A NON-LTE ANALYSIS OF A SAMPLE OF O STARS
SELECTED FROM GALACTIC OB ASSOCIATIONS

Thesis by
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I am particularly grateful to Ann for arranging a very productive trip to the Institute for Astronomy of the University of Hawaii, whose hospitality I wish to acknowledge.

Many of the computations for this research were made at the San Diego Supercomputer Center, whose support I also wish to acknowledge.
ABSTRACT

The tables of non-LTE line profiles and equivalent widths published by Mihalas and his collaborators [33], [7], [35] have been revised and extended to four different values of the abundance ratio He/H. Bolometric corrections have been calculated for V magnitudes. The theoretical line profiles have been fit to echelle spectrograms of 22 galactic O stars by $\chi^2$ minimization. It is found that the stars with the lowest surface gravities are fitted best by theoretical spectra with unexpectedly high helium abundances (He/H ~ 0.50), while the stars with higher surface gravities are fitted best by theoretical spectra with He/H~ 0.10, the accepted cosmic ratio. This suggests a systematic failure of conventional non-LTE, plane-parallel models for the more luminous O stars, probably as a result of the neglect of geometrical dilution.

The formula, log He/H = 1.1234-0.4791 log g, gives a good fit to the relation between the apparent helium abundance and log g. Using this relationship, the apparent abundances have been reduced to what are probably true abundances relative to the normal cosmic abundance. It is found that there is no significant difference in the average helium abundances of the associations observed. However, the stars HD 12993, HD 242908, and HD 193595 may be blue stragglers with moderately enhanced helium abundance (He/H ~ 0.19).

Relative carbon abundances have been determined empirically by comparison of the CIV 5812Å and HeII 4542Å equivalent widths. It is found that the association Cyg OB2 is overabundant in carbon by ~ 50%. Likewise, the blue straggler HD 236894 is underabundant in carbon by a factor of two.

The estimated effective temperatures of the sample are compared to the previously accepted calibration of MK spectral types to the effective temperature. Estimates of the radii and masses of the stars in the sample have been calculated from their physical parameters and their absolute visual magnitudes.
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1

1. INTRODUCTION

The evolution of very young stellar populations is of great interest, since these stars have a decisive influence on the interstellar medium and the chemical evolution of the universe and are generally believed to be the precursors of Type II supernovae.

However, while young, massive stars are bright and easily observed, the observations are difficult to interpret. This is unfortunate, since recent developments in the theory of stellar evolution have led to detailed predictions of the evolution of the stellar parameters and surface chemical abundances of such stars [14], [30] that beg to be confirmed observationally.

This situation is changing. Advances in computational methods and capacity have made it possible to calculate efficiently model stellar atmospheres in which the approximation of local thermodynamic equilibrium (LTE) is not made [27]. Since departures from LTE give rise to many of the difficulties in analyzing the spectra of very hot stars, the new computational methods promise to revolutionize the interpretation of such spectra.

In addition, advances in instrumentation have made it possible to observe large numbers of moderately bright objects in a short time. Faint objects that were previously inaccessible may now be observed. For example, the McCarthy echelle spectrograph at the Palomar 2m telescope [29] can obtain spectrograms of 12th magnitude stars with a moderately high signal-to-noise ratio (~ 100) in the best orders in less than two hours. Thus, one can build up statistics by observing a large and varied sample.

1.1 MASS LOSS AND EVOLUTION OF YOUNG POPULATIONS

In a recent review [14], Chiosi and Maeder have summarized the results of recent theoretical calculations of the evolution of massive stars in which both convective overshoot and mass loss have been taken into account. They come to the following important conclusions:

1. Convective overshoot in the cores of evolving main sequence O stars results in the availability of significantly more hydrogen for core burning than previously thought. This results in the observed
extension of the main-sequence band to supergiants of type A0 [11], [32].

2. Mass loss explains the large numbers of red supergiants observed in the initial mass range from 20 to 50 M⊙ and the absence of any red supergiants brighter than M_{bol} < -9.5 [24] and may explain the compositional peculiarities of Wolf-Rayet stars that are not contact binaries. The statistics on red supergiants vs. blue supergiants are given in Table 1.

They find that models calculated with a moderate degree of overshooting and average observed mass-loss rates have the following properties:

1. For stars initially more massive than 60 M⊙, the mass-loss rates are so great that the outer layers of the stars are entirely peeled away, resulting in a bare helium core, quasi-homogeneous evolution, and no red supergiants. The stars pass through a luminous blue variable (LBV) phase and become Wolf-Rayet stars.

The abundance changes associated with this evolutionary scheme are very marked: The surface hydrogen abundance is reduced by a factor of 2 by the time the star reaches its lowest surface temperature of about 11000K, and hydrogen disappears completely as the star returns to the left side of the color-magnitude diagram. Later, triple-α products appear, and the surface helium mass fraction is reduced by a factor of two at the end of the carbon-abundant Wolf-Rayet (WC) phase.

2. For stars with initial masses in the range of 25 to 60 M⊙, the evolution of the star is sensitive to the exact rate of mass loss at different evolutionary phases. Mass loss on the main sequence favors the formation of red supergiants by suppressing the intermediate convection zone and thus reducing the amount of core hydrogen available. Mass loss during the red supergiant phase, on the other hand, shortens the red supergiant phase. If mass loss during the red supergiant phase is sufficiently great, the star becomes a Wolf-Rayet star.

During the evolution from O star to red supergiant, CNO-processed material comes to the surface; the carbon-to-nitrogen ratio thus goes from the cosmic value of 4 prior to the red supergiant phase to the CNO equilibrium value of 0.025 after the star returns to the left side of the color-magnitude diagram. The surface hydrogen abundance drops abruptly to zero halfway through
Table 1. Theoretical Luminosities and Lifetimes (in units of $10^6$ years)

<table>
<thead>
<tr>
<th>Initial mass (M/$\odot$)</th>
<th>$\log L/L_\odot$</th>
<th>H-burning lifetime</th>
<th>He-burning lifetime</th>
<th>Fraction of He phase at $\log T_{eff} &gt; 4.2$ (%)</th>
<th>Fraction of He phase at $\log T_{eff} &lt; 3.8$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>4.25</td>
<td>11.582</td>
<td>2.344</td>
<td>1</td>
<td>55</td>
</tr>
<tr>
<td>25</td>
<td>4.85</td>
<td>6.624</td>
<td>1.222</td>
<td>16</td>
<td>38</td>
</tr>
<tr>
<td>40</td>
<td>5.34</td>
<td>4.530</td>
<td>0.856</td>
<td>58</td>
<td>14</td>
</tr>
<tr>
<td>60</td>
<td>5.70</td>
<td>3.708</td>
<td>0.707</td>
<td>93</td>
<td>0</td>
</tr>
<tr>
<td>85</td>
<td>5.98</td>
<td>3.253</td>
<td>0.760</td>
<td>100</td>
<td>0</td>
</tr>
<tr>
<td>120</td>
<td>6.23</td>
<td>2.810</td>
<td>0.840</td>
<td>100</td>
<td>0</td>
</tr>
</tbody>
</table>

After Chiosi and Maeder [14]
the nitrogen-abundant Wolf-Rayet (WN) phase, accounting for the transition from WN stars with hydrogen (WNL) to WN stars without hydrogen (WNE). Finally, triple-\(\alpha\) products appear very abruptly, the helium abundance goes to zero, and the star becomes a WC star.

3. Less massive stars always become red supergiants, but if the mass-loss rates are low, the star makes a blueward loop during the red supergiant phase and may cross the Cepheid instability strip repeatedly. Larger mass-loss rates tend to suppress this loop.

As with more massive stars, CNO-cycled material appears during the red supergiant phase and produces marked abundance changes. However, for stars of 15 M\(_\odot\) or less, the C/N ratio does not drop below 1 during the first red supergiant phase and equilibrium CNO abundances are not yet established during the blueward loop.

1.1.1 Observational Consequences

The theoretical predictions described by Chiosi and Maeder may be checked observationally on several points. First, one may look for the surface abundance changes predicted for the more massive stars. For the most massive, one may expect to see a significant increase in the helium content while the star is still near the main sequence. At lower masses, an increase of the helium abundance will be evident when the star returns to the left side of the color-magnitude diagram. Unfortunately, the high excitation of the optical helium spectrum makes it impossible to trace the helium abundance during the cooler phases of the star’s evolution, as we would otherwise wish to do.

The carbon-to-nitrogen ratio should change markedly at the same evolutionary phases at which the helium abundance changes. Unfortunately, although molecules of both elements are visible in red supergiants, the molecular data and model atmospheres are in a very primitive state at present and one cannot hope to trace accurately the abundances at cooler temperatures. One is restricted to an analysis of the atomic spectra at the same temperatures at which the helium abundance may be studied.

Finally, one may attempt to determine the stellar parameters \(T_{\text{eff}}, \log g,\) and \(M_{\text{bol}}\) with suf-
ficient accuracy to make a reasonable estimate of the stellar radii and masses. One then detects the effects of mass loss in the same way that one detects mass exchange in binary systems: The stars that have experienced mass loss will be overluminous for their masses. However, since both the bolometric magnitude $M_{\text{bol}}$ and $\log g$ are difficult to determine accurately, this procedure is of limited usefulness.

The determination of $T_{\text{eff}}$ and $\log g$ for a sufficiently large sample of stars also permits an accurate calibration of the mapping of the ($T_{\text{eff}}$, $\log g$) plane to the two-dimensional MK spectral types. This is of value for studies in which the observed spectral types are used to construct theoretical temperature-luminosity diagrams for OB associations with known distance moduli [24], [25].

1.2 THE ANALYSIS OF O STARS USING SIMPLE NON-LTE MODELS

Rapid progress is being made in the computation of self-consistent models of radiation-driven stellar winds [2], [16] and in the application of the effects of wind blanketing to photosphere models [1], [12], [47]. Likewise, the new computational techniques are making possible an attack on the difficult problem of line blanketing in non-LTE model atmospheres [5], [48]. One may anticipate that it will soon be possible to calculate efficiently non-plane-parallel non-LTE models as well.

These refinements have the unfortunate effect of greatly increasing the computational cost of analyzing a particular star. Not only does each model computation take more computer time than one for a plane-parallel, unblanketed, non-LTE model, but the fact that such models require additional parameters prevents the computation of a master model grid for use in the analysis. One must perform a series of computations for each individual star analyzed. Since preliminary indications are that the effects of blanketing (both wind- and line-) and of departures from plane-parallel geometry are small for many O stars, it is reasonable to investigate what can be learned, using a grid of the simpler non-LTE models.

With these motivations, a sample of O stars stars selected from a number of galactic OB
associations [24] has been observed with the McCarthy echelle at the Palomar 2m telescope. The observed line profiles have been compared with a grid of theoretical line profiles calculated at the San Diego Supercomputer Center, using non-LTE model atmospheres with a range of effective temperatures, surface gravities, and helium abundance fraction. The method of $\chi^2$ minimization has been used to determine the choice of stellar parameters, giving the best fit of theoretical profiles to the observed profiles for each star.
2. OBSERVATIONS

2.1 OBJECT SELECTION

A sample of 36 stars from eight galactic associations was chosen for study. The particular OB associations sampled were selected to cover a range of ages (based on the relative numbers of O, B and M supergiants known to be members of each association) and galactocentric distances [24]. Table 2 lists the associations and stars selected for study. Figure 1 gives the theoretical H-R diagrams for the selected associations. In the diagram at upper left, circles represent members of Cyg OB2 and triangles, members of Aur OB2. In the upper right diagram, circles represent members of Cyg OB1 and triangles denote members of Cep OB2. In the lower left diagram, circles denote Gem OB1 and triangles denote Per OB1. The final diagram is a composite for all the associations observed. In all diagrams, filled symbols indicate stars for which parameters were eventually derived by the method of analysis described here. Parameters for other stars are taken from the paper by Humphreys [24].

The stars analyzed all fall in the region of moderate-luminosity O stars; cooler objects and Of stars were not observed or were dropped from the sample. The associations themselves appear to be of slightly different ages, with Aur OB2 and Cyg OB2 being the youngest and Per OB1 and Gem OB1 being the oldest.

The stars selected for analysis included no known binaries, and where estimates of $v \sin i$ were available, no stars with $v \sin i > 160$ km/sec. However, such data are scanty, and a number of the objects selected were found to have excessive $v \sin i$ and were not included in the final analysis. Likewise, stars showing strong Of characteristics were eventually dropped from the sample because the plane-parallel models described later were found to be completely inadequate to describe such stars. Those O stars observed but not analyzed are indicated in italics in Table 2.

Spectroscopic binarity is a more difficult problem, since for most companions bright enough to affect the measurements, the spectra of the two components would be nearly indistinguishable unless separated by large orbital Doppler shifts. Thus, it is possible that a number of spectroscopic
Table 2. O Stars Observed

<table>
<thead>
<tr>
<th>Star</th>
<th>Spectrum</th>
<th>V</th>
<th>B-V</th>
<th>Mv</th>
<th>Remarks</th>
</tr>
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<tbody>
<tr>
<td>Per OB1</td>
<td>R=11.73kpc</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>236894</td>
<td>O8 V</td>
<td>9.37</td>
<td>0.19</td>
<td>-3.9</td>
<td></td>
</tr>
<tr>
<td>12993</td>
<td>O6.5V</td>
<td>8.95</td>
<td>0.20</td>
<td>-4.4</td>
<td></td>
</tr>
<tr>
<td>13022</td>
<td>O9.5 II-III</td>
<td>8.76</td>
<td>0.32</td>
<td>-4.9</td>
<td></td>
</tr>
<tr>
<td>13268</td>
<td>O7</td>
<td>8.18</td>
<td>0.13</td>
<td>-5.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Large vsin i</td>
</tr>
<tr>
<td>Aur OB2</td>
<td>R=13.14kpc</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>242908</td>
<td>O4 V</td>
<td>9.04</td>
<td>0.28</td>
<td>-5.3</td>
<td>NGC 1893</td>
</tr>
<tr>
<td>242926</td>
<td>O7 V</td>
<td>9.35</td>
<td>0.34</td>
<td>-5.1</td>
<td>NGC 1893</td>
</tr>
<tr>
<td>242935</td>
<td>O7 V</td>
<td>9.43</td>
<td>0.20</td>
<td>-4.6</td>
<td>NGC 1893</td>
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<td>35619</td>
<td>O7 V</td>
<td>8.55</td>
<td>0.24</td>
<td>-5.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gem OB1</td>
<td>R=11.49kpc</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>42088</td>
<td>O6.5</td>
<td>7.55</td>
<td>0.07</td>
<td>-4.5</td>
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<tr>
<td>254755</td>
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<td>8.84</td>
<td>0.60</td>
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<tr>
<td>256035</td>
<td>O9 Vp</td>
<td>9.16</td>
<td>0.55</td>
<td>-4.3</td>
<td>Large vsin i</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cyg OB1</td>
<td>R=9.71kpc</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>193504</td>
<td>O7 Ibf</td>
<td>7.40</td>
<td>0.45</td>
<td>-6.2</td>
<td>Of</td>
</tr>
<tr>
<td>193595</td>
<td>O7</td>
<td>8.72</td>
<td>0.36</td>
<td>-6.6</td>
<td></td>
</tr>
<tr>
<td>193682</td>
<td>O5</td>
<td>8.41</td>
<td>0.51</td>
<td>-5.4</td>
<td>Large vsin i</td>
</tr>
<tr>
<td>194094</td>
<td>O9 III</td>
<td>9.02</td>
<td>0.59</td>
<td>-5.0</td>
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</tr>
<tr>
<td>194280</td>
<td>OC9.7 lb</td>
<td>8.39</td>
<td>0.76</td>
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<tr>
<td>229841</td>
<td>O6.5 V</td>
<td>8.94</td>
<td>0.56</td>
<td>-5.0</td>
<td>Large vsin i</td>
</tr>
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<td>229254</td>
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<td>8.92</td>
<td>0.77</td>
<td>-5.6</td>
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<td>1364063</td>
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<td>9.71</td>
<td>1.14</td>
<td>-5.9</td>
<td>Confused</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cyg OB2</td>
<td>R=9.85kpc</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td># 1</td>
<td>O9 V</td>
<td>11.09</td>
<td>1.42</td>
<td>-5.4</td>
<td>Large vsin i</td>
</tr>
<tr>
<td># 3</td>
<td>O9:</td>
<td>10.22</td>
<td>1.61</td>
<td>-6.8</td>
<td>Large vsin i</td>
</tr>
<tr>
<td># 4</td>
<td>O7 III</td>
<td>10.22</td>
<td>1.17</td>
<td>-5.6</td>
<td>+40 4219</td>
</tr>
<tr>
<td># 6</td>
<td>O8 V</td>
<td>10.67</td>
<td>1.22</td>
<td>-5.2</td>
<td>Large vsin i</td>
</tr>
<tr>
<td># 7</td>
<td>O3 If</td>
<td>10.50</td>
<td>1.44</td>
<td>-6.1</td>
<td>Of</td>
</tr>
<tr>
<td># 8A</td>
<td>O6 Iab</td>
<td>8.98</td>
<td>1.29</td>
<td>-7.2</td>
<td>+40 4227 Large vsin i</td>
</tr>
<tr>
<td># 8B</td>
<td>O8:</td>
<td>10.31</td>
<td>1.35</td>
<td>-6.6</td>
<td></td>
</tr>
<tr>
<td># 8C</td>
<td>O5 III</td>
<td>10.08</td>
<td>1.35</td>
<td>-6.2</td>
<td>Large vsin i</td>
</tr>
<tr>
<td># 9</td>
<td>O5 If</td>
<td>10.80</td>
<td>1.93</td>
<td>-7.3</td>
<td>Of</td>
</tr>
<tr>
<td># 10</td>
<td>O9.5 Ia</td>
<td>10.04</td>
<td>1.43</td>
<td>-6.5</td>
<td>+41 3804</td>
</tr>
<tr>
<td># 11</td>
<td>O5 If</td>
<td>10.04</td>
<td>1.43</td>
<td>-6.5</td>
<td>+41 3807 Of</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cep OB2</td>
<td>R=10.21kpc</td>
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<td></td>
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<tr>
<td>204827</td>
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<td>7.95</td>
<td>0.81</td>
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<td>Tr 37</td>
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<tr>
<td>207198</td>
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<td>0.31</td>
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<td>0.33</td>
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<tr>
<td>209975</td>
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<td>-5.7</td>
<td>19 Cep</td>
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<tr>
<td>Miscellaneous</td>
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</tr>
<tr>
<td>9 Sgr</td>
<td>O4V</td>
<td>5.97</td>
<td>0.03</td>
<td>-6.1</td>
<td></td>
</tr>
<tr>
<td>λ Ori</td>
<td>O8</td>
<td>3.66</td>
<td>-0.19</td>
<td>-5.2</td>
<td></td>
</tr>
</tbody>
</table>
Figure 1. H-R diagram of observed associations. See text for explanation of symbols.
binaries have crept into the sample.

The selection of stars with a low $v \sin i$ will bias the sample towards slow rotators. Since the ultimate objective of this research is to test the models of Chiosi and Maeder [14], in which rotation is neglected, this bias may actually be advantageous.

2.2 DATA COLLECTION AND REDUCTIONS

The sample of stars was observed with the McCarthy echelle spectrograph on the Palomar 2m telescope [29]. This instrument covers the entire optical spectrum from about 3650Å to 8000Å, with partial coverage to 10000Å. Each order covers from 100Å (in the near infrared) to 50Å (in the violet). The detector is a Texas Instruments 800 x 800-pixel charge-coupled device (CCD) cooled with liquid nitrogen. It is routinely soaked in oxygen and flooded with ultraviolet light prior to use to improve the quantum efficiency at short wavelengths.

For each observation, the signal-to-noise ratio for the optimal orders, those covering the wavelength range from about 5850Å to 6550Å, was better than 100. The signal-to-noise ratio usually decreased rapidly farther towards the blue, both because of the decreased sensitivity of the CCD detector and because most of the objects observed show significant reddening from interstellar dust. The stars from OB2 Cyg were particularly difficult in this respect, with a typical reddening of $E(B-V) \sim 1.5$, or greater. In most cases it was impossible to obtain a high signal in the blue orders without saturating the red orders and ruining the exposure. As a result, the analysis was restricted to lines longward of the Hγ line at 4342Å.

Flat fields for calibration were prepared by summing frames obtained by exposing the echelle to a diffuse incandescent source through a series of broad-band filters. This made it possible to obtain a satisfactory exposure level in the blue orders of the echelle without overexposing the orders in the red. A thorium-argon lamp was used to obtain a comparison spectrum for the wavelength calibration.

The spectrograms were reduced using the echelle routines in the FIGARO data processing
The flat field, comparison, and object spectrograms were first remapped to remove curvature from the orders (using the FIGARO routine CDIST). A normalized flat field was then obtained by dividing the raw flat field by a copy of the flat field that had been smoothed in the direction parallel to the orders; this ensured that the flat field was close to unity everywhere (while retaining pixel-to-pixel variations and interference fringes), so that noisier, low-signal rows in each order were not artificially amplified when the flat field was used to calibrate the object spectra. After the observed spectrograms were divided by the normalized flat field, the rows making up each order were summed and an estimate of the crosstalk between orders was subtracted from each order (using the FIGARO routine ECHTRACT).

The profiles of the hydrogen and helium lines were obtained by fitting a polynomial to the two orders adjacent to each order containing a line of interest; the central order was then divided by the average of the two polynomials. This provided a way of estimating the continuum level even in the presence of very strong wings, as illustrated by the profile obtained this way for Hβ in Vega (Figure 2). Unfortunately, the results were rarely this good for the spectrograms of O stars presented here; the Stark wings are much shallower in O stars, and confusion from stellar and interstellar lines and bands resulted in some uncertainty in the continuum level.

2.3 DATA QUALITY AND SYSTEMATIC ERRORS

The chief source of uncertainty in the observations is ambiguity in the continuum level, rather than Poisson noise. The technique of interpolating the continuum from adjacent orders is most effective for the Balmer lines, with their strong wings. The much narrower neutral and ionized helium lines are much more sensitive to small, local errors in the continuum-level determination.

Such errors arise primarily from two sources: imperfect flat-field calibration and confusion with stellar or interstellar lines and bands. The former effect is noticeable for the HeI 4471Å line and for the red wing of the Hγ Balmer line (which is located near the end of an echelle order). Here one sees that the local continuum level is not flat. The effect is reproducible from night to night despite
Figure 2. Continuum-flattened data for H\(\beta\) in Vega. The line profile has been normalized to the continuum level interpolated from the adjacent two echelle orders.
the fact that fresh flat fields were obtained and used each night.

The second effect is seen, e.g., with the HeI 6678Å line and the Balmer lines. In the case of HeI 6678Å, a diffuse feature (probably intrinsic to the star rather than an interstellar feature) badly confuses the red wing of the line. Likewise, stellar OII lines confuse the already uncertain calibration of the red wing of Hγ.

In general, the effects of poor flat-field calibration are more troublesome than the effects of interstellar bands. Future work on these objects would best be done on an instrument with superior photometric characteristics, even at the expense of a lower signal-to-noise ratio and/or resolution. However, the confusion from lines and bands sets an ultimate limit on the quality of observational line profiles.

Another uncertainty in the data is the absolute wavelength calibration. The FIGARO software for carrying out the calibration is computationally expensive; since little information about the physical parameters is contained in the wavelength of the line centers, it was decided to use a single wavelength calibration for all spectrograms. However, thorium-argon comparison spectra were obtained each night for possible future use in determining radial velocities.

Finally, a particular difficulty with echelle spectrograms is the problem of removing crosstalk between orders and accounting for scattered light in the instrument. The McCarthy software [29] for reducing echelle data does an excellent job of accounting for both effects for spectra that are well focused on nights of fair-to-excellent seeing. It is unlikely that such background light has significantly affected the line residual intensities.

2.4 OBSERVED EQUIVALENT WIDTHS

Although profiles were used in the fit of theory to data described in Chapter 4, the equivalent widths of helium lines contain useful information in a concise form. Table 3 gives equivalent widths (in mÅ) for lines of neutral and ionized helium, along with equivalent widths of the prominent CIII emission line at 5696Å and the CIV absorption lines at 5801Å and 5812Å. Some qualitative analysis
Table 3. Equivalent Widths of Helium and Carbon Lines

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<td>770 ± 30</td>
<td>160 ± 50</td>
<td>598 ± 50</td>
<td>267 ± 10</td>
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<tr>
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of the carbon features is presented in Chapter 5. The detectability limit for weak lines was \(~ 80 \text{ mÅ}\) for the stars with \(v \sin i > 100 \text{ km/sec}\) and \(~ 20 \text{ mÅ}\) for stars with \(v \sin i \sim 60 \text{ km/sec}\).

The equivalent widths were measured using the FIGARO routine GAUSS. This routine determines the continuum level by fitting a polynomial to the continuum with iterative rejection of outlier points. Equivalent widths may then be obtained both by simple integration and by fitting of Gaussian profiles. The values quoted here were obtained by simple integration and compared with the results from fitting Gaussian profiles to estimate the uncertainties in the values. This allows for the effects of imperfect continuum normalization and blends and the uncertainty in the wings of the Stark-broadened ionized helium lines.

The Balmer lines, since they are dominated by the shallow \(\Delta \nu^{-5.2}\) Stark wings, are difficult to measure equivalent widths for. It was quite common to measure values for the equivalent widths that were up to a factor of 2 smaller than those of the theoretical profiles that best matched the observed profiles. Hence, no observed equivalent widths for the Balmer lines are presented here. The profiles are presented later, along with the helium line profiles and the corresponding best theoretical fits.
3. THEORY

3.1 BACKGROUND

It is generally recognized that model atmospheres and synthetic spectra for hot stars cannot be approximated usefully under the assumption of local thermodynamic equilibrium [34]. The calculation of non-LTE model atmospheres is considerably more difficult than the calculation of LTE model atmospheres, primarily because of the detailed dependence of the source function at each frequency on the radiation field at all frequencies.

An LTE calculation may be thought of as a very restricted scattering problem in which the source function at each frequency is uniquely determined by a single weighted integral of the radiation field, the constraint of radiative equilibrium, which is characterized by a single quantity, the temperature. That is, at each depth point,

\[ S(\nu) = B_\nu(T) \]  

subject to the condition

\[ \int_0^\infty (J_\nu - B_\nu(T)) \kappa_\nu d\nu = 0. \]  

(Convective energy transport is negligible in the atmospheres of O stars.) Thus, it is relatively easy to organize the transfer equations describing the model atmosphere by frequency in such a way that the resulting computational algorithm scales linearly with the number of frequencies [41]. One determines (to first order) the perturbation to the single integral of interest, the condition of radiative transfer, resulting from the perturbation of the radiation field at each frequency and depth: Since the condition of radiative equilibrium is only approximately satisfied by the starting model atmosphere (obtained by a gray atmosphere calculation or some other simple analytic approximation), one sets the perturbation in the condition of radiative equilibrium equal to the opposite of the current value of this integral (which should be, but is not yet, equal to zero):

\[ - \int_0^\infty (J_\nu^0 - B_\nu^0(T^0)) \kappa_\nu^0 d\nu = \Delta \int_0^\infty (J_\nu - B_\nu(T)) \kappa_\nu d\nu = \int_0^\infty (\Delta J_\nu - \frac{\partial B_\nu}{\partial T} \Delta T) \kappa_\nu d\nu, \]
which, after the integral is replaced by a quadrature sum, has the form

\[ A = \sum_N W_N \Delta J_\nu - \sum_N X_N \Delta T, \]  

(4)

where \( A, W_N, \) and \( X_N \) are scalars. These coefficients are calculated for each depth point, requiring of order \( ND \) operations (where \( N \) is the number of frequency points in the quadrature sum and \( D \) the number of depth points). Here the opacity is assumed to be constant; this approximation may be dropped (as was done for the actual calculations) without changing the form of the last equation.

The transfer equation may then be used to determine the perturbations in the radiation field resulting from a perturbation to \( T \); one gets equations of the form

\[ \Delta J_\nu = \sum_D Y_D \Delta T_D. \]  

(5)

The scalar coefficients \( Y_D \) are calculated for each frequency, and \( \Delta J_\nu \) is eliminated from Equation 4; this takes of order \( ND^3 \) operations. One is left with the system of equations

\[ A = M \Delta T, \]  

(6)

where \( A \) and \( \Delta T \) represent vectors over all depths and \( M \) is a \( D \times D \) matrix \[34\]. This system is solved for the corrections to \( T \) (and thus the source function at each depth) in of order \( D^3 \) operations. The computational cost is dominated by the calculation of the coefficients to Equation 5 so that the calculation time scales as \( ND^3 \).

In the case of a non-LTE calculation, on the other hand, the source function is defined by a very large number of radiation field integrals, each with a different weighting function, in addition to the temperature; that is,

\[ S(\nu) = S_\nu(T, N_L), \]  

(7)

subject to the same constraint of radiative equilibrium (Equation 2), and additional constraints of the general form

\[ N_L \left( \sum_{L' \neq L} A_{L,L'} \int_0^\infty J_\nu \kappa_{\nu,L-L'} dv + C_{L-L'}(T) \right) = \sum_{L' \neq L} N_{L'} \left( B_{L,L'} \int_0^\infty J_\nu \kappa_{\nu,L'-L} dv + C_{L'-L}(T) \right). \]  

(8)
Here $L$ represents the number of atomic levels and $N_L$ represents the occupation numbers for these levels, which characterize the constraint equations. The quantity $C_{L' \rightarrow L}(T)$ includes spontaneous radiative de-excitation or recombination.

If one attempted to proceed as with the LTE calculation, organizing by frequency, one would eventually end up with equations of the form

$$A = M \Delta N,$$

where $A$ and $\Delta N$ represent vectors over all depths and all constraints and $M$ is the corresponding square matrix. $M$ will have ~ 500-5000 rows and columns (since for a typical non-LTE calculation, there will be ~ 50 depth points and ~ 10 - 100 constraints), and the computational cost becomes astronomical.

Thus, one cannot organize the problem by frequency, and one is forced to organize it by depth; the resulting equations have the form

$$Q = A \Delta \psi_{d-1} + B \Delta \psi_d + C \Delta \psi_{d+1}$$

at each depth point $d$ [33]; here $\psi$ represents a vector over all frequencies and constraint equations at a single depth point. The only full matrices that must be inverted are $(N + L) \times (N + L)$ matrices. Thus, the computation time scales as $(N + L)^3 D$. Although this is much more practical than the organization by frequency, it puts a severe limit on the number of frequencies and atomic levels that may included in the calculation. The models calculated by Mihalas, Auer, and Heasley [36] (hereafter MAH) were restricted to 105 frequencies and 11 atomic levels and were expensive to compute even for such a simple description of the radiation field and atomic physics.

Recently Anderson [6] has pointed out that it should be possible to sum many transfer equations describing the same line or continuum into a single equation, approximately describing the total radiative energy density in that line or continuum. Thus, the number of equations linearized is greatly reduced, since many quantities $\Delta J_\nu$ are reduced to a few quantities $\Delta E_b$ representing the
total energy density in a “block” of frequencies describing one line or continuum. In addition, the presence of both the occupation numbers (each characterizing a constraint equation) and the energy densities in the solution vector \( \psi \) is redundant, since the corrections to the one are given by the corrections in the other (to the same order of approximation as the overall computation); thus, the large solution vector \( \psi \) containing corrections to all frequencies and occupation numbers may be replaced by a much smaller vector \( \psi_{\text{and}} \) containing only corrections to the temperature and a few energy densities \( E_b \). The temperature could, in principle, be eliminated as well, since, like the other variables of constraint, it is uniquely defined by the radiation field; but since its presence would introduce non-linearities into the subsequent calculation of the new values for the constraint variables (through collision terms), it is treated explicitly.

The actual numerical approximation made is that the detailed distribution of the radiation field in a particular block of frequencies dominated by a single line or continuum and formed at similar depths is fixed. One then solves (to first order) for the factor by which all the mean intensities in each frequency block should be multiplied in order to better satisfy the transfer and constraint equations. The resulting equations are similar in form to Equation 10. These are solved and the mean intensities in each block are multiplied by the correcting factor for that block. The level populations are then revised using the modified mean intensities and temperatures, the transfer equations for all frequencies are solved using the resulting source function, and the distribution of the radiation field in each frequency block is updated. The whole procedure is iterated to convergence.

The resulting method converges linearly rather than quadratically (as is characteristic of the complete linearization procedure), but the convergence rate is acceptable for moderate error tolerances. It typically requires less than fifteen iterations to reach a tolerance of 0.01% in the surface flux. The number of operations per iteration scales as \( DB^3 \), where \( B \) is the number of frequency blocks.
3.2 MODEL ATMOSPHERE AND SYNTHETIC SPECTRUM CALCULATIONS

The calculation of theoretical line profiles proceeds in several steps. A gray model atmosphere is first calculated, using an approximate T-τ relationship. This model is then used as the starting approximation for an LTE model atmosphere code. The resulting LTE model is then used as the starting approximation for a non-LTE code employing the Anderson algorithm.

At this point, the temperature and electron density at each depth in the model atmosphere is fixed. However, an effort is made to improve the accuracy of the hydrogen and helium level populations further by carrying out a calculation in which the level populations of one element are refined while holding the populations of the other element and the temperature and electron density fixed. This permits an approximate treatment of a larger number of transitions for each element, using more detailed line profiles.

Finally, profiles for selected lines are calculated, using the most accurate available theoretical line broadening data.

The whole set of computer codes is written in FORTRAN 77 for use on a CRAY or other compatible vector processor. The codes proved to be well suited for vector optimization, and it was usually possible to vectorize by frequency index rather than by depth index (the number of frequencies being much greater than the number of depths).

3.2.1 Approximations

The chief approximations made in the theoretical calculations are (1) the approximation of plane-parallel geometry; (2) the neglect of metallic line blanketing; and (3) the approximations in the atomic physics.

The use of plane-parallel models has a number of practical advantages. First, it is considerably more difficult and computationally expensive to calculate models with spherical symmetry than to calculate plane-parallel models, because one is obliged to use many more angle points in the moment sums. Second, the use of spherical models introduces an additional physical parameter, since $T_{\text{eff}}$
and log $g$ are replaced by the total luminosity, mass, and radius at the base of the atmosphere. Since the plane-parallel models described here already have three physical parameters, the introduction of a fourth would make it impractical to calculate a grid of models, and one would be forced to make calculations for individual stars.

In any case, an analysis using spherical geometry would need starting estimates of the stellar parameters, and these would be best provided by the plane-parallel analysis described here.

It cannot be denied that atmospheric extension and stellar winds have important effects. The most obvious effect is that opaque transitions will arise from a larger radiating area, resulting in greater flux in the line. This is generally recognized as the mechanism whereby the prominent emission lines of supergiant stars, including the Of stars, originate. In particular, it will be seen later that the HeII 4686Å line is much weaker in most of the observed spectra than in the theoretical spectra calculated here.

The other important effect of atmospheric extension is the geometric dilution of the radiation field in the outer regions of the atmosphere. This has the effect of reducing the source function in strong lines. In particular, as was first pointed out by Ghobros [18], the population of the $2^3S$ level of neutral helium is most strongly overpopulated relative to a non-LTE plane-parallel model. Voels et al. [47] find that the the 6678Å, 5876Å, and 4471Å lines are all suspect. It will be seen later that the 5876Å line reproduces poorly the observational material presented here, but that the fits to the other two lines seem satisfactory (except for the 6678Å line at higher $T_{\text{eff}}$).

The effects of neglecting winds are difficult to estimate at present. Although rapid progress is being made in the theory of radiation-driven stellar winds, practical computations of stellar spectra (such as, e.g., Voels et al. [47]) use an assumed value for the mass-loss rate. This, in turn, must be estimated from observations of P Cygni profiles of ultraviolet resonance lines that are not available for the bulk of the stars observed here. Two of the five stars studied in detail by the Colorado group [12], [47] show significant effects from wind blanketing: ζ Pup, spectral type O4f, and α Cam, spectral type O9.5 Ia. For the other objects (ζ Ori A, spectral type O9.7 Ib; δ Ori, spectral
type O9.5 II; and AE Aur, spectral type O9.5 V), the effects of wind blanketing were found to be negligible. Thus, for the most luminous supergiant and Of stars, the neglect of wind blanketing may be serious, while for less luminous objects, the effects are not important.

The second approximation, the neglect of metallic line blanketing, is made for the same reasons as the approximation of plane-parallel geometry. Non-LTE metallic line blanketing greatly increases the computational cost of a model and introduces at least one additional free parameter, the metallicity. The main physical consequences of metallic line blanketing in non-LTE models are a slight reduction in the effects of departures from LTE (because the mean thermalization depth in ionization continua is reduced) and heating of the atmosphere through backscattering. Since backscattering by stellar winds has a similar effect, the neglect of metallic line blanketing may be no worse an approximation than the neglect of spherical geometry.

Werner [48] has calculated plane-parallel non-LTE model atmospheres that treat detailed line blanketing by hydrogen, helium, and carbon. Although his models cover a somewhat different temperature range than those described here (60000K to 100000K), his general conclusions may be relevant. He finds that the optical lines of hydrogen and helium are only marginally affected, the changes in the line profiles being limited to the line cores. The models with line blanketing show shallower line cores for the combined H/HeI and H/HeII lines and the HeII 4686Å line and deeper line cores for all other lines. The effects, however, are not great.

The atomic data used are somewhat uncertain. Although the radiative rates are generally reliable (those for hydrogen and ionized helium being exact, and those for neutral helium being excellent approximations), the collision rates are uncertain even for the hydrogenic atoms because of the difficulty of the theoretical calculation. Those for the lowest levels ($n \leq 3$ for hydrogen and neutral helium and $n \leq 5$ for ionized helium) are from fairly sophisticated theoretical calculations and/or laboratory measurements. Those for higher levels are much more uncertain. However, since the collision rates are important mainly for determining the thermalization depth of line transitions, the uncertainty in these rates is unimportant when the thermalization of the corresponding lines
is dominated by the overlapping continuum absorption (for which the cross sections are reliable). This is certainly the case for infrared transitions, since the continuum absorption increases rapidly towards lower frequencies.

3.2.2 The Gray Atmosphere Calculation

The gray atmosphere program, GRAY, is a highly modified version of the MAH code written for the same purpose. The main differences are in the formats of the input and output files and in the neutral helium bound-free cross sections used. The file format was developed with the intention that it be as general as possible, so that models calculated with different approximations, e.g., LTE vs. non-LTE, could be represented in the same format (Table 4).

The neutral helium bound-free cross sections for the lowest states are represented as Kramers' cross sections modified by Gaunt factors. The Gaunt factors were approximated by fitting rational functions to values calculated from the tables of Stewart [44], Jacobs [26], and Steward and Webb [45]. The resulting approximations are quite good close to the absorption edge, but are less accurate at higher frequencies where autoionization levels give a complex structure to the cross section. Since the lowest autoionizing state has a rather high excitation (55.4 eV), no autoionizing states have been included in the neutral helium model atom, and the structure these levels give to the photoionization cross sections are probably of little importance. The relative contribution of the radiation field at such high frequencies to the bound-free rates for neutral helium is small.

The program GRAY optionally includes negative hydrogen ion opacities [17], [19], although these were not used for the O star models described here (since they are negligible at temperatures characteristic of O star atmospheres).

3.2.3 The LTE Calculation

The gray model atmospheres are used as starting approximations for an LTE atmosphere code (LTE), which uses the highly efficient Rybicki method described above [34], [41]. This LTE calculation improved the convergence of the subsequent non-LTE calculation by providing a first
Table 4. Format of Machine-Readable Model Atmospheres

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<th>FORTRAN Format</th>
<th>Explanation</th>
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<tr>
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<td>(2I5)</td>
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</tr>
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<td>(5E15.7)</td>
<td>Frequency grid</td>
</tr>
<tr>
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<td>(2I5)</td>
<td>Frequency quadrature rule and grid point: first value is 2 for trapezoid rule and 3 for Simpson’s rule, second value gives the grid point for which the rule applies. The final line has zero for both values.</td>
</tr>
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<td>(2I5)</td>
<td>First value flags use of negative hydrogen ion opacities; second flags inclusions of lines</td>
</tr>
<tr>
<td>20+</td>
<td>(I5)</td>
<td>Atomic number of an element whose model and occupation numbers are given by the succeeding lines. The final line has zero as the value.</td>
</tr>
<tr>
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<td>Gives number of levels and lines for each ion of the particular element being described, starting with the negative ion.</td>
</tr>
<tr>
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<td>Ionization frequency of each level starting with those of the negative ion; a new line is started for each ion.</td>
</tr>
<tr>
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<td>(2I5)</td>
<td>Lower and upper state of each line transition</td>
</tr>
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<td>(5E15.7)</td>
<td>Occupation numbers of all levels of all ions at each depth in the atmosphere, listed in that order without any breaks.</td>
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</table>
approximation with an accurate temperature and electron-density stratification at large optical depths. The continuum opacities used are identical with those in the gray model calculation, and line opacities have been added to the calculation. The line profiles used are depth-dependent Doppler profiles. It is assumed that microturbulence is negligible.

3.2.4 The Non-LTE Calculations

The MAH non-LTE model atmosphere code was modified to use the Anderson algorithm and to treat many more transitions and continua. Whereas the original calculations were made with model helium ions with only two levels and with six hydrogen line transitions (and none of helium), the modified code handles ten hydrogen levels, all neutral helium levels with a principal quantum number of five or less, and fifteen ionized helium levels. In addition to continuum radiative transition rates, the program handles ten hydrogen line transitions and fourteen neutral helium line transitions (all those connecting levels with principal quantum number \( n \leq 5 \)) and ten ionized helium transitions (all those connecting levels with principal quantum number \( 2 \leq n \leq 6 \)). More transitions are used for neutral helium than hydrogen because of the non-degeneracy of the \( nl \) levels of the two spin systems. The code includes an automatic scheme for allocating frequency blocks; the criteria described by Anderson [6] are used to determine the frequency block assignment. Since the resonance lines of ionized helium are extremely opaque [22], they are assumed to be in detailed balance; the lines arising from the first excited level are treated as if they were resonance lines for purposes of determining block assignment.

As a test of the algorithm, a continuum-only model (non-LTE, no lines) was calculated, using complete linearization and compared with one calculated by the Anderson algorithm using an identical frequency grid and identical atomic data. The resulting level populations were identical to within the tolerance of the calculations.

The opacities used in the non-LTE calculations were identical with those used in the gray and LTE calculations. The collisional excitation rates for transitions between the lower states of
hydrogen were taken from Aggarwal [3]. Collisional excitation rates for transitions between lower states of neutral helium were taken from Aggarwal et al. [4] and Berrington et al. [10]. Collision strengths for ionization from lower states of hydrogen, neutral helium, and ionized helium are from Lennon et al. [28]. All other collisional rates were identical with those of the original code. These are represented as the product of a Boltzmann term, \( \exp \left( \frac{-E}{kT} \right) \), a power of \( T \) (usually \( T^{-1/2} \)), and a rational function of \( T \) determined by a least-squares fit.

Generally, model convergence was reasonably rapid. However, for a small number of models (roughly 10% of all those calculated), it was necessary to employ a radiative/collisional switching method [23]. The calculations using the switching method were carried out after normal calculations had been attempted for all points in the model grid, and it was later discovered that the switched calculations had inadvertently been made with a slightly modified set of ionization frequencies for the upper states of neutral helium. This did not appear to have had any significant effect on the calculations, which is not surprising, considering that the associated continua are very weak.

With a suitable grid of models, the next step was to refine the individual line spectra for hydrogen and helium by carrying out a more detailed calculation for each spectrum while holding the temperature, electron density, and level populations of the other element fixed. The hydrogen spectrum code replaces the Doppler profiles with more accurate line profiles that include the Stark effect, and allows for the effects of the overlapping ionized helium lines. Ten transitions are included explicitly, and the rates of all other transitions connecting the first ten levels of hydrogen are estimated at the start of the calculation using the equivalent two-level atom approach [34].

A similar calculation is used to refine the helium lines. The line profiles used are Voigt profiles with a damping width that is the sum of the natural damping width and the quadratic Stark damping width [20]. The effects of the overlapping hydrogen lines are taken into account for the ionized helium lines.

For the model at \( T_{\text{eff}} = 30000 \text{K} \), \( \log g = 3.0 \), \( \text{He}/\text{H}=0.20 \), the equivalent widths of the HeII 4686Å and He I 5016Å lines were vanishingly small. In the case of the HeII 4686Å line, this was due
to a flux in the line wings that exceeded the continuum flux; the profile itself appeared reasonable. The tiny equivalent width for the HeI 5016Å line reflected the actual line profile. All other lines for this model were consistent with those of the adjacent models in the grid. The reasons for this inconsistency in the two lines is unclear, although it may have something to do with the low gravity of the model (close to the Eddington limit for this effective temperature). The equivalent widths and line profiles of these two lines were interpolated from adjacent models for use in the tables and fits presented here.

3.2.5 Line Synthesis

For the final line synthesis, the Balmer line profiles are calculated using theoretical absorption profiles from the tables of Vidal, Cooper, and Smith [46]. The ionized helium line profiles are taken from the very recent unified-theory calculations of Schöning and Butler [43]. For neutral helium, the Voigt profiles are replaced by unified-theory profiles for the lines with forbidden components (the 4471Å and 4922Å lines) at densities in excess of $10^{13}$ electrons/cm$^2$ [8], [9].

3.2.6 Computational Costs

The gray model computation is extremely fast and represents a negligible fraction of the total computation cost. The LTE calculation takes less than a minute of processor time on the CRAY to complete a model calculation. The non-LTE code is somewhat more expensive, taking slightly less than one minute per iteration for a total of up to 12 minutes per model. The code for refining the hydrogen populations takes less than a minute per model, but that for helium is quite expensive (more than 10 minutes per model) and is also expensive in memory usage. In light of the computational cost, the benefits of the refined population codes are probably insufficient to warrant their use for future calculations. They are included here primarily to rule out the possibility that discrepancies between theory and observation arise from too simplistic a model atom.
3.3 RESULTS

Figure 3 gives the profile of the H$\beta$ line for a model with $T_{\text{eff}} = 35000$, $\log g = 4.0$, and [He/H]=0.10 at each stage of the calculation. The profiles, in order of increasing depth, correspond to the gray model, the LTE model, the non-LTE model, and the non-LTE model with refined treatment of the hydrogen spectrum. It is evident that the effects of departures from LTE are sizable, as was noted two decades ago by Auer and Mihalas [7]. However, the more refined non-LTE calculation has little effect outside the line core.

The temperature structure for the same model is given in Figure 4, along with the temperature structure of the Mihalas model with the same effective temperature, surface gravity, and helium abundance fraction [33]. It is evident that while the structures are identical at depth, the temperature is significantly higher in the outermost layers of the atmosphere in the new model. Since heating by photoionizations from the ground state of hydrogen largely determines the temperature structure in the upper atmosphere [34], it is likely that the higher temperature results from the additional transitions included in the model hydrogen atom. These permit electrons to cascade freely into the ground state. Although the change in the temperature structure is pronounced, it does not have a large effect on the calculated line profiles, the effects being restricted to the cores of the stronger lines.

3.3.1 Theoretical Equivalent Widths and Profiles

The equivalent widths of the synthesized optical lines are found in Table 5. Since the equivalent widths of the hydrogen Balmer lines are of limited practical value, complete profiles have been given in Figure 5 for He/H=0.10, the normal cosmic abundance. (The hydrogen lines themselves are not very sensitive to composition, although the overlapping ionized helium lines are.) These are in general agreement with the results of the MAH calculations, the greatest differences being at the highest effective temperatures modeled and for the ionized helium lines.
Figure 3. Theoretical profiles of H/β at different points in the calculation. The profiles are, in order of increasing depth: for a gray model atmosphere; for an LTE model atmosphere; for a non-LTE model atmosphere; and for a non-LTE model atmosphere with improved profiles and approximate treatment of all transitions between states with \( n \leq 10 \).
Figure 4. Temperature structure of a typical model atmosphere. The model chosen has $T_{\text{eff}} = 35000\,\text{K}$, $\log g = 4.5$, and $\text{He/H}=0.10$. The bottom curve is the temperature profile for the MAH model with these parameters; the top curve is the temperature profile for the author's model.
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Table 5-10. Theoretical Equivalent Widths of HeI 5016Å

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Table 5-11. Theoretical Equivalent Widths of HeI 4713Å

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Figure 5. Theoretical hydrogen Balmer profiles. The profiles illustrated are for the composition He/H=0.10, the normal cosmic abundance.
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
Figure 5. (Continued)
3.3.2 Bolometric Corrections

A very useful quantity is the bolometric correction, which, for stars of known $T_{\text{eff}}$ and $\log g$, permits one to convert the visual magnitude $M_v$ to the bolometric magnitude $M_{\text{bol}}$.

Code et al. [15] give the following formula for calculating the bolometric correction:

$$B.C. = 2.5 \log \left( \frac{\int_0^\infty f_\lambda S_V(\lambda)d\lambda}{\int_0^\infty f_\lambda d\lambda} \right) + 0.958,$$

(11)

where the zero point constant 0.958 has been determined empirically. The sensitivity function $S_V$ is given by Matthews and Sandage [31].

Table 6 gives the bolometric corrections obtained using this formula for the models calculated here. One finds that the bolometric correction is rather insensitive to $\log g$ and quite insensitive to He/H; the values quoted here are for He/H=0.05, which differ by less than 0.06 magnitude from the values for He/H=0.50. These values show good agreement with the values obtained empirically by Code et al. [15] for stars with effective temperatures in the range of the theoretical calculations presented here.
Table 6. Bolometric Corrections

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4. DETERMINATION OF STELLAR PARAMETERS

4.1 THE FITTING OF LINE PROFILES BY $\chi^2$ MINIMIZATION

The parameters of each star observed were determined by the method of $\chi^2$ minimization. The $\chi^2$ parameter is a weighted sum of the squares of the differences between the observed data $D(\lambda)$ and theoretical profiles $T(\lambda)$, which are characterized by the parameters $T_{\text{eff}}$, $\log g$, He/H, and the projected rotational velocity $v \sin i$. The values of the parameters for which the value of $\chi^2$ is a minimum is found using the implementation of the Levenberg-Marquardt algorithm given by Press et al. [40].

The chief advantage of this method of fitting is that it eliminates most of the personal bias that unconsciously creeps into any fit obtained by simple inspection of the observational profile superimposed on a grid of theoretical profiles. Some personal bias remains, since the user specifies which wavelength regions are too contaminated by blends or continuum errors to be included in the fit; but it is felt that this is much less than the personal bias in a fit by inspection.

Another advantage of the $\chi^2$ minimization is that it allows information from all parts of all the line profiles to be taken into account simultaneously. The human eye and brain cannot do this for eleven detailed line profiles, and so the human observer must pick a subset of lines sensitive to each parameter and estimate each parameter iteratively from a limited subset of the data.

As a result of the uncertainty of the continuum level and wavelength calibration, the actual fit of theoretical profiles to the observed profiles must allow a certain amount of flexibility in the assumed continuum level and wavelength zero point. This is introduced through three free parameters for each line that are allowed to vary with the physical parameters in the fit by $\chi^2$ minimization. If $T_0(\lambda)$ is the theoretical profile of a given line, the profile used in the actual fit has the form

$$T(\lambda) = (a + b\lambda)T_0(\lambda + c),$$

where it is assumed that $a \sim 1.0$ and $b$ and $c$ are small.
Some justification for this use of a rather large number of "fudge parameters" is in order. The parameter \( c \) destroys the information contained in the central wavelength of each line. Since the central wavelengths are only very weakly dependent on the physical parameters, the information contained in the wavelength scale is swamped by noise resulting from the imperfect wavelength calibration. It is therefore reasonable to eliminate both the signal and noise by permitting the zero point of the wavelength scale for each line to be a free parameter in the \( \chi^2 \) minimization. The continuum flux level (and the information in it) have already been eliminated by the normalization of the line profiles to the continuum level. This normalization is "fine-tuned" by the parameter \( a \) with no loss of information.

The hydrogen and ionized helium line profiles are symmetric through the properties of the linear Stark effect; the neutral helium line profiles are approximately symmetric for all but the lines with forbidden components (the 4471Å and 4922Å lines), and these are approximately symmetric after convolution with the rotational and instrumental profiles. Thus, an expansion of the line profiles about their centers is dominated by even terms, whereas local errors in the continuum normalization may be expected to be dominated by a linear term. The parameter \( b \) eliminates the noise from the lead term in the continuum level with little loss of information about the line profile.

The use of the line-fitting program, SPECTRUM, is as follows. SPECTRUM first prompts for a video-display device name, which is passed to the PGPLOT graphics library [39] initialization routines. The user then gives the names of the files containing the observed profiles. SPECTRUM plots the data and prompts the user for limits on the shoulders of the profile and the profile center; these are used to fit a Gaussian to the line profile and to obtain good starting values for \( a \), \( b \), and \( c \). The user then supplies the program with starting estimates of the physical parameters \( T_{\text{eff}} \), \( \log g \), and He/H. For the stars analyzed here, the starting estimates of \( T_{\text{eff}} \) and \( \log g \) were obtained from the calibration of Humphreys [24], and He/H was assumed to be equal to 0.11, close to the cosmic ratio. The program then determines which grid points enclose the starting estimates and reads the corresponding eight theoretical profiles from disk libraries. The user then gives the estimated
$v \sin i$ for the object, and SPECTRUM calculates the convolution of the theoretical profiles with a rotational profile. Mihalas and Auer [35] have shown that because of the reduced limb darkening in non-LTE atmospheres, this is a sufficient approximation of the effects of rotation.

The user then instructs SPECTRUM to carry out iterations of the $\chi^2$ minimization. After each iteration, SPECTRUM returns the current value of $\chi^2$ and asks the user whether to make another iteration. When the user is satisfied that the minimum has been found, SPECTRUM uses the covariance matrix from the minimization to give a conservative estimate of the uncertainty of the fit. The user may try a different set of initial values for the parameters (if, for example, the minimum that has been found lies outside the mesh in parameter space enclosing the initial guess) or may make a revised estimate of the value of $v \sin i$. Since the latter parameter is very insensitive to the estimates of the three physical parameters, it is not included in the $\chi^2$ minimization.

When the user is satisfied with the fit, SPECTRUM prompts for a hardcopy- device type and produces plot files of the final fit.

4.2 RESULTS FOR THE SAMPLE OF O STARS

Estimated parameters for the objects observed are given in Table 7. Figure 6 gives the actual fits obtained. It seems clear from these profiles and fits that the introduction of the three continuum variables was necessary. In most cases the resulting fits are quite good, particularly for the ionized helium lines, indicating that the Schöning-Butler ionized helium profiles are satisfactory.

The values of the projected rotational velocity $v \sin i$ include the effects of the instrumental profile; given the lowest values of $v \sin i$ measured, it appears that rotational velocities less than about 50 km/sec are not resolved.

It is important to determine the ambiguity of the fit (i.e., the range of parameters over which the fit remains good). SPECTRUM quotes errors calculated by determining the change in the parameters that would increase the value of $\chi^2$ by 30%. These errors appear to be much too conservative; this is understandable, since most of the data points will be insensitive to one or more of the physical
Table 7. Estimated Parameters of Objects Observed

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<td>3.97 ± 0.46</td>
<td>0.16 ± 0.07</td>
<td>132</td>
<td>0.11 ± 0.03</td>
</tr>
<tr>
<td>12993</td>
<td>42900 ± 1100</td>
<td>3.78 ± 0.13</td>
<td>0.36 ± 0.05</td>
<td>101</td>
<td>0.17 ± 0.03</td>
</tr>
<tr>
<td>13022</td>
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<td>3.07 ± 0.09</td>
<td>0.35 ± 0.04</td>
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<td>0.08 ± 0.03</td>
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<td>Aur OB2</td>
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</tr>
<tr>
<td>242908</td>
<td>47900 ± 1100</td>
<td>3.82 ± 0.11</td>
<td>0.34 ± 0.10</td>
<td>110</td>
<td>0.09 ± 0.02</td>
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<tr>
<td>242926</td>
<td>40800 ± 1400</td>
<td>4.02 ± 0.24</td>
<td>0.12 ± 0.02</td>
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<tr>
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<tr>
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<td>0.11 ± 0.04</td>
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<td>0.08 ± 0.02</td>
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<td>Cyg OB1</td>
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<tr>
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<td>0.08 ± 0.02</td>
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<td>0.09 ± 0.02</td>
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<tr>
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<tr>
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</tr>
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<td>0.13 ± 0.02</td>
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<tr>
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<td></td>
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<td></td>
</tr>
<tr>
<td>9 Sgr</td>
<td>50500 ± 2300</td>
<td>4.44 ± 0.05</td>
<td>0.10 ± 0.06</td>
<td>92</td>
<td>0.10 ± 0.02</td>
</tr>
<tr>
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<td>4.00 ± 0.17</td>
<td>0.18 ± 0.11</td>
<td>74</td>
<td>0.11 ± 0.02</td>
</tr>
</tbody>
</table>
parameters and since the continuum parameters are held fixed. Another approach is to hold one parameter fixed at a value somewhat different from that for the best fit, and to recalculate the minimum with all other parameters allowed to vary. This method has been used to determine the errors quoted here, with $v \sin i$ being the parameter held fixed at a non-optimal value. The resulting change in $\chi^2$ is used to estimate the change in $v \sin i$ that would significantly degrade the fit, and the corresponding change in the best fit for the physical parameters is quoted as the error.

