8786E20*SQRT((AMASS*T(J))**3)
      GO TO 140
  135 ID=CODE(JMOL)
      DO 136 J=1,NRHOX
      CALL PFSAHA(J,ID,NCOMP,3,FRAC)
  136 XNMOL(J,JMOL)=XNMOL(J,JMOL)/FRAC(J,1)
  140 CONTINUE
  149 IF(IFPNCH(ITER).NE.5)RETURN
      WRITE(6,150)
  150 FORMAT(1H120X38HNUMBER DENSITIES / PARTITION FUNCTIONS)
      WRITE(6,151)NUMMOL
      WRITE(7,151)NUMMOL
  151 FORMAT(I5,10H MOLECULES)
      DO 155 JMOL=1,NUMMOL
      WRITE(6,152)CODE(JMOL),(XNMOL(J,JMOL),J=1,NRHOX)
      WRITE(7,152)CODE(JMOL),(XNMOL(J,JMOL),J=1,NRHOX)
  152 FORMAT(F20.2/(1P8E10.3))
C 152 FORMAT(F20.2/(0P8E10.3))
  155 CONTINUE
      WRITE(6,158)(XNATOM(J),RHO(J),J=1,NRHOX)
      WRITE(7,158)(XNATOM(J),RHO(J),J=1,NRHOX)
  158 FORMAT(11H XNATOM,RHO/(1P8E10.3))
C 158 FORMAT(11H XNATOM,RHO/(0P8E10.3))
      RETURN
      END
```

```
      SUBROUTINE KAPP(N,NSTEPS,STEPWT)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /IFOP/IFOP(20)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/AHYD(40),AH2P(40),AHMIN(40),SIGH(40),AHE1(40),
     1       AHE2(40),AHEMIN(40),SIGHE(40),ACOOL(40),ALUKE(40),AHOT(40),
     2            SIGEL(40),SIGH2(40),AHLINE(40),ALINES(40),SIGLIN(40),
     3            AXLINE(40),SIGXL(40),AXCONT(40),SIGX(40),SHYD(40),
     4            SHMIN(40),SHLINE(40),SXLINE(40),SXCONT(40)
      COMMON /OPTOT/ACONT(40),SCONT(40),ALINE(40),SLINE(40),SIGMAC(40),
     1              SIGMAL(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION DUMMY(40,25)
      EQUIVALENCE (AHYD(1),DUMMY(1))
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 90
      ITEMP1=ITEMP
      IF(IFOP(1).EQ.1)CALL POPS(1.01,11,XNFPH)
      IF(IFOP(5)+IFOP(7).GT.0)CALL POPS(2.02,11,XNFPHE)
   90 STEPWT=1.
      NSTEPS=1
      IF(N.GT.1)GO TO 200
      DO 91 J=1,NRHOX
      DO 91 I=1,25
   91 DUMMY(J,I)=0.
      IF(IFOP(1).EQ.1)CALL HOP
      IF(IFOP(2).EQ.1)CALL H2PLOP
      IF(IFOP(3).EQ.1)CALL HMINOP
      IF(IFOP(4).EQ.1)CALL HRAYOP
      IF(IFOP(5).EQ.1)CALL HE1OP
      IF(IFOP(6).EQ.1)CALL HE2OP
      IF(IFOP(7).EQ.1)CALL HEMIOP
      IF(IFOP(8).EQ.1)CALL HERAOP
      IF(IFOP(9).EQ.1)CALL COOLOP
      IF(IFOP(10).EQ.1)CALL LUKEOP
      IF(IFOP(11).EQ.1)CALL HOTOP
      IF(IFOP(12).EQ.1)CALL ELECOP
      IF(IFOP(13).EQ.1)CALL H2RAOP
      IF(IFOP(14).EQ.1.AND.N.GT.0)CALL HLINOP
      IF(IFOP(15).EQ.1.AND.N.GT.0)CALL LINOP(N,NSTEPS,STEPWT)
      IF(IFOP(16).EQ.1.AND.N.GT.0)CALL LINSOP(N,NSTEPS,STEPWT)
      IF(IFOP(17).EQ.1.AND.N.GT.0)CALL XLINOP
      IF(IFOP(18).EQ.1.AND.N.GT.0)CALL XLISOP
      IF(IFOP(19).EQ.1)CALL XCONOP
      IF(IFOP(20).EQ.1)CALL XSOP
      DO 100 J=1,NRHOX
      A=AH2P(J)+AHE1(J)+AHE2(J)+AHEMIN(J)+ACOOL(J)+ALUKE(J)+AHOT(J)
      ACONT(J)=A+AHYD(J)+AHMIN(J)+AXCONT(J)
      SCONT(J)=BNU(J)
      IF(ACONT(J).GT.0.)SCONT(J)=(A*BNU(J)+AHYD(J)*SHYD(J)+AHMIN(J)*
     1SHMIN(J)+AXCONT(J)*SXCONT(J))/ACONT(J)
      ALINE(J)=AHLINE(J)+ALINES(J)+AXLINE(J)
      SLINE(J)=BNU(J)
      IF(ALINE(J).GT.0.)SLINE(J)=(AHLINE(J)*SHLINE(J)+ALINES(J)*BNU(J)+
     1AXLINE(J)*SXLINE(J))/ALINE(J)
      SIGMAC(J)=SIGH(J)+SIGHE(J)+SIGEL(J)+SIGH2(J)+SIGX(J)
  100 SIGMAL(J)=SIGLIN(J)+SIGXL(J)
      RETURN
```

```
  200 IF(IFOP(15).EQ.1)CALL LINOP(N,NSTEPS,STEPWT)
      IF(IFOP(16).EQ.1)CALL LINSOP(N,NSTEPS,STEPWT)
      DO 201 J=1,NRHOX
      ALINE(J)=AHLINE(J)+ALINES(J)+AXLINE(J)
      IF(ALINE(J).GT.0.)SLINE(J)=(AHLINE(J)*SHLINE(J)+ALINES(J)*BNU(J)+
     1AXLINE(J)*SXLINE(J))/ALINE(J)
  201 SIGMAL(J)=SIGLIN(J)+SIGXL(J)
      RETURN
      END


      SUBROUTINE HOP
C     REQUIRES FUNCTIONS COULX AND COULFF
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/AHYD(40),D1(40,19),SHYD(40),D2(40,4)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION CONT(8),BOLT(40,8),EXLIM(40),FREET(40),BOLTEX(40)
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      ITEMP1=ITEMP
      DO 15 J=1,NRHOX
      DO 11 N=1,8
   11 BOLT(J,N)=EXP(-(13.595-13.595/FLOAT(N*N))/TKEV(J))*2.*FLOAT(N*N)*
     1XNFPH(J,1)/RHO(J)
      DO 12 N=1,6
   12 BOLT(J,N)=BOLT(J,N)*BHYD(J,N)
      FREET(J)=XNE(J)*XNFPH(J,2)/RHO(J)/SQRT(T(J))
      XR=XNFPH(J,1)*(2./2./13.595)*TKEV(J)/RHO(J)
      BOLTEX(J)=EXP(-13.427/TKEV(J))*XR
   15 EXLIM(J)=EXP(-13.595/TKEV(J))*XR
   20 DO 21 N=1,8
   21 CONT(N)=COULX(N,FREQ,1.)
      FREQ3=FREQ**3
      CFREE=3.6919E8/FREQ3
      C=2.815E29/FREQ3
      DO 32 J=1,NRHOX
      EX=BOLTEX(J)
      IF(FREQ.LT.4.05933E13)EX=EXLIM(J)/EHVKT(J)
      H=(CONT(7)*BOLT(J,7)+CONT(8)*BOLT(J,8)+(EX-EXLIM(J))*C+
     1COULFF(J,1)*FREET(J)*CFREE)*STIM(J)
      S=H*BNU(J)
      DO 31 N=1,6
      H=H+CONT(N)*BOLT(J,N)*(1.-EHVKT(J)/BHYD(J,N))
   31 S=S+CONT(N)*BOLT(J,N)*BNU(J)*STIM(J)/BHYD(J,N)
      AHYD(J)=H
   32 SHYD(J)=S/H
      RETURN
      END
```

```
      FUNCTION COULX(N,FREQ,Z)
      DIMENSION A(6),B(6),C(6)
      DATA A/.9916,1.105,1.101,1.101,1.102,1.0986/
      DATA B/2.719E13,-2.375E14,-9.863E13,-5.765E13,-3.909E13,-2.704E13/
      DATA C/-2.268E30,4.077E28,1.035E28,4.593E27,2.371E27,1.229E27/
      IF(FREQ.LT.Z*Z*3.28805E15/FLOAT(N*N))GO TO 1
      COULX=2.815E29/FREQ/FREQ/FREQ/FLOAT(N**5)*Z**4
      IF(N.GT.6)RETURN
      COULX=COULX*(A(N)+(B(N)+C(N)*(Z*Z/FREQ))*(Z*Z/FREQ))
      RETURN
    1 COULX=0.
      RETURN
      END


      FUNCTION COULFF(J,NZ)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION Z4LOG(6),A(11,12)
      DATA Z4LOG/0.,1.20412,1.90849,2.40824,2.79588,3.11261/
      DATA A/
     15.53,5.49,5.46,5.43,5.40,5.25,5.00,4.69,4.48,4.16,3.85,
     24.91,4.87,4.84,4.80,4.77,4.63,4.40,4.13,3.87,3.52,3.27,
     34.29,4.25,4.22,4.18,4.15,4.02,3.80,3.57,3.27,2.98,2.70,
     43.64,3.61,3.59,3.56,3.54,3.41,3.22,2.97,2.70,2.45,2.20,
     53.00,2.98,2.97,2.95,2.94,2.81,2.65,2.44,2.21,2.01,1.81,
     62.41,2.41,2.41,2.41,2.41,2.32,2.19,2.02,1.84,1.67,1.50,
     71.87,1.89,1.91,1.93,1.95,1.90,1.80,1.68,1.52,1.41,1.30,
     81.33,1.39,1.44,1.49,1.55,1.56,1.51,1.42,1.33,1.25,1.17,
     90.90,0.95,1.00,1.08,1.17,1.30,1.32,1.30,1.20,1.15,1.11,
     A0.45,0.48,0.52,0.60,0.75,0.91,1.15,1.18,1.15,1.11,1.08,
     B0.33,0.36,0.39,0.46,0.59,0.76,0.97,1.09,1.13,1.10,1.08,
     C0.19,0.21,0.24,0.28,0.38,0.53,0.76,0.96,1.08,1.09,1.09/
C     GAMLOG=ALOG10(158000*Z*Z/T)*2
      GAMLOG=10.39638-TLOG(J)/1.15129+Z4LOG(NZ)
      IGAM=MAX0(MIN0(IFIX(GAMLOG+7.),10),1)
C     HVKTLG=ALOG10(HVKT)*2
      HVKTLG=(FREQLG-TLOG(J))/1.15129-20.63764
      IHV<T=MAX0(MIN0(IFIX(HVKTLG+9.),11),1)
      P=GAMLOG-FLOAT(IGAM-7)
      Q=HVKTLG-FLOAT(IHVKT-9)
      COULFF=(1.-P)*((1.-Q)*A(IGAM,IHVKT)+Q*A(IGAM,IHVKT+1))+
     1P*((1.-Q)*A(IGAM+1,IHVKT)+Q*A(IGAM+1,IHVKT+1))
      RETURN
      END


      SUBROUTINE HRAYOP
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,3),SIGH(40),D2(40,21)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      WAVE=2.997925E18/AMIN1(FREQ,2.463E15)
      WW=WAVE**2
      SIG=(5.799E-13+1.422E-6/WW+2.784/(WW*WW))/(WW*WW)
      DO 2 J=1,NRHUX
    2 SIGH(J)=SIG*XNFPH(J,1)*2.*BHYD(J,1)/RHO(J)
      RETURN
      END
```

```
      SUBROUTINE H2PLOP
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40),AH2P(40),D2(40,23)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      IF(FREQ.GT.3.28805E15)RETURN
      FR=-3.0233E3+(3.7797E2+(-1.82496E1+(3.9207E-1-3.1672E-3*FREQLG)*
     1FREQLG)*FREQLG)*FREQLG
      ES=-7.342E-3+(-2.409E-15+(1.028E-30+(-4.230E-46+(1.224E-61-
     1 1.351E-77*FREQ)*FREQ)*FREQ)*FREQ)*FREQ
      DO 10 J=1,NRHOX
   10 AH2P(J)=EXP(-ES/TKEV(J)+FR)*XNFPH(J,1)*2.*BHYD(J,1)*XNFPH(J,2)/
     1RHO(J)*STIM(J)
      RETURN
      END


      SUBROUTINE HMINOP
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,2),AHMIN(40),D2(40,18),SHMIN(40),D3(40,3)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION XHMIN(40)
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      ITEMP1=ITEMP
      DO 11 J=1,NRHOX
   11 XHMIN(J)=EXP(.7552/TKEV(J))/(2.*2.4148E15*T(J)*SQRT(T(J)))*
     1BMIN(J)*BHYD(J,1)*XNFPH(J,1)*XNE(J)
   20 B=(1.3727E-25+4.3748E-10/FREQ)/FREQ
      C=-2.5993E-7/FREQ**2
      IF(FREQ.LE.1.8259E14)GO TO 23
      IF(FREQ.GE.2.111E14)GO TO 22
      HMINBF=3.695E-16+(-1.251E-1+1.052E13/FREQ)/FREQ
      GO TO 30
   22 HMINBF=6.801E-20+(5.358E-3+(1.481E13+(-5.519E27+4.808E41/FREQ)/
     1FREQ)/FREQ)/FREQ
      GO TO 30
   23 HMINBF=0.
   30 DO 31 J=1,NRHOX
      HMINFF=(B+C/T(J))*XNFPH(J,1)*2.*BHYD(J,1)*XNE(J)/RHO(J)
      H=HMINBF*(1.-EHVKT(J)/BMIN(J))*XHMIN(J)/RHO(J)
      AHMIN(J)=H+HMINFF
   31 SHMIN(J)=(H*BNU(J)*STIM(J)/(BMIN(J)-EHVKT(J))+HMINFF*BNU(J))/
     1AHMIN(J)
      RETURN
      END
```

```
      SUBROUTINE HE1OP
C     REQUIRES FUNCTIONS COULX AND COULFF
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,4),AHE1(40),D2(40,20)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION CHI(10),BOLT(40,10),EXLIM(40),HEFREQ(10),TRANS(10),G(10)
      DIMENSION BOLTEX(40),FREET(40)
      DATA G/1.,3.,1.,9.,3.,3.,1.,9.,20.,3./
      DATA HEFREQ/5.945209E15,1.152844E15,.9603331E15,.8761076E15,
     1 .8147104E15,.4519048E15,.4030971E15,.3821191E15,.3660215E15,
     2 .3627891E15/
      DATA CHI/0.,19.819,20.615,20.964,21.217,22.718,22.920,23.006,
     1 23.073,23.086/
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 10
      ITEMP1=ITEMP
      DO 5 J=1,NRHOX
      DO 4 N=1,10
    4 BOLT(J,N)=EXP(-CHI(N)/TKEV(J))*G(N)*XNFPHE(J,1)/RHO(J)
      FREET(J)=XNE(J)*XNFPHE(J,2)/RHO(J)/SQRT(T(J))
      XR=XNFPHE(J,1)*(4./2./13.595)*TKEV(J)/RHO(J)
      BOLTEX(J)=EXP(-23.730/TKEV(J))*XR
    5 EXLIM(J)=EXP(-24.587/TKEV(J))*XR
   10 FREQ3=FREQ**3
      CFREE=3.6919E8/FREQ3
      C=2.815E29/FREQ3
      DO 15 NMIN=1,10
      TRANS(NMIN)=0.
      IF(HEFREQ(NMIN).LE.FREQ)GO TO 16
   15 CONTINUE
      GO TO 40
   16 GO TO (21,22,23,24,25,26,27,28,29,30),NMIN
   21 TRANS(1)=EXP(33.32-2.*FREQLG)
   22 TRANS(2)=EXP(-390.026+(21.035-.318*FREQLG)*FREQLG)
   23 TRANS(3)=EXP(26.83-1.91*FREQLG)
   24 TRANS(4)=EXP(61.21-2.9*FREQLG)
   25 TRANS(5)=EXP(81.35-3.5*FREQLG)
   26 TRANS(6)=EXP(12.69-1.54*FREQLG)
   27 TRANS(7)=EXP(23.85-1.86*FREQLG)
   28 TRANS(8)=EXP(49.30-2.60*FREQLG)
   29 TRANS(9)=EXP(85.20-3.69*FREQLG)
   30 TRANS(10)=EXP(58.81-2.89*FREQLG)
   40 DO 45 J=1,NRHOX
      EX=BOLTEX(J)
      IF(FREQ.LT.2.055E14)EX=EXLIM(J)/EHVKT(J)
      HE1=(EX-EXLIM(J))*C
      DO 41 N=1,10
   41 HE1=HE1+TRANS(N)*BOLT(J,N)
   45 AHE1(J)=(HE1+COULFF(J,1)*FREET(J)*CFREE)*STIM(J)
      RETURN
      END
```

```
      SUBROUTINE HE2OP
C     REQUIRES FUNCTIONS COULX AND COULFF
C     FREQUENCIES ARE 4X HYDROGEN,CHI ARE FOR ION POT=54.403
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,5),AHE2(40),D2(40,19)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION CONT(9),BOLT(40,9),EXLIM(40),FREET(40),BOLTEX(40)
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      ITEMP1=ITEMP
      DO 15 J=1,NRHOX
      DO 14 N=1,9
   14 BOLT(J,N)=EXP(-(54.403-54.403/FLOAT(N*N))/TKEV(J))*2.*FLOAT(N*N)*
     1XNFPHE(J,2)/RHO(J)
      FREET(J)=XNE(J)*XNFPHE(J,3)/RHO(J)/SQRT(T(J))
      XR=XNFPHE(J,2)*(2./2./13.595)*TKEV(J)/RHO(J)
      BOLTEX(J)=EXP(-53.859/TKEV(J))*XR
   15 EXLIM(J)=EXP(-54.403/TKEV(J))*XR
   20 DO 21 N=1,9
   21 CONT(N)=COULX(N,FREQ,2.)
      FREQ3=FREQ**3
      CFREE=3.6919E8/FREQ3*4.
      C=2.815E29*2.*2./FREQ3
      DO 35 J=1,NRHOX
      EX=BOLTEX(J)
      IF(FREQ.LT.1.31522E14)EX=EXLIM(J)/EHVKT(J)
      HE2=(EX-EXLIM(J))*C
      DO 31 N=1,9
   31 HE2=HE2+CONT(N)*BOLT(J,N)
   35 AHE2(J)=(HE2+COULFF(J,2)*CFREE*FREET(J))*STIM(J)
      RETURN
      END


      SUBROUTINE HEMIOP
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,6),AHEMIN(40),D2(40,18)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      A=3.397E-46+(-5.216E-31+7.039E-15/FREQ)/FREQ
      B=-4.116E-42+(1.067E-26+8.135E-11/FREQ)/FREQ
      C=5.081E-37+(-8.724E-23-5.659E-8/FREQ)/FREQ
      DO 3 J=1,NRHOX
    3 AHEMIN(J)=(A*T(J)+B+C/T(J))*XNE(J)*XNFPHE(J,1)/RHO(J)
      RETURN
      END
```

```
      SUBROUTINE HERAOP
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,7),SIGHE(40),D2(40,17)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      WAVE=2.997925E18/AMIN1(FREQ,5.15E15)
      WW=WAVE**2
      SIG=5.484E-14/WW/WW*(1.+(2.44E5+5.94E10/(WW-2.90E5))/WW)**2
      DO 2 J=1,NRHOX
    2 SIGHE(J)=SIG*XNFPHE(J,1)/RHO(J)
      RETURN
      END


      SUBROUTINE COOLOP
C     SI1,MG1,AL1,C1
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /OPS/D1(40,8),ACOOL(40),D2(40,16)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION XNFPC(40),XNFPMG(40),XNFPAL(40),XNFPSI(40)
      REAL MG1OP
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 10
      ITEMP1=ITEMP
      CALL POPS(6.,11,XNFPC)
      CALL POPS(12.,11,XNFPMG)
      CALL POPS(13.,11,XNFPAL)
      CALL POPS(14.,11,XNFPSI)
   10 DO 20 J=1,NRHOX
   20 ACOOL(J)=(C1OP(J)*XNFPC(J)+MG1OP(J)*XNFPMG(J)+AL1OP(J)*XNFPAL(J)+
     1SI1OP(J)*XNFPSI(J))*STIM(J)/RHO(J)
      RETURN
      END
```

```
      FUNCTION C1OP(J)
C     CROSS-SECTION TIMES THE PARTITION FUNCTION
      COMMON /FREQ/FREQ.FREQLG.EHVKT(40).STIM(40).BNJ(40)
      COMMON /RHOX/RHOX(40).NRHOX
      COMMON /TEMP/T(40).TKEV(40).TK(40).HKT(40).TLOG(40).ITEMP
      DIMENSION C1240(40).C1444(40)
      DATA FREQ1.ITEMP1/0..0/
      IF(ITEMP.EQ.ITEMP1)GO TO 30
      ITEMP1=ITEMP
      DO 20 K=1.NRHOX
      C1240(K)=5.*EXP(-1.264/TKEV(K))
   20 C1444(K)=EXP(-2.683/TKEV(K))
   30 IF(FREQ.EQ.FREQ1)GO TO 40
      X1444=0.
      X1240=0.
      X1100=0.
      IF(FREQ.GE.2.7254E15)X1100=SEATON(2.7254E15.1.219E-17.2..3.317)
      IF(FREQ.GE.2.4196E15)X1240=SEATON(2.4196E15.1.03E-17.1.5.2.789)
      IF(FREQ.GE.2.0761E15)X1444=SEATON(2.0761E15.9.59E-18.1.5.3.501)
      FREQ1=FREQ
   40 C1OP=X1100*9.+X1240*C1240(J)+X1444*C1444(J)
      RETURN
      END
```

```
      FUNCTION SEATON(FREQ0.XSECT.POWER.A)
      COMMON /FREQ/FREQ.FREQLG.EHVKT(40).STIM(40).BNJ(40)
      SEATON=XSECT*(A+(1.-A)*(FREQ0/FREQ))*
     1SQRT((FREQ0/FREQ)**(IFIX(2.*POWER+.01)))
      RETURN
      END
```