Generally, the errors so obtained are close to the scatter one sees in the values of the physical parameters when the fit is repeated for different choices of the portion of the line spectra to fit. Occasionally, the errors seem not to be conservative enough; in these cases, the error is taken from the scatter in repeated fits, using different portions of the line profiles.

It must be emphasized that the quoted uncertainties are from the ambiguity of the fit alone; uncertainties arising from the theory are not included.
Figure 6. Observed line profiles with the best theoretical fit shown for HD 236894.
Figure 6. (Continued) HD 236894
Figure 6. (Continued) HD 236894
Figure 6. (Continued) HD 12993
Figure 6. (Continued) HD 12993
Figure 6. (Continued) HD 12993
Figure 6. (Continued) HD 13022
Figure 6. (Continued) HD 13022
Figure 6. (Continued) HD 13022
Figure 6. (Continued) HD 242908
Figure 6. (Continued) HD 242908
Figure 6. (Continued) HD 242908
Figure 6. (Continued) HD 242926
Figure 6. (Continued) HD 242926
Figure 6. (Continued) HD 242926
Figure 6. (Continued) HD 242935
Figure 6. (Continued) HD 242935
Figure 6. (Continued) HD 242935
Figure 6. (Continued) HD 35619
Figure 6. (Continued) HD 35619
Figure 6. (Continued) HD 35619
Figure 6. (Continued) HD 42088
Figure 6. (Continued) HD 42088
Figure 6. (Continued) HD 42088
Figure 6. (Continued) HD 254755
Figure 6. (Continued) HD 254755
Figure 6. (Continued) HD 254755
Figure 6. (Continued) HD 193595
Figure 6. (Continued) HD 193595
Figure 6. (Continued) HD 193595
Figure 6. (Continued) HD 194094
Figure 6. (Continued) HD 194094
Figure 6. (Continued) HD 194094
Figure 6. (Continued) HD 194280
Figure 6. (Continued) HD 194280
Figure 6. (Continued) HD 194280
Figure 6. (Continued) HD 229234
Figure 6. (Continued) HD 229234
Figure 6. (Continued) HD 229234
Figure 6. (Continued) #4 OB2 Cyg (BD +40 4219)
Figure 6. (Continued) #4 OB2 Cyg
Figure 6. (Continued) #4 OB2 Cyg
Figure 6. (Continued) #8B OB2 Cyg
Figure 6. (Continued) #8B OB2 Cyg
Figure 6. (Continued) #8B OB2 Cyg
Figure 6. (Continued) #10 OB2 Cyg (BD +41 3804)
Figure 6. (Continued) #10 OB2 Cyg
BD +41 3804

Figure 6. (Continued) #10 OB2 Cyg
Figure 6. (Continued) HD 204827
Figure 6. (Continued) HD 204827
Figure 6. (Continued) HD 204827
Figure 6. (Continued) HD 207198
Figure 6. (Continued) HD 207198
Figure 6. (Continued) HD 207198
Figure 6. (Continued) HD 207538
Figure 6. (Continued) HD 207538
Figure 6. (Continued) HD 207538
Figure 6. (Continued) HD 209975 (19 Cep)
Figure 6. (Continued) HD 209975
Figure 6. (Continued) HD 209975
Figure 6. (Continued) 9 Sgr
Figure 6. (Continued) 9 Sgr
Figure 6. (Continued) 9 Sgr
Figure 6. (Continued) Λ Ori
Figure 6. (Continued) \( \lambda \) Ori
Figure 6. (Continued) λ Ori
5. CONCLUSIONS

5.1 COMPARISON OF THEORY TO OBSERVATION

In examining the fits for individual lines, one sees that two of the lines are not well reproduced by the theoretical calculations. The HeII 4686Å line is found in emission in the Of stars, and Auer and Mihalas [7] showed that this could not be explained by fluorescence arising from the overlap of the hydrogen Balmer and helium Pickering series. They concluded that the emission was likely a result of atmospheric extension. The analysis here shows that the theoretical calculations produce a line that is too strong even for normal O stars.

Auer and Mihalas also noted that the HeI 5876Å line was somewhat stronger in their small sample of stars than was predicted by their theoretical work, although the extent and severity of the discrepancy was unclear. The analysis here confirms the discrepancy. It is found that the effect is strongest in the cooler and more luminous stars in the sample; it is most pronounced in BD +41° 3804, HD 13022, HD 194280, HD 229234, HD 194094, HD 207198, and 19 Cephei, all of which have $T_{\text{eff}} < 36000K$ and $\log g < 3.7$. This discrepancy probably arises from the geometrical dilution effect described by Ghobros [18], as noted by Voels et al. [47]. However, the effect seems not to be significant for other neutral helium lines. As a check, a second fit to the observed profiles for BD +41° 3804 was made with the HeI 6678Å, 5876Å, and 4471Å lines omitted. The change in the fit parameters was not significant.

Because the theory poorly reproduces the HeII 4686Å and HeI 5876Å lines, these were given one-tenth the normal weight in the $\chi^2$ fit.

Another discrepancy between theory and observations is that the theory predicts emission lines of HeI 6678Å and 4922Å in the hottest stars that are not observed. This is most evident for 9 Sagittarii, which is slightly hotter than 50000K. Since 9 Sagittarii appears to have a rather high surface gravity, this discrepancy probably does not arise from the assumption of plane-parallel geometry.
5.2 HELIUM ABUNDANCES

One disturbing tendency in the fitted parameters is the almost perfect correlation between low gravity (or high luminosity) and high He/H (Figure 7). Although the more luminous stars lose mass at a great rate, so that they are the most likely members of the sample to show a large He/H, it seems very unlikely that all the high-luminosity stars should show large He/H, since the associations chosen are not all of the same age. These fitted abundances most likely reflect a systematic failure of the theory rather than the actual compositions of the stars involved.

However, such a failure of the theory is not suggested by the quality of the fits, which are generally quite good. In this respect, the "normal" O stars analyzed differ from the Of stars that were dropped from the sample; attempts to analyze the Of stars by the method described yielded obviously poor fits, with, e.g., indications that the cores of the Balmer lines are much shallower in the observed profiles than in any of the theoretical profiles.

It is of note that Voels et al. [47] do not find a large value for He/H for the O supergiants they have analyzed (although two of their objects, ζ Pup and α Cam, show somewhat enhanced He). The only substantial difference between their models and the models used here is the inclusion of the effects of wind blanketing. It is surprising that neglect of wind blanketing should result in systematic overestimates of He/H, particularly since some of the O supergiants for which Voels et al. find cosmic He/H show negligible effects from the wind blanketing. Unfortunately, there is no overlap between their sample of objects and the sample of objects analyzed here, which makes a direct comparison difficult. Likewise, they do not present tables of profiles and their illustrations containing profiles do not have labels on the Y-axis. Thus no direct comparison is possible.

A final point that should be raised is that many of the objects with low values for log g are off the original model grid, and the values for the stellar parameters are extrapolated. In the case of the two lowest-gravity objects, HD 194280 and BD +41° 3804, the model grid was extended to $T_{\text{eff}}=28000\text{K}$ and $\log g=3.75$ for He/H of $0.20$ and $0.50$, to reduce the amount of the extrapolation. The result was that the estimated value of He/H actually increased, which would seem to rule
Figure 7. Correlation of Derived He/H with log\(g\). Error bars are indicated. See Figure 1 for explanation of symbols.
out the extrapolation of the theoretical profiles as the cause for the overestimation of He/H. (The parameters given for these objects are those obtained with the extended model grid.)

5.2.1 Semi-Empirical Helium Abundances

If the correlation of He/H with log\textit{g} is, in fact, the result of a failure of the theory, we may account for this failure by fitting a curve through the plotted points in the (log\textit{g}, He/H) plane and using it to reduce all values for He/H determined by our method of analysis. The data shown are well represented by the formula, log(He/H) = 1.1264 – 0.4791 log\textit{g}. The reduced helium abundances calculated using this formula and assuming a cosmic He/H of 0.10 are given in the table of estimated parameters under the column labeled \textit{"(He/H)_0"}, along with association averages. Figure 8 plots these corrected values against effective temperature.

When this reduction is made, we find that there is no object in the sample with an obviously high value for \textit{(He/H)_0}. The three stars near log\textit{g} = 3.8, He/H=0.4, HD 242908, HD 12993, HD 193595, are the likeliest candidates for a moderate helium overabundance \textit{((He/H)_0 ~ 0.19)}. It may be significant that HD 12993 is certainly a blue straggler, while the other two stars are also possibly blue stragglers (being the hottest objects in each of their respective associations). Although this apparent helium overabundance may be a temperature effect, the normal abundances for HD 40800, HD 242935, HD 35619, HD 42088, #4 OB2 Cyg, and \textit{\lambda} Ori argue against this.

One may also conclude from the plotted points and association averages and probable errors that there is no significant difference in the primordial helium abundance between the associations studied. This agrees with the results obtained by Wolf and Heasley [50]but does not agree with those of Nissin [38].

5.3 RADII AND MASSES

If one knows \textit{T_{eff}}, log\textit{g}, and the bolometric magnitude \textit{M_{bol}} for a star, one can derive the radii and masses. Although the analysis here has not determined these quantities with high precision, one can at least make rough estimates of the values of these parameters. These are given in Table 8.
Figure 8. Corrected He/H vs. $T_{eff}$. See Figure 1 for explanation of symbols.
Table 8. Radii and Masses of the Stars in the Sample

<table>
<thead>
<tr>
<th>Object</th>
<th>B.C.</th>
<th>(M_{\text{bol}})</th>
<th>Radius ((R_\odot))</th>
<th>Mass ((M_\odot))</th>
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</table>
The visual magnitudes $M_v$ and bolometric corrections used in this calculation are those reported by Humphreys [24]. Since $T_{\text{eff}}$ is well determined, the uncertainty in the radii depends mainly on the uncertainty in the absolute bolometric magnitudes and is probably of order 30%. The uncertainty in the masses is greater, as it depends on the uncertainty of both the bolometric magnitude and the surface gravity, and is probably as large as a factor of two. Although the radii and masses seem generally to be of the right order of magnitude, some of the individual values are highly questionable. In particular, the mass for 9 Sgr is unacceptable. It is likely that log $g$ for this object has been badly overestimated. The sensitivity of the hydrogen and helium lines to log $g$ is not great at high $T_{\text{eff}}$.

Stars that have lost particularly large fractions of their mass should be overluminous. However, since an overestimate of the luminosity of a particular star leads to an overestimate of the mass as well, a much more accurate determination of the luminosities is needed than is available for the stars in this sample or, indeed, for any O star. A plot of $M_{\text{bol}}$ vs. the logs of the masses would show far too much scatter to permit any conclusions about the presence or absence of overluminous stars.

Voels et al. [47] also estimate masses spectroscopically for their sample of O supergiants. They find values ranging from 19 to 36 M$_\odot$, in rough agreement with the values found here but with less scatter.

5.4 THE MAPPING OF SPECTRAL TYPES TO PHYSICAL PARAMETERS

Figure 9 shows the ($T_{\text{eff}}$, log $g$) diagram of all the stars in the sample. The MK spectral class, or closest estimate, is given for each star. The estimated temperature calibration for MK spectral types is given in Table 9. For comparison, the calibration employed by Humphreys [24] is also listed. There is considerable discrepancy, particularly near spectral types O7 and O8, with the new calibration giving a considerably higher effective temperature. Unfortunately, because of the scantiness of the data, our calibration is probably not much more reliable than the Humphreys calibration.
Figure 9. Spectral types vs. physical parameters.
Table 9. Calibration of $T_{\text{eff}}$ to MK Spectral Type

<table>
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</table>

Upper value is from the analysis here; lower value is the calibration given by Humphreys [24].
5.5 CARBON AND NITROGEN FEATURES

Although no detailed analysis of carbon is attempted here, it is worth noting that the CIV 5801Å and 5812Å features are stronger for the three members of the Cyg OB2 association than for stars of similar spectral type belonging to other associations. Figure 10 shows the correlation between the equivalent width of a prominent ionized helium line, HeII 4542Å, and the equivalent width of one member of the C IV doublet at 5812Å. (This member of the doublet was chosen because it is less confused with diffuse interstellar bands than the component at 5801Å.) The open points corresponding to the three stars analyzed from Cyg OB2 definitely lie above the average curve for this correlation, indicating a carbon overabundance for this association. The carbon line is roughly 0.35 dex stronger than normal for these stars. If we assume that the carbon line equivalent widths obey the well-known square-root law for a strong line with a Voigt absorption profile, this corresponds to an approximate carbon overabundance of 50%.

Since the carbon overabundance is detected in three quite dissimilar O stars in Cyg OB2, it must be regarded as a primordial carbon enrichment. Charles et al. [13] find that the entire region around Cygnus OB2 is disturbed, and they attribute this to the explosion of 30-100 supernovae in the last few million years. These supernovae might account for the local carbon enrichment.

It should also be pointed out that HD 236894 is clearly carbon-deficient, the carbon abundance indicated by the line strength being about half normal. It would be very interesting to estimate the relative nitrogen abundance of this object, as this might confirm that the carbon underabundance is evolutionary. Such an estimate could not be made with the echelle spectrograms presented here, since the only detectable nitrogen lines are too close to the blue for accurate measurements. It would be interesting to examine the nitrogen abundances of the stars in OB2 Cyg as well.

It is probably worthwhile to mention the findings of Schild and Berthet [42]. Three of the objects for which they present nitrogen spectra are included in the analysis here. These are HD 42088 and HD 254755, for which they report enhanced nitrogen, and HD 12993, for which they report moderately enhanced nitrogen. HD 12993 is one of the three blue stragglers in the sample for
Figure 10. Equivalent Widths of C IV 5812Å vs. HeII 4542Å. See Figure 1 for explanation of symbols.
which a helium overabundance is suspected. No helium overabundance is suspected for the others, but this is not incompatible with the nitrogen overabundance; evolutionary changes in the nitrogen abundance may be expected to appear before changes in the helium abundance. It should be kept in mind that the helium overabundance of HD 12993 is only suspected and must be confirmed by a more careful analysis, using the best possible data and the most accurate available atmospheric models.

5.6 SUMMARY

Although reasonable values for the effective temperatures and gravities of O stars may be obtained by an analysis of their line spectra, using non-LTE, plane-parallel models, the helium abundances so obtained show a strong correlation with log $g$; the stars with higher log $g$ show an abundance ratio near the accepted cosmic value (He/H $\sim$ 0.10), but at lower gravities the ratio increases to unreasonable values (He/H $\sim$ 0.50). This failure of the theory probably arises from the approximation of plane-parallel geometry. The correlation is well fit by the relation log He/H = 1.1234-0.4791 log $g$.

If this correlation is divided out of the fitted helium abundances, one obtains "corrected" abundances that probably correspond to the true helium-to-hydrogen ratio. It is found that there is no systematic difference in the helium abundance from association to association. However, the stars HD 12993, HD 242908, and HD 193595 may be blue stragglers with an enhanced helium abundance (He/H$\sim$0.19). The enhanced helium abundance would arise from the same mixing that explains their status as blue stragglers.

A strong correlation exists between the equivalent widths of the CIV 5812Å line and the HeII 4342Å line. Using this correlation, it is possible to estimate the approximate carbon abundance of different O stars relative to the average cosmic value. It is found that the association Cyg OB2 is carbon-rich by $\sim$ 50%. This carbon enrichment may be a result of heavy supernova activity in the Cygnus Superbubble [13]. The blue straggler HD 236894, on the other hand, is found to have
roughly half the normal carbon abundance.

The calibration of physical parameters to the MK spectral classification is still very uncertain, with discrepancies between previous calibrations and the calibration given here being as great as 6200K. Many more MK-classified stars must be analyzed before an improved calibration can be given.
REFERENCES

19. Gingerich, O. 1969. *Theory and Observation of Normal Stellar Atmospheres*, (Gin-
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Institute of Technology.


Appendix. Selected Listings of Computer Programs

The following pages list portions of the FORTRAN source codes used to carry out the calculations described in this dissertation. Wherever possible, this code has adhered strictly to the ANSI 1977 standard. The listings are not complete; omissions are noted in the introduction to each code and in certain places in the code listings themselves. Readers interested in obtaining the full listings in machine-readable format are encouraged to contact the author at the following address:

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Organization 1531
Sandia National Laboratory
Albuquerque, NM 87185
A. Program GRAY

GRAY is listed in its entirety.

The program takes an input file in standard atmosphere format, but no lines after the opacity specification line are used. The output file is also in standard atmosphere format, and includes the LTE populations of hydrogen and helium for standard model ions. It may be read directly into the program LTE if the default number of iterations (15) is acceptable, as is usually the case.

The subroutines LINK and EXIT are CRAY FORTLIB routines to create a dropfile and initial I/O links and to exit the program. EXIT(n) is equivalent to a Fortran STOP n statement, while LINK has no normal FORTRAN equivalent.
PROGRAM GRAY

COMMON BLOCK MACROS FOR ALL GLOBAL DATA IN PROGRAM
(CRAY PRECOMPILER)

COMMON PARAMETERS:

MNDEPTH  MAXIMUM NUMBER OF PHYSICAL DEPTHS IN MODEL
MNJ      MAXIMUM NUMBER OF FREQUENCIES
MQHE1    MAXIMUM HYDROGEN LEVELS FOR PARTITION FUNCTION
MLH      NUMBER OF HYDROGEN LEVELS TREATED EXPLICITLY
MLHE1    NUMBER OF SINGLY-IONIZED HYDROGEN LEVELS TREATED EXPLICITLY
MLHE2    NUMBER OF SINGLY-IONIZED HELIUM LEVELS TREATED EXPLICITLY
MK       PLANCK'S CONSTANT OVER BOLTZMANN'S CONSTANT
MHYD     1./AVOGADRO'S NUMBER = MASS OF HYDROGEN NUCLEUS
SIGE     THOMPSON CROSS-SECTION FOR FREE ELECTRONS

COMMON VARIABLES:

MNDEPTH  NUMBER OF DEPTH POINTS
MNJ      NUMBER OF FREQUENCY POINTS
CHI      EXTINCTION COEFFICIENT
FF       FREE-FREE CUTOFF FREQUENCY
FREQ     FREQUENCY GRID
FRQB     HYDROGEN IONIZATION FREQUENCIES
FRQHE1   NEUTRAL HELIUM IONIZATION FREQUENCIES
FRQHE2   IONIZED HELIUM IONIZATION FREQUENCIES
GB       HYDROGEN LEVEL STATISTICAL WEIGHTS
GHE1     NEUTRAL HELIUM LEVEL STATISTICAL WEIGHTS
GHE2     IONIZED HELIUM LEVEL STATISTICAL WEIGHTS
GRAV     SURFACE GRAVITY
N        MASS GRID (DIFFERENCES)
MU       MEAN MOLECULAR WEIGHT
MU1      NUCLEI PER PROTON
W        HYDROGEN NUMBER DENSITY
WE       ELECTRON NUMBER DENSITY
NHE1     NEUTRAL HELIUM NUMBER DENSITY
NHE2     IONIZED HELIUM NUMBER DENSITY
NHE3     DOPLY-IONIZED HELIUM NUMBER DENSITY
NPUP     IONIZED HYDROGEN NUMBER DENSITY
NPUP1    TOTAL PARTICLE NUMBER DENSITY
SIGH     HYDROGEN PHOTOIONIZATION CROSS-SECTIONS
SIGHE1   NEUTRAL HELIUM PHOTOIONIZATION CROSS-SECTIONS
SIGHE2   IONIZED HELIUM PHOTOIONIZATION CROSS-SECTIONS
SUMH     PARTITION FUNCTION OF HYDROGEN
SUMHE1   PARTITION FUNCTION OF NEUTRAL HELIUM
SUMHE2   PARTITION FUNCTION OF IONIZED HELIUM
TEMP     ELECTRON TEMPERATURE
WT       QUADRATURE WEIGHTS FOR FREQUENCY GRID
Y        NUMBER RATIO OF HELIUM TO HYDROGEN

CLICHE PLIST

INTEGER MNDEPTH, MNJ, MQHE1, MLH, WLHE1, WLHE2
REAL DELQUAD, HK, MHYD, SIGE
PARAMETER (MNDEPTH=100, MNJ=105, MQHE1=31, MLH=10)
PARAMETER (WLHE1=25, WLHE2=15, DELQUAD=0.6, HK=4.798E-11)
PARAMETER (MHYD=1.660538E-24, SIGE=0.664E-24)

POINTERS FOR STATE MATRIX

INTEGER IHHE2, IWHE3, IMPROT, INTOT, MWWW
PARAMETER (IHHE2=1, IWHE3=2, IMPROT=3, INTOT=4, MWWW=4)

ENDCLICHE

CLICHE BLANK

REAL CHI(MNJ)

COMMON //CHI

ENDCLICHE
CLICHEL ROOT

INTEGER MDEPTH, NJ

REAL FF(NMJ,3), FREZ(NMJ), GRAV, M(MDEPTH), MJ, MJ1

REAL WE(MDEPTH), WKL(M, MDEPTH), WE1(WLE1, MDEPTH)

REAL RHE2(RHE2, MDEPTH), WE2(MDEPTH)

REAL NPRT(MDEPTH), WT0T(MDEPTH), SIGEN(NMJ)

REAL SIG(N+1, MJ), SIGE1(WLE1, MJ), SIGE2(WLE2, MJ)

REAL SUME(MDEPTH), SUME1(WLE1, MDEPTH), SUME2(WLE2, MDEPTH)

REAL TEFF, TEMP(MDEPTH), WT(MJ), Y

LOGICAL RULE(2)

COMMON /ROOTI/MJ, MJ1, FF, FREZ, GRAV, MJ, MJ1, MJ, NE,
: WE1, WE2, WE3, NPRT, WT0T, SIG, SIG1E1, SIGEN,
: SIGE2, SUME, SUME1, SUME2, TEFF, TEMP, WT, Y, RULE

ENDCLICHE

CLICHEL ROOT

REAL FRQBM, FRQH(MQB), FRQBE1(MQBE1), FRQBE2(MQB)

REAL GB(MQB), GBE1(MQBE1), GBE2(MQB)

COMMON /ROOTI/FRQBM, FRQH, FRQBE1, FRQBE2, GB, GBE1, GBE2

ENDCLICHE

PROGRAM GRAY

CREATE A GRAY MODEL ATMOSPHERE FOR USE AS FIRST APPROXIMATION

IN MORE SOPHISTICATED CODES

IMPLICIT NONE

PLIST

ROOT

LOCAL VARIABLES

REAL ERR, FLUX, KAP1, KAP2, M2(70), MASS(99), MEID, MSTART, MSTEP

REAL TAU(99), TEID, TSTART, TSRO(70), TSTEP

LOGICAL SECOID, STDGRID

DATA TSTD/1.000E-07, 3.162E-07, 1.000E-06, 1.334E-06, 1.778E-06,
: 2.371E-06, 3.162E-06, 4.217E-06, 5.623E-06, 7.499E-06, 1.000E-05,
: 1.334E-05, 1.778E-05, 2.371E-05, 3.162E-05, 4.217E-05, 5.623E-05,
: 7.499E-05, 1.000E-04, 1.334E-04, 1.778E-04, 2.371E-04, 3.162E-04,
: 4.217E-04, 5.623E-04, 7.499E-04, 1.000E-03, 1.334E-03, 1.778E-03,
: 2.371E-03, 3.162E-03, 4.217E-03, 5.623E-03, 7.499E-03, 1.000E-02,
: 1.334E-02, 1.778E-02, 2.371E-02, 3.162E-02, 4.217E-02, 5.623E-02,
: 7.499E-02, 1.000E-01, 1.334E-01, 1.778E-01, 2.371E-01, 3.162E-01,
: 4.217E-01, 5.623E-01, 7.499E-01, 1.000E-00, 1.334E-00, 1.778E-00,
: 2.371E-00, 3.162E-00, 4.217E-00, 5.623E-00, 7.499E-00, 1.000E+00,
: 1.334E+00, 1.778E+00, 2.371E+00, 3.162E+00, 4.217E+00, 5.623E+00,
: 7.499E+00, 1.000E+01, 1.334E+01, 1.778E+01, 2.371E+01, 3.162E+01,
: 4.217E+01, 5.623E+01, 7.499E+01, 1.000E+02, 1.334E+02, 1.778E+02

DATA MASS/1.000E-08, 1.259E-07, 1.585E-07, 1.995E-07, 2.512E-07,
: 3.162E-07, 3.981E-07, 5.012E-07, 6.316E-07, 8.000E-07, 1.000E-06,
: 1.259E-06, 1.585E-06, 1.995E-06, 2.512E-06, 3.162E-06, 3.981E-06,
: 5.012E-06, 6.310E-06, 7.943E-06, 1.000E-05, 1.259E-05, 1.585E-05,
: 1.995E-05, 2.512E-05, 3.162E-05, 3.981E-05, 5.012E-05, 6.316E-05,
: 7.943E-05, 1.000E-04, 1.259E-04, 1.585E-04, 1.995E-04, 2.512E-04,
: 3.162E-04, 3.981E-04, 5.012E-04, 6.310E-04, 7.943E-04, 1.000E-03,
: 1.259E-03, 1.585E-03, 1.995E-03, 2.512E-03, 3.162E-03, 3.981E-03,
: 5.012E-03, 6.310E-03, 7.943E-03, 1.000E-02, 1.259E-02, 1.585E-02,
: 1.995E-02, 2.512E-02, 3.162E-02, 3.981E-02, 5.012E-02, 6.310E-02,
: 7.943E-02, 1.000E-01, 1.259E-01, 1.585E-01, 1.995E-01, 2.512E-01,
: 3.162E-01, 3.981E-01, 5.012E-01, 6.310E-01, 7.943E-01, 1.000E+00,
: 1.259E+00, 1.585E+00, 1.995E+00, 2.512E+00, 3.162E+00, 3.981E+00,
: 5.012E+00, 6.310E+00, 7.943E+00, 1.000E+01, 1.259E+01, 1.585E+01,
: 1.995E+01, 2.512E+01, 3.162E+01, 3.981E+01, 5.012E+01, 6.310E+01,
: 7.943E+01, 1.000E+02, 1.259E+02, 1.585E+02, 1.995E+02, 2.512E+02,
: 3.162E+02, 3.981E+02, 5.012E+02, 6.310E+02

EXTERNALS
REAL EXIT, FIT, LINK, MASINT, PUTOUT, SETUP, STATE
EXTERNAL EXIT, FIT, LINK, MASINT, PUTOUT, SETUP, STATE

C CRAY DROPFILE LINK FUNCTION
C CALL LINK("UNITS=(input,OPEN,TEXT),UNIT12=
    :output,CREATE,TEXT),UNIT10=TERMINAL/"
C
C PREPARE MASS DIFFERENCE GRID
C M(1)=MASS(1)
DO 10 I=2,99
   M(I)=MASS(I)-MASS(I-1)
CONTINUE
C
C READ IN PARAMETER/WAVELENGTH FILE AND PREPARE FOR COMPUTATION
C CALL SETUP
C
C CALCULATE SURFACE BOUNDARY CONDITIONS
C FLUX=5.6697E-5*TEFF**4/2.99792E10
TEMP(1)=FIT(0.)
SECOND=.FALSE.
M0=99
20 WTOT(I)=GRAV*M(I)/(1.38E-16*TEMP(I))
30 CALL STATE(I,KAP1)
   TAU(I)=KAP1*M(I)
   TEMP(I)=FIT(TAU(I))
   ERR=WTOT(I)
   WTOT(I)=MAX(WTOT(I)+.1,M(I)+(GRAV-KAP1*FLUX)/TEMP(I)/1.38065E+16)
   ERR=ABS((ERR-WTOT(I))/WTOT(I))
   IF (ERR.GT.0.0005) GO TO 30
KAP1=KAP1
50 CONTINUE
IF (SECOND) GO TO 80
C FIRST CYCLE--CALCULATE MASS GRID CORRESPONDING TO DEPTH GRID
C CALL MASINT(TAU,M0,M99,TSTD,M2,NDEPTB)
DO 60 I=1,NDEPTB
   MASS(I)=M2(I)
60 CONTINUE
M(1)=MASS(1)
DO 70 I=2,NDEPTB
   M(I)=MASS(I)-MASS(I-1)
70 CONTINUE
SECON=.TRUE.
DO=600
GO TO 20
C SECOND CYCLE COMPLETE--WRITE OUT GRAY MODEL
C CALL PUTOUT
CALL EXIT(0)
END

SUBROUTINE MASINT (TO,M0,M1,T1,M1,W1)
C INTERPOLATE TO DEFINED AT POINTS M0 TO T1 DEFINED AT POINTS M1
C ADAPTED FROM AUEX/MIBALAS CODE
C REAL TO(M0), MO(M0), T1(M1), M1(W1)
IF (T0(1).GT.T1(1)) GO TO 40
IF (T0(IO).LT.T1(IO)) GO TO 40
IID=2
DO 30 I1=1,11
    DO 10 ID=IID,10
        IF (T0(ID).GT.T1(I1)) GO TO 20
    10 CONTINUE
    IID=ID-1
    M1(I1)=MO(ID)+
    (MO(IID)-MO(ID))*(T1(I1)-T0(ID))/(T0(IID)-T0(ID))
30 CONTINUE
RETURN
WRITE (6,*) 'INTERPOLATION TABLE TOO SMALL: T0(1)=',T0(1),
', T0(MAX)=',T0(NO)
STOP
END

SUBROUTINE FRE(SKK,ID)
C
C CALCULATE FREE-FREE CROSS SECTIONS
C ADAPTED FROM AUEH/MINHALAS CODE
C
C IMPLICIT NONE
C
C PLIST
ROOT
C
C LOCAL VARIABLES
C
INTEGER ID, IJ
REAL SKK(4,IIIJ)
REAL EX, EXT, EXGF, EXGFT, GF, GFT, HKT, BKTF, HKTFT, SRT

C EXTERNAL PROCEDURE
C
REAL GFREE, HMFREE
EXTERNAL GFREE, HMFREE
SRT=1.0/SQRT(TEMP(ID))
HKT=HK/TEMP(ID)
DO 10 IJ=1,IJ
    C HYDROGEN CONTRIBUTION
    C THE EXPONENTIAL TERM REFLECTS THE UPPER-STATE BOUND-FREE
    C CONTRIBUTIONS (BOTH ABOVE AND BELOW, FOR HELIUM).
    C
    BKTF=HKT*FF(IJ,1)
    EX=EXP(BKTF)
    SKK(1,IJ)=SIG(ILB+1,IJ)*SRT*EXGF

    C SINGLY IONIZED HELIUM CONTRIBUTION
    C (NO GAUNT FACTOR USED.)
    C
    BKTF=HKT*FF(IJ,2)
    EX=EXP(BKTF)
    SKK(2,IJ)=SIG(WLH+1,IJ)*SRT*EX

    C IONIZED HELIUM CONTRIBUTION.
    C (NO GAUNT FACTOR USED.)
    C
    BKTF=HKT*FF(IJ,3)
    EX=EXP(BKTF)
    SKK(3,IJ)=4.0*SIG(WLH+1,IJ)*SRT*EX

    C NEGATIVE HYDROGEN ION FREE-FREE
    C
    SKK(4,IJ)=HMFREE(TEMP(ID),FREQ(IJ))
10 CONTINUE
RETURN
END
REAL FUNCTION GAUNT(NW,QF)
C
RETURNS GAUNT FUNCTIONS OF HYDROGENIC ATOMS
ADAPTED FROM AUEA/MIRALAS CODE
C
IMPLICIT NONE
C
REAL CO(11)
DATA CO/1.2302628,1.1595421,1.1450949,1.1306695,1.1190904,
1.1168376,1.1128632,1.1093137,1.1078717,1.1052734,1.1/
C REAL C1(11)
DATA C1/-2.9094219E-3,-2.0735860E-3,-1.9366592E-3,-1.3428273E-3,
-1.0401085E-3,-8.9465734E-4,-7.4332606E-4,-6.2019148E-4,
-5.493392E-4,-4.34157E-4,0./
C REAL C2(11)
DATA C2/7.5939579E-6,2.0323565E-6,-4.649424E-6,-6.994888E-6,
-8.839133E-6,-1.0244504E-5,-1.1128632E-5,-1.128632E-5,
-1.134206E-5,-1.139905E-5,0./
C REAL C3(11)
DATA C3/-8.7356966E-9,0.,0.,2.3546378E-8,
2.8496742E-8,3.4696786E-8,3.9568771E-8,4.1477231E-8,4.3796716E-8,4.7003140E-8,0./
C REAL CM(11)
DATA CM/-5.757885,-1.270945,-.5936432,-.3110730,-.16051018,
-.13075417,-.9.5441161E-2,-.7.101056E-2,-.5.604566E-2,
-.4.726379E-2,0./
C REAL CW(11)
DATA CW/12.8083223,2.1328684,5.4271924,19.638684,5.554091E-2,
4.1218185E-2,2.335012E-2,1.320411E-2,0.5139736E-3,0.151565E-3,0./
C REAL CWS(11)
DATA CWS/0.,-2.0244141,-.23387156,-.4.418565E-2,-.8.918584E-3,
-.5.3630574E-3,2.276281E-3,-9.7200274E-4,-.4.967046E-4,
-2.3907933E-4,0./
C
INTEGER NW, N
REAL QF, X
C
X=QF/0.29979315
N=MIN(NW,11)
GAUNT=CO(N)+X*(C1(N)+X*(C2(N)+X*C3(N)))+CM(N)+CP1(N)+CP2(N)
RETURN
END

REAL FUNCTION GFREE(FRQ,T)
C
C CALCULATES HYDROGENIC FREE-FREE GAUNT FACTORS
IDENTICAL WITH AUEA/MIRALAS CODE
C
IMPLICIT NONE
C
REAL FRQ, T, THET, X, C1, C2, C3, C4
C THET=0.04003/T
IF (THET.LT.4.0E-2)THET=4.0E-2
X=FRQ/0.29979315
IF (X.GT.1.0)GO TO 10
IF (X.LT.0.2)X=0.2
GFREE=(1.0823+2.98E-2/THET)+(6.71E-3+1.12E-2/THET)/X
RETURN
10 C1=(3.9999167E-3-3.7862289E-5/THET)/THET+1.070192
C2=(6.94628601E-2-6.198313E-4/THET)/THET+2.8061249E-1
C3=(1.3903474E-3-5.7542343E-2)/THET+6.7917786E-1
C4=-3.4195006E-1+1.8522364E-2/T
GFREE=((C4/X-C3)/X+C2)/X+C1
RETURN
END

REAL FUNCTION HEGAUNT(IL,LA)
C
C NEUTRAL HELIUM BOUND-FREE GAUNT FACTORS APPROXIMATED FROM
C
IMPLICIT NONE
C
INTEGER IL
REAL A, X
REAL RYD, CUT(25), CM2(5), CO(5), CP1(5), CP2(5)
C
PARAMETER (RYD=3.2880E15)

DATA CUT/32.0, 4*2.40, 20*1.E38/
DATA CM1/S1.5909,3.07758,-.022590913,-.2224690,-.4675104/
DATA CO/26.40076,25.32980,-1.213830,1.033202,*.4675104/
DATA CP1/.1051292,-12.04806,6.419941,-.1599973,.6149698/
DATA CP2/-2.058184229,4.235189,-.472744,.060324013,.3983392/

REAL FUNCTION HMFREE(T,FREQ)
C IEGATIVE HYDROGEN FREE-FREE OPACITY FORMULA FROM GINGERICH (1969)
C
REAL LAMBDA
LAMBDA=2.99792E16/FREQ
C
CO=0.005366+TETRA*(-0.011493+TETRA*0.027039)
C1=1.000-(3.2062+TETRA*11.924+TETRA*1.9390)
C2=1.000-(0.40192+TETRA*7.0388+TETRA*0.34592)
HMFREE=1.00E-28*(CO+LAMBDA*C1+LAMBDA*C2)*T*1.3806E-16
RETURN
END

REAL FUNCTION HMIIUS(FREQ)
C IEGATIVE HYDROGEN BOUND-FREE OPACITY APPROXIMATED FROM TABLE
C OF GELTMAN (1962)
C
REAL LAMBDA
LAMBDA=2.99792E16/FREQ
HMIIUS=1.00E-17*LAMBDA*(1.103927109E-3+LAMBDA*(2.7792168339E-2+
LAMBDA*(1.68296722E-4+LAMBDA*(5.570765568E-5+LAMBDA*
(-1.7683406278E-6+LAMBDA*(2.301357777E-8+LAMBDA*
(-1.5666817662E-10+LAMBDA*7.55981817662E-16)))))))
RETURN
END

SUBROUTINE IURATE(LHS,RHS,ID)
C CALCULATE THE RATE MATRIX FOR LTE GIVEN TEMPERATURE
C AND ELECTRON DENSITY.
C
INTEGER I, ID, IL, J, L, U
REAL LHS(MWWW,MWWW), RHS(MWWW)
REAL SUM, T, VI, VIT
REAL SB, SBHE1, SBHE2
SB(I,T)=2.0706E-16*GH(I)*EIP(HK*FRQH(I)/T)/T/SQRT(T)
SBHE1(I,T)=2.0706E-16*GHE1(I)*EIP(HK*FRQH(I)/T)/T/SQRT(T)/2.
SBHE2(I,T)=2.0706E-16*GHE2(I)*EIP(HK*FRQH(I)/T)/T/SQRT(T)
END

REAL FUNCTION X=MIL(CUT(IL),A/RYD)
IF (IL.LE.S) THEN
HEGAU=CO(IL)+(CM1(IL)+CK2(IL))/X/X+(CP1(IL)+X*CP2(IL))
ELSE
HEGAU=1.00
ENDIF
RETURN
END
```
SUMB(ID) = SUMB(ID) + VX

CONTINUE
SUMBE1(ID) = 0.0
DO 20 IL = 1, MQBE1
    VX = SBBE1(IL, TEMP(ID))
    SUMBE1(ID) = SUMBE1(ID) + VX
20 CONTINUE
SUMBE2(ID) = 0.0
DO 30 IL = 1, IIQB2
    VX = SBBE2(IL, TEMP(ID))
    SUMBE2(ID) = SUMBE2(ID) + VX
30 CONTINUE
DO 40 I = 1, MHI
    RBS(I) = 0.0
    DO 40 J = 1, MIII
        LBS(I, J) = 0.0
40 CONTINUE
DO 50
    I = 1, MHI
    RBS(I) = -IE(ID)
    LBS(I, IIProt) = -1.0
    LBS(I, IIBE3) = 1.0 + IE(ID) * SUMB(ID)
50 CONTINUE
DO 60
    I = 1, MHI
    RBS(I) = 1.0
    LBS(I, IIProt) = 1.0
    LBS(I, IIBE2) = 2.0 + IE(ID) * SUMBE2(ID)
60 CONTINUE
RETURN
END

SUBROUTINE GEIER(ID)
C CALCULATES LTE OPACITIES
C
C IMPLICIT NONE
C
C PLIST
C ROOT
C BLANK
C ROUTI
C
C INTEGER I, ID, IJ, IL, IT, J, L, U
C REAL C, E, SIGMA, T, VX, XO
C REAL EX(MIJ), BKT
C REAL SKK(4,MIJ), SRT, X1
C REAL FRE
C EXTERIAL FRE
C REAL SB, SBBE1, SBBE2, SBBM
C SB(I, T) = 2.0706E-16 * GB(I) * EXP(BK * FREQ(I)/T)/T/SQRT(T)
C SBBE1(I, T) = 2.0706E-16 * GB(E1(I)) * EXP(BK * FREQBE1(I)/T)/T/SQRT(T)/2.
C SBBE2(I, T) = 2.0706E-16 * GB(E2(I)) * EXP(BK * FREQBE2(I)/T)/T/SQRT(T)
C SBBM(T) = 2.0706E-16 * 0.5 * EXP(BK * FREQM/T)/T/SQRT(T)
C
C START OF EXECUTABLE STATEMENTS
C
C FREQUENCY-INDEPENDENT CALLS AND STATEMENTS
C
C BKT = BK/TEMP(ID)
C CALL FRE(SKK, ID)
C DO 10 J = 1, MJ
        CHE(J) = 0.0
        EX(J) = EXP(-BKT * FREQ(J))
10 CONTINUE
DO 50 IL = 1, MHE1
```
DO 40 IJ=1,NJ
   C=SIGNE1(IL,IJ)*WHE1(IL,ID)
   CHI(IJ)=CHI(IJ)+C
40 CONTINUE
DO 90 IL=1,NLHE2
   DO 80 IJ=1,NJ
      C=SIGNE2(IL,IJ)*WHE2(IL,ID)
      CHI(IJ)=CHI(IJ)+C
80 CONTINUE
90 CONTINUE
DO 130 IJ=1,NJ
   C=SKK(2,IJ)*WE(ID)*WHE3(ID)*SUMBE2(ID)
   CHI(IJ)=CHI(IJ)+C
   C=SIGBE2(IL,IJ)*WHE2(ID)*SKK(3,IJ)
   CHI(IJ)=CHI(IJ)+C
   C=WPROT(ID)*WE(ID)*SKK(1,IJ)
   CHI(IJ)=CHI(IJ)+C
130 CONTINUE
C NEGATIVE HYDROGEN ION
IF (RULE(1)) THEN
   DO 140 IJ=1,NJ
      CHI(IJ)=CHI(IJ)+SKK(4,IJ)*L(1,ID)*IE(ID)
      CHI(IJ)=CHI(IJ)+L(1,ID)*IE(ID)*SIGBE(IJ)
140 CONTINUE
ENDIF
DO 200 IL=1,NL
   DO 190 IJ=1,NJ
      C=SIG(IL,IJ)*L(IL,ID)
      CHI(IJ)=CHI(IJ)+C
190 CONTINUE
200 CONTINUE
DO 240 IJ=1,NJ
   CHI(IJ)=CHI(IJ)+(1.-EX(IJ))*WE(ID)*SIGE
240 CONTINUE
RETURN
END

SUBROUTINE PUTOUT
WRITE OUT A COMPLETED MODEL TO DISK
IMPLICIT NONE
PLIST
ROUT ROUTI
LOCAL VARIABLES
LOGICAL LINES
INTEGER I, ID, IL
REAL ABUND(92)
REAL T
INTEGER LOWERB(10),UPPERB(10),LOWERBE1(14),UPPERBE1(14)
INTEGER LOWERBE2(10),UPPERBE2(10)
DATA LOWERB/1,1,1,2,2,3,3,4/ DATA LOWERBE1/1,1,2,2,3,3,4,4,5,5,5,5/ DATA LOWERBE2/2,2,2,2,3,3,3,4,4,5,5,5,5,5,5,5,6,6,6/DATA LOWERH/1,1,1,1,1,2,2,3,3,4/ DATA UPPERH/2,3,4,5,6,7,8,9,10,11,12,13,14/ DATA UPPERBE1/1,1,2,2,3,3,4,4,4,4,5,5,5,5,5,5,5,6,6,6,6/ DATA UPPERBE2/2,2,3,3,3,3,3,4,4,4,5,5,5,5,5,5,5,6,6,6,6/ START OF EXECUTABLE STATEMENTS
PREVIOUS OUTPUT LINES WERE ALREADY TAKEN CARE OF IN SETUP
WRITE (12,1007)(M(ID),TEMP(ID),WTOT(ID),WE(ID),ID=1,NDEPTH)
HYDROGEN OCCUPATION NUMBERS
WRITE (12,1005)1
WRITE (12,1005)10,10,0,5,10
WRITE (12,1005)FRQH(IL),IL=1,10
DO 10 IL=1,10
   WRITE (12,1005)LOWERH(IL),UPPERH(IL)
10 CONTINUE
HELIUM OCCUPATION NUMBERS

WRITE (12,1005) 2
WRITE (12,1005) 0,0,19,14,10,10
WRITE (12,1006) (FRQHE1(IL), IL=1,19)
DO 20 IL=1,14
WRITE (12,1005) LOWERHE1(IL), UPPERHE1(IL)
20 CONTINUE
WRITE (12,1006) (HE1(IL,ID), IL=1,19), (HE2(IL,ID), IL=1,10), HE3(ID), ID=1,IDEPTH
WRITE (12,1005) 0
WRITE (12,1005) 0
RETURN

FORMAT STATEMENTS

1005 FORMAT (16I5)
1006 FORMAT (5E15.7)
1007 FORMAT (4E15.7)

SUBROUTINE SETUP

READ IN THE APPROXIMATE MODEL MAKE ALL INITIAL CALCULATIONS

IMPLICIT NONE

PLIST
ROOT
ROOTI

LOCAL VARIABLES

CHARACTER*80 HEADER
INTEGER I, ID, II, IJ, IL, IT, J, NO, W1, W2, W3, W4, W5, WITER
LOGICAL LIIES
REAL ABUID(92)
REAL ALPHA, BETA, DUMMY, FCOI, GLOG, T, TLIIE, VX, Z

TABLE OF ATOMIC WEIGHTS

REAL WEIGHT(92)
DATA WEIGHT/1.0,4.0,6.9,9.0,10.8,12.0,14.0,16.0,19.0,20.2,23.0,
: 24.3,27.0,28.1,31.0,32.1,35.5,39.0,39.1,40.1,44.0,47.9,50.9,52.0,
: 54.8,56.5,58.9,58.7,63.5,65.4,69.7,72.6,74.9,79.9,83.8,85.8,
: 87.6,88.9,89.2,90.9,98.9,99.9,101.1,102.9,106.4,107.9,112.4,
: 114.8,118.7,121.8,127.6,126.9,131.3,132.9,137.3,138.9,140.1,
: 140.9,144.2,145.0,150.4,152.0,157.3,158.9,162.5,164.9,167.3,
: 169.9,173.0,175.0,179.5,180.9,183.9,186.2,190.2,192.2,195.1,
: 197.0,200.6,204.4,207.2,209.0,209.0,210.0,222.0,223.0,226.0,
: 227.0,232.0,231.0,238.0/

TABLE GIVING QUANTUM NUMBER OF ACTIVE ELECTRON OF EACH NEUTRAL
HELIUM STATE TREATED BY THE PROGRAM

INTEGER QW(25)
DATA QW/1,4*2,8*3,8*4,5,6,7,8,9,10/

EXTERNAL PROCEDURES

REAL EXIT, HEGAU1T, GAU1T, HMINUS
EXTERNAL EXIT, HEGAU1T, GAU1T, HMINUS

START OF EXECUTABLE STATEMENTS

READ COMMENT LINE OF INPUT MODEL

READ (5,1001) HEADER
WRITE (8,1001) HEADER
WRITE (12,1001) 'GRAY MODEL'

READ BASIC MODEL PARAMETERS
READ (6,1002)TEFF,TLIME,GLOG,Y,Z,IITER
WRITE (12,1002)TEFF,TLIME,GLOG,Y,Z,IITER,5.0,20.0

C CALCULATE EDDINGTON FLUX AND SURFACE GRAVITY FROM PARAMETERS
C
GRAV=EXP(2.302585093*GLOG)
WRITE (6,1003)TEFF,TLIME,GLOG,Y,Z,IITER

C READ COMPOSITION, WHICH TAKES THE FORM OF LOG NUMBER RELATIVE
C TO HYDROGEN=12.0
C
READ (5,1004)ABUND
WRITE (12,1004)ABUND

C CALCULATE MEAN MOLECULAR WEIGHT (MU) AND NUCLEI PER PROTON (MU1)
C
MU=1.0+4.0*Y
MU1=1.0+Y
DO 10 I=3,92
VX=1.E-12*EXP(2.302585093*ABUND(I))*Z
MU=MU+VX*WEIGHT(I)
MU1=MU1+VX
CONTINUE
M=MU/MU1

C READ NUMBER OF DEPTH POINTS AND FREQUENCIES
C AND THEN READ THE FREQUENCIES
C
READ (5,1005)NDEPTH,NJ
READ (5,1006)(FREQ(IJ),IJ=1,NJ)
WRITE (12,1005)NDEPTH,NJ
WRITE (12,1006)(FREQ(IJ),IJ=1,NJ)

C CALCULATE FREQUENCY QUADRATURE WEIGHTS
C NO CORRECTION IS MADE FOR LINES; I.E. IT IS
C ASSUMED THAT THE LINES ARE NARROW.
C
DO 20 IJ=1,NJ
WT(IJ)=0.0
CONTINUE

C READ IN FREQUENCY INTERVAL NUMBER AND RULE
C
READ (5,1005)NO,W1
WRITE (12,1005)NO,W1
IF (NO.EQ.2)THEN
C TRAPEZOIDAL RULE: W1 IS NUMBER OF FIRST FREQUENCY
C
VX=0.5*ABS(FREQ(W1)-FREQ(W1+1))
WT(W1)=WT(W1)+VX
WT(W1+1)=WT(W1+1)+VX
GO TO 30
ELSE IF (NO.EQ.3)THEN
C SIMPSON'S RULE: W1 IS NUMBER OF CENTRAL FREQUENCY
C **NOTE THAT NO CHECK IS MADE TO BE SURE THAT THE
C TWO FREQUENCY SUBINTERVALS ARE EQUAL, AS THEY NEED
C TO BE.**
C
VX=ABS(FREQ(W1+1)-FREQ(W1-1))/6.0
WT(W1+1)=WT(W1)+VX
WT(W1-1)=WT(W1-1)+VX
WT(W1)=WT(W1)+4.0*VX
GO TO 30
ELSE IF (NO.NE.0)THEN
C PROGRAM DOESN'T RECOGNIZE THE RULE
C WRITE (6,*) 'ERROR IN FREQUENCY QUADRATURE RULE'
CALL EXIT(1)
ENDIF
C
READ OPACITY RULE
READ (5,1005)RULE
WRITE (12,1005)RULE

C REMAINDER OF DECK IS IGNORED
CALCULATE CONTINUUM ABSORPTION COEFFICIENTS

DO 70 IJ=1,NI

BOUND-FREE ABSORPTION

FCOM=FREQ(IJ)

DO 40 IL=1,ILHE2

SIGHE2(IL,IJ)=0.0

IF (FCOM.GT.FRQHE2(IL)) SIGHE2(IL,IJ)=45.04E29*GAUWT(IL,FCOM)/FLOAT(IL)**5/FCOM**3

CONTINUE

DO 50 IL=1,ILHE1

SIGHE1(IL,IJ)=0.0

IF (FCOM.GT.FRQHE1(IL)) SIGHE1(IL,IJ)=2.815E29*GAUWT(IL,FCOM)/FLOAT(IL)**5/FCOM**3

CONTINUE

SINGLY-IONIZED HELIUM IS HYDROGENIC AND THUS USES SCALED HYDROGEN EXPRESSIONS.

DO 60 IL=1,ILHE2

SIGBI(IL,IJ)=0.0

IF (FCOM.GT.FRQHE2(IL)) SIGBI(IL,IJ)=2.815E29*GAUWT(IL,FCOM)/FLOAT(IL)**5/FCOM**3

CONTINUE

FREE-FREE ABSORPTION

SIGH(ILH+1,IJ)=3.69E8/FCOM**3

CONTINUE

NEGATIVE HYDROGEN ION

IF (RULE(IJ)) THEN

DO 80 IL=1,NI

SIGHMM(IL,IJ)=0.0

IF (FREQ(IJ).GT.FRQM) SIGHMM(IJ)=MAX(0.,MINUS(FREQ(IJ)))

CONTINUE

ENDIF

DETERMINE CUTOFF FREQUENCIES FOR FREE-FREE OPACITY.

THESE ALLOW THE INCLUSION OF BOUND LEVELS ABOVE THOSE ACCOUNTED FOR EXPLICITLY AS PART OF THE FREE-FREE OPACITY.

DO 90 IL=1,NI

FF(IJ,1)=MIN(FRQH(ILH)*(MQH/(MQH+1))**2,FREQ(IJ))

FF(IJ,2)=MIN(FRQHE1(ILHE1)*(MQHE1/(MQHE1+1))**2,FREQ(IJ))

FF(IJ,3)=MIN(FRQHE2(ILHE2)*(2*MQH/(2*MQH+1))**2,FREQ(IJ))

CONTINUE

RETURN

C CONTAINS ALL DATA STATEMENTS FOR COMMON BLOCKS, IN ACCORDANCE WITH THE ANSI STANDARD

PLIST

HYDROGEN STATISTICAL WEIGHTS

DATA GH/2. ,8. ,18. ,32. ,50. ,72. ,98. ,128. ,162. ,200. ,242. ,288. ,338. ,392. ,450. ,512./

NEUTRAL HELIUM STATISTICAL WEIGHTS

END
DATA GHE1/1.,3.,1.,9.,3.,1.,9.,5.,15.,3.,1.,9.,5.,15.,3.,
  21.,7.,100.,144.,196.,256.,324.,400.,484.,576.,676.,784.,900.,
  1024./

IONIZED HELIUM STATISTICAL WEIGHTS

  1352.,1458.,1568.,1682.,1800.,1922.,2048./

NEGATIVE HYDROGEN ION IONIZATION FREQUENCY

DATA FIIQH/1.874E14/

HYDROGEN IONIZATION FREQUENCIES

DATA FIIQH/3.28799E1S,0.821997E1S,0.365332E1S,0.205499E1S,
  0.131519E15,0.0913329E15,0.0671018E15,0.0513740E15,
  0.0405924E15,0.0328799E15,0.0271735E15,0.0228333E15,
  0.0194566E15,0.0167755E15,0.0146133E15,0.0128437E15/

NEUTRAL HELIUM IONIZATION FREQUENCIES

DATA FQHE1/5.04520E1S,1.1520E15,0.957430E15,0.876230E15,
  0.81774E15,0.451890E15,0.400142E15,0.381976E15,0.362850E15,
  0.366032E15,0.362408E15,0.240134E15,0.217774E15,0.212670E15,
  0.202058E15,0.202703E15,0.199689E15,0.191520E15,
  0.0913331E15,0.0871018E15,0.08384532E15,0.0813748E15,
  0.0778222E15,0.0748035E15,0.0720574E15,0.0698695E15,
  0.0686020E15,0.0671018E15,0.0657105E15,0.0648607E15,
  0.0640678E15,0.063322E15,0.0625290E15,0.0617735E15,
  0.0610431E15,0.0603508E15,0.0596566E15,0.0589437E15/

IONIZED HELIUM IONIZATION FREQUENCIES

DATA FQHE2/13.1520E15,3.28799E1S,1.46133E15,0.821997E1S,
  0.526078E15,0.365332E15,0.268407E15,0.205499E15,0.162270E15,
  0.131519E15,0.108694E15,0.0913329E15,0.0778222E15,
  0.0671018E15,0.0584532E15,0.0513740E15,0.0465058E15,
  0.0405924E15,0.0364320E15,0.0271735E15,0.0228333E15,
  0.0210431E15,0.020574E15,0.0202703E15,0.0199689E15,
  0.0194566E15,0.0180411E15,0.0167755E15,0.0156385E15,
  0.0146133E15,0.0136857E15,0.0128437E15/

EXTERNAL REAL FUNCTION FWT(DUM)

APPROXIMATE T-TAU RELATIONSHIP

PLOT ROOT

REAL DUM

FWT=TEFF*SQRT(SQRT(75*(-1.331+EXP(-3.4488*DUM))))
RETURN

END

SUBROUTINE STATE(ID,KAP)

MAIN ROUTINE FOR CALCULATING STATE VARIABLES

IMPLICIT NONE

COMMON INCLUSION

PLOT ROOT

LOCAL VARIABLES

INTEGER I, II, IJ, IL, J, K, ID
REAL ENR, DEL, CLSR(MNNN,NNN), RHO
REAL RHS(MNNN), LHS(MNNN,NNN), T, VX
REAL AMN(MNNN), AN(MNNN), KAP, BSUM

C

C

C

C

C

C
REAL LIMSILV, MATINV, MURATE, GEN
EXTERNAL LIMSILV, MATINV, MURATE, GEN
C
REAL SB, SHBE1, SHBE2
SB(I,T)=2.0706E-16*SH(I)*EXP(HE*FREQ(I)/T)/T/SQRT(T)
SHBE1(I,T)=2.0706E-16*SHBE1(I)*EXP(HE*FREQ(I)/T)/T/SQRT(T)/2.
SHBE2(I,T)=2.0706E-16*SHBE2(I)*EXP(HE*FREQ(I)/T)/T/SQRT(T)
C
START OF EXECUTABLE
C
INITIAL GUESS OF ELECTRON DENSITY
C
IF (ID.EQ.1) THEN
    NE(ID)=1.
ELSE
    NE(ID)=NE(ID-1)
ENDIF
C
DO 40 II=1,30
    CALL MURATE(LBS,RBS,II)
    DO 10 I=1,NMNN
        DO 5 J=1,NJIIJ
            CLBS(I,J)=LBS(I,J)
    10 CONTINUE
C
DO 20 I=1,NJIIJ
    CALL LIJISLV(CLBS,RBS,ANS,NMNN,NMNN)
A(4)=-1.-ANS(INPROT)*MU1+SUMH(ID)
A(3)=1.-ANS(INHE3)+SUMH2(ID)
A(1)=ANS(INHE3)+SHBE2(1,TEMP(ID))
A(2)=ANS(INHE3)+SUMH3(ID)-Y*ANS(INPROT)+SUMH(ID)
    CALL MATINV(LBS,NMNN,NMNN)
    DEL=0.
    DO 10 II=1,4
        DEL=DEL+LBS(4,II)*A(II)
10 CONTINUE
C
DO 30 II=1,ILB
    NG=WT(I)+FREQ(I)•3/(EXP(BK•FREQ(I)/TENP(ID))-1.)
    BSUN=BSUN+NG
    KAP=KAP+NG/CBI(I)
30 CONTINUE
C
RBD=NU•(ITOT(ID)-IE(ID))/6.022E23
KAP=BSUN/KAP/RBD
RETURN
END
C
SUBROUTINE LINSILV(A,B,T,W,WR)
C
SOLVE SET OF LINEAR EQUATIONS
C
FROM AVER/MISHALAS CODE
C
IMPLICIT NONE
C
INTEGER NQW
PARAMETER (NQW=4)
INTEGER J, JTEMP, JP1, N, I, NR, K, IP1, MR1, KP1, R, P(NR, I)
REAL W, SUM, D(NR, I)
REAL A(NR, NR), B(NR), X(NR)

REAL EXIT
EXTERNAL EXIT

IF (W.GT.NR) THEN
   WRITE (6,20) 'M TOO BIG IN LINSLV; = ', W
   CALL EXIT(1)
ENDIF

DO 70 R = 1, N
   DO 10 K = 1, R
      D(K) = A(K, R)
   CONTINUE
   IIR1 = R - 1
   IF (IIR1.LT.1) GO TO 40
   DO 30 J = 1, IIR1
      ITEMP = P(J)
      A(J, R) = D(ITEMP)
      D(ITEMP) = D(J)
      JP1 = J + 1
      DO 20 I = JP1, R
         D(I) = D(I) - A(I, J) * A(J, R)
      CONTINUE
   CONTINUE
   30 CONTINUE
   40 ll = ABS(D(R))
   P(R) = R
   DO 50 I = R, 1, 1
      IF (ll.GE.ABS(D(I))) GO TO 50
      P(R) = I
      ll = ABS(D(I))
   CONTINUE
   50 CONTINUE
   ITEMP = P(R)
   A(R, R) = D(ITEMP)
   D(ITEMP) = D(R)
   IIR1 = R + 1
   IF (IIR1.GT.N) GO TO 80
   DO 60 J = IIR1, R
      A(J, R) = D(J) / A(R, R)
   CONTINUE
   70 CONTINUE
   80 DO 100 I = 1, N
      ITEMP = P(I)
      X(I) = B(ITEMP)
      B(ITEMP) = B(I)
      IP1 = I + 1
      IF (IP1.GT.N) GO TO 110
      DO 90 J = IP1, N
         B(J) = B(J) - A(J, I) * X(I)
      CONTINUE
   100 CONTINUE
   110 DO 140 I = 1, N
      K = I - 1
      SUM = 0.0
      KP1 = K + 1
      IF (KP1.GT.N) GO TO 130
      DO 120 J = KP1, N
         SUM = SUM + A(K, J) * X(J)
      CONTINUE
   130 X(K) = (X(K) - SUM) / A(K, K)
   140 CONTINUE

RETURN
END

SUBROUTINE MATINV(A, N, NR)
C
C     INVERT MATRIX IN PLACE
C     FROM AUE/MIHALLS CODE
C
C     IMPLICIT NONE
C
INTEGER N, K, NR, I, L, KO, II, J, JJ
REAL A(NR, NR), DIV, SUM

DO 60 I = 2, N
   DIV = A(I, I)
   A(I, I) = A(I, I) / DIV
   DO 30 J = 2, I - 1
      A(J, I) = A(J, I) / A(I, I)
      DO 10 K = J + 1, N
         A(K, I) = A(K, I) - A(K, J) * A(J, I)
      CONTINUE
   30 CONTINUE
   60 CONTINUE
DIV=A(J,J)
SUM=0.
DO 10 L=1,J-1
   SUM=SUM+A(I,L)*A(L,J)
10 CONTINUE
A(I,J)=(A(I,J)-SUM)/DIV
30 CONTINUE
DO 50 J=I,N
   SUM=0.
   DO 40 L=1,J-1
      SUM=SUM+A(I,L)*A(L,J)
40 CONTINUE
A(I,J)=A(I,J)-SUM
50 CONTINUE
DO 60 J=I,I-1
   SUM=0.
   DO 50 L=1,J-1
      SUM=SUM+A(I,L)*A(L,J)
50 CONTINUE
A(I,J)=A(I,J)-SUM
60 CONTINUE
DO 100 I=1,2,-1
   DO 90 J=I-1,1,-1
      SUM=0.
      DO 70 K=J+1,I-1
         SUM=SUM+A(I,K)*A(K,J)
70 CONTINUE
A(I,J)=-A(I,J)-SUM
90 CONTINUE
100 CONTINUE
A(N,N)=1.0/A(N,N)
DO 140 I=1,1,-1
   DIV=A(I,I)
   DO 120 J=I,I-1,-1
      SUM=0.
      DO 110 K=I+1,J
         SUM=SUM+A(I,K)*A(K,J)
110 CONTINUE
A(I,J)=-SUM/DIV
120 CONTINUE
A(I,I)=1.0/A(I,I)
140 CONTINUE
DO 190 I=1,N
   DO 180 J=I,1,-1
      SUM=0.0
      DO 150 K=I,J
         SUM=SUM+A(I,K)*A(K,J)
150 CONTINUE
A(I,J)=SUM
180 CONTINUE
DO 170 K=J+1,N
   DO 160 J=I,J
      SUM=0.0
      DO 150 K=J+1,N
         SUM=SUM+A(I,K)*A(K,J)
150 CONTINUE
A(I,J)=SUM
170 CONTINUE
180 CONTINUE
RETURN
END
B. Program LTE

LTE is listed in its entirety, except for those program units that are essentially identical to the ones in GRAY. These are:

FRE
GAUNT
GENER
HEGAUNT
HMINUS
LINSLV
MATINV
PROGRAM LTE

COMMON BLOCK MACROS FOR ALL GLOBAL DATA IN PROGRAM
(CRAY PRECOMPILED)

BASIC PARAMETERS

CLICHE PLIST
INTEGER MDEPTH, MJJC, MNTRB, MTRBE1, MTRBE2, MQB, MQBE1, WLB
INTEGER MLBE1, MLBE2, SQUAD
PARAMETER (MDEPTH=70, MJJC=105, MNTRB=10, MTRBE1=14)
PARAMETER (MTRBE2=10, MQB=16, MQBE1=31, WLB=10)
PARAMETER (MLBE1=25, MLBE2=15, SQUAD=7)

INTEGER MJJC
PARAMETER (MJJC=MJJC+MQBE1*(MTRBE2+MTRBE1+MTRBE2))

REAL CC, DELQUAD, EMASS, ESU, HP, KB, MBYD, PI
PARAMETER (CC=2.99792E10, DELQUAD=0.6, EMASS=9.10953E-28)
PARAMETER (ESU=4.80325E-10, HP=6.62618E-27, KB=1.38066E-16)
PARAMETER (MBYD=1.66058E-24, PI=3.141592654)

REAL ACCOF, BBCOF, DOPCOF, BK, HYDCOF, PIE2MC, SDCOF, SIGE
PARAMETER (ACCOF=2.074E-16, BBCOF=2.*HP/(CC*CC), DOPCOF=4.286E-7)
PARAMETER (BK=HP/KB, HYDCOF=4.*PI/CC)
PARAMETER (PIE2MC=PI*ESU/EMA, SDCOF=4.*PI/HP)
PARAMETER (SIGE=8.*PI*ESU*ESU/EMA):

EIDCLICHE

CLICHE BLANK

REAL CHI(NMJ), ETA(NMJ), FK(MDDEPTB), RAD(MDDEPTB)

COMMON //CHI, ETA, FK, RAD

EIDCLICHE

CLICHE ROOT

INTEGER ITPTRB, ITPTRBE1, ITPTRBE2, MDEPTH, MJJC, MTRBE1
INTEGER MTRBE2

LOGICAL RULE(2)

REAL DSBDT(MDDEPTB), DSBE1(MDDEPTB), DSBE2(MDDEPTB), FF(MMJ,3)
REAL FB, FREQ(MMJ), GRAV, HO, M(MDDEPTB), MU, MJJ
REAL WE(MDDEPTB), W(MJJC,MDDEPTB), WHE1(WHE1,MDDEPTB)
REAL WHE2(WHE2,MDDEPTB), WHE3(MMDDEPTB)
REAL WM(MMDDEPTB), WPRT(MMDDEPTB), WTUT(MMDDEPTB), SIGEM(MMJ)
REAL SIGE(MMJ,3), SIGE1(SIGE1,3), SIGE2(SIGE2,3)
REAL SUMM(MMDDEPTB), SUMH1(MMDDEPTB), SUMH2(MMDDEPTB)
REAL TEMP(MMDDEPTB), TLINE, WT(NMJ), Y

COMMON /ROOT//ITPTRB, ITPTRBE1, ITPTRBE2, MDEPTH, MJJC, MTRBE1
INTEGER NTRBE1, NTRBE2, RULE, DSBDT, DSBE1, DSBE2, FF, FB, FREQ, GRAV,
: HO, M, MU, MJJC, W, WE, WHE1, WHE2, WHE3, WM, WPRT, WTUT, SIG,
: SIGE1, SIGE2, SIGEM, SUMM, SUMH1, SUMH2, TEMP, TLINE, WT, Y

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CLICHE ROOTI

INTEGER ITRB(5,5), ITRE1(19,19), ITRE2(10,10), LOWERE(MNTRB)
INTEGER LOWERE1(MNTRBE1, LOWERE2(MNTRBE2), LWR(NMJ)
INTEGER LOWERE1(MNTRBE1), LOWERE2(MNTRBE2), LWR(NMJ)
INTEGER LOWERE1(MNTRBE1), LOWERE2(MNTRBE2), LWR(NMJ)
INTEGER LOWERE1(MNTRBE1), LOWERE2(MNTRBE2)
REAL FHQM, FHQB(MQB), FHQE1(MQBE1), FHQE2(MQBE2), GH(MGQB)
REAL GHE1(GHE1, MOCB(10), MOCH(104), MOCH(104))

COMMON /ROOT//ITRE1, ITRE2, LOWERE, LOWERE1, LOWERE2,
: LOWE, LOWE1, LOWE2, UPHE, UPHE1, UPHE2, UPHERE, UPHERE1,
: UPHERE2, FHQEM, FHQE, FHQIE1, FHQIE2, GH, GHE1, GHE2, GHE3, GHE4,
: GHE5, GHE6, GHE7, GHE8, GHE9, GHE10, GHE11, GHE12, GHE13

EIDCLICHE

CLICHE SIGS

END
POINTERS FOR STATE MATRIX

INTEGER INHE2, INHE3, IMPROT, INTOT, NWWW

PARAMETER (INHE2=1, INHE3=2, IMPROT=3, INTOT=4, NWWW=4)

REAL DW(NWWW,NDEP), DT(NWWW,NDEP)

COMMON /SEG/DW, DT

ENDCLICHE

PROGRAM LTE

CALCULATE AN LTE ATMOSPHERE OF HYDROGEN AND HELIUM.

THE PROGRAM UTILIZES THE OUTPUT MODEL OF PROGRAM GRAY
AS A FIRST APPROXIMATION.

IMPLICIT NONE

LOCAL VARIABLES

INTEGER I, WITER
REAL ERR, TEFF, Z

EXTERNAL PROCEDURES

REAL EXIT, LK, LTESTEP, PUTOUT, SETUP
EXTERNAL EXIT, LK, LTESTEP, PUTOUT, SETUP

START OF EXECUTABLE STATEMENTS

THE NEXT LINE MAY BE DELETED ON NON-CRAY IMPLEMENTATIONS

THE FILE input HOLDS THE FIRST APPROXIMATION MODEL.
THE FILE output RECEIVES THE CALCULATED MODEL.
THE FILE monitor RECEIVES VARIOUS PROGRAM-GENERATED REMARKS.

CALL LK("UNITS=(input,OPEN,TEXT),UNIT12=(output,CREATE,TEXT),
:UNIT6=(monitor,CREATE,TEXT)/")

READ THE FIRST APPROXIMATION MODEL AND CALCULATE QUANTITIES
DEPENDENT ONLY ON THE FREQUENCY MESS AND IONIZATION ENERGIES.

CALL SETUP(WITER,TEFF,Z)

MAIN LOOP:

DO 10 I=1,WITER

PERFORM AN LTE COMPLETE LINEARIZATION ITERATION

CALL LTESTEP(ERR)

TELL THE USER HOW WE'RE COMING ALONG.

WRITE (6,1008) I, ERR

SUCCESS! EXIT THE LOOP AND SAVE THE POLISHED MODEL.

IF (ERR.LT.1.E-4)GO TO 20

CONTINUE

SAVE THE COMPLETED MODEL

20 CALL PUTOUT(TEFF,Z)

CALL EXIT(0)

FORMAT STATEMENTS

1008 FORMAT (' * ITERATION*,I3,' COMPLETE WITH ERR = ',F9.4)

END

SUBROUTINE EDDFAC(IJ)

SOLVE EQUATION OF TRANSFER FOR A GIVEN SOURCE FUNCTION AND
CALCULATE VARIABLE EDDINGTON FACTORS

IMPLICIT NONE
INTEGER I, ID, IJ, IMU, J
REAL A(3), AA, B(3,3), BB, C(3), CCC, D(3,3,NDP), DD(MPD)
REAL DIV, DP, DT(MPD), DTO, DIV, E, EJ, EE, L, MU(MPD), P
REAL PHI(3,MDP), Q(3), QQ, QS, RO

C GAUSSIAN INTEGRATION ORDINATES AND WEIGHTS
C
REAL WTMU(3)
DATA WTMU/.5,77777777777778,.44444444444444,
: .5,77777777777778/

C START OF EXECUTABLE STATEMENTS
C
C CALCULATE OPTICAL DEPTH SCALE
C
DO 20 ID=T,IDEPTH-1
DT(ID)=0.5*(CBI(ID+1)/IM(ID+1)+CBI(ID)/IM(ID))*
M(ID+1)/MYD
20 CONTINUE
C
C UPPER BOUNDARY CONDITIONS
C
QQ=ETA(1)/CBI(1)
QS=IE(ID)*SIGE/CBI(1)
DO 60 I=1,3
PSI(I,1)=0.
DIV=0.5*DT(ID)/AMU(I)
Q(I)=DIV*QQ
C(I)=AMU(I)/DT(ID)
60 CONTINUE
B(I,I)=WTMU(I)*QS*DIV
B(I,1)=B(I,1)+1.0+C(I)+DIV
B(2,1)=B(2,1)/B(1,1)
B(2,2)=B(2,2)-B(2,1)*B(1,2)
B(2,3)=B(2,3)-B(2,1)*B(1,3)
B(3,1)=B(3,1)/B(1,1)
B(3,2)=B(3,2)-B(3,1)*B(1,2)/B(2,2)
B(3,3)=B(3,3)-B(3,1)*B(1,3)-B(3,2)*B(2,3)
B(3,2)=B(3,2)
B(3,1)=B(3,1)-B(3,2)*B(2,1)
B(2,1)=B(2,1)
B(3,3)=1.0/B(3,3)
B(2,3)=B(2,3)*B(3,3)/B(2,2)
B(2,2)=1.0/B(2,2)
B(1,3)=B(1,2)*B(2,3)+B(1,3)*B(3,3)/B(1,1)
B(1,2)=B(1,2)/B(2,2)/B(1,1)
B(1,1)=1.0/B(1,1)
B(1,1)=B(1,1)+B(1,2)*B(2,1)*B(1,3)*B(3,1)
B(1,2)=B(1,2)+B(1,3)*B(3,2)
B(2,1)=B(2,2)+B(2,1)*B(3,3)/B(3,1)
B(2,2)=B(2,2)+B(3,3)/B(3,2)
B(3,1)=B(3,1)+B(3,2)
B(3,2)=B(3,3)*B(3,2)
DO 80 J=1,3
70 CONTINUE
D(I,J)=B(I,J)+C(I)*J
PSI(I,J)=PSI(I,J)+B(I,J)*Q(J)
80 CONTINUE
C
C INVERT MATRIX (DONE EXPLICITLY SINCE SMALL MATRIX)
C
B(2,1)=B(2,1)/B(1,1)
B(2,2)=B(2,2)-B(2,1)*B(1,2)
B(2,3)=B(2,3)-B(2,1)*B(1,3)
B(3,1)=B(3,1)/B(1,1)
B(3,2)=B(3,2)-B(3,1)*B(1,2)/B(2,2)
B(3,3)=B(3,3)-B(3,1)*B(1,3)-B(3,2)*B(2,3)
B(3,2)=B(3,2)
B(3,1)=B(3,1)-B(3,2)*B(2,1)
B(2,1)=B(2,1)
B(3,3)=1.0/B(3,3)
B(2,3)=B(2,3)*B(3,3)/B(2,2)
B(2,2)=1.0/B(2,2)
B(1,3)=B(1,2)*B(2,3)+B(1,3)*B(3,3)/B(1,1)
B(1,2)=B(1,2)/B(2,2)/B(1,1)
B(1,1)=1.0/B(1,1)
B(1,1)=B(1,1)+B(1,2)*B(2,1)*B(1,3)*B(3,1)
B(1,2)=B(1,2)+B(1,3)*B(3,2)
B(2,1)=B(2,2)+B(2,1)*B(3,3)/B(3,1)
B(2,2)=B(2,2)+B(3,3)/B(3,2)
B(3,1)=B(3,1)+B(3,2)
B(3,2)=B(3,3)*B(3,2)
DO 80 J=1,3
70 CONTINUE
D(I,J)=B(I,J)+C(J)
PSI(I,J)=PSI(I,J)+B(I,J)*Q(J)
80 CONTINUE
C
C NORMAL DEPTH POINTS
C
DO 130 ID=2,MDP-1
DTO=0.5*(DT(ID-1)+DT(ID))
QQ=ETA(ID)*SIGE/CBI(ID)
QS=MY(ID)*SIGE/CBI(ID)
DO 120 J=1,3
A(I,J)=AMU(I)*QQ*DT(ID)/DTO
C(I,J)=AMU(I)*QQ*DT(ID)/DTO
Q(J)=QQ*A(I,J)*PSI(I,J)
120 CONTINUE
130 CONTINUE
C
C END OF EXECUTABLE STATEMENTS
DO 70 J=1,3
   B(I,J)=-WTMU(J)*QS
   CONTINUE
B(I,I)=B(I,I)+A(I)+C(I)
CONTINUE
DO 100 I=1,3
   DO 90 J=1,3
      B(I,J)=B(I,J)-A(I)*D(I,J,ID-1)
   CONTINUE
B(2,1)=B(2,1)/B(1,1)
B(2,2)=B(2,2)/B(1,1)
B(2,3)=B(2,3)/B(1,1)
B(3,1)=B(3,1)/B(1,1)
B(3,2)=B(3,2)/B(1,1)
B(3,3)=B(3,3)/B(1,1)
B(3,2)=-B(3,2)
B(3,1)=-B(3,1)
B(2,1)=-B(2,1)
B(3,3)=1.0/B(3,3)
B(2,2)=1.0/B(2,2)
B(1,3)=-(B(1,2)*B(2,3)+B(1,3)*B(3,3))/B(1,1)
B(1,2)=B(1,2)+B(2,2)/B(1,1)
B(1,1)=B(1,1)
B(1,2)=B(1,2)+B(2,1)+B(1,3)*B(3,1)
B(2,2)=B(2,2)+B(2,1)+B(2,3)*B(3,1)
B(2,2)=B(2,2)+B(2,3)*B(3,2)
B(3,1)=B(3,1)*B(3,1)
B(3,2)=B(3,2)*B(3,2)
DO 120 I=1,3
   PSI(I,ID)=0.
   DO 110 J=1,3
      PSI(I,ID)=PSI(I,ID)+B(I,J)*Q(J)
   CONTINUE
DO 110 J=1,3
   PSI(I,ID)=PSI(I,ID)+B(I,J)*Q(J)
   CONTINUE
C
LOWER BOUNDARY CONDITIONS
C
RO=BBCCF*FREQ(I)**3
P=RO/(EXP(BK*FREQ(I))/TEMP(WDEPTH))**1.)
DP=RO/(EXP(BK*FREQ(I))/TEMP(WDEPTH)-1.)
DO 150 I=1,3
   A(I)=AMU(I)/DT(WDEPTH-1)
   Q(I)=AMU(I)*DP+A(I)*PSI(I,WDEPTH-1)
DO 140 J=1,3
   B(I,J)=0.
CONTINUE
B(I,I)=B(I,I)+A(I)
CONTINUE
DO 170 I=1,3
   DO 160 J=1,3
      B(I,J)=B(I,J)-A(I)*D(I,J,WDEPTH-1)
   CONTINUE
B(I,I)=B(I,I)+A(I)*D(I,I,WDEPTH-1)
BACKSUBSTITUTION TO DETERMINE SPECIFIC INTENSITIES

DO 190 I=1,3
PSI(I, IDPETH)=0.
DO 180 J=1,3
PSI(I, IDPETH)=PSI(I, IDPETH)+B(I, J)*Q(J)
CONTINUE
DO 190 I=1,3
PSI(I, IDPETH)=0.
DO 180 J=1,3
PSI(I, IDPETH)=PSI(I, IDPETH)+B(I, J)*Q(J)
CONTINUE
DO 230 IDPETH=1,-1
EJ=0.
DO 220 I=1,3
IF (ID.EQ.IDPETH) GO TO 210
DO 200 J=1,3
PSI(I, ID)=PSI(I, ID)+D(I, J)*PSI(J, ID)
CONTINUE
210 EJ=EJ+VTM(I)*PSI(I, ID)
END
DO 240 I=1,3
EB=EB+VTM(I)*AMU(I)**2*PSI(I, 1)
CONTINUE
FB=EB/EJ
DO 250 ID=2, IDPETH-1
DT0=0.5*(DT(ID-1)+DT(ID))
AA=FK(ID-1)/(DT(ID-1)*DT0)
CCC=FK(ID+1)/(DT(ID+1)*DT0)
L=ETA(ID)/CHI(ID)
BB=BB+AA*DD(ID-1)
CONTINUE
BB=BB+AA*(IDPETH-1)*DT0
AAA=FK(IDPETH-1)/(DT(IDPETH-1)*DT0)
BB=BB+AAA/DD(IDPETH-1)
L=0.5*P/3.0
RAD(ID)=(L+AAA*IDPETH-1)/BB
CONTINUE
RAD(ID)=UID(ID)+DD(ID)*RAD(ID+1)
RETURN
END

SUBROUTINE LSTATE(WTM, WTT, BSUM, BSUMW, BSUMT)
CALCULATES WTOT DERIVATIVES AND LOWER BOUNDARY SUMS FOR LTESTEP

IMPLICIT NONE
PLIST
BLARK
ROOT
ROOTI
SIGM
INTEGER I, ID, IJ, IL, IT, J, L, U
REAL BSUM, BSUMW, BSUMT, C, DOP, E, FRQO, HKT
REAL HKT, SIGMA, SIGMAT, SRT, SRT2, T, IO, II, IX1, X1T, VX, VIT
REAL CBIL(MIII), CHIT(MIII), CLHS(MIII,MIII), DELTA(MIII)
REAL DSKK(4,IIIJ), ETAl(MIII), ETAT(IIIJ)
REAL EX(IIIJ), LHS(MIII,MIII), LT(MDEPTB), RHS(MIII)
REAL Rl(MIII), RT(MIII), SKK(4,IIIJ)

EXTERNAL
REAL FRE, MATINV, MURATE
EXTERNAL FRE, MATINV, MURATE

STATEMENT FUNCTIONS
REAL BB, BBT, BBT, FQ, TQ
REAL SB, SBBE1, SBBE2, SBH, SBBE2T
REAL SBM, SBMT
SBM(T)=ACCOF*0.5*EXP(HK*FRQH/T)/T/SQRT(T)
SBMT(T)=-1.5*HK*FRQH(T)/T
SBH(I,I)=ACCOF*GHI(I)*EXP(HK*FRQH(I)/T)/T/SQRT(T)
SBH(I,T)=(-1.5*HK*FRQH(I)/T)/T
SBH(I,T)=ACCOF*GHE1(I)*EXP(HK*FRQH1(I)/T)/T/SQRT(T)/2.
SBH2T(I,T)=(-1.5*HK*FRQH2(T)/T)/T
SBH2T(I,T)=ACCOF*GHE1(I)*EXP(HK*FRQH2(T)/T)/T/SQRT(T)
SBH2T(I,T)=-1.5*HK*FRQH2(T)/T
BB(FQ,TQ)=BB(FQ,TQ)*BK*FQ/TQ/TQ/(1.0-EXP(-BK*FQ/TQ))
BBT(FQ,TQ)=BBT(FQ,TQ)=-BK*FQ*(1.0-EXP(-BK*FQ/TQ))/
(1.0-EXP(-BK*FQ/TQ))/TQ-2.0)/TQ

START OF EXECUTABLE STATEMENTS
ESTABLISH LTE POPULATIONS AND DERIVATIVES
DO 120 ID=1,NDEPTB
CALL MURATE(LHS,Ll,LT,RHS,Rl,RT,ID)
CALL MATINV(LH,NS,NS,NS,NS,NS,NS)
DO 20 I=1,NS
DN(I,ID)=0.0
DT(I,ID)=0.0
DO 10 J=1,NS
CLHS(I,J)=LHS(I,J)
10 CONTINUE
20 CONTINUE
DO 30 J=1,NS
DO 35 I=1,NS
DELTA(I)=DELTA(I)-LHS(I,J)*RHS(J)
35 CONTINUE
30 CONTINUE
MTOT(ID)=MTOT(ID)+LHS(I,J)*RHS(ID)
NPRT(ID)=NPRT(ID)+ME(ID)+MNE(ID)
MHE2(ID)=MHE2(ID)+ME(ID)*MHE2(ID)
MHE3(ID)=MHE3(ID)+ME(ID)*MHE3(ID)
DO 50 IL=1,ILBE1
MLBE1(IL,ID)=MLBE1(IL,TEMP(ID))*ME(ID)+MNPRT(ID)
50 CONTINUE
DO 60 IL=1,ILBE2
MLBE2(IL,ID)=MLBE2(IL,TEMP(ID))*ME(ID)*MHE2(ID)
60 CONTINUE
DO 70 IL=1,ILBE2
MLBE2(IL,ID)=MLBE2(IL,TEMP(ID))*ME(ID)*MHE3(ID)
70 CONTINUE
DO 80 I=1,NS
DO 80 J=1,NS
RL(I)=RL(I)-LHS(I,J)*DELTA(J)
RT(I)=RT(I)-LHS(J,I)*DELTA(J)
80 CONTINUE
80 CONTINUE
DO 110 I=1,NS
DO 100 J=1,NS
DN(I,ID)=DN(I,ID)+LHS(I,J)*RHS(J)
DT(I,ID)=DT(I,ID)+CLHS(I,J)*RT(J)
100 CONTINUE
110 CONTINUE
NRM(ID)=NRM(ID)*MTOT(ID)*ME(ID)
NRM(ID)=NRM(ID)*MTOT(ID)
NRM(ID)=NRM(ID)*MTOT(ID)
120 CONTINUE
CALCULATE LOWER BOUNDARY OPACITIES AND DERIVATIVES

SRT = SQRT(TLIME/TEMP(WDEPTH))
SRT2 = SQRT(TEMP(WDEPTH))
CALL FREQ(SK,FSK,WDEPTH)
HKT = H/T/TEMP(WDEPTH)
BKT = BKT/TEMP(WDEPTH)

ELECTRON SCATTERING

DO 130 IJ=1,NJ
CHI(IJ) = NE(WDEPTH) * SIGE
CHI(IJ) = SIGE
EX(IJ) = EXP(-HKT * FREQ(IJ))
ETA(IJ) = 0.0
ETAT(IJ) = 0.0
CHIT(IJ) = 0.0
130 CONTINUE

BOUND-FREE OPACITIES

DO 150 IL=1,NLE
DO 140 IJ=1,NJ
C = SIG(IL,IJ) * W(IL,WDEPTH)
E = C * EX(IJ)
ETA(IJ) = ETA(IJ) + E
EX(IJ) = ETA(IJ) + E * (SBT(IL, TEMP(WDEPTH)) - HKT * FREQ(IJ))
CHI(IJ) = CHI(IJ) + C
CHIT(IJ) = CHIT(IJ) + C
140 CONTINUE
150 CONTINUE

FREE-FREE OPACITIES

XO = IBE3(1,DEPTB) * IE(IDEPTB) * 2
X1 = XO * SUMBE2(1,DEPTB)
X1T = XO * DSHE2(1,DEPTB)

C0 = SIGE2(IL,IJ) * WHE1(IL,WDEPTH)
E = C0 * EX(IJ)
ETA(IJ) = ETA(IJ) + E
EX(IJ) = ETA(IJ) + E * (SBHE1T(IL, TEMP(WDEPTH)) - HKT * FREQ(IJ))
CHI(IJ) = CHI(IJ) + C
CHIT(IJ) = CHIT(IJ) + C
170 CONTINUE
180 CONTINUE

DO 200 IL=1,NHE2
DO 190 IJ=1,NJ
C = SIGE2(IL,IJ) * WHE2(IL,WDEPTH)
E = C0 * EX(IJ)
ETA(IJ) = ETA(IJ) + E
EX(IJ) = ETA(IJ) + E * (SBHE2T(IL, TEMP(WDEPTH)) - HKT * FREQ(IJ))
CHI(IJ) = CHI(IJ) + C
CHIT(IJ) = CHIT(IJ) + C
190 CONTINUE
200 CONTINUE

C0 = WHE3(WDEPTH) * WE(WDEPTH) * 2
X1 = XO * SUMHE2(WDEPTH)
X1T = XO * DSHE2(WDEPTH)
\texttt{X1W=2.0*X1/\text{WE}(\text{WDEPTH})}

\texttt{DO 210 IJ=1,WJ}
\texttt{C=X1*SKK(2,IJ)}
\texttt{E=E*(X1/X1+DSKK(2,IJ))}
\texttt{ETA(IJ)=ETA(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{ETAM(IJ)=ETAM(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{CBI(IJ)=CBI(IJ)+C}
\texttt{CBIT(IJ)=CBIT(IJ)+C*(X1/X1+DSKK(2,IJ))}
\texttt{ETAM(IJ)=ETAM(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{ETAM(IJ)=ETAM(IJ)+E*(X1/X1+DSKK(2,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(2,IJ))}

\texttt{DO 220 IJ=1,WJ}
\texttt{C=XHE3(\text{WDEPTH})+WE(\text{WDEPTH})+SKK(3,IJ)}
\texttt{E=E*(X1/X1+DSKK(3,IJ))}
\texttt{ETA(IJ)=ETA(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{ETAM(IJ)=ETAM(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{CBI(IJ)=CBI(IJ)+C}
\texttt{CBIT(IJ)=CBIT(IJ)+C*(X1/X1+DSKK(3,IJ))}
\texttt{ETAM(IJ)=ETAM(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{ETAM(IJ)=ETAM(IJ)+E*(X1/X1+DSKK(3,IJ))}
\texttt{ETAT(IJ)=ETAT(IJ)+E*(X1/X1+DSKK(3,IJ))}

\texttt{DO 230 IJ=ITPTRB,ITPTRBE1-1}
\texttt{L=LOWB(IJ)}
\texttt{U=UPBH(IJ)}
\texttt{IT=ITRH(L,U)}
\texttt{FRQO=FRQB(L)-FRQB(U)}
\texttt{DOP=SRT2*FRQO*DOPCOF} 
\texttt{VI=DELQUAD*NOD(IJ-ITPTRB,IQUAD)*SRT} 
\texttt{SIGNA=PIE2NC*OSCBE1(IT)*EIP(-VI)*VI)/DOP/1.7724539} 
\texttt{SIGNAT=(VI*VI-0.5)/\text{TEMP}(\text{WDEPTH})} 
\texttt{E=GB(L)*SIGNA\quad(\text{U,\text{WDEPTH})}} 
\texttt{C=SIGNA\quad(\text{L,\text{WDEPTH})}} 
\texttt{ETA(IJ)=ETA(IJ)+E} 
\texttt{CBI(IJ)=CBI(IJ)+C} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 

\texttt{DO 240 IJ=ITPTRBE1,ITPTRBE2-1}
\texttt{L=LOWBE1(IJ)}
\texttt{U=UPBE1(IJ)}
\texttt{IT=ITREH(L,U)}
\texttt{FRQO=FRQBE1(L)-FRQBE1(U)}
\texttt{DOP=SRT2*FRQO*DOPCOF*0.5} 
\texttt{VI=DELQUAD*NOD(IJ-ITPTRBE1,IQUAD)*SRT} 
\texttt{SIGNA=PIE2MC*OSCE1(IT)*EXP(-VI)*VI)/DOP/1.7724539} 
\texttt{SIGNAT=(VI*VI-0.5)/\text{TEMP}(\text{WDEPTH})} 
\texttt{E=GB(L)*SIGNA\quad(\text{U,\text{WDEPTH})}} 
\texttt{C=SIGNA\quad(\text{L,\text{WDEPTH})}} 
\texttt{ETA(IJ)=ETA(IJ)+E} 
\texttt{CBI(IJ)=CBI(IJ)+C} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]} 
\texttt{ETAT(IJ)=ETAT(IJ)+E*SIGNAT/(\text{TEMP}(\text{WDEPTH})]}
E = GBE(L) \times \Sigma \times \text{IBE}(U, IDEPTB) / GBE(U)
C = \Sigma \times \text{IBE}(L, IDEPTB)
\eta(I,J) = \eta(I,J) + E
\text{CB}(I,J) = \text{CB}(I,J) + C
\eta(I,J) = \eta(I,J) + E \times (\Sigma + \text{SBB}(U, IDEPTB))
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(L, IDEPTB))
\eta(I,J) = \eta(I,J) + E / \text{IE}(IDEPTB)
\eta(I,J) = \eta(I,J) + E \times (\Sigma + \text{SBB}(U, IDEPTB)) / \text{IBE}(1, IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C / \text{IE}(IDEPTB)
\eta(I,J) = \eta(I,J) + E \times (\Sigma + \text{SBB}(L, IDEPTB)) / \text{IBE}(1, IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(U, IDEPTB)) / \text{IBE}(1, IDEPTB)
\eta(I,J) = \eta(I,J) + E \times \text{IE}(IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(L, IDEPTB)) / \text{IBE}(1, IDEPTB)
\eta(I,J) = \eta(I,J) + E \times \text{IE}(IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(U, IDEPTB)) / \text{IBE}(1, IDEPTB)
\eta(I,J) = \eta(I,J) + E \times \text{IE}(IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(L, IDEPTB)) / \text{IBE}(1, IDEPTB)
\eta(I,J) = \eta(I,J) + E \times \text{IE}(IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(U, IDEPTB)) / \text{IBE}(1, IDEPTB)
\eta(I,J) = \eta(I,J) + E \times \text{IE}(IDEPTB)
\text{CB}(I,J) = \text{CB}(I,J) + C \times (\Sigma + \text{SBB}(L, IDEPTB)) / \text{IBE}(1, IDEPTB)
\eta(I,J) = \eta(I,J) + E \times \text{IE}(IDEPTB)
ETAM(IJ) = ETAM(IJ) * VX

CONTINUE

LOWER BOUNDARY SUMS

BSUM = 0.0
BSUN = 0.0
BSUNT = 0.0
DO 280 IJ = 1, N

VX = WT(IJ) * BBT(FREQ(IJ), TEMP(WDEPTB)) / CBI(IJ)
BSUM = BSUM + VX
BSUM = BSUM + VX / CHI(IJ)
BSUN = BSUN + VX * CHI(IJ)
BSUNT = BSUNT + VX * CHI(IJ) * WT(IJ) *:

BBT(FREQ(IJ), TEMP(WDEPTB)) / CHI(IJ)

CONTINUE
RETURN
END

SUBROUTINE LTESTEP(ERR)

SUBROUTINE TO PERFORM LTE RYBICKI STEP.

IMPLICIT NONE

PLIST
BLANK
ROOT

INTEGER INDX(2*MIDPTB)
INTEGER I, J, K
REAL CHIN(MIDPTB), CHIT(MIDPTB)
REAL DWTUW(MIDPTB), DWTUTT(MIDPTB)
REAL ETAK(MIDPTB), ETAT(MIDPTB)
REAL MB(2*MIDPTB,2*MIDPTB), ML(2*MIDPTB)
REAL MW(2*MIDPTB), MWE(MIDPTB, MWEPTB)
REAL MV(MIDPTB, MIDPTB), NV(MIDPTB, MIDPTB)
REAL NK(2*NIDPTB)
REAL BSUN, BSUM, BSUMT, DET, DTC, DTM, DTP
REAL ERR, FLUX, MW, MW
REAL EDDFAC, LIISLV, LSTATE, GEIER

EXTERNAL EDDFAC, LIISLV, LSTATE, GENER

STATEMENTS

CALL DWTUW(DWTUW, DWTUWT, BSUN, BSUN, BSUNT)
FLUX = 0.
DO 20 I = 1, NDEPTB
ML(I) = 0.0
DO 10 J = 1, NDEPTB
MS(J) = 0.0
10 CONTINUE
20 CONTINUE

SOLVE TRANSFER EQUATION AND CALCULATE DERIVATIVES AT EACH FREQUENCY

DO 280 IJ = 1, N
CALL GENER(IJ, ETAM, ETAT, CHIN, CHIT)
CALL EDDFAC(IJ)
DO 40 I = 1, NDEPTB
MS(I) = 0.0
DO 30 J = 1, NDEPTB
MWE(I, J) = 0.0
NV(I, J) = 0.0
30 CONTINUE
CONTINUE
  RH01=MN(1)*MYHD
  RH01=(DTOTM(1)-1.0)*MYHD+MU
  OMEGA1=CHI(1)/RH01
  OMEGA1=CHI(1)/RH01-OMEGA1*RHO1/RH01
  OMEGA1=CHI(1)/RH01-OMEGA1*RHO1/RH01
  OMEGA2=CHI(2)/RH02
  OMEGA2=CHI(2)/RH02-OMEGA2*RHO2/RH02
  DTP=0.5*(OMEGA1+OMEGA2)*M(2)
  VALPHA=(FK(2)/RAD(2)-FK(1)/RAD(1))/DTP
  S=(ETAT(1)-S*CHI(1)/CHI(1))/CHI(1)
  ST=(ETAT(1)-S*CHI(1)/CHI(1))/CHI(1)
  VB=(VALPHA*0.5*DTP*(RAD(1)-S)+DTP/VALPHA)
  NT(1,2)=FK(1)/DTP-FB*0.5*(1.0-SIGE*WE(1))/CHI(1)
  NT(1,3)=FK(2)/DTP
  MUE(1,1)=FB+OMEGA1+0.5*DTP+ST
  MUE(1,2)=FB+OMEGA2
  NV(1,1)=FB+OMEGA1+0.5*DTP+ST
  NV(1,2)=FB+OMEGA2
  DO 50 ID=2,NDPTB-1
  DTM=DTP
  RH03=MN(ID+1)*MYHD
  RH03=(DTOTM(ID+1)-1.0)*MYHD+MU
  OMEGA3=CHI(ID+1)/RH03
  OMEGA3=CHI(ID+1)/RH03-OMEGA3*RHO3/RH03
  DTP=0.5*(OMEGA3+OMEGA2)*M(ID+1)
  DTM=DTP
  VALPHA=(FK(ID)/RAD(ID)-FK(ID-1)/RAD(ID-1))/DTP
  VGAMMA=(FK(ID)/RAD(ID)-FK(ID+1)/RAD(ID+1))/DTP
  V=VALPHA+VGAMMA
  VA=VALPHA+0.5*V/DTM/DTP
  VC=VGAMMA+0.5*V/DTM/DTP
  VB=VA+VC
  MK(ID)=FB+RAD(ID)-WE(ID)*S*CHI(ID)/CHI(ID)
  NT(ID,1)=FK(ID-1)/DTP/DTC
  NT(ID,2)=(FK(ID)/DTC+1.0-WE(ID)*S*CHI(ID))/CHI(ID)
  NT(ID,3)=FK(ID+1)/DTP/DTC
  MUE(ID,1)=FB+OMEGA1
  MUE(ID,2)=FB+OMEGA2
  MUE(ID,3)=FB+OMEGA3
  MUE(ID,1)=FB+OMEGA1
  MUE(ID,2)=FB+OMEGA2
  MUE(ID,3)=FB+OMEGA3
  MV(ID,ID)=FB+OMEGA2
  MV(ID,ID)=FB+OMEGA2
  MV(ID,ID)=FB+OMEGA3
  MV(ID,ID)=FB+OMEGA2
  MV(ID,ID)=FB+OMEGA2
  MV(ID,ID)=FB+OMEGA3
  CONTINUE
  DTM=DTP
  ID=DEPTB
  VALPHA=(FK(ID)/RAD(ID)-FK(ID-1)/RAD(ID-1))/DTP
  VB=VALPHA
  VC=0.5*BBT(FREQ(IJ),TEMPIP(IDC))/CHI(IDC)/BSUM
  MK(ID)=VC+VALPHA
MT(ID,1) = -FK(ID)/DTN
MT(ID,2) = FK(ID)/DTM
MUE(ID,ID-1) = VB • OMEGA11
MUE(ID,ID) = VB • OMEGA21 + VC • (CBi(ID)/CBI(ID) + BSUMI/BSUM)
MV(ID,ID-1) = VB • OMEGA1T
MV(ID,ID) = VB • OMEGA2T - VC • (BBT(FREQ(IJ), TEIIP(ID))/BBT(FREQ(IJ), TEMP(ID)) - CBIT(ID)/CBI(ID) - BSUMT/BSUM)
MT(1,3) = MT(1,3)/MT(1,2)
MV(1,1) = MV(1,1)/MT(1,2)
MV(1,2) = MV(1,2)/MT(1,2)
MUE(1,1) = MUE(1,1)/MT(1,2)
MUE(1,2) = MUE(1,2)/MT(1,2)
MK(1) = MK(1)/MT(1,2)
MT(2,2) = MT(2,2) - MT(2,1) • MT(1,3)
MV(2,1) = MV(2,1) - MT(2,1) • MV(1,1)
MV(2,2) = MV(2,2) - MT(2,1) • MV(1,2)
MUE(2,1) = MUE(2,1) - MT(2,1) • MUE(1,1)
MUE(2,2) = MUE(2,2) - MT(2,1) • MUE(1,2)
MK(2) = MK(2) - MK(1) • MT(2,1)
DO 80 J = 2, NDEPTH - 1
MT(J,3) = MT(J,3)/MT(J,2)
MV(J,1) = MV(J,1)/MT(J,2)
MV(J,2) = MV(J,2)/MT(J,2)
MUE(J,1) = MUE(J,1)/MT(J,2)
MUE(J,2) = MUE(J,2)/MT(J,2)
MK(J) = MK(J)/MT(J,2)
MK(J) = MK(J) - MK(1) • MK(J)
DO 70 K = 1, J + 1
MV(J+1,K) = MV(J+1,K) - MT(J+1,1) • MV(J,K)
MUE(J+1,K) = MUE(J+1,K) - MT(J+1,1) • MUE(J,K)
MK(J+1) = MK(J+1) - MT(J+1,1) • MK(J)
80 CONTINUE

CONTINUE
DO 90 J = 1, NDEPTH
MV(IDEPTB,J) = MV(IDEPTB,J)/MT(IDEPTB,2)
MUE(IDEPTB,J) = MUE(IDEPTB,J)/MT(IDEPTB,2)
MK(IDEPTB) = MK(IDEPTB)/MT(IDEPTB,2)
90 CONTINUE

C RADIATION FIELD DERIVATIVES OF HYDROSTATIC EQUATION
C
MI = M(1) • (4 • PI/CC) • WT(IJ) • CBI(1) • FB/IM(1)/MBYD
DO 120 K = 1, NDEPTH
MB(1,K+IDEPTB) = MB(1,K+IDEPTB) - MX • MV(1,K)
MB(1,K) = MB(1,K) - MX • MUE(1,K)
120 CONTINUE
ML(1) = ML(1) - MX • MK(1)
MI = FK(1) • WT(IJ) • (4 • PI/CC)
DO 150 J = 2, NDEPTH
DO 130 K = 1, NDEPTH
MB(J,K) = MB(J,K) - MX • MUE(J,K)
MB(J,K+IDEPTB) = MB(J,K+IDEPTB) - MX • MV(J,K)
130 CONTINUE
ML(J) = ML(J) - MX • MK(J)
MI = FK(J) • WT(IJ) • (4 • PI/CC)
DO 140 K = 1, NDEPTH
MB(J,K) = MB(J,K) - MX • MUE(J,K)
MB(J,K+IDEPTB) = MB(J,K+IDEPTB) - MX • MV(J,K)
140 CONTINUE
ML(J) = ML(J) - MX • MK(J)
150 CONTINUE
C RADIATION FIELD DERIVATIVES OF CONSTRAINT OF RADIATIVE EQUILIBRIUM
C
DO 170 J = 1, NDEPTH
MW • WT(IJ) • CHI(I) • WE(J) • SIGE
DO 160 K = 1, NDEPTH
MB(J,K+IDEPTB) = MB(J,K+IDEPTB) - MW • MUE(J,K)
MB(J,K) = MB(J,K) - MW • MK(J)
160 CONTINUE
ML(J) = ML(J) - MW • MK(J)
170 CONTINUE
**RADIATIVE EQUILIBRIUM**

```fortran
DO 180 ID = 1, IDEPTH
   ML(ID+IDEPTB) = ML(ID+IDEPTB) + WT(IJ) • (ETA(ID) - (CHI(ID) - IE(ID) • SIGE) • RAD(ID))
   NB(ID+IDEPTB, ID) = NB(ID+IDEPTB, ID) - WT(IJ) • (ETA(ID) - (CHI(ID) - SIGE) • RAD(ID))
   NB(ID+IDEPTB, ID+IDEPTB) = NB(ID+IDEPTB, ID+IDEPTB) - WT(IJ) • (ETA(ID) - (CHI(ID) - SIGE) • RAD(ID))
180 CONTINUE

**HYDROSTATIC EQUILIBRIUM**

```fortran
RH01 = NH(1) • NHYD
RH01 = (DITOT(1) - 1.0) • NHYD • MU
RHO1 = DITOT(1) • NHYD • MU
VA = (4. • PI/CC) • M(1) • WT(IJ) • FB • RAD(1) • CHI(1) / RH01
ML(1) = ML(1) - VA
NB(1,1) = NB(1,1) + VA • (CH1(1) / CH(1) - RB01 / RH01)
NB(1,1+IDEPTB) = NB(1,1+IDEPTB) + VA • (CH1(1) / CH(1) - RB01 / RH01)
DO 190 ID = 2, IDEPTH
   ML(ID) = ML(ID) - (4. • PI/CC) • WT(IJ) • (FK(ID) • RAD(ID) - FK(ID-1) • RAD(ID-1))
190 CONTINUE
```

**SURFACE FLUX CHECK**

```fortran
WRITE (6,1000) FLUX, HO
```

**SOLVE THE SYSTEM OF EQUATIONS**

```fortran
CALL LINSOL(NB, NL, NK, 2•IDEPTB, 2•NIDEPTB)
```

**SCALE DOWN CORRECTIONS IF VERY LARGE TO IMPROVE HYPERCIRCLE OF CONVERGENCE**