```
      FUNCTION AL1OP(J)
C     CROSS-SECTION TIMES THE PARTITION FUNCTION
      COMMON /FREQ/FREQ.FREQLG.EHVKT(40).STIM(40).BNJ(40)
      AL1OP=0.
      IF(FREQ.GE.1.443E15)AL1OP=2.1E-17*(1.443E15/FREQ)**3*6.
      RETURN
      END
```

```
      REAL FUNCTION MG1OP(J)
C     CROSS-SECTION TIMES THE PARTITION FUNCTION
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION FLOG(9),FREQMG(7),PEACH(7,15),X(7),TLG(7),DT(40),NT(40)
      DATA PEACH/
C        4000      5000      6000      7000      8000      9000     10000     WAVE(A)
     1 -42.474, -42.350, -42.109, -41.795, -41.467, -41.159, -40.883,   1500
     2 -41.808, -41.735, -41.582, -41.363, -41.115, -40.866, -40.631,   1550
     3 -41.273, -41.223, -41.114, -40.951, -40.755, -40.549, -40.347,   1621
     4 -45.583, -44.008, -42.957, -42.205, -41.639, -41.198, -40.841,   1622
     5 -44.324, -42.747, -41.694, -40.939, -40.370, -39.925, -39.566,   2513
     6 -50.969, -48.388, -46.630, -45.344, -44.355, -43.568, -42.924,   2514
     7 -50.633, -48.026, -46.220, -44.859, -43.803, -42.957, -42.264,   3756
     8 -53.028, -49.643, -47.367, -45.729, -44.491, -43.520, -42.736,   3757
     9 -51.785, -48.352, -46.050, -44.393, -43.140, -42.157, -41.363,   6549
     T -52.285, -48.797, -46.453, -44.765, -43.486, -42.480, -41.668,   6550
     1 -52.028, -48.540, -46.196, -44.507, -43.227, -42.222, -41.408,   7234
     2 -52.384, -48.876, -46.513, -44.806, -43.509, -42.488, -41.660,   7235
     3 -52.363, -48.856, -46.493, -44.786, -43.489, -42.467, -41.639,   7291
     4 -54.704, -50.772, -48.107, -46.176, -44.707, -43.549, -42.611,   7292
     5 -54.359, -50.349, -47.643, -45.685, -44.198, -43.027, -42.418/   9000
      DATA FREQMG/1.9341452E15,1.8488510E15,1.1925797E15,7.9804046E14,
     1 4.5772110E14,4.1440977E14,4.1113514E14/
      DATA FLOG/35.23123,35.19844,35.15334,34.71490,34.31318,33.75728,
     1 33.65788,33.64994,33.43947/
      DATA TLG/8.29405,8.51719,8.69951,8.85367,8.98720,9.10498,9.21034/
      DATA FREQ1,ITEMP1/0.,0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      ITEMP1=ITEMP
      DO 11 K=1,NRHOX
      N=MAX0(MIN0(6,IFIX(T(K)/1000.)-3),1)
      NT(K)=N
   11 DT(K)=(TLOG(K)-TLG(N))/(TLG(N+1)-TLG(N))
      GO TO 21
   20 IF(FREQ.EQ.FREQ1)GO TO 30
   21 FREQ1=FREQ
      DO 22 N=1,7
      IF(FREQ.GT.FREQMG(N))GO TO 23
   22 CONTINUE
      N=8
   23 D=(FREQLG-FLOG(N))/(FLOG(N+1)-FLOG(N))
      IF(N.GT.2)N=2*N-2
      D1=1.-D
      DO 24 IT=1,7
   24 X(IT)=PEACH(IT,N+1)*D+PEACH(IT,N)*D1
   30 N=NT(J)
      MG1OP=EXP(X(N)*(1.-DT(J))+X(N+1)*DT(J))
      RETURN
      END
```

```
      FUNCTION SI1OP(J)
C     CROSS-SECTION TIMES THE PARTITION FUNCTION
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION FLOG(11),FREQSI(9),X(9),TLG(9),DT(40),NT(40)
      DIMENSION PEACH(9,19)
      DATA PEACH/
C       4000   5000   6000   7000   8000   9000   10000  11000  12000   WAVE(A)
     1 38.136,38.138,38.140,38.141,38.143,38.144,38.144,38.145,38.145,  1200
     2 37.834,37.839,37.843,37.847,37.850,37.853,37.855,37.857,37.858,  1400
     3 37.898,37.898,37.897,37.897,37.897,37.896,37.895,37.895,37.894,  1519
     4 40.737,40.319,40.047,39.855,39.714,39.604,39.517,39.445,39.385,  1520
     5 40.581,40.164,39.893,39.702,39.561,39.452,39.366,39.295,39.235,  1676
     6 45.521,44.456,43.753,43.254,42.878,42.580,42.332,42.119,41.930,  1677
     7 45.520,44.455,43.752,43.251,42.871,42.569,42.315,42.094,41.896,  1978
     8 55.068,51.783,49.553,47.942,46.723,45.768,44.997,44.360,43.823,  1979
     9 53.868,50.369,48.031,46.355,45.092,44.104,43.308,42.652,42.100,  5379
     T 54.133,50.597,48.233,46.539,45.261,44.262,43.456,42.790,42.230,  5380
     1 54.051,50.514,48.150,46.454,45.176,44.175,43.368,42.702,42.141,  5624
     2 54.442,50.854,48.455,46.733,45.433,44.415,43.592,42.912,42.340,  5625
     3 54.320,50.722,48.313,46.583,45.277,44.251,43.423,42.738,42.160,  6260
     4 55.691,51.965,49.444,47.615,46.221,45.119,44.223,43.478,42.848,  6261
     5 55.661,51.933,49.412,47.582,46.188,45.085,44.189,43.445,42.813,  6349
     6 55.973,52.193,49.630,47.769,46.349,45.226,44.314,43.555,42.913,  6350
     7 55.922,52.141,49.577,47.715,46.295,45.172,44.259,43.500,42.858,  6491
     8 56.828,52.821,50.110,48.146,46.654,45.477,44.522,43.730,43.061,  6492
     9 56.657,52.653,49.944,47.983,46.491,45.315,44.360,43.569,42.901/  6900
C     3P,1D,1S,1D,3D,3F,1D,3P
      DATA FREQSI/2.1413750E15,1.9723165E15,1.7879689E15,1.5152920E15,
     1 5.5723927E14,5.3295914E14,4.7886458E14,4.7216422E14,4.6185133E14/
      DATA FLOG/35.45438,35.30022,35.21799,35.11986,34.95438,33.95402,
     1 33.90947,33.80244,33.78835,33.76626,33.70518/
      DATA TLG/8.29405,8.51719,8.69951,8.85367,8.98720,9.10498,9.21034,
     1 9.30565,9.39266/
      DATA FREQ1,ITEMP1/0.,0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      ITEMP1=ITEMP
      DO 11 K=1,NRHOX
      N=MAX0(MIN0(8,IFIX(T(K)/1000.)-3),1)
      NT(K)=N
   11 DT(K)=(TLOG(K)-TLG(N))/(TLG(N+1)-TLG(N))
      GO TO 21
   20 IF(FREQ.EQ.FREQ1)GO TO 30
   21 FREQ1=FREQ
      DO 22 N=1,9
      IF(FREQ.GT.FREQSI(N))GO TO 23
   22 CONTINUE
      N=10
   23 D=(FREQLG-FLOG(N))/(FLOG(N+1)-FLOG(N))
      IF(N.GT.2)N=2*N-2
      D1=1.-D
      DO 24 IT=1,9
   24 X(IT)=PEACH(IT,N+1)*D+PEACH(IT,N)*D1
   30 N=NT(J)
      SI1OP=EXP(-(X(N)*(1.-DT(J))+X(N+1)*DT(J)))*9.
      RETURN
      END
```

```
      SUBROUTINE LUKEOP
C     SI2,MG2,CA2,N1,O1
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /OPS/D1(40,9),ALUKE(40),D2(40,15)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION XNFPN(40),XNFPO(40),XNFPMG(40),XNFPSI(40),XNFPCA(40)
      REAL N1OP,MG2OP
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 10
      ITEMP1=ITEMP
      CALL POPS(7.,1,XNFPN)
      CALL POPS(8.,1,XNFPO)
      CALL POPS(12.01,1,XNFPMG)
      CALL POPS(14.01,1,XNFPSI)
      CALL POPS(20.01,1,XNFPCA)
   10 DO 11 J=1,NRHOX
   11 ALUKE(J)=(N1OP(J)*XNFPN(J)+O1OP(J)*XNFPO(J)+MG2OP(J)*XNFPMG(J)+
     1SI2OP(J)*XNFPSI(J)+CA2OP(J)*XNFPCA(J))*STIM(J)/RHO(J)
      RETURN
      END


      REAL FUNCTION N1OP(J)
C     CROSS-SECTION TIMES PARTITION FUNCTION
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION C1130(40),C1020(40)
      DATA FREQ1,ITEMP1/0.,0/
      IF(ITEMP.EQ.ITEMP1)GO TO 30
      ITEMP1=ITEMP
      DO 20 K=1,NRHOX
      C1130(K)=6.*EXP(-3.575/TKEV(K))
   20 C1020(K)=10.*EXP(-2.384/TKEV(K))
   30 IF(FREQ.EQ.FREQ1)GO TO 40
      X1130=0.
      X1020=0.
      X853=0.
      IF(FREQ.GE.3.517915E15)X853=SEATON(3.517915E15,1.142E-17,2.,4.29)
      IF(FREQ.GE.2.941534E15)X1020=SEATON(2.941534E15,4.41E-18,1.5,3.85)
      IF(FREQ.GE.2.653317E15)X1130=SEATON(2.653317E15,4.2E-18,1.5,4.34)
      FREQ1=FREQ
   40 N1OP=X853*4.+X1020*C1020(J)+X1130*C1130(J)
      RETURN
      END


      FUNCTION O1OP(J)
C     CROSS-SECTION TIMES PARTITION FUNCTION
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      DATA FREQ1/0./
      IF(FREQ.EQ.FREQ1)GO TO 1
      X911=0.
      IF(FREQ.GE.3.28805E15)X911=SEATON(3.28805E15,2.94E-18,1.,2.66)
      FREQ1=FREQ
    1 O1OP=X911*9.
      RETURN
      END
```

```
      REAL FUNCTION MG2OP(J)
C     CROSS-SECTION TIMES PARTITION FUNCTION
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION C1169(40)
      DATA FREQ1,ITEMP1/0.,0/
      IF(ITEMP.EQ.ITEMP1)GO TO 30
      ITEMP1=ITEMP
      DO 20 K=1,NRHOX
   20 C1169(K)=6.*EXP(-4.43/TKEV(K))
   30 IF(FREQ.EQ.FREQ1)GO TO 40
      X1169=0.
      X824=0.
      IF(FREQ.GE.3.635492E15)X824=SEATON(3.635492E15,1.40E-19,4.,6.7)
      IF(FREQ.GE.2.564306E15)X1169=5.11E-19*(2.564306E15/FREQ)**3
      FREQ1=FREQ
   40 MG2OP=X824*2.+X1169*C1169(J)
      RETURN
      END


      FUNCTION CA2OP(J)
C     CROSS-SECTION TIMES THE PARTITION FUNCTION
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION C1218(40),C1420(40)
      DATA FREQ1,ITEMP1/0.,0/
      IF(ITEMP.EQ.ITEMP1)GO TO 30
      ITEMP1=ITEMP
      DO 20 K=1,NRHOX
      C1218(K)=10.*EXP(-1.697/TKEV(K))
   20 C1420(K)=6.*EXP(-3.142/TKEV(K))
   30 IF(FREQ.EQ.FREQ1)GO TO 40
      X1420=0.
      X1218=0.
      X1044=0.
      IF(FREQ.GE.2.870454E15)X1044=5.4E-20*(2.870454E15/FREQ)**3
      IF(FREQ.GE.2.460127E15)X1218=1.64E-17*SQRT(2.460127E15/FREQ)
      IF(FREQ.GE.2.110779E15)X1420=SEATON(2.110779E15,4.13E-18,3.,.69)
      FREQ1=FREQ
   40 CA2OP=X1044*2.+X1218*C1218(J)+X1420*C1420(J)
      RETURN
      END
```

```
            FUNCTION SI2OP(J)
      C     CROSS-SECTION TIMES THE PARTITION FUNCTION
            COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
            COMMON /RHOX/RHOX(40),NRHOX
            COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
            DIMENSION FLOG(9),FREQSI(7),PEACH(6,14),X(6),TLG(6),DT(40),NT(40)
            DATA PEACH/
C          10000     12000     14000     16000     18000     20000       WAVE(A)
     1   -43.8941, -43.8941, -43.8941, -43.8941, -43.8941, -43.8941,       500
     2   -42.2444, -42.2444, -42.2444, -42.2444, -42.2444, -42.2444,       600
     3   -40.6054, -40.6054, -40.6054, -40.6054, -40.6054, -40.6054,       759
     4   -54.2389, -52.2906, -50.8799, -49.8033, -48.9485, -48.2490,       760
     5   -50.4108, -48.4892, -47.1090, -46.0672, -45.2510, -44.5933,      1905
     6   -52.0936, -50.0741, -48.5999, -47.4676, -46.5649, -45.8246,      1906
     7   -51.9548, -49.9371, -48.4647, -47.3340, -46.4333, -45.6947,      1975
     8   -54.2407, -51.7319, -49.9178, -48.5395, -47.4529, -46.5709,      1976
     9   -52.7355, -50.2218, -48.4059, -47.0267, -45.9402, -45.0592,      3245
     T   -53.5387, -50.9189, -49.0200, -47.5750, -46.4341, -45.5082,      3246
     1   -53.2417, -50.6234, -48.7252, -47.2810, -46.1410, -45.2153,      3576
     2   -53.5097, -50.8535, -48.9263, -47.4586, -46.2994, -45.3581,      3577
     3   -54.0561, -51.2365, -49.1980, -47.6497, -46.4302, -45.4414,      3900
     4   -53.8469, -51.0256, -48.9860, -47.4368, -46.2162, -45.2266/      4200
            DATA FREQSI/4.9965417E15,3.9466738E15,1.5736321E15,1.5171539E15,
           1 9.2378947E14,8.3825004E14,7.6869872E14/
      C     2P,2D,2P,2D,2P
            DATA FLOG/36.32984,36.14752,35.91165,34.99216,34.95561,34.45951,
           1 34.36234,34.27572,34.20161/
            DATA TLG/9.21034,9.39266,9.54681,9.68034,9.79813,9.90349/
            DATA FREQ1,ITEMP1/0.,0/
            IF(ITEMP.EQ.ITEMP1)GO TO 20
            ITEMP1=ITEMP
            DO 11 K=1,NRHOX
            N=MAXO(MINO(5,IFIX(T(K)/2000.)-4),1)
            NT(K)=N
         11 DT(K)=(TLOG(K)-TLG(N))/(TLG(N+1)-TLG(N))
            GO TO 21
         20 IF(FREQ.EQ.FREQ1)GO TO 30
         21 FREQ1=FREQ
            DO 22 N=1,7
            IF(FREQ.GT.FREQSI(N))GO TO 23
         22 CONTINUE
            N=8
         23 D=(FREQLG-FLOG(N))/(FLOG(N+1)-FLOG(N))
            IF(N.GT.2)N=2*N-2
            IF(N.EQ.14)N=13
            D1=1.-D
            DO 24 IT=1,6
         24 X(IT)=PEACH(IT,N+1)*D+PEACH(IT,N)*D1
         30 N=NT(J)
            SI2OP=EXP(X(N)*(1.-DT(J))+X(N+1)*DT(J))*6.
            RETURN
            END
```

```
                SUBROUTINE HOTOP
                COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
                COMMON /OPS/D1(40,10),AHOT(40),D2(40,14)
                COMMON /RHOX/RHOX(40),NRHOX
                COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
                COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
                DIMENSION XNFP(40,21)
                DIMENSION A(420)
                DIMENSION A1(63),A2(63),A3(63),A4(63),A5(63),A6(63),A7(42)
                EQUIVALENCE (A(1),A1(1)),(A(64),A2(1)),(A(127),A3(1))
                EQUIVALENCE (A(190),A4(1)),(A(253),A5(1)),(A(316),A6(1))
                EQUIVALENCE (A(379),A7(1))
                DATA A1/
     1 4.149945E15, 6.90E-18, 1.000, 6.,  6.,  13.71,  2.,                   6.01
     2 4.574341E15, 2.50E-18, 1.000, 4.,  2.,  11.96,  2.,                   6.01
     3 5.220770E15, 1.08E-17, 1.000, 4., 10.,   9.28,  2.,                   6.01
     4 5.222307E15, 5.35E-18, 3.769, 2.,  1.,   0.00, 16.,                   10.00
     5 5.892577E15, 4.60E-18, 1.950, 6.,  6.,   0.00,  2.,                   6.01
     6 6.177022E15, 3.50E-18, 1.000, 4., 12.,   5.33,  2.,                   6.01
     7 6.181062E15, 6.75E-18, 3.101, 5.,  1.,   4.05,  6.,                   7.01
     8 6.701879E15, 6.65E-18, 2.789, 5.,  5.,   1.90,  6.,                   7.01
     9 7.158382E15, 6.65E-18, 2.860, 6.,  9.,   0.00,  6./                   7.01
                DATA A2/
     1 7.284488E15, 3.43E-18, 4.174, 5.,  6.,   5.02, 11.,                   8.01
     2 7.693612E15, 3.53E-18, 3.808, 5., 10.,   3.33, 11.,                   8.01
     3 7.885955E15, 2.32E-18, 3.110, 5.,  6.,   5.02, 11.,                   8.01
     4 8.295079E15, 3.97E-18, 3.033, 5., 10.,   3.33, 11.,                   8.01
     5 8.497686E15, 7.32E-18, 3.837, 5.,  4.,   0.00, 11.,                   8.01
     6 8.509966E15, 2.00E-18, 1.750, 7.,  3.,  12.69,  3.,                   6.02
     7 8.572854E15, 1.68E-18, 3.751, 5.,  6.,   5.02, 11.,                   8.01
     8 9.906370E15, 4.16E-18, 2.717, 3.,  6.,   0.00, 17.,                   10.01
     9 1.000693E16, 2.40E-18, 1.750, 7.,  9.,   6.50,  3./                   6.02
                DATA A3/
     1 1.046078E16, 4.80E-18, 1.000, 4., 10.,  12.53,  7.,                   7.02
     2 1.067157E16, 2.71E-18, 2.148, 3.,  6.,   0.00, 17.,                   10.01
     3 1.146734E16, 2.06E-18, 1.626, 6.,  6.,   0.00,  7.,                   7.02
     4 1.156813E16, 5.20E-19, 2.126, 3.,  6.,   0.00, 17.,                   10.01
     5 1.157840E16, 9.10E-19, 4.750, 4.,  1.,   0.00,  3.,                   6.02
     6 1.177220E16, 5.30E-18, 1.000, 4., 12.,   7.10,  7.,                   7.02
     7 1.198813E16, 3.97E-18, 2.780, 6.,  1.,   5.35, 12.,                   8.02
     8 1.267503E16, 3.79E-18, 2.777, 6.,  5.,   2.51, 12.,                   8.02
     9 1.327649E16, 3.65E-18, 2.014, 6.,  9.,   0.00, 12./                   8.02
                DATA A4/
     1 1.361466E16, 7.00E-18, 1.000, 2.,  5.,   7.48, 12.,                   8.02
     2 1.365932E16, 9.30E-19, 1.500, 7.,  6.,   8.00,  4.,                   6.03
     3 1.481487E16, 1.10E-18, 1.750, 7.,  3.,  16.20,  8.,                   7.03
     4 1.490032E16, 5.49E-18, 3.000, 5.,  1.,   6.91, 18.,                   10.02
     5 1.533389E16, 1.80E-18, 2.277, 4.,  9.,   0.00, 18.,                   10.02
     6 1.559452E16, 8.70E-19, 3.000, 6.,  2.,   0.00,  4.,                   6.03
     7 1.579688E16, 4.17E-18, 2.074, 4.,  5.,   3.20, 18.,                   10.02
     8 1.643205E16, 1.39E-18, 2.792, 5.,  5.,   3.20, 18.,                   10.02
     9 1.656208E16, 2.50E-18, 2.346, 5.,  9.,   0.00, 18./                   10.02
                DATA A5/
     1 1.671401E16, 1.30E-18, 1.750, 7.,  9.,   8.35,  8.,                   7.03
     2 1.719725E16, 1.48E-18, 2.225, 5.,  9.,   0.00, 18.,                   10.02
     3 1.737839E16, 2.70E-18, 1.000, 4., 10.,  15.74, 13.,                   8.03
     4 1.871079E16, 1.27E-18,  .831, 6.,  6.,   0.00, 13.,                   8.03
     5 1.873298E16, 9.10E-19, 3.000, 4.,  1.,   0.00,  8.,                   7.03
     6 1.903597E16, 2.90E-18, 1.000, 4., 12.,   8.88, 13.,                   8.03
     7 2.060738E16, 4.60E-18, 1.000, 3., 12.,  22.84, 19.,                   10.03
```