```fortran
VA = MIN(0.95, 0.1 / ERR)
WRITE (6,*)
WRITE (6,1001)
```

**END**

1000 FORMAT (' CALCULATED FLUX IS ', E12.5, /
          ' EXPECTED FLUX IS ', E12.5)
1001 FORMAT ('TEMPERATURE AND ELECTRON DENSITY STRATIFICATION AND ERRORS:')
SUBROUTINE WURATE(LHS,LW,LT,RHS,RM,RT,ID)

CALCULATE THE RATE MATRIX FOR PSEUDO-LTE GIVEN DEPARTURE COEFFICIENTS, TEMPERATURE, AND ELECTRON DENSITY

IMPLICIT NONE

PLIST
ROOT
ROOTI
SEGHR

INTEGER I, ID, IL, J, L, U
REAL LS((NNNN,NNNN), LM(NNNN,NNNN), LT(NNNN,NNNN)
REAL RS(NNNN), RM(NNNN), RT(NNNN)

REAL SB, SBHE1, SBHE2, SBHE1T, SBHE2T

SB(I,T)=ACCOF•GB(I)•EXP(BK•FBQB(I)/T)/T/SQRT(T)
SBT(I,T)=-(BK•FBQB(I)/T+1.5)/T
SBHE1(I,T)=ACCOF•GBE1(I)•EXP(BK•FBQBE1(I)/T)/T/SQRT(T)/2.
SBHE1T(I,T)=-(BK•FBQBE1(I)/T+1.5)/T
SBHE2(I,T)=ACCOF•GBE2(I)•EXP(BK•FBQBE2(I)/T)/T/SQRT(T)
SBHE2T(I,T)=-(BK•FBQBE2(I)/T+1.5)/T

C START OF EXECUTABLE STATEMENTS

C PARTITION FUNCTIONS

SUMH(ID)=0.0
DSHDT>ID)=0.0
DO 10 IL=1,MQH
  VIX=SBH(Il,TEMP(ID))
  VIT=VIX•SBHET(Il,TEMP(ID))
  SUMH(ID)=SUMH(ID)+VIX
  DSHDT(ID)=DSHDT(ID)+VIT
10 CONTINUE

SUMBE1(ID)=0.0
DSBE1(ID)=0.0
DO 20 IL=1,MQHE1
  VIX=SBHE1(Il,TEMP(ID))
  VIT=VIX•SBHE1T(Il,TEMP(ID))
  SUMBE1(ID)=SUMBE1(ID)+VIX
  DSBE1(ID)=DSBE1(ID)+VIT
20 CONTINUE

SUMBE2(ID)=0.0
DSBE2(ID)=0.0
DO 30 IL=1,MQH+2
  VIX=SBHE2(Il,TEMP(ID))
  VIT=VIX•SBHE2T(Il,TEMP(ID))
  SUMBE2(ID)=SUMBE2(ID)+VIX
  DSBE2(ID)=DSBE2(ID)+VIT
30 CONTINUE

DO 50 I=1,MNNN
  RBS(I)=0.0
  RM(I)=0.0
  RT(I)=0.0
  DO 40 J=1,NNNN
    LHS(I,J)=0.0
    LM(J,I)=0.0
    LT(I,J)=0.0
40 CONTINUE
50 CONTINUE

C PARTICLE CONSERVATION

RBS(1)=WE(ID)
RM(1)=1.0
LHS(1,IMPRT)=1.
LHS(1,IMPRT)=MU1+(1.+WE(ID)•SUMH(ID))
LM(1,IMPRT)=MU1•SUMH(ID)
LT(1,IMPRT)=MU1•WE(ID)•DSHDT(ID)

C CHARGE CONSERVATION EQUATION

RBS(2)=WE(ID)
RM(2)=1.0
LHS(2,IMPRT)=1.0
LHS(2,IIBE3)=2.0+WE(ID)*SUMHE2(ID)
LW(2,IIBE3)=SUMHE2(ID)
LT(2,IIBE3)=WE(ID)*OSHE2(ID)

STATISTICAL EQUILIBRIUM

SINGLY-IONIZED HELIUM

LW(3,IIBE3)=SBHE2(1,TEMP(ID))
LHS(3,IIBE3)=LW(3,IIBE3)*WE(ID)
LT(3,IIBE3)=LHS(3,IIBE3)*SBHE2T(1,TEMP(ID))
LBS(3,IIBE3)=1.0

HELIUM ABUNDANCE EQUATION

LHS(4,IIME3)=WE(ID)+SUMHE1(ID)+1.0
LW(4,IIME3)=SUMHE1(ID)
LT(4,IIME3)=WE(ID)+OSHE1(ID)
LHS(4,IIME3)=WE(ID)+SUMHE2(ID)+1.0
LW(4,IIME3)=SUMHE2(ID)
LT(4,IIME3)=WE(ID)+OSHE2(ID)
LHS(4,IIPROT)=-Y•(1.0+WE(ID)*SUMB(ID))
LW(4,IIPROT)=-Y•SUMB(ID)
LT(4,IIPROT)=-Y•WE(ID)+DSHDY(ID)
RETURN
END

SUBROUTINE PUTOUT(TEFF,Z)
WRITE OUT A COMPLETED MODEL TO DISK

IMPLICIT NONE
PLIST ROOT ROOTI
LOCAL VARIABLES
LOGICAL .LIES
INTEGER I, ID, IL
REAL ABUID(92)
REAL T, TEFF, Z

START OF EXECUTABLE STATEMENTS
PREVIOUS OUTPUT LINES WERE ALREADY TAKEN CARE OF IN SETUP
WRITE (12,1007)(M(ID),TEIIP(ID),ITOT(ID),IE(ID),ID=1,IDEPTB)
BYDROGEI OCCUPATION IUMBERS
WRITE (12,1005)0,0,5,ITRB
WRITE (12,1006)(FRQB(IL),IL=1,5)
DO 10 IL=1,ITRB
WRITE (12,1005)LOWERB(IL),UPPERB(IL)
10 CONTINUE
HELIUM OCCUPATION NUMBERS
WRITE (12,1005)2
WRITE (12,1006)0,0,19,ITRBE1,10,ITRBE2
WRITE (12,1006)(FRQBE1(IL),IL=1,19)
DO 20 IL=1,ITRBE1
WRITE (12,1005)LOWERBE1(IL),UPPERBE1(IL)
20 CONTINUE
WRITE (12,1006)(FRQBE2(IL),IL=1,10)
DO 30 IL=1,ITRBE2
WRITE (12,1005)LOWERBE2(IL),UPPERBE2(IL)
30 CONTINUE
HELIUM OCCUPATION NUMBERS
WRITE (12,1005)2
WRITE (12,1005)0,0,19,TRHE1,10,TRHE2
WRITE (12,1006)(FRQHE1(IL),IL=1,19)
DO 20 IL=1,TRHE1
WRITE (12,1005)LOWERHE1(IL),UPPERHE1(IL)
20 CONTINUE
WRITE (12,1006)(FRQHE2(IL),IL=1,10)
DO 30 IL=1,TRHE2
WRITE (12,1005)LOWERHE2(IL),UPPERHE2(IL)
30 CONTINUE
WRITE (12,1006)(((HE1(IL,ID),IL=1,19),(HE2(IL,ID),IL=1,10),(HE3(ID),ID=1,NDEPTB))
WRITE (12,1005)0
WRITE (12,1005)0
RETURN

FORMAT STATEMENTS

1005 FORMAT (16I5)
SUBROUTINE SETUP(IITER,TEFF,Z)
READ IN THE APPROXIMATE MODEL MAKE ALL INITIAL CALCULATIONS
IMPLICIT NONE
PLIST ROOT ROOTI
LOCAL VARIABLES
CHARACTER*80 HEADER
INTEGER I, ID, II, IL, IT, J, NO, N1, N2, N3, N4, N5, NITER
REAL ALPH, BET!, CO!, COll1, DOP, DUMMY, FCOI, FRQ3, GLOG, T
REAL TEFF, VI, Z, SRT
TABLE OF ATOMIC WEIGHTS
REAL WEIGHT(92)
DATA WEIGHT/1.0,4.0,6.9,9.0,10.8,12.0,14.0,16.0,19.0,20.2,23.0,
: 24.3,27.0,28.1,31.0,32.1,35.5,39.9,40.1,45.0,47.9,50.9,52.0,
: 54.9,55.8,58.9,58.7,63.5,65.4,69.7,72.6,74.9,79.0,79.9,83.8,85.5,
: 87.6,88.9,91.2,92.9,95.9,98.9,101.1,102.9,106.4,107.9,112.4,
: 114.8,116.7,121.6,127.6,126.9,131.3,132.9,137.3,138.9,140.1,
: 140.9,144.2,145.0,150.4,152.0,157.3,158.9,162.5,164.9,167.3,
: 168.9,173.0,175.0,180.9,183.9,186.2,190.2,192.2,195.1,
: 197.0,200.6,204.4,207.2,209.0,209.0,210.0,222.0,223.0,226.0,
: 227.0,232.0,231.0,238.0/
TABLE GIVING QUANTUM NUMBER OF ACTIVE ELECTRON OF EACH NEUTRAL HELIUM STATE TREATED BY THE PROGRAM
INTEGER Q(25)
DATA Q/1,4*2,6*3,8*4,5,6,7,8,9,10/
EXTERI!L PROCEDURES
REAL EXIT, HEG!UIT, G!UIT, SB, SBHE1, SBHE2, HMINUS
EXTERNAL EXIT, HEG!UIT, G!UIT, HMINUS
LOCAL STATEMENT FUNCTIONS
THESE FUNCTIONS GIVE ACTIVITIES OF THE VARIOUS STATES OF HYDROGEN (SB), NEUTRAL HELIUM (SBHE1), AND IONIZED HELIUM (SBHE2).
SB(I,T)=ACCF*GH1(I)*EXP(BK*FRQH(I)/T)/T/SQRT(T)
SBHE1(I,T)=ACCF*GHE1(I)*EXP(BK*FRQHE1(I)/T)/T/SQRT(T)/2.
SBHE2(I,T)=ACCF*GHE1(I)*EXP(BK*FRQHE2(I)/T)/T/SQRT(T)
START OF EXECUTABLE STATEMENTS
WRITE (6,*)'LTE MODEL CALCULATION PROGRAM'
READ COMMENT LINE OF INPUT MODEL
READ (5,1001)HEADER
WRITE (6,1001)HEADER
WRITE (12,1001)'LTE MODEL WITHOUT LINES'
READ BASIC MODEL PARAMETERS
READ (5,1002)TEFF,TLINE,GLOG,Y,Z,NITER
WRITE (12,1002)TEFF,TLINE,GLOG,Y,Z,NITER,-1,0,0
CALCULATE EDDINGTON FLUX AND SURFACE GRAVITY FROM PARAMETERS
BO=5.6692E-5*TEFF**4/12.5663708
GRAV=EXP(2.302585093*GLOG)
WRITE (6,1003)TEFF,TLINE,GLOG,Y,Z,NITER
READ COMPOSITION, WHICH TAKES THE FORM OF LOG NUMBER RELATIVE TO HYDROGEN=12.0
C
READ (5,1004) ABUND
WRITE (12,1004) ABUND
C
CALCULATE MEAN MOLECULAR WEIGHT (MU) AND NUCLEI PER PROTON (MU1)
C
MU=1.0+4.0*Y
MU1=1.0+Y
DO 10 I=3,92
   VI=1.0E-12*EXP(2.302585093*ABUND(I))*Z
   MU=MU+VI*WEIGHT(I)
   MU1=MU1+VI
10 CONTINUE
MU=MU/MU1
C
C READ NUMBER OF DEPTH POINTS AND FREQUENCIES
C AND THEN READ THE FREQUENCIES
C
READ (5,1005) NDEPTHS, NJ
READ (5,1006)(FREQ(IJ), IJ=1,NJ)
WRITE (12,1005) NDEPTHS, NJ
WRITE (12,1006)(FREQ(IJ), IJ=1,NJ)
C
C CALCULATE FREQUENCY QUADRATURE WEIGHTS
C NO CORRECTION IS MADE FOR LINES; I.E. IT IS
C ASSUMED THAT THE LINES ARE NARROW.
C
DO 20 IJ=1,NJ
   WT(IJ)=0.0
20 CONTINUE
C
C READ IN FREQUENCY INTERVAL NUMBER AND RULE
C
READ (5,1005) IO, I1
WRITE (12,1005) IO, I1
IF (IO.EQ.2) THEN
   C TRAPEZOIDAL RULE: I1 IS NUMBER OF FIRST FREQUENCY
   VI=0.5*ABS(FREQ(I1)-FREQ(I1+1))
   WT(I1)=WT(I1)+VI
   WT(I1+1)=WT(I1+1)+VI
   GO TO 30
ELSE IF (IO.EQ.3) THEN
   C SIMPSON'S RULE; I1 IS NUMBER OF CENTRAL FREQUENCY
   **NOTE THAT NO CHECK IS MADE TO BE SURE THAT THE
   TWO FREQUENCY SUBINTERVALS ARE EQUAL, AS THEY NEED
   TO BE.**
   VI=ABS(FREQ(I1+1)-FREQ(I1-1))/6.0
   WT(I1+1)=WT(I1+1)+VI
   WT(I1-1)=WT(I1-1)+VI
   WT(I1)=WT(I1)+4.0*VI
   GO TO 30
ELSE IF (IO.NE.0) THEN
   C PROGRAM DOESN'T RECOGNIZE THE RULE
   WRITE (6,*) 'ERROR IN FREQUENCY QUADRATURE RULE'
   CALL EXIT(1)
ENDIF
C
C READ OPACITY RULE AND DISCARD IT
C
READ (5,1005) RULE
WRITE (12,1005) RULE
IF (RULE(2)) THEN
   WRITE (6,*) 'LINES INCLUDED IN MODEL'
ENDIF
C
C READ MODEL
C
READ (5,1007)(M(ID), TEMP(ID), WTOT(ID), WE(ID), ID=1,NDEPTHS)
C
BE SURE MASS VARIABLE IS MASS DIFFERENCE, NOT COLUMN MASS.
THIS IS INDICATED BY LOOKING AT LAST TWO ENTRIES; THE LAST
MASS DIFFERENCE SHOULD ALWAYS BE VERY SMALL.
C
IF (M(NDEPTHS).GT.M(NDEPTHS-1)) THEN
   DO 40 ID=NDEPTHS,2,-1
      M(ID)=M(ID)-M(ID-1)
40 CONTINUE
CONTINUE
ENDIF

READ ATOMIC OCCUPATION NUMBERS

READ (5,1005) I
IF (I.EQ.1) THEN
READ NUMBER OF HYDROGEN LEVELS TO USE FOR EACH IONIZATION.
ALSO READ LINES TO USE.

READ (5,1005) N0, N1, N2, NTRH
IF (N1.NE.0) THEN
WRITE (6,*) 'PLEASE DO NOT SPECIFY ANY H- LINES.'
CALL EXIT(1)
ENDIF

THROW AWAY NEGATIVE HYDROGEN IONIZATION FREQUENCY.

IF (N0.NE.0) THEN
READ (5,1006) CNW
READ NEUTRAL HYDROGEN IONIZATION FREQUENCIES.

READ (5,1006) (FREQ(N), IL=1, N2)
READ LIST OF LINES TO USE FOR HYDROGEN

IF (NTRH.GT.0) THEN
READ (5,1011) (LOWER(N), UPPER(N), IL=1, NTRH)
READ ALL HYDROGEN OCCUPATION NUMBERS.
NEGATIVE HYDROGEN ION OCCUPATION IS THROWN AWAY.

READ (5,1006) ((CNW, IL=1, N0), (N(N), IL=1, N2),
IF (NTRH1.GT.0) THEN
READ (5,1011) (LOWER1(N), UPPER1(N), IL=1, NTRH1)
READ (5,1006) (FREQ1(N), IL=1, N4)
READ (5,1011) (LOWER2(N), UPPER2(N), IL=1, NTRH2)
READ (5,1006) (CNW, IL=1, N0), (N(N), IL=1, N2),

CALCULATE LTE POPULATIONS FOR LEVELS NOT INCLUDED IN APPROXIMATE
INPUT MODEL.

DO 70 ID=1, NDEPTH
DO 60 IL=1, NLEH
W(N, IL) = WPROT(ID)*WE(ID)*SB(IL, TEMP(ID))
CONTINUE
70 CONTINUE
GO TO 50
ELSE IF (I.EQ.2) THEN
TREAT HELIUM THE SAME WAY AS HYDROGEN.

READ (5,1006) NO, N1, N2, NTRHE1, N4, NTRHE2
IF (N1.NE.0) THEN
WRITE (6,*) 'PLEASE DO NOT SPECIFY ANY HE- LINES.'
CALL EXIT(1)
ENDIF
IF (N0.NE.0) THEN
READ (5,1006) CNW
READ (5,1006) (FREQHE1(IL), IL=1, N2)
READ (5,1011) (LOWERHE1(IL), UPPERHE1(IL), IL=1, NTRHE1)
READ (5,1006) (FREQHE2(IL), IL=1, N4)
READ (5,1011) (LOWERHE2(IL), UPPERHE2(IL), IL=1, NTRHE2)
READ (5,1006) ((CNW, IL=1, N0), (NHE1(IL, ID), IL=1, N2,

DO 100 ID=1, NDEPTH
DO 80 IL=1, NLEH
WHE1(IL, ID) = WPROT(ID)*WE(ID)*SBHE1(IL, TEMP(ID))
CONTINUE
80 CONTINUE
GO TO 50
ELSE IF (I.NE.0) THEN
OTHER ELEMENTS INCLUDED BUT NOT WANTED.
PARDOM THE ANACHRONISTIC USE OF THE TERMS "CARDS" AND "DECK." THESE ARE PROBABLY REALLY LINES IN AN EDITOR-CREATED DISK FILE.

WRITE (6,*) 'PLEASE REMOVE HEAVY ION CARDS FROM DECK'
CALL EXIT(1)
ENDIF
C REMAINDER OF DECK IS IGNORED.
C PREPARE PRECALCULATED QUANTITIES.
C
ITPTRH=I+1
ITPTRHE1=ITPTRH
ITPTRHE2=ITPTRH
IF (RULE(2)) THEN
SRT=SQT(TLINE)
ENDIF
C HYDROGEN LINES
C
W1=WTRH
DO 130 IL=1,W1
C GET UPPER AND LOWER LEVEL NUMBERS.
C
I=UPPERH(IL)
J=LOWERH(IL)
IT=ITRH(I,J)
C REJECT LINE IF FORBIDDEN
C
IF (IT.EQ.0) THEN
WRITE (6,*) 'H LINE ',I,' TO ',J,' IS FORBIDDEN.'
GO TO 130
ENDIF
C CALCULATE LINE CENTRAL FREQUENCY AND DOPPLER WIDTH.
C NOTE THAT THIS PROGRAM ASSUMES LINE BROADENING IS DOMINATED
C BY DOPPLER BROADENING.
C
FCO=FQRH(I)-FQRH(J)
DOP=SRT*FCO*DOPCOF
IF (FCO.LE.0) THEN
WRITE (6,*) 'H IONIZATION FREQUENCY ERROR FOR LINE ',
I,' TO ',J,'.'
FCO=-FCO
ENDIF
C ADD FREQUENCIES TO FREQUENCY LIST FOR THE LINE.
C
DO 110 II=1,QUAD
FREQ(II+IJ)=FCO
UPH(II+IJ)=J
LOWH(II+IJ)=I
110 CONTINUE
C CALCULATE WEIGHTS FOR THE LINE FREQUENCIES.
C NOTE THAT SIMPSON'S RULE IS USED; THUS QUAD SHOULD BE ODD.
C
DO 120 I=1,QUAD-2,2
WT(I+IJ)=WT(I+IJ)+2.0*DELQUAD*DOP/3.0
WT(I+IJ+1)=WT(I+IJ+1)+8.0*DELQUAD*DOP/3.0
WT(I+IJ+2)=WT(I+IJ+2)+2.0*DELQUAD*DOP/3.0
120 CONTINUE
C NOW DO ALL THE SAME FOR NEUTRAL AND SIMPLY IONIZED HELIUM.
C
ITPTRHE1=ITPTRH+1
W1=WTRHE1
DO 160 IL=1,W1
J=UPPERHE1(IL)
I=LOWERHE1(IL)
IT=ITRHE1(I,J)
IF (IT.EQ.0) THEN
WRITE (6,*) 'HE1 LINE ',I,' TO ',J,' IS FORBIDDEN.'
GO TO 160
ENDIF
FCO=FQHE1(I)-FQHE1(J)
DOP=SRT*FCO*DOPCOF
IF (FCO.LE.0) THEN
WRITE (6,*) 'HE1 IONIZATION FREQUENCY ERROR FOR LINE ',
I,' TO ',J,'.'
FCO=-FCO
ENDIF
DO 140 II=1,QUAD
FREQ(II+IJ)=FC01
UPHE2(II+IJ)=J
LOWHE2(II+IJ)=I
CONTINUE
DO 150 I=1,NQUAD,2
WT(I+IJ)=WT(I+IJ)+2.0*DELQUAD*DOP/3.0
WT(I+IJ+1)=WT(I+IJ+1)+8.0*DELQUAD*DOP/3.0
WT(I+IJ+2)=WT(I+IJ+2)+2.0*DELQUAD*DOP/3.0
CONTINUE
N0=NBI+NQUAD
CONTINUE
IPTMPHE2=N0+1
N1=NPTRHE2
DO 190 II=1,N1
J=UPPERHE2(II)
I=LOWERHE2(II)
I0=ITRHE2(I,II)
IF (IT.EQ.0) THEN
WRITE (6,*)'HE2 LINE ',I,' TO ',J,' IS FORBIDDEN.'
GO TO 190
ENDIF
FC0W=FRQHE2(II)-FRQHE2(J)
DOP=SRT*FC0W*FC0W0.5
IF (FC0W.LE.0) THEN
WRITE (6,*)'HE2 IONIZATION FREQUENCY ERROR FOR LINE ',
I1',',I',',J'
FC0W=-FC0W
ENDIF
DO 170 II=1,NQUAD
FREQ(II+N0)=FC0W
UPHE2(II+N0)=J
LOWHE2(II+N0)=I
CONTINUE
DO 180 I=1,NQUAD-2,2
WT(I+IJ)=WT(I+IJ)+2.0*DELQUAD*DOP/3.0
WT(I+IJ+1)=WT(I+IJ+1)+8.0*DELQUAD*DOP/3.0
WT(I+IJ+2)=WT(I+IJ+2)+2.0*DELQUAD*DOP/3.0
CONTINUE
ENDIF
IF (IJ.GT.N0) THEN
WRITE (6,*)
'TOO MANY FREQUENCY POINTS'
CALL EXIT(1)
ENDIF
WRITE (6,*)' TOO MANY FREQUENCY POINTS = ',N0
IF (RULE(1)) THEN
DO 200 II=1,N0
IF (FC0W.GT.FRQHE2(II)) SIGHE2(I,II)=0.
IF (FC0W.GT.FRQHE2(II)) SIGHE2(I,II)=N0.*GAUWT(I,FC0W,FC0W)/FLOAT(I)**5
200 CONTINUE
ENDIF
C BOUND-FREE CROSS SECTIONS
C DO 240 IJ=1,N0
FC0W=FRQH(IJ)
FRQ3=FC0W**3
COM=2.815E29/FRQ3
COM1=FC0W/4.0
DO 210 I=1,NLHE2
SIGHE2(I,IJ)=0.
IF (FC0W.GT.FRQHE2(IJ))
SIGHE2(I,IJ)=16.*COM*GAUWT(I,COM1)/FLOAT(I)**5
210 CONTINUE
DO 220 I=1,NLHE1
SIGHE1(I,IJ)=0.
IF (FC0W.GT.FRQHE2(IJ))
SIGHE1(I,IJ)=COM*HEGAWT(I,FC0W)/FLOAT(W(I))***5
220 CONTINUE
DO 230 I=1,NLH
SIG(I,IJ)=0.
IF (FC0W.GT.FRQH(I)) SIG(I,IJ)=COM*GAUWT(I,FC0W)/FLOAT(QW(I))***5
230 CONTINUE
SIG(NLH+1,IJ)=3.69E8/FRQ3
240 CONTINUE
C DETERMINE CUTOFF FREQUENCIES FOR FREE-FREE OPAcity.
C THESE ALLOW THE INCLUSION OF BOUND LEVELS ABOVE THOSE
C ACCOUNTED FOR EXPLICITLY AS PART OF THE FREE-FREE OPAcity.
DO 250 IJ=1,IJ
FF(IJ,1)=MIN(FRQH(WLH)*(MQH/(MQH+1))**2,FREQ(IJ))
FF(IJ,2)=MIN(FRQHE1(WLHE1)*(MQHE1/(MQHE1+1))**2,FREQ(IJ))
FF(IJ,3)=MIN(FRQHE2(WLHE2)*(2*MQH/(2*MQH+1))**2,FREQ(IJ))
250 CONTINUE
C
C CALCULATE AUAER/MIHANAS PSEUDO HEAVY PARTICLE DENSITY
C
DO 260 ID=1,IDEPTH
IM(ID)=MU•(ITOT(ID)-IE(ID))
260 CONTINUE
RETURN
C
1001 FORMAT (A80)
1002 FORMAT (F9.0,F8.2,F8.5,4I5)
1003 FORMAT (' EFFECTIVE TEMPERATURE = ',F9.0,/,': LINE TEMPERATURE = ',F9.0,/,': LOG SURFACE GRAVITY = ',F8.2,/,': HELIUM/HYDROGEN = ',F8.3,/,': Z SCALE FACTOR = ',F8.5,/,': ITERATION LIMIT = ',I5,/)!
1004 FORMAT (8F10.6)
1005 FORMAT (16IS)
1006 FORMAT (4E15.7)
1007 FORMAT (SE15.7)
C
BLOCK DATA TABLES
C
C CONTAINS ALL DATA STATEMENTS FOR COMMON BLOCKS, IN ACCORDANCE
C WITH THE ANSI STANDARD
C
PLIST
ROOTI
C
NEUTRAL HELIUM STATISTICAL WEIGHTS
C
DATA GHE1/1.,3.,1.,9.,3.,3.,3.,1.,9.,3.,1.,9.,3.,1.,9.,3.,1.,9.,3.,1./
: 21.,7.,100.,146.,196.,256.,326.,400.,484.,576.,676.,784.,900.,
: 1024. /
C
HYDROGEN/IONIZED HELIUM STATISTICAL WEIGHTS
C
: 1352.,1456.,1568.,1682.,1800.,1922.,2048. /
C
HYDROGENIC OSCILLATOR STRENGTHS
C
DATA OSCB/4.162E-1,7.910E-2,2.899E-2,1.394E-2,6.408E-1,1.193E-1,4.467E-2,8.420E-1,1.506E-1,1.038/
C
HYDROGEN TRANSITION MATRIX
C
DATA (ITRH(1,I),I=1,5)/0,1,2,3,4/
DATA (ITRH(2,I),I=1,5)/1,5,1,0,0/
DATA (ITRH(3,I),I=1,5)/0,0,0,0,0/
DATA (ITRH(4,I),I=1,5)/0,0,0,0,0/
DATA (ITRH(5,I),I=1,5)/0,0,0,0,0/
DATA (ITRH(6,I),I=1,5)/0,0,0,0,0/
DATA (ITRH(7,I),I=1,5)/0,0,0,0,0/
DATA (ITRH(8,I),I=1,5)/0,0,0,0,0/
DATA (ITRH(9,I),I=1,5)/0,0,0,0,0/
C
NEUTRAL HELIUM OSCILLATOR STRENGTHS
C
DATA OSCHE1/0.2762.,0.0734.,0.5391.,0.06446.,0.0231.,0.3764.,1514.,
: 0.0507.,0.0693.,0.0900.,0.0118.,0.1250.,0.0480.,0.7110.,0.0034.,
: 0.1220.,0.0960.,0.429.,0.6290.,0.1110.,0.1450.,0.4820.,0.0139.,
: 0.0058.,0.1000.,0.0205.,0.1020.,0.1030.,0.6470.,1.2100.,0.8530.,0.2000./
C
NEUTRAL HELIUM TRANSITION MATRIX
C
DATA (ITRHE1(1,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(8,I),I=1,19)/0,0,0,0,0,22,0,0,0,22,0,23,0,0,0,24,0,30/
DATA (ITRBE1(9,I),I=1,19)/0,0,0,0,15,0,0,0,0,0,25,0,0,0,0,0,26,0,27/
DATA (ITRBE1(10,I),I=1,19)/0,0,0,11,0,0,0,22,0,0,0,0,0,28,0,0,0,29/
DATA (ITRBE1(11,I),I=1,19)/2,0,8,0,0,0,20,0,25,0,0,0,30,0,31,40/
DATA (ITRBE1(12,I),I=1,19)/0,0,0,12,0,0,0,23,0,0,0,0,0,32,0,0,0,30/
DATA (ITRBE1(13,I),I=1,19)/0,0,0,0,16,0,0,0,0,0,30,0,0,0,0,0,33,0,0/
DATA (ITRBE1(14,I),I=1,19)/0,6,0,0,0,19,0,0,0,28,0,32,0,0,0,30,0,0/
DATA (ITRBE1(15,I),I=1,19)/0,0,0,0,17,0,0,0,0,0,31,0,0,0,0,0,0,0,0/
DATA (ITRBE1(16,I),I=1,19)/0,0,0,13,0,0,0,24,0,0,0,0,0,34,0,0,0,0,0/
DATA (ITRBE1(17,I),I=1,19)/0,0,0,0,0,21,0,26,0,0,0,33,0,0,0,0,0,0/
DATA (ITRBE1(18,I),I=1,19)/0,0,0,0,0,0,0,29,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(19,I),I=1,19)/0,0,0,0,0,0,0,0,27,0,0,0,0,0,0,0,0,0/

IONIZED HELIUM OSCILLATOR STRENGTHS

DATA (ITRBE2(1,I),I=1,10)/ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9/
DATA (ITRBE2(2,I),I=1,10)/ 1, 0,10,11,12,13,14,15,16,17/
DATA (ITRBE2(3,I),I=1,10)/ 2,10, 0,18,19,20,21,22,23,24/
DATA (ITRBE2(4,I),I=1,10)/ 3, 11, 18,25,26,27,28,29,30,31/
DATA (ITRBE2(5,I),I=1,10)/ 4,12,19,26,31,32,33,34,35,36/
DATA (ITRBE2(6,I),I=1,10)/ 5,13,20,27,32,36,40,41,43,45/
DATA (ITRBE2(7,I),I=1,10)/ 6,14,21,27,32,36,40,41,43,45/
DATA (ITRBE2(8,I),I=1,10)/ 7,15,22,28,33,37,40,43,45,47/
DATA (ITRBE2(9,I),I=1,10)/ 8,16,23,29,34,38,41,43,45,47/
DATA (ITRBE2(10,I),I=1,10)/9,17,24,30,35,39,42,44,46,49/

NEGATIVE HYDROGEN IONIZATION FREQUENCIES

DATA FRQBN/1.874E14/

IONIZED HELIUM TRANSITION MATRIX

DATA FRQBE1/5.94520E15,1.15305E15,0.957439E15,0.876230E15,0.817746E15,0.519896E15,0.400142E15,0.381976E15,0.362850E15,0.363023E15,0.362480E15,0.240134E15,0.217774E15,0.212670E15,0.202699E15,0.200574E15,0.202703E15,0.199699E15,0.191520E15,0.187737E15,0.182637E15,0.181177E15,0.131592E15,0.128437E15,

NEUTRAL HELIUM IONIZATION FREQUENCIES

DATA FRQBE/13.1520E15,3.28799E15,1.46133E15,0.821997E15,0.528672E15,0.365332E15,0.268407E15,0.254899E15,0.254899E15,0.214375E15,0.205699E15,0.191987E15,0.182637E15,0.173861E15,0.131520E15,0.108694E15,0.093329E15,0.087822E15,0.082199E15,0.077822E15,0.073849E15,0.069345E15,0.064832E15,0.061374E15,0.056382E15,0.051374E15,0.046857E15,0.042437E15,0.038017E15,0.033598E15,0.029179E15,0.024833E15,0.020431E15,0.016037E15,0.011643E15,0.007250E15,0.002857E15,0.000437E15/
C. Program ANDERS

ANDERS is listed in its entirety, except for those routines that are essentially identical to ones in GRAY and LTE and for a very large number of DATA statements in COLRAT, whose inclusion would not contribute to the understanding of the program. The location of the omitted data statements is indicated in the listing. The omitted subroutines are:

- DFRE  (differs from FRE in that the temperature derivative is calculated)
- EDDFAC
- FRE
- GAUNT
- GENER
- HEGAUNT
- HMINUS
- LINSLV
- MATINV

In addition, use is made of the following CRAY FORTLIB routines: CREATE, which creates a file; DESTROY, which deletes a file; USERINFO, which returns information about the user's account and job (it is called here so that disk scratch-file names will be unique); IOSTATUS, which has the effect of halting the CPU until a buffered I/O operation is complete; RDABS and WRABS, which perform a function similar to that of the disk I/O routines employed in the MAH code [36]; and XTENDABS, which is used here to extend the disk scratch files to the proper size.
PROGRAM ANDERS

AN ADAPTATION OF PORTIONS OF THE MIHALAS (1975) CODE TO THE
ANDERSON ALGORITHM FOR THE EFFICIENT SOLUTION OF LARGE NUMBERS OF
TRANSFER EQUATIONS IN NON-LTE.

THIS CODE ALSO Optionally EMPLOYS THE RADIATIVE/COLLISIONAL

PARAMETERS:

PARAMETERS:

MWB  MAXIMUM NUMBER OF FREQUENCY BLOCKS
MD2P  MAXIMUM NUMBER OF DEPTH POINTS
M2J  MAXIMUM TOTAL NUMBER OF FREQUENCIES
M2Jc  MAXIMUM NUMBER OF CONTINUUM FREQUENCY POINTS
MNN  NUMBER OF VARIABLES LINEARIZED
MNTR  MAXIMUM NUMBER OF HYDROGEN TRANSITIONS
MNTRHE1 MAXIMUM NUMBER OF NEUTRAL HELIUM TRANSITIONS
MNTRHE2 MAXIMUM NUMBER OF IONIZED HELIUM TRANSITIONS
Mmax  MAXIMUM QUANTUM NUMBER IN PARTITION SUMS OF HYDROGEN
MNORHE1 MAXIMUM QUANTUM NUMBER IN PARTITION SUMS OF HELIUM I
NEN  TOTAL NUMBER OF ATOMIC STATES
Nquad  NUMBER OF QUADRATURE POINTS PER LINE.
      SINCE SIMPSON'S RULE IS USED, THIS MUST BE ODD.
NLE  NUMBER OF NON-LTE HYDROGEN LEVELS
NLEHE1 NUMBER OF NON-LTE HELIUM LEVELS
NLEHS  TOTAL HELIUM LEVELS
NLEHE2 NUMBER OF NON-LTE IONIZED HELIUM LEVELS
NLEHE2S TOTAL IONIZED HELIUM LEVELS
NLS  TOTAL HYDROGEN LEVELS

ACCOF  Saha ACTIVITY COEFFICIENT
BBCCF  PLANCK FUNCTION COEFFICIENT
CC  VELOCITY OF LIGHT
DELQUAD  FRACTION OF DOPPLER WIDTH PER LINE INTEGRATION INTERVAL
DDPCOF  DOPPLER WIDTH COEFFICIENT
EMASS  ELECTRON MASS
ESU  ELECTRON CHARGE
HK  PLANCK'S CONSTANT OVER BOLTZMANN'S CONSTANT
HP  PLANCK'S CONSTANT
HYDCF  HYDROSTATIC EQUATION RADIATIVE COEFFICIENT
KB  BOLTZMANN'S CONSTANT
MHYD  MASS OF HYDROGEN ATOM
PI  PI
PIE2MC  CLASSICAL ELECTRON ABSORPTION COEFFICIENT
SCOF  RADIATIVE RATE COEFFICIENT
SIE  ELECTRON THOMPSON CROSS SECTION

VARIABLES:

FEXIT  FLAG TO EXIT
FLTE  FLAG TO ASSUME LTE
FPRIIT  FLAG TO PRINT DIAGNOSTICS
FSWITCH  EMPLOY RADIATIVE-COLLISIONAL SWITCHING
RULE  FLAG TO INCLUDE VARIOUS OPACITIES
       ONLY CURRENT USE IS RULE(2) TO INCLUDE LINES

BLOCK  BLOCK ASSIGNMENTS

ITPTRH POINTS TO HYDROGEN LINE FREQUENCIES
ITPTRHE1 POINTS TO NEUTRAL HELIUM LINE FREQUENCIES
ITPTRHE2 POINTS TO IONIZED HELIUM LINE FREQUENCIES
ITR  TRANSITION INDICES FOR HYDROGEN
      I.E. ITR(1) IS TRANSITION INDEX OF
      HYDROGEN L LEVEL TO U LEVEL.
ITRHE1 TRANSITION INDICES OF NEUTRAL HELIUM
ITRHE2 TRANSITION INDICES OF IONIZED HELIUM
LOWH  LOWER LEVEL OF DOMINANT HYDROGEN TRANSITION AT THE
       SPECIFIED FREQUENCY
LOWHE1 " OF NEUTRAL HELIUM
LOWHE2 " OF IONIZED HELIUM
LOWERR LOWER LEVEL OF HYDROGEN TRANSITIONS REQUESTED BY USER
LOWHERHE1 " OF NEUTRAL HELIUM
LOWHERHE2 " OF IONIZED HELIUM
NB  NUMBER OF FREQUENCY BLOCKS
MDP  NUMBER OF DEPTH POINTS
NITER  NUMBER OF ITERATIONS TO MAKE
NJ  NUMBER OF FREQUENCIES
ME  POINTER TO ELECTRON NUMBER IN MATRICES
MW " TO END OF MATRIX
**Compiler Directives:** Numerous short loop directives are present in the program. These assume that $\text{MMNW}$ is less than 64.
CLICHE COMA

INCLUDES PARAMETERS

INTEGER NM, NDMPTE, NJC, MQB, MQHE1, MLB, MLHE1, MLHE2, MLE2, MLE2S, MLEQ, MQUAD
PARAMETER (NM=80, NDMPTE=70, NJC=105, MQB=16, MQHE1=31, MLB=5)
PARAMETER (MLH=19, MLHE1=26, MLE2=10, MLHE2=15, MLHE3=15, MLHE4=10)
PARAMETER (MQUAD=7)

INTEGER NWTR, MNTRHE1, MNTRHE2
PARAMETER (NWTR=10, MNTRHE1=14, MNTRHE2=10)

INTEGER NJ
PARAMETER (NJ=NJ+MQUAD*(NWTR+MNTRHE1+MNTRHE2))

INTEGER NEQW, NWWW
PARAMETER (NEQW=MLH+1+MLE2+MLB+2, NWWW=NM+2)

REAL CC, DELQUAD, EMAS, ESU, HP, KB, MHOY, PI
PARAMETER (CC=2.997925E10, DELQUAD=0.6, EMAS=9.10953E-28)
PARAMETER (ESU=4.8032E-10, HP=6.62618E-27, KB=1.38066E-16)
PARAMETER (MHOY=1.67265E-24, PI=3.141592654)

REAL ACHEF, BHEF, DHEF, HKHE1, HKHE2, HYDHE1, HYDHE2
PARAMETER (ACHEF=2.074E-16, BHEF=2.*HP/(CC*CC), DHEF=4.286E-7)
PARAMETER (HKHE1=HP/KB, HYDHE1=4.*PI/(CC*KB))
PARAMETER (PIE21HE1=PI*ESU*ESU/(EHE1*CC), SCOF=4.*PI/HP)
PARAMETER (SIGHE1=8.*PI*ESU*ESU*ESU*ESU/(3.*EHE1*EMHE1*CC*CC*CC*CC))

INTEGER BLOCK(NM), ITPTRH, ITPTRHE1, ITPTRHE2, IB, IDEMPTE, IITER

LOGICAL FEIIT, FLTE, FPRIIT, FSWITCH, RULE

REAL B(NWWW, NWWW), CHI(NNJ, NM), HO, IE, IE
PARAMETER (B=2.11E-14, CHI=1.0)

REAL DRH(NML+1, NML+1), DRHE1(MLHE1+1, MLHE1+1), DRHE2(MLHE2+1, MLHE2+1)
PARAMETER (DRH=0.0, DRHE1=0.0, DRHE2=0.0)

REAL ETA(NNJ, NM), FF(NNJ, 3), FH(NNJ)
PARAMETER (ETA=0.0, FF=0.0, FH=0.0)

REAL FK(NNJ, NDMPTE), FREQ(NNJ), GRAV, GR, GQ(NWWW), LAMC

REAL LAML, LAMR, M(NDMPTE), MS(NDMPTE), NS(NDMPTE)
REAL NHE1(NLH1, NDMPTE), NHE1S(NLHE1S, NDMPTE), NHE2(NLH2, NDMPTE)
REAL NHE3(NLH3, NDMPTE), NHE4(NLH4, NDMPTE), NHE5(NLH5, NDMPTE)
REAL NH(NDMPTE), NHHE1, NHHE2, NHHE3, NHHE4, NHHE5, NHHE6
REAL RAD(NNJ, NDMPTE), RH(NML+1, NML+1)
REAL RHE1(NLH1+1, NLE2S+1, NLE1+1), RHE2(NLH2+1, NLE2S+1, NLE1+1)
REAL SIG(NLH1+1, NJ), SIGHE1(MLHE1+1), SIGHE2(MLHE2+1)
REAL SIGHE3(MLHE3+1, NJ), SUMH(NDMPTE), SUMHE(NNJ)
REAL TEMP(NDMPTE), TLINE, VS(VNJ), WT(NNJ), Y, ZTOT

COMMON //ITPTRH, ITPTRHE1, ITPTRHE2, BLOCK, IB, IDEMPTE, IITER,
MJ, NW, MNN, MJ, MJ, MTB, MTBE1, MTBE2, FEIIT, FLTE, FPRIIT,
FSWITCH, RULE, Q, G, CH, DRH, DRE1, DRE2,
DSMTE1, DSMTE2, ETA, FF, FB, FK, FREQ, GRAV, GR, GQ, LAMC,
LAML, LAMR, M, NE, NH1, NH1S, NH2, NH2S, NH3, NH4, NH5, NH6,
RS, WTOT, RAD, RE, RHE1, RHE2, SIG, SIGHE1, SIGHE2, SUMH,
SUMHE, TEMP, TLINE, VS, WT, Y, ZTOT

ENDCLICHE

CLICHE COMA

INTEGER ITRB(NML, NMB), ITEBE1(NLH1, NLH1), ITBE2(NLH2, NLHE2)
INTEGER LOWER(MNJ), LOWERHE1(MNJ), LOWERHE2(MNJ)
INTEGER LOWER(NML), LOWER2(NML), UPPER(MNJ), UPPERHE1(MNJ)
INTEGER UPPER2(NMN), FRQHE1(NHE1), FRQHE2(2*MHE1), GQ(NMQ)
REAL GHE1(NMHE1), GHE2(2*MHE1), OSCHE1(34), OSCHE2(46)
EQUIVALENCE (GHE2(1), GQ(1))

COMMON //COMA1/ITRB, ITBR1, ITBE2, LOWER, LOWERHE1, LOWERHE2,
LOWER2, LOWER3, UPPER, UPPERHE1, UPPER2, FRQHE1, FRQHE2, GQ(NMQ)
REAL GHE1(NMHE1), GHE2(2*MHE1), OSCHE1(34), OSCHE2(46)
EQUIVALENCE (GHE2(1), GQ(1))

ENDCLICHE

CLICHE COMDC
REAL AN(NEQW,NEQH), ANS(NEQW), BN(NEQW), CR(NLB,NLB+1)
REAL CRHE1(NLHE1,NLHE1+1), CRHE2(NLHE2,NLHE2+1)
REAL DCRDT(NLB,NLB+1), DCRHE1(NLHE1,NLHE1+1)
REAL DCRHE2(NLHE2,NLHE2+1)

COMMON /COMAN/, ANS, BN, CR, CRHE1, CRHE2, DCRDT, DCRHE1, DCRHE2

ENDCLICHE

C LICHE CONF
REAL A(MWNN,MWWN), C(MWWN,MWWN)

COMMON /CONF/A, C

ENDCLICHE

C LICHE COMM

REAL WTO(MWW)
COMMON /COMM/WTO

ENDCLICHE

PROGRAM AIDERS

C ENTRY POINT
C IMPLICIT NONE

MACRO

C LOCAL VARIABLES

CHARACTER USER*6, !CC*6, DROP*8, SUFFIX*1
INTEGER LENGTH

EXTERNAL PROCEDURES

REAL BLOCKS, CONTROL, CREATE, DESTROY, EXIT, LINK, PUTOUT, SETUP
REAL USERINFO

EXTERNAL BLOCKS, CONTROL, CREATE, DESTROY, EXIT, LINK, PUTOUT
EXTERNAL SETUP, USERINFO

START OF EXECUTABLE STATEMENTS.

C THE FILE input CONTAINS A FIRST-APPROXIMATION MODEL.
C THE FILE output CONTAINS THE MODEL HEREIN CALCULATED.
C THE FILE monitor CONTAINS ALL OTHER OUTPUT.

CALL LINK("UNIT=(input,OPEN,TEXT),UNIT12=(output,CREATE,TEXT),
: UNIT6=(monitor,CREATE,TEXT)//")

READ IN THE FIRST APPROXIMATION AND SET UP EVERYTHING
PREPARATORY TO BEGINNING CALCULATIONS.

CALL SETUP

GET USER SUFFIX (SO THAT SCRATCH FILES CAN BE UNIQUELY NAMED)

CALL USERINFO(USER,ACC,DROP,SUFFIX)

CREATE SCRATCH FILES

LENGTH=MWWN*(MWWN+1)*(NDEPTH-1)
CALL CREATE(9,'%acrr8'/SUFFIX,4,LENGTH)

LENGTH=MWWN*NDEPTH
CALL CREATE(9,'%acrr8'/SUFFIX,4,LENGTH)

SET UP FREQUENCY BINNING.

CALL BLOCKS

ENTER MAIN CONTROL ROUTINE AND CARRY OUT THE CALCULATIONS.

CALL CONTROL
WRITE THE RESULTS.
CALL PUTOUT
DELETE SCRATCH FILES AND EXIT.
CALL DESTROY('xcr8'/SUFFIX)
CALL DESTROY('xcr9'/SUFFIX)
CALL EXIT(0)

SUBROUTINE BLOCKS
SET UP BLOCK ASSIGNMENTS FOR FREQUENCIES

IMPLICIT NONE
MACROS
COMA
COMAI
LOCAL VARIABLES
INTEGER I, I1, I2, I3, ID, IJ, IL, INDI(100), K
REAL DEPTH, RAT
PARAMETER DETERMINING THE MASS RANGE OVER WHICH TO BIN FREQUENCIES.
PARAMETER (MRAT=10.0)
EXTERNAL PROCEDURES
REAL EXIT, GERE, IIDEXI
EXTERNAL EXIT, GERE, IIDEXI
START OF EXECUTABLE STATEMENTS
DO 10 IJ=1,IJ
BLnCK(IJ)=0
CONTINUE
CALCULATE OPACITIES
CALL GERE
CALCULATE DEPTH OF FORMATION FOR EACH FREQUENCY
DO 30 IJ=1,IJ
DEPTH=CHI(IJ,1)*M(1)
DO 20 ID=2,DEPTH
DEPTH=DEPTH+0.5*(CHI(IJ,ID+1)+CHI(IJ,ID))*(M(ID+1)-M(ID))
IF (DEPTH.GT.(2./3.))THEN
VV(IJ)=M(ID)
GO TO 30
ENDIF
CONTINUE
WRITE (6,*)'M.ISS GRID TOO SHALLOW'
CALL EXIT(1)
CONTINUE
CONTINUUM POINTS FIRST
ALL FREQUENCIES IN THE SAME IONIZATION CONTINUUM AND WITH A FORMATION DEPTH WITHIN A FACTOR OF MRAT OF EACH OTHER ARE GROUPED TOGETHER.
WB=1
I2=1
I3=1
DEPTH=VV(I)
DO 40 IJ=1,ITPTRB-1
ARE WE AT THE EDGE OF A NEW IONIZATION CONTINUUM?
IF SO, START A NEW BIN.
NOTE THAT THE PROGRAM ASSUMES THAT ALL HYDROGEN IONIZATION
CONTINUOUS START AT THE SAME FREQUENCIES THAT CORRESPONDING
HELIUM-II CONTINUUM START. (THIS IS VERY NEARLY TRUE.)
HYDROGEN AND HELIUM-II LINE TRANSITIONS, ON THE OTHER HAND,
ARE TREATED AS HAVING NO OVERLAP.

IF (SIGBE1(I2,IJ).EQ.0.AND.SIGHE1(I2,MAX(1,IJ-1)).NE.0) THEN
  WB=WB+1
  DEPTH=VV(IJ)
  I2=I2+1
ELSE
  IF (SIGBE2(I3,IJ).EQ.0.AND.SIGHE2(I3,MAX(1,IJ-1)).NE.0) THEN
    WB=WB+1
    DEPTH=VV(IJ)
    I3=I3+1
ENDIF

SEE IF THE DEPTH OF FORMATION HAS CHANGED ENOUGH TO WARRANT
STARTING A NEW BIN.

RAT=MAX(VV(IJ),DEPTH)/MIN(VV(IJ),DEPTH)
IF (RAT.GT.MRAT) THEN
  WB=WB+1
  DEPTH=VV(IJ)
ENDIF
BLOCK(IJ)=WB

40 CONTINUE
IF (.NOT.RULE(2)) GO TO 260

LINE POINTS
WE DIVIDE THE LINES INTO THREE CLASSES: RESONANCE, LOW
EXCITATION, AND HIGH EXCITATION. THE DIVISIONS ARE SOMEWHAT
ARBITRARY.

RESONANCE LINES FIRST: TREAT EACH LINE SEPARATELY.

IF (ITRBE1.LT.1) GO TO 85
I=ITPTRBE
50 IF (LOWH(I).EQ.1) THEN
  WB=WB+1
  DEPTH=VV(I+IQUAD-1)
  BLOCK(I+IQUAD-1)=WB
  DO 60 IJ=I+IQUAD-2,I,-1
    RAT=MAX(VV(IJ),DEPTH)/MIN(VV(IJ),DEPTH)
    IF (RAT.GT.MRAT) THEN
      WB=WB+1
      DEPTH=VV(IJ)
    ENDIF
    BLOCK(IJ)=WB
    CONTINUE
  I=I+IQUAD
  GO TO 50
ENDIF
I=I
65 IF (ITRBE1.LT.1) GO TO 85
I=ITPTRBE1
70 IF (LOWHE1(I).EQ.1) THEN
  WB=WB+1
  DEPTH=VV(I+IQUAD-1)
  BLOCK(I+IQUAD-1)=WB
  DO 80 IJ=I+IQUAD-2,I,-1
    RAT=MAX(VV(IJ),DEPTH)/MIN(VV(IJ),DEPTH)
    IF (RAT.GT.MRAT) THEN
      WB=WB+1
      DEPTH=VV(IJ)
    ENDIF
    BLOCK(IJ)=WB
    CONTINUE
  I=I+IQUAD
  GO TO 70
ENDIF
I=I
85 IF (ITRBE2.LT.1) GO TO 105

SINCE RESONANCE HELIUM LINES ARE USUALLY ASSUMED TO BE IN DETAILED
BALANCE, LINES FROM THE N=2 LEVEL MAY BE TREATED AS RESONANCE LINES.
The PROGRAM DETERMINES WHETHER OR NOT TO DO THIS BASED ON THE LOW
LEVEL OF THE FIRST HELIUM LINE READ IN.
I=ITPTRBE2
I3=LOWHE2(I)
90 IF (LOWHE2(I).EQ.I3) THEN
   NB=NB+1
   DEPTH=VV(I+IQUAD-1)
   BLOCK(I+IQUAD-1)=NB
   DO 100 IJ=I+IQUAD-2,I,-1
      RAT=MAX(VV(IJ),DEPTH)/MIN(VV(IJ),DEPTH)
      IF (RAT.GT.NRAT) THEN
         NB=NB+1
         DEPTH=VV(IJ)
      ENDIF
   BLOCK(IJ)=NB
   CONTINUE
   I=I+IQUAD
   GO TO 90
   ENDFI
100 CONTINUE
110 CONTINUE
I3=I
C SUBORDINATE LINES
C BIN ALL MODERATE-EXCITATION LINES WITH SAME LOWER LEVEL TOGETHER.
C FOR HYDROGEN, ONLY THE N=2 LEVEL IS SO TREATED.
C DETERMINE WHICH SET OF FREQUENCIES CORRESPOND TO A SINGLE LOWER
C LEVEL.
105 IF (WTRH.LT.1) GO TO 140
   DO 110 I=I1,ITPTRBE1-1,IQUAD
      IF (LOWB(I).IE.2) THEN
         K=I
         GO TO 120
      ENDIF
   CONTINUE
C NOW PRODUCE AN INDEX ARRAY
C CALL INDEX(K-I1,VV(I1),INDX)
C NOW SET UP BINS
   NB=NB+1
   IJ=INDX(K-I1)+I1-1
   DEPTH=VV(IJ)
   BLOCK(IJ)=NB
   DO 130 I=K-I1-1,1,-1
      IJ=INDX(I)+I1-1
      RAT=MAX(VV(IJ),DEPTH)/MIN(VV(IJ),DEPTH)
      IF (RAT.GT.NRAT) THEN
         NB=NB+1
         DEPTH=VV(IJ)
      ENDIF
      BLOCK(IJ)=NB
   CONTINUE
110 CONTINUE
120 CONTINUE
C SAME IDEA FOR HELIUM IONS, EXCEPT THAT HERE LEVELS 2 THROUGH 5
C ARE SO TREATED (ALL OF WHICH CORRESPOND TO A PRINCIPAL QUANTUM
C NUMBER OF 2).
140 IF (WTRHE1.LT.1) GO TO 180
   DO 150 I=I2,ITPTRHE2,IQUAD
      IF (LOWHE1(I).NE.LOWHE1(I2)) THEN
         K=I
         GO TO 160
      ENDIF
   CONTINUE
C NOW PRODUCE AN INDEX ARRAY
C CALL INDEX(K-I2,VV(I2),INDX)
C NOW SET UP BINS
   NB=NB+1
   IJ=INDX(K-I2)+I2-1
   DEPTH=VV(IJ)
   BLOCK(IJ)=NB
   DO 170 I=K-I2-1,1,-1
      IJ=INDX(I)+I2-1
\[ R\_LT = \frac{\text{MAX}(VV(IJ), \text{DEPTH})}{\text{MIN}(VV(IJ), \text{DEPTH})} \]

\[ \text{IF} (R\_LT > NR\_LT) \text{THEN} \]
\[ WB = WB + 1 \]
\[ \text{DEPTH} = VV(IJ) \]
\[ \text{ENDDIF} \]
\[ \text{BLOCK}(IJ) = WB \]

170 \text{CONTINUE} \]

\text{NOW LOOP BACK FOR THE NEXT LINE} \\

I2 = K  \\
\text{IF} (\text{LOWBE2}(K) .LT. 6 .AND. K .LT. IPTTREE2) \text{GO TO 140} \\

\text{NOW IONIZED HELIUM; HERE LEVELS 2 THROUGH 4 ARE SO TREATED.}  \\
\text{(OR LEVELS 3 THROUGH 4 IF LEVEL 2 LINES ARE TREATED AS RESONANCE.)} \\

180 \text{IF} (\text{WTRHE2}(I) .LT. 1) \text{GO TO 215}  \\
\text{IF} (I3+\text{QUAD} .GT. WJ) \text{THEN}  \\
K = WJ + 1  \\
\text{GO TO 200} \]
\[ \text{ENDDIF} \]
\[ \text{DO 190} \text{I} = I3, IJ, I\text{QUAD} \]
\[ \text{IF} (\text{LOWHE2}(I) .LE. \text{LOWBE2}(I3)) \text{THEN} \]
\[ K = I \]
\[ \text{GO TO 200} \]
\[ \text{ENDDIF} \]

190 \text{CONTINUE} \\

\text{NOW PRODUCE AN INDEX ARRAY} \\

200 \text{CALL INDEX}(K-I3, VV(I3), INDX) \\

\text{NOW SET UP BINS} \\

WB = WB + 1  \\
I3 = INDEX(K-I3) + I3 - 1  \\
\text{DEPTH} = VV(IJ)  \\
\text{BLOCK}(IJ) = WB  \\
\text{DO 210} \text{I} = K-I3+1, I3, -1  \\
I3 = INDEX(I) + I3 - 1  \\
\text{RAT} = \frac{\text{MAX}(VV(IJ), \text{DEPTH})}{\text{MIN}(VV(IJ), \text{DEPTH})} \text{IF} (R\_LT > NR\_LT) \text{THEN}  \\
WB = WB + 1  \\
\text{DEPTH} = VV(IJ) \]
\[ \text{ENDDIF} \]
\[ \text{BLOCK}(IJ) = WB \]

210 \text{CONTINUE} \]

\text{NOW LOOP BACK FOR THE NEXT LINE} \\

I3 = K  \\
\text{IF} (\text{LOWHE2}(K) .LT. 5.0 .AND. K .LT. WJ) \text{GO TO 180} \\

\text{NOW FOR HIGH-EXCITATION LINES.} \\
\text{THESE ARE ALL BINNED TOGETHER BY IOW.} \\

\text{PRODUCE AN INDEX ARRAY} \\

215 \text{IF} (\text{WTRH}.LT.1) \text{GO TO 225}  \\
\text{CALL INDEX}(\text{IPTTREE1}-I1, VV(I1), INDX) \\

\text{NOW SET UP BINS} \\

WB = WB + 1  \\