```
8 2.125492E16, 5.90E-19, 1.000, 6.,  6.,   9.99,  9.,               7.04
9 2.162610E16, 1.69E-18, 1.937, 5.,  6.,   7.71, 19./               10.03
         DATA A6/
1 2.226127E16, 1.69E-18, 1.841, 5., 10.,   5.08, 19.,               10.03
2 2.251163E16, 9.30E-19, 2.455, 6.,  6.,   7.71, 19.,               10.03
3 2.278001E16, 7.90E-19, 1.000, 6.,  9.,  10.20, 14.,               8.04
4 2.317678E16, 1.65E-18, 2.277, 6., 10.,   5.08, 19.,               10.03
5 2.348946E16, 3.11E-18, 1.963, 6.,  4.,   0.00, 19.,               10.03
6 2.351911E16, 7.30E-19, 1.486, 5.,  6.,   7.71, 19.,               10.03
7 2.366973E16, 5.00E-19, 1.000, 4.,  2.,   0.00,  9.,               7.04
8 2.507544E16, 6.90E-19, 1.000, 6.,  3.,  19.69, 14.,               8.04
9 2.754065E16, 7.60E-19, 1.000, 2.,  1.,   0.00, 14./               8.04
         DATA A7/
1 2.864850E16, 1.54E-18, 2.104, 6.,  1.,   7.92, 20.,               10.04
2 2.965598E16, 1.53E-18, 2.021, 6.,  5.,   3.76, 20.,               10.04
3 3.054151E16, 1.40E-18, 1.471, 6.,  9.,   0.00, 20.,               10.04
4 3.085141E16, 2.80E-18, 1.000, 4.,  5.,  11.01, 20.,               10.04
5 3.339687E16, 3.60E-19, 1.000, 6.,  2.,   0.00, 15.,               8.05
6 3.818757E16, 4.90E-19, 1.145, 6.,  6.,   0.00, 21./               10.05
         DATA NUM/60/
         DATA ITEMP1/0/
         IF(ITEMP.EQ.ITEMP1)GO TO 95
         ITEMP1=ITEMP
         CALL POPS(6.03,11,XNFP)
         CALL POPS(7.04,11,XNFP(1,5))
         CALL POPS(8.05,11,XNFP(1,10))
         CALL POPS(10.05,11,XNFP(1,16))
      95 L=-6
         DO 20 I=1,NUM
         L=L+7
         IF(FREQ.LT.A(L))GO TO 20
         XSECT=A(L+1)*(A(L+2)+(A(L)/FREQ)-A(L+2)*(A(L)/FREQ))*
        1 SQRT((A(L)/FREQ)**IFIX(A(L+3)))
         ID=A(L+6)
         DO 10 J=1,NRHOX
         XX=XSECT*XNFP(J,ID)*A(L+4)
         IF(XX.GT.AHOT(J)/100.)AHOT(J)=AHOT(J)+XX/EXP(A(L+5)/TKEV(J))
      10 CONTINUE
      20 CONTINUE
         DO 30 J=1,NRHOX
      30 AHOT(J)=AHOT(J)*STIM(J)/RHOX(J)
         RETURN
         END
```

```
      SUBROUTINE ELECOP
      COMMON /OPS/D1(40,11),SIGEL(40),D2(40,13)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      DO 1 J=1,NRHOX
    1 SIGEL(J)=.6653E-24*XNE(J)/RHO(J)
      RETURN
      END


      SUBROUTINE H2RAOP
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,12),SIGH2(40),D2(40,12)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION XNH2(40)
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      ITEMP1=ITEMP
      DO 11 J=1,NRHOX
   11 XNH2(J)=(XNFPH(J,1)*2.*BHYD(J,1))**2*EXP(4.477/TKEV(J)-4.6628E1+
     1(1.8031E-3+(-5.0239E-7+(8.1424E-11-5.0501E-13*T(J))*T(J))*T(J))*
     2T(J)-1.5*TLOG(J))/RHO(J)
   20 WAVE=2.997925E18/AMIN1(FREQ,2.922E15)
      WW=WAVE**2
      SIG=(8.14E-13+1.28E-6/WW+1.61/(WW*WW))/(WW*WW)
      DO 21 J=1,NRHOX
   21 SIGH2(J)=SIG*XNH2(J)
      RETURN
      END
```

```
      SUBROUTINE HLINOP
C     REQUIRES STARK AND COULX
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /OPS/D1(40,13),AHLINE(40),D2(40,8),SHLINE(40),D3(40,2)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION BOLT(40,4),MLAST(40)
      DATA ITEMP1/0/
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      DO 10 J=1,NRHOX
      MLAST(J)=1100./XNE(J)**.133333333
      DO 10 N=1,4
   10 BOLT(J,N)=EXP(-(13.595-13.595/FLOAT(N*N))/TKEV(J))*2.*FLOAT(N*N)*
     1BHYD(J,N)*XNFPH(J,1)/RHO(J)
      ITEMP1=ITEMP
   20 N=SQRT(3.28805E15/FREQ)
      IF(N.EQ.0.OR.N.GT.4)RETURN
      GO TO (21,22,30,30),N
   21 IF(FREQ.LT.2.E15)RETURN
      GO TO 30
   22 IF(FREQ.LT.4.44E14)RETURN
   30 MFREQ=SQRT(3.28805E15/(3.28805E15/FLOAT(N*N)-FREQ))
      DO 50 J=1,NRHOX
      M1=MFREQ
      M2=M1+1
      M1=MAX0(M1,N+1)
      H=0.
      S=0.
      IF(M1.LE.6)GO TO 39
      IF(M1.GT.MLAST(J))GO TO 45
      M1=M1-1
      M2=M2+3
      IF(N.LT.4.OR.M1.GT.8)GO TO 39
      H=STARK(3,4,J)*(1.-EHVKT(J)*BHYD(J,4)/BHYD(J,3))*BOLT(J,3)
      S=H*BNU(J)*STIM(J)/(BHYD(J,3)/BHYD(J,4)-EHVKT(J))
   39 DO 40 M=M1,M2
      BHYDJM=1.
      IF(M.LE.6)BHYDJM=BHYD(J,M)
C     ASSUMING FREQ APROXIMATELY FREQNM
      A=STARK(N,M,J)*(1.-EHVKT(J)*BHYDJM/BHYD(J,N))*BOLT(J,N)
      H=H+A
   40 S=S+A*BNU(J)*STIM(J)/(BHYD(J,N)/BHYDJM-EHVKT(J))
      AHLINE(J)=H
      SHLINE(J)=S/H
      GO TO 50
   45 AHLINE(J)=COULX(N,3.28806E15/FLOAT(N*N),1.)*(1.-EHVKT(J)/
     1BHYD(J,N))*BOLT(J,N)
      SHLINE(J)=BNU(J)*STIM(J)/(BHYD(J,N)-EHVKT(J))
   50 CONTINUE
      RETURN
      END
```

```
      FUNCTION STARK(N,M,J)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNJ(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      DIMENSION FO(40)
      DIMENSION KNMTAB(5,4),FSTARK(10,4)
      REAL NN,MM,IMPACT,KNM,KNMTAB
      DATA KNMTAB/.000356,.000523,.00109,.00149,.00225,.0125,.0177,.028,
     1.0348,.0493,.124,.171,.223,.261,.342,.683,.866,1.02,1.19,1.46/
      DATA FSTARK/.1387,.07910,.02126,.01394,.006462,.004814,.002779,
     1 .002216,.001443,.001201,.3921,.1193,.03766,.02209,.01139,
     2 .008036,.005007,.003850,.002658,.002151,.6103,.1506,.04931,
     3 .02768,.01485,.01023,.006588,.004996,.003542,.002838,.8163,.1788,
     4 .05985,.03189,.01762,.01196,.007825,.005882,.004233,.003375/
C     IF YOUR RYDBERG IS DIFFERENT YOU MAY GET LINES IN STRANGE PLACES
      DATA RYD/3.28805E15/
      DATA ITEMP1/0/
      EXINT(X)=-ALOG(X)-.57516+(.97996-(.21654-(.033572-(.0029222-
     1 1.05439E-4*X)*X)*X)*X)*X
      IF(ITEMP.EQ.ITEMP1)GO TO 20
      DO 10 K=1,NRHOX
   10 FO(K)=1.25E-9*XNE(K)**.6666667
      ITEMP1=ITEMP
   20 XN=N
      XM=M
      X=XN/XM
      XX=X**2
      NN=N*N
      MM=M*M
      MMINN=M-N
      IF(MMINN.GT.5)GO TO 21
      KNM=KNMTAB(MMINN,N)
      GO TO 22
   21 KNM=5.5E-5*(NN*MM)**2/(MM-NN)
   22 IF(MMINN.GT.10)GO TO 23
      FNM=FSTARK(MMINN,N)
      GO TO 30
   23 FNM=FSTARK(10,N)*((20.*XN+100.)/(XN+10.)/XM/(1.-XX))**3
   30 FREQNM=RYD*(1./NN-1./MM)
      DEL=ABS(FREQ-FREQNM)
      DBETA=2.997925E18/FREQNM**2/FO(J)/KNM
      BETA=DBETA*DEL
      Y1=MM*DEL*HKT(J)/2.
      Y2=(3.14159*3.14159/2./.0265384/2.997925E10)*DEL**2/XNE(J)
      QSTAT=1.5+.5*(Y1**2-1.384)/(Y1**2+1.384)
      IMPACT=0.
      IF(Y1.GT.8..OR.Y1.GE.Y2)GO TO 40
      EXY2=0.
      IF(Y2.LE.8.)EXY2=EXINT(Y2)
      IMPACT=1.438*SQRT(Y1*(1.-XX))*(.4*EXP(-Y1)+EXINT(Y1)-.5*EXY2)
   40 IF(BETA.GT.20.)GO TO 45
      PROF=8./(80.+BETA**3)
      RATIO=QSTAT+IMPACT
      GO TO 50
   45 PROF=1.5/BETA/BETA/SQRT(BETA)
      DIOI=6.28*1.48E-25*(2.*MM*RYD/DEL)*XNE(J)*(SQRT(2.*MM*RYD/DEL)*
     1(1.3*QSTAT+.30*IMPACT)-3.9*RYD*HKT(J))
      RATIO=QSTAT*AMIN1(1.+DIOI,1.25)+IMPACT
   50 STARK=.0265384*FNM*PROF*DBETA*RATIO
      RETURN
      END
```

```
      SUBROUTINE LINOP(J,NSTEPS,STEPWT)
C     DUMMY FOR LINE ABSORPTION DISTRIBUTION FUNCTIONS
      COMMON /OPS/D1(40,14),ALINES(40),D2(40,10)
      RETURN
      END


      SUBROUTINE LINSOP(J,NSTEPS,STEPWT)
      COMMON /OPS/D1(40,15),SIGLIN(40),D2(40,9)
C     DUMMY FOR LINE ABSORPTION DISTRIBUTION FUNCTIONS    S=J
      RETURN
      END


      SUBROUTINE XLINOP
      COMMON /OPS/D1(40,16),AXLINE(40),D2(40,6),SXLINE(40),D3(40)
C     DUMMY LINE OPACITY ROUTINE
      RETURN
      END


      SUBROUTINE XLISOP
      COMMON /OPS/D1(40,17),SIGXL(40),D2(40,7)
C     DUMMY LINE SCATTERING ROUTINE
      RETURN
      END


      SUBROUTINE XCONOP
      COMMON /OPS/D1(40,18),AXCONT(40),D2(40,5),SXCONT(40)
C     DUMMY CONTINUOUS OPACITY ROUTINE
      RETURN
      END


      SUBROUTINE XSOP
      COMMON /OPS/D1(40,19),SIGX(40),D2(40,5)
C     DUMMY SCATTERING ROUTINE
      RETURN
      END
```

```
      SUBROUTINE JOSH(IFSCAT,IFSURF)
C     IFSCAT=1  SOLVE INTEGRAL EQUATION FOR SOURCE FUNCTION
C     IFSCAT=0  SET SNU=SBAR
C     IFSURF=0  CALCULATE J AND H
C     IFSURF=1  CALCULATE SURFACE FLUX
C     IFSURF=2  CALCULATE SURFACE SPECIFIC INTENSITY
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
C     COMMON /MATX/COEFJ(43,43),COEFH(43,43),XTAU(43),NXTAU
      COMMON /MATX/C1(43),C2(43),C3(43),C4(43),C5(43),C6(43),C7(43),
     1             C8(43),C9(43),C10(43),C11(43),C12(43),C13(43),
     2             C14(43),C15(43),C16(43),C17(43),C18(43),C19(43),
     3             C20(43),C21(43),C22(43),C23(43),C24(43),C25(43),
     4             C26(43),C27(43),C28(43),C29(43),C30(43),C31(43),
     5             C32(43),C33(43),C34(43),C35(43),C36(43),C37(43),
     6             C38(43),C39(43),C40(43),C41(43),C42(43),C43(43),
C    7             COEFH(43,43),XTAU(43),NXTAU
     7             D1(43),D2(43),D3(43),D4(43),D5(43),D6(43),D7(43),
     8             D8(43),D9(43),D10(43),D11(43),D12(43),D13(43),
     9             D14(43),D15(43),D16(43),D17(43),D18(43),D19(43),
     T             D20(43),D21(43),D22(43),D23(43),D24(43),D25(43),
     1             D26(43),D27(43),D28(43),D29(43),D30(43),D31(43),
     2             D32(43),D33(43),D34(43),D35(43),D36(43),D37(43),
     3             D38(43),D39(43),D40(43),D41(43),D42(43),D43(43),
     4             XTAU(43),NXTAU
      DIMENSION COEFJ(43,43)
      DIMENSION COEFH(43,43)
      EQUIVALENCE (COEFJ(1),C1(1))
      EQUIVALENCE (COEFH(1),D1(1))
      COMMON /MUS/ANGLE(20),SURFI(20),NMU
      COMMON /OPTOT/ACONT(40),SCONT(40),ALINE(40),SLINE(40),SIGMAC(40),
     1              SIGMAL(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNU,JMINS
      DIMENSION XS(43),XSBAR(43),XALPHA(43),DIAG(43),XH(43),XJS(43)
      EQUIVALENCE (XSBAR(1),XH(1)),(XALPHA(1),XJS(1))
      DIMENSION A(40),B(40),C(40),SNUBAR(40)
      EQUIVALENCE (A(1),HNU(1)),(B(1),JNU(1)),(C(1),JMINS(1))
      REAL NEW
      DO 10 J=1,NRHOX
      ABTOT(J)=ACONT(J)+ALINE(J)+SIGMAC(J)+SIGMAL(J)
      ALPHA(J)=(SIGMAC(J)+SIGMAL(J))/ABTOT(J)
   10 SNUBAR(J)=(ACONT(J)*SCONT(J)+ALINE(J)*SLINE(J))/
     1(ACONT(J)+ALINE(J))
      RHOX0=RHOX(1)
      RHOX(1)=0.
      CALL INTEG(RHOX,ABTOT,TAUNU,NRHOX)
      RHOX(1)=RHOX0
      IF(IFSCAT.EQ.1)GO TO 30
      DO 20 J=1,NRHOX
   20 SNU(J)=SNUBAR(J)
      IF(IFSURF.EQ.2)GO TO 70
      MAXJ=MAP1(TAUNU,SNU,NRHOX,XTAU,XS,NXTAU)
      IF(IFSURF.EQ.1)GO TO 60
      DO 21 J=1,NRHOX
   21 ALPHA(J)=0.
   30 MAXJ=MAP1(TAUNU,SNUBAR,NRHOX,XTAU,XSBAR,NXTAU)
      MAXJ=MAP1(TAUNU,ALPHA,NRHOX,XTAU,XALPHA,NXTAU)
      DO 31 L=1,NXTAU
C     IN CASE OF BAD INTERPOLATION
```

```
      IF(XALPHA(L).LT.0.)XALPHA(L)=0.
      XS(L)=XSBAR(L)
      DIAG(L)=1.-XALPHA(L)*COEFJ(L,L)
   31 XSBAR(L)=(1.-XALPHA(L))*XSBAR(L)
C     THE LIMIT ON DO 34, THE MAXIMUM NUMBER OF ITERATIONS, IS ARBITRARY
      DO 34 L=1,NXTAU
      IFERR=0
      K=NXTAU+1
      DO 33 KK=1,NXTAU
      K=K-1
      DELXS=C1(K)*XS(1)+C2(K)*XS(2)+C3(K)*XS(3)+C4(K)*XS(4)+C5(K)*XS(5)+
     1C6(K)*XS(6)+C7(K)*XS(7)+C8(K)*XS(8)+C9(K)*XS(9)+C10(K)*XS(10)+
     2C11(K)*XS(11)+C12(K)*XS(12)+C13(K)*XS(13)+C14(K)*XS(14)+
     3C15(K)*XS(15)+C16(K)*XS(16)+C17(K)*XS(17)+C18(K)*XS(18)+
     4C19(K)*XS(19)+C20(K)*XS(20)+C21(K)*XS(21)+C22(K)*XS(22)+
     5C23(K)*XS(23)+C24(K)*XS(24)+C25(K)*XS(25)+C26(K)*XS(26)+
     6C27(K)*XS(27)+C28(K)*XS(28)+C29(K)*XS(29)+C30(K)*XS(30)+
     7C31(K)*XS(31)+C32(K)*XS(32)+C33(K)*XS(33)+C34(K)*XS(34)+
     8C35(K)*XS(35)+C36(K)*XS(36)+C37(K)*XS(37)+C38(K)*XS(38)+
     9C39(K)*XS(39)+C40(K)*XS(40)+C41(K)*XS(41)+C42(K)*XS(42)+
     TC43(K)*XS(43)
C     DELXS=0.
C     DO 32 M=1,NXTAU
C  32 DELXS=DELXS+COEFJ(K,M)*XS(M)
      DELXS=(DELXS*XALPHA(K)+XSBAR(K)-XS(K))/DIAG(K)
      ERROR=ABS(DELXS/XS(K))
      IF(ERROR.GT..00001)IFERR=1
   33 XS(K)=XS(K)+DELXS
   39 IF(IFERR.EQ.0)GO TO 35
   34 CONTINUE
C
   35 IF(IFSURF.EQ.1)GO TO 60
      MDUMMY=MAP1(XTAU,XS,NXTAU,TAUNU,SNU,MAXJ)
      IF(MAXJ.EQ.NRHOX)GO TO 46
      MAXJ1=MAXJ+1
      DO 40 J=MAXJ1,NRHOX
   40 SNU(J)=SNUBAR(J)
      M=MAX0(MAXJ-1,1)
      NM1=NRHOX-M+1
      NMJ=NRHOX-MAXJ+1
C     THE LIMIT ON DO 45 IS ARBITRARY
      DO 45 L=1,NXTAU
      ERROR=0.
      CALL DERIV(TAUNU(M),SNU(M),HNU(M),NM1)
      DO 41 J=M,NRHOX
   41 HNU(J)=HNU(J)/3.
      CALL DERIV(TAUNU(MAXJ),HNU(MAXJ),JMINS(MAXJ),NMJ)
      DO 43 J=MAXJ1,NRHOX
      JNU(J)=JMINS(J)+SNU(J)
      SNEW=(1.-ALPHA(J))*SNUBAR(J)+ALPHA(J)*JNU(J)
      ERROR=ABS(SNEW-SNU(J))/SNEW+ERROR
   43 SNU(J)=SNEW
      IF(ERROR.LT..00001)GO TO 46
   45 CONTINUE
   46 IF(IFSURF.EQ.2)GO TO 70
C
C  50 DO 51 L=1,NXTAU
C     XJS(L)=-XS(L)
C     XH(L)=0.
C     DO 51 M=1,NXTAU
```

```
C     XJS(L)=XJS(L)+COEFJ(L,M)*XS(M)
C  51 XH(L)=XH(L)+COEFH(L,M)*XS(M)
   50 DO 51 K=1,NXTAU
      XJ    =C1(K)*XS(1)+C2(K)*XS(2)+C3(K)*XS(3)+C4(K)*XS(4)+C5(K)*XS(5)+
     1C6(K)*XS(6)+C7(K)*XS(7)+C8(K)*XS(8)+C9(K)*XS(9)+C10(K)*XS(10)+
     2C11(K)*XS(11)+C12(K)*XS(12)+C13(K)*XS(13)+C14(K)*XS(14)+
     3C15(K)*XS(15)+C16(K)*XS(16)+C17(K)*XS(17)+C18(K)*XS(18)+
     4C19(K)*XS(19)+C20(K)*XS(20)+C21(K)*XS(21)+C22(K)*XS(22)+
     5C23(K)*XS(23)+C24(K)*XS(24)+C25(K)*XS(25)+C26(K)*XS(26)+
     6C27(K)*XS(27)+C28(K)*XS(28)+C29(K)*XS(29)+C30(K)*XS(30)+
     7C31(K)*XS(31)+C32(K)*XS(32)+C33(K)*XS(33)+C34(K)*XS(34)+
     8C35(K)*XS(35)+C36(K)*XS(36)+C37(K)*XS(37)+C38(K)*XS(38)+
     9C39(K)*XS(39)+C40(K)*XS(40)+C41(K)*XS(41)+C42(K)*XS(42)+
     TC43(K)*XS(43)
      XJS(K)=XJ-XS(K)
      XH(K)=D1(K)*XS(1)+D2(K)*XS(2)+D3(K)*XS(3)+D4(K)*XS(4)+D5(K)*XS(5)+
     1D6(K)*XS(6)+D7(K)*XS(7)+D8(K)*XS(8)+D9(K)*XS(9)+D10(K)*XS(10)+
     2D11(K)*XS(11)+D12(K)*XS(12)+D13(K)*XS(13)+D14(K)*XS(14)+
     3D15(K)*XS(15)+D16(K)*XS(16)+D17(K)*XS(17)+D18(K)*XS(18)+
     4D19(K)*XS(19)+D20(K)*XS(20)+D21(K)*XS(21)+D22(K)*XS(22)+
     5D23(K)*XS(23)+D24(K)*XS(24)+D25(K)*XS(25)+D26(K)*XS(26)+
     6D27(K)*XS(27)+D28(K)*XS(28)+D29(K)*XS(29)+D30(K)*XS(30)+
     7D31(K)*XS(31)+D32(K)*XS(32)+D33(K)*XS(33)+D34(K)*XS(34)+
     8D35(K)*XS(35)+D36(K)*XS(36)+D37(K)*XS(37)+D38(K)*XS(38)+
     9D39(K)*XS(39)+D40(K)*XS(40)+D41(K)*XS(41)+D42(K)*XS(42)+
     TD43(K)*XS(43)
   51 CONTINUE
      MDUMMY=MAP1(XTAU,XJS,NXTAU,TAUNU,JMINS,MAXJ)
      MDUMMY=MAP1(XTAU,XH,NXTAU,TAUNU,HNU,MAXJ)
      DO 52 J=1,MAXJ
   52 JNU(J)=JMINS(J)+SNU(J)
      RETURN
C
   60 HNU(1)=0.
      DO 61 M=1,NXTAU
   61 HNU(1)=HNU(1)+COEFH(1,M)*XS(M)
      RETURN
   70 CALL PARCOE(SNU,TAUNU,A,B,C,NRHOX)
      N1=NRHOX-1
      DO 74 MU=1,NMU
      OLD=1.
      SUM=0.
      DO 73 J=1,N1
      NEW=0.
      TANGLE=TAUNU(J+1)/ANGLE(MU)
      IF(TANGLE.LT.50.)NEW=EXP(-TANGLE)
      D=TANGLE-TAUNU(J)/ANGLE(MU)
      IF(D.LE..03)GO TO 72
      SUM=SUM+OLD*(SNU(J)+((B(J)+2.*C(J)*TAUNU(J))+2.*C(J)*
     1ANGLE(MU))*ANGLE(MU))-NEW*(SNU(J+1)+((B(J)+2.*C(J)*TAUNU(J+1))+
     2 2.*C(J)*ANGLE(MU))*ANGLE(MU))
      GO TO 73
   72 SUM=SUM+NEW*(SNU(J)+(SNU(J)+(B(J)+2.*C(J)*TAUNU(J))*ANGLE(MU)+
     1(SNU(J)+(B(J)+2.*C(J)*TAUNU(J)+2.*C(J)*ANGLE(MU))*ANGLE(MU))*
     2((((((D/9.+1.)*D/8.+1.)*D/7.+1.)*D/6.+1.)*D/5.+1.)*D/4.+1.)*
     3D/3.)*D/2.)*D
   73 OLD=NEW
   74 SURFI(MU)=SUM+OLD*(SNU(NRHOX)+((B(NRHOX)+2.*C(NRHOX)*
     1TAUNU(NRHOX))+2.*C(NRHOX)*ANGLE(MU))*ANGLE(MU))
      RETURN
      END
```

```
      SUBROUTINE BLOCKJ
C     CAN BE BLOCK DATA INSTEAD OF SUBROUTINE
      COMMON /MATX/CJ(1849),CH(1849),XTAU(43),NXTAU
      DIMENSION CJ   1(36),CJ   2(36),CJ   3(36),CJ   4(36),CJ   5(36)
      DIMENSION CJ   6(36),CJ   7(36),CJ   8(36),CJ   9(36),CJ  10(36)
      DIMENSION CJ  11(36),CJ  12(36),CJ  13(36),CJ  14(36),CJ  15(36)
      DIMENSION CJ  16(36),CJ  17(36),CJ  18(36),CJ  19(36),CJ  20(36)
      DIMENSION CJ  21(36),CJ  22(36),CJ  23(36),CJ  24(36),CJ  25(36)
      DIMENSION CJ  26(36),CJ  27(36),CJ  28(36),CJ  29(36),CJ  30(36)
      DIMENSION CJ  31(36),CJ  32(36),CJ  33(36),CJ  34(36),CJ  35(36)
      DIMENSION CJ  36(36),CJ  37(36),CJ  38(36),CJ  39(36),CJ  40(36)
      DIMENSION CJ  41(36),CJ  42(36),CJ  43(36),CJ  44(36),CJ  45(36)
      DIMENSION CJ  46(36),CJ  47(36),CJ  48(36),CJ  49(36),CJ  50(36)
      DIMENSION CJ  51(36),CJ  52(13)
      EQUIVALENCE (CJ   1(1),CJ (   1)),(CJ   2(1),CJ (  37))
      EQUIVALENCE (CJ   3(1),CJ (  73)),(CJ   4(1),CJ ( 109))
      EQUIVALENCE (CJ   5(1),CJ ( 145)),(CJ   6(1),CJ ( 181))
      EQUIVALENCE (CJ   7(1),CJ ( 217)),(CJ   8(1),CJ ( 253))
      EQUIVALENCE (CJ   9(1),CJ ( 289)),(CJ  10(1),CJ ( 325))
      EQUIVALENCE (CJ  11(1),CJ ( 361)),(CJ  12(1),CJ ( 397))
      EQUIVALENCE (CJ  13(1),CJ ( 433)),(CJ  14(1),CJ ( 469))
      EQUIVALENCE (CJ  15(1),CJ ( 505)),(CJ  16(1),CJ ( 541))
      EQUIVALENCE (CJ  17(1),CJ ( 577)),(CJ  18(1),CJ ( 613))
      EQUIVALENCE (CJ  19(1),CJ ( 649)),(CJ  20(1),CJ ( 685))
      EQUIVALENCE (CJ  21(1),CJ ( 721)),(CJ  22(1),CJ ( 757))
      EQUIVALENCE (CJ  23(1),CJ ( 793)),(CJ  24(1),CJ ( 829))
      EQUIVALENCE (CJ  25(1),CJ ( 865)),(CJ  26(1),CJ ( 901))
      EQUIVALENCE (CJ  27(1),CJ ( 937)),(CJ  28(1),CJ ( 973))
      EQUIVALENCE (CJ  29(1),CJ (1009)),(CJ  30(1),CJ (1045))
      EQUIVALENCE (CJ  31(1),CJ (1081)),(CJ  32(1),CJ (1117))
      EQUIVALENCE (CJ  33(1),CJ (1153)),(CJ  34(1),CJ (1189))
      EQUIVALENCE (CJ  35(1),CJ (1225)),(CJ  36(1),CJ (1261))
      EQUIVALENCE (CJ  37(1),CJ (1297)),(CJ  38(1),CJ (1333))
      EQUIVALENCE (CJ  39(1),CJ (1369)),(CJ  40(1),CJ (1405))
      EQUIVALENCE (CJ  41(1),CJ (1441)),(CJ  42(1),CJ (1477))
      EQUIVALENCE (CJ  43(1),CJ (1513)),(CJ  44(1),CJ (1549))
      EQUIVALENCE (CJ  45(1),CJ (1585)),(CJ  46(1),CJ (1621))
      EQUIVALENCE (CJ  47(1),CJ (1657)),(CJ  48(1),CJ (1693))
      EQUIVALENCE (CJ  49(1),CJ (1729)),(CJ  50(1),CJ (1765))
      EQUIVALENCE (CJ  51(1),CJ (1801)),(CJ  52(1),CJ (1837))
      DATA CJ   1/
     1 8.14986025E-05, 7.31538254E-05, 6.71178656E-05, 6.24581491E-05,
     2 5.79414138E-05, 5.36599004E-05, 4.95677731E-05, 4.53702132E-05,
     3 4.11409031E-05, 3.70180419E-05, 3.30221502E-05, 2.88995437E-05,
     4 2.55766809E-05, 2.24455861E-05, 1.88519709E-05, 1.58867744E-05,
     5 1.33092440E-05, 1.09509308E-05, 8.86744834E-06, 6.98752785E-06,
     6 5.33944478E-06, 4.00549621E-06, 3.06255733E-06, 2.30471158E-06,
     7 1.70829464E-06, 1.22756917E-06, 8.97423163E-07, 6.17580912E-07,
     8 4.31441568E-07, 2.84814120E-07, 1.90447891E-07, 1.28648434E-07,
     9 7.72171575E-08, 4.14502255E-08, 2.00042982E-08, 8.21662923E-09/
      DATA CJ   2/
     1 2.04916539E-09, 3.36821047E-10, 2.97451696E-11, 1.98489427E-12,
     2 1.37287283E-13, 9.73803273E-15, 7.03780218E-16, 1.50153547E-04,
     3 1.69998410E-04, 1.49551568E-04, 1.33114548E-04, 1.22341492E-04,
     4 1.12691930E-04, 1.03789120E-04, 9.48288272E-05, 8.58965958E-05,
     5 7.72399845E-05, 6.88765300E-05, 6.02632697E-05, 5.33275330E-05,
     6 4.67953579E-05, 3.93007243E-05, 3.31179453E-05, 2.77440975E-05,
     7 2.28276312E-05, 1.84843096E-05, 1.45654595E-05, 1.11299644E-05,
     8 8.34933442E-06, 6.38378621E-06, 4.80407272E-06, 3.56085984E-06,
     9 2.55880582E-06, 1.87063082E-06, 1.28731302E-06, 8.99315117E-07/
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 DATA CJ    3/
1 5.93678149E-07, 3.96977081E-07, 2.68159722E-07, 1.60954311E-07,
2 8.64003431E-08, 4.16976593E-08, 1.71270216E-08, 4.27134786E-09,
3 7.02080564E-10, 6.20017576E-11, 4.13737418E-12, 2.86165744E-13,
4 2.02982455E-14, 1.46698029E-15, 1.38762226E-04, 1.52892603E-04,
5 1.73973599E-04, 1.48361768E-04, 1.27782783E-04, 1.16648599E-04,
6 1.06792177E-04, 9.72270010E-05, 8.78857753E-05, 7.89334108E-05,
7 7.03363020E-05, 6.15124360E-05, 5.44199981E-05, 4.77466096E-05,
8 4.00947229E-05, 3.37846547E-05, 2.83013360E-05, 2.32853712E-05,
9 1.88545261E-05, 1.48569320E-05, 1.13525420E-05, 8.51622518E-06/
 DATA CJ    4/
1 6.51134817E-06, 4.90004469E-06, 3.63198185E-06, 2.60990507E-06,
2 1.90798268E-06, 1.31301454E-06, 9.17268607E-07, 6.05529102E-07,
3 4.04901009E-07, 2.73512100E-07, 1.64166733E-07, 8.81246833E-08,
4 4.25298033E-08, 1.74688037E-08, 4.35658139E-09, 7.16089755E-10,
5 6.32388810E-11, 4.21992498E-12, 2.91875343E-13, 2.07032318E-14,
6 1.49624885E-15, 2.56894537E-04, 2.68265016E-04, 2.82680119E-04,
7 3.20147632E-04, 2.71320447E-04, 2.33081797E-04, 2.11908717E-04,
8 1.91950967E-04, 1.73009337E-04, 1.55132197E-04, 1.38103891E-04,
9 1.20705419E-04, 1.06754481E-04, 9.36443364E-05, 7.86242175E-05/
 DATA CJ    5/
1 6.62442877E-05, 5.54893860E-05, 4.56528336E-05, 3.69646972E-05,
2 2.91266743E-05, 2.22560211E-05, 1.66953761E-05, 1.27648716E-05,
3 9.60600474E-06, 7.12006931E-06, 5.11638732E-06, 3.74034592E-06,
4 2.57398256E-06, 1.79817365E-06, 1.18705058E-06, 7.93747494E-07,
5 5.36178620E-07, 3.21823317E-07, 1.72754489E-07, 8.33728443E-08,
6 3.42447430E-08, 8.54035678E-09, 1.40377384E-09, 1.23969092E-10,
7 8.27244054E-12, 5.72171358E-13, 4.05851067E-14, 2.93313638E-15,
8 4.28478661E-04, 4.38774832E-04, 4.48007290E-04, 4.74192405E-04,
9 5.41887599E-04, 4.55714232E-04, 3.88809427E-04, 3.48834558E-04/
 DATA CJ    6/
1 3.12498628E-04, 2.79274670E-04, 2.48145814E-04, 2.16625539E-04,
2 1.91470492E-04, 1.67889720E-04, 1.40916781E-04, 1.18707073E-04,
3 9.94231585E-05, 8.17917639E-05, 6.62222043E-05, 5.21781154E-05,
4 3.98685750E-05, 2.99067370E-05, 2.28655892E-05, 1.72069282E-05,
5 1.27538260E-05, 9.16465428E-06, 6.69979937E-06, 4.61055441E-06,
6 3.22090046E-06, 2.12624430E-06, 1.42175560E-06, 9.60397422E-07,
7 5.76444952E-07, 3.09434371E-07, 1.49335410E-07, 6.13382136E-08,
8 1.52972066E-08, 2.51438798E-09, 2.22048435E-10, 1.48172404E-11,
9 1.02484777E-12, 7.26941783E-14, 5.25369629E-15, 6.81346357E-04/
 DATA CJ    7/
1 6.90881617E-04, 6.98754282E-04, 7.15098172E-04, 7.61797143E-04,
2 8.79148724E-04, 7.30251690E-04, 6.11067387E-04, 5.42551009E-04,
3 4.82001904E-04, 4.26857352E-04, 3.71876580E-04, 3.28350939E-04,
4 2.87718988E-04, 2.41367155E-04, 2.03264175E-04, 1.70210809E-04,
5 1.40006824E-04, 1.13344596E-04, 8.93004808E-05, 6.82295010E-05,
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2-1.21476176E-09,-1.21508339E-09,-1.21567326E-09,-1.21674650E-09,
3-1.21862695E-09,-1.22185740E-09,-1.22780229E-09,-1.23595589E-09,
4-1.24828859E-09,-1.27192260E-09,-1.30461649E-09,-1.35002457E-09,
5-1.41565584E-09,-1.50763296E-09,-1.64151023E-09,-1.83746665E-09,
6-2.11003211E-09,-2.43680651E-09,-2.87773197E-09,-3.47545902E-09,
7-4.34090389E-09,-5.42383519E-09,-7.16876756E-09,-9.48085809E-09,
8-1.32707815E-08,-1.85935498E-08,-2.60775219E-08,-4.10071712E-08,
9-7.24179015E-08,-1.43956009E-07,-3.42506712E-07,-1.40134936E-06/
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      DATA CJ  51/
     1-9.70094682E-06,-1.65409793E-04,-9.75158564E-03, 9.41592324E-02,
     2 8.42018552E-01, 2.00443013E-02,-9.09966467E-11,-9.09998056E-11,
     3-9.10021749E-11,-9.10065186E-11,-9.10144169E-11,-9.10282406E-11,
     4-9.10519432E-11,-9.10954140E-11,-9.11745054E-11,-9.13130813E-11,
     5-9.15511324E-11,-9.19891800E-11,-9.25899129E-11,-9.34984102E-11,
     6-9.52389670E-11,-9.76457687E-11,-1.00986696E-10,-1.05811883E-10,
     7-1.12567016E-10,-1.22385705E-10,-1.36730202E-10,-1.56634264E-10,
     8-1.80431063E-10,-2.12441329E-10,-2.55678370E-10,-3.18012771E-10,
     9-3.95642810E-10,-5.20035550E-10,-6.83820118E-10,-9.50336363E-10/
      DATA CJ  52/
     1-1.32157045E-09,-1.83904531E-09,-2.86022274E-09,-4.97692943E-09,
     2-9.70293516E-09,-2.24631475E-08,-8.71919425E-08,-5.48748367E-07,
     3-7.48344600E-06,-1.80376685E-04,-1.01123390E-02, 7.39345544E-02,
     4 9.89887661E-01/
      DATA XTAU/0.,              .000032,.000056,.0001,.00018,.00032,
     1.00056,.001,.0018,.0032,.0056,.01,.016,.025,.042,.065,
     2.096,.139,.196,.273,.375,.5,.63,.78,.95,1.15,1.35,1.6,1.85,2.15,
     32.45,2.75,3.15,3.65,4.25,5.0,6.2,7.8,10.,12.5,15.,17.5,20./
      DATA NXTAU/43/
      END