I1 = INDEX(\text{IPTTREE1}-I1) + I1 - 1  \\
\text{DEPTH} = VV(IJ)  \\
\text{BLOCK}(IJ) = WB  \\
\text{DO 220} \text{I} = \text{IPTTREE1}-I1+1, I1, -1  \\
I1 = INDEX(I) + I1 - 1  \\
\text{RAT} = \frac{\text{MAX}(VV(IJ), \text{DEPTH})}{\text{MIN}(VV(IJ), \text{DEPTH})} \text{IF} (R\_LT > NR\_LT) \text{THEN}  \\
WB = WB + 1  \\
\text{DEPTH} = VV(IJ) \]
\[ \text{ENDDIF} \]
\[ \text{BLOCK}(IJ) = WB \]

220 \text{CONTINUE} \\

\text{SAME FOR OTHER IONS} \\

\text{PRODUCE AN INDEX ARRAY}
IF (ITRHE1.LT.1) GO TO 240
IF (ITPTRHE2-I2.LE.0) GO TO 240
CALL INDEXX(ITPTRHE2-I2,VV(I2),INDX)

NOW SET UP BINS

WB=WB+1
I2=INDX(ITPTRHE2-I2)+I2-1
DEPTH=VV(I2)
BLOCK(I2)=WB
DO 230 I=ITPTRHE2-I2-1,1,-1
   J2=INDX(I)+I2-1
   RAT=MAX(VV(I2),DEPTH)/MIN(VV(I2),DEPTH)
   IF (RAT.GT.MRAT) THEN
      WB=WB+1
      DEPTH=VV(I2)
   ENDIF
   BLOCK(I2)=WB
230 CONTINUE

NOW IONIZED HELIUM

PRODUCE AN INDEX ARRAY

IF (ITRHE2.LT.1) GO TO 260
IF (WJ+1-I3.LE.0) GO TO 260
CALL INDEXX(WJ+1-I3,VV(I3),INDX)

NOW SET UP BINS

WB=WB+1
I3=INDX(WJ-I3+1)+I3-1
DEPTH=VV(I3)
BLOCK(I3)=WB
DO 250 I=WJ-I3,1,-1
   J3=INDX(I)+I3-1
   RAT=MAX(VV(I3),DEPTH)/MIN(VV(I3),DEPTH)
   IF (RAT.GT.MRAT) THEN
      WB=WB+1
      DEPTH=VV(I3)
   ENDIF
   BLOCK(I3)=WB
250 CONTINUE

SUBROUTINE COLRAT(T,C,CHE1,CHE2)

CALCULATE COLLISION RATE COEFFICIENTS

IMPLICIT NONE

LOCAL VARIABLES

INTEGER I, J
REAL C(NLH,NLH+1), CHE1(NLHE1,NLHE1+1), CHE2(NLHE2,NLHE2+1)
REAL CA, CCMW, CCR, E1, E5, EX, GAM, ERT, SRT, T, U0, U1, U2, V
REAL XX
PARAMETER (CCM=5.465E-11, CA=4.3144E-6)

HYDROGEN LINE GAMMA COEFFICIENTS

REAL A18(NLH,MQH), A28(NLH,MQH), A38(NLH,MQH), A48(NLH,MQH)
REAL A58(NLH,MQH)
(106 lines of DATA statements omitted)

**NEUTRAL HELIUM GAMMA COEFFICIENTS**

REAL A1HE1(WLHE1,MQHE1), A2HE1(WLHE1,MQHE1), A3HE1(WLHE1,MQHE1), A4HE1(WLHE1,MQHE1), A5HE1(WLHE1,MQHE1)

(848 lines of DATA statements omitted)

**IONIZED HELIUM GAMMA COEFFICIENTS**

(461 lines of DATA statements omitted)

**HYDROGEN IONIZATION WIDTH COEFFICIENTS**

REAL COH(5), C1H(5), C2H(5), C3H(5), C4H(5), C5H(5)

DATA COH/4.99256853566402E+3, 3.99644687573465E+5, 3.88203823242319E+5, 
: 5.78364340343856E+5, 9.01892625624507E+5/

DATA C1H/-4.11942376702136E+3, 3.76618400049636E+5, 4.16239306165835E+5, 
: -6.70825392728656E+5, -2.43449002577712E+6/

data C2H/-3.31759642620004E+3, 1.35841239372724E+5, 1.75607300195952E+5, 
: 3.30851970000000E+6, 1.63566251543658E+6/

DATA C3H/4.9351199736847E+3, -2.28353902477235E+4, 4.63241388463064E+4, 1.15074682397601E+5, 
: -6.8774629291332E+5, -5.36682142076778E+5/

DATA C4H/-4.44335358358851E+3, 1.76194565100000E+6, 3.05991327554483E+6, 
: 7.12736329505883E+6, 5.66229543979763E+6/

DATA C5H/5.50514583961151E+3, -4.74391293104158E+5, -1.47537595031046E+5, 
: 3.01051976118922E+5, -2.64683515928094E+5/

**NEUTRAL HELIUM IONIZATION WIDTH COEFFICIENTS**

REAL COHE1(19), C1HE1(19), C2HE1(19), C3HE1(19), C4HE1(19), C5HE1(19)

DATA COHE1/-4.91489194654352E-6, 4.52575319554019E+3, 6.19427179888361E+5, 8.98300097829758E-6,
: 1.92215936524694E+3, 4.45876055360785E-5/

DATA C1HE1/-4.57165360736388E-6, 5.62950496624053E-5, 6.95268999507597E-5, 8.19238907237432E-5,
: 1.15810671348136E-4, 1.90865278386069E-4, 8.98170530058522E-4,
: 5.74800893543380E-4, 1.62679285167244E-4, 3.56938876712160E-4, 8.17994634033470E-4,
: 1.38388905019199E-3, 3.23707184136869E-3, 1.85313948952327E-3, 8.15067303401430E-3,
: 8.65724188081018E-8, 0.00000000000000E+0, 1.17873552725727E-8, 6.75652198881018E-9/ 

**IONIZED HELIUM IONIZATION WIDTH COEFFICIENTS**

REAL COHE2(10), C1HE2(10), C2HE2(10), C3HE2(6), C4HE2(8), C5HE2(6)

DATA COHE2/-7.982502484, 4.1840431549916, 1.96634691767181, 1.18133516427340,
: 1.4401016249221260, 4.6653121923821760, 3.9873516432297382, 
: -8.79065.12522636, -1.591432227411, -2.289146.11997632, -2.007.11914,
: -2.507.7581, 8.248.43875, -1.390.1250/

DATA C1HE2/-1.722.036570026580.7599.439998198, 
: 3.860022972999, 6.9164.12399282, 1.03961.96662899, 2.40, 30.105526,
: 97.9747874/

DATA C2HE2/-4.2582386343433, -1.722.036570026580.7599.439998198, 
: 3.860022972999, 6.9164.12399282, 1.03961.96662899, 2.40, 30.105526,
: 97.9747874/

DATA C3HE2/-3.562032948247, 4.037229638371, -1.467.056585238, 
: -7.452.392601514, -1.4662.3021131, -2.2877.34946565, 
: -1.923825868069, -4.6202585731757, 1.256.6977110972, 
: 7.432.637181628, 1.517.485430160, 2.466.673087330, -2.810.7812, 
: -1.283.5625/

DATA C4HE2/0.000000000000000, 2.061471799965, 4.324390597780, 
: -2.14243384304, -6.152929455881, -1.022217157435/

**START OF EXECUTABLE STATEMENTS**

START=SQRT(T)
BK=TR/T
XI=LODI(T)

CLEAR RATE COEFFICIENTS

DO 20 I=1,NLHN
DO 10 J=1,NLHN+1
C1(I,J)=0
CONTINUE

10 CONTINUE

DO 40 I=1,NLHNE
DO 30 J=1,NLHNE+1
C1(I,J)=0.0
CONTINUE

DO 60 I=1,ILHE2
DO 60 J=1,ILHE2+1
CHE2(I,J)=0.0
CONTINUE

C HYDROGEN IONIZATION RATES
C FROM LENNOM e.a. (1986)

DO 70 I=1,ILNL
GAM=MAX(1.E-15,(COH(I)/XX+C1H(I))/XX+C2H(I)+XX*(C3H(I)+
II*(C4H(I)+II*C5H(I))))
C(I,ILNL+1)=CCON*SRT*GAM*EXP(-HKT*FRQH(I))
CONTINUE

C HYDROGEN EXCITATION RATES
C GROUND STATE TO 2ND AND 3RD LEVEL FROM AGGARWAL (1983)
C 2ND TO 3RD LEVEL FROM BATA et al. (1980)
C OTHERS FROM MIBALAS (1978).

DO 100 I=1,ILNL
DO 80 J=I+1,ILNL
UO=FRQH(I)-FRQH(J)
UO=UO*HKT
EX=EXP(-UO)
GAM=MAX(1.E-15,(A1H(I,J)+T*(A2H(I,J)+T*A3H(I,J)))/
(1.0+T*(A4H(I,J)+T*A5H(I,J))))
CCR=CA*EX*GAM/SRT
C(I,J)=CCR
C(J,I)=GCH(I)*CCR/(GCH(J)*EX)
CONTINUE

DO 90 J=ILNL+1,MBH
UO=FRQH(I)-FRQH(J)
UO=UO*HKT
EX=EXP(-UO)
GAM=MAX(1.E-15,(A1H(I,J)+T*(A2H(I,J)+T*A3H(I,J)))/
(1.0+T*(A4H(I,J)+T*A5H(I,J))))
CCR=CA*EX*GAM/SRT
C(I,ILNL)=C(I,ILNL)+CCR
CONTINUE

C HELIUM IONIZATION RATE COEFFICIENTS FROM LENNOM et al. (1986).

DO 110 I=1,ILHE1
GAM=MAX(1.E-15,(COHE1(I)/XX+C1HE1(I))/XX+C2HE1(I)+XX*(C3HE1(I)+
II*(C4HE1(I)+II*C5HE1(I))))
CHE1(I,ILHE1+1)=CCON*SRT*GAM*EXP(-HKT*FRQHE1(I))
CONTINUE

C HELIUM EXCITATION RATES FROM AGGARWAL et al. (1978) FOR
C GROUND LEVEL TO FIRST FOUR EXCITED LEVELS.
C OTHER RATES FROM BERRITOT ET AL. (1985) OR FROM MIBALAS
C ET AL. (1976).

DO 140 J=I+1,ILHE1
UO=FRQHE1(I)-FRQHE1(J)
UO=UO*HKT
EX=EXP(-UO)
V=GHE1(I)/GHE1(J)
(1.0+T*(A4HE1(I,J)+T*A5HE1(I,J))))
CCR=CA*EX*GAM/SRT
CHE1(I,J)=CCR
CHE1(J,I)=V*CCR/EX
CONTINUE

DO 150 J=ILHE1+1,MBHE1
UO=FRQHE1(I)-FRQHE1(J)
UO=UO*HKT
EX=EXP(-UO)
V=GHE1(I)/GHE1(J)
(1.0+T*(A4HE1(I,J)+T*A5HE1(I,J))))
CCR=CA*EX*GAM/SRT
CONTINUE
CHE1(I,WLBH=1+1)=CHE1(I,WLBH=1+1)+CCR

CONTINUE

ICHEMIZED HELIUM IONIZATION RATE COEFFICIENTS
FROM LENNOW et al. (1986)

DO 150 I=1,6
GAM=MAXI(1.E-15,(CBE2I(I)/II+CBE2I(II))*/II*(CBE2I(I)+
II*(CBE2I(I)/I+II*CBE2I(II))))
CHE2I(I,WLBH+1)=CCQM*SRT*GAM*EXP(-HKT*FRQHE2I(I))

CONTINUE

IONIZATION RATES FROM MINALAS et al. (1975)

DO 160 I=7,WLB2
GAM=MAXI(1.E-15,COBE2I(I)+C1BE2I(I)+C2BE2I(I)*II*
C4BE2I(I)/II/II)
UO=HKT*FRQHE2I(I)
CHE2I(I,WLBH+1)=CCQM*SRT*EXP(-UO)*GAM

CONTINUE

IONIZATION RATES FROM MINALAS et al. (1975)

DO 190 I=1,7,WLB2
DO 170 J=I+1,7,WLB2
UO=FRQHE2(i,J)-FRQHE2(I,J)
UO=HKT*UO
EX=EXP(-UO)
1.0+T*(A4BE2(I,J)+A5BE2(I,J)))
CCR=CA*EX*GAN/SRT
CHE2I(J,J)=GHN(I,J)*CCR/GAN

CONTINUE

DO 180 J=1,12,WNB
UO=FRQHE2I(I,J)-FRQHE2I(I,J)
UO=HKT*UO
EX=EXP(-UO)
1.0+T*(A4BE2(I,J)+A5BE2(I,J)))
CCR=CA*EX*GAN/SRT
CHE2I(I,J)=CHE2|1,ILBEH+1)=CHE2I(I,WLBH+1)+CCR

CONTINUE

RETURN

END

SUBROUTINE CONTROL

OVERALL CONTROL SUBROUTINE FOR LINEARIZATION AND
LAMBDA ITERATION

IMPLICIT NONE

COMMON COMMON

INTEGER ID, I

REAL EDFAC, EXIT, GAB, GEIER, LINEAR, LIMIT, NUPOP
EXTERNAL EDFAC, EXIT, GAB, GEIER, LINEAR, LIMIT, NUPOP

EXIT=.FALSE.
DO 30 I=1,ITER
CALL GEIER
CALL EDFAC
CALL LINEAR
CALL LIMIT(I)
WRITE (6,*)'LINE= ',LINEAR,' LANL= ',LANL

DO 10 ID=1,IDEPTH
CALL NUPOP(ID)

CONTINUE

RETURN

END
DIAGNOSTICS
IF (FPRINT) CALL GAB

DIRECT LINEARIZATION
CALL LINEAR
DO 20 ID=1,NDEPTB
CALL BUPOP(ID)
CONTINUE
IF (EXIT) GO TO 40
30 CONTINUE
WRITE (6,*) 'ITERATIONS FAILED TO CONVERGE'
40 CALL GAB
RETURN
END

SUBROUTINE DGENER(IDD,PR)
CALCULATE OPACITIES AND DERIVATIVES
IMPLICIT NONE
MACROS

LOCAL VARIABLES
INTEGER I, IR, II, ID, IDD, IL, IJ, L, IT, U, J, JJ, NO
REAL DD(IEQI,NIB+2), DSKKDT(NIJ,3), PR(MIJ+1), SKK(NIJ,3)
REAL C(MIJ), DC, DE, DOP, DQPT, DT, E(MIJ), FRQO, HKT
REAL HKT2, S, SIGMA, SIGMAT, SRT, SRT2, T1, X, X0, XI
EXTERNAL PROCEDURES
REAL COLRAT, DFRE, MATINV, RATEQ
EXTERNAL COLRAT, DFRE, MATINV, RATEQ
ID=IDD
CALL DFRE(ID,SKK,DSKKDT)
T1=1.0/TEMP(ID)
BKT=T1
BKTT=T1
SRT=SQRT(TIME/TEMP(ID))
SRT2=SQRT(TEMP(ID))

GENERATE COLLISION RATES AND DERIVATIVES.
CALL COLRAT(TEMP(ID),CR,CRBE1,CRBE2)
DT=1.E-4/TEMP(ID)
CALL COLRAT(TEMP(ID)+DT,DCRDT,DCRBE1,DCRBE2)
DO 20 I=1,ILB
DO 10 J=1,ILB+1
DCRDT(I,J)=(DCRDT(I,J)-CR(I,J))/DT
10 CONTINUE
20 CONTINUE
DO 40 I=1,ILBE1
DO 30 J=1,ILBE1+1
DCRBE1(I,J)=(DCRBE1(I,J)-CRBE1(I,J))/DT
30 CONTINUE
40 CONTINUE
DO 60 I=1,ILBE2
DO 50 J=1,ILBE2+1
DCRBE2(I,J)=(DCRBE2(I,J)-CRBE2(I,J))/DT
50 CONTINUE
60 CONTINUE
DO 80 I=1,NEQN
DO 70 J=1,NWW
DD(I,J)=0.0
70 CONTINUE
80 CONTINUE
DO 90 I=1,NWW
PR(I)=0.0
90 CONTINUE

OBTAIN RATE EQUATION MATRIX AND INVERT.
CALL RATEQ(ID, NEQD, BW, RD)
CALL MATINV(AN, NEQW, NEQM)

CALL NATIV(ID, NEQL, NEQI)

DO 100 IJ = 1, IJ
EX(IJ) = EXP(-BKT • FREQ(IJ))
CONTINUE
IF (PLTE) GO TO 180
DO 170 IJ = 1, IJ
DO 160 I = 1, IEQI
Bl(I) = 0.
110 CONTINUE
S = SCDF • WT(IJ) / FREQ(IJ)
IF (I.J. LT. ITTPRBE) THEN
DO 120 IJ = 1, IJ
Bl(IJ) = WLCM • (WHEIS(I, ID) • EX(IJ) - WHE1(I, ID)) • SIGE1(I, IJ)
120 CONTINUE
DO 130 I = 1, ILE1
II = MLHE1
Bl(II) = WLCM • (WHE2(I, ID) • EX(IJ) - WHE2(I, ID)) • SIGE2(I, IJ)
130 CONTINUE
ELSE IF (IJ. LT. ITPTRBE1) THEN
I = LOWH(IJ)
J = UPB(IJ)
IT = ITRB(I, J)
JJ = J + ILE1 + ILB + 1
II = I + ILE1 + ILB + 1
FRQO = FRQB(I) - FRQB(J)
DOP = SQRT(2 • FRQO • DOPCOF)
X = DELQUAD • NOD(IJ - ITPTRB, IQUAD) • SQRT(SIGNA)
X = S • SIGNA • (IHE1(I, ID) - GB(I) • IHE2(J, ID) / GB(J))
Bl(II) = -X
Bl(JJ) = +X
140 CONTINUE
ELSE IF (IJ. LT. ITPTRBE2) THEN
I = LOWBE1(IJ)
J = UPBE1(IJ)
IT = ITRBE1(I, J)
JJ = J + MLBE1
II = I + MLBE1
FRQO = FRQBE1(I) - FRQBE1(J)
DOP = SQRT(2 • FRQO • DOPCOF • 0.5)
X = DELQUAD • MOD(IJ - ITPTRBE1, WQUAD) • SQRT(SIGNA)
X = S • SIGNA • (IHE1(I, ID) - GBE1(I) • IHE2(J, ID) / GBE1(J))
Bl(I) = -X
Bl(J) = +X
150 CONTINUE
ELSE
I = LOWBE2(IJ)
J = UPBE2(IJ)
IT = ITRBE2(I, J)
JJ = J + MLBE1
II = I + MLBE1
FRQO = FRQBE2(I) - FRQBE2(J)
DOP = SQRT(2 • FRQO • DOPCOF • 0.5)
X = DELQUAD • MOD(IJ - ITPTRBE2, WQUAD) • SQRT(SIGNA)
X = S • SIGNA • (IHE1(I, ID) - GBE2(I) • IHE2(J, ID) / GBE2(J))
Bl(II) = -X
Bl(JJ) = +X
160 CONTINUE
END IF
IB = BLOCK(IJ)
DO 160 IL = 1, NEQW
DO 150 J = 1, NEQW
DD(IL, IB) = DD(IL, IB) + AN(IL, J) • BN(J) • RAD(IJ, ID)
150 CONTINUE
160 CONTINUE
170 CONTINUE
CALL RADIUS FIELD PERTURBATIONS
180 DO 190 I = 1, MLBE1
BN(I) = WHEIS(I, ID) • (WDEIS(MLBE1 + 1, I) -
((1.6 • BKT • FRQBE1(I)) / TEMP(ID)) •
DO 190 I = 1, MLBE1
BN(I) = WHEIS(I, ID) • (WDEIS(MLBE1 + 1, I) -
((1.6 • BKT • FRQBE1(I)) / TEMP(ID)) •
DO 190 I = 1, MLBE1
BN(I) = WHEIS(I, ID) • (WDEIS(MLBE1 + 1, I) -
((1.6 • BKT • FRQBE1(I)) / TEMP(ID)) •
202

: (RHE1(WLHE1+1,I)+WE(ID)*CRHE1(I,WLHE1+1))+
  WE(ID)*DCRHE1(I,WLHE1+1)*((RHE1S(I,ID)-WHE1(I,ID))

199 CONTINUE
DO 230 I=1,WLHE1
DO 200 J=1,WLHE1
  BM(I)=BM(I)+WE(ID)*
    (DCRHE1(I,J)*WHE1(J,ID)-DCRHE1(I,J)*WHE1(I,ID))

200 CONTINUE
DO 210 J=1,I-1
  FRQ0=FRQHE1(J)-FRQHE1(I)
  X=FRQHE1(I)*EXP(BKT*FRQ0)/FRQHE1(I)
  XO=X*BKT*FRQ0
  BM(I)=BM(I)*FRQ0(I,ID)*X+RHE1(I,J)+XO*
  RHE1(I,J)+X0*

210 CONTINUE
DO 220 J=I+1,WLHE1
  FRQ0=FRQHE1(J)-FRQHE1(I)
  X=FRQHE1(I)*EXP(BKT*FRQ0)/FRQHE1(I)
  X0=X*BKT*FRQ0
  BM(I)=BM(I)*FRQ0(I,ID)*X+RHE1(I,J)+

220 CONTINUE
DO 230 I=1,WLHE2
II=I+WLHE1
  BM(I)=BM(I)+WE(ID)*
    (DCRHE2(I,I)*WHE2(I,ID)-DCRHE2(I,I)*WHE2(I,ID))

230 CONTINUE
DO 260 J=1,WLHE2
II=I+WLHE1
  BM(J)=BM(J)+WE(ID)*
    (DCRHE2(I,J)*WHE2(J,ID)-DCRHE2(I,J)*WHE2(I,ID))

260 CONTINUE
DO 270 J=1,WLHE2
II=I+WLHE1
  BM(J)=BM(J)+WE(ID)*
    (DCRHE2(I,J)*WHE2(J,ID)-DCRHE2(I,J)*WHE2(I,ID))

270 CONTINUE
DO 290 I=1,WLH
II=I+WLHE1+WLE2+1
  BM(I)=BM(I)+(DRH(WLH+1,I)-(1.5+BKT*FRQH(I))/TEMP(ID)) *
    (RHE(WLH+1,I)+WE(ID)*CR(WLH+1,I))+
  WE(ID)*DCRHT(I,WLH+1)*((DSBDT(I,ID)-WHE2(I,ID))

290 CONTINUE
DO 330 I=1,WLH
II=I+WLHE1+WLE2+1
  BM(I)=BM(I)+WE(ID)*
    (DCRHT(I,J)*W(J,ID)-DCRHT(I,J)*W(I,ID))

330 CONTINUE
Bl(IEQI) = -IE(ID) * BE3(ID) * DSHEDT(2,ID)
DO 350 IL=1,IEQI
DO 340 J=1,IEQI
       DD(IL,J) = DD(IL,J) + AJL(IL,J) * Bl(J) * TEMP(ID)
340 CONTINUE
350 CONTINUE

C ELECTRON DENSITY DERIVATIVES.
C
DO 360 I=1,ILBE1
       Bl(I) = (ibe1s(I,ID)/ie(ID) * (rbe1(1lbe1+1,I) + 2.0 * ie(ID) * crbe1(I,lbe1+1)) -
               be1(I,ID) * crbe1(I,lbe1+1)
360 CONTINUE
DO 370 J=1,ILBE1
       Bl(J) = Bl(J) + crbe1(J,I) * be1(J,ID) - crbe1(I,J) * be1(I,ID)
370 CONTINUE
DO 380 I=1,ILBE2
       Bl(I) = (ibe2s(I,ID)/ie(ID) * (rbe2(1lbe2+1,I) + 2.0 * ie(ID) * crbe2(I,lbe2+1)) -
               be2(I,ID) * crbe2(I,lbe2+1)
380 CONTINUE
DO 390 I=1,ILBE2
       II=I+ILBE1
       Bl(II) = (ibe2s(I,ID)/ie(ID) * (rbe2(1lbe2+1,I) + 2.0 * ie(ID) * crbe2(I,lbe2+1)) -
               be2(I,ID) * crbe2(I,lbe2+1)
390 CONTINUE

Bl(IEQI) = 1.0 - BE3(ID) * SUMBE(2,ID)
DO 400 I=1,IEQI
       DD(IL,IIE) = DD(IL,IIE) + AJL(IL,J) * Bl(J) * IE(ID)
400 CONTINUE

C TOT AND DERIVATIVES THEREOF
C
PR(111+1) = ye(id)
PR(WNE) = we(id)
DO 470 IL=1,NLBE1
       PR(111+1) = PR(111+1) + WHE1(IL,ID)
470 CONTINUE
DO 480 IL=1,NWNE
       PR(J) = PR(J) + DD(IL,J)
480 CONTINUE
DO 500 IL=1,NLBE2
       PR(111+1) = PR(111+1) + WHE2(IL,ID)
500 CONTINUE
DO 520 IL=1,NWNE
       PR(J) = PR(J) + DD(IL,J)
520 CONTINUE

PR(111+1) = PR(111+1) + WHE1(1,ID) * SUMBE(1,ID) * WE(ID)
PR(WNT) = PR(WNT) + WHE2(1,ID) * DSHEDT(1,ID) * WE(ID) * TEMP(ID)
PR(WNE) = PR(WNE) + WHE2(1,ID) * SUMBE(1,ID) * WE(ID)
DO 530 J=1,NWNE
       PR(J) = PR(J) + DD(WHE1+1,J) * SUMBE(1,ID) * WE(ID)
530 CONTINUE
PR(111+1) = PR(111+1) + WHE3(ID) * (1.0 + SUMHE(2,ID) * WE(ID))
PR(WNT) = PR(WNT) + WHE3(ID) * DSHEDT(2,ID) * WE(ID) * TEMP(ID)
PR(WNE) = PR(WNE) + WHE3(ID) * SUMBE(2,ID) * WE(ID)
DO 540 J=1,NWW
PR(J)=PR(J)+DD(WLHEE1+WLHE2+1,J)*(1.0+SUMHE(2,ID)*WE(ID))
540 CONTINUE
DO 550 IL=1,NLH
PR(NWW+1)=PR(NWW+1)*W(IL,ID)
550 CONTINUE
DO 570 IL=1,NLH
DO 560 J=1,NWW
PR(J)=PR(J)+DD(IL+WLHE1+WLHE2+1,J)
560 CONTINUE
DO 580 IL=1,ILB
PR(111+1)=PR(111+1)+1(IL,ID)
580 CONTINUE
DO 590 J=1,III
PR(J)=PR(J)+DD(IL+ILBE1+ILBE2+1,J)•(1.0+SUMBE(2,ID)•IE(ID))
590 CONTINUE
DO 600 J=1,III
PR(IIT)=PR(IIT)+IPROT(ID)•DSBDT(ID)•IE(ID)•TEMP(ID)
PR(IIE)=PR(IIE)+IPROT(ID)*SUMB(ID)•IE(ID)
DO 610 J=1,III
PR(J)=PR(J)+DD(ILBE1+ILBE2+1LBE2+2,J)•(1.0+SUNB(ID)•IE(ID))
610 CONTINUE
ITOT(ID)=PR(111+1)
C
C ELECTRON SCATTERING
C
10=111+1
DO 620 J=1,III
DO 630 IJ=1,IJ
CBI(IJ,J)=0.0
ETA(IJ,J)=0.0
630 CONTINUE
620 CONTINUE
DO 640 J=1,NWW
DO 650 IJ=1,IJ
E(IJ)=SIGBE1(IL,IJ)•WBE1S(IL,ID)•EI(IJ)
ETA(IJ,IO)=ETA(IJ,IO)+E(IJ)
CBI(IJ,IO)=CBI(IJ,IO)+SIGBE1(IL,IJ)•WBE1S(IL,ID)
ETA(IJ,IIT)=ETA(IJ,IIT)+E(IJ)•(-1.5+BKT•(FREQ(IJ)-FRQBE1(IL))-
ETA(IJ,NWE)=ETA(IJ,NWE)+E(IJ)
650 CONTINUE
640 CONTINUE
DO 660 IJ=1,IJ
E(IJ)=SIGBE2(IL,IJ)•WBE2S(IL,ID)•EI(IJ)
ETA(IJ,IO)=ETA(IJ,IO)+E(IJ)
CBI(IJ,IO)=CBI(IJ,IO)+SIGBE2(IL,IJ)•WBE2S(IL,ID)
ETA(IJ,IRT)=ETA(IJ,IRT)+E(IJ)•(-1.5+BKT•(FREQ(IJ)-FRQBE2(IL))-
CBI(IJ,NWE)=CBI(IJ,NWE)•C(IJ)
ETA(IJ,NWE)=ETA(IJ,NWE)+E(IJ)
660 CONTINUE
DO 670 IJ=1,IJ
ETA(IJ,J)=ETA(IJ,J)+E(IJ)•DD(ILBE1+1,J)/IBE2(1,ID)
CBI(IJ,J)=CBI(IJ,J)+SIGBE1(IL,IJ)•DD(IL,J)
670 CONTINUE
680 CONTINUE
DO 690 IJ=1,IJ
E(IJ)=SIGBE1(IL,IJ)•WBE1S(IL,ID)•EI(IJ)
ETA(IJ,IO)=ETA(IJ,IO)+E(IJ)
CBI(IJ,IO)=CBI(IJ,IO)+SIGBE1(IL,IJ)•WBE1S(IL,ID)
ETA(IJ,IIT)=ETA(IJ,IIT)+E(IJ)•(-1.5+BKT•(FREQ(IJ)-FRQBE1(IL))-
CBI(IJ,NWE)=CBI(IJ,NWE)•C(IJ)
690 CONTINUE
DO 700 IJ=1,IJ
ETA(IJ,J)=ETA(IJ,J)+E(IJ)•DD(ILBE1+1,J)/IBE2(1,ID)
CBI(IJ,J)=CBI(IJ,J)+SIGBE1(IL,IJ)•DD(IL,J)
700 CONTINUE
DO 720 J=1,NW
  ETA(I,J)=ETA(I,J)+E(I,J)*DD(WLHE1+WLHE2+1,J)/WE3(ID)
  CBI(I,J)=CBI(I,J)+SIGHE2(IL,II)*DD(WLHE1+IL,II)
END

CONTINUE

710 CONTINUE

720 CONTINUE

730 CONTINUE

DO 770 IL=WLHE2+1,WLHE2
DO 740 J=1,NW
  C(IJ)=SIGHE2(IL,II)*WE2S(IL,ID)
  E(IJ)=C(IJ)*EX(IJ)
  ETA(I,J,X)=E(I,J)*(-1.5+HKT*(FREQ(IJ)-FRQHE2(IL)))
  CBI(I,J,X)=CBI(I,J,X)+SIGHE2(IL,II)*E(I,J)
END

CONTINUE

740 CONTINUE

DO 760 J=1,NW
  ETA(I,J)+E(I,J)*DD(WLHE1+WLHE2+1,J)/WE3(ID)
END

CONTINUE

760 CONTINUE

770 CONTINUE

C FREE-FREE OPACITIES
C
I0=WE3(ID))*WE(ID)**2
I=0*SUMHE2(2,ID)
DO 780 IL=1,ILHE2
  X=X*WE(II,ID)
DO 790 IJ=1,IJ

C
DC=(I0)*IE(ID)*SKK(IJ,2)*DD(ILHE1+IL,II)
CBI(I,J)=CBI(I,J)+DC
ETA(I,J)=ETA(I,J)+DC*EX(IJ)
END

CONTINUE

800 CONTINUE

DO 850 IJ=1,IJ

DC=(I0)*IPROT(ID)*IE(ID)*SKK(IJ,1)
CBI(I,J)=CBI(I,J)+DC
ETA(I,J)=ETA(I,J)+DC*EX(IJ)
END

CONTINUE
DSKDT(I J, I)*EX(I J)*TEMP(ID)
CHI(I J, WNT)=CHI(I J, WNT)*NPROT(ID)*WE(ID)*DSKDT(I J, I)*TEMP(ID)
ETA(I J, WNE)=ETA(I J, WNE)*E(I J)
CHI(I J, WNE)=CHI(I J, WNE)*C(I J)

850 CONTINUE
DO 870 I=1, W
DO 860 J=1, W
DC=SKK(I J, 3)*DD(ILBE1+1LBE2+1J)*E(I J)
CHI(I J, W0)=CHI(I J, W0)*DC
ETA(I J, WNT)=ETA(I J, WNT)*E(I J)*(-1.5+BKT*(FREQ(I J)-
FRQB(IL)))/IPROT(ID)
CBI(I J, WNT)=CBI(I J, WNT)*DC

860 CONTINUE
870 CONTINUE
C HYDROGEN BOUND-FREE OPACITIES
C DO 910 IL=1, WB
DO 880 IJ=1, IJ
E(I J)=SIG(IL, IJ)*IS(IL, ID)*E(I J)
ETA(I J, IO)=ETA(I J, IO)*E(I J)
CBI(I J, IO)=CBI(I J, IO)*C(I J)
ETA(I J, IIT)=ETA(I J, IIT)*E(I J)*(-1.5+BKT*(FREQ(I J)-
FRQB(IL)))*IPROT(ID)
CBI(I J, IIT)=CBI(I J, IIT)*C(I J)*(-1.5-BKT*FRQB(IL))

880 CONTINUE
DO 900 J=1, W
DO 890 IJ=1, IJ
ET(I J, J)=ETA(I J, J)*E(I J)*DD(ILBE1+1LBE2+2J)*IPROT(ID)
CBI(I J, J)=CBI(I J, J)*E(I J)*DD(ILBE1+1LBE2+2J)/IPROT(ID)

890 CONTINUE
900 CONTINUE
910 CONTINUE
DO 950 IL=WB+1, W
DO 920 IJ=1, IJ
E(I J)=SIG(IL, IJ)*IS(IL, ID)
ET(I J, IO)=ETA(I J, IO)+GB(L)*SIGM1*G(U)/GB(U)
CBI(I J, IO)=CBI(I J, IO)*GB(G)
ET(I J, IIT)=ETA(I J, IIT)+GB(L)*SIGM1T*G(U)/GB(U)
CBI(I J, IIT)=CBI(I J, IIT)*GB(G)

920 CONTINUE
DO 940 J=1, W
DO 930 IJ=1, IJ
ET(I J, J)=ETA(I J, J)*E(I J)*DD(WLEH1+WLEH2+WLE2+J)*IPROT(ID)
CBI(I J, J)=CBI(I J, J)*E(I J)*DD(WLEH1+WLEH2+WLE2+1J)/IPROT(ID)

930 CONTINUE
940 CONTINUE
950 CONTINUE
C LINE OPACITIES
C DO 960 IJ=ITPTRH,ITPTRHE-1
L=LOWB(I J)
U=UPB(I J)
IT=ITM(L, U)
FRQO=FRQB(L)-FRQB(U)
DGF=SRT2*FRQ0+DOPCDF
I=DEQD(L, M(I J-ITPTRH, quad))*SRT
SIGMA=PIE2MC*OSCB(L)*EIP(-X*I)*DOP/1. 7724539
C(I J)=SIGMA
SIGMAT=SIGMA*(X*I-0.5)
ET(I J, W0)=ETA(I J, W0)*CHI(L, U)*SIGMA*W(U, ID)/G(U)
CHI(I J, W0)=CHI(I J, W0)*SIGMA*W(L, ID)
ET(I J, WNT)=ETA(I J, WNT)*CHI(L, U)*SIGMA*W(U, ID)/G(U)
CHI(I J, WNT)=CHI(I J, WNT)*SIGMA*W(L, ID)

960 CONTINUE
DO 980 IJ=ITPTRH,ITPTRHE-1
L=LOWB(I J)
U=UPB(I J)
DO 970 J=1, W
ET(I J, J)=ETA(I J, J)*G(L)*C(I J)*DD(WLEH1+WLEH2+1J)/
G(U)
CBI(I,J) = CBI(I,J) + C(I,J) * DD(WLHE1 + WLHE2 + 1 + L, J)

CONTINUE

DO 990 IJ = ITPTRBE1, ITPTRBE2 - 1
  L = LOWHE1(IJ)
  UPHE1(IJ) = L
  IT = ITRHE1(L, U)
  FREQ0 = FREQHE1(L) - FREQHE1(U)
  DOP = SRT2 * FREQ0 * DOPCF0 * 0.6
  X = DELQUAD + MOD(IJ - ITPTRBE1, NQUAD) * SAT
  SIGMA = PIE2 * GCHE1(IT) * EXP(-X^2) / DOP / 1.7724539
  C(I,J) = SIGMA
  SIGMA = SIGMA * (1 - X^2)
  ETA(I,J, NO) = ETA(I,J, NO) + GHE1(L) * SIGMA *mue(I(J) / GHE1(U) / GHE1(L)
  ETA(I,J, WNT) = ETA(I,J, WNT) + GHE1(L) * SIGMA *mue(I(J) / GHE1(U) / GHE1(L)

CONTINUE

DO 1010 IJ = ITPTRBE1, ITPTRBE2 - 1
  L = LOWHE1(IJ)
  UPHR1(IJ) = L
  DO 1000 J = 1, NWW
    ETA(I,J) = ETA(I,J) + GHE1(L) * C(I,J) + DD(U, J) / GHE1(U)
    CBI(I,J) = CBI(I,J) + C(I,J) * DD(L, J)

CONTINUE

DO 1020 IJ = ITPTRBE2, NJ
  L = LOWHE2(IJ)
  UPHR2(IJ) = L
  FREQ0 = FREQHE2(L) - FREQHE2(U)
  DOP = SRT2 * FREQ0 * DOPCF0 * 0.6
  X = DELQUAD + MOD(IJ - ITPTRBE2, NQUAD) * SAT
  SIGMA = PIE2 * GCHE2(IT) * EXP(-X^2) / DOP / 1.7724539
  C(I,J) = SIGMA
  SIGMA = SIGMA * (1 - X^2)
  ETA(I,J, NO) = ETA(I,J, NO) + GHE2(L) * SIGMA *mue(I(J) / GHE2(U) / GHE2(L)
  ETA(I,J, WNT) = ETA(I,J, WNT) + GHE2(L) * SIGMA *mue(I(J) / GHE2(U) / GHE2(L)

CONTINUE

DO 1040 IJ = ITPTRBE2, NJ
  L = LOWHE2(IJ)
  UPHR2(IJ) = L
  DO 1030 J = 1, NWW
    ETA(I,J) = ETA(I,J) + GHE2(L) * C(I,J) + DD(U, J) / GHE2(U)
    CBI(I,J) = CBI(I,J) + C(I,J) * DD(L, J)

CONTINUE

DO 1050 IJ = ITPTRBE2, NJ
  L = LOWHE2(IJ)
  UPHR2(IJ) = L
  EX(I,J) = BBCDF * FREQE2(IJ) * 3

CONTINUE

DO 1060 IJ = 1, NJ
  EX(I,J) = BBCDF * FREQE2(IJ) * 3

CONTINUE

C CONVERT OPACITIES TO MASS COEFFICIENTS

DO 1080 J = 1, NWW
  DO 1070 IJ = 1, NJ
    ETA(I,J) = ETA(I,J) - ETA(I,J, NO) * MU1 * PR(J) / WM(J)
    ETA(I,J) = ETA(I,J) - ETA(I,J, WNT) * MU1 * PR(J) / WM(J)
    ETA(I,J) = ETA(I,J) - ETA(I,J) * ETA(I,J, WNT)
    ETA(I,J) = ETA(I,J) - ETA(I,J, NO)

RETURN

END

SUBROUTINE GAB
BE VERBOSE
INTER
IMPLICIT NONE
INTEGER I, ID, IJ, IL, J, NO, W1
REAL DIS, SUM
PRINT BOUND-FREE JUMPS
WRITE (6,1001)
WRITE (6,1002)
WRITE (6,1003)
IL=1
DO 10 IJ=2,ITPTRB-1
IF (SIG(IJ).EQ.0)THEN
  DIS=-2.5*LOG10(FB(IJ-1)*RAD(IJ-1,1)/FB(IJ)/RAD(IJ,1))
  WRITE (6,1004)IL,DIS
  IL=IL+1
ENDIF
IF (IL.GT.ILB)GO TO 20
10 CONTINUE
20 WRITE (6,1005)
IL=1
DO 30 IJ=2,ITPTRB-1
IF (SIGBE1(IJ).EQ.0)THEN
  DIS=-2.5*LOG10(FB(IJ-1)*RAD(IJ-1,1)/FB(IJ)/RAD(IJ,1))
  WRITE (6,1004)IL,DIS
  IL=IL+1
ENDIF
IF (IL.GT.ILBE1)GO TO 40
30 CONTINUE
40 WRITE (6,1006)
IL=1
DO 50 IJ=2,ITPTRB-1
IF (SIGBE2(IJ).EQ.0)THEN
  DIS=-2.5*LOG10(FB(IJ-1)*RAD(IJ-1,1)/FB(IJ)/RAD(IJ,1))
  WRITE (6,1004)IL,DIS
  IL=IL+1
ENDIF
IF (IL.GT.ILBE2)GO TO 60
50 CONTINUE
C
C PRINT TOTAL FLUX
C
SUM=0.
60 DO 70 I=1,W1
  SUM=SUM+WT(I)*FB(I)*RAD(I,1)
70 CONTINUE
WRITE (6,1007)SUM
C
C PRINT BASIC MODEL PARAMETERS AND POPULATIONS
C
WRITE (6,1001)
WRITE (6,1008)
WRITE (6,1009)(M(I),TEMP(I),WTOT(I),WE(I),WPROT(I),I=1,WDEPTH)
C
C PRINT POPULATIONS
C
WRITE (6,1010)
W1=MIN(WLH,3)
80 WRITE (6,1011) (I,I,I=W0,W1)
DO 90 ID=1,WDEPTH
  WRITE (6,1015)M(ID),(W(I,ID),M(I,ID)/WS(I,ID),I=0,W1)
90 CONTINUE
IF (W1.LT.WLH)THEN
  W1=W1+1
  W1=MIN(WLH,W1+3)
  GO TO 80
ENDIF
WRITE (6,1012)
W1=MIN(WLHE1,3)
100 WRITE (6,1011) (I,I,I=W0,W1)
DO 110 ID=1,WDEPTH
WRITE (6,1015)M(ID),WHE1(I,ID),WHE1(I,ID)/WHE1S(I,ID),
I=NO,NI)
110 CONTINUE
IF (NI.LT.WLHE1)THEN
  NO=NI+1
  NI=MIN(WLHE1,NI+3)
  GO TO 100
ENDIF
WRITE (6,1013)
NO=1
NI=MIN(WLHE2,3)
120 WRITE (6,1011) (I,I=NO,NI)
DO 130 ID=1,NDEPT
WRITE (6,1015)M(ID),WHE2(I,ID),WHE2(I,ID)/WHE2S(I,ID),
I=NO,NI)
130 CONTINUE
IF (NI.LT.WLHE2)THEN
  NO=NI+1
  NI=MIN(NI+3,WLHE2)
  GO TO 120
ENDIF
WRITE (6,1014)
DO 140 ID=1,NDEPT
WRITE (6,1015)M(ID),WHE3(ID)
140 CONTINUE
C C PRINT RATES AS A DIAGNOSTIC
C IF (.NOT.FPRINT)RETURN
WRITE (6,1001)
WRITE (6,1016)
WRITE (6,1017)
DO 150 I=1,MLH
WRITE (6,1018)(CR(I,J),J=1,MLH+1)
150 CONTINUE
WRITE (6,1019)
DO 160 I=1,MLHE1
WRITE (6,1018)(CRHE1(I,J),J=1,MLHE1+1)
160 CONTINUE
WRITE (6,1020)
DO 170 I=1,MLHE2
WRITE (6,1018)(CRHE2(I,J),J=1,MLHE2+1)
170 CONTINUE
WRITE (6,1001)
WRITE (6,1021)
WRITE (6,1017)
DO 180 I=1,MLH+1
WRITE (6,1018)(RS(I,J),J=1,MLH+1)
180 CONTINUE
WRITE (6,1019)
DO 190 I=1,MLHE1+1
WRITE (6,1018)(RSHE1(I,J),J=1,MLHE1+1)
190 CONTINUE
WRITE (6,1020)
DO 200 I=1,MLHE2+1
WRITE (6,1018)(RSHE2(I,J),J=1,MLHE2+1)
200 CONTINUE
WRITE (6,1001)
RETURN
C 1001 FORMAT (IH1)
1002 FORMAT (H BOUND-FREE JUMPS: )
1003 FORMAT (H HYDROGEN )
1004 FORMAT (H ,I2, ':', F6.2)
1005 FORMAT (H HELIUM I )
1006 FORMAT (H HELIUM II )
1007 FORMAT (H TOTAL SURFACE FLUX = ',E14.6)
1008 FORMAT (4X,'MASS',SX,'TEMPERATURE',6X,'TOTAL W',11X,'WE',13X,'MP')
1009 FORMAT (E11.3,4E15.8)
1010 FORMAT (1H ,0.6X, 'HYDROGEN POPULATIONS')
1011 FORMAT (6X,'MASS',3(6X,'(',I2,')',SX,'NS(',I2,')'))
1012 FORMAT (1H ,32X, 'BELIUM I POPULATIONS')
1013 FORMAT (1H ,32X, 'BELIUM II POPULATIONS')
1014 FORMAT (1H ,32X, 'BELIUM III POPULATION'//6X,'MASS',6X,'W')
1015 FORMAT (E11.3,6E11.3)
1016 FORMAT (1X,'COLLISION RATES AT DEPTHS')
1017 FORMAT (4X,'HYDROGEN')
1018 FORMAT (1X,7E11.4)
1019 FORMAT (4X,'NEUTRAL HELIUM')
1020 FORMAT (4X,'IONIZED HELIUM')
SUBROUTINE INDEXI(W,ARRIN,INDI)

C FROM "NUMERICAL RECIPES"
C
C CREATES AN INDEX ARRAY FOR A VECTOR ARRIN.
C
REAL ARRIN(W)
INTEGER INDI(W)
DO 10 J=1,W
INDI(J)=J
10 CONTINUE
L=W/2+1
IR=W
20 CONTINUE
IF (L.GT.1) THEN
   L=L-1
   INDI=L
   Q=ARRIN(INDI)
ELSE
   INDI=INDI(IR)
   Q=ARRIN(INDI)
   INDEX(IR)=INDEX(1)
   IR=IR-1
   IF (IR.EQ.1) THEN
      INDEX(1)=INDI
      RETURN
   ENDIF
   I=L
   J=L+L
30 IF (J.LE.IR) THEN
   IF (J.LT.IR) THEN
      IF (ARRIN(INDI(J)).LT.ARRIN(INDI(J+1))) J=J+1
   ENDIF
   IF (Q.LT.ARRIN(INDI(J))) THEN
      INDEX(J)=INDEX(J)
      I=J
   ELSE
      J=IR+1
   ENDIF
   GO TO 30
ENDIF
GO TO 20
END

SUBROUTINE LINEAR

C MAIN LINEARIZATION ROUTINE
C
C IMPLICIT NONE
C
C MACROS
C
C COMA
COMF
C
LOCAL VARIABLES
C
INTEGER I, IBASE, ID, J, K
REAL D(NWNN,NWNN+1), NU(NWNN), Nuo(NWNN)
EQUIVALENCE (D(1,NWNN+1), NU(1))
C
INTEGER IOSTATUS
REAL MATGEN, MATINV, OUT, RDABS, WRABS, XTMEDARS
EXTERNAL IOSTATUS, MATGEN, MATINV, OUT, RDABS, WRABS, XTMEDARS
C
DO 130 ID=1,NDEPHS
C
GENERATE LEVEL MATRICES
C
CALL MATGEN(ID)
   IF (ID.EQ.150 TO 50)
   DO 40 I=1,NWNN
   DO 10 K=1,NWNN
      Q(I)=Q(I)+A(I,K)*NU(K)
CONTINUE
DO 30 J=1,III
DO 20 K=1,III
B(I,J)=B(I,J)-A(I,K)*D(K,J)
CONTINUE
CONTINUE
CONTINUE
DO 50 CALL MATINV(B,III,III)
IBASE=IOSTATUS(8,I)
DO 60 I=1,III
NU(I)=0.0
CONTINUE
DO 60 I=1,III
DO 70 J=1,III
NU(I)=NU(I)+B(I,J)*Q(J)
CONTINUE
CONTINUE
IF (ID.EQ.IDECPTB)GO TO 130
DO 120 J=1,III
DO 90 I=1,III
D(I,J)=0.
DO 110 I=1,III
DO 100 K=1,III
D(I,J)=D(I,J)+B(I,K)*C(K,J)
CONTINUE
CONTINUE
CONTINUE
IBASE=(ID-1)*KIII*(MIII+1)
CALL WRABS(8,D,KIII*(MIII+1),IBASE)
CONTINUE
CONTINUE
DO 130 ID=IDECPTB,1,-1
IBASE=IOSTATUS(8,I)
IF (ID.EQ.IDECPTB)GO TO 160
DO 150 I=1,III
DO 140 J=1,III
U(I,O)=U(I,O)+D(I,J)*UO(J)
CONTINUE
CONTINUE
CONTINUE
IBASE=IOSTATUS(9,I)
DO 170 I=1,III
UO(I)=U(I)
CONTINUE
CALL WRABS(9,UO,III,MIII*(ID-1))
IF (ID.EQ.IDEPTB)GO TO 190
IBASE=(ID-2)*KIII*(MIII+1)
CALL RDABS(8,D,MIII*(MIII+1),IBASE)
CONTINUE
CONTINUE
CALL OUT
RETURN
END

SUBROUTINE LIMIT(ITER)
C CALCULATE VALUE FOR SWITCHING PARAMETER
C IMPLICIT NONE
C COMA
C COMC
C INTEGER I, ITER, J
C REAL FAC
C REAL COLRAT, NURATE, WTSET
C EXTERNAL COLRAT, NURATE, WTSET
C KEEP LAMBDA=1.0 IF NO SWITCHING EMPLOYED
C IF ((.NOT.FSWITCH).AND.(ITER.GT.1))RETURN
C INITIALIZE IF FIRST ITERATION
C IF (ITER.LE.1)THEN
C SET LAMBDA=1.0 IF NO SWITCHING EMPLOYED.
C IF (.NOT.FSWITCH)THEN
LAM=1.0
LAM=1.0
ELSE

LAMBDA NOT SPECIFIED IN INPUT FILE

LAML=1.0
IF (LAML.LE.0.) THEN

FIND MAXIMUM OF R/C (NOT MIN C/R SINCE R MAY BE ZERO)

CALL WSET(1.)
LAML=1.
CALL CURAT(TEMP(1),CR,CRBE1,CRBE2)
CALL URATE(1)
LAML=0.
DO 20 I=1,ILH
   DO 10 J=I+1,ILH+1
      LAML=MAX(LAML,DB(I,J)/CR(I,J))
   CONTINUE
20 CONTINUE
DO 40 I=1,ILBE1
   DO 30 J=I+1,ILBE1+1
      LAML=MAX(LAML,DBE1(I,J)/CRBE1(I,J))
   CONTINUE
30 CONTINUE
DO 60 I=1,ILBE2
   DO 50 J=I+1,ILBE2+1
      LAML=MAX(LAML,DBE2(I,J)/CRBE2(I,J))
   CONTINUE
50 CONTINUE
LAML=1.0
ELSE

SUBSEQUENT ITERATIONS WHEN EMPLOYING SWITCHING

FAC=10.
IF (LINERR.GT.(.02))FAC=2.
IF (LINERR.GT.(.10))FAC=1.
LAML=FAC•LAML
IF (LAML.GT.(.1))LAML=1.0
ENDIF
CALL WSET(LAML)
RETURN
END

SUBROUTINE MATGEN(IDD)

GENERATE LINEARIZATION MATRICES

IMPLICIT NONE

MACROS
COMA
COMAI
CONC
CONF

LOCAL VARIABLES

INTEGER IB, ID, IDD, IJ, J
REAL BETO(NWB), BETO(NWB,NWW), BETP(NWB,NWW)
REAL CHI(NWJ,NWW+1), CHL(NWJ,NWW+1), ETAO(NWJ,NWW+1)
REAL CHIP(NWJ,NWDEPT), ETAP(NWJ,NWDEPT)
REAL DEL(NWB), DELO(NWB,NWW), GAMMA(NWB)
REAL GAM(NWB,NWW), GANO(NWB,NWW), GANO(NWB,NWW)
REAL KAP(NWB), KAPP(NWB), KAPPA(NWB)
REAL PSI(NWB), PARM(NWB+3)
REAL PEP(NWB+3), PRO(NWB+3), RHO(NWB)
REAL TT(NWW)
REAL XIOPPO(NWB), XIOPPO(NWB,NWW), XIOPPP(NWB,NWW)
REAL XIOPO(NWB), XIOPO(NWB,NWW), XIOPPOP(NWB,NWW)
REAL XIOMO(NWB), XIOMO(NWB,NWW), XIOMO(NWB,NWW)
REAL XIOMN(NWB), XIOMN(NWB,NWW), XIOMN(NWB,NWW)
REAL CONE, DELM, DELP, DELTA, VX, VY, VZ, V21, V22
EQUIVALENCE (CHIP, CHI), (ETAP, ETA), (BETA, GAMMA, DEL)
EQUIVALENCE (BETO, GAMO, OELO), (BETP, GAMP)

BE SURE ALL THE LOCAL VARIABLES ARE RETAINED FOR THE NEXT CALL.

SAVE

EXTERNAL PROCEDURES

REAL OGEIER
EXTERNAL OGEIER

START OF EXECUTABLE STATEMENTS

CLEAR EVERYTHING FIRST

ID=100
Q(E)=Q(W)/(E)/W/ID/MYD
DO 10 I=1,NN
Q(I)=0.0
10 CONTINUE
DO 20 I=1,NN
B(I,J)=0.0
A(I,J)=0.0
C(I,J)=0.0
20 CONTINUE
DO 30 I=1,NN
30 CONTINUE

TRANSFER EQUATIONS

FIRST DEPTH POINT

IF (ID.GT.1) GO TO 210

CLEAR SUMMATIONS

DO 40 IB=1,NB
KAPPA(IB)=0.
RHO(IB)=0.
PHI(IB)=0.
BETO(IB, J)=0.
XIOPO(IB,J)=0.
40 CONTINUE
DO 60 IB=1,NB
DO 50 J=1,NN
BETO(IB,J)=0.
BETP(IB,J)=0.
XIOPO(IB,J)=0.
50 CONTINUE
60 CONTINUE

ACCUMULATE SOURCE TERMS

DO 70 IJ=1,NN
IB=BLOCK(IJ)
KAPPA(IB)=KAPPA(IB)+WT(IJ)*FK(IJ,1)*RAD(IJ,1)
KAPP(IB)=KAPP(IB)+WT(IJ)*FK(IJ,2)*RAD(IJ,2)
RHO(IB)=RHO(IB)+WT(IJ)*RAD(IJ,1)
PHI(IB)=PHI(IB)*WT(IJ)*RAD(IJ,1)*FS(IJ)
70 CONTINUE
CALL DGNER(1,PRO)

SAVE LOWER LEVEL OPECITIES

DO 80 IJ=1,NN+1
CHI0(IJ,J)=CHI(IJ,J)
ETA0(IJ,J)=ETA(IJ,J)
80 CONTINUE

CALL DGNER(2,PRP)
C SOURCE SUMS

DO 110 IJ=1,BJ
IB=BLOCK(IJ)
VY=WT(IJ)*((CHIO(IJ,BBB+1)-COBE)*RAD(IJ,1)-ETAO(IJ,BBB+1))
  /CBIO(IJ,BBB+1)
VZ=CHIO(IJ,BBB+1)+CHIP(IJ,BBB+1)
BETA(IB)=BETA(IB)+VY*VZ
DO 100 I=1,BBB
  VX=-COBE*MU1*PRO(I)/BM(1)
  BETO(IB,I)=BETO(IB,I)+WT(IJ)*((CHIO(IJ,I)-VI)*RAD(IJ,1)-ETAO(IJ,I))
     *VZ/CHIO(IJ,BBB+1)+VY*CHIO(IJ,I)*(1-VZ/CHIO(IJ,BBB+1))
  BETP(IB,I)=BETP(IB,I)+VY*CHIP(IJ,I)
100 CONTINUE

VI=COBE*(1.0+MU1*BE(1)/BM(1))
BETO(IB,BB)=BETO(IB,BB)-WT(IJ)*VI*RAD(IJ,1)*VZ/CHIO(IJ,BBB+1)
BETO(IB,IB)=BETO(IB,IB)+WT(IJ)*(CHIO(IJ,BBB+1)-COBE)*RAD(IJ,1)*
     VZ/CHIO(IJ,BBB+1)
110 CONTINUE

C OPACITY SUMS

DO 130 IJ=1,BJ
IB=BLOCK(IJ)
VI1=CHIP(IJ,BBB+1)+CHIO(IJ,BBB+1)
VI=WT(IJ)*FK(IJ,2)*RAD(IJ,2)/VX1
IIOPP(IB)=IIOPP(IB)+VX
VY=WT(IJ)*FK(IJ,1)*RAD(IJ,1)/VX1
IIOPO(IB)=IIOPO(IB)+VY
DO 120 I=1,BBB
  IIOPPO(IB,I)=IIOPPO(IB,I)-VX*CBIO(IJ,I)/VX1
  IIOPPP(IB,I)=IIOPPP(IB,I)-VX*CHIP(IJ,I)/VI1
  IIOPOO(IB,I)=IIOPOO(IB,I)-VY*CHIO(IJ,I)/VI1
  IIOPOP(IB,I)=IIOPOP(IB,I)-VY*CHIP(IJ,I)/VX1
120 CONTINUE

130 CONTINUE

C BORMALIZE

DO 150 IB=1,NB
  IIOPP(IB)=2.*IIOPP(IB)/KAPP(IB)
  IIOPO(IB)=2.*IIOPO(IB)/KAPPA(IB)
  PHI(IB)=PHI(IB)/RHO(IB)
  BETA(IB)=0.5*BETA(IB)
150 CONTINUE

DO 160 IB=1,BB
  DO 150 I=1,BBB
    BETO(IB,I)=0.5*BETO(IB,I)
    BETP(IB,I)=0.5*BETP(IB,I)
    IIOPPO(IB,I)=2.*IIOPPO(IB,I)/KAPP(IB)
    IIOPPP(IB,I)=2.*IIOPPP(IB,I)/KAPP(IB)
    IIOPOO(IB,I)=2.*IIOPOO(IB,I)/KAPPA(IB)
    IIOPOP(IB,I)=2.*IIOPOP(IB,I)/KAPPA(IB)
160 CONTINUE

170 CONTINUE

C MOVE SUMS DOWN IF NOT AT SURFACE

DO 210 IB=1,NB
  KAPM(IB)=KAPPA(IB)
210 CONTINUE

C SOURCE SUMS

DO 110 IJ=1,NJ
IB=BLOCK(IJ)
VY=WT(IJ)*((CHIO(IJ,NWW+1)-COBE)*RAD(IJ,1)-ETAO(IJ,NWW+1))
  /CHIO(IJ,NWW+1)
VZ=CHIO(IJ,NWW+1)+CHIP(IJ,NWW+1)
BETA(IB)=BETA(IB)+VY*VZ
DO 100 I=1,NWW
  VX=COBE*MU1*PRO(I)/NW(1)
  BETO(IB,I)=BETO(IB,I)+WT(IJ)*((CHIO(IJ,I)-VI)*RAD(IJ,1)-
     ETAO(IJ,I))*VZ/CHIO(IJ,I,NWW+1)+VY*CHIO(IJ,I,NWW+1)
     *(1-VZ/CHIO(IJ,I,NWW+1))
  BETP(IB,I)=BETP(IB,I)+VY*CHIP(IJ,I)
100 CONTINUE

VI=COBE*(1.0+MU1*WE(1)/NW(1))
BETO(IB,BB)=BETO(IB,BB)-WT(IJ)*VI*RAD(IJ,1)*VZ/CHIO(IJ,I,NWW+1)
BETO(IB,IB)=BETO(IB,IB)+WT(IJ)*(CHIO(IJ,I,NWW+1)-COBE)*RAD(IJ,1)*
     VZ/CHIO(IJ,I,NWW+1)
110 CONTINUE

C OPACITY SUMS

DO 130 IJ=1,NJ
IB=BLOCK(IJ)
VI1=CHIP(IJ,NWW+1)+CHIO(IJ,NWW+1)
VI=WT(IJ)*FK(IJ,2)*RAD(IJ,2)/VX1
IIOPP(IB)=IIOPP(IB)+VX
VY=WT(IJ)*FK(IJ,1)*RAD(IJ,1)/VX1
IIOPO(IB)=IIOPO(IB)+VY
DO 120 I=1,NWW
  IIOPPO(IB,I)=IIOPPO(IB,I)-VX*CBIO(IJ,I)/VX1
  IIOPPP(IB,I)=IIOPPP(IB,I)-VX*CHIP(IJ,I)/VI1
  IIOPOO(IB,I)=IIOPOO(IB,I)-VY*CHIO(IJ,I)/VI1
  IIOPOP(IB,I)=IIOPOP(IB,I)-VY*CHIP(IJ,I)/VX1
120 CONTINUE

130 CONTINUE

C BORMALIZE

DO 150 IB=1,NB
  IIOPP(IB)=2.*IIOPP(IB)/KAPP(IB)
  IIOPO(IB)=2.*IIOPO(IB)/KAPPA(IB)
  PHI(IB)=PHI(IB)/RHO(IB)
  BETA(IB)=0.5*BETA(IB)
150 CONTINUE

DO 160 IB=1,BB
  DO 150 I=1,NWW
    BETO(IB,I)=0.5*BETO(IB,I)
    BETP(IB,I)=0.5*BETP(IB,I)
    IIOPPO(IB,I)=2.*IIOPPO(IB,I)/KAPP(IB)
    IIOPPP(IB,I)=2.*IIOPPP(IB,I)/KAPP(IB)
    IIOPOO(IB,I)=2.*IIOPOO(IB,I)/KAPPA(IB)
    IIOPOP(IB,I)=2.*IIOPOP(IB,I)/KAPPA(IB)
160 CONTINUE

170 CONTINUE

C NOW CALCULATE THE ACTUAL LINEARIZATION MATRIX ELEMENTS

DELP=M(2)-M(1)
DO 190 IB=1,NB
  DO 180 I=1,NWW