      SUBROUTINE BLOCKH
C     CAN BE BLOCK DATA INSTEAD OF SUBROUTINE
      COMMON /MATX/CJ(1849),CH(1849),XTAU(43),NXTAU
      DIMENSION CH   1(36),CH   2(36),CH   3(36),CH   4(36),CH   5(36)
      DIMENSION CH   6(36),CH   7(36),CH   8(36),CH   9(36),CH  10(36)
      DIMENSION CH  11(36),CH  12(36),CH  13(36),CH  14(36),CH  15(36)
      DIMENSION CH  16(36),CH  17(36),CH  18(36),CH  19(36),CH  20(36)
      DIMENSION CH  21(36),CH  22(36),CH  23(36),CH  24(36),CH  25(36)
      DIMENSION CH  26(36),CH  27(36),CH  28(36),CH  29(36),CH  30(36)
      DIMENSION CH  31(36),CH  32(36),CH  33(36),CH  34(36),CH  35(36)
      DIMENSION CH  36(36),CH  37(36),CH  38(36),CH  39(36),CH  40(36)
      DIMENSION CH  41(36),CH  42(36),CH  43(36),CH  44(36),CH  45(36)
      DIMENSION CH  46(36),CH  47(36),CH  48(36),CH  49(36),CH  50(36)
      DIMENSION CH  51(36),CH  52(13)
      EQUIVALENCE (CH   1(1),CH (   1)),(CH   2(1),CH (  37))
      EQUIVALENCE (CH   3(1),CH (  73)),(CH   4(1),CH ( 109))
      EQUIVALENCE (CH   5(1),CH ( 145)),(CH   6(1),CH ( 181))
      EQUIVALENCE (CH   7(1),CH ( 217)),(CH   8(1),CH ( 253))
      EQUIVALENCE (CH   9(1),CH ( 289)),(CH  10(1),CH ( 325))
      EQUIVALENCE (CH  11(1),CH ( 361)),(CH  12(1),CH ( 397))
      EQUIVALENCE (CH  13(1),CH ( 433)),(CH  14(1),CH ( 469))
      EQUIVALENCE (CH  15(1),CH ( 505)),(CH  16(1),CH ( 541))
      EQUIVALENCE (CH  17(1),CH ( 577)),(CH  18(1),CH ( 613))
      EQUIVALENCE (CH  19(1),CH ( 649)),(CH  20(1),CH ( 685))
      EQUIVALENCE (CH  21(1),CH ( 721)),(CH  22(1),CH ( 757))
      EQUIVALENCE (CH  23(1),CH ( 793)),(CH  24(1),CH ( 829))
      EQUIVALENCE (CH  25(1),CH ( 865)),(CH  26(1),CH ( 901))
      EQUIVALENCE (CH  27(1),CH ( 937)),(CH  28(1),CH ( 973))
      EQUIVALENCE (CH  29(1),CH (1009)),(CH  30(1),CH (1045))
      EQUIVALENCE (CH  31(1),CH (1081)),(CH  32(1),CH (1117))
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 EQUIVALENCE (CH  33(1),CH (1153)),(CH  34(1),CH (1189))
 EQUIVALENCE (CH  35(1),CH (1225)),(CH  36(1),CH (1261))
 EQUIVALENCE (CH  37(1),CH (1297)),(CH  38(1),CH (1333))
 EQUIVALENCE (CH  39(1),CH (1369)),(CH  40(1),CH (1405))
 EQUIVALENCE (CH  41(1),CH (1441)),(CH  42(1),CH (1477))
 EQUIVALENCE (CH  43(1),CH (1513)),(CH  44(1),CH (1549))
 EQUIVALENCE (CH  45(1),CH (1585)),(CH  46(1),CH (1621))
 EQUIVALENCE (CH  47(1),CH (1657)),(CH  48(1),CH (1693))
 EQUIVALENCE (CH  49(1),CH (1729)),(CH  50(1),CH (1765))
 EQUIVALENCE (CH  51(1),CH (1801)),(CH  52(1),CH (1837))
 DATA CH    1/
1 7.15468111E-06,-7.63518254E-06,-7.15194190E-06,-7.14908817E-06,
2-7.14434126E-06,-7.13655915E-06,-7.12412582E-06,-7.10337944E-06,
3-7.06894113E-06,-7.01450683E-06,-6.93090638E-06,-6.79555793E-06,
4-6.63291776E-06,-6.41788366E-06,-6.06957067E-06,-5.67267991E-06,
5-5.22293773E-06,-4.70482715E-06,-4.14396013E-06,-3.53845938E-06,
6-2.91564752E-06,-2.33731168E-06,-1.88157141E-06,-1.48246502E-06,
7-1.14445670E-06,-8.53997483E-07,-6.43477679E-07,-4.56544435E-07,
8-3.26945808E-07,-2.21153320E-07,-1.50877193E-07,-1.03653072E-07,
9-6.33945709E-08,-3.46862852E-08,-1.70494808E-08,-7.13023297E-09/
 DATA CH    2/
1-1.81676142E-09,-3.04652954E-10,-2.74072641E-11,-1.85486483E-12,
2-1.29572640E-13,-9.25877958E-15,-6.72963730E-16, 1.49104109E-05,
3-3.90201199E-06,-1.61388810E-05,-1.49037775E-05,-1.48935421E-05,
4-1.48771099E-05,-1.48514527E-05,-1.48079226E-05,-1.47359130E-05,
5-1.46223031E-05,-1.44479043E-05,-1.41656379E-05,-1.38265136E-05,
6-1.33781866E-05,-1.26520376E-05,-1.18246559E-05,-1.08871250E-05,
7-9.80709529E-06,-8.63795420E-06,-7.37578617E-06,-6.07754325E-06,
8-4.87201699E-06,-3.92204193E-06,-3.09012066E-06,-2.38555751E-06,
9-1.78010945E-06,-1.34129184E-06,-9.51639673E-07,-6.81498671E-07/
 DATA CH    3/
1-4.60980408E-07,-3.14494034E-07,-2.16058241E-07,-1.32141902E-07,
2-7.23012998E-08,-3.55385179E-08,-1.48624949E-08,-3.78691638E-09,
3-6.35028248E-10,-5.71285479E-11,-3.86633654E-12,-2.70085094E-13,
4-1.92992751E-14,-1.40274544E-15, 1.52026574E-05, 1.68173785E-05,
5 4.09890951E-06,-1.75587254E-05,-1.51942778E-05,-1.51773709E-05,
6-1.51506530E-05,-1.51059123E-05,-1.50322201E-05,-1.49160857E-05,
7-1.47379368E-05,-1.44497640E-05,-1.41036562E-05,-1.36461842E-05,
8-1.29053252E-05,-1.20612605E-05,-1.11048794E-05,-1.00031765E-05,
9-8.81060628E-06,-7.52317033E-06,-6.19895694E-06,-4.96932846E-06/
 DATA CH    4/
1-4.00036789E-06,-3.15182512E-06,-2.43318816E-06,-1.81564832E-06,
2-1.36806808E-06,-9.70635957E-07,-6.95101755E-07,-4.70181345E-07,
3-3.20770911E-07,-2.20370321E-07,-1.34779083E-07,-7.37441757E-08,
4-3.62477144E-08,-1.51590763E-08,-3.86248133E-09,-6.47699272E-10,
5-5.82684230E-11,-3.94347888E-12,-2.75473821E-13,-1.96843285E-14,
6-1.43073233E-15, 2.97896810E-05, 2.97980436E-05, 3.02862105E-05,
7 5.50647710E-06,-3.39987917E-05,-2.97607355E-05,-2.97074452E-05,
8-2.96191403E-05,-2.94741216E-05,-2.92456743E-05,-2.88957424E-05,
9-2.83301186E-05,-2.76510734E-05,-2.67537628E-05,-2.53008644E-05/
 DATA CH    5/
1-2.36457701E-05,-2.17705777E-05,-1.96105587E-05,-1.72724667E-05,
2-1.47484513E-05,-1.21523844E-05,-9.74178213E-06,-7.84222059E-06,
3-6.17873953E-06,-4.76993351E-06,-3.55932255E-06,-2.68189971E-06,
4-1.90278810E-06,-1.36264217E-06,-9.21718380E-07,-6.28821467E-07,
5-4.32001343E-07,-2.64212927E-07,-1.44563571E-07,-7.10577364E-08,
6-2.97168721E-08,-7.57175055E-09,-1.26970521E-09,-1.14225320E-10,
7-7.73051375E-12,-5.40018920E-13,-3.85877188E-14,-2.80470236E-15,
8 5.33166565E-05, 5.33305336E-05, 5.33411719E-05, 5.45903541E-05,
9 9.45344282E-06,-5.98750876E-05,-5.32380787E-05,-5.30767814E-05/
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 DATA CH   6/
1-5.28138232E-05,-5.24019312E-05,-5.17726512E-05,-5.07570460E-05,
2-4.95388096E-05,-4.79297869E-05,-4.53254263E-05,-4.23593245E-05,
3-3.89992680E-05,-3.51292236E-05,-3.09404208E-05,-2.64187551E-05,
4-2.17681883E-05,-1.74499821E-05,-1.40472898E-05,-1.10675313E-05,
5-8.54399479E-06,-6.37549656E-06,-4.80383043E-06,-3.40827054E-06,
6-2.44075547E-06,-1.65097143E-06,-1.12633544E-06,-7.73792885E-07,
7-4.73252449E-07,-2.58938632E-07,-1.27276602E-07,-5.32279265E-08,
8-1.35622540E-08,-2.27424725E-09,-2.04595667E-10,-1.38465591E-11,
9-9.67257493E-13,-6.91165342E-14,-5.02365045E-15, 9.11154271E-05/
 DATA CH   7/
1 9.11373857E-05, 9.11540613E-05, 9.11851613E-05, 9.35975905E-05,
2 1.47063981E-05,-1.03462545E-04,-9.08852056E-05,-9.04268240E-05,
3-8.97143108E-05,-8.86303376E-05,-8.68853571E-05,-8.47952605E-05,
4-8.20369956E-05,-7.75751291E-05,-7.24955321E-05,-6.67426582E-05,
5-6.01176981E-05,-5.29478997E-05,-4.52090066E-05,-3.72500018E-05,
6-2.98601473E-05,-2.40372258E-05,-1.89381774E-05,-1.46199094E-05,
7-1.09092379E-05,-8.21988044E-06,-5.83189075E-06,-4.17635691E-06,
8-2.82495145E-06,-1.92724820E-06,-1.32401640E-06,-8.09767079E-07,
9-4.43060175E-07,-2.17777566E-07,-9.10757716E-08,-2.32056491E-08/
 DATA CH   8/
1-3.89133110E-09,-3.50070669E-10,-2.36919192E-11,-1.65500706E-12,
2-1.18260370E-13,-8.59560278E-15, 1.61084638E-04, 1.61120455E-04,
3 1.61147523E-04, 1.61197627E-04, 1.61290471E-04, 1.65663480E-04,
4 3.12833419E-05,-1.84767459E-04,-1.60383513E-04,-1.59095624E-04,
5-1.57151776E-04,-1.54037375E-04,-1.50316852E-04,-1.45414273E-04,
6-1.37492118E-04,-1.28479528E-04,-1.18276734E-04,-1.06530685E-04,
7-9.38212441E-05,-8.01050512E-05,-6.60003185E-05,-5.29053047E-05,
8-4.25875346E-05,-3.35527875E-05,-2.59017163E-05,-1.93273550E-05,
9-1.45626021E-05,-1.03318579E-05,-7.39883160E-06,-5.00464369E-06/
 DATA CH   9/
1-3.41426413E-06,-2.34558186E-06,-1.43454739E-06,-7.84901321E-07,
2-3.85800856E-07,-1.61343209E-07,-4.11091944E-08,-6.89352042E-09,
3-6.20149585E-10,-4.19700385E-11,-2.93182374E-12,-2.09496329E-13,
4-1.52269488E-14, 2.95118055E-04, 2.95178254E-04, 2.95223603E-04,
5 2.95307214E-04, 2.95460869E-04, 2.95735398E-04, 3.02765668E-04,
6 5.58676946E-05,-3.37573853E-04,-2.93054976E-04,-2.89397455E-04,
7-2.83590510E-04,-2.76688690E-04,-2.67619892E-04,-2.52994639E-04,
8-2.36378122E-04,-2.17582125E-04,-1.95954621E-04,-1.72562085E-04,
9-1.47323476E-04,-1.21375266E-04,-9.72882826E-05,-7.83117813E-05/
 DATA CH  10/
1-6.16962878E-05,-4.76263106E-05,-3.55369461E-05,-2.67755473E-05,
2-1.89963282E-05,-1.36034154E-05,-9.20135573E-06,-6.27727001E-06,
3-4.31241145E-06,-2.63742438E-06,-1.44303115E-06,-7.09283125E-07,
4-2.96621802E-07,-7.55764702E-08,-1.26731441E-08,-1.14008132E-09,
5-7.71570818E-11,-5.38979485E-12,-3.85131719E-13,-2.79926878E-14,
6 5.27450267E-04, 5.27548209E-04, 5.27621866E-04, 5.27757352E-04,
7 5.28005236E-04, 5.28444092E-04, 5.29212980E-04, 5.42982886E-04,
8 9.43257262E-05,-5.94289095E-04,-5.21949858E-04,-5.11218869E-04,
9-4.98593743E-04,-4.82097986E-04,-4.55597512E-04,-4.25563821E-04/
 DATA CH  11/
1-3.91641331E-04,-3.52647471E-04,-3.10500866E-04,-2.65051281E-04,
2-2.18341644E-04,-1.74994619E-04,-1.40851146E-04,-1.10959921E-04,
3-8.56508809E-05,-6.39065263E-05,-4.81490961E-05,-3.41589441E-05,
4-2.44608124E-05,-1.65448705E-05,-1.12868617E-05,-7.75380763E-06,
5-4.74205493E-06,-2.59450211E-06,-1.27523489E-06,-5.33293310E-07,
6-1.35875428E-07,-2.27840386E-08,-2.04962735E-09,-1.38710531E-10,
7-9.68951630E-12,-6.92367014E-13,-5.03233504E-14, 8.67939527E-04,
8 8.68086519E-04, 8.68196952E-04, 8.68399838E-04, 8.68770151E-04,
9 8.69422777E-04, 8.70555854E-04, 8.72685043E-04, 9.00316827E-04/
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 DATA CH  12/
1 1.18726820E-04,-1.05068040E-03,-8.51640282E-04,-8.30180001E-04,
2-8.02328557E-04,-7.57838031E-04,-7.07603820E-04,-6.50991942E-04,
3-5.86013815E-04,-5.15855799E-04,-4.40257134E-04,-3.62606802E-04,
4-2.90576808E-04,-2.33857067E-04,-1.84211669E-04,-1.42183646E-04,
5-1.06079989E-04,-7.99196360E-05,-5.66953416E-05,-4.05972023E-05,
6-2.74581721E-05,-1.87312937E-05,-1.28676222E-05,-7.86932554E-06,
7-4.30539149E-06,-2.11610499E-06,-8.84915842E-07,-2.25456988E-07,
8-3.78043305E-08,-3.40075163E-09,-2.30144881E-10,-1.60763829E-11,
9-1.14873131E-12,-8.34926889E-14, 1.61498414E-03, 1.61522856E-03/
 DATA CH  13/
1 1.61541206E-03, 1.61574893E-03, 1.61636286E-03, 1.61744182E-03,
2 1.61930543E-03, 1.62277036E-03, 1.62924770E-03, 1.68333458E-03,
3 3.60899757E-04,-1.82730765E-03,-1.58410667E-03,-1.52899488E-03,
4-1.44234855E-03,-1.34546950E-03,-1.23689296E-03,-1.11271628E-03,
5-9.78971597E-04,-8.35109934E-04,-6.87538020E-04,-5.50779439E-04,
6-4.43161682E-04,-3.49011624E-04,-2.69337615E-04,-2.00915634E-04,
7-1.51349791E-04,-1.07355641E-04,-7.68658545E-05,-5.19840976E-05,
8-3.54597507E-05,-2.43579442E-05,-1.48953901E-05,-8.14890300E-06,
9-4.00495346E-06,-1.67469957E-06,-4.26647390E-07,-7.15352259E-08/
 DATA CH  14/
1-6.43470743E-09,-4.35448549E-10,-3.04166311E-11,-2.17336083E-12,
2-1.57962724E-13, 2.50720905E-03, 2.50755068E-03, 2.50780708E-03,
3 2.50827754E-03, 2.50913426E-03, 2.51063770E-03, 2.51322757E-03,
4 2.51801809E-03, 2.52687709E-03, 2.54289614E-03, 2.63774332E-03,
5 1.76260416E-04,-2.78126196E-03,-2.45704320E-03,-2.31262955E-03,
6-2.15394575E-03,-1.97774832E-03,-1.77739883E-03,-1.56245308E-03,
7-1.33188374E-03,-1.09584644E-03,-8.77427902E-04,-7.05726344E-04,
8-5.55621605E-04,-4.28668973E-04,-3.19696027E-04,-2.40783539E-04,
9-1.70762699E-04,-1.22247776E-04,-8.26646695E-05,-5.63817215E-05/
 DATA CH  15/
1-3.87261829E-05,-2.36795672E-05,-1.29532571E-05,-6.36557648E-06,
2-2.66157673E-06,-6.77995222E-07,-1.13667632E-07,-1.02237148E-08,
3-6.91813611E-10,-4.83219157E-11,-3.45263538E-12,-2.50935807E-13,
4 3.20994276E-03, 3.21034034E-03, 3.21063867E-03, 3.21118592E-03,
5 3.21218201E-03, 3.21392850E-03, 3.21693250E-03, 3.22247328E-03,
6 3.23266196E-03, 3.25087011E-03, 3.28333413E-03, 3.52880121E-03,
7 2.90599435E-04,-3.99201557E-03,-3.07880403E-03,-2.86239707E-03,
8-2.62426711E-03,-2.35540482E-03,-2.06836350E-03,-1.76152461E-03,
9-1.44821000E-03,-1.15882208E-03,-9.31623746E-04,-7.33184814E-04/
 DATA CH  16/
1-5.65473991E-04,-4.21599458E-04,-3.17461291E-04,-2.25092147E-04,
2-1.61113538E-04,-1.08927603E-04,-7.42843836E-05,-5.10170507E-05,
3-3.11911486E-05,-1.70601847E-05,-8.38286988E-06,-3.50466057E-06,
4-8.92642574E-07,-1.49636185E-07,-1.34574290E-08,-9.10558142E-10,
5-6.35972818E-11,-4.54388504E-12,-3.30236900E-13, 5.61912502E-03,
6 5.61974854E-03, 5.62021633E-03, 5.62107432E-03, 5.62263546E-03,
7 5.62537113E-03, 5.63007179E-03, 5.63872596E-03, 5.65458361E-03,
8 5.68273038E-03, 5.73223829E-03, 5.82772200E-03, 6.17039808E-03,
9 1.43639190E-03,-6.68103918E-03,-5.37711410E-03,-4.91201049E-03/
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3-7.78728323E-04,-5.86104634E-04,-4.15382293E-04,-2.97210854E-04,
4-2.00873337E-04,-1.36950183E-04,-9.40333957E-05,-5.74765590E-05,
5-3.14294076E-05,-1.54399049E-05,-6.45358275E-06,-1.64330990E-06,
6-2.75407226E-07,-2.47632234E-08,-1.67526173E-09,-1.16994342E-10,
7-8.35829727E-12,-6.07419294E-13, 8.60872637E-03, 8.60958456E-03,
8 8.61022836E-03, 8.61140900E-03, 8.61355681E-03, 8.61731911E-03,
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3-6.43680809E-03,-5.45363991E-03,-4.46443150E-03,-3.56017279E-03,
4-2.85517842E-03,-2.24242398E-03,-1.72651510E-03,-1.28528029E-03,
5-9.66674652E-04,-6.84627687E-04,-4.89594200E-04,-3.30726916E-04,
6-2.25387410E-04,-1.54703712E-04,-9.45251600E-05,-5.16691993E-05,
7-2.53739882E-05,-1.06022757E-05,-2.69865726E-06,-4.52114678E-07,
8-4.06387087E-08,-2.74859164E-09,-1.91919631E-10,-1.37094058E-11,
9-9.96203776E-13, 1.04706488E-02, 1.04715868E-02, 1.04722905E-02/
 DATA CH  19/
1 1.04735808E-02, 1.04759277E-02, 1.04800379E-02, 1.04870926E-02,
2 1.05000549E-02, 1.05237187E-02, 1.05654328E-02, 1.06378618E-02,
3 1.07738115E-02, 1.09663337E-02, 1.12726017E-02, 1.26399636E-02,
4 1.00257118E-03,-1.32448573E-02,-1.02003884E-02,-8.84301595E-03,
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6-3.02952045E-03,-2.32888278E-03,-1.73132600E-03,-1.30078168E-03,
7-9.20311543E-04,-6.57610360E-04,-4.43884672E-04,-3.02318135E-04,
8-2.07403662E-04,-1.26655650E-04,-6.91945397E-05,-3.39630183E-05,
9-1.41841204E-05,-3.60829257E-06,-6.04192720E-07,-5.42826409E-08/
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2 1.33110352E-02, 1.33121192E-02, 1.33129323E-02, 1.33144233E-02,
3 1.33171350E-02, 1.33218831E-02, 1.33300305E-02, 1.33449935E-02,
4 1.33722851E-02, 1.34203163E-02, 1.35034721E-02, 1.36586923E-02,
5 1.38764431E-02, 1.42174069E-02, 1.49161828E-02, 1.68840513E-02,
6 1.68049676E-03,-1.75585958E-02,-1.31968210E-02,-1.10288702E-02,
7-8.93226417E-03,-7.06568073E-03,-5.63477235E-03,-4.40515439E-03,
8-3.37877289E-03,-2.50692076E-03,-1.88069912E-03,-1.32869378E-03,
9-9.48354161E-04,-6.39452497E-04,-4.35142460E-04,-2.98317864E-04/
 DATA CH  21/
1-1.82035567E-04,-9.93745215E-05,-4.87418148E-05,-2.03423910E-05,
2-5.17079894E-06,-8.65204519E-07,-7.76821776E-08,-5.24960379E-09,
3-3.66338380E-10,-2.61574502E-11,-1.90012484E-12, 1.62635669E-02,
4 1.62647788E-02, 1.62656879E-02, 1.62673547E-02, 1.62703861E-02,
5 1.62756934E-02, 1.62847988E-02, 1.63015153E-02, 1.63319866E-02,
6 1.63855544E-02, 1.64781138E-02, 1.66502535E-02, 1.68902874E-02,
7 1.72624926E-02, 1.80097009E-02, 1.91301740E-02, 2.20507234E-02,
8 1.60598467E-03,-2.29301685E-02,-1.64041170E-02,-1.31520191E-02,
9-1.03269818E-02,-8.19508155E-03,-6.38158993E-03,-4.87910449E-03/
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3-1.41505510E-04,-6.93399826E-05,-2.89124421E-05,-7.34137704E-06,
4-1.22720877E-06,-1.10088386E-07,-7.43470144E-09,-5.18589035E-10,
5-3.70162362E-11,-2.68824340E-12, 1.90288838E-02, 1.90301864E-02,
6 1.90311635E-02, 1.90329549E-02, 1.90362129E-02, 1.90419163E-02,
7 1.90517000E-02, 1.90696574E-02, 1.91023759E-02, 1.91598480E-02,
8 1.92590133E-02, 1.94429574E-02, 1.96983785E-02, 2.00918628E-02,
9 2.08715613E-02, 2.20119512E-02, 2.37371486E-02, 2.83114149E-02/
 DATA CH  23/
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2-1.20287271E-02,-9.31144019E-03,-7.08564280E-03,-5.22193919E-03,
3-3.89775767E-03,-2.74046750E-03,-1.94871813E-03,-1.30935747E-03,
4-8.88519151E-04,-6.07746487E-04,-3.69934554E-04,-2.01457063E-04,
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6-1.55703706E-07,-1.05059482E-08,-7.32366100E-10,-5.22518089E-11,
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8 2.18920464E-02, 2.18955065E-02, 2.19015636E-02, 2.19119529E-02,
9 2.19310185E-02, 2.19657448E-02, 2.20267078E-02, 2.21317887E-02/
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3 2.92743075E-03,-3.73647840E-02,-2.38681375E-02,-1.85748279E-02,
4-1.42447859E-02,-1.07616185E-02,-7.88376564E-03,-5.85888497E-03,
5-4.10243568E-03,-2.90808105E-03,-1.94826632E-03,-1.31904346E-03,
6-9.00545180E-04,-5.47062546E-04,-2.97330725E-04,-1.45238774E-04,
7-6.03779764E-05,-1.52779792E-05,-2.54593371E-06,-2.27744155E-07,
8-1.53482999E-08,-1.06903513E-09,-7.62254979E-11,-5.53125955E-12,
9 2.36015431E-02, 2.36029258E-02, 2.36039630E-02, 2.36058645E-02/
 DATA CH  25/
1 2.36093224E-02, 2.36153754E-02, 2.36257567E-02, 2.36448050E-02,
2 2.36794912E-02, 2.37403567E-02, 2.38451879E-02, 2.40390035E-02,
3 2.43067409E-02, 2.47159813E-02, 2.55150365E-02, 2.66539649E-02,
4 2.83052241E-02, 3.08509749E-02, 3.47923899E-02, 4.46119530E-02,
5 3.20503910E-03,-4.47187614E-02,-2.99247790E-02,-2.25420281E-02,
6-1.68110438E-02,-1.21916112E-02,-8.99598614E-03,-6.25826949E-03,
7-4.41481615E-03,-2.94457279E-03,-1.98669550E-03,-1.35260584E-03,
8-8.19247514E-04,-4.43981117E-04,-2.16298007E-04,-8.96923905E-05,
9-2.26304235E-05,-3.76143506E-06,-3.35701359E-07,-2.25853298E-08/
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1-1.57126337E-09,-1.11939888E-10,-8.11753486E-12, 2.10819534E-02,
2 2.10831118E-02, 2.10839807E-02, 2.10855737E-02, 2.10884705E-02,
3 2.10935411E-02, 2.11022372E-02, 2.11181919E-02, 2.11472395E-02,
4 2.11981948E-02, 2.12859096E-02, 2.14479200E-02, 2.16713789E-02,
5 2.20121631E-02, 2.26748079E-02, 2.36128573E-02, 2.49588564E-02,
6 2.69994181E-02, 3.00695593E-02, 3.50546660E-02, 4.82036877E-02,
7-7.97111783E-04,-4.87438566E-02,-3.09328678E-02,-2.26544845E-02,
8-1.62047269E-02,-1.18463299E-02,-8.17351975E-03,-5.73132332E-03,
9-3.80196984E-03,-2.55452966E-03,-1.73345966E-03,-1.04625341E-03/
 DATA CH  27/
1-5.65090551E-04,-2.74450106E-04,-1.13476006E-04,-2.85368603E-05,
2-4.72921747E-06,-4.20972316E-07,-2.82677419E-08,-1.96399356E-09,
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4 1.80361500E-02, 1.80374397E-02, 1.80397849E-02, 1.80438900E-02,
5 1.80509298E-02, 1.80638448E-02, 1.80873553E-02, 1.81285880E-02,
6 1.81995382E-02, 1.83304906E-02, 1.85109119E-02, 1.87856137E-02,
7 1.93181999E-02, 2.00685569E-02, 2.11377479E-02, 2.27412677E-02,
8 2.51123942E-02, 2.88515368E-02, 3.50495187E-02, 5.16632021E-02,
9 3.00500586E-03,-5.10502016E-02,-3.11834652E-02,-2.18472301E-02/
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2-3.29037961E-03,-2.22343494E-03,-1.33610350E-03,-7.18622045E-04,
3-3.47694325E-04,-1.43252461E-04,-3.58817234E-05,-5.92553698E-06,
4-5.25827462E-07,-3.52284403E-08,-2.44380886E-09,-1.73737228E-10,
5-1.25787831E-11, 1.64786075E-02, 1.64794279E-02, 1.64800433E-02,
6 1.64811715E-02, 1.64832231E-02, 1.64868141E-02, 1.64929723E-02,
7 1.65042692E-02, 1.65248325E-02, 1.65608906E-02, 1.66229198E-02,
8 1.67373508E-02, 1.68948904E-02, 1.71344875E-02, 1.75980955E-02,
9 1.82492013E-02, 1.91727468E-02, 2.05483911E-02, 2.25612944E-02/
 DATA CH  29/
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2 1.38016993E-03,-5.70339351E-02,-3.20806211E-02,-2.27479574E-02,
3-1.52901387E-02,-1.05291477E-02,-6.87599889E-03,-4.56641458E-03,
4-3.07072472E-03,-1.83601908E-03,-9.82842417E-04,-4.73524685E-04,
5-1.94334826E-04,-4.84650274E-05,-7.97307566E-06,-7.05164855E-07,
6-4.71286473E-08,-3.26392278E-09,-2.31762737E-10,-1.67645871E-11,
7 1.49382707E-02, 1.49389835E-02, 1.49395182E-02, 1.49404985E-02,
8 1.49422810E-02, 1.49454010E-02, 1.49507513E-02, 1.49605658E-02,
9 1.49784293E-02, 1.50097490E-02, 1.50636142E-02, 1.51629417E-02/
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3 2.68624659E-02, 3.32277631E-02, 4.20505558E-02, 6.32993021E-02,
4 4.77638112E-03,-6.19856622E-02,-3.71436880E-02,-2.42903955E-02,
5-1.64402688E-02,-1.05882308E-02,-6.96335960E-03,-4.64839913E-03,
6-2.75889880E-03,-1.46685643E-03,-7.02504829E-04,-2.86746026E-04,
7-7.10852755E-05,-1.16341887E-05,-1.02437882E-06,-6.82424944E-08,
8-4.71587304E-09,-3.34334041E-10,-2.41552083E-11, 1.19676523E-02,
9 1.19682039E-02, 1.19686175E-02, 1.19693759E-02, 1.19707550E-02/
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1 1.19731688E-02, 1.19773080E-02, 1.19849008E-02, 1.19987195E-02,
2 1.20229452E-02, 1.20646023E-02, 1.21413936E-02, 1.22469917E-02,
3 1.24073222E-02, 1.27166280E-02, 1.31489715E-02, 1.37581127E-02,
4 1.46565416E-02, 1.59520156E-02, 1.79155963E-02, 2.09638003E-02,
5 2.55738576E-02, 3.17370854E-02, 4.13539855E-02, 6.47330583E-02,
6-3.13002439E-03,-6.64300268E-02,-3.38972397E-02,-2.25383908E-02,
7-1.42927434E-02,-9.29930308E-03,-6.15889710E-03,-3.62688409E-03,
8-1.91468013E-03,-9.11336795E-04,-3.69930636E-04,-9.11557818E-05,
9-1.48423565E-05,-1.30108568E-06,-8.64017699E-08,-5.95801290E-09/
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1-4.21745668E-10,-3.04351150E-11, 9.90213654E-03, 9.90257751E-03,
2 9.90290825E-03, 9.90351464E-03, 9.90461728E-03, 9.90654721E-03,
3 9.90985662E-03, 9.91592702E-03, 9.92697457E-03, 9.94634027E-03,
4 9.97963508E-03, 1.00409936E-02, 1.01253323E-02, 1.02533023E-02,
5 1.04998993E-02, 1.08439750E-02, 1.13275447E-02, 1.20382071E-02,
6 1.30576130E-02, 1.45908932E-02, 1.69430759E-02, 2.04359677E-02,
7 2.49835860E-02, 3.18044908E-02, 4.24883980E-02, 7.17810122E-02,
8 8.67332704E-03,-6.89895852E-02,-3.75877207E-02,-2.31267135E-02,
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7 8.93367940E-03, 9.32067034E-03, 9.88797957E-03, 1.06988496E-02,
8 1.19121548E-02, 1.37590627E-02, 1.64702835E-02, 1.99453256E-02,
9 2.50435890E-02, 3.27774721E-02, 4.59347375E-02, 7.42013248E-02/
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3-8.02224334E-04,-1.94269373E-04,-3.11778855E-05,-2.70011013E-06,
4-1.77780823E-07,-1.21896014E-08,-8.59347250E-10,-6.18247844E-11,
5 6.11252521E-03, 6.11278293E-03, 6.11297622E-03, 6.11333061E-03,
6 6.11397502E-03, 6.11510290E-03, 6.11703692E-03, 6.12058433E-03,
7 6.12703979E-03, 6.13835434E-03, 6.15780263E-03, 6.19362889E-03,
8 6.24284199E-03, 6.31744633E-03, 6.46097742E-03, 6.66074206E-03,
9 6.94051524E-03, 7.34963242E-03, 7.93233789E-03, 8.79983611E-03/
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1 1.01105399E-02, 1.20139653E-02, 1.44190263E-02, 1.78794221E-02,
2 2.29776191E-02, 3.12457639E-02, 4.32092822E-02, 8.03682628E-02,
3 7.96504037E-03,-7.77435659E-02,-3.82082769E-02,-2.39372959E-02,
4-1.33928966E-02,-6.77602270E-03,-3.11640595E-03,-1.22867876E-03,
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8 4.84235409E-03, 4.84385235E-03, 4.84660042E-03, 4.85160115E-03,
9 4.86036555E-03, 4.87542922E-03, 4.90317432E-03, 4.94127798E-03/
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2 5.79563422E-03, 6.24351713E-03, 6.90795579E-03, 7.90675700E-03,
3 9.34685632E-03, 1.11498855E-02, 1.37134602E-02, 1.74284831E-02,
4 2.33075143E-02, 3.15464164E-02, 4.71303961E-02, 8.31860584E-02,
5-1.39809080E-03,-8.27387920E-02,-4.26914313E-02,-2.30114305E-02,
6-1.13291684E-02,-5.10872289E-03,-1.98326793E-03,-4.67128039E-04,
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9 3.06099849E-03, 3.06116847E-03, 3.06147755E-03, 3.06201853E-03/
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1 3.06294614E-03, 3.06464754E-03, 3.06774352E-03, 3.07316939E-03,
2 3.08249429E-03, 3.09966707E-03, 3.12324631E-03, 3.15896846E-03,
3 3.22761787E-03, 3.32299780E-03, 3.45626012E-03, 3.65047653E-03,
4 3.92579238E-03, 4.33292826E-03, 4.94215751E-03, 5.81499105E-03,
5 6.89908541E-03, 8.42487188E-03, 1.06056083E-02, 1.39880458E-02,
6 1.85952310E-02, 2.69222098E-02, 3.97570231E-02, 8.17551485E-02,
7-2.09131453E-03,-8.11066235E-02,-3.25775813E-02,-1.56223141E-02,
8-6.89366661E-03,-2.63175306E-03,-6.10107245E-04,-9.46532067E-05,
9-7.97870666E-06,-5.15774840E-07,-3.49442591E-08,-2.44287458E-09/
 DATA CH  38/
1-1.74654400E-10, 2.40512571E-03, 2.40522114E-03, 2.40529272E-03,
2 2.40542396E-03, 2.40566258E-03, 2.40608023E-03, 2.40679639E-03,
3 2.40810991E-03, 2.41050005E-03, 2.41468874E-03, 2.42188700E-03,
4 2.43514190E-03, 2.45333866E-03, 2.48089982E-03, 2.53384359E-03,
5 2.60735450E-03, 2.70997012E-03, 2.85933438E-03, 3.07069863E-03,
6 3.38249757E-03, 3.84744668E-03, 4.51040248E-03, 5.32899596E-03,
7 6.47276667E-03, 8.09200038E-03, 1.05707708E-02, 1.38891885E-02,
8 1.97365176E-02, 2.84560234E-02, 4.53047976E-02, 8.93548007E-02,
9 1.14633644E-02,-8.50321604E-02,-2.84309792E-02,-1.22811274E-02/
 DATA CH  39/
1-4.58861788E-03,-1.04252349E-03,-1.59353873E-04,-1.32809492E-05,
2-8.52138923E-07,-5.74588777E-08,-4.00355036E-09,-2.85539274E-10,
3 2.01712685E-03, 2.01720552E-03, 2.01726451E-03, 2.01737268E-03,
4 2.01756936E-03, 2.01791361E-03, 2.01850388E-03, 2.01958652E-03,
5 2.02155648E-03, 2.02500871E-03, 2.03094102E-03, 2.04186369E-03,
6 2.05685634E-03, 2.07955939E-03, 2.12315372E-03, 2.18364614E-03,
7 2.26801810E-03, 2.39068326E-03, 2.56398272E-03, 2.81904874E-03,
8 3.19818241E-03, 3.73643021E-03, 4.39752935E-03, 5.31530603E-03,
9 6.60386497E-03, 8.55456517E-03, 1.11290500E-02, 1.55742879E-02/
 DATA CH  40/
1 2.20122110E-02, 3.39250844E-02, 5.36878777E-02, 9.95979074E-02,
2 7.38783044E-03,-9.50072179E-02,-2.79356771E-02,-1.01851683E-02,
3-2.24587849E-03,-3.36029960E-04,-2.75671564E-05,-1.75095562E-06,
4-1.17317849E-07,-8.13872981E-09,-5.78618369E-10, 1.33691378E-03,
5 1.33696491E-03, 1.33700326E-03, 1.33707358E-03, 1.33720143E-03,
6 1.33742520E-03, 1.33780889E-03, 1.33851262E-03, 1.33979310E-03,
7 1.34203698E-03, 1.34589263E-03, 1.35299095E-03, 1.36273259E-03,
8 1.37748057E-03, 1.40578764E-03, 1.44504138E-03, 1.49974151E-03,
9 1.57916833E-03, 1.69118670E-03, 1.85566113E-03, 2.09931507E-03/
 DATA CH  41/
1 2.44365704E-03, 2.86428333E-03, 3.44438938E-03, 4.25209311E-03,
2 5.46149607E-03, 7.03592367E-03, 9.70370806E-03, 1.34682349E-02,
3 2.01665716E-02, 3.06303250E-02, 4.73318755E-02, 1.06574541E-01,
4 6.58083280E-03,-9.85451697E-02,-2.41064074E-02,-5.12218188E-03,
5-7.41842410E-04,-5.94664130E-05,-3.72309705E-06,-2.47259455E-07,
6-1.70506064E-08,-1.20694890E-09, 7.78854591E-04, 7.78883836E-04,
7 7.78905770E-04, 7.78945986E-04, 7.79019109E-04, 7.79147093E-04,
8 7.79366544E-04, 7.79769034E-04, 7.80501380E-04, 7.81784680E-04,
9 7.83989647E-04, 7.88048628E-04, 7.93618284E-04, 8.02048402E-04/
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 DATA CH  42/
1 8.18222883E-04, 8.40638968E-04, 8.71850601E-04, 9.17120249E-04,
2 9.80866557E-04, 1.07426366E-03, 1.21221123E-03, 1.40639039E-03,
3 1.64246567E-03, 1.96622437E-03, 2.41386451E-03, 3.07813259E-03,
4 3.93352139E-03, 5.36225587E-03, 7.34083699E-03, 1.07710625E-02,
5 1.59396774E-02, 2.38349433E-02, 4.14797560E-02, 1.10667846E-01,
6 6.69476806E-03,-1.00490686E-01,-8.34055502E-03,-1.38819796E-03,
7-1.12607643E-04,-7.04375324E-06,-4.66733399E-07,-3.21186259E-08,
8-2.26965265E-09, 4.45876399E-04, 4.45892830E-04, 4.45905154E-04,
9 4.45927749E-04, 4.45968832E-04, 4.46040738E-04, 4.46164033E-04/
 DATA CH  43/
1 4.46390164E-04, 4.46801609E-04, 4.47522568E-04, 4.48761254E-04,
2 4.51041255E-04, 4.54169369E-04, 4.58903016E-04, 4.67981895E-04,
3 4.80557056E-04, 4.98052784E-04, 5.23401307E-04, 5.59042637E-04,
4 6.11155327E-04, 6.87908451E-04, 7.95544891E-04, 9.25829005E-04,
5 1.10358370E-03, 1.34780443E-03, 1.70733573E-03, 2.16596771E-03,
6 2.92284891E-03, 3.95529451E-03, 5.71016659E-03, 8.28724061E-03,
7 1.21018809E-02, 2.02805452E-02, 3.94082016E-02, 1.19326015E-01,
8 2.58470846E-02,-9.46027264E-02,-2.39823456E-03,-3.28979558E-04,
9-2.15337590E-05,-1.44104765E-06,-9.94313398E-08,-7.02990926E-09/
 DATA CH  44/
1 1.91892428E-04, 1.91899370E-04, 1.91904577E-04, 1.91914122E-04,
2 1.91931479E-04, 1.91961858E-04, 1.92013946E-04, 1.92109479E-04,
3 1.92283299E-04, 1.92587867E-04, 1.93111123E-04, 1.94074172E-04,
4 1.95395272E-04, 1.97394042E-04, 2.01226243E-04, 2.06531377E-04,
5 2.13906976E-04, 2.24582219E-04, 2.39571298E-04, 2.61445769E-04,
6 2.93578931E-04, 3.38486848E-04, 3.92625716E-04, 4.66147726E-04,
7 5.66593618E-04, 7.13435719E-04, 8.99238192E-04, 1.20277877E-03,
8 1.61173826E-03, 2.29607918E-03, 3.28165543E-03, 4.70753692E-03,
9 7.66612215E-03, 1.42774187E-02, 3.06073228E-02, 1.11348077E-01/
 DATA CH  45/
1 9.05174743E-03,-9.10890130E-02, 4.23839019E-03, 6.52943626E-05,
2 1.76371806E-06, 4.67683038E-08, 4.29648844E-10, 3.88348135E-05,
3 3.88361829E-05, 3.88372100E-05, 3.88390931E-05, 3.88425171E-05,
4 3.88485098E-05, 3.88587853E-05, 3.88776307E-05, 3.89119188E-05,
5 3.89719962E-05, 3.90752038E-05, 3.92651340E-05, 3.95256307E-05,
6 3.99196469E-05, 4.06747385E-05, 4.17193111E-05, 4.31701504E-05,
7 4.52672436E-05, 4.82063665E-05, 5.24848668E-05, 5.67483530E-05,
8 6.74626885E-05, 7.79135491E-05, 9.20210692E-05, 1.11156157E-04,
9 1.38882621E-04, 1.73609351E-04, 2.29633624E-04, 3.03982032E-04/
 DATA CH  46/
1 4.26086041E-04, 5.97959532E-04, 8.40167451E-04, 1.32446578E-03,
2 2.34418068E-03, 4.64229330E-03, 1.03060732E-02, 1.02579871E-01,
3 1.40535965E-02,-8.03045607E-02, 5.76840587E-03, 1.50710934E-04,
4 6.92153933E-06, 3.81045304E-07, 4.55312566E-06, 4.55328223E-06,
5 4.55339966E-06, 4.55361495E-06, 4.55400643E-06, 4.55469159E-06,
6 4.55586639E-06, 4.55802098E-06, 4.56194105E-06, 4.56880930E-06,
7 4.58060760E-06, 4.60231729E-06, 4.63208792E-06, 4.67710664E-06,
8 4.76334352E-06, 4.88256254E-06, 5.04800120E-06, 5.28683607E-06,
9 5.62100286E-06, 6.10633382E-06, 6.81460776E-06, 7.79601868E-06/
 DATA CH  47/
1 8.96748562E-06, 1.05404093E-05, 1.26603932E-05, 1.57087088E-05,
2 1.94936487E-05, 2.55363991E-05, 3.34578555E-05, 4.62779780E-05,
3 6.40158596E-05, 8.85481005E-05, 1.36412175E-04, 2.33722148E-04,
4 4.43310225E-04, 9.62549398E-04, 2.23092560E-03, 8.73151804E-02,
5 2.71444166E-03,-7.68157795E-02, 5.10252445E-03, 1.27671125E-04,
6 5.67396829E-06,-7.73402679E-08,-7.73434165E-08,-7.73457781E-08,
7-7.73501078E-08,-7.73579807E-08,-7.73717602E-08,-7.73953878E-08,
8-7.74387240E-08,-7.75175795E-08,-7.76557706E-08,-7.78932455E-08,
9-7.83305118E-08,-7.89307593E-08,-7.98398026E-08,-8.15856703E-08/
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 DATA CH  48/
1-8.40089168E-08,-8.73898190E-08,-9.23069411E-08,-9.92561203E-08,
2-1.09485909E-07,-1.24687480E-07,-1.46242275E-07,-1.72647247E-07,
3-2.09135396E-07,-2.59971094E-07,-3.35959627E-07,-4.34381901E-07,
4-5.99372871E-07,-8.27837373E-07,-1.22141783E-06,-1.80526801E-06,
5-2.67343677E-06,-4.52838449E-06,-8.80740898E-06,-1.97946979E-05,
6-5.57319213E-05,-3.16220538E-04,-4.67708855E-03, 7.98809888E-02,
7-1.74424993E-03,-7.73015278E-02, 5.08110768E-03, 1.26415472E-04,
8-2.35229915E-08,-2.35238254E-08,-2.35244508E-08,-2.35255975E-08,
9-2.35276826E-08,-2.35313319E-08,-2.35375891E-08,-2.35490651E-08/
 DATA CH  49/
1-2.35699450E-08,-2.36065296E-08,-2.36693794E-08,-2.37850421E-08,
2-2.39436824E-08,-2.41836442E-08,-2.46435373E-08,-2.52798064E-08,
3-2.61636631E-08,-2.74414620E-08,-2.92327810E-08,-3.18412956E-08,
4-3.56617144E-08,-4.09799727E-08,-4.73618779E-08,-5.59823597E-08,
5-6.76834284E-08,-8.46519064E-08,-1.05922602E-07,-1.40270863E-07,
6-1.85900967E-07,-2.60930271E-07,-3.66694583E-07,-5.16006631E-07,
7-8.15470672E-07,-1.45050597E-06,-2.91340829E-06,-7.04558759E-06,
8-2.99192566E-05,-2.26323937E-04,-5.82515447E-03, 7.79801956E-02,
9 2.64981937E-05,-7.72380706E-02, 5.08455687E-03,-1.10721562E-09/
 DATA CH  50/
1-1.10725448E-09,-1.10728363E-09,-1.10733706E-09,-1.10743423E-09,
2-1.10760428E-09,-1.10789586E-09,-1.10843063E-09,-1.10940360E-09,
3-1.11110836E-09,-1.11403694E-09,-1.11942618E-09,-1.12681742E-09,
4-1.13799643E-09,-1.15941759E-09,-1.18904619E-09,-1.23018909E-09,
5-1.28963998E-09,-1.37292604E-09,-1.49409450E-09,-1.67133328E-09,
6-1.91765674E-09,-2.21268824E-09,-2.61035604E-09,-3.14876883E-09,
7-3.92717721E-09,-4.89960462E-09,-6.46347526E-09,-8.53112373E-09,
8-1.19118032E-08,-1.66462726E-08,-2.32831944E-08,-3.64734820E-08,
9-6.40818411E-08,-1.26528298E-07,-2.98194168E-07,-1.19785294E-06/
 DATA CH  51/
1-8.01992633E-06,-1.26283859E-04,-5.07820452E-03, 7.73783206E-02,
2 5.35582696E-03,-1.43906176E-01,-8.42356555E-11,-8.42385674E-11,
3-8.42407515E-11,-8.42447557E-11,-8.42520365E-11,-8.42647795E-11,
4-8.42866291E-11,-8.43267015E-11,-8.43996095E-11,-8.45273508E-11,
5-8.47467877E-11,-8.51505756E-11,-8.57043109E-11,-8.65417017E-11,
6-8.81459237E-11,-9.03639825E-11,-9.34424940E-11,-9.78878527E-11,
7-1.04109656E-10,-1.13150043E-10,-1.26351379E-10,-1.44658354E-10,
8-1.66530972E-10,-1.95930758E-10,-2.35606951E-10,-2.92748415E-10,
9-3.63830105E-10,-4.77578458E-10,-6.27122117E-10,-8.70043981E-10/
 DATA CH  52/
1-1.20775676E-09,-1.67755564E-09,-2.60232678E-09,-4.51267404E-09,
2-8.75886974E-09,-2.01539927E-08,-7.73451278E-08,-4.77509588E-07,
3-6.26368061E-06,-1.38811220E-04,-5.35582696E-03, 6.66666667E-02,
4 1.38689160E-01/
 END
```

```
      SUBROUTINE CONVEC
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1               GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2               IFCONV
      REAL MIXLTH
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /PTOTAL/PTOTAL(40)
      COMMON /RAD/ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /TEFF/TEFF,GRAV,GLOG
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1                 IFTURB
      COMMON /XABUND/XABUND(99),WTMOLE
      DIMENSION EQ(4),DEQ(4,4),DUMMY(4)
      DIMENSION TNEW(4),PNEW(4),ENERGY(4),RHON(4)
      DIMENSION DTDRHX(40)
      EQUIVALENCE (DTDRHX(1),DLTDLP(1))
      CALL DERIV(RHOX,T,DTDRHX,NRHOX)
C     CALCULATE DERIVATIVES BY EVALUATING FUNCTIONS AT + AND - .001
C     FIRST GUESSES
      XH=AMAX1(XABUND(1),1.E-20)
      XHE=AMAX1(XABUND(2),1.E-20)
      XNHE1=XNATOM(1)*XHE
      XNH1=XNFPH(1,1)*2.
      XNAT=XNATOM(1)
      XNEL=XNE(1)
      DO 30 J=1,NRHOX
      TNEW(1)=T(J)*1.001
      PNEW(1)=P(J)
      TNEW(2)=T(J)*.999
      PNEW(2)=P(J)
      TNEW(3)=T(J)
      PNEW(3)=P(J)*1.001
      TNEW(4)=T(J)
      PNEW(4)=P(J)*.999
      DO 15 I=1,4
      TN=TNEW(I)
      TKN=TN*1.3804E-16
      TKEVN=TN*8.6171E-5
      XNTOT=PNEW(I)/TKN
      CT32=2.4148E15*TN*SQRT(TN)
      CEQH2=CT32*EXP(-13.595/TKEVN)
      CEQHH=0.
      IF(TN.LT.10000.)CEQHH=EXP(4.477/TKEVN-4.6628E1+(1.8031E-3+
     1(-5.0239E-7+(8.1424E-11-5.0501E-15*TN)*TN)*TN)*TN-1.5*ALOG(TN))
C     THE AMIN IS FOR ANY UNFORTUNATE WHO HAS A 360
      CEQHE2=4.*CT32*EXP(-AMIN1(24.580/TKEVN,150.))
      CEQHE3=4.*CT32**2*EXP(-AMIN1(78.983/TKEVN,150.))
      DO 13 K=1,100
      XNH2=XNH1*CEQH2/XNEL
      XNHH=XNH1**2*CEQHH
      XNHE2=XNHE1*CEQHE2/XNEL
      XNHE3=XNHE1*CEQHE3/XNEL**2
      EQ(1)=XNH1+XNH2+2.*XNHH-XH*XNAT
      EQ(2)=XNHE1+XNHE2+XNHE3-XHE*XNAT
      EQ(3)=XNH2+XNHE2+2.*XNHE3-XNEL
      EQ(4)=XNH1+XNH2+XNHH+XNHE1+XNHE2+XNHE3+XNEL-XNTOT
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```
      DEQ(1,1)=(XNH1+XNH2+4.*XNHH)/XNH1
      DEQ(1,2)=0.
      DEQ(1,3)=-XH
      DEQ(1,4)=-XNH2/XNEL
      DEQ(2,1)=0.
      DEQ(2,2)=(XNHE1+XNHE2+XNHE3)/XNHE1
      DEQ(2,3)=-XHE
      DEQ(2,4)=(-XNHE2-2.*XNHE3)/XNEL
      DEQ(3,1)=XNH2/XNH1
      DEQ(3,2)=(XNHE2+XNHE3)/XNHE1
      DEQ(3,3)=0.
      DEQ(3,4)=(-XNH2-XNHE2-4.*XNHE3-XNEL)/XNEL
      DEQ(4,1)=(XNH1+XNH2+2.*XNHH)/XNH1
      DEQ(4,2)=(XNHE1+XNHE2+XNHE3)/XNHE1
      DEQ(4,3)=0.
      DEQ(4,4)=(-XNH2-XNHE2-2.*XNHE3+XNEL)/XNEL
C     CALL SOLVIT(DEQ,4,EQ,DUMMY)
      Q1311=DEQ(1,3)/DEQ(1,1)
      Q1411=DEQ(1,4)/DEQ(1,1)
      E111=EQ(1)/DEQ(1,1)
      Q2322=DEQ(2,3)/DEQ(2,2)
      Q2422=DEQ(2,4)/DEQ(2,2)
      E222=EQ(2)/DEQ(2,2)
      Q3431=DEQ(3,4)/DEQ(3,1)
      Q3231=DEQ(3,2)/DEQ(3,1)
      E331=EQ(3)/DEQ(3,1)
      Q4441=DEQ(4,4)/DEQ(4,1)
      Q4241=DEQ(4,2)/DEQ(4,1)
      E441=EQ(4)/DEQ(4,1)
      QQQ3=Q1311+Q2322*Q3231
      QQQ4=Q1311+Q2322*Q4241
      QQQQ3=(Q1411+Q2422*Q3231-Q3431)/QQQ3
      EQQQ3=(E111+E222*Q3231-E331)/QQQ3
      QQQQ4=(Q1411+Q2422*Q4241-Q4441)/QQQ4
      EQQQ4=(E111+E222*Q4241-E441)/QQQ4
      EQ(4)=(EQQQ4-EQQQ3)/(QQQQ4-QQQQ3)
      EQ(3)=EQQQ3-QQQQ3*EQ(4)
      EQ(2)=E222-Q2422*EQ(4)-Q2322*EQ(3)
      EQ(1)=E111-Q1411*EQ(4)-Q1311*EQ(3)
      ERROR=ABS(EQ(1)/XNH1)+ABS(EQ(2)/XNHE1)+ABS(EQ(3)/XNAT)+
     1ABS(EQ(4)/XNEL)
      XNH1=XNH1-EQ(1)
      XNHE1=XNHE1-EQ(2)
      XNAT=XNAT-EQ(3)
      XNEL=XNEL-EQ(4)
      IF(ERROR.LT..00001)GO TO 14
   13 CONTINUE
      CALL EXIT
   14 XNH2=XNH1*CEQH2/XNEL
      XNHH=XNH1**2*CEQHH
      XNHE2=XNHE1*CEQHE2/XNEL
      XNHE3=XNHE1*CEQHE3/XNEL**2
      EHH=-4.476/TKEVN+(1.*(1.8031E-3)+(2.*(-5.0739E-7)+(3.*(8.1424E-11)
     1+4.*(-5.0501E-15)*TN)*TN)*TN)*TN
      RHON(I)=XNAT*WTMOLE*1.660E-24
   15 ENERGY(I)=((1.5*XNTOT+13.595/TKEVN*XNH2+EHH*XNHH+
     1 24.580/TKEVN*XNHE2+78.983/TKEVN*XNHE3)*TKN+
     2 3.*PRAD(J)*(TN/T(J))**4)/RHON(I)
      DEDT=(ENERGY(1)-ENERGY(2))/T(J)*500.
      DRDT=(RHON(1)-RHON(2))/T(J)*500.
```