    B(IB,I)=(XIOPPO(IB,I)*KAPP(IB)-XIOPOO(IB,I)*KAPPA(IB))/DELP+
      0.5*DELP*BETO(IB,I)
    C(IB,I)=(XIOPPP(IB,I)*KAPP(IB)-XIOPOPP(IB,I)*KAPPA(IB))/DELP+
      0.5*DELP*BETP(IB,I)
180 CONTINUE

190 CONTINUE

DO 200 IB=1,NB
  B(IB,IB)=K(IP(IB),IB)*RHO(IB)/DELP+PHI(IB)*RHO(IB)
  C(IB,IB)=C(IP(IB),IB)*KAPPA(IB)/DELP
200 CONTINUE

GO TO 540

C MOVE SUMS DOWN IF NOT AT SURFACE

DO 210 IB=1,NB
  KAPM(IB)=KAPPA(IB)
210 CONTINUE

C BORMALIZE

DO 150 IB=1,NB
  IIOPP(IB)=2.*IIOPP(IB)/KAPP(IB)
  IIOPO(IB)=2.*IIOPO(IB)/KAPPA(IB)
  PHI(IB)=PHI(IB)/RHO(IB)
  BETA(IB)=0.5*BETA(IB)
150 CONTINUE

DO 160 IB=1,BB
  DO 150 I=1,NWW
    BETO(IB,I)=0.5*BETO(IB,I)
    BETP(IB,I)=0.5*BETP(IB,I)
    IIOPPO(IB,I)=2.*IIOPPO(IB,I)/KAPP(IB)
    IIOPPP(IB,I)=2.*IIOPPP(IB,I)/KAPP(IB)
    IIOPOO(IB,I)=2.*IIOPOO(IB,I)/KAPPA(IB)
    IIOPOP(IB,I)=2.*IIOPOP(IB,I)/KAPPA(IB)
160 CONTINUE

170 CONTINUE

C NOW CALCULATE THE ACTUAL LINEARIZATION MATRIX ELEMENTS

DELP=M(2)-M(1)
DO 190 IB=1,NB
  DO 180 I=1,NWW
    B(IB,I)=(XIOPPO(IB,I)*KAPP(IB)-XIOPOO(IB,I)*KAPPA(IB))/DELP+
      0.5*DELP*BETO(IB,I)
    C(IB,I)=(XIOPPP(IB,I)*KAPP(IB)-XIOPOPP(IB,I)*KAPPA(IB))/DELP+
      0.5*DELP*BETP(IB,I)
180 CONTINUE

190 CONTINUE

DO 200 IB=1,NB
  B(IB,IB)=K(IP(IB),IB)*RHO(IB)/DELP+PHI(IB)*RHO(IB)
  C(IB,IB)=C(IP(IB),IB)*KAPPA(IB)/DELP
200 CONTINUE

GO TO 540

C MOVE SUMS DOWN IF NOT AT SURFACE

DO 210 IB=1,NB
  KAPM(IB)=KAPPA(IB)
KAPPA(IB)=KAPPA(IB)
KAPP(IB)=0.
GANMA(IB)=0.
XIOMO(IB)=XIOPP(IB)
XIOPP(IB)=0.0
XIOM(IB)=XIOPO(IB)
XIOPO(IB)=0.0
220 CONTINUE
DO 240 IB=1,IB
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IB
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
220 CONTINUE
DO 240 IB=1,IBM
DO 230 J=1,IBM
GANN(IB,J)=0.
GANO(IB,J)=0.
GANO(IB,J)=GANO(IB,J)
GANO(IB,J)=GANO(IB,J)
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
XIN0N(IB,J)=XIOPP(IB,J)
XIOPP(IB,J)=0.
VX1 = CBIP(I,J,111+1) + cBIO(I,J,111+1)
VX = IIT(I,J) • FK(I,J,ID+1) • RAD(I,J,ID+1) / VX1
XIOPP(IB) = XIOPP(IB) + VX
VY = IIT(I,J) • FK(I,J,ID) • RAD(I,J,ID) / VX1
XIOPO(IB) = XIOPO(IB) + VY
DO 300 I = 1, III
216 XIOPPO(IB,I) = XIOPPO(IB,I) - VX • CBIO(I,J,I) / VX1
XIOPPP(IB,I) = XIOPPP(IB,I) - VX * CBIP(I,J,I) / VX1
XIOPOO(IB,I) = XIOPOO(IB,I) - VY • CBIO(I,J,I) / VX1
XIOPOP(IB,I) = XIOPOP(IB,I) - VY • CBIP(I,J,I) / VX1
300 CONTINUE
310 CONTINUE
C C NORMALIZE
C DO 320 IB = 1, NB
XIOPP(IB) = 2. • XIOPP(IB) / KAPP(IB)
XIOPO(IB) = 2. • XIOPO(IB) / KAPPA(IB)
GAMMA(IB) = 0.25 • GAMMA(IB)
320 CONTINUE
C C NOW CALCULATE THE ACTUAL LINEARIZATION MATRIX ELEMENTS
C DO 360 IB = 1, NB
A(IB,J) = (XIMOMN(IB,J) • KAPM(IB) - XIMOM(IB,J) • KAPPA(IB)) / DELM - GAMM(IB,J)
B(IB,J) = -(XIOPPO(IB,J) • KAPP(IB) - XIOPOO(IB,J) • KAPPA(IB)) / DELP + (XINO0O(IB,J) • KAPPA(IB) - XINOMO(IB,J) • KAPN(IB)) / DELN - GAMO(IB,J)
C(IB,J) = (XIOPPP(IB,J) • KAPP(IB) - XIOPOP(IB,J) • KAPPA(IB)) / DELP - GAMP(IB,J)
350 CONTINUE
360 CONTINUE
DO 370 IB = 1, NB
A(IB,IB) = A(IB,IB) + XIMON(IB) • KAPN(IB) / DELN
B(IB,IB) = B(IB,IB) + XIOPO(IB) • KAPPA(IB) / DELP + XIMOO(IB) • KAPPA(IB) / DELM
C(IB,IB) = C(IB,IB) - XIOPO(IB) • KAPPA(IB) / DELP - (XIMOM(IB) • KAPPA(IB) - XINOM(IB) • KAPM(IB)) / DELM - GAMM(IB)
370 CONTINUE
GO TO 540
C C TRANSFER EQUATION AT LOWER BOUNDARY
C 380 DO 400 IB = 1, NB
DELO(IB) = 0.
390 CONTINUE
DO 410 IB = 1, NB
DELO(IB,J) = 0.
400 CONTINUE
410 CONTINUE
DO 430 IJ = 1, N
IB = BLOCK(IJ)
VI = B*FREQ(IJ) / TEMP(NDEPTB)
VI1 = EXP(VI)
C C PLANK FUNCTION
C VZ = BCOF * FREQ(IJ) ** 3 / (VI1 - 1.0)
C C DERIVATIVE OF PLANK FUNCTION WITH TEMPERATURE
C VZ1 = VZ + VX * VI1 / (VI1 - 1.0) / TEMP(ID)
C C DERIVATIVE OF (DERIVATIVE OF PLANK FUNCTION WITH TEMPERATURE) WITH
C LOG TEMPERATURE
C
VZ2=VZ1*(-2.0-VX1+2.0*VX1/(VX1-1.0))
VY=WT(IJ)+VZ1/CHIO(IJ,NNN+1)
DELO(IB)=DELO(IB)+VY
DO 420 IB=1,NNN
DELO(IB,J)=DELO(IB,J)-VY*CHIO(IJ,NNN+1)
CONTINUE
420 CONTINUE
DELO(IB,NWT)=DELO(IB,NWT)+WT(IJ)+VZ2/CHIO(IJ,NNN+1)
CONTINUE
430 CONTINUE
VY=0.
DO 440 IB=1,NNN
VY=VY+DELO(IB)
440 CONTINUE
DO 450 J=1,NNN
TT(J)=0.
450 CONTINUE
DO 470 IB=1,NNN
DELO(IB,J)=DELO(IB,J)-VY*CBIO(IJ,J)/CBIO(IJ,111+1)
470 CONTINUE
DO 480 IB=1,NNN
DELO(IB,IIT)=DELO(IB,IIT)+WT(IJ)/CBIO(IJ,111+1)
480 CONTINUE
VY=0.
DO 490 IB=1,IB
VY=VY+DELO(IB)
490 CONTINUE
DO 500 J=1,111
TT(J)=0.
500 CONTINUE
DO 510 IB=1,IB
DO 520 J=1,111
DELO(IB,J)=-(DELO(IB)*TT(J)+BO*DELO(IB,J))/VY
520 CONTINUE
510 CONTINUE
DELM=DELP
DO 530 IB=1,IB
DO 540 J=1,111
A(IB,J)=-(XIMOMM(IB,J)*KAPM(IB)-XIMOMM(IB,J)*KAPPA(IB))/DELM
B(IB,J)=(XIMOOO(IB,J)*KAPPA(IB)-XIMOMO(IB,J)*KAPM(IB))/DELM
Q(IB)=DELO(IB,J)-(-DELO(IB)*TT(J)+BO*DELO(IB,J))/VY
540 CONTINUE
530 CONTINUE
DO 550 IJ=1,IJ
VI=WT(IJ)+((CHIO(IJ,NNN+1)-COIE)*RAD(IJ,1)-ETAO(IJ,1))/Q(NWT)+VX
550 CONTINUE
DO 570 IB=1,IB
DO 560 J=1,JS
B(NWT,J)=B(NWT,J)-((CHIO(IJ,J)-VZ)*RAD(IJ,ID)-ETAO(IJ,J))/Q(NWT)+VX
560 CONTINUE
570 CONTINUE
VZ=VZ1+(-2.0-VX1+2.0*VX1/(VX1-1.0))
DO 610 IJ=1,IB
IB=BLOCK(IJ)
VX=BYDCOF*IB+NE(ID)/NNN
DO 580 IJ=1,IB
B(NWT,NNN)=B(NWT,NNN)+VZ*RAD(IJ,ID)
580 CONTINUE
590 CONTINUE
DO 600 IJ=1,IB
IB=BLOCK(IJ)
B(NWT,IB)=B(NWT,IB)-((CHIO(IJ,NNN+1)-COIE)*RAD(IJ,ID)-ETAO(IJ,1))/Q(NWT)+VX
600 CONTINUE
610 CONTINUE
C BUILD LINEARIZATION MATRICES
DELM=DELP
DO 520 IB=1,IB
DO 540 J=1,111
A(IB,J)=-(XIMOMM(IB,J)*KAPM(IB)-XIMOMM(IB,J)*KAPPA(IB))/DELM
B(IB,J)=(XIMOOO(IB,J)*KAPPA(IB)-XIMOMO(IB,J)*KAPM(IB))/DELM
Q(IB)=DELO(IB,J)-(-DELO(IB)*TT(J)+BO*DELO(IB,J))/VY
540 CONTINUE
530 CONTINUE
DO 550 IJ=1,IJ
VI=WT(IJ)+((CHIO(IJ,NNN+1)-COIE)*RAD(IJ,1)-ETAO(IJ,1))/Q(NWT)+VX
550 CONTINUE
DO 570 IB=1,IB
DO 560 J=1,JS
B(NWT,J)=B(NWT,J)-((CHIO(IJ,J)-VZ)*RAD(IJ,ID)-ETAO(IJ,J))/Q(NWT)+VX
560 CONTINUE
570 CONTINUE
VZ=VZ1+(-2.0-VX1+2.0*VX1/(VX1-1.0))
DO 610 IJ=1,IB
IB=BLOCK(IJ)
VX=BYDCOF*IB+NE(ID)/NNN
DO 580 IJ=1,IB
B(NWT,NNN)=B(NWT,NNN)+VZ*RAD(IJ,ID)
580 CONTINUE
590 CONTINUE
DO 600 IJ=1,IB
IB=BLOCK(IJ)
B(NWT,IB)=B(NWT,IB)-((CHIO(IJ,NNN+1)-COIE)*RAD(IJ,ID)-ETAO(IJ,1))/Q(NWT)+VX
600 CONTINUE
610 CONTINUE
C RADIATIVE EQUILIBRIUM
C
IF (ID.GT.1)GO TO 630
DO 610 IJ=1,IB
IB=BLOCK(IJ)
VX=BYDCOF*WT(IJ)+NE(ID)*RAD(IJ,1)
Q(NWT)=Q(NWT)+V*(CHIO(IJ,NNN+1)-COIE)*RAD(IJ,ID)
DO 600 IJ=1,IB
610 CONTINUE
C HYDROSTATIC EQUILIBRIUM
C
C SURFACE
C
B(NWW, I) = B(NWW, I) + VX * CHIO(IJ, I)

CONTINUE
B(NWW, IB) = B(NWW, IB) + VX * CHIO(IJ, NW + I)

CONTINUE
B(NWW, NWT) = B(NWW, NWT) + PRO(NWW + I) * TEMP(ID) / M(1)
CONTINUE
Q(NWW) = PRO(NWW + 1) * TEMP(ID) / M(1) + CHAV / KB
RETURN

COITIIIUE

DO 620 I = 1, NW
B(NWW, I) = B(NWW, I) + PR0(I) * TEP1P(ID) / M(1)
CONTINUE
Q(NWW) = PRO(I + 1) * TEMP(ID) / M(1)
IF (ABS(Q(NWW)) .GT. GRW / KB) WRITE (6, *) 'EDDINGTON LIMIT WARNING'
RETURN

COITIIIUE

DO 630 IB = 1, NW
A(NWW, IB) = PRM(IB) * TEMP(ID-1) + HYCOF * KAPM(IB)
B(NWW, IB) = PRO(IB) * TEMP(ID) + HYCOF * KAPPA(IB)
Q(NWW) = HYCOF * (KAPPA(IB) - KAPM(IB))
RETURN

END

SUBROUTINE NUPOP(IDD)

RECALCUUTE POPULATIONS BASED ON RADIATION FIELD

IMPLICIT NONE

INTEGER IDD, ID, I
REAL COLR, TOT, RATEQ
EXTERNAL COLR, TOT, RATEQ
REAL SB, SBBE1, SBBE2

SB(I, ID) = ACCOF * EXP(HK * FRQH(I) / TEMP(ID)) * CH1(I) / TEMP(ID) / 
SQRT(TEMP(ID))
SBBE1(I, ID) = ACCOF * EXP(HK + FRQBE1(I) / TEMP(ID)) * CH1(I) / 
TEMP(ID) / SQRT(TEMP(ID))/2.
SBBE2(I, ID) = ACCOF * EXP(HK + FRQBE2(I) / TEMP(ID)) * CH1(I) / 
TEMP(ID) / SQRT(TEMP(ID))

ID = IDD
CALL COLRAT(TEMP(ID), CR, CRBE1, CRBE2)
CALL RJ.TEQ(ID, IE(ID), A1, B1)
CALL LIISLV(A1, B1, AIS, IEQ1, IEQ2)
ITOT(ID) = IE(ID)
DO 10 I = 1, ILB
AIS(I, ID) = AIS(I) + AIS(I+ILBE1+1) + AIS(I+ILBE2+1)
ITOT(ID) = ITOT(ID) + A1(I, ID)
10 CONTINUE
PROTOT(ID) = PROTOT(ID) * SBBE1(I, ID)
PROTOT(ID) = PROTOT(ID) * SBBE2(I, ID)
DO 20 I = 1, ILBE1
WB(I, ID) = AIS(I) + WB(I, ID) + AIS(I+ILBE2+1)
ITOT(ID) = ITOT(ID) + WB(I, ID)
20 CONTINUE
DO 30 I = 1, ILBE2
WB(I, ID) = AIS(I) + WB(I, ID) + AIS(I+ILBE2+1)
ITOT(ID) = ITOT(ID) + WB(I, ID)
30 CONTINUE
DO 40 I = 1, ILBS
IS(I, ID) = IE(ID) * IPROT(ID) * SB(I, ID)
40 CONTINUE
DO 50 I = 1, ILBE1S
IBE1S(I, ID) = IE(ID) * IBE1(I, ID) * SBBE1(I, ID)
50 CONTINUE
DO 60 I = 1, ILBE2S
IBE2S(I, ID) = IE(ID) * IBE2S(I, ID) * SBBE2(I, ID)
60 CONTINUE
CONTINUE
BM(ID)=(XTOT(ID)-WM(ID))\*MU1
RETURN
END

SUBROUTINE WURATE(IDD)
C
CALCULATE RADIATIVE RATE BRACKETS
C
IMPLICIT NONE
C
MACROS
C
CONA
CONAI
C
LOCAL VARIABLES
C
INTEGER I, IDD, ID, IJ, IL, IT, J
REAL DOP, DOPT, EX, FREQ, EKT, BT, P, S, SIGMA, SIGMAT, SIGR, SRT
REAL SRT2, I
REAL DSPIDT(I), SPI(I), SR(I)
C
EXTERNAL PROCEDURE
C
REAL PARTI
EXTERNAL PARTI
C
START OF EXECUTABLE STATEMENTS
C
ID=IDD
SRT=SQRT(PTID/TEMP(ID))
SRT2=SQRT(TEMP(ID))
EKT=EKT/TEMP(ID)
BT=BT/TEMP(ID)
C
CLEAR RATES
C
DO 20 I=1,ILB+1
DO 10 J=1,ILB+1
RB(I,J)=0.
DRB(I,J)=0.
10 CONTINUE
20 CONTINUE
DO 40 I=1,ILBE1+1
DO 30 J=1,ILBE1+1
RBE1(I,J)=0.
DRBE1(I,J)=0.
30 CONTINUE
40 CONTINUE
DO 60 I=1,ILBE2+1
DO 50 J=1,ILBE2+1
RBE2(I,J)=0.
DRBE2(I,J)=0.
50 CONTINUE
60 CONTINUE
C
PREPARE FREQUENCY-DEPENDENT VECTORS
C
IF (FLTE)GO TO 260
DO 70 IJ=1,IJ
S=LANC**SCOF**WT(IJ)/FREQ(IJ)
EX=EXP(-EKT**FREQ(IJ))
P=BCOF**FREQ(IJ)**3*RAD(IJ,ID)
SR(IJ)=S*RAD(IJ,ID)
SPI(IJ)=S*P*EI
DSPIDT(IJ)=EKT*FREQ(IJ)*SPI(IJ)
70 CONTINUE
C
TEMPERATURE DERIVATIVE OF RATE
C
DO 90 IL=1,ILB
DO 80 IJ=1,IPTRB-1
DRH(ILB+1,IL)=DRH(ILB+1,IL)+SIG(IJ)*DSPIDT(IJ)
80 CONTINUE
90 CONTINUE
C
SOME OF THE FOLLOWING LOOPS ARE DONE IN A CLUMSY WAY
C
IN ORDER TO ENHANCE VECTORIZATION.
C
DO 120 IT=1,ILB
DO 100 IJ=1,ITPTRB-1
  RR(IT,MLB+1)+RR(IT,MLB+1)+SIG(IT,IJ)*SR(IJ)
100 CONTINUE

DO 110 IJ=1,ITPTRB-1
  RR(MLB+1,IT)+RR(MLB+1,IT)+SIG(IT,IJ)*SPX(IJ)
110 CONTINUE

DO 120 IJ=1,ITPTRB-1
  DRBE1(MLBE1+1,IT)+DRBE1(MLBE1+1,IT)+SIGBE1(IT,IJ)*SR(IJ)
120 CONTINUE

DO 130 IJ=1,ITPTRB-1
  DRBE1(MLBE1+1,IT)+DRBE1(MLBE1+1,IT)+SIGBE1(IT,IJ)*SPX(IJ)
130 CONTINUE

DO 140 IL=1,ILBE1
  DO 150 IJ=1,ITPTRB-1
    DRBE1(ILBE1+1,IL)+DRBE1(ILBE1+1,IL)+SIGBE1(IL,IJ)*DSPXDT(IJ)
  150 CONTINUE

DO 160 IJ=1,ITPTRB-1
  DRBE1(ILBE1+1,IL)+DRBE1(ILBE1+1,IL)+SIGBE1(IL,IJ)*SPX(IJ)
160 CONTINUE

DO 170 IL=1,ILBE2
  DO 180 IJ=1,ITPTRB-1
    DRBE2(ILBE2+1,IL)+DRBE2(ILBE2+1,IL)+SIGBE2(IL,IJ)*DSPXDT(IJ)
  180 CONTINUE

DO 190 IL=1,ILBE2
  DO 200 IJ=1,ITPTRB-1
    DRBE2(ILBE2+1,IL)+DRBE2(ILBE2+1,IL)+SIGBE2(IL,IJ)*SPX(IJ)
  200 CONTINUE

DO 210 IJ=ITPTRB,ITPTRBE1-1
  I=LOWB(IJ)
  J=UPB(IJ)
  IT=ITRBE1(I,J)
  FRQO=FRQBE1(I)-FRQBE1(J)
  DOP=SRT2*FRQO*0.5
  I=DELQUAD(MOD(I1-ITPTRBE1,NQUAD))*SAT
  SIGMA=PIE2MC*OSCB(IT)•EXP(-X*X)/DOP/1.7724539
  SIGMA=SIGMA*(X*X-0.5)/TEIIP(ID)
  RR(I,J)=RR(I,J)*SIGMA*SR(IJ)
  DRBE1(I,J)=DRBE1(I,J)*SIGMA*SR(IJ)
  RBE1(I,J)=RBE1(I,J)+SIGMA*SR(IJ)
  DRBE1(I,J)=DRBE1(I,J)*SIGMA*SR(IJ)
210 CONTINUE

DO 220 IJ=ITPTRBE1,ITPTRBE2-1
  I=LOWBE1(IJ)
  J=UPBE1(IJ)
  IT=ITRBE2(I,J)
  FRQO=FRQBE2(I)-FRQBE2(J)
  DOP=SRT2*FRQO*0.5
  I=DELQUAD(MOD(I1-ITPTRBE2,NQUAD))*SAT
  SIGMA=PIE2MC*OSCB2(IT)•EXP(-X*X)/DOP/1.7724539
  SIGMA=SIGMA*(X*X-0.5)/TEIIP(ID)
  RBE2(I,J)=RBE2(I,J)+SIGMA*SR(IJ)
  DRBE2(I,J)=DRBE2(I,J)*SIGMA*SR(IJ)
  RBE2(I,J)=RBE2(I,J)+SIGMA*SR(IJ)
  DRBE2(I,J)=DRBE2(I,J)*SIGMA*SR(IJ)
220 CONTINUE

DO 230 IJ=ITPTRBE2,NJ
  I=LOWBE2(IJ)
  J=UPBE2(IJ)
  IT=ITRBE2(I,J)
  FRQO=FRQBE2(I)-FRQBE2(J)
  DOP=SRT2*FRQO*0.5
  I=DELQUAD(MOD(I1-ITPTRBE2,NQUAD))*SAT
  SIGMA=PIE2MC*OSCB2(IT)•EXP(-X*X)/DOP/1.7724539
  SIGMA=SIGMA*(X*X-0.5)/TEIIP(ID)
  RBE2(I,J)=RBE2(I,J)+SIGMA*SR(IJ)
  DRBE2(I,J)=DRBE2(I,J)*SIGMA*SR(IJ)
  RBE2(I,J)=RBE2(I,J)+SIGMA*SR(IJ)
  DRBE2(I,J)=DRBE2(I,J)*SIGMA*SR(IJ)
230 CONTINUE

CALL PARTI(ID)
RETURN
SUBROUTINE OUT
C APPLY CORRECTIONS CALCULATED IN LINEAR.
C ONLY RAD, NE, AND TEMP CORRECTIONS ARE BOthered WITH
C SINCE THE REST ARE DEFINED BY THE SUBSEQUENT LAMBDA ITERATION.
C IMPLICIT NONE
C COMA
C COMAI
C REAL ERRMAI, ERRJMAX, ERRMAX, ERRTOT, NU(MMWW)
C INTEGER IB, ID, IJ, IL
C REAL DEL, DELJ
C INTEGER IOSTATUS
C REAL RABS
C EXTERNAL
C IOSTATUS, RABS
C ERRMAX=0.
C ERRMAI=0.
C ERRJMAX=0.
C ERRTOT=0.
DO 20 ID=1, NDEPTH
CALL RABS(9, NU, WW, (ID-1)*MMWW)
IJ=IOSTATUS(9, IL)
OT=0.
DO 20 ID=1, NDEPTH
CALL RABS(9, NU, WW, (ID-1)*MMWW)
IJ=IOSTATUS(9, IL)
DO 10 IB=1, NB
ERRMAX=MAX(ABS(NU(IB)), ERRJMAX)
10 CONTINUE
ERRJMAX=MAX(ERRJMAX, ABS(NU(WN)))
ERRMAX=MAX(ERRMAX, ABS(NU(WN)))
20 CONTINUE
WRITE (6, *)'MAXIMUM J ERROR = ', ERRJMAX
WRITE (6, *)'MAXIMUM NE ERROR = ', ERRMAX
WRITE (6, *)'MAXIMUM T ERROR = ', ERRMAX
EXIT=.FALSE.
ERRTOT=MAX(ERRTOT, ERRMAX)
IF (ERRTOT.LT.(.0001).AID.LAMC.EQ.(1.).AIO.LAML.EQ.(1.))
: EXIT=.TRUE.
LINERR=ERRTOT
C SCALE DOWN LARGE CORRECTIONS TO INCREASE CIRCLE OF CONVERGENCE
C DEL=MIN(0.2/ERRTOT,1.0)
WRITE (6, *)'USING CORRECTION FACTOR OF ', DEL
C NOW APPLY CORRECTIONS
C DO 60 ID=1, NDEPTH
CALL RABS(9, NU, WW, (ID-1)*MMWW)
IJ=IOSTATUS(9, IL)
DO 50 IB=1, NB
IB=BLOCK(IJ)
RAD(IJ,ID)=RAD(IJ,ID)*MAX(0.1,1.0+DEL*NU(IB))
50 CONTINUE
TEMP(ID)=TEMP(ID)*(1.0+DEL*NU(WNT))
NE(ID)=NE(ID)*(1.0+DEL*NU(WNE))
60 CONTINUE
RETURN
END
SUBROUTINE PartI(IDD)
C CALCULATE UPPER-STATE SUMS
C IMPLICIT NONE
C COMA
C COMAI
C INTEGER IDD, ID, IL, IT
C REAL HKT, X
C REAL SB, SBHE1, SBHE2
SUBB(E1,ID)=ACCL*EXP(BK*FRQBE1(ID)/TEMP(ID))*G(E1(ID)/TEMP(ID)/
: SQRT(TEMP(ID))
SBBE2(ID)=ACCL*EXP(BK*FRQBE2(ID)/TEMP(ID))*G(E2(ID)/TEMP(ID)/
: SQRT(TEMP(ID))

END

SUBROUTINE PUTOUT
C
C PUNCH OUT RESULT
C
IMPLICIT NONE
C
INTEGER ID, I
C
WRITE (12,1001) (W(ID),TEMP(ID),WTOT(ID),WE(ID),ID=1,1DEPT)
WRITE (12,1002) 1
WRITE (12,1002) 0,0,MLB,MA
WRITE (12,1003) (FRQBE(I),I=1,ILB)
DO 10 I=1,1MA
WRITE (12,1002) (LOWERBE(I),UPPERBE(I))
10 CONTINUE
WRITE (12,1003) (FRQBE1(I),I=1,ILBE1)
DO 20 I=1,1BE1
WRITE (12,1002) (LOWERBE1(I),UPPERBE1(I))
20 CONTINUE
WRITE (12,1003) (FRQBE2(I),I=1,ILBE2)
DO 30 I=1,1BE2
WRITE (12,1002) (LOWERBE2(I),UPPERBE2(I))
30 CONTINUE
WRITE (12,1003) (NBE1(ID),I=1,1BE1),(NBE2(ID),I=1,1BE2),
: NBE3(ID),ID=1,1DEPT
WRITE (12,1002) 0
RETURN
C
1001 FORMAT (4E15.7)
1002 FORMAT (16I5)
1003 FORMAT (5E15.7)
END

SUBROUTINE RATEQ(IDD,ECALL,1AA,1BB)
C
C PRODUCE RATE EQUATIONS
C
IMPLICIT NONE
C
COMM
REAL AAB(WEQW,WEQW), SBB(WEQW)
INTEGER ID, IDD, I, II, JJ, J, J, NO
REAL ELECI, K, X

REAL SBBE1, SBBE2
SBE1(I,ID)=ACOF•EXP(HK•FRQBE1(I)/TEMP(ID))•GB(I)/TEIIP(ID)/
SQR(TEMP(ID))
SBE2(I,ID)=ACOF•EXP(HK•FRQBE2(I)/TEMP(ID))•GB(I)/
TEMP(ID)/SQR(TEMP(ID))/2.

DO 10 I=1,IEQI
BBI(I)=0.
10 CONTINUE
DO 30 J=1,IEQJ
AAN(I,J)=0.
30 CONTINUE
HKT=HK/TEMP(ID)
DO 40 I=1,ILHE1
AAl(I,I)=RHE1(I,ILHE1+1)+ELEC•CRHE1(I,ILHE1+1)
AAl(I,ILHE1+1)=ELEC•SBHE1(I,ID)•(RHE1(1LHE1+1,I)+
ELEC•CRHE1(I,ILHE1+1))
40 CONTINUE
DO 60 I=1,ILHE1
DO 50 J=1,I-1
JJ=ILBE1+J
AAl(I,II)=AAl(I,II)+ELEC•CRHE2(I,J)
AAl(I,II)=ELEC•CRHE2(I,J)
50 CONTINUE
DO 80 J=I+1,ILHE2
JJ=J+ILHE1
AAl(I,II)=AAl(I,II)+ELEC•CRHE2(I,J)
AAl(I,II)=ELEC•CRHE2(I,J)
80 CONTINUE
DO 100 I=1,ILBE2
II=I+ILHE1
AAl(I,II)=RHE2(I,ILBE2+1)+ELEC•CRHE2(I,ILBE2+1)
AAl(I,ILBE2+1)=ELEC•SBHE2(I,ID)•(RHE2(ILBE2+1,I)+
ELEC•CRHE2(I,ILBE2+1))
100 CONTINUE
DO 110 J=1,ILHE1
JJ=J+ILHE1
AAl(I,II)=AAl(I,II)+ELEC•CRHE1(I,J)
AAl(I,II)=ELEC•CRHE1(I,J)
110 CONTINUE
DO 120 J=J+1,ILHE2
JJ=J+ILHE1
AAl(I,II)=AAl(I,II)+ELEC•CRHE2(I,J)
AAl(I,II)=ELEC•CRHE2(I,J)
120 CONTINUE
! 224

CONTINUE
AAN(NLBE1+NLBE2+1,NEQM)=AAN(NLBE1+NLBE2+1,NEQM)-Y*ELEC*SUMBE(ID)
DO 150 I=1,NLB
 II=NLBE1+NLBE2+1
 AAN(II,II)=RH(I,NLB+1)+ELEC*CR(I,NLB+1)
DO 130 J=1,I-1
 JJ=J+NLBE1+NLBE2+1
 AAN(II,II)=AAN(II,II)+ELEC*CR(I,J)
 AAN(II,JJ)=-ELEC*CR(J,I)
 X=GB(J)*EXP(HKT*(FRQB(J)-FRQB(I)))/GB(I)
 AAN(II,II)=AAN(II,II)+X*RB(I,J)
 AAN(II,JJ)=AAN(II,JJ)-X*RB(J,I)
CONTINUE
DO 140 J=I+1,NLB
 JJ=J+NLBE1+NLBE2+1
 AAN(II,II)=AAN(II,II)+ELEC*CR(I,J)
 AAN(II,JJ)=-ELEC*CR(J,I)
 X=GB(I)*EXP(HKT*(FRQB(I)-FRQB(J)))/GB(J)
 AAN(II,II)=AAN(II,II)+RB(I,J)
 AAN(II,JJ)=AAN(II,JJ)-X*RB(J,I)
CONTINUE
AAN(II,NEQM)=ELEC*SB(I,ID)*(RB(NLB+1,I)+ELEC*CR(I,NLB+1))
CONTINUE
DO 160 I=1,NLBE2
 J=NLBE1
 AAN(NEQM,J)=1.0
CONTINUE
AAN(NEQM,NLBE1+NLBE2+1)=2.0+ELEC*SUMBE(2,ID)
AAN(NEQM,NEQM)=1.0
RETURN
END
SUBROUTINE SETUP
C
C READ IN MODEL APPROXIMATION
C PERFORM ALL PRECALCULATIONS (E.G. OF CROSS-SECTIONS)
C
IMPLICIT NONE
C
MACROS
C
COMA
COMAI
COMN
C
LOCAL VARIABLES
C
CHARACTER*80 HEADER
INTEGER I, II, ID, IJ, IL, IT, J, W0, M1, M2, M3
REAL ARUNB(92)
REAL CW, DOP, FCW, FRQ3, GLOG, SRT, TEFF, V1, Z
C
TABLE OF ATOMIC WEIGHS
C
REAL WEIGHT(92)
DATA WEIGHT/1.0,4.0,6.9,9.0,10.8,12.0,14.0,16.0,18.0,20.2,23.0,  
: 24.3,27.0,28.1,31.0,35.5,39.9,39.9,40.1,44.5,47.9,50.9,52.0,  
: 54.9,55.8,58.9,58.9,63.5,65.4,69.7,72.6,74.9,79.0,79.9,83.8,85.5,  
: 87.6,88.9,91.2,92.9,96.9,98.9,101.1,102.9,106.4,107.9,112.4,  
: 114.8,118.7,121.8,127.6,126.9,131.3,132.9,137.3,138.9,140.1,  
: 146.9,144.2,145.0,150.4,152.0,157.3,158.8,162.5,164.9,167.3,  
: 168.9,173.0,175.0,178.5,180.9,183.9,186.2,190.2,192.2,196.1,  
: 197.0,200.6,204.4,207.2,209.0,210.0,222.0,223.0,226.0,  
: 227.0,232.0,231.0,238.0/
C
TABLE GIVING QUANTUM NUMBER OF ACTIVE ELECTRON OF EACH NEUTRAL  
HELIUM STATE TREATED BY THE PROGRAM
C
INTEGER QN(25)
DATA QN/1,4*2,6*3,8*4,5,6,7,8,9,10/
C
EXTERNAL PROCEDURES
REAL CREATE, EXIT, GAUWT, HEGAUWT, WUPAP, PARTI
EXTERNAL CREATE, EXIT, GAUWT, HEGAUWT, WUPAP, PARTI
C
STATEMENT FUNCTIONS
REAL SB, SBHE1, SBHE2
SB(IL,ID)=ACCF+EXP(BK*FRQ3(IL)/TEMP(ID))*GN(IL)/TEMP(ID)/


225

SQRT(TEMP(ID))

SBE1(IL,ID)=ACCOF*EXP(BK*FRQBE1(IL)/TEMP(ID))*GHE1(IL)/TEMP(ID)/

: SQRT(TEMP(ID))/2.

SBE2(IL,ID)=ACCOF*EXP(BK*FRQBE2(IL)/TEMP(ID))*GHE1(IL)/TEMP(ID)/

: SQRT(TEMP(ID))

START OF EXECUTABLE STATEMENTS

WRITE (6,*)'NON-LTE ATMOSPHERE PROGRAM'

READ (5,1001)HEADER

WRITE (12,1001)HEADER

READ (5,1002)TEFF,TLINE,GLOG,Y,Z,NITER,FLTE,FPRIIT,FSWITCH

WRITE (12,1002)TEFF,TLINE,GLOG,Y,Z,NITER,FLTE,FPRIIT,0

IF (FSWITCH) READ (5,1007)LANC

IF (FLTE) THEN

WRITE (6,*)'LTE MODEL'

ELSE

WRITE (6,*)'NON-LTE MODEL'

ENDIF

READ (5,1006)(ABUND(i),I=1,92)

WRITE (12,1006)(ABUND(i),I=1,92)

MU1=1.+4.*Y

ZTOT=1.+Y

IF (FPRIIT) WRITE (6,*)'ELEMENTAL ABUNDANCES'

DO 10 I=3,92

V1=1.E-12*EXP(2.302585093*ABUND(i))

IF (FPRIIT) WRITE (6,*)I,V1

ZTOT=ZTOT+V1

MU1=MU1+Z*WEIGHT(I)

CONTINUE

MU1=MU1/ZTOT

WRITE (6,*)'MEAN MOLECULAR WEIGHT = ',MU1

WRITE (6,*)'NUCLEI PER PROTON = ',ZTOT

C WAVELENGTH GRID

READ (5,1003)(DEPTH(I),I=1,1J)

WRITE (12,1003)(DEPTH(I),I=1,1J)

WRITE (6,*)'DEPTH POINTS = ',IDEPTH

READ (5,1006)(FREQ(I),I=1,1J)

WRITE (12,1006)(FREQ(I),I=1,1J)

C QUADRATURE WEIGHTS

DO 20 IJ=1,1J

WT0(IJ)=0.

CONTINUE

READ (5,1003)IO,11

WRITE (12,1003)IO,11

IF (IO.EQ.1) THEN

GO TO 30

ELSE IF (IO.EQ.2) THEN

TRAPEZOIDAL RULE

V1=ABS(FREQ(I1+1)-FREQ(I1))

WT0(I1+1)=WT0(I1+1)+0.5*V1

WT0(I1)=WT0(I1)+0.5*V1

GO TO 30

ELSE IF (IO.EQ.3) THEN

SIMPSON'S RULE

V1=ABS(FREQ(I1+1)-FREQ(I1-1))

WT0(I1+1)=WT0(I1+1)+V1/6.

WT0(I1)=WT0(I1)+2.*V1/3.

WT0(I1-1)=WT0(I1-1)+V1/6.

GO TO 30

ELSE IF (IO.EQ.4) THEN

GO TO 30

ENDIF
READ OPACITY RULE
READ (5,1003)RULE
WRITE (12,1003)RULE
IF (RULE(2))THEN
WRITE (6,'*') 'LINES INCLUDED'
ELSE
WRITE (6,'*') 'CONTINUUM ONLY'
ENDIF
READ (5,1007)(M(I),TEMP(I),WTOT(I),WE(I),I=1,NDEPTB)

MASS GRID OR MASS DIFFERENCE GRID? MAKE SURE OF THE FORMER
IF (M(NDEPTB).LE.M(NDEPTB-1))THEN
DO 40 ID=2,NDEPTB
N(ID)=N(ID)+N(ID-1)
40 CONTINUE
ENDIF

READ ATOMIC OCCUPATION NUMBERS
READ (5,1003)I
IF (I.EQ.1)THEN
READ (5,1006)COI
READ (5,1006)(FRQB(IL),IL=1,12)
READ LIST OF LINES TO USE FOR HYDROGEN
IF (ITRB.GT.0)
READ (5,1008)(LOWERB(J),UPPERB(J),J=1,ITRB)
C
CALCULATE LTE POPULATIONS FOR LEVELS INCLUDED IN APPROXIMATE INPUT MODEL.
DO 70 ID=1,NDEPTB
DO 60 IL=W2+1,ILB
L(IL,ID)=IPROT(ID)*IE(ID)*SB(IL,ID)
60 CONTINUE
70 CONTINUE
ELSE IF (I.EQ.2)THEN
TREAT HELIUM THE SAME WAY AS HYDROGEN.
READ (5,1003)W0,W1,W2,WTRHE1,W3,WTRHE2
IF (W1.WE.0)THEN
WRITE (6,'*') 'PLEASE DO NOT SPECIFY ANY HE- LINES.'
CALL EXIT(1)
ENDIF
READ (5,1008)(FQHE1(IL),IL=1,13)
READ (5,1008)(LOWERHE1(J),UPPERHE1(J),J=1,WTRHE1)
READ (5,1008)(FQHE2(IL),IL=1,13)
READ (5,1008)(LOWERHE2(J),UPPERHE2(J),J=1,WTRHE2)
READ (5,1008)(CWH,IL=1,W0),(#HE1(IL,ID),IL=1,13),
DO 100 ID=1,IDEPTH
   DO 80 IL=I2+1,ILBE1
     IHE1(IL,m) = IBE2(1,ID) * IE(ID) * SBHE1(IL,ID)
   80 CONTINUE
   DO 90 IL=I3+1,ILBE2
     IBE2(IL,m) = IBE3(ID) * IE(ID) * SBHE2(IL,ID)
   90 CONTINUE
100 CONTINUE
GO TO 50

ELSE IF (I.IE.0) THEN
   WRITE (6,*), 'PLEASE REMOVE HEAVY ION CARDS FROM DECK'
   CALL EXIT(1)
ENDIF

REMINDER OF DECK IS IGNORED.
PREPARE PRECALCULATED QUANTITIES.
ITPTRH=I3+1
ITPTRH1=ITPTRH
ITPTRH2=ITPTRH
IF (RULE(2)) THEN
   SRT=SQR(TLINE)
ENDIF

HYDROGEN LINES
W=WTAB
DO 130 IL=I1,W1
J=UPPERH(IL)
I=LOWERS(IL)
IT=ITRH(I,J)
REJECT LINE IF FORBIDDEN
IF (IT.EQ.0) THEN
   WRITE (6,*) 'LINE ',I,' TO ',J,' IS FORBIDDEN.'
   GO TO 130
ENDIF

CALCULATE LINE CENTRAL FREQUENCY AND DOPPLER WIDTH.
NOTE THAT THIS PROGRAM ASSUMES LINE BROADENING IS DOMINATED
BY DOPPLER BROADENING.
FCOM=FRQH(I)-FRQH(J)
DOP=SRT*FCOM*GDP0CF
IF (FCOM.LE.0) THEN
   WRITE (6,*), 'IONIZATION FREQUENCY ERROR FOR LINE ',I,' TO ',J,'
   FCOM=FCOM
ENDIF
IF (FPRINT) WRITE (6,*), 'LINE ',I,' TO ',J,'
   FREQ = ',FCOM,
   DOP = ',DOP
ADD FREQUENCIES TO FREQUENCY LIST FOR THE LINE.
DO 110 II=1,WQUAD
   FREQ((II+W1)=FCOM
   UPH((II+W1)=J
   LOW((II+W1)=I
110 CONTINUE
CALCULATE WEIGHTS FOR THE LINE FREQUENCIES.
NOTE THAT SIMPSON'S RULE IS USED; THUS WQUAD SHOULD BE ODD.
DO 120 I=W1,WQUAD-2,2
   WTO((I+W1)=WTO((I+W1)) + 2.0*DELQUAD*DOP/3.0
120 CONTINUE
W1=W1+WQUAD
C NOW DO ALL THE SAME FOR NEUTRAL AND SINGLE IONIZED HELIUM.

C

ITPTRL1=IJ+1
NI=ITNRI1
DO 160 IL=1,N1
J=UPPERB1(IL)
I=LOWERB1(IL)
IT=ITRBL1(I,J)
IF (IT.EQ.0) THEN
WRITE (6,*) 'HE1 LINE ',I,' TO ',J,' IS FORBIDDEN.'
GO TO 160
ENDIF
FCO1=FRQBE1(I)-FRQBE1(J)
DOP=SRT*FCO1*GDPDCF*0.5
IF (FCO1.LE.0) THEN
WRITE (6,*) 'HE1 IONIZATION FREQUENCY ERROR FOR LINE ',
I,','','J
FCO1=-FCO1
ENDIF
IF (FPRIIT) WRITE (6,*) 'HE1 ',I,' TO ',J,' FREQUENCY = ',FCO1,
'DOP = ',DOP
DO 140 II=1,1QUAD
FRQBE1(II+IJ)=FCO1
UPBE1(II+IJ)=J
LOWBE1(II+IJ)=I
140 CONTINUE
DO 150 I=1,1QUAD-2,2
WTO(I+IJ)=WTO(I+IJ)+2.0*DELQUAD*DOP/3.0
WTO(I+IJ+1)=WTO(I+IJ+1)+8.0*DELQUAD*DOP/3.0
WTO(I+IJ+2)=WTO(I+IJ+2)+2.0*DELQUAD*DOP/3.0
150 CONTINUE
IJ=IJ+IQUAD
160 CONTINUE
ITPTRL2=IJ+1
NI=ITNRI2
DO 190 IL=1,N1
J=UPPERB2(IL)
I=LOWERB2(IL)
IT=ITRBL2(I,J)
IF (IT.EQ.0) THEN
WRITE (6,*) 'HE2 LINE ',I,' TO ',J,' IS FORBIDDEN.'
GO TO 190
ENDIF
FCO1=FRQBE2(I)-FRQBE2(J)
DOP=SRT*FCO1*GDPDCF*0.5
IF (FCO1.LE.0) THEN
WRITE (6,*) 'HE2 IONIZATION FREQUENCY ERROR FOR LINE ',
I,','','J
FCO1=-FCO1
ENDIF
IF (FPRIIT) WRITE (6,*) 'HE2 ',I,' TO ',J,' FREQUENCY = ',FCO1,
'DOP = ',DOP
DO 170 II=1,1QUAD
FRQBE2(II+IJ)=FCO1
UPBE2(II+IJ)=J
LOWBE2(II+IJ)=I
170 CONTINUE
DO 180 I=1,1QUAD-2,2
WTO(I+IJ)=WTO(I+IJ)+2.0*DELQUAD*DOP/3.0
WTO(I+IJ+1)=WTO(I+IJ+1)+8.0*DELQUAD*DOP/3.0
WTO(I+IJ+2)=WTO(I+IJ+2)+2.0*DELQUAD*DOP/3.0
180 CONTINUE
IJ=IJ+IQUAD
190 CONTINUE
ENDIF
IF (I.J/.GT.NWJ) THEN
WRITE (6,*) 'TOO MANY FREQUENCY POINTS'
CALL EXIT(1)
ENDIF
WRITE (6,*) 'FREQUENCY POINTS = ',NWJ
IF (FPRIIT) THEN
WRITE (6,*) 'FREQUENCIES AND WEIGHTS'
WRITE (6,1007)(FRQ(IJ),WTO(IJ),IJ=1,NWJ)
ENDIF
DO 200 IJ=1,NWJ
WTO(IJ)=WTO(IJ)
190 CONTINUE
DO 240 IJ=1,NWJ
FRQ3=FRQ(IJ)**3
200 CONTINUE
DO 210 IL=1,ILBE2S
SIGBE2(IL,IL)=0.
IF (FREQ(IJ).GT.FRQBE2(IL))
SIGBE2(IL,IL)=VI*GAUWT(IL,FREQ(IJ))/FLOAT(IL)**5
CONTINUE
DO 210 IL=1,ILBE2S
SIGBE2(IL,IL)=0.
IF (FREQ(IJ).GT.FRQBE1(IL))
SIGBE1(IL,IJ)=VI*GAUWT(IL,FREQ(IJ))/FLOAT(IL)**5
CONTINUE
DO 210 IL=1,ILBE2S
SIG(IL,IL)=0.
IF (FREQ(IJ).GT.FRQB(IL))
SIG(IL,IJ)=VI*GAUWT(IL,FREQ(IJ))/FLOAT(IL)**5
CONTINUE
SIG(ILBS+1,IJ)=3.69E8/FRQ3
CONTINUE
DO 250 I=1,IDEPTB
FF(I,1)=MIN(FQH(ILBS+1),FREQ(I))
FF(I,2)=MIN(FQH1(ILBE1S+1),FREQ(I))
FF(I,3)=MIN(FQH2(ILBE2S+1),FREQ(I))
CONTINUE
DO 290 ID=1,IDEPTB
IF (FLTE)TBEIT
CALL IUPOP(ID)
ELSE
CALL PARTI(ID)
CONTINUE
DO 260 IL=1,ILBS
W1(IL,ID)=IE(ID)*JIPROT(ID)*SB(IL,ID)
CONTINUE
DO 270 IL=1,ILBS
W2S(IL,ID)=WE3(ID)*WB2E2(IL,ID)
CONTINUE
DO 280 IL=1,ILBS
W1S(IL,ID)=WE2(ID)*WB1E1S(IL,ID)
CONTINUE
W1(ID)=(ITOT(ID)-JIE(ID))*NU1
CONTINUE
RETURN

C 1001 FORMAT (A80)
1002 FORMAT (2F9.0,F8.2,F8.3,F8.5,4I5)
1003 FORMAT (16I5)
1004 FORMAT (2F9.0,F8.2,F8.3,F8.5,4I5)
1005 FORMAT (2F10.6)
1006 FORMAT (5E15.7)
1007 FORMAT (4E15.7)
1008 FORMAT (2I5)
END

BLOCK DATA TABLES
C CONTAINS ALL DATA STATEMENTS FOR COMMON BLOCKS, IN ACCORDANCE
C WITH THE ANSI STANDARD
C COMA
COMAI
: 1024./
: 1352.,1458.,1568.,1682.,1800.,1922.,2048./
C DATA OSCB/4.162E-1,7.910E-2,2.899E-2,1.394E-2,6.408E-1,1.193E-1,
: 4.467E-2,8.420E-1,1.506E-1,1.038/
DATA (ITRBE1(I),I=1,19)/0,0,0,0,1,0,0,0,0,0,2,0,0,0,0,0,3,0,0,0/
DATA (ITRBE1(2,I),I=1,19)/0,0,0,0,1,1,1,1,0,0,0,1,0,0,0,0,0,0,0,0/
DATA (ITRBE1(3,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(4,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(5,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(6,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(7,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(8,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(9,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(10,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(11,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(12,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(13,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(14,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(15,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(16,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(17,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(18,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
DATA (ITRBE1(19,I),I=1,19)/0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/


DATA (ITRBE2(I),I=1,10)/0,1,2,3,4,5,6,7,8,9/
DATA (ITRBE2(1,I),I=1,10)/1,0,10,11,12,13,14,15,16,17/
DATA (ITRBE2(3,I),I=1,10)/2,0,18,19,20,21,22,23,24,25/
DATA (ITRBE2(4,I),I=1,10)/3,11,18,19,20,21,22,23,24,25/
DATA (ITRBE2(5,I),I=1,10)/4,12,18,19,20,21,22,23,24,25/
DATA (ITRBE2(6,I),I=1,10)/5,13,20,21,22,23,24,25,26,27/
DATA (ITRBE2(7,I),I=1,10)/6,14,21,27,32,33,34,35,36,37/
DATA (ITRBE2(8,I),I=1,10)/7,15,22,28,33,34,35,36,37,38/
DATA (ITRBE2(9,I),I=1,10)/8,16,23,29,34,35,36,37,38,39/
DATA (ITRBE2(10,I),I=1,10)/9,17,24,30,35,36,37,38,39,40/

DATA FRQBE/3.28799E15,0.821997E15,0.365332E15,0.205499E15,0.131519E15,0.0913329E15,0.0671018E15,0.0513748E15,0.0405924E15,0.0328799E15,0.0271735E15,0.0228333E15,0.0194556E15,0.0167755E15,0.0146133E15,0.0128437E15/

DATA FRQBE1/5.94520E15,1.15305E15,0.957439E15,0.876230E15,0.811774E15,0.651896E15,0.526078E15,0.365332E15,0.268407E15,0.240134E15,0.217774E15,0.212670E15,0.205704E15,0.200575E15,0.199699E15,0.195205E15,0.190348E15,0.181735E15,0.177555E15,0.146133E15,0.128437E15/

DATA FRQBE2/13.1520E15,3.28799E15,1.46133E15,0.821997E15,0.526078E15,0.365332E15,0.268407E15,0.240134E15,0.217774E15,0.212670E15,0.205704E15,0.200575E15,0.199699E15,0.195205E15,0.190348E15,0.181735E15,0.177555E15,0.146133E15,0.128437E15/

C DATA FRQBE/3.28799E15,0.821997E15,0.365332E15,0.205499E15,0.131519E15,0.0913329E15,0.0671018E15,0.0513748E15,0.0405924E15,0.0328799E15,0.0271735E15,0.0228333E15,0.0194556E15,0.0167755E15,0.0146133E15,0.0128437E15/

C SUBROUTINE WTSET(LLAN)
C SET THE INTEGRATION WEIGHTS
C
C IMPLICIT NONE
C
C COMA
COMW
C
INTEGER IJ
REAL LLAM
C
DO 10 IJ=ITPTRN,HJ
   WT(IJ)=LLAM*WT(IJ)
10 CONTINUE
RETURN
END
D. Program HYD

Only those portions of HYD that differ significantly from ANDERS are listed here.
PROGRAM BYD

AN ADAPTATION OF PORTIONS OF THE MIRALAS et al. (1975) CODE TO THE
ANDERSON ALGORITHM FOR THE EFFICIENT SOLUTION OF LARGE NUMBERS OF
TRANSFER EQUATIONS IN NON-LTE.

PARAMETERS:

MNB  MAXIMUM NUMBER OF FREQUENCY BLOCKS
MDEPTH MAXIMUM NUMBER OF DEPTH POINTS
MNH  MAXIMUM TOTAL NUMBER OF FREQUENCIES
MNC  MAXIMUM NUMBER OF CONTINUUM FREQUENCY POINTS
MNTRBE1 MAXIMUM NUMBER OF NEUTRAL HELIUM TRANSITIONS
MNTRBE2 MAXIMUM NUMBER OF IONIZED HELIUM TRANSITIONS
MNCQ MAXIMUM QUANTUM NUMBER IN PARTITION SUMS OF HYDROGEN
MEQI  MAXIMUM QUANTUM NUMBER IN PARTITION SUMS OF HELIUM I
NQEW  TOTAL NUMBER OF ATOMIC STATES
NQUAD SPECIFIES NUMBER OF QUADRATURE POINTS ON EACH SIDE
OF PROFILE.
NLB  NUMBER OF NON-LTE HYDROGEN LEVELS
NLBE1 NUMBER OF NON-LTE HELIUM LEVELS
NLBE1S TOTAL HELIUM LEVELS
NLBE2 NUMBER OF NON-LTE IONIZED HELIUM LEVELS
NLBE2S TOTAL IONIZED HELIUM LEVELS
NLBS TOTAL HYDROGEN LEVELS
ACCOF SABA ACTIVITY COEFFICIENT
BCCOF PLANCK FUNCTION COEFFICIENT
CC VELOCITY OF LIGHT
DELQUAD FRACTION OF DOPPLER WIDTH PER LINE INTEGRATION INTERVAL
DDPCOF DOPPLER WIDTH COEFFICIENT
ERASS ELECTRON MASS
ESI ELECTRON CHARGE
EK PLANCK'S CONSTANT OVER BOLTZMANN'S CONSTANT
EP PLANCK'S CONSTANT
HYDCOF HYDROSTATIC EQUATION RADIATIVE COEFFICIENT
KB BOLTZMANN'S CONSTANT
MBYD MASS OF HYDROGEN ATOM
PI PI
PIE2MC CLASSICAL ELECTRON ABSORPTION COEFFICIENT
SCOF RADIATIVE RATE COEFFICIENT
SIGE ELECTRON THOMPSON CROSS-SECTION

VARIABLES:

FEXIT FLAG TO EXIT
RULE FLAG TO INCLUDE VARIOUS OPACITIES
BLOCK BLOCK ASSIGNMENTS
ITPRB POINTS TO HYDROGEN LINE FREQUENCIES
ITRH TRANSITION INDICES FOR HYDROGEN;
I.E. ITRH(L,U) IS TRANSITION INDEX OF
HYDROGEN L LEVEL TO U LEVEL.
LOWE LOWER LEVEL OF DOMINANT HYDROGEN TRANSITION AT THE
SPECIFIED FREQUENCY
LOWERBE1 LOWER LEVEL OF HYDROGEN TRANSITIONS REQUESTED BY USER
LOWERBE2 " OF NEUTRAL HELIUM
LOWERBE2 " OF IONIZED HELIUM
NB NUMBER OF FREQUENCY BLOCKS
NDEPTH NUMBER OF DEPTH POINTS
NITER NUMBER OF ITERATIONS TO MAKE
NJ NUMBER OF FREQUENCIES
NTRBE1 NUMBER OF HYDROGEN TRANSITIONS
NTRBE2 " OF NEUTRAL HELIUM TRANSITIONS
NTRBE2 " OF IONIZED HELIUM TRANSITIONS
UPBE UPPER LEVEL OF DOMINANT HYDROGEN TRANSITION AT THE
FREQUENCY SPECIFIED.
UPPERBE1 UPPER HYDROGEN LEVELS OF TRANSITIONS REQUESTED BY USER
UPPERBE2 " OF NEUTRAL HELIUM
UPPERBE2 " OF IONIZED HELIUM
A A MATRIX OF LINEARIZATION
AN LHS OF POPULATION EQUATIONS
ANS RESULT OF POPULATION CALCULATION
B B MATRIX OF LINEARIZATION
BN RHS OF POPULATION EQUATIONS
C C-MATRIX OF LINEARIZATION
CHI OPACITY MATRIX
C

CHIOV  MATRIX OF NO->HYDROGEN OPACITY
C
C
CR  COLLISION RATES FOR HYDROGEN
C
C
ETA  EMISSIVITY MATRIX
C
C
ETA0V  MATRIX OF NO->HYDROGEN EMISSIVITY
C
C
FF  FREE-FREE CUTOFF (TO ACCOUNT FOR UPPER STATES)
C
C
FH  EDDINGTON FACTOR FOR FLUX
C
C
FK  EDDINGTON FACTOR FOR RADIATIVE PRESSURE
C
C
FREQ  FREQUENCY GRID
C
C
FREQH  IONIZATION FREQUENCIES OF HYDROGEN
C
C
FREQHE1  " OF NEUTRAL HELIUM
C
C
FREQHE2  " OF IONIZED HELIUM
C
C
GH  STATISTICAL WEIGHS OF HYDROGENIC LEVELS
C
C
GHE1  " OF NEUTRAL HELIUM
C
C
NO  SURFACE FLUX
C
C
OSCH  HYDROGEN OSCILLATOR STRENGTHS LISTED BY TRANSITION INDEX
C
C
M  MASS GRID
C
C
MU1  MOLECULE PER PROTON
C
C
N  HYDROGEN NUMBER DENSITIES
C
C
NE  ELECTRON DENSITY
C
C
NHE1  NEUTRAL HELIUM DENSITIES
C
C
NHE1S  LTE NEUTRAL HELIUM DENSITIES
C
C
NHE2  IONIZED HELIUM DENSITIES
C
C
NHE2S  LTE IONIZED HELIUM DENSITIES
C
C
NHE3  DOUBLY-IONIZED HELIUM DENSITIES
C
C
NM  FICTIONAL MASSIVE PARTICLE DENSITY
C
C
NP0T  PHOTON DENSITY
C
C
NS  LTE HYDROGEN DENSITIES
C
C
NTOT  TOTAL PARTICLE DENSITY
C
C
Q  RHS OF LINEARIZATION
C
C
RAD  MEAN INTENSITY OF RADIATION
C
C
RH  HYDROGEN RADIATIVE BRACKETS
C
C
RNSD  SECONDARY RATES OF HYDROGEN DOWN
C
C
RBUU  SECONDARY RATES OF HYDROGEN UP
C
C
SIG  HYDROGEN CROSS-SECTIONS PLUS FREE-FREE
C
C
SIGRE  FREE-FREE HYDROGEN OPACITY
C
C
SIGL  BOUND-BOUND CROSS SECTION FOR HYDROGEN
C
C
SUNH  HYDROGEN UPPER STATE SUM
C
C
SUMH  HELIUM UPPER STATE SUMS
C
C
TEMP  TEMPERATURE
C
C
tLINE  TEMPERATURE ASSUMED TO DETERMINE LINE FREQUENCY GRID
C
C
WT  FREQUENCY QUADRATURE WEIGHTS MODIFIED BY SWITCHING
C
C
WTO  UNMODIFIED FREQUENCY QUADRATURE WEIGHTS
C
C
Y  RATIO OF HELIUM TO HYDROGEN BY NUMBER
C
C
ZTOT  PHOTONS PER NUCLEUS
C
C
CLICHE COLA
C
C
INCLUDES PARAMETERS
C
C
INTEGER NMB, NMDEPTH, NJC, MUB, MQUE1, NLH, NLHE1, NLHE2
C
INTEGER NQUAD
PARAMETER (NMB=60, NMDEPTH=70, NJC=105, MUB=16, MQUE1=37)
PARAMETER (NLH=10, NLHE1=31, NLHE2=16, NQUAD=6)
C
INTEGER NTRB, NTRBE1, NTRBE2
PARAMETER (NTRB=10, NTRBE1=14, NTRBE2=10)
C
INTEGER MJ,
PARAMETER (MJ=NJJC+(2*MQUAD+1)*NTRB)
C
INTEGER NEQW
PARAMETER (NEQW=NLH+1)
C
REAL CC, DELQUAD, EMSS, ESU, HP, KB, MBYD, PI
PARAMETER (CC=2.997925E10, DELQUAD=0.6, EMSS=9.10935E-28)