```
      DEDPG=(ENERGY(3)-ENERGY(4))/P(J)*500.
      DRDPG=(RHON(3)-RHON(4))/P(J)*500.
C
C     CALCULATE THERMODYNAMIC QUANTITIES AND CONVECTIVE FLUX
C     IGNORING PTURB AND ASSUMING PRAD PROPORTIONAL TO T**4
      DPDPG=1.
      DPDT=4.*PRAD(J)/T(J)
      DLTDLP(J)=PTOTAL(J)/T(J)/GRAV*DTDRHX(J)
      HEATCV=DEDT-DEDPG*DRDT/DRDPG
      HEATCP(J)=DEDT-DEDPG*DPDT/DPDPG-PTOTAL(J)/RHO(J)**2*(DRDT-
     1DRDPG*DPDT/DPDPG)
      VELSND(J)=SQRT(HEATCP(J)/HEATCV*DPDPG/DRDPG)
      DLRDLT(J)=T(J)/RHO(J)*(DRDT-DRDPG*DPDT/DPDPG)
      GRDADB(J)=-PTOTAL(J)/RHO(J)/T(J)*DLRDLT(J)/HEATCP(J)
      HSCALE(J)=PTOTAL(J)/RHO(J)/GRAV
      VCONV(J)=0.
      FLXCNV(J)=0.
      IF(MIXLTH.EQ.0.)GO TO 30
      DEL=DLTDLP(J)-GRDADB(J)
      IF(DEL.LT.0.)GO TO 30
      VCO=.5*MIXLTH*SQRT(-.5*PTOTAL(J)/RHO(J)*DLRDLT(J))
      FLUXCO=.5*RHO(J)*HEATCP(J)*T(J)*MIXLTH/12.5664
      D=8.*5.6697E-5*T(J)**4/(ABROSS(J)*HSCALE(J)*RHO(J))/
     1(FLUXCO*12.5664)/VCO
      D=D**2/2.
      DDD=(DEL/(D+DEL))**2
      IF(DDD.LT..5)GO TO 24
      DELTA=(1.-SQRT(1.-DDD))/DDD
      GO TO 26
   24 DELTA=.5
      TERM=.5
      JP=-1.
      DOWN=2.
   25 JP=JP+2.
      DOWN=DOWN+2.
      TERM=JP/DOWN*DDD*TERM
      DELTA=DELTA+TERM
      IF(TERM.GT.1.E-6)GO TO 25
   26 DELTA=DELTA*DEL**2/(D+DEL)
      VCONV(J)=VCO*SQRT(DELTA)
      FLXCNV(J)=FLUXCO*VCONV(J)*DELTA
   30 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE HIGH
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /HEIGHT/HEIGHT(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      DIMENSION RHOINV(40)
      EQUIVALENCE (RHOINV(1),ABTOT(1))
      DO 1 J=1,NRHOX
    1 RHOINV(J)=1.E-5/RHO(J)
      CALL INTEG(RHOX,RHOINV,HEIGHT,NRHOX)
      RETURN
      END


      SUBROUTINE TURB
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1              GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2              IFCONV
      REAL MIXLTH
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1                IFTURB
      DO 10 J=1,NRHOX
      VTURB(J)=(TRBFDG*RHO(J)**TRBPOW+TRBSND*VELSND(J)/1.E5+TRBCON)*1.E5
   10 PTURB(J)=RHO(J)*VTURB(J)**2*0.5
      RETURN
      END
```

9. UTILITY PROGRAMS

9.1 FRESET

Given a list of frequencies, FRESET (pages 1 to 3 in the listing in Section 9.5) computes least-squares parabolic integration coefficients, which are defined in Section 2.6. FRESET punches the frequencies and integration coefficients in a format that can be read by READIN.

Below we list a sample input deck for FRESET. First comes the name of the frequency set and then the list of frequencies or wavelengths that FRESET reads using subroutines FREEFR and FREEFF from ATLAS5. Negative numbers represent discontinuities, which FRESET divides into two, one frequency on each side of the discontinuity. The end of the data is marked with a 0.

```
COOL
H -3.28805E15,-.8220125E15,-3.6533889E14,-.205503125E15,-.131522E15,
 -9.1334722E13,-6.7103061E13,-5.1375781E13,-4.0593210E13,-3.28805E13
HMINUS -1641.9
C -2.7254E15,-2.4196E15,-2.0761E15
AL -1.443E15
MG -1.8488510E15,-1.1925797E15,-7.9804046E14
SI -1.9723165E15,-1.7879689E15,-1.5152920E15
.195E15,.23E15,.26E15,.30E15,.33E15,        .4E15,.45E15,.5E15,.55E15,
.6E15,.65E15,.7E15,.75E15,.85E15,.9E15,
.95E15,1.E15,1.05E15,1.1E15,1.15E15,
1.25E15,1.3E15,1.35E15,1.4E15,1.55E15,1.6E15,1.65E15,1.75E15,
1.82E15,1.9E15,2.02E15
2.2E15,2.3E15,2.5E15,2.6E15,2.8E15,3.E15
0.
```

The easiest way to use FRESET is to start by reading in all the discontinuities required. FRESET will print them out in order with integration weights indicative of their spacing. With this information, intermediate frequencies can be chosen easily.

9.2 PRETAB

PRETAB (pages 4 to 10) computes integration matrices for the radiation field as described in Section 2.6. The dimensions are set for a maximum of 80 τ's, which are listed in the statement DATA TAU. Instructions are given by defining the variables NTAU, IFJ, IFH, and IFPUN. PRETAB also requires subroutine EXPI from ATLAS5.

9.3 ATLAS5 for TTAUP

This is a modified version of ATLAS5 (pages 11 and 12) that produces an opacity table for TTAUP. It is run just as if ATLAS5 were computing a model.

9.4 REDIME

REDIME redimensions all the arrays in ATLAS5 that are dimensioned 40 to any dimension up to 99. A card with the new dimension precedes the deck to be converted. The deck is followed by a card with 0 in column 1.

9.5 Listing of Programs

```
      PROGRAM FRESET(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,
     1TAPE7=PUNCH)
      DIMENSION FREQIN(1000),FREQ(1000),RCO(1000)
      DIMENSION A(1000)
      COMMON /FREE/WORD(6),NUMCOL,LETCOL,LAST,MORE,IFFAIL,MAXPOW
      DIMENSION CARD(81)
      DATA CARD/81*1H /
      MAXPOW=99
      LAST=81
      NUMCOL=1
   90 DO 1 I=1,1000
    1 RCO(I)=0.
      READ (5,2)ALABEL
    2 FORMAT(A6)
      WRITE(6,80)
   80 FORMAT(1H1)
C
      IN=1
   10 FREQIN(IN)=FREEFR(CARD)
      IF(FREQIN(IN).EQ.0.)GO TO 11
      IF(ABS(FREQIN(IN)).LT.1.E6)FREQIN(IN)=2.997925E17/FREQIN(IN)
      IN=IN+1
      GO TO 10
   11 DO 12 I=1,IN
      A(I)=ABS(FREQIN(I))
   12 WRITE(6,70)I,FREQIN(I),A(I)
   70 FORMAT(I5,2E20.8)
C
      DO 16 LAST=2,IN
      LAST1=IN-LAST+2
      DO 15 I=2,LAST1
      IF(A(I).GE.A(I-1))GO TO 15
      SAVE=A(I-1)
      A(I-1)=A(I)
      A(I)=SAVE
      SAVE=FREQIN(I-1)
      FREQIN(I-1)=FREQIN(I)
      FREQIN(I)=SAVE
   15 CONTINUE
   16 CONTINUE
      WRITE(6,80)
      DO 17 I=1,IN
   17 WRITE(6,70)I,FREQIN(I),A(I)
C
      WRITE(6,80)
      J=1
      DO 22 I=1,IN
      FREQ(J)=A(I)
      J=J+1
      IF(FREQIN(I).GE.0.)GO TO 22
      IF(I.EQ.IN)GO TO 22
      FREQ(J)=A(I)
      J=J+1
   22 CONTINUE
      NJ=J-1
      DO 23 J=1,NJ
   23 WRITE(6,70)J,FREQ(J)
C
      K1=1
      DO 39 J=1,NJ
```

```
      IF(J.EQ.NJ)GO TO 32
      IF(FREQ(J+1).NE.FREQ(J))GO TO 39
   32 K2=J
      NUM=K2-K1+1
      IF(NUM.GT.2)GO TO 33
      W=(FREQ(J)-FREQ(J-1))/2.
      RCO(J)=W
      RCO(J-1)=W
      K1=K2+1
      GO TO 39
   33 K21=K2-1
      DO 35 K=K1,K21
      M=K-K1+1
      DO 34 L=K1,K2
      N=L-K1+1
      RCO(L)=RCO(L)+(FREQ(K+1)-FREQ(K))*PARCO(M,1,N,FREQ(K1),NUM)+
     1(FREQ(K+1)**2-FREQ(K)**2)/2.*PARCO(M,2,N,FREQ(K1),NUM)+
     2(FREQ(K+1)**3-FREQ(K)**3)/3.*PARCO(M,3,N,FREQ(K1),NUM)
   34 CONTINUE
   35 CONTINUE
      K1=K2+1
   39 CONTINUE
C
      NJ1=NJ-1
      DO 45 J=1,NJ1
      IF(FREQ(J+1).NE.FREQ(J))GO TO 45
      FREQ(J)=FREQ(J)*.999999
      FREQ(J+1)=FREQ(J+1)*1.000001
   45 CONTINUE
      IF(FREQIN(IN).LT.0.)FREQ(NJ)=FREQ(NJ)*.999999
      WRITE(6,80)
      WRITE(6,77)NJ1,NJ1,ALABEL
      WRITE(7,77)NJ1,NJ1,ALABEL
   77 FORMAT(17H READ FREQUENCIES,I5,29H VALUES.  INTEGRATE FROM 1 TO,
     1I5, 3H.  A6,11H IS THE ID.)
      DO 41 J=2,NJ
      J1=J-1
      WRITE(7,70)J1,FREQ(J),RCO(J)
   41 WRITE(6,70)J1,FREQ(J),RCO(J)
      CALL EXIT
      END



      FUNCTION PARCO(J,K,I,TAU,NTAU)
      DIMENSION TAU(1)
      PARCO=0.
      JI2=I-J+2
      IF(JI2.LT.1.OR.JI2.GT.4)RETURN
      IF(J.EQ.1)GO TO 100
      IF(J.EQ.NTAU-1)GO TO 200
      X1=TAU(J-1)
      X2=TAU(J)
      X3=TAU(J+1)
      X4=TAU(J+2)
      D=X1**2+X4**2-(X2+X3)*(X1+X4)+2.*X2*X3
      XXD=(X2-X3)*D
```

```
      GO TO (10,20,30,40),JI2
   10 GO TO (11,12,13),K
   11 PARCO=X2*X3/D
      RETURN
   12 PARCO=-(X2+X3)/D
      RETURN
   13 PARCO=1./D
      RETURN
   20 GO TO (21,22,23),K
   21 PARCO=X3*(-X1**2-X4**2+X3*X1+X3*X4)/XXD
      RETURN
   22 PARCO=(X1**2-2.*X3**2+X4**2)/XXD
      RETURN
   23 PARCO=(-X1+2.*X3-X4)/XXD
      RETURN
   30 GO TO (31,32,33),K
   31 PARCO=X2*(X1**2+X4**2-X2*X1-X2*X4)/XXD
      RETURN
   32 PARCO=(-X1**2+2.*X2**2-X4**2)/XXD
      RETURN
   33 PARCO=(X1-2.*X2+X4)/XXD
      RETURN
   40 GO TO (41,42,43),K
   41 PARCO=X2*X3/D
      RETURN
   42 PARCO=-(X2+X3)/D
      RETURN
   43 PARCO=1./D
      RETURN
  100 X1=TAU(1)
      X2=TAU(2)
      X3=TAU(3)
      GO TO (110,120,130),I
  110 GO TO (111,112,113),K
  111 PARCO=X2*X3/(X1-X2)/(X1-X3)
      RETURN
  112 PARCO=-(X2+X3)/(X1-X2)/(X1-X3)
      RETURN
  113 PARCO=1./(X1-X2)/(X1-X3)
      RETURN
  120 GO TO(121,122,123),K
  121 PARCO=X1*X3/(X2-X1)/(X2-X3)
      RETURN
  122 PARCO=-(X1+X3)/(X2-X1)/(X2-X3)
      RETURN
  123 PARCO=1./(X2-X1)/(X2-X3)
      RETURN
  130 GO TO(131,132,133),K
  131 PARCO=X1*X2/(X3-X1)/(X3-X2)
      RETURN
  132 PARCO=-(X1+X2)/(X3-X1)/(X3-X2)
      RETURN
  133 PARCO=1./(X3-X1)/(X3-X2)
      RETURN
  200 X1=TAU(NTAU-2)
      X2=TAU(NTAU-1)
      X3=TAU(NTAU)
      I3=I-NTAU+3
      GO TO (110,120,130),I3
      END
```

```
      PROGRAM PRETAB(OUTPUT,PUNCH,TAPE6=OUTPUT,TAPE7=PUNCH)
      COMMON COEF(80,80)
      DIMENSION CO(6400),S(80),TAU(81),F(80),EXACT(80),ERROR(80)
        EQUIVALENCE(COEF,CO)
      DIMENSION LABEL(2)
      DIMENSION A(4),B(4),C(4),D(4)
      DATA TAU/0.,                  .000032,.000056,.0001,.00018,.00032,
     1.00056,.001,.0018,.0032,.0056,.01,.016,.025,.042,.065,
     2.096,.139,.196,.273,.375,.5,.63,.78,.95,1.15,1.35,1.6,1.85,2.15,
     32.45,2.75,3.15,3.65,4.25,5.0,6.2,7.8,10.,12.5,15.,17.5,20./
      DATA LABEL/3HCJ ,3HCH /
      DATA A,B,C,D/1.,0.,0.,1.,0.,1.,0.,1.,0.,0.,1.,0.,0.,0.,0.,1./
      NTAU=43
      IFJ=1
      IFJ=0
      IFH=0
      IFH=1
      IFPUN=0
      IFPUN=1
      TAU(NTAU+1)=TAU(NTAU)+1000.
      NFIRST=1
      NLAST=2
      IF(IFJ.EQ.0)NFIRST=2
      IF(IFH.EQ.0)NLAST=1
      DO 50 N=NFIRST,NLAST
      CALL INTCO(COEF,TAU,NTAU,N)
      WRITE(6,200)
  200 FORMAT(1H1)
      DO 201 L=1,NTAU
  201 WRITE(6,202)(COEF(L,J),J=1,NTAU)
  202 FORMAT(/(X10E13.5))
      DO 70 M=1,4
      DO 3 L=1,NTAU
      CALL ANALYT(TAU(L),S(L),EJ,EH,A(M),B(M),C(M),D(M))
      EXACT(L)=EJ
      IF(N.EQ.2)EXACT(L)=EH
    3 CONTINUE
      DO 9 L=1,NTAU
      F(L)=0.
      DO 1 J=1,NTAU
    1 F(L)=F(L)+COEF(L,J)*S(J)
    9 ERROR(L)=(F(L)-EXACT(L))/EXACT(L)
      N1=A(M)
      N2=B(M)
      N3=C(M)
      N4=D(M)
      WRITE(6,29)N1,N2,N3,N4
   29 FORMAT(19H1ANALYTIC TEST    S=,I1,1H+,I1,4HTAU+,I1,7HTAU**2-,I1,
     A9HEXP(-TAU)//
     15X,9X3HTAU9X,10X1HS10X,5X11HFUNCTION N=I1,4X,8X5HEXACT8X,
     28X5HERROR)
      WRITE(6,30)(L,TAU(L),S(L),F(L),EXACT(L),ERROR(L),L=1,NTAU)
   30 FORMAT(I5,5E21.14)
   70 CONTINUE
      IF(IFPUN.EQ.0)GO TO 50
      I=0
      DO 4 J=1,NTAU
      DO 4 L=1,NTAU
      I=I+1
    4 CO(I)=COEF(L,J)
```

```
      CALL PUNDAT(CO,NTAU**2,LABEL(N))
   50 CONTINUE
      CALL EXIT
      END


      FUNCTION EXPIDI(TAUL,TAUJ,TAUJ1,K,KK,N)
      DIMENSION FACT(11),PSI(6)
      DATA ALOGD,ALOGD1/0.,0./
      DATA FACT/1.,1.,2.,6.,24.,120.,720.,5040.,40320.,362880.,3628800./
      DATA PSI/-.577215664901533,.422784335098467,.922784335098467,
     11.256117668431800,1.506117668431800,1.706117668431800/
      DATA SAVED,SAVED1/1.E30,1.E30/
      D=ABS(TAUL-TAUJ)
      D1=ABS(TAUL-TAUJ1)
      IF(D.EQ.SAVED.AND.D1.EQ.SAVED1)GO TO 1
      IF(D.GT.0.)ALOGD=ALOG(D)
      IF(D1.GT.0.)ALOGD1=ALOG(D1)
      SAVED=D
      SAVED1=D1
    1 D=-D
      D1=-D1
      NKK=N+KK
      KKK=K-KK
      TERM=0.
      IF(TAUJ.GT.0.)TERM=TAUJ**KKK
      IF(TAUJ.EQ.0..AND.KKK.EQ.0)TERM=1.
      TERM1=TAUJ1**KKK
      C=PSI(NKK)-ALOGD
      C1=PSI(NKK)-ALOGD1
      SUM=(TERM-TERM1)/FLOAT(NKK-1)
      DO 5 MM=2,11
      TERM=TERM*D
      TERM1=TERM1*D1
      IF(MM.EQ.NKK)GO TO 3
      SUM=SUM-(TERM-TERM1)/FLOAT(MM-NKK)/FACT(MM)
      GO TO 5
    3 SUM=SUM+(TERM*C-TERM1*C1)/FACT(NKK)
    5 CONTINUE
      EXPIDI=SUM
      RETURN
      END


      SUBROUTINE INTCO(COINT,TAU,NTAU,N)
      DIMENSION COINT(80,80)
      DO 1 L=1,NTAU
      DO 1 J=1,NTAU
      SUM=0.
      DO 2 K=1,3
      DO 2 I=1,NTAU
      P=PARCO(I,K,J,TAU,NTAU)
      IF(P.EQ.0.)GO TO 2
      E=ETA(N,K,I,L,TAU,NTAU)
      SUM=SUM+E*P
    2 CONTINUE
    1 COINT(L,J)=SUM
      RETURN
      END
```