PARAMETER (ESU=4.803258E-10, HP=6.62618E-27, KB=1.38066E-16)
PARAMETER (MBYD=1.6726E-24, PI=3.141592654)
C
REAL ACCOF, BBCOF, DPCOF, BK, KYDCOF, PIE2MC, SCOF, SIGE
PARAMETER (ACCOF=2.0742E-16, BBCOF=2.0E/(CC*CC), DPCOF=4.2065E-7)
PARAMETER (BK=HP/KB, KYDCOF=4.*PI/(CC*KB))
PARAMETER (PIE2MC=PI/ESU/(EMSS*CC), SCOF=4.*PI/HP)
PARAMETER (SIGE=8.*PI*ESU*ESU*ESU/(3.*EMSS*EMSS*CC*CC*CC*CC))
C
INTEGER BLOCK(MJ), TTTRB, WB, WDEPTH, WITER
INTEGER MJ, WTRB, WTRBE1, WTRBE2
C
LOGICAL FEIT, RULE(2)
THE SECOND DIMENSION OF THE VARIABLES CHI AND ETA MUST BE THE GREATER OF NMB+3 OR NWDPHT.

REAL B(NWBB,NWBB), CHI(NWBB,NWDPHT), CHIOV(NWBB,NWDPHT)
REAL ETA(NWBB,NWDPHT), ETAOV(NWBB,NWDPHT)
REAL F(B(NWBB), FK(NWBB,NWDPHT), FREQ(NWBB), HO, Q(NWBB)
REAL W(NWDPHT), MW(NWDPHT), ME(NWDPHT)
REAL WHE1(NWHE1,NWDPHT), WHE1S(NWHE1,NWDPHT)
REAL WHE2(NWHE2,NWDPHT), WHE2S(NWHE2,NWDPHT), WHE3(NWDPHT)
REAL WM(NWDPHT), WROV(NWDPHT), WS(NWLS,NWDPHT), WTOT(NWDPHT)
REAL RAD(NWJ,NWDPHT), RH(NWLS+1,NWLS+1), RHDS(NWDS,NWDPHT)
REAL RHUS(NWDS,NWDPHT), SIG(NWLS+1,NWJ), SIGL(NWJ,NWDPHT)
REAL SIGFRE(NWJ,NWDPHT)
REAL TMLS(NWDPHT), TMLM2(NWDPHT), TLMW(NWDPHT), TLMZ
REAL WT(NWJ), Y, ZTOT

COMMON //ITP98, BLOCK, NW, NWDPHT, WI8, W18, WTRH, WTRHE1,
    : WTRHE2, FEXIT, NUL8, Q, B, CHI, CHIOV, ETA, ETAOV, FR, FK,
    : FREQ, HO, NW, W18, W8, WHE1, WHE1S, WHE2, WHE2S, WHE3, WM,
    : WPROT, WS, WTOT, RAD, RH, RHDS, RHUS, SIG, SIGL, SIGFRE,
    : SUME, SUME, TEMP, TLIME, WT, Y, ZTOT

ENDCLICHE

CLICHE CDNC
REAL AQ(NWQ8,NWQ8), ANS(NWQ8), BN(NWQ8), CR(NWLS,NW8+1,NWDPHT)

COMMON //CDNC/AN, ANS, BN, CR

ENDCLICHE

CLICHE COMF
REAL A(NWBB,NWBB), C(NWBB,NWBB)

COMMON //COMF/A, C

ENDCLICHE

CLICHE COMM
REAL A1B(NWLB,NWQ8), A2B(NWLB,NWQ8), A3L(NWLB,NWQ8), A3H(NWLB,NWQ8)
REAL A3L(NWLB,NWQ8)
REAL C0B(NWLB), C1B(NWLB), C2L(NWLB), C3B(NWLB), C4B(NWLB), C5B


ENDCLICHE

CLICHE CONT
LOGICAL FSH(105), FSET

COMMON //CONT/FSH, FSET

ENDCLICHE

PROGRAM HYD

END

ENTRY POIT

IMPLICIT NONE
MACROS

INTERNAL PROCEDURES

REAL BLOCKS, CONTROL, CREATE, DESTROY, EXIT, LINK, PUTOUT, SETUP
REAL USERINFO, OPEN

EXTERNAL BLOCKS, CONTROL, CREATE, DESTROY, EXIT, LINK, PUTOUT
EXTERNAL SETUP, USERINFO, OPEN

START OF EXECUTABLE STATEMENTS.

THE FILE input CONTAINS A FIRST-APPROXIMATION MODEL.
THE FILE output CONTAINS THE MODEL HERE CALCULATED.
THE FILE monitor CONTAINS ALL OTHER OUTPUT.

CALL LINK("UIUTs=(input,OPEN,TEXT),UIUT12=(output,CREATE,TEXT),
: : UIUT6=(monitor,CREATE,TEXT)"")

SET UP STARK TABLES

LENGTH=50+21*4+105
CALL OPEN(10,\"stark.t\",4,LENGTH)

READ IN THE FIRST APPROXIMATION AND SET UP EVERYTHING
PREPARATORY TO BEGINNING CALCULATIONS.

CALL SETUP

GET USER SUFFIX (SO THAT SCRATCH FILES CAN BE UNIQUELY NAMED)

CALL USERINFO(USER,ACC,DROP,SUFFIX)

CREATE SCRATCH FILES

LENGTH=MB*(MB+1)*(NDEPT-1)
CALL CREATE(8,\"Xscr8\"//SUFFIX,4,LENGTH)
LENGTH=MB*NDEPT
CALL CREATE(9,\"Xscr9\"//SUFFIX,4,LENGTH)

SET UP FREQUENCY BINNING.

CALL BLOCKS

ENTER MAIN CONTROL ROUTINE AND CARRY OUT THE CALCULATIONS.

CALL CONTROL

WRITE THE RESULTS.

CALL PUTOUT

DELETE SCRATCH FILES AND EXIT.

CALL DESTROY(\"Xscr8\"//SUFFIX)
CALL DESTROY(\"Xscr9\"//SUFFIX)
CALL EXIT(0)

END

REAL FUNCTION ASY(WL,WU,ALPHA,TEMP,DEM)

IMPLICIT NONE

CALCULATES QUASI-STATIC STARK BROADENING OF HYDROGEN.
THE DOPPLER CONVOLUTION IS IGNORED; THIS FUNCTION IS VALID
ONLY FOR THE WINGS OF THE LINE.

INTEGER I, J, K, WL, MSC(10,9), WU

REAL ALAM, ALPHA, B, CKMAX, CKMIN, CORE, DEM, DWU, DOP, FO, FAC
REAL FAC1, SHIELD, TEMP, XI, X2, X3, Y1, Y2, Y3
REAL CK(127,10,9), FF(127,10,9), FIELD(301), W(300,5), IX(300)
REAL XY(5), IZ(5), YARR(301)
REAL WFLD
EXTERNAL WFLD

COMMON /MICRO/W, SHIELD

START OF EXECUTABLE STATEMENTS

SHIELD=0.0898*DEl**(1./6.)/SQRT(TEMP)
ALAM=1.E8/(109678.758•((1./IL)**2-(1./IU)**2))
FAC=0.

DO 10 K=2,ISC(IU,IL)
FAC=FAC+FF(K,IU,IL)•WFLD(ALPHA/CK(K,IU,IL))/CK(K,IU,IL)
10 CONTINUE
ASY=FAC
RETURN
END

REAL FUNCTION HELIPOP(L,U,DWU,T,DEI)

C CALCULATE HELIUM II QUASISTATIC PROFILE

IMPLICIT NONE

LOCAL VARIABLES

INTEGER I, IT, L, U
REAL CORE, DADIU, DEI, DIU, FO, FRQO, STARK, STREIGTB, T, VO

DATA (ITRBE2(1,I),I=1,10)/ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9/
DATA (ITRBE2(2,I),I=1,10)/ 1, 0, 1, 12, 13, 14, 15, 16, 17/
DATA (ITRBE2(3,I),I=1,10)/ 2.10, 0.18, 19, 20, 21, 22, 23, 24/
DATA (ITRBE2(4,I),I=1,10)/ 3.1118, 0.25, 26, 27, 28, 29, 30/
DATA (ITRBE2(5,I),I=1,10)/ 4.12, 18, 26, 31, 30, 31, 32, 33, 34, 35/
DATA (ITRBE2(6,I),I=1,10)/ 5.13, 20, 26, 31, 0.36, 37, 38, 39/
DATA (ITRBE2(7,I),I=1,10)/ 6.14, 21, 27, 32, 36, 0.40, 41, 42/
DATA (ITRBE2(8,I),I=1,10)/ 7.15, 22, 28, 33, 37, 40, 0.43, 44/

EXTERNALS

REAL ASY
EXTERNAL ASY

START OF EXECUTABLE STATEMENTS

IT=ITRBE2(L,U)
STREIGTB=OSCHE2(IT)•PIE2MC
FRQO=FRQHE2(L)-FRQHE2(U)
FO=1.25E-9•DEl**(2./3.)

DOPPLER CORE

VO=DOPCOF•FRQO•SQRT(T)•0.5
CORE=EXP(-(DIU/VO)**2)/VO/1.7724539

HYDROGENIC STARK PROFILE
STARK = 0.

IF (DNW GT VO) THEN
    DADNU = 3.2E9 + CC/FO/FRQ0/FRQ0
    STARK = DADNU * ASY(L, U, AB5(DNW - FRQ0 + 4.03E-4) * DADNU, T, DEI)
ENDIF

NOW DECIDE WHICH TO USE: WE ASSUME DOPPLER PROFILE FOR
DNW < VO, AND TAKE THE GREATER OF THE DOPPLER OR STARK PROFILES
FOR DNW > VO

BE uncovered = STRENGTH * MAX(STARK, CORE)
RETURN
END

REAL FUNCTION HPROFILE(L, U, DNW, T, WEL)

CALCULATE H LINE PROFILES

HYDROGEN LINES 1-2 TO 2-5 ARE TREATED USING THE FULL UNIFIED
STARK THEORY WITH LOWER STATE INTERACTIONS AS OUTLINED BY VIDAL,

ALL OTHER LINES ARE TREATED APPROXIMATELY USING THE QUASI-STATIC
STARK THEORY.

IMPLICIT NONE

MACRO

LOCAL VARIABLES

INTEGER I, J, K, IAO, IMO, IT, L, U, TRCUR
REAL ALPHA, CORE, DADIU, LALPBA, DNW, FO, FRQ0, WEL, LT, WEL
REAL STARK, STRENGTH, T, VO
REAL SPROF(S0,21,4), SPI(4), SPl(4), SPT(4), IT(4), IIE(21)
REAL XALPHA(50)

EXTERNALS

REAL POLY, ASY, RDABS
INTEGER IOSTATUS
EXTERNAL POLY, ASY, RDABS, IOSTATUS

PROFILE DATA

LOG TEMPERATURES

DATA IT/4.0, 4.30103, 4.60206, 4.90309/

LOG ELECTRON NUMBER DENSITIES

DATA WME/
    : 8.0, 8.5, 9.0, 9.5, 10.0, 10.5, 11.0, 11.5, 12.0, 12.5,
    : 13.0, 13.5, 14.0, 14.5, 15.0, 15.5, 16.0, 16.5, 17.0, 17.5,
    : 18.0/

LOG ALPHA (=WAVELENGTH OVER NORMALIZED FIELD STRENGTH)

DATA XALPHA/
    : -5.8, -5.6, -5.4, -5.2, -5.0, -4.8, -4.6, -4.4, -4.2, -4.0,
    : -3.8, -3.6, -3.4, -3.2, -3.0, -2.8, -2.6, -2.4, -2.2, -2.0,
    : -1.8, -1.6, -1.4, -1.2, -1.0, -0.8, -0.6, -0.4, -0.2, 0.0,
    : 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0,
    : 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0/

TRANSITION 1 TO 2 10000. 8.0 (INITIAL TABLE IN MEMORY)

(1061 lines of DATA statements omitted.)

INDICATE THAT THE DATA FOR THE FIRST TRANSITION ARE
ALREADY IN THE ARRAY SPROF. OTHER TRANSITION TABLES
ARE READ INTO MEMORY AS REQUIRED.

DATA TRCUR/1/

BE SURE THE PROGRAM SAVES TRCUR AND SPROF. THIS IS A NO-OP
FOR MOST COMPILERS, SINCE VERY FEW FORTRAN COMPILERS USE
ANYTHING BUT STATIC MEMORY FOR VARIABLES.

SAVE

CALCULATE TOTAL LINE OPACITY AND FREQUENCY

IT=ITRB(L,U)

IF NECESSARY, READ IN THE TABLES FOR THE NEXT TRANSITION.

IF (IT.NE.TRCUR) THEN
  TRCUR=IT
  I=60+21*I
  CALL RDABS(10,SPROF,I,J)
  I=ISTATUS(10,J)
ENDIF

STRENGTH=QSCN(IT)+PIE2MC
FRQO=FRQR(L)-FRQR(U)

CALCULATE NORMALIZED FIELD STRENGTH AND CONVERSION FACTOR FROM FREQUENCY TO THE DIMENSIONLESS QUANTITY ALPHA.

FO=1.25E-9*1EL**(2./3.)
DADU=1.E8*CC/FO/FRQO/FRQO
ALPHA=ABS(DADU*DADU)

PREPARE TO INTERPOLATE FROM TABLE

LT=LOG10(T)
LWEL=LOG10(WEL)
LALPHA=LOG10(MAX(1.E-6,ALPHA))

CHECK INPUT QUANTITIES TO SEE IF THEY ARE ON THE TABLE GRID. IF NOT, FOLLOW APPROXIMATE PROCEDURES FOR EACH CASE.

IF (LT.LT.ILT(1)) THEN
  WRITE (6,*)'TEMPERATURE TOO LOW: U=',U,' L=',L,' T=',T
  STOP
ELSE IF (LT.GT.ILT(4).OR.LIEL.GT.IE(21)) THEN
  WRITE (6,*)'TEMPERATURE OR ELECTRON DENSITY OFF THE TOP OF THE SCALE; THIS HAPPENS ONLY AT GREAT OPTICAL DEPTH, THUS AN ACCURATE TREATMENT IS OF NO IMPORTANCE. WE USE THE QUASI-STATIC PROFILE WITHOUT DOPPLER CONVOLUTION; THIS GIVES ACCURATE WINGS, WHICH ARE THE ONLY PART OF THE PROFILE THAT MIGHT POSSIBLY BE IMPORTANT AT SUCH GREAT DEPTHS.
  STARK=ASY(L,U,ALPHA,T,LIEL)
  HPROFILE=STRENGTH*STARK*DADU
ELSE IF (LWEL.LT.ILX(1)) THEN
  WRITE (6,*)'VERY LOW ELECTRON DENSITY; WE USE THE DOPPLER PROFILE, SINCE WINGS WILL BE UNIMPORTANT AT SUCH LOW DENSITY.
  VO=DOPCOF*FBQO*SQRT(T)
  HPROFILE=STRENGTH*EXP(-(DNU/VO)**2)/VO/1.7724539
ELSE IF (LALPHA.GT.IALPHA(SO)) THEN
  WRITE (6,*)'WAY OUT IN THE WINGS. WE TAKE THE GREATER OF THE DOPPLER PROFILE OR THE STARK PROFILE.
  VO=DOPCOF*FRQO*SQRT(T)
  CORE=EXP(-(DNU/VO)**2)/VO/1.7724539
  STARK=DNU*ASY(L,U,ALPHA,T,WEL)
  HPROFILE=STRENGTH*MAX(CORE,STARK)
ELSE
  WRITE (6,*)'TEMPERATURE AND ELECTRON NUMBER ARE BOTH ON THE SCALE.'
FIRST CHECK AND SEE IF ALL THE GRID POINTS REQUIRED ARE THERE.

IMO=MAX(1,MIN(18,INT(2*(LWEL-.0))))
IAO=MAX(1,MIN(47,INT(5*(LALPHA+.8))))
DO 20 I=1,4
  DO 10 J=IMO,IMO+3
    IF (SPROF(I,J,1).EQ.(0.)) GO TO 60
240

10 CONTINUE
20 CONTINUE
DO 50 I=1,4
DO 40 J=1,4
DO 30 K=1,4
30 CONTINUE
SPP(K)=SPROF(IAO+I-1,IAO+K-1,J)
40 CONTINUE
SPT(J)=POLY(4,XT,SPW,LT)
50 CONTINUE
SPI(I)=POLY(4,XT,SPT,LT)
STARK=POLY(4,XALPHA(IAO),SPI,ULPBA)
PROFILE=STRENGTH*EXP(2.302585093*STARK)*DADU
ENDIF
RETURN
60 PROFILE=STRENGTH*DADU*ASY(L,U,ALPHA,T,WE)
END

BLOCK DATA MFIELD
C
C MICROFIELD DISTRIBUTION
C
REAL W(300,6)
COMMON /MICRO/W, SHIELD
C
(659 lines of DATA statements omitted)
C
END

REAL FUNCTION POLY(W,X,Y,Z)
C
C WH-PT POLYNOMIAL INTERPOLATION
C
REAL XT(W),YT(W)
C
SUM=0.
DO 20 I=1,W
TERM=YT(I)
DO 10 J=1,W
IF (I.NE.J)TERM=TERM*(X-XT(J))/(XT(I)-XT(J))
10 CONTINUE
SUM=SUM+TERM
20 CONTINUE
POLY=SUM
RETURN
END

BLOCK DATA COMMT
C
C DATA STATEMENTS FOR COMMON BLOCK COMMT
C
IMPLICIT NONE
C
MACROS
C
COMMT
C
DATA FSET/.FALSE./
DATA FSBR/105*.TRUE./
C
END

SUBROUTINE TRIDAG(A,W,WR)
C
C INVERT TRIDIAGONAL MATRIX IN PLACE
C
REAL A(WR,WR)
C
A(1,2)=A(1,2)/A(1,1)
A(1,1)=1./A(1,1)
DO 30 I=2,W-1
A(I,1)=A(I,1)-A(I-1,1)*A(I-1,1)
DO 10 J=1,W-1
A(I,J)=A(I,J)-A(I,J-1)*A(I-1,J)
10 CONTINUE
RETURN
END
A(I,J) = -A(I,I-1)*A(I-1,J)

CONTINUE

DIV = A(I,1)
DO 20 J = 1, I-1
A(I,J) = A(I,J)/DIV

CONTINUE

A(I,1) = 1./DIV
A(I+1,1) = A(I+1,1)/DIV

CONTINUE

B(N,N) = A(N,N) - A(N,N-1) + A(N-1,N)

DO 40 J = 1, N-1

A(I,J) = A(N,N-1) + A(N-1,J)/A(N,N)

CONTINUE

A(N,N) = 1./A(N,N)
DO 50 J = N-1, 1, -1
DIV = A(I,1)
DO 30 J = 1, I
A(I,J) = A(I,J) - DIV*A(I+1,J)

CONTINUE

A(N,1) = -DIV*A(I+1,1)

CONTINUE

RETURN

END

SUBROUTINE TWOATM

ESTIMATES RATE BRACKETS FOR A LINE TRANSITION USING AN EQUIVALENT TWO-LEVEL ATOM APPROACH. ONLY THE RATE COEFFICIENTS ARE ACTUALLY SAVED FOR USE IN THE MAIN CALCULATION.

THIS ROUTINE IS CALLED ONCE ONLY TO MAKE AN INITIAL ESTIMATE OF THE RELEVANT RATES. THIS IS DONE AFTER THE RATES FOR EXPLICIT TRANSITIONS ARE CALCULATED FROM THE INPUT MODEL, WHICH SHOULD BE A NOME-LTE MODEL ATMOSPHERE WITH THE MOST IMPORTANT LINES ALREADY REPRESENTED.

IMPLICIT NONE

MACROS

do, cona, conb, cont

LOCAL VARIABLES AND PARAMETERS

INTEGER NNU
PARAMETER (NNU=3)

INTEGER I, INU, J, ID, IJ, IT, IIT, L, LL, U, UU
REAL A1(NNDPHTS), A2(NNDPHTS), A3(NNDPHTS), A4(NNDPHTS)
REAL CHIC(NNDPHTS), CHIL(NNDPHTS), ETAC(NNDPHTS), ETAL(NNDPHTS)
REAL FCH(NNDPHTS), MAC(NNDPHTS, NNDPHTS), MAV(NNDPHTS)
REAL MAK(NNDPHTS, NNDPHTS), MAV(NNDPHTS), MAQ(NNDPHTS)
REAL MAV(NNDPHTS, NNDPHTS), MAV(NNDPHTS, NNDPHTS), MAV(MAV(NNDPHTS, NNDPHTS))
REAL BB, CHIT, DOP, DTC, E, F, FNU
REAL PR, MAYSUM(NNDPHTS), SIGMA(NQUAD, NNDPHTS)
REAL VX, VY, VZ

REAL W(NNU), WTNU(NNU)
DATA WTNU/.2777777777777778, .44444444444444, .2777777777777778/

REAL FWT(0:NQUAD-1)
DATA FWT/.6888867, 2.8866667, 1.3333333, 2.6688687, .8866667/

SAVE

EXTERNALS

REAL TEDDFAC, HPROFILE, LIISLV, TGEMER, TRIDAG
EXTERNAL TEDDFAC, HPROFILE, LIISLV, TGEMER, TRIDAG

FUNCTIONS

REAL SB, SBHE1, SBHE2
SB(I, ID) = ACDP*EXP(NU*FRQH(I)/TEMP(ID))*GH(I)/TEMP(ID)
\begin{verbatim}
: SQRT(TEMP(ID))
SBHE1(I,ID)=ACCOF*EXP((HK*FRQHE1(I)/TEMP(ID))*GHE1(I)/
TEMP(ID)/SQRT(TEMP(ID))
: SQRT(TEMP(ID))
SBHE2(I,ID)=ACCOF*EXP((HK*FRQHE2(I)/TEMP(ID))*GHE2(I)/
TEMP(ID)/SQRT(TEMP(ID))
C C START OF EXECUTABLE STATEMENTS C C IF NOT ALREADY DONE (I.E. THIS IS FIRST ITERATION) SET UP FS'S IF (.NOT.FSET) THEN DO 10 I=1,ITRB L=LOWERB(I) U=UPPERB(I) IT=ITRB(L,U) FSH(IT)=-.FALSE. 10 CONTINUE ENDIF C C BEGIN ESTIMATING RATES OF SECONDARY TRANSITIONS INVOLVING C UPPERMOST LEVELS (N>WLH), WHICH ARE ADDED TO THE CONTINUUM C RATES. DO 350 LL=1,WLH-1 DO 340 UU=LL+1,WLH L=LL U=UU IT=ITRB(L,U) IF (.NOT.FSH(IT)) THEN FRQO=FRQH(L)-FRQH(U) IF (FRQO.LT .0) THEN FRQO=ABS(FRQO) L=UU U=LL ENDIF C C CALCULATE LINE PROFILE C DOP=SQRT(TLINE)*FRQO*DCPCOF DO 30 IJ=1,IQUAD DO 20 ID=1,IDEPTB SIGMA(IJ,ID)=HPROFILE(L,U,DOP*DELQUAD*(IJ-1), TEMP(ID),WE(ID)) 20 CONTINUE 30 CONTINUE C C ACCUMULATE RATES TO/FROM CONTINUUM C DO 40 ID=1,WEPTH A1(ID)=RHUS(ITRH(L,MQH+1),ID)+WE(ID)*CR(L,WLH+1,ID) A2(ID)=WS(L,ID)*(RED5(ITRH(L,MQH+1),ID)+WE(ID)* CR(L,WLH+1,ID)) A3(ID)=RHUS(ITRH(U,MQH+1),ID)+WE(ID)*CR(U,WLH+1,ID) A4(ID)=WS(U,ID)*(RED5(ITRH(U,MQH+1),ID)+WE(ID)* CR(U,WLH+1,ID)) 40 CONTINUE C C ACCUMULATE RATES TO/FROM LEVELS OTHER THAN L AND U C DO 70 I=1,L-1 DO 50 ID=1,WEPTH A1(ID)=A1(ID)+WE(ID)*CR(L,I,ID) A2(ID)=A2(ID)+WE(ID)*CR(I,L,ID) 50 CONTINUE ITT=ITRH(I,L) IF (ITT.WE.0) THEN DO 60 ID=1,WEPTH V=WS(I,ID)/WS(L,ID) A1(ID)=A1(ID)+V*RHDS(ITT,ID) A2(ID)=A2(ID)+V*WS(I,ID) 60 CONTINUE ENDIF 70 CONTINUE DO 100 I=L+1,ULB IF (I.WE.U) THEN DO 80 ID=1,WEPTH A1(ID)=A1(ID)+WE(ID)*CR(L,I,ID) A2(ID)=A2(ID)+WE(ID)*CR(I,L,ID) 80 CONTINUE ITT=ITRH(L,I)
\end{verbatim}
IF (ITT.NE.0) THEN
  DO 90 ID=1,NDEPT
    VX=WS(L,ID)/WS(I,ID)
    A1(ID)=A1(ID)+RHUS(ITT,ID)
    A2(ID)=A2(ID)+#(I,ID)*VX*RHDS(ITT,ID)
  CONTINUE
90 CONTINUE
ENDIF

DO 130 I=1,U-1
  IF (I.NE.L) THEN
    DO 110 ID=1,NDEPT
      A3(ID)=A3(ID)+WE(ID)*CR(U,I,ID)
      A4(ID)=A4(ID)+#(I,ID)*WE(ID)*CR(I,U,ID)
    CONTINUE
110 CONTINUE
  ITT=ITRB(I,U)
  IF (ITT.NE.0) THEN
    DO 120 ID=1,NDEPT
      VX=WS(U,ID)/WS(I,ID)
      A3(ID)=A3(ID)+VX*RHDS(ITT,ID)
      A4(ID)=A4(ID)+#(I,ID)*VX*RHUS(ITT,ID)
    CONTINUE
120 CONTINUE
  ENDIF
130 CONTINUE

DO 160 I=U+1,ILB
  DO 140 ID=1,NDEPT
    A3(ID)=A3(ID)+WE(ID)*CR(U,I,ID)
    A4(ID)=A4(ID)+#(I,ID)*WE(ID)*CR(I,U,ID)
  CONTINUE
140 CONTINUE
  ITT=ITRB(U,I)
  IF (ITT.NE.0) THEN
    DO 150 ID=1,NDEPT
      VX=WS(U,ID)/WS(I,ID)
      A3(ID)=A3(ID)+VX*RHDS(ITT,ID)
      A4(ID)=A4(ID)+#(I,ID)*VX*RHUS(ITT,ID)
    CONTINUE
150 CONTINUE
  ENDIF
160 CONTINUE

C INTEGRATE PROFILE
C
DO 180 ID=1,NDEPT
  MAVSUM(ID)=0.
  DO 170 IJ=1,NQUAD
    MAVSUM(ID)=MAVSUM(ID)+
      STORM(IJ,ID)*DELQUAD*DGDFWT(IJ-1)
170 CONTINUE
180 CONTINUE
C CALCULATE TERMS REPRESENTING LINE SCATTERING AND LINE THERMAL
C TERMS.
C
BB=BBBCOF*FRQO*FRQO*FRQO
DO 190 ID=1,NDEPT
  EX=EXP(BB*FRQO/TEMP(ID))
  VX=VX=WE(ID)*CR(L,U,ID)+EX*SCOF+MAVSUM(ID)+BB*FRQO-
      NE(ID)*CR(L,U,ID)+GH(U)*A2(ID)*A3(ID)/GH(L)-
      A1(ID)*A4(ID)
  VZ=VZ=WE(ID)*CR(L,U,ID)+A1(ID)*A4(ID)/VY
  VY=VY=SCOF*FRQO/VY
  A1(ID)=BB=VY
  A2(ID)=BB=VZ
190 CONTINUE
C A1 NOW CONTAINS SCATTERING LINE SOURCE TERM; A2 IS THERMAL
C (OR OTHER TRANSITION) SOURCE TERM.
C CALCULATE CONTINUUM OPACITIES FOR THIS TRANSITION.
C CALL TGENNER(FRQO,CHIC,ETAC)
C CLEAR RYBICKI MATRICES
C
DO 210 I=1,NDEPT
  DO 200 J=1,NDEPT
    NAW(I,J)=0.
200 CONTINUE
210 CONTINUE
DO 220 I=1,NDEPTH
  MAV(I,1)=1.
  MAQ(I)=0.
220 CONTINUE
DO 320 JJ=0,NQUAD-1
C CALCULATE FREQUENCY INTEGRAL WEIGHTS AND LINE OPACITY
C FROM PROFILE CALCULATED EARLIER.
C
DO 230 ID=1,NDEPTH
  MAV(ID)=DELQUD*DELQ*FWT(JJ)*SIIA(I+1,ID)
  ETAL(ID)=SIIA(I+1,ID)*(ETAL(ID)+SIIA(ID))
  CHIL(ID)=SIIA(I+1,ID)*CHIL(ID)
  ETA(I)=ETA(ID)*BB/ETA(ID)
230 CONTINUE
C GENERATE MOCUMENT FACTORS
C CALL TESSFAC(FRQO,CHIC,ETAC,CHIL,ETAL,F1)
C
C OPTICAL DEPTHS
DO 240 ID=1,NDEPTH-1
  DT(ID)=( ETA(ID+1)-ETA(ID))/0.5*(CHIL(ID+1)+CHIL(ID)+
        CHIC(ID+1)+CHIC(ID))
240 CONTINUE
C SET UP SOURCE MATRICES
MAV(I)=0.
MAQ(I)=0.
DO 250 ID=2,NDEPTH-1
  CHIC(ID)=CHIC(ID)+CHIL(ID)
  MAV(ID)=CHIL(ID)*(CHIC(ID))/CHIT
  MAQ(ID)=(ETAC(ID)+A2(ID)*CHIL(ID))/CHIT
250 CONTINUE
MAV(NDEPTH)=0.
MAQ(NDEPTH)=BB/(EXP(N*FRQO/TEMP(NDEPTH))-1.)
C SET UP DIFFERENCE OPERATOR MATRIX
DO 270 ID=1,NDEPTH
  DO 260 JJ=1,NDEPTH
    MAT(I,J)=0.
 260 CONTINUE
270 CONTINUE
C SURFACE
MAT(1,1)=FM(1)/DT(1)-FM
MAT(1,2)=FM(1)/DT(1)
C ORDINARY DEPTH POINT
DO 280 ID=2,NDEPTH-1
  DTC=0.5*(DT(ID)+DT(ID-1))
  MAT(ID,1)=FM(ID-1)/DT(ID-1)/DTC
  MAT(ID,2)=FM(ID-1)/DT(ID-1)/DTC
  MAT(ID,3)=MAT(ID,ID-1)-MAT(ID,ID+1)-1.0+
             NE(ID)*SIIA(CHIC(ID)+CHIL(ID))/
             ETA(ID)/ETA(ID)
280 CONTINUE
C LOWER BOUNDARY CONDITION
MAT(NDEPTH,NDEPTH-1)=0.
MAT(NDEPTH,NDEPTH)=1.0
C NOW ACCUMULATE CONTRIBUTION OF THIS (ANGLE,FREQUENCY) POINT
CALL TRIDAG(MAT,NDEPTH,NDEPTH)
DO 300 I=1,NDEPTH
  MAV(J,1)=MAW(J,1)-MAT(J,I)*MAQ(I)
  MAV(J)=MAQ(J)*MAW(J)*MAT(I,J)
  MAQ(J)=MAQ(J)*MAW(J)*MAT(I,J)
300 CONTINUE
CONTINUE
C NOW SOLVE FOR MEAN SOURCE FUNCTION
C CALL LINSLV(MAW,MAQ,MEANJ,MDEPTH,NMDEPTH)
C NORMALIZE MEANJ USING MAVSUM AND CALCULATE RATES.
C DO 330 ID=1,MDEPTH
  EX=EXP(-FRQO*BB/TEMP(ID))
  RMSU(IT,ID)=SCDF*MEANJ(ID)/FRQO
  RMSD(IT,ID)=SCDF*(MAVSUM(ID)*BB+MEANJ(ID))/EX/FRQO
330 CONTINUE
ENDIF
340 CONTINUE
350 CONTINUE
FSET=.TRUE.
RETURN
END

FUNCTION WFLD(B)
C INTERPOLATION OF MICROFIELD DISTRIBUTION TABLE
C COMMON /MICRO/W(300,5), SHIELD
REAL SPT(5), II(5)
DATA II/0.0, 0.2, 0.4, 0.6, 0.8/
C
WFLD=0.0
IF (B.LE.30.0)GO TO 10
SBS=1./B/SQRT(B)
WFLD=((21.6*SBS+7.639)*SBS+1.496)*SBS/B
RETURN
10 IF (B.LE.0.)RETURN
  J=(B+0.2)*10.0
  L=J-1
  IF (J.GT.2)L=J-2
  IF (J.GT.3)L=J-3
  IF (J.GT.300)L=297
  LLL=L+4
  DO 50 I=1,5
    SPT(I)=0.
    DO 40 K=L,LLL
      AK=K-1
      TERN=W(K,I)
      DO 30 N=L,LLL
        IF (K.NE.M)THEN
          AM=M-1
          TERM=TERM+(10.*B-AM)/(AK-AM)
        ENDIF
30 CONTINUE
    SPT(I)=SPT(I)+TERM
  40 CONTINUE
  50 CONTINUE
WFLD=POLY(5,II,SPT,SHIELD)
RETURN
END
E. Program HE

Only the profile functions for neutral helium have been listed for HE, as all other subroutines are similar to ones already listed.
REAL FUNCTION VOIGT(A,V)

VOIGT FUNCTION CALCULATION; THIS IS SUFFICIENTLY CLEVER TO HANDLE
A VALUE OF A, NOT JUST SMALL A. THIS IS DONE BY MEANS OF AN
ASYMPTOTIC EXPANSION FOR LARGE A AND A SERIES EXPANSION FOR SMALL
A.

PARAMETER (PI=3.141592654)

REAL TERM(100)

COMMON /COMCON/A1,V1

REAL CONINT
EXTERNAL CONINT

I=V/A
T=0.25*(A/A)
DET=0.25*X*X/T
IF (DET.LT.49.)THEN

SERIES REGIME

THE FIRST TERM IN THE SEQUENCE IS A BIT TRICKY;
WE MUST USE A SERIES EXPRESSION FOR VERY SMALL T.
OTHERWISE THE EXPONENTIAL FACTOR OVERFLOWS AS THE ERFC
FACTOR UNDERFLOWS.

IF (T.GT.(.001S))THEN

ELSE

ENDIF

S1=SO
W=1
FAC=1.1

N=N+1
SO=(1.0-SO)*0.5/(2.*W-1)/T
FAC=FAC*DET/W
TERM(N)=SO+FAC
IF (TERM(N).GT.(1.E-8*S1).AND.W.LT.100)GO TO 10
SUM=0.
DO 10 I=W,1,-1
SUM=SUM+TERM(I)
10 CONTINUE
SUM=SUM+1
UO=SUM*EXP(-DET)
ELSE IF (X.GT.10.)THEN

ASYMPTOTIC REGIME

S1=.A.
SO=.1/X
W=1
TERM(I)=SO
SIGA=1.

N=N+1
S3=S1
S2=SO
S1=S2/X-2.*T*(W-1)*S3/X/X
W=W+1
SO=S1/X-2.*T*(W-1)*S2/X/X
SIGA=SIGA
TERM(N)=SIGA*SO
IF (ABS(SO*X).GT.1.E-8.AND.W.LT.99)GO TO 30
SUM=0.
DO 30 I=W,1,-2
SUM=SUM+TERM(I)
30 CONTINUE
UO=SUM/X
ELSE

INTEGRATION REGIME

A1=A
V1=V
CALL QROMB(CONINT,0.,1.,UO)
UO=SO*A*A/1.7724539
ENDIF
REAL FUNCTION COMINT(X)
C COMMON /CUWO/ A, V
C IF (X.LE.O) THEN
   COMINT = 0.
ELSE
   COMINT = X/((V+LOG(X))**2+A*A)+1./((V-LOG(X))**2+A*A)
ENDIF
RETURN
END

SUBROUTINE QROMB(FUIC,A,B,SS)
PARAMETER (EPS=1.E-6, JMAX=20, JMAXP=JMAX+1, K=5, KM=K-1)
REAL S(JMAXP), H(JMAXP)
C H(1)=1.
DO 11 J=1,JMAX
   CALL TRAPZD(FUIC,A,B,J,SYM)
   IF (J.GE.K) THEN
      CALL POLINT(H(J-KM),S(J-KM),K,0.,55,DSS)
      IF (ABS(DSS).LT.EPS*ABS(SS)) RETURN
      S(J+1)=S(J)
      B(J+1)=0.25*B(J)
11 CONTINUE

SUBROUTINE POLINT(XA,YA,M,X,Y,DY)
PARAMETER (IMAX=10)
DIMENSION XA(1), YA(1), C(IMAX), D(IMAX)
C M=1
   DF=ABS(X-XA(1))
   DO 11 I=1,M
      DIFT=ABS(X-XA(I))
      IF (DIFT.LT.DF) THEN
         MS=I
         DF=DIFT
      ENDIF
      C(I)=YA(I)
      D(I)=YA(I)
11 CONTINUE
   Y=YA(MS)
   MS=MS-1
   DO 13 M=1,M-1
      DO 12 I=1,M-M
         BO=XA(I)-X
         BP=XA(I+M)-X
         W=C(I+1)-D(I)
         DEN=BO*BP
         IF (DEN.EQ.0.) STOP 'FATAL ERROR IN POLINTERP'
         DEN=W/DEN
         D(I)=BP*DEN
         C(I)=BO*DEN
12 CONTINUE
      IF (2*MS.LT.M) THEN
         DY=C(MS+1)
      ELSE
         DY=0.DS
         MS=MS-1
      ENDIF
13 CONTINUE
RETURN
END

FUNCTION ERFC(X)
ERROR FUNCTION CALCULATION, FROM "NUMERICAL RECIPES."

ERFC=GAMMQ(.5,X**2)
RETURN
END

FUNCTION GAMMLN(XX)

LOG OF GAMMA FUNCTION; ALSO FROM "NUMERICAL RECIPES."

REAL*8 COF(6),STP,SAF,TMP,SEIL
DATA COF,STP/76.1809173DD0,-86.50532033DD0,24.01409822DD0/  
* -1.231739516DD0, .53638205, 2.5066282746DD0/
DATA SAF/0.5DD0,1.0DD0,0.5DD0/
X=XX-ONE
TMP=X+SAF
TMP=(X+HALF)+LOG(TMP)-TMP
SER=ONE
DO 11 J=1,6
   X=X+ONE
   SER=SER+COF(J)/X
11 CONTINUE
GAMMLN=TMP+LOG(STP*SER)
RETURN
END

FUNCTION GAMMQ(A,X)

PARTIAL GAMMA FUNCTION FROM "NUMERICAL RECIPES."

IF(X.LT.0..OR.A.LE.0.)PAUSE
IF(X.LT.A+1.)THEN
   CALL GSEIL(GAMSEIL,A,X,GLI)
   GAMMQ=1.-GAMSEIL
   ELSE
   CALL GCF(GAMMQ,A,X,GLI)
ENDIF
RETURN
END

SUBROUTINE GCF(GAMMCF,A,X,GLI)

CONTINUED FRACTION REPRESENTATION OF PARTIAL GAMMA FUNCTION,  
FROM "NUMERICAL RECIPES."

PARAMETER (ITMAX=100,EPS=3.E-7)
GLI=GAMMLN(A)
GOLD=0.
AO=1.
AI=1.
BO=0.
BI=1.
FAC=1.
DO 11 N=1,ITMAX
   AB=FLOAT(N)
   ABA=A+1.
   AO=(AI+AO*ABA)*FAC
   BO=(BI+BO*ABA)*FAC
   ARF=AB+FAC
   AI=AB+FAC
   BI=BO+FAC
   IF(A1.NE.0.)THEN
      FAC1=A1/G
      G=FAC1
   ELSE
      IF(ABS((G-GOLD)/G).LT.EPS)GO TO 1
      GOLD=G
   ENDF
11 CONTINUE
PAUSE 'A too large, ITMAX too small'
1 GAMMCF=EXP(-A+1.0+LOG(1)-GLI)*G
RETURN
END

SUBROUTINE GSEIL(GAMSEIL,A,X,GLI)
SERIES REPRESENTATION OF PARTIAL GAMMA FUNCTION, FROM
"NUMERICAL RECIPES."

PARAMETER (ITMAX=100, EPS=3.E-7)
GLN=GAMMLN(A)
IF(X.LE.0.) THEN
  GAMSER=0.
  RETURN
ENDIF
AP=A
SUM=1./A
DEL=SUM
DO 11 I=1,ITMAX
  AP=AP+1.
  DEL=DEL*X/AP
  SUM=SUM+DEL
  IF(ABS(DEL).LT.ABS(SUM)*EPS) GO TO 1
1 CONTINUE
  PAUSE 'A too large, ITMAX too small'
  GAMSER=SUM*EXP(-X*A+LOG(X)-GLN)
  RETURN
END

SUBROUTINE TRAPZD(FUNC,A,B,S,IT)
REAL FUNC
EXTERNAL FUNC

SAVE IT

IF (IT.EQ.1) THEN
  S=0.5*(B-A)*(FUNC(A)+FUNC(B))
  IT=1
ELSE
  TWM=IT
  DEL=(B-A)/TWM
  X=A+0.5*DEL
  SUM=0.
  DO 11 J=1,IT
    SUM=SUM+FUNC(X)
    X=X+DEL
 11 CONTINUE
  S=0.5*(S+(B-A)*SUM/TWM)
  IT=2*IT
ENDIF
RETURN
END
F. Program SPECTRUM

The program SPECTRUM is listed here in its entirety. All subroutines beginning with ICH are part of the Caltech Astronomy character function library ICH. All subroutines beginning with PG are part of the PGPLOT package [39].
PROGRAM SPECTRUM

S P E C T R U M

Takes a set of line data tables and a directory full of theoretical line profiles and allows the user to interactively fit the observed data to the theoretical profiles by chi-square minimization.

Input files:

Line data are read from files whose names are prompted for by the program.

Theoretical data are contained in numerous disk files whose names are in the format '<grav><abund><wave>', where <grav> is a two-numeral string specifying gravity, <abund> is a single numeral specifying ratio of helium to hydrogen, and <wave> is a four-numeral string specifying the line. Thus, 't4514863' is a file containing theoretical profiles of the hydrogen 4863 angstrom line (B beta) for log g of 4.5 and He/H of 0.1. The profiles are listed within the file by temperature; the data consist of a record that starts with the temperature (the remainder of the record may be discarded) followed by a record containing the number of points in the profile, followed by the wavelengths and data for those points.

If the specified library file does not contain a profile at the appropriate temperature, the program attempts to interpolate in abundance first and then in log gravity. If neither works, the program so notifies the user.

Output files:

The user specifies a soft device (must be something with a cursor) on which lines are displayed and fits may be made.

The user is also prompted for a hard device type; when he finishes determining his fit, the final results are written to the disk in a format suitable for the specified hard-device type. The user may specify the hard device to be a soft device if he wishes to eyeball the fit before making a hard-output plot.

The remainder of the program is menu-driven.

IMPLICIT NONE

Functions

INTEGER ICLEN, LOCATE, PGBEGIN

Parameters

INTEGER NPIX, ML
PARAMETER (NPIX=801, ML=12)

Local variables

CHARACTER CC*1, CVALUE*32, CWAVE*4, FILE*32, HARD*8, OPTION*1
CHARACTER SOFT*32, TITLE*50, XLABEL*20, YLABEL*13

LOGICAL EXIST, FETCHED, IFAIL, ROTATED

INTEGER I, IA1, IA2, ICENTER(ML), ICLEFT1(ML), ICLEFT2(ML)
INTEGER ICRIGHT1(ML), ICRIGHT2(ML), IDENEM, IDUMMY, IGI
INTEGER IG2, IT1, IT2, J, JJ, K, L, LISTA(40), LTITLE
INTEGER NA, NFIT, IDPIX(ML), OLDVALUES, PLN

REAL ABUND, AGRID(4), CONTA(ML), CONTR(ML), DEV, FITA, FITB
REAL FITC, FITD, GBRID(5), GRAV, HABUND, MGRAV, WROT, WTEFF
REAL OLDROT, OSIG(NPIX,ML)
REAL ORX(NPIX,ML), OY(NPIX,ML), ROT, SIG, SIGFIT(NPIX)
REAL SUM, SUM2, SUMG, SUM2G, SUMT, SUM2T, SUMW, SUMWG, SUMWT
REAL TO00(NPIX,ML), TO01(NPIX,ML), TO10(NPIX,ML), TO11(NPIX,ML)
REAL T100(NPIX,ML), T101(NPIX,ML), T110(NPIX,ML), T111(NPIX,ML)
REAL TCENTER(ML), TEFF, TGRID(8), WAVE(ML), WEIGHT(ML), WT, X
REAL X1, X2, X3, X4, ICENTER(ML), YFIT(NPIX,1), YFIT(NPIX,2)
REAL YFIT2(NPIX), YFIT3(NPIX), XPLT(NPIX), Y, Y1, Y2, YPLT(NPIX)
REAL YFil1(MPII), YFil2(MPII), YFil3(MPII), YFil4(MPII)
REAL YFil5(MPII)

C

C
REAL•S CPROJ(40,40), DALPU(40,40), DCOVAR(40,40), DERR, DET
REAL•S DFIT(40), DLAMBDA, DRIIS, DIPLOT(MPII), DYPLOT(MPII)
REAL•S OLDLAMBDA, OLDRMS, PERR(4)
REAL•S SUMI, SUMI2, SUMY, SUMIY

C Main data COMMON block
C
C
INTEGER DPII(ML), ILIIES
REAL•S DOSIG(MPII,ML), DOI(MPII,ML), DOY(MPII,ML)
REAL•S RT0000(MPII,ML), RT0001(MPII,ML), RT0100(MPII,ML)
REAL•S RT0011(MPII,ML), RT0101(MPII,ML), RT1000(MPII,ML)
REAL•S RT0100(MPII,ML), RT1001(MPII,ML), RT1010(MPII,ML)
REAL•S RT1100(MPII,ML), RT1101(MPII,ML), RT1110(MPII,ML)
REAL•S RT1111(MPII,ML)
COMMON /MAIN/DPII, ILIIES, DOSIG, DOI, DOY, RT0000, RT0001,
: RT0010, RT0011, RT0100, RT0101, RT0110, RT0111, RT1000,
: RT1001, RT1010, RT1011, RT1100, RT1101, RT1110, RT1111

C PLOTFUNC common block
C
COMMON /PLOTFUNC/DIPLOT, DYPLOT, PLE
C
Data statements
C
DATA ILABEL/'Wavelength/Anstroms'/
DATA YLABEL/'Relative Flux'/
DATA AGRID/0.05, 0.1, 0.2, 0.5/
DATA GGRID/2.75, 3.0, 3.5, 4.0, 4.5/
DATA TGRID/28000., 30000., 32500., 35000., 37500., 40000., 45000.,
: 50000./
C
Exterals
EXTERNAL GAUSS, ROTFUNC, PHYSFUNC, PLOTFUNC

* Start of executable statements *
C
C
N0=0
OLDN0=0
I1=0
IG=0
RHT=0.
FETCHED=.FALSE.
ROTATE=.FALSE.
C
Get the top label for all plots
C
70 WRITE (6,*)'Object name? '
READ (5,2000,ERR=70)TITLE
LTITLE=ICHLEN(TITLE)
C
Query user for soft device type
C
10 WRITE (6,*)'Soft device type? '
READ (5,2000,ERR=10)SOFT
CALL PQINF('CURSOR',CVALUE,I)
IF (CVALUE(1).EQ.'l')THEN
WRITE (6,*)'Please select a device with a cursor.'
GO TO 10
ENDIF
C
Open soft device
C
CALL PGBEGIN(0,SOFT,1,1)
C
Get option
C
15 WRITE (6,*)'Option? '
READ (5,2000)OPTION
IF (OPTION.EQ.'?')THEN
List the options
WRITE (6,*)'Options are:'
WRITE (6,*)
WRITE (6,*) 'Print this message'
WRITE (6,*) 'Read in an observed profile'
WRITE (6,*) 'Choose values for the three parameters'
WRITE (6,*) 'Rotate theoretical profiles'
WRITE (6,*) 'Measure VSIII'
WRITE (6,*) 'Measure parameters'
WRITE (6,*) 'Produce hardcopy'
WRITE (6,*) 'Exit'
GO TO 15

ELSE IF (OPTION.EQ.'0'.OR.OPTION.EQ.'o') THEN

Prompt user for data file

I=NINES+1
30 WRITE (6,1000)I
1000 FORMAT (1X,'Data file for line ',I2,'?')
READ (5,2000,ERR=30)FILE
OPEN (UNIT=1,FILE=FILE, ACCESS='SEQUENTIAL', STATUS='OLD',
READONLY, ERR=30)

Read data records to end of file

READ (1,*)
DO J=1,800
READ (1,*,END=40)OX(J,1),OY(J,1)
ENDDO
WRITE (6,*) 'Warning -- not all of file read'
CLOSE (1)

WARNING: 'Wavelength of line?'
READ (5,*,ERR=51)WAVE(I)
WRITE (CWave,1001)IIT(WAVE(I))
INQUIRE (FILE='f450'//CWAVE//'.',EXIST=EXIST)
IF (.NOT.EXIST) THEN
WRITE (6,*) 'That line is not in the library.'
GO TO 15
ENDIF
IDP=IDP+1
DO J=1,IDP(I)
YPLOT(J)=OY(IDP(I)-J+1,1)
XPLT(J)=OX(IDP(I)-J+1,1)
ENDDO
DO J=1,IDP(I)
OX(J,1)=XPLT(J)
OY(J,1)=YPLOT(J)
ENDDO
ENDIF

Reverse the order of the arrays if necessary.
(Try to be ordered from lowest wavelength to highest.)

DO J=1,IDP(I)
VPLT(J)=OY(IDP(I)-J+1,1)
XPLT(J)=OX(IDP(I)-J+1,1)
ENDDO
DO J=1,IDP(I)
OX(1,I)=XPLT(J)
OY(J,1)=VPLT(J)
ENDDO
ENDIF

Now throw up the plots and let the user take a look at them.
The user must specify the "shoulders" of the plots, e.g.,
the region around the line that will be used to fine-tune
the continuum level. The user is then prompted for the
line center; the program tries to refine this guess by
fitting a Gaussian to the line.

CALL PSCSI(I)
CALL PGTV(WAVE(I)=20.0, WAVE(I)=20.0, 0.0, 1.1, 0, 0)
CALL PGLABEL(XLABEL,YLABEL,TITLE,IITLE))
CALL PGIN(WDPFX(I),OY(I,1),OY(1,1),.TRUE.)
WRITE (6,*) 'Indicate limits of left shoulder:'
CALL PGCURSE(I,Y,CC)
ICLEFT1(I)=LOCATE(OY(I,1),IDP(I),I)
CALL PGCURSE(I,Y,CC)
ICLEFT2(I)=LOCATE(OY(I,1),IDP(I),I)
WRITE (6,*) 'Indicate limits of right shoulder:'
CALL PGCURSE(I,Y,CC)
ICRIGHT1(I)=LOCATE(OY(I,1),IDP(I),I)
CALL PGCURSE(I,Y,CC)
ICRIGHT2(I)=LOCATE(OY(I,1),IDP(I),I)

Make REAL=8 copy of trimmed profile.

DO J=ICLEFT1(I),ICRIGHT2(I)
JJ=J-ICLEFT1(I)+1
DOX(JJ,I)=OX(J,I)
DOY(JJ,I)=OY(J,I)
ENDO
DPIX(I)=ICRIGHT2(I)-ICLEFT1(I)+1

Calculate line through shoulders.

CALL LINEFIT(ICLEFT1(I),ICLEFT2(I),ICRIGHT1(I),ICRIGHT2(I),
OX(1,I),OY(1,I),COITA(I),COITB(I))
CALL PGSCI(2)
X=OX(ICLEFT1(I),I)
Xt=OX(ICRIGHT2(I),I)
Y=COITA(I)•X+COITB(I)
Yt=COITA(I)•Xt+COITB(I)
CALL PMOVE(X,Y)
CALL PGDRAW(X1,Y1)
CALL PGSCI(1)

Now get approximate line center.

WRITE (6,*)'Indicate approximate line center.'
WRITE (6,*)'(Be sure both I and Y are indicated.)'
CALL PGCURSE(X,Y,CC)

Evaluate best Gaussian fit to line center.

DFIT(1)=X
DFIT(2)=1.-Y
DFIT(3)=1.0
DFIT(4)=COITA(I)
DFIT(5)=COITB(I)
DLAMBDA=1.
DO J=1,5
USU(J)=J
ENDO
CALL NRQNIL(DOX(1,I),DOY(1,I),DPIX(I),DFIT,
5,LISTA,3,DCOVAR,DALPHA,40,OLDRNS,GAUSS,DLAMBDA)

75 CALL NRQNIL(DOX(1,I),DOY(1,I),DPIX(I),DFIT,
5,LISTA,3,DCOVAR,DALPHA,40,OLDRNS,GAUSS,DLAMBDA)
IF (MAX(ABS((DRNS-OLDRNS)/DRNS),ABS(DRNS-OLDRNS)).GT.
(1.E-3))THEN
75
OLDRNS=DRNS
GO TO 75
ENDIF
XCEITER(I)=DFIT(1)
ICEITER(I)=LOCATE(OX(t,I),DPIX(I),XCEITER(I))
WRITE (6,*)'Line center calculated as ',XCEITER(I)

Toss up the line so that the user can see if he likes it.

DO J=1,DPIX(I)
XPLOT(J)=DOX(J,I)
YPLOT(J)=DFIT(4)•XPLOT(J)+DFIT(5)
YPLOT(J)=YPLOT(J)•(1.0-DFIT(2)*EXP(-((DFIT(1)-XPLOT(J))/
DFIT(3))**2))
ENDO
CALL PGSCI(3)
CALL PGLINE(ICRIGHT2(I)-ICLEFT1(I)+1,XPLOT,YPLOT)

Estimate V sin I and the equivalent width.

WRITE (6,*)'Line center calculated as ',XCEITER(I)
WRITE (6,*)'Estimated V sin I is ',ABS(DFIT(3))•3.E5/WAVE(I)
WRITE (6,*)'Equivalent width is ',DFIT(2)•ABS(DFIT(3))•1.77245
WRITE (6,*)'Keep this line?'
READ (5,2001)OPTIOI
IF (OPTIOI.EQ.'t'.OR.OPTIOI.EQ.'n')GO TO 15
77 WRITE (6,*)'Theoretical weight factor?'
READ (5,•,ERR=77)WEIGBT(I)

Estimate the errors in the flux across the profile.

DO J=1,DPIX(I)
K=0
SUMX=0.
SUMX2=0.
SUMY=0.
SUMXY=0.

ENDO
DO JJ=J-2,J+2
IF (JJ.GT.0.AND.JJ.LE.DPIX(I))THEN
  E=K+1
  SUMX=SUMX+DOX(JJ,I)
  SUMX2=SUMX2+DOX(JJ,I)**2
  SUMY=SUMY+DOY(JJ,I)
  SUMXY=SUMXY+DOX(JJ,I)*DOY(JJ,I)
ENDIF
ENDDO
DET=K*SUMX2-SUMX*SUMX
FITA=(SUMY*SUMX2-SUMXY*SUMX)/DET
FITB=(K*SUMXY-SUMX*SUMY)/DET
SUMX2=0.
DO JJ=J-2,J+2
IF (JJ.GT.0.AND.JJ.LE.DPIX(I))THEN
  SUMX2=SUMX2+(DOY(JJ,I)-FITA-FITB*DOX(JJ,I))**2
ENDIF
ENDDO
DOSIG(J,I)=SQRT(SUMX2/(K-1))/KAX(1.E-25,WEIGHT(I))
ENDDO
{GET Coil