```
      FUNCTION ETA(N,K,I,L,TAU,NTAU)
      DIMENSION TAU(1)
      IF(I.GT.NTAU)GO TO 1
      IF(I.EQ.0)GO TO 1
      TI=TAU(I)
      TI1=TAU(I+1)
      TL=TAU(L)
      Z=SIGN(1.,TI-TL)**(N-1)
      S=ISIGN(1,I-L)
      TIL=ABS(TI-TL)
      TI1L=ABS(TI1-TL)
      K1=K-1
      K2=K-2
      K3=K-3
      X1=K1
      X2=K2
      N1=N+1
      N2=N+2
      N3=N+3
      TT=TI
      IF(TI.EQ.0.)TT=1.E-40
      IF(TI1.GT.1.)GO TO 7
      IF(TL.LE.20..AND.TI1.LT.TL/10.)GO TO 9
      IF(TL.GT.20..AND.TI1.LT..0001)GO TO 1
    7 IF(TIL.LT..16.AND.TI1L.LT..16)GO TO 2
      C1=TT**K1*EXPI(N1,TIL)
      C2=S*X1*TT**K2*EXPI(N2,TIL)
      C3=X1*X2*TT**K3*EXPI(N3,TIL)
      D1=TI1**K1*EXPI(N1,TI1L)
      D2=S*X1*TI1**K2*EXPI(N2,TI1L)
      D3=X1*X2*TI1**K3*EXPI(N3,TI1L)
      GO TO 8
    9 C1=TT**K1*EXPIS(TL,TI,N,1)
      C2=S*X1*TT**K2*EXPIS(TL,TI,N,2)
      C3=X1*X2*TT**K3*EXPIS(TL,TI,N,3)
      D1=TI1**K1*EXPIS(TL,TI1,N,1)
      D2=S*X1*TI1**K2*EXPIS(TL,TI1,N,2)
      D3=X1*X2*TI1**K3*EXPIS(TL,TI1,N,3)
    8 ETA=Z/2.*ABS(C1+C2+C3-D1-D2-D3)
      RETURN
    2 ETA=Z/2.*ABS(EXPIDI(TL,TI,TI1,K,1,N)+S*X1*EXPIDI(TL,TI,TI1,K,2,N)+
     1X1*X2*EXPIDI(TL,TI,TI1,K,3,N))
      RETURN
    1 ETA=0.
      RETURN
      END
```

```
      FUNCTION EXPIS(X,Y,N,NN)
      DIMENSION E(10)
      DATA X1/-1./
      IF(X.EQ.X1)GO TO 2
      X1=X
      EX=EXP(-X)
      DO 1 I=1,6
    1 E(I)=EXPI(I,X)
    2 IF(Y.EQ.0.)GO TO 10
      SUM=0.
      TERM=Y**(NN-1)
      IF(NN.EQ.3)TERM=TERM/2.
      DO 3 I=1,N
      TERM=TERM*Y/FLOAT(NN+I-1)
      NI1=N-I+1
    3 SUM=SUM+TERM*E(NI1)
      TERM=TERM*EX*Y/FLOAT(NN+N)/X
      SUM=SUM+TERM
      DO 4 M=1,100
      TERM=TERM*FLOAT(M)/FLOAT(NN+N+M)*Y/X
      S=1.
      T=1.
      DO 5 MM=1,M
      T=T*X/FLOAT(MM)
    5 S=S+T
      SUM1=SUM+S*TERM
      IF(SUM.EQ.SUM1)GO TO 9
    4 SUM=SUM1
    9 EXPIS=SUM1
      RETURN
   10 EXPIS=0.
      RETURN
      END


      SUBROUTINE ANALYT(X,S,AJ,H,A,B,C,D)
      S=A+B*X+C*X**2+D*EXP(-X)
      E1=EXPI(1,X)
      E2=EXPI(2,X)
      E3=EXPI(3,X)
      E4=EXPI(4,X)
      E5=EXPI(5,X)
      AJ=A*(1.-E2/2.)+B*(X+E3/2.)+C*(2./3.+X**2-E4)
      H=A*E3/2.+B*(1./3.-E4/2.)+C*(2./3.*X+E5)
      IF(X.GT.0) GO TO 3
      AJ=ALOG(2.)/2.*D+AJ
      H=(1.-ALOG(2.))/2.*D+H
      RETURN
    3 AJ=AJ+D*(EXP(-X)/2.*(ALOG(2.*X)+.577215664901533)+E1/2.)
      H=H+D*(EXP(-X)/2.*(2.-.577215664901533-ALOG(2.*X))-(E2+E1)/2.)
      RETURN
      END
```

```
      FUNCTION PARCO(J,K,I,TAU,NTAU)
      DIMENSION TAU(1)
      PARCO=0.
      JI2=I-J+2
      IF(JI2.LT.1.OR.JI2.GT.4)RETURN
      IF(J.EQ.NTAU-1)GO TO 100
      IF(J.EQ.1)GO TO 200
      IF(J.EQ.NTAU)GO TO 300
      X1=TAU(J-1)
      X2=TAU(J)
      X3=TAU(J+1)
      X4=TAU(J+2)
      D=X1**2+X4**2-(X2+X3)*(X1+X4)+2.*X2*X3
      XXD=(X2-X3)*D
      GO TO (10,20,30,40),JI2
   10 GO TO (11,12,13),K
   11 PARCO=X2*X3/D
      RETURN
   12 PARCO=-(X2+X3)/D
      RETURN
   13 PARCO=1./D
      RETURN
   20 GO TO (21,22,23),K
   21 PARCO=X3*(-X1**2-X4**2+X3*X1+X3*X4)/XXD
      RETURN
   22 PARCO=(X1**2-2.*X3**2+X4**2)/XXD
      RETURN
   23 PARCO=(-X1+2.*X3-X4)/XXD
      RETURN
   30 GO TO (31,32,33),K
   31 PARCO=X2*(X1**2+X4**2-X2*X1-X2*X4)/XXD
      RETURN
   32 PARCO=(-X1**2+2.*X2**2-X4**2)/XXD
      RETURN
   33 PARCO=(X1-2.*X2+X4)/XXD
      RETURN
   40 GO TO (41,42,43),K
   41 PARCO=X2*X3/D
      RETURN
   42 PARCO=-(X2+X3)/D
      RETURN
   43 PARCO=1./D
      RETURN
  100 X1=TAU(J-1)
      X2=TAU(J)
      X3=TAU(J+1)
      X4=2.*TAU(J+1)-TAU(J)
      D=X1**2+X4**2-(X2+X3)*(X1+X4)+2.*X2*X3
      XXD=(X2-X3)*D
      GO TO (10,120,130,333),JI2
  120 GO TO (121,122,123),K
  121 PARCO=X3*(-X1**2-X4**2+X3*X1+X3*X4)/XXD-X2*X3/D
      RETURN
  122 PARCO=(X1**2-2.*X3**2+X4**2)/XXD+(X2+X3)/D
      RETURN
  123 PARCO=(-X1+2.*X3-X4)/XXD-1./D
      RETURN
  130 GO TO (131,132,133),K
  131 PARCO=X2*(X1**2+X4**2-X2*X1-X2*X4)/XXD+2.*X2*X3/D
```

```
      RETURN
  132 PARCO=(-X1**2+2.*X2**2-X4**2)/XXD-2.*(X2+X3)/D
      RETURN
  133 PARCO=(X1-2.*X2+X4)/XXD+2./D
      RETURN
  200 X1=2.*TAU(J)-TAU(J+1)
      X2=TAU(J)
      X3=TAU(J+1)
      X4=TAU(J+2)
      D=X1**2+X4**2-(X2+X3)*(X1+X4)+2.*X2*X3
      XXD=(X2-X3)*D
      GO TO(333,220,230,40),JI2
  220 GO TO(221,222,223),K
  221 PARCO=X3*(-X1**2-X4**2+X3*X1+X3*X4)/XXD+2.*X2*X3/D
      RETURN
  222 PARCO=(X1**2-2.*X3**2+X4**2)/XXD-2.*(X2+X3)/D
      RETURN
  223 PARCO=(-X1+2.*X3-X4)/XXD+2./D
      RETURN
  230 GO TO (231,232,233),K
  231 PARCO=X2*(X1**2+X4**2-X2*X1-X2*X4)/XXD-X2*X3/D
      RETURN
  232 PARCO=(-X1**2+2.*X2**2-X4**2)/XXD+(X3+X2)/D
      RETURN
  233 PARCO=(X1-2.*X2+X4)/XXD-1./D
      RETURN
  300 X1=TAU(J-1)
      X2=TAU(J)
      GO TO (310,320,333,333),JI2
  310 GO TO(311,312,333),K
  311 PARCO=X2/(X2-X1)
      RETURN
  312 PARCO=1./(X1-X2)
      RETURN
  320 GO TO(321,322,333),K
  321 PARCO=X1/(X1-X2)
      RETURN
  322 PARCO=1./(X2-X1)
  333 RETURN
      END
```

```
      SUBROUTINE PUNDAT(X,NUMB,TITLE)
C     X IS AN ARRAY TO BE PUNCHED IN DATA STATEMENTS
C     NUMB IS ITS LENGTH
C     TITLE IS A 3 LETTER DUMMY NAME FOR THE OUTPUT ARRAYS
      DIMENSION X(1)
      DIMENSION IDIM(300),COMMAS(300),A(81),B(81)
      DATA B/1H1,8*1H,,1H2,8*1H,,1H3,8*1H,,1H4,8*1H,,1H5,8*1H,,
     1 1H6,8*1H,,1H7,8*1H,,1H8,8*1H,,1H9,8*1H,/
      DATA QCOMMA,QBLANK,QSLASH,QPAREN/1H,,1H ,1H/,1H(/
      NARRAY=(NUMB+35)/36
      LAST=NUMB-NARRAY*36+36
C     DIMENSIONS
      DO 10 I=1,NARRAY
      IDIM(I)=36
   10 COMMAS(I)=QCOMMA
      DO 11 I=5,NARRAY,5
   11 COMMAS(I)=QBLANK
      COMMAS(NARRAY)=QBLANK
      IDIM(NARRAY)=LAST
      WRITE(6,12)(TITLE,I,IDIM(I),COMMAS(I),I=1,NARRAY)
      WRITE(7,12)(TITLE,I,IDIM(I),COMMAS(I),I=1,NARRAY)
   12 FORMAT(6X,10HDIMENSION ,5(A3,I3,1H(,I2,1H),A1))
C     EQUIVALENCES
      DO 20 I=1,NARRAY
      IDIM(I)=(I-1)*36+1
   20 COMMAS(I)=QCOMMA
      DO 21 I=2,NARRAY,2
   21 COMMAS(I)=QBLANK
      COMMAS(NARRAY)=QBLANK
      WRITE(6,22)(QPAREN,TITLE,I,TITLE,IDIM(I),COMMAS(I),I=1,NARRAY)
      WRITE(7,22)(QPAREN,TITLE,I,TITLE,IDIM(I),COMMAS(I),I=1,NARRAY)
   22 FORMAT(6X,12HEQUIVALENCE ,2(A1,A3,I3,4H(1),A3,1H(,I4,2H)),A1))
C     DATA STATEMENTS
      L=0
      DO 33 ISTART=1,NUMB,36
      L=L+1
      IEND=MINO(NUMB,ISTART+35)
      DO 30 K=1,81
   30 A(K)=B(K)
      K=1
      DO 31 I=ISTART,IEND
      IF(I-I/4*4.EQ.1)K=K+1
      A(K)=X(I)
   31 K=K+2
      K=K-1
      A(K)=QSLASH
      WRITE(7,32)TITLE,L,(A(J),J=1,K)
   33 WRITE(6,32)TITLE,L,(A(J),J=1,K)
   32 FORMAT(6X,5HDATA ,A3,I3,1H/(5XA1,4(E15.8,A1)))
      RETURN
      END
```

```
      PROGRAM ATLAS5(INPUT=513,OUTPUT=513,PUNCH=513,TAPE5=INPUT,
     1TAPE6=OUTPUT,TAPE7=PUNCH)
      COMMON /ABROSS/ABROSS(40),TAUROS(40)
      COMMON /ABTOT/ABTOT(40),ALPHA(40)
      COMMON /CONV/DLTDLP(40),HEATCP(40),DLRDLT(40),VELSND(40),
     1               GRDADB(40),HSCALE(40),FLXCNV(40),VCONV(40),MIXLTH,
     2               IFCONV
      REAL MIXLTH
      COMMON /DEPART/BHYD(40,6),BMIN(40),NLTEON
      COMMON /ELEM/ABUND(99),ATMASS(99),ELEM(99)
      COMMON /FLUX/ FLUX,FLXERR(40),FLXDRV(40),FLXRAD(40)
      COMMON /FREQ/FREQ,FREQLG,EHVKT(40),STIM(40),BNU(40)
      COMMON /FRESET/FRESET(500),RCOSET(500),NULO,NUHI,NUMNU
      COMMON /HEIGHT/HEIGHT(40)
      COMMON /IF/IFCORR,IFPRES,IFSURF,IFSCAT,IFMOL
      COMMON /IFOP/IFOP(20)
      COMMON /IONS/XNFPH(40,2),XNFPHE(40,3)
      COMMON /ITER/ ITER,IFPRNT(15),IFPNCH(15),NUMITS
      COMMON /JUNK/TITLE(74),FREQID(6),WLTE,XSCALE
      COMMON /MUS/ANGLE(20),SURFI(20),NMU
      COMMON /OPS/AHYD(40),AH2P(40),AHMIN(40),SIGH(40),AHE1(40),
     1        AHE2(40),AHEMIN(40),SIGHE(40),ACOOL(40),ALUKE(40),AHOT(40),
     2              SIGEL(40),SIGH2(40),AHLINE(40),ALINES(40),SIGLIN(40),
     3              AXLINE(40),SIGXL(40),AXCONT(40),SIGX(40),SHYD(40),
     4              SHMIN(40),SHLINE(40),SXLINE(40),SXCONT(40)
      COMMON /OPTOT/ACONT(40),SCONT(40),ALINE(40),SLINE(40),SIGMAC(40),
     1                 SIGMAL(40)
      COMMON /PTOTAL/PTOTAL(40)
      COMMON /PUT/PUT,IPUT
      COMMON /RAD/ ACCRAD(40),PRAD(40)
      COMMON /RHOX/RHOX(40),NRHOX
      COMMON /STATE/P(40),XNE(40),XNATOM(40),RHO(40)
      COMMON /TAUSHJ/TAUNU(40),SNU(40),HNU(40),JNU(40),JMINS(40)
      REAL JNU,JMINS
      COMMON /TEFF/TEFF,GRAV,GLOG
      COMMON /TEMP/T(40),TKEV(40),TK(40),HKT(40),TLOG(40),ITEMP
      COMMON /TURBPR/VTURB(40),PTURB(40),TRBFDG,TRBCON,TRBPOW,TRBSND,
     1                 IFTURB
      COMMON /WAVEY/WBEGIN,DELTAW,IFWAVE
      COMMON /XABUND/XABUND(99),WTMOLE
      DIMENSION ABNORM(40)
      DIMENSION KABROS(40)
      EQUIVALENCE (ABROSS(1),KABROS(1))
      DIMENSION TABT(30),TABP(30)
      DATA NT,NP/30,30/
      DATA TABT/3.5,3.525,3.55,3.575,3.6,3.625,3.65,3.675,3.7,3.725,
     1 3.75,3.775,3.8,3.825,3.85,3.875,3.9,3.925,3.95,3.975,4.,4.05,4.1,
     2 4.15,4.2,4.25,4.3,4.35,4.4,4.45/
      DATA TABP/-2.,-1.5,-1.,-.5,0.,.5,1.,1.25,1.5,1.75,2.,2.25,2.5,
     1 2.75,3.,3.2,3.4,3.6,3.8,4.,4.2,4.4,4.6,4.8,5.,5.2,5.4,5.6,5.8,6./
      EXP10(X)=EXP(X*2.302585092994E0)
      CALL READIN(1)
      WRITE(6,75)TABT,TABP
      WRITE(7,75)TABT,TABP
   75 FORMAT(6X10HDATA TABT/4X,7(F6.3,1H,)/5X1H1,9(F6.3,1H,)/
     1 5X1H2,9(F6.3,1H,)/5X1H3,4(F6.3,1H,),F6.3,1H//
     2        6X10HDATA TABP/4X,7(F6.3,1H,)/5X1H1,9(F6.3,1H,)/
     3 5X1H2,9(F6.3,1H,)/5X1H3,4(F6.3,1H,),F6.3,1H/)
      NRHOX=NT
      ITER=1
```

```
      DO 1 J=1,NRHOX
      T(J)=EXP10(TABT(J))
      TK(J)=1.38054E-16*T(J)
      HKT(J)=6.6256E-27/TK(J)
      TKEV(J)=8.6171E-5*T(J)
    1 TLOG(J)=ALOG(T(J))
      ITEMP=0
      DO 100 K=1,NP
      ITEMP=ITEMP+K
      DO 2 J=1,30
      ABNORM(J)=0.
      ABROSS(J)=0.
    2 P(J)=EXP10(TABP(K))
      CALL POPS(0.,1,XNE)
C
C     FREQUENCY INTEGRATION SECTION
      DO 25 NU=NULO,NUHI
      IF(IFWAVE.EQ.0)GO TO 21
      WAVE=WBEGIN+FLOAT(NU-NULO)*DELTAW
      FREQ=2.997925E17/WAVE
      RCO=ABS(DELTAW/WAVE*FREQ)
      GO TO 22
   21 FREQ=FRESET(NU)
      RCO=RCOSET(NU)
   22 FREQLG=ALOG(FREQ)
      DO 20 J=1,NRHOX
      EHVKT(J)=EXP(-FREQ*HKT(J))
      STIM(J)=1.-EHVKT(J)
   20 BNU(J)=1.47439E-47*FREQ**3*EHVKT(J)/STIM(J)
      N=0
   24 N=N+1
      CALL KAPP(N,NSTEPS,STEPWT)
      RCOWT=RCO*STEPWT
      DO 23 J=1,NRHOX
      ABTOT(J)=ACONT(J)+ALINE(J)+SIGMAC(J)+SIGMAL(J)
      DBDT=BNU(J)*FREQ*HKT(J)/T(J)/STIM(J)
      ABNORM(J)=ABNORM(J)+DBDT*RCOWT
   23 ABROSS(J)=ABROSS(J)+DBDT/ABTOT(J)*RCOWT
      IF(N.LT.NSTEPS)GO TO 24
   25 CONTINUE
      DO 29 J=1,NRHOX
C     NORMALIZATION IS PERFORMED WITH AN INTEGRAL SO THAT A
C        MONOCHROMATIC OPACITY CAN BE FOUND BY INTEGRATING OVER ONLY ONE
C        FREQUENCY
      ABROSS(J)=ABNORM(J)/ABROSS(J)
   29 KABROS(J)=ALOG10(ABROSS(J))*1000.
      K1=K/10
      K2=K-K1*10
      WRITE(6,77)K1,K2,TABP(K),(KABROS(J),J=1,10),TABP(K),
     1(KABROS(J),J=11,20),TABP(K),(KABROS(J),J=21,30),TABP(K)
      WRITE(7,77)K1,K2,TABP(K),(KABROS(J),J=1,10),TABP(K),
     1(KABROS(J),J=11,20),TABP(K),(KABROS(J),J=21,30),TABP(K)
   77 FORMAT(6X9HDATA KTAB,2I1,1H/,54X,F6.3/5X1H1,10(I5,1H,),6XF6.3/
     1 5X1H2,10(I5,1H,),6XF6.3/5X1H3,9(I5,1H,),I5,1H/,6XF6.3)
  100 CONTINUE
      CALL EXIT
      END
```

```
      PROGRAM REDIME(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,
     1TAPE7=PUNCH)
      DIMENSION A(80)
C     BCD CHARACTERS
      DATA QA,QB,QC,QD,QE,QF,QG,QH,QI,QJ,QK,QL,QM,QN,QO,QP,QQ,QR,QS,
     1QT,QU,QV,QW,QX,QY,QZ,Q0,Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8,Q9,QPLUS,QMINUS,
     2QSTAR,QSLASH,QPARL,QPARR,QDOLL,QEQUAL,QBLANK,QCOMMA,QPOINT/
     3 1HA,1HB,1HC,1HD,1HE,1HF,1HG,1HH,1HI,1HJ,1HK,1HL,1HM,1HN,1HO,1HP,
     4 1HQ,1HR,1HS,1HT,1HU,1HV,1HW,1HX,1HY,1HZ,1H0,1H1,1H2,1H3,1H4,1H5,
     5 1H6,1H7,1H8,1H9,1H+,1H-,1H*,1H/,1H(,1H),1H$,1H=,1H ,1H,,1H./
      IFCONT=0
      READ(5,11)QDIM1,QDIM2
   11 FORMAT(80A1)
   10 READ(5,11)A
      IF(A(1).EQ.QO)CALL EXIT
      IF(A(1).NE.QBLANK)GO TO 100
      IF(A(6).NE.QBLANK.AND.IFCONT.NE.0)GO TO 25
      IFCONT=0
      IF(A(7).EQ.QC)GO TO 20
      IF(A(7).EQ.QD)GO TO 21
      GO TO 100
   20 IF(A(8).NE.QO)GO TO 100
      IF(A(9).NE.QM)GO TO 100
      IF(A(10).NE.QM)GO TO 100
      IF(A(11).NE.QO)GO TO 100
      IF(A(12).NE.QN)GO TO 100
      N=13
      IFCONT=1
      GO TO 30
   21 IF(A(8).NE.QI)GO TO 22
      IF(A(9).NE.QM)GO TO 100
      IF(A(10).NE.QE)GO TO 100
      IF(A(11).NE.QN)GO TO 100
      IF(A(12).NE.QS)GO TO 100
      IF(A(13).NE.QI)GO TO 100
      IF(A(14).NE.QO)GO TO 100
      IF(A(15).NE.QN)GO TO 100
      N=16
      IFCONT=1
      GO TO 30
   22 IF(A(8).NE.QA)GO TO 100
      IF(A(9).NE.QT)GO TO 100
      IF(A(10).NE.QA)GO TO 100
      N=11
      IFCONT=2
      GO TO 40
   25 GO TO (30,40),IFCONT
   29 N=N-1
   30 DO 31 I=N,69
      IF(A(I).EQ.QPARL.OR.A(I).EQ.QCOMMA)GO TO 35
   31 CONTINUE
      N=7
      GO TO 100
   35 N=I+1
      IF(A(N).NE.Q4)GO TO 30
      N=N+1
      IF(A(N).NE.Q0)GO TO 29
      N=N+1
      IF(A(N).NE.QPARR.AND.A(N).NE.QCOMMA)GO TO 29
```

```
      A(I+1)=QDIM1
      A(I+2)=QDIM2
      GO TO 29
   39 N=N-1
   40 DO 41 I=N,69
      IF(A(I).EQ.Q4)GO TO 45
   41 CONTINUE
      N=7
      GO TO 100
   45 N=N+1
      IF(A(N).NE.Q0)GO TO 40
      N=N+1
      IF(A(N).NE.QSTAR)GO TO 39
      A(I)=QDIM1
      A(I+1)=QDIM2
      GO TO 39
  100 WRITE(6,101)A
  101 FORMAT(1X,80A1)
      WRITE(7,11)A
      GO TO 10
      END
```

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