C ELSE IF (OPTION.EQ.'P'.OR.OPTION.EQ.'p') THEN

C GET the estimate of stellar parameters

80  WRITE (6,*)'Estimate of TEFF ?'
  READ (5,*,ERR=80)TEFF
  I=LOCATE(TGRID,8,TEFF)
  IF (I.LT.1.0R.I.GE.8)TBEB
    WRITE (6,*)'Unacceptable temperature range'
    GO TO 80
  ENDIF
91  WRITE (6,*)'Estimate of LOG G ?'
  READ (5,*,ERR=91)GRAV
  J=LOCATE(GGRID,5,GRAV)
  IF (J.LT.1.0R.J.GE.5)TBEB
    WRITE (6,*)'Unacceptable gravity range'
    GO TO 91
  ENDIF
101 WRITE (6,*)'Estimate of Be/B ?'
  READ (5,*,ERR=101)ABUID
  K=LOCATE(AGRID,4,ABUID)
  IF (K.LT.1.0R.K.GT.4)TBEB
    WRITE (6,*)'Unacceptable abundance range'
    GO TO 101
  ENDIF

C NOW try getting the needed libraries.

C IF (I.EQ.IT1.AND.J.EQ.IG1.AND.K.EQ.IA1.AND.OLDILIIES.EQ.
  OLDILIIES)GO TO 15
  OLDILIIES=ILIIES
  IT1=I
  IT2=I+1
  IG1=J
  IG2=J+1
  IA1=K
  IA2=K+1
  IFAIL=.FALSE.
  DO I=1,ILIIES
    WRITE (CWAVE,1001)IIT(WAVE(I))
    CALL FETCH(IT1,IG1,IA1,CWAVE,I,T000(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT1,IG2,IA1,CWAVE,I,T010(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT2,IG1,IA1,CWAVE,I,T100(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT2,IG2,IA1,CWAVE,I,T110(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT1,IG1,IA2,CWAVE,I,T001(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT1,IG2,IA2,CWAVE,I,T011(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT2,IG1,IA2,CWAVE,I,T101(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
    CALL FETCH(IT2,IG2,IA2,CWAVE,I,T111(1,I),FETCBED)
    IFAIL=IFAIL.OR.. NOT.FETCBED
IF (IFAIL) TBEI
   WRITE (6,*) 'Try a different set of parameters'
   FETCHED=.FALSE.
   GO TO 15
ENDIF

K=0
X=1.3E8
DO J=1,DOI(I)
   IF (TOO0(J,I).LT.X) TBEI
      K=J
      X=TOO0(J,I)
   ENDIF
ENDDO

TCENTER(I)=GXX(K,I)
ENDDO

FETCHED=.TRUE.

ROTATED=.FALSE.
GO TO 15
ELSE IF (OPTION.EQ.'V'.OR.OPTION.EQ.'v') THEN
   GET a good measure of the rotational velocity by chi-square
   minimisation. In practice this does not work very well; the
   user is almost always better off to eyeball it by using
   the R and H commands to adjust the rotation parameter.
ENDIF

IF (.NOT.FETCHED) THEN
   WRITE (6,*) 'Please estimate parameters first.'
   GO TO 15
ENDIF

WRITE (6,*) 'Value of VSINI to bracket?'
READ (5,*) ROT

C Calculate profiles for given rotation.

DO I=1,NLINES
   CALL ROTATE(I,TOO0(1,I),TO0000(1,I),.8333*ROT)
   CALL ROTATE(I,TO01(1,I),TO0010(1,I),.8333*ROT)
   CALL ROTATE(I,TO10(1,I),TO1000(1,I),.8333*ROT)
   CALL ROTATE(I,TO11(1,I),TO1010(1,I),.8333*ROT)
   CALL ROTATE(I,T100(1,I),T10000(1,I),.8333*ROT)
   CALL ROTATE(I,T101(1,I),T10010(1,I),.8333*ROT)
   CALL ROTATE(I,T110(1,I),T11000(1,I),.8333*ROT)
   CALL ROTATE(I,T111(1,I),T11010(1,I),.8333*ROT)
   CALL ROTATE(I,TO000(1,I),TO0001(1,I),1.1667*ROT)
   CALL ROTATE(I,TO001(1,I),TO0011(1,I),1.1667*ROT)
   CALL ROTATE(I,TO010(1,I),TO0101(1,I),1.1667*ROT)
   CALL ROTATE(I,TO011(1,I),TO0110(1,I),1.1667*ROT)
   CALL ROTATE(I,T1001(1,I),T10011(1,I),1.1667*ROT)
   CALL ROTATE(I,T1010(1,I),T10101(1,I),1.1667*ROT)
   CALL ROTATE(I,T1100(1,I),T11001(1,I),1.1667*ROT)
   CALL ROTATE(I,T1110(1,I),T11101(1,I),1.1667*ROT)
ENDDO

C Now find the best fit.

MIFIT=3*NLINES+1
DO I=1,NLINES
   DFIT(3*I-2)=CONTA(I)
   DFIT(3*I-1)=CONB(I)
   DFIT(3*I)=XCENTER(I)-TCENTER(I)
ENDDO

DFIT(3*NLINES+1)=(TEFF-TGRID(IT1))/(TGRID(IT2)-TGRID(IT1))
DFIT(3*NLINES+2)=(GRAV-GGRID(IG1))/(GGRID(IG2)-GGRID(IG1))
DFIT(3*NLINES+3)=LOG(ABUND/AGRID(IA1))/LOG(AGRID(IA2))
 : AGRID(IA1)
 : AGRID(IA2)
DFIT(3*NLINES+4)=0.5
DCLA=1.0
DO I=1,3*NLINES
   LISTA(I)=I
ENDDO

LISTA(MIFIT)=3*NLINES+4
CALL MRQMIN2(DFIT,MIFIT,3,LISTA,DFIT,DCOVAR,DALPHA,40,DRMS,
   DLA=,NOTFUNC)

IF (OPTIOI.EQ.'Y'.OR.OPTION.EQ.'y') GO TO 261

WRITE (6,*) 'Iterate again?'
READ (5,2OO1) OPTIOI
IF (OPTIOI.EQ.'Y'.OR.OPTIOI.EQ.'y') GO TO 261

NROT=DFIT(MIFIT+3)
Now estimate probable error.

CALL MRQMINW2(DFIT,NFIT+1,LISTA,DFIT,DCOVAR,DALPHA,40,DRNS,

DLAMBA,DRTFUNC)

PERR(4)=SQRT(DCOVAR(NFIT+3,NFIT+3)*.3*DRNS)*.3333*Rot

WRITE (6,*,'(s3,1x,e15.8)') 'DRNS='.,DRNS,'.' P.E. = ',PERR(4)

ROTATED=.FALSE.

GO TO 15

ELSE IF (OPTION.EQ.'R'.OR.OPTION.EQ.'r') THEN

Rotate the profiles fetched from the libraries.

WRITE (6,*,'(a15,1x)') 'Value of VSIII to use?'

READ (5,*) ROT

DO I=1,ILIIES

CALL ROTATE(I,T000(I),RT000(I),ROT)

CALL ROTATE(I,T010(I),RT010(I),ROT)

CALL ROTATE(I,T100(I),RT100(I),ROT)

CALL ROTATE(I,T110(I),RT110(I),ROT)

E100

ROTATED=.TRUE.

GO TO 15

ELSE IF (OPTION.EQ.'F'.OR.OPTION.EQ.'f') THEN

Do the big fit by chi-square minimization.

NFIT=ILIIES+3+3

DO I=1,ILIIES

Initial estimate of the continuum and wavelength zero point parameters.

DFIT(3*I-2)=COITA(I)

DFIT(3*I-1)=COITB(I)

DFIT(3*I)=ICEITER(I)-TCEITER(I)

E100

Initial estimates of temperature, gravity, and abundance.

DFIT(3*ILIIES+1)=(TEFF-TGRID(IT1))/(TGRID(IT2)-TGRID(IT1))

DFIT(3*ILIIES+2)=(GRAV-GGRID(IG1))/(GGRID(IG2)-GGRID(IG1))

DFIT(3*ILIIES+3)=LOG(ABUND/AGRID(I1))/LOG(AGRID(I2))/

AGRID(I1))

DLAMBA=-1.

Set up and execute the minimization.

DO I=1,NFIT+1

LISTA(I)=I

E100

CALL MRQMINW2(DFIT,NFIT+1,LISTA,DFIT,DCOVAR,DALPHA,40,DRNS,

DLAMBA,PSYSFUNC)

Let the user decide if he is satisfied with current minimization.

WRITE (6,*,'(a15,1x)') 'Do the big fit again?'

READ (5,2001) OPTION

IF (OPTION.EQ.'Y'.OR.OPTION.EQ.'y') GO TO 260

DO I=1,ILIIES

COITA(I)=DFIT(3*I-2)

COITB(I)=DFIT(3*I-1)

ICEITER(I)=DFIT(3*I)+TCEITER(I)

E100

ITEFF=DFIT(3*ILIIES+1)

IGRAV=DFIT(3*ILIIES+2)

IABUID=DFIT(3*ILIIES+3)

Now estimate probable error from covariance matrix.

DLAMBA=0.0

CALL MRQMINW2(DFIT,NFIT+1,LISTA,DFIT,DCOVAR,DALPHA,40,DRNS,
DUIIBDA,PBYSFUIC)

DO I=1,3*1LIIES+3
    DO J=1,3*1LIIES+3
        CPROJ(I,J)=DCOVAR(I,J)
    ENDDO
ENDDO
CALL MATINV(CPROJ,3*1LIIES+3,40)
J=3*1LIIES+3
TEFF=TEFF+TGRID(IT2)+(1.-TEFF)*TGRID(IT1)
PERR(1)=SQRT(.3*DRMS/CPROJ(J+1,J+1))*(TGRID(IT2)-TGRID(IT1))
MGRAV=MGRAV+GRID(GIG2)+(1.-MGRAV)*GRID(GIG1)
PERR(2)=SQRT(.3*DRMS/CPROJ(J+2,J+2))*(GRID(GIG2)-GRID(GIG1))
MABUND=MABUND*(LOG(AGRID(IAI)+1.-MABUND)*LOG(AGRID(IAI)))
PERR(3)=SQRT(.3*DRMS/CPROJ(J+3,J+3))*LOG(AGRID(IAI)+1.-MABUND)
       ENDIF
WRITE (6,*)'Parameters estimated as:'
WRITE (6,*)'TEFF = ',ITEFF,' P.E. = ',PERR(1)
WRITE (6,*)'GRAV = ',MGRAV,' P.E. = ',PERR(2)
WRITE (6,*)'ABUID = ',IABUID,' P.E. = ',PERR(3)
WRITE (6,*)'Inverse covariance matrix:'
WRITE (6,*)'CHISQ = ',DRMS
DO I=1,3
    WRITE (6,*)('CPROJ(I,J),J=1,3')
ENDDO
GO TO 15
ELSE IF (OPTION.EQ.'B') THEN
C
C Make a hard plot of the current fit.
C
IF (.NOT.FETCHED) THEN
    WRITE (6,*)'Please specify parameters first'
    GO TO 15
ELSE IF (.NOT.ROTATED) THEN
    WRITE (6,*)'Please specify rotation first'
    GO TO 15
ENDIF
READ (6,2000,ERR=270) HARD
WRITE (6,*)'TEFF, GRAV, ABUID to use?'
READ (6,*)TEFF,GRAV,ABUID
CALL PGBEGIN(0,HARD,1,1)
DO I=1,3*1LIIES
    CALL PGEIV(WAVE(I)-20.0, WAVE(I)+20.0, 0.0, 1.1, 0, 0)
    CALL PGUBEL(IUBEL,YUBEL,TITLE(:LTITLE))
    CALL PGBel(IDPII(I),01(1,I),OY{l,I),.TRUE.)
C Calculate the profile to use.
C
X=(WTEFF-(GRID(IT2)-TGRID(IT1)))
DO J=1,DPFIX(I)
    YFIN1(J)=X*RT100(J,J)+(1.-X)*RT000(J,J)
    YFIN2(J)=X*RT010(J,J)+(1.-X)*RT001(J,J)
    YFIN3(J)=X*RT110(J,J)+(1.-X)*RT011(J,J)
    YFIN4(J)=X*RT111(J,J)+(1.-X)*RT011(J,J)
ENDDO
X=(MGRAV-(GRID(GIG2)-GRID(GIG1)))
DO J=1,DPFIX(I)
    YFIN1(J)=YFIN1(J)+(1.-YFIN1(J))
    YFIN2(J)=YFIN2(J)+(1.-YFIN2(J))
ENDDO
X=LOG(MABUND/(AGRID(IAI)))*LOG(AGRID(IAI))/LOG(AGRID(IAI))
DO J=1,DPFIX(I)
    DXPLOT(J)=DOX(J,J)
    DYPLOT(J)=YFIN2(J)+(1.-X)*YFIN1(J)
    YPLOT(J)=DYPLOT(J)
ENDDO
PL=DPFIX(I)
C
Now fit the continuum parameters to the data.
C
DFIT(1)=CONTA(I)
DFIT(2)=CONTB(I)
DFIT(3)=0.
DLAMBDAX=1.
DO J=1,3
    LISTA(J)=J
ENDDO
CALL MRQMIN((DOX(1,I),DOY(1,I),DPIX(I),DFIT,3,LISTA,3,DCOVAR,
DALPHA,40,OLDRMS,PLOTFUNC,DLAMBDA)
CALL MRQMIN((DOX(1,I),DOY(1,I),DPIX(I),DFIT,3,LISTA,3,
DCOVAR,DALPHA,40,OLDRMS,PLOTFUNC,DLAMBDA)
ENDIF
DO J=1,DPIX(I)
XPLOT(J)=XPLOT(J)+DFIT(3)
YPLOT(J)=YPLOT(J)•(DFIT(1)•XPLOT(J)+DFIT(2))
ENDDO
CALL PGLINE(DPIX(I),XPLOT,YPLOT)
ENDDO
C Restore the soft device.
C CALL PGEND
CALL PGBEGIN(0,SOFT,1,1)
GO TO 15
ELSE IF (OPTIO.EQ.'X')TBEI
C C EXIT
CALL PGEND
CALL EXIT
ELSE
GO TO 15
ENDIF
C 1001 FORMAT (I4)
2000 FORMAT (A)
2001 FORMAT (Ai)
ENDIF
INTEGER FUNCTION DLOCATE(XX,I,X)
C This is essentially the Numerical Recipes routine LOCATE,
C but here defined as a function rather than subroutine.
C Also, the real arguments are REAL*8.
C REAL*8 XX(I), X
JL=0
JU=I+1
10 IF (JU-JL.GT.1)TBEI
JN=(JU+JL)/2
IF ((XX(JU).GT.XX(1)).EQV.(X.GT.XX(JN)))THEN
JL=JN
ELSE
JU=JN
ENDIF
GO TO 10
ENDIF
DLOCATE=MAX(1,MIN(JL,JU))
RETURN
END
SUBROUTINE LINEFIT(I1,I2,I3,I4,X,Y,A,B)
C Fit a line through two regions of a profile.
C IMPLICIT NONE
C Compiler parameters
C INTEGER MPIX
PARAMETER (MPIX=801)
C Parameters
C INTEGER I1,I2,I3,I4
REAL I(MPIX),Y(MPIX),A,B
C Local variables
C INTEGER I,J
REAL*8 SUMX, SUMY, SUMX2, N, RMS, DET
C Start of executable statements

C

SUMY=0.0
SUMXY=0.0
SUMX=0.0
SUMX2=0.0
N=I4-I3+I2-I1+2
DO I=I1,I2
  SUMY=SUMY+Y(I)
  SUMXY=SUMXY+Y(I)*X(I)
  SUMX=SUMX+X(I)
  SUMX2=SUMX2+X(I)*X(I)
ENDD
DO I=I3,I4
  SUMY=SUMY+Y(I)
  SUMXY=SUMXY+Y(I)*X(I)
  SUMX=SUMX+X(I)
  SUMX2=SUMX2+X(I)*X(I)
ENDD
DET=SUMX*SUMX-SUMX2*11
A=(SUMY•SUMX-SUMXY•ll)/DET
B=(SUMX•SUMXY-SUMX2*SUMY)/DET
RETURN

INTEGER FUNCTION LOCATE(XX,N,X)
C
C  This is essentially the Numerical Recipes routine by the
C  same name, but here defined as a function rather than subroutine.
C
DIMENSION XX(N)
JL=0
JU=1
10 IF (JU-JL.GT.1)THEII
  JN=(JU+JL)/2
  IF (XX(JN).GE.VX(JL))THEII
    JL=JN
  ELSE
    JU=JN
  ENDIF
  GO TO 10
ENDIF
LOCATE=MAX(1,MIN(N,JL))
RETURN
END

SUBROUTINE ROTATE(NL,FLUX,ROT,VVSINI)
C
C  Convolve profile with rotational profile corresponding
C  to VVSINI=ROT. It incidentally reverses the order of
C  the profile points if they are not in ascending order.
C
IMPLICIT NONE
C
INTEGER MPIX, ML
REAL PI
PARAMETER (MPIX=801, ML=12, PI=3.141592654D0)
C
Parameters
C
INTEGER ML
REAL FLUX(MPIX), VVSINI
REAL•S ROT(MPIX)
C
Functions
C
INTEGER DLOCATE
C
Local variables
C
INTEGER I, LL, LH, J, N
REAL A, AA, BB, A1, B, B1, VSINI
REAL•S XHI, XLO
C
Main data COMMON block
C
INTEGER DPIX(ML), BLINES
REAL*8 DOSIG(MPII,NL), DOI(MPII,NL), DOY(MPII,NL)
REAL*8 RT0000(MPII,ML), RT000T(MPII,ML), RT0010(MPII,ML)
REAL*8 RT0011(MPII,ML), RT0100(MPII,ML), RT0101(MPII,ML)
REAL*8 RT0110(MPII,ML), RT1000(MPII,ML), RT1001(MPII,ML)
REAL*8 RT1010(MPII,ML), RT1100(MPII,ML), RT1101(MPII,ML)
REAL*8 RT1110(MPII,ML)
COMMON /MAII/DPII, ILINES, DOSIG, DOI, DOY, RTO000, RT000T,
: RT0010, RT0011, RT0100, RT0101, RT0110, RT0111,
: RT1001, RT1010, RT1100, RT1101, RT1110, RT1111

C Prepare to convolve semi-analytically.

DO I=1,N
  VSIII=DOSIG(I,NL)/2.997925
  IF (VSIII.EQ.0.) THEN
    DO J=1,N
      ROT(J)=FLUI(J)
    ENDDO
    RETURN
  ENDIF

  A=(DOI(I,IL)-DOI(I,IL))/VSIII
  B=(DOI(I+1,IL)-DOI(I,IL))/VSIII
  BB=(FLUX(I+1)-FLUX(I))/A-B
  AA=FLUX(J)-BB*B
  A=ACOS(MAX(-1.,MIN(1.,A)))
  B=ACOS(MAX(-1.,MIN(1.,B)))
  ROT(I)=AA*0.5*(A+B-0.5*(SSQ(2*A)-SSQ(2*B)))
  A=SQRT(1.-MIN(1.,A*A))
  B=SQRT(1.-MIN(1.,B*B))
  ROT(I)=ROT(I)+BB*(A+B)/3.
ENDDO

C Main portion of convolution

DO J=1,L-1
  A=(DOI(J,IL)-DOI(I,IL))/VSIII
  B=(DOI(J+1,IL)-DOI(I,IL))/VSIII
  BB=(FLUX(J+1)-FLUX(J))/B-A
  AA=FLUX(J)-BB*A
  A=ACOS(MAX(-1.,MIN(1.,A)))
  B=ACOS(MAX(-1.,MIN(1.,B)))
  ROT(I)=ROT(I)+AA*0.5*(A+B-0.5*(SSQ(2*A)-SSQ(2*B)))
  A=SQRT(1.-MIN(1.,A*A))
  B=SQRT(1.-MIN(1.,B*B))
  ROT(I)=ROT(I)+BB*(A+B)/3.
ENDDO

C High end of convolution

IF (VSIII.EQ.0.) THEN
  A=(DOI(I,IL)-DOI(I,IL))/VSIII
  B=(DOI(I+1,IL)-DOI(I,IL))/VSIII
  BB=(FLUX(I+1)-FLUX(I))/B-A
  AA=FLUX(J)-BB*B
  A=ACOS(MAX(-1.,MIN(1.,A)))
  B=ACOS(MAX(-1.,MIN(1.,B)))
  ROT(I)=AA*0.5*(A+B-0.5*(SSQ(2*A)-SSQ(2*B)))
  A=SQRT(1.-MIN(1.,A*A))
  B=SQRT(1.-MIN(1.,B*B))
  ROT(I)=ROT(I)+BB*(A+B)/3.
ENDDO
A = MAX(-1.0, MIN(1.0, A))

ROT(I) = ROT(I) + FLUX(I) * 0.5 * (0.5 * PI - ASIN(A) - A * SQRT(1 - A * A))

ELSE

A = (DOX(LB, NL) - DOX(I, NL)) / VSIII
BB = (FLUX(LB+1) - FLUX(LB)) / VSIII / (DOX(LB+1, NL) - DOX(LB, NL))
AA = FLUX(LB) - BB * A

ROT(I) = ROT(I) + A * 0.5 * (ACOS(MAX(-1.0, MIN(1.0, A))) -
    A * SQRT(1 - MIN(1.0, A * A)))

A1 = SQRT(1 - MIN(1.0, A * A))


ENDIF

CONTINUE
ENDG

Normalized

DO I = 1, N
    ROT(I) = ROT(I) * 2. / 3.141592654
ENDDO
RETURN
END

SUBROUTINE NRQMIN(X, Y, NDATA, A, NA, LISTA, NFIT,
                    COVAR, ALPHA, NCA, CHISQ, FWC, ALANDA)

NUMERICAL RECIPES routine to perform chi-square minimization.

IMPLICIT REAL*A-H-Z
PARAMETER (MMAX = 5)
DIMENSION X(NDATA), Y(NDATA), A(NA), LISTA(NFIT),
        COVAR(NCA, NCA), ALPHA(NCA, NCA), ATRY(NMAX), BETA(NMAX), DA(NMAX)

IF (AUNDA.LT.0.) THEN
    KK = NFIT + 1
    DO 12 J = 1, NA
        IBIT = 0
        DO 11 K = 1, NFIT
            IF (LISTA(K) .EQ. J) IBIT = IBIT + 1
        11 CONTINUE
        IF (IBIT .EQ. 0) THEN
            LISTA(KK) = J
            KK = KK + 1
        ELSE IF (IBIT .GT. 1) THEN
            PAUSE 'Improper permutation in LISTA'
        END IF
        CONTINUE
    12 CONTINUE
    IF (KK .NE. (NA + 1)) PAUSE 'Improper permutation in LISTA'
    ALANDA = 0.001
    CALL NRQCOF(X, Y, NDATA, A, NA, LISTA, NFIT, ALPHA, NCA, CHISQ, F
        OCHISQ = CHISQ
        DO 13 J = 1, NA
            ATRY(J) = A(J)
        13 CONTINUE
    ENDIF
    DO 16 J = 1, NFIT
        DO 14 K = 1, NFIT
            COVAR(J, K) = ALPHA(J, K)
        14 CONTINUE
        DO 15 J = 1, NFIT
            DA(J) = BETA(J)
        15 CONTINUE
    CALL GAUSSJ(COVAR, NFIT, NCA, DA, 1, 1)
    IF (ALANDA .EQ. 0.) THEN
        CALL COVSVT(COVAR, NCA, NA, LISTA, NFIT)
    ELSEIF DO 16 J = 1, NFIT
        ATRY(LISTA(J)) = ATRY(LISTA(J)) + DA(J)
    16 CONTINUE
    CALL NRQCOF(X, Y, NDATA, ATRY, NA, LISTA, NFIT, COVAR, NCA, CHISQ, F
        OCHISQ = CHISQ
        DO 18 J = 1, NFIT
            DA(J) = OCHISQ
        18 CONTINUE
    CALL NRQCOF(X, Y, NDATA, ATRY, NA, LISTA, NFIT, COVAR, NCA, CHISQ, F
        OCHISQ = CHISQ
        DO 18 J = 1, NFIT
            DA(J) = OCHISQ
        18 CONTINUE
    ENDIF
CONTINUE
ELSE
  ALAMDA=10.*ALAMDA
  CHISQ=GCHISQ
ENDIF
RETURN
END

SUBROUTINE NRQCOF(X,Y,MDATA,A,MA,LISTA,MFIT,ALPHA,BETA,WALP,CH
  *ISQ,FUNC)
  IMPLICIT REAL*8(A-H,O-Z)
  PARAMETER (NMA=40)
  DIMENSION X(MDATA),Y(MDATA),ALPHA(WALP,WALP),BETA(MA),
  *DYDA(NMA),LISTA(MFIT)
  DO 12 J=1,MFIT
    DO 11 K=1,J
      ALPBA(J,K)=O.
    11 CONTINUE
    BETA(J)=O.
  12 CONTINUE
  CBISQ=O.
  DO 15 I=1,IDATA
    CALL FUNC(I,Y(I),A,YNOD,DYDA)
    DY=Y(I)-YNOD
    DO 14 J=1,MFIT
      WT=DYDA(LISTA(J))
      DO 13 K=1,J
        ALPBA(J,K)=ALPBA(J,K)+WT*DYDA(LISTA(K))
      13 CONTINUE
      BETA(J)=BETA(J)+DY*WT
    14 CONTINUE
    CBISQ=CBISQ+DY*DY
  15 CONTINUE
  DO 17 J=2,MFIT
    DO 16 K=1,J-1
      ALPBA(K,J)=ALPBA(J,K)
    16 CONTINUE
  17 CONTINUE
  RETUIUI
END

SUBROUTINE COVSRT(COVAR,ICVM,MA,LISTA,MFIT)
  IMPLICIT REAL*8(A-H,O-Z)
  DIMENSION COVAR(ICVM,ICVM),LISTA(MFIT)
  DO 12 J=1,MA-1
    DO 11 I=J+1,NA
      COVAR(I,J)=O.
    11 CONTINUE
  12 CONTINUE
  DO 14 I=1,MFIT-1
    DO 13 J=I+1,MFIT
      IF(LISTA(J).GT.LISTA(I)) THEN
        COVAR(LISTA(J),LISTA(I))=COVAR(I,J)
      ELSE
        COVAR(LISTA(I),LISTA(J))=COVAR(I,J)
      ENDIF
    13 CONTINUE
  14 CONTINUE
  SWAP=COVAR(1,1)
  DO 15 J=2,MA
    COVAR(1,J)=COVAR(J,J)
    COVAR(J,J)=O.
  15 CONTINUE
  COVAR(LISTA(1),LISTA(1))=SWAP
  DO 16 J=2,MFIT
    COVAR(LISTA(J),LISTA(J))=COVAR(1,J)
  16 CONTINUE
  DO 18 J=2,NA
    DO 17 I=1,J-1
      COVAR(I,J)=COVAR(J,I)
    17 CONTINUE
  18 CONTINUE
  RETURN
END

SUBROUTINE GAUSSJ(A,MA,MA,B,MA,MA)
  IMPLICIT REAL*8(A-H,O-Z)
PARAMETER (MNAX=60)
DIMENSION A(NP,NP),B(NP,NP),IPIV(NMAX),INDX(NMAX),INDXC(NMAX)
DO 11 J=1,N
IPIV(J)=0
11 CONTINUE
DO 22 I=1,N
BIG=0.
DO 13 J=1,N
IF(IPIV(J).NE.1)THEN
DO 12 K=1,N
IF (IPIV(K).EQ.0) THEN
IF (ABS(A(J,K)).GE.BIG) THEN
BIG=ABS(A(J,K))
IROW=J
ICOL=K
ENDIF
ELSE IF (IPIV(K).GT.1) THEN
PAUSE 'Singular matrix'
ENDIF
12 CONTINUE
13 CONTINUE
ENDIF
14 CONTINUE
IPIV(ICOL)=IPIV(ICOL)+1
IF (IROW.NE.ICOL) THEN
DO 15 L=1,M
DUM=A(IROW,L)
A(IROW,L)=A(ICOL,L)
A(ICOL,L)=DUM
15 CONTINUE
DO 17 L=1,M
B(IROW,L)=B(ICOL,L)
B(ICOL,L)=DUM
17 CONTINUE
18 CONTINUE
ENDIF
INDX(I)=IROW
INDXC(I)=ICOL
IF (A(ICOL,ICOL).EQ.O.) PAUSE 'Singular matrix.'
PIVIIV=1./A(ICOL,ICOL)
A(ICOL,ICOL)=1.
DO 19 L=1,I
A(ICOL,L)=A(ICOL,L)*PIVIIV
19 CONTINUE
DO 21 L=1,M
B(ICOL,L)=B(ICOL,L)*PIVIIV
21 CONTINUE
22 CONTINUE
DO 24 L=1,M-1
IF (INDX(L).NE.INDXC(L)) THEN
DO 23 K=1,N
DUM=A(K,INDX(L))
A(K,INDX(L))=A(K,INDXC(L))
A(K,INDXC(L))=DUM
23 CONTINUE
ENDIF
24 CONTINUE
RETURN
END

SUBROUTINE GAUSS(X,A,YFIT,DYDA,MA)
C
C Generate Gaussian and derivatives for fit to line profiles.
C
IMPLICIT REAL*8(A-E,0-Z)
DIMENSION A(5),DYDA(3)
C
C Start of executable statements
C
DEL=A(1)-X
CONT=A(4)*X*A(5)
EX=EXP(-DEL/A(3))**2
YFIT=CONT*(1.0D0-A(2)*EX)
DYDA(1)=+2.0D0*DEL*A(2)*CONT*EX/A(3)/A(3)
DYDA(2)=-COIT*EX
DYDA(3)=-2.0D0*DEL*DEL*A(2)*CONT*EX/A(3)/A(3)/A(3)
RETURN
END

SUBROUTINE FETCH(IT,IG,IA,CWAVE,ML,T,FETCHED)
C
C Fetch a theoretical profile from the library directory.
C
IMPLICIT NONE
C
Compiler parameters
C
INTEGER ML, MPIX
PARAMETER (ML=12, MPIX=801)
C
Functions
C
INTEGER LOCATE
C
Parameters
C
INTEGER IT,IG,IA,ML
CHARACTER*4 CWAVE
LOGICAL FETCHED
REAL T(MPIX)
C
Local variables
C
INTEGER I, J, L, M1, FILE
CHARACTER*2 GGRID(5)
CHARACTER*1 AGRID(4)
CHARACTER FILE*9
REAL TGRID(MPIX,4), TGRID(MPIX), TEFF, VX1
REAL VX2, VY1, VY2, WAVE, X1(MPIX), X2(MPIX), XX, YY
C
Main data COMMON block
C
INTEGER DPIX(ML), NLIINES
REAL*8 DOSIG(MPIX,ML), DQI(MPIX,ML), DQY(MPIX,ML)
REAL*8 RT0000(MPIX,ML), RT0001(MPIX,ML), RT0010(MPIX,ML)
REAL*8 RT0011(MPIX,ML), RT0100(MPIX,ML), RT0101(MPIX,ML)
REAL*8 RT0110(MPIX,ML), RT0111(MPIX,ML), RT1000(MPIX,ML)
REAL*8 RT0100(MPIX,ML), RT1010(MPIX,ML), RT1100(MPIX,ML)
REAL*8 RT1011(MPIX,ML), RT1110(MPIX,ML), RT1111(MPIX,ML)
COMMON /MAIN/DPIX, NLIINES, DOSIG, DQI, DQY, RT0000, RT0001,
: RT0010, RT0011, RT0100, RT0101, RT0110, RT0111, RT1000,
: RT1001, RT1010, RT1011, RT1100, RT1101, RT1110, RT1111
C
Data statements
C
DATA GGRID/"27", "30", "35", "40", "45"/
DATA AGRID/"0", "1", "2", "5"/
DATA TGRID/28000., 30000., 32500., 35000., 37500., 40000., 45000.,
: 50000. /
C
Start of executable statements
C
Construct filename
C
FILE="f"/GGRID(IG)/AGRID(IA)/CWAVE/"
C
Try opening the file
C
OPEN (UNIT=1,FILE=FILE,STATUS='OLD',ACCESS='SEQUENTIAL',ERR=600)
C
Look for the temperature desired.
C
10 READ (1,*,END=30)TEFF
IF (TEFF.EQ.TGRID(IT))GO TO 20
READ (1,*)IT
DO I=1,IT
READ (1,*)TINT(I,1)
ENDDO
GO TO 10

C Read in the library profile.
C
20 READ (1,*)IT
   DO I=1,IT
      READ (1,*)X1(I),TINT(I,1)
   ENDDO
GO TO 100

C Try to interpolate the necessary profile; first try to do
C it by abundance.
C
30 WRITE (6,*)'Cannot find entry for ',TGRID(IT),'K in '/FILE
   WRITE (6,*)'Will attempt to interpolate profile.'
   CLOSE(1)
   IF (IA.EQ.1.OR.IA.EQ.4)GO TO 200
   DO IFILE=IA-1,IA+1,2
      FILE='/GGRID(IG)//AGRID(IFILE)//CWAVE//'.
      OPEN (UNIT=1,FILE=FILE,STATUS='OLD',ACCESS='SEQUENTIAL',
         ERR=600)
   END
   READ (1,*,EID=200)TEFF
   IF (TEFF.EQ.TGRID(IT-1))GO TO 50
   READ (1,*)IT
   DO I=t,IT
      READ (1,*)TINT(I,IFILE)
   ENDDO
   GO TO 40

C Read in the library profile.
C
50 READ (1,*)IT
   DO I=1,IT
      READ (1,*)X1(I),TINT(I,IFILE)
   ENDDO

C Now interpolate.
C
   DO I=1,IT
      TINT(I,1)=0.5*(TINT(I,IA-1)+TINT(I,IA+1))
   ENDDO
GO TO 100

C Abundance interpolation fails--try gravity next.
C
200 IF (IG.EQ.1.OR.IG.EQ.4)THEN
   GO TO 590
END IF
   DO IFILE=IG-1,IG+1,2
      FILE='/GGRID(IFILE)//AGRID(IA)//CWAVE//'.
   END
   OPEN (UNIT=1,FILE=FILE,STATUS='OLD',ACCESS='SEQUENTIAL',
         ERR=600)
   READ (1,*,EID=590)TEFF
   IF (TEFF.EQ.TGRID(IT))GO TO 250
   READ (1,*)IT
   DO I=1,IT
      READ (1,*)TINT(I,IFILE)
   ENDDO
   GO TO 240

C Read in the library profile.
C
250 READ (1,*)IT
   DO I=1,IT
      READ (1,*)X1(I),TINT(I,IFILE)
   CLOSE (1)
   ENDDO

C Now interpolate.
C
   DO I=1,IT
      TINT(I,1)=0.5*(TINT(I,IG-1)+TINT(I,IG+1))
   ENDDO
Successful read or interpolate. Now regrid the profile onto the scale used for the data.

IF (X1(1).GT.X1(2)) THEN
REVERSE ORDER OF ARRAYS IF NECESSARY.
DO I=T,IT
X2(I)=X1(IT-I+1)
TINT(I,2)=TINT(IT-I+1,1)
ENDDO
DO I=1,WT
X1(I)=X2(I)
TINT(I,1)=TINT(I,2)
ENDDO
ENDIF

FIND THEORETICAL PROFILE MINIMUM.
J=0
WAVE=.99.
DO I,WT
IF (TINT(I,1).LT.WAVE) THEN
WAVE=TINT(I,1)
J=I
ENDIF
ENDDO
WAVE=X1(J)
W=X(DPIX(I,WT))
DO I,11
IF (DOX(I,W).LT.X1(1)) THEN
INTERPOLATE OFF ENDS OF THEORETICAL PROFILE BY ASSUMING -2.5 WINGS.
XX=ABS((DOX(I,W)-WAVE)/(X1(1)-WAVE))
T(I)=1.-(1.-TINT(1,1))/XX/XX/SQRT(XX)
ELSE IF (DOX(I,W).GT.X1(1)) THEN
XX=ABS((DOX(I,W)-WAVE)/(X1(1)-WAVE))
T(I)=1.-(1.-TINT(1,1))/XX/XX/SQRT(XX)
ELSE
L=LOCATE(X1,WT,REAL(DOX(I,W)))
I=MAX(2,MIN(WT-2,L))
XX=DOX(I,W)
VX1=X1(L)
VY1=TINT(L,1)
VX2=X1(L+1)
VY2=TINT(L+1,1)
T(I)=VY1*(XX-VX2)/(VX1-VX2)+VY2*(XX-VX1)/(VX2-VX1)
ENDIF
ENDDO
FETCHED=.TRUE.
RETURN

WRITE (6,*)'Unable to interpolate'
CLOSE (1)
FETCHED=.FALSE.
RETURN
WRITE (6,*)'Cannot find file '//FILE
GO TO 590

SUBROUTINE MQMIN2(A,MA,LISTA,NFIT,COVAR,ALPHA, NCA, CHISQ, ALANDA,
: FUNCS)

Chi-square minimization, from "Numerical Recipes"
IMPLICIT REAL*8(A-H,0-Z)
PARAMETER (MINMAX=40)
Parameters
DIMENSION A(MA), LISTA(NFIT), COVAR(NCA,NCA), ALPHA(NCA,NCA)
DIMENSION ATRY(MINMAX), BETA(MINMAX), DA(MINMAX)
IF(ALANDA.LT.0.) THEN
KK=MFIT+1
DO 12 J=1,MFIT
IBIT=0
DO 11 K=1,MFIT
IF(LIST1(K).EQ.J)IBIT=IBIT+1
CONTINUE
IF (IBIT.EQ.0) THEN
LIST1(KK)=J
KK=KK+1
ELSE IF (IBIT.GE.1) THEN
PAUSE 'Improper permutation in LISTA'
ENDIF
CONTINUE
IF (KK.NE.(M1+1))) PAUSE 'Improper permutation in LISTA'
ALAMDA=0.001
CALL MRQCOF2(A,MA,LISTA,MFIT,ALPHA,BETA,WCA,CHISQ,FUNCS)
OCBISQ=CHISQ
DO 13 J=1,MA
ATRY(J)=A(J)
CONTINUE
ENDIF
DO 14 J=1,MFIT
DO 13 K=1,MFIT
COV1R(J,K)=1LPB1(J,K)
CONTINUE
DO 14 J=1,MFIT
DO 13 K=1,MFIT
1LPB1(J,K)=COVAR(J,K)
CONTINUE
ELSE
ALAMDA=10.*ALAMDA
CHISQ=OCBISQ
ENDIF
RETURN
END

SUBROUTINE MRQCOF2(A,MA,LISTA,MFIT,ALPHA,BETA,WALP,CHISQ,FUNCS)

IMPLICIT REAL*8 (A-H,O-Z)
PARAMETER (ML=12, MMAX=40, MPII=801)
DIMENSION ALPHA(ML), WCA(MFIT), LISTA(MFIT), DAT(MFIT)
DIMENSION A(ML)

DO 12 J=1,MFIT
DO 11 K=1,MFIT
1LPB1(J,K)=O.
CONTINUE
IF (CHISQ.LT.OCBISQ) THEN
ALAMDA=0.1*ALAMDA
OCBISQ=CHISQ
DO 15 J=1,MFIT
DO 14 K=1,MFIT
1LPB1(J,K)=COVAR(J,K)
CONTINUE
ENDIF
DO 16 J=1,MFIT
ATRY(LISTA(J))=ATRY(LISTA(J))
CONTINUE
CALL MRQCOF2(ATTRY,MA,LISTA,MFIT,COVAR,DA,VALP,CHISQ,FUNCS)
IF (CHISQ.LT.OCBISQ) THEN
ALAMDA=0.1*ALAMDA
OCBISQ=CHISQ
DO 17 K=1,MFIT
BETA(J)=DA(J)
ATRY(LISTA(J))=ATRY(LISTA(J))
CONTINUE
ELSE
ALAMDA=10.*ALAMDA
CHISQ=OCBISQ
CONTINUE
ENDIF
RETURN
END
BETA(J) = 0.

CONTINUE
CHISQ = 0.

DO IL = 1, NXLINES
  DO 15 I = 1, DPII(IL)
    CALL FUNCS(IL, DOI(IL), A, YMOD, DYDA, MA)
    SIG2I = 1./
      (DOSIG(I, IL)*DOSIG(I, IL))
    DT = DY(I, IL) - YMOD
    DO 14 J = 1, NFIT
      WT = DYDA(LISTA(J)) * SIG2I
    DO 13 K = 1, J
      ALPBA(J, K) = ALPBA(J, K) + WT * DYDA(LISTA(K))
    CONTINUE
  CONTINUE
BETA(J) = BETA(J) + DT * WT
  CONTINUE
  CHISQ = CHISQ + WT * WT * SIG2I
15 CONTINUE
ENDDO
17 CONTINUE
RETURN
END

SUBROUTINE PHYSFUNC(IL, XI, A, YMOD, DYDA, MA)

Model function subroutine for MRQMIN used in main parameter fitting.

IMPLICIT REAL*8 (A-Z, 0-2)

Compiler parameters
PARAMETER (ML = 12, MPI = 801)

Parameters
INTEGER IL, MA
DIMENSION A(MA), DYDA(MA)

Main data COMMON block

INTEGER DPII(ML), NXLINES
REAL*8 DOSIG(MPII, ML), DOI(MPII, ML), DOY(MPII, ML)
REAL*8 RTO000(MPII, ML), RTO001(MPII, ML), RTO010(MPII, ML)
REAL*8 RTO011(MPII, ML), RTO100(MPII, ML), RTO101(MPII, ML)
REAL*8 RTO110(MPII, ML), RTO111(MPII, ML), RT1000(MPII, ML)
REAL*8 RT1001(MPII, ML), RT1010(MPII, ML), RT1011(MPII, ML)
REAL*8 RT1100(MPII, ML), RT1101(MPII, ML), RT1110(MPII, ML)
REAL*8 RT1111(MPII, ML)
COMMON /MAIN/DPII, NXLINES, DOSIG, DOI, DOY, RTO000, RTO001,
: RTO010, RTO011, RTO100, RTO101, RTO110, RTO111, RT1000,
: RT1001, RT1010, RT1011, RT1100, RT1101, RT1110, RT1111

Functions

INTEGER DLOCATE

Start of executable statements

DO I = 1, MA
  DYDA(I) = 0.
ENDDO

XI = XI - A(3 + IL)
L = DLOCATE(DOX(1, IL), DPII(IL), XI)
L = MIN(DPIX(IL) - 2, MAX(2, L))
L = DOX(L - 1, IL)
2 = DOX(L, IL)
3 = DOX(L + 1, IL)
4 = DOX(L + 2, IL)

Calculate interpolant for each mesh point.

Y1 = RTO000(L - 1, IL)
Y2 = RTO000(L, IL)
Y3 = RTO000(L + 1, IL)
Y4 = RTO000(L + 2, IL)
Y000 = Y1*(X - X2)*(X - X3)*(X - X4)/((X1 - X2)*(X1 - X3)*(X1 - X4))*
\[
\begin{align*}
Y_{100} &= Y_1 \cdot (X-x_2) \cdot (X-x_3) \cdot (X-x_4)/((X_1-x_2) \cdot (X_1-x_3) \cdot (X_1-x_4)) + \\
Y_2 &= Y_2 \cdot (X-x_1) \cdot (X-x_4)/((X_2-x_1) \cdot (X_2-x_3) \cdot (X_2-x_4)) + \\
Y_3 &= Y_3 \cdot (X-x_1) \cdot (X-x_2)/((X_3-x_1) \cdot (X_3-x_2) \cdot (X_3-x_4)) + \\
Y_4 &= Y_4 \cdot (X-x_1)/((X_4-x_1) \cdot (X_4-x_2) \cdot (X_4-x_3)) + \\
DY_{100d3} &= -Y_1 \cdot ((X-I_3) \cdot (X-I_4)+(X-I_2) \cdot (X-I_4)+(X-I_2) \cdot (X-I_3))/((I_1-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4)) + \\
&\quad -Y_2 \cdot ((I-I_3) \cdot (I-I_4)+(I-I_1) \cdot (I-I_4)+(I-I_1) \cdot (I-I_3))/((I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)) + \\
&\quad -Y_3 \cdot ((I-I_2) \cdot (I-I_4)+(I-I_1) \cdot (I-I_4)+(I-I_1) \cdot (I-I_2))/((I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)) + \\
&\quad -Y_4 \cdot ((I-I_2) \cdot (I-I_3)+(I-I_1) \cdot (I-I_3)+(I-I_1) \cdot (I-I_2))/((I_4-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3)) \\
Y_1 &= RT0010(L-1, I_L) \\
Y_2 &= RT0010(L, I_L) \\
Y_3 &= RT0010(L+1, I_L) \\
Y_4 &= RT0010(L+2, I_L) \\
DY_{010d3} &= Y_1 \cdot (X-I_3) \cdot (X-I_4)+(X-I_2) \cdot (X-I_4)+(X-I_2) \cdot (X-I_3))/((X_1-X_2) \cdot (X_1-X_3) \cdot (X_1-X_4)) + \\
&\quad -Y_2 \cdot ((X-X_3) \cdot (X-X_4)+(I-I_1) \cdot (X-X_4)+(X-X_1) \cdot (I-X_3))/((X_2-X_1) \cdot (X_2-I_3) \cdot (X_2-I_4)) + \\
&\quad -Y_3 \cdot ((X-X_2) \cdot (X-X_4)+(X-X_1) \cdot (X-X_4)+(X-X_1) \cdot (X-X_2))/((X_3-X_1) \cdot (X_3-X_2) \cdot (X_3-X_4)) + \\
&\quad -Y_4 \cdot ((X-X_2) \cdot (X-X_3)+(I-X_1) \cdot (X-X_3)+(X-X_1) \cdot (X-X_2))/((X_4-X_t) \cdot (X_4-I_2) \cdot (X_4-X_3)) \\
Y_1 &= RT0100(L-1, I_L) \\
Y_2 &= RT0100(L, I_L) \\
Y_3 &= RT0100(L+1, I_L) \\
Y_4 &= RT0100(L+2, I_L) \\
DY_{011d3} &= Y_1 \cdot (X-I_3) \cdot (X-I_4)+(X-I_2) \cdot (X-I_4)+(X-I_2) \cdot (X-I_3))/((X_1-X_2) \cdot (X_1-X_3) \cdot (X_1-X_4)) + \\
&\quad -Y_2 \cdot ((X-X_3) \cdot (X-X_4)+(X-X_1) \cdot (X-X_4)+(X-X_1) \cdot (X-X_2))/((X_2-X_1) \cdot (X_2-X_3) \cdot (X_2-X_4)) + \\
&\quad -Y_3 \cdot ((X-X_2) \cdot (X-X_4)+(X-X_1) \cdot (X-X_4)+(X-X_1) \cdot (X-X_2))/((X_3-X_1) \cdot (X_3-X_2) \cdot (X_3-X_4)) + \\
&\quad -Y_4 \cdot ((X-X_2) \cdot (X-X_3)+(I-X_1) \cdot (X-X_3)+(X-X_1) \cdot (X-X_2))/((X_4-X_t) \cdot (X_4-X_2) \cdot (X_4-X_3)) \\
Y_1 &= RT0110(L-1, I_L) \\
Y_2 &= RT0110(L, I_L) \\
Y_3 &= RT0110(L+1, I_L) \\
Y_4 &= RT0110(L+2, I_L) \\
DY_{101d3} &= Y_1 \cdot (X-I_3) \cdot (X-I_4)+((X-I_2) \cdot (X-I_3) \cdot (X-I_4))/((I_1-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4)) + \\
&\quad -Y_2 \cdot ((I-I_3) \cdot (I-I_4)+(I-I_2) \cdot (I-I_4)+(I-I_2) \cdot (I-I_3))/((I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)) + \\
&\quad -Y_3 \cdot ((X-I_2) \cdot (X-I_4)+(I-I_1) \cdot (X-I_4)+(X-X_1) \cdot (I-X_3))/((I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)) + \\
&\quad -Y_4 \cdot ((X-X_2) \cdot (X-I_3)+(I-X_1) \cdot (X-X_3)+(X-X_1) \cdot (X-X_2))/((X_4-X_t) \cdot (X_4-I_2) \cdot (X_4-X_3)) \\
Y_1 &= RT1000(L-1, I_L) \\
Y_2 &= RT1000(L, I_L) \\
Y_3 &= RT1000(L+1, I_L) \\
Y_4 &= RT1000(L+2, I_L) \\
DY_{101d3} &= Y_1 \cdot (X-I_3) \cdot (X-I_4)+((X-I_2) \cdot (X-I_3) \cdot (X-I_4))/((I_1-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4)) + \\
&\quad -Y_2 \cdot ((I-I_3) \cdot (I-I_4)+(I-I_2) \cdot (I-I_4)+(I-I_2) \cdot (I-I_3))/((I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)) + \\
&\quad -Y_3 \cdot ((X-I_2) \cdot (X-I_4)+(I-I_1) \cdot (X-I_4)+(X-X_1) \cdot (I-X_3))/((I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)) + \\
&\quad -Y_4 \cdot ((X-X_2) \cdot (X-I_3)+(I-X_1) \cdot (X-X_3)+(X-X_1) \cdot (X-X_2))/((X_4-X_t) \cdot (X_4-I_2) \cdot (X_4-X_3)) \\
Y_1 &= RT1010(L-1, I_L) \\
Y_2 &= RT1010(L, I_L) \\
Y_3 &= RT1010(L+1, I_L) \\
Y_4 &= RT1010(L+2, I_L) \\
Y_{101} &= Y_1 \cdot (X-X_2)+(X-X_3)+(X-X_4)/((X_1-X_2)+(X_1-X_3)+(X_1-X_4)) + \\
&\quad -Y_2 \cdot ((X-X_3)+(X-X_4)+(X-X_1)+(X-X_4))/((X_2-X_1)+(X_2-X_3)+(X_2-X_4)) + \\
&\quad -Y_3 \cdot ((X-X_2)+(X-X_4)+(X-X_1)+(X-X_2))/((X_3-X_1)+(X_3-X_2)+(X_3-X_4)) + \\
&\quad -Y_4 \cdot ((X-X_2)+(X-X_3)+(X-X_1)+(X-X_2))/((X_4-X_t)+(X_4-X_2)+(X_4-X_3)) \\
\end{align*}
\]
\[
Y_2 = \frac{(X - X_1)(X - X_3)(X - X_4)}{(X_2 - X_1)(X_2 - X_3)(X_2 - X_4)} + \\
Y_3 = \frac{(X - X_1)(X - X_2)(X - X_4)}{(X_3 - X_1)(X_3 - X_2)(X_3 - X_4)} + \\
Y_4 = \frac{(X - X_1)(X - X_2)(X - X_3)}{(X_4 - X_1)(X_4 - X_2)(X_4 - X_3)}
\]

\[
DY_{101}D_3 = -Y_1 \frac{(X - X_3)(X - X_4) + (X - X_2)(X - X_4) + (X - X_2)(X - X_3)}{(X_1 - X_2)(X_1 - X_3)(X_1 - X_4)} + \\
-Y_2 \frac{(X - X_3)(X - X_4) + (X - X_1)(X - X_4) + (X - X_1)(X - X_3)}{(X_2 - X_1)(X_2 - X_3)(X_2 - X_4)} + \\
-Y_3 \frac{(X - X_2)(X - X_4) + (X - X_1)(X - X_4) + (X - X_1)(X - X_2)}{(X_3 - X_1)(X_3 - X_2)(X_3 - X_4)} + \\
-Y_4 \frac{(X - X_2)(X - X_3) + (X - X_1)(X - X_3) + (X - X_1)(X - X_2)}{(X_4 - X_1)(X_4 - X_2)(X_4 - X_3)}
\]

\[
Y_1 = RT_{1100}(L-1, IL) \\
Y_2 = RT_{1100}(L, IL) \\
Y_3 = RT_{1100}(L+1, IL) \\
Y_4 = RT_{1100}(L+2, IL)
\]

\[
Y_{111} = Y_1 \frac{(X - X_2)(X - X_3)(X - X_4)}{(X_1 - X_2)(X_1 - X_3)(X_1 - X_4)} + \\
Y_2 \frac{(X - X_1)(X - X_3)(X - X_4)}{(X_2 - X_1)(X_2 - X_3)(X_2 - X_4)} + \\
Y_3 \frac{(X - X_1)(X - X_2)(X - X_4)}{(X_3 - X_1)(X_3 - X_2)(X_3 - X_4)} + \\
Y_4 \frac{(X - X_1)(X - X_2)(X - X_3)}{(X_4 - X_1)(X_4 - X_2)(X_4 - X_3)}
\]

\[
DY_{110}D_3 = -Y_1 \frac{(X - X_3)(X - X_4) + (X - X_2)(X - X_4) + (X - X_2)(X - X_3)}{(X_1 - X_2)(X_1 - X_3)(X_1 - X_4)} + \\
-Y_2 \frac{(X - X_3)(X - X_4) + (X - X_1)(X - X_4) + (X - X_1)(X - X_3)}{(X_2 - X_1)(X_2 - X_3)(X_2 - X_4)} + \\
-Y_3 \frac{(X - X_2)(X - X_4) + (X - X_1)(X - X_4) + (X - X_1)(X - X_2)}{(X_3 - X_1)(X_3 - X_2)(X_3 - X_4)} + \\
-Y_4 \frac{(X - X_2)(X - X_3) + (X - X_1)(X - X_3) + (X - X_1)(X - X_2)}{(X_4 - X_1)(X_4 - X_2)(X_4 - X_3)}
\]

\[
Y_1 = RT_{1110}(L-1, IL) \\
Y_2 = RT_{1110}(L, IL) \\
Y_3 = RT_{1110}(L+1, IL) \\
Y_4 = RT_{1110}(L+2, IL)
\]

Now calculate YFIT

Abundance interpolant

I = \# of LINES
A1 = 1 - A(I)
A2 = A(I)
Y00 = A1 * Y00 + A2 * Y01
DY00D = A1 * DY00D + A2 * DY01D3
DY00D = Y01 - Y00
Y10 = A1 * Y10 + A2 * Y01
DY10D3 = A1 * DY10D3 + A2 * DY01D3
DY10D = Y10 - Y01
Y11 = A1 * Y110 + A2 * Y110
DY11D = Y110 - Y110

Gravity interpolant

I = \# of LINES
A1 = 1 - A(I)
A2 = A(I)
Y0 = A1 * Y00 + A2 * Y01
DY0D = A1 * DY0D + A2 * DY01D3
DY0D = Y01 - Y00
Y1 = A1 * Y10 + A2 * Y01
DY1D3 = A1 * DY1D3 + A2 * DY01D3
DY1D = Y10 - Y01

Temperature interpolant
I=3*NLINES+1
A1=1.-A(I)
A2=A(I)
Y=A1*Y0+A2*Y1
DYD3=A1*DYOD3+A2*DY1D3
DYDA=A1*DYODA+A2*DY1DA
DYDG=A1*DYODG+A2*DY1DG
DYDT=Y1-Y0
C
Continuum fit
C
A1=a(3*IL-2)
A2=a(3*IL-1)
YC=a1*X+a2
YMDD=Y*YC
DYDA(3*IL-2)=X*Y
DYDA(3*IL-1)=Y
DYDA(3*IL)=YC*DYDS
DYDA(3*NLINES+1)=YC*DYDT
DYDA(3*NLINES+2)=YC*DYDG
DYDA(3*NLINES+3)=YC*DYDAA
RETURN
END
SUBROUTINE MATINV(A,W,NR)
C
Invert matrix in place by LU decomposition; routine
C
originally from Aser-Mihalas codes.
C
IMPLICIT REAL*(8)
C
INTEGER W, K, NR, I, L, KO, II, J, JJ
DIMENSION A(NR,NR)
C
DO 60 I=2,W
DIV=A(I,1)
A(I,1)=A(I,1)/DIV
DO 30 J=2,I-1
DIV=A(J,J)
SUM=0.
DO 10 L=1,J-1
SUM=SUM+A(I,L)*A(L,J)
10 CONTINUE
A(I,J)=(A(I,J)-SUM)/DIV
30 CONTINUE
DO 50 J=I,W
SUM=0.
DO 40 L=1,I-1
SUM=SUM+A(I,L)*A(L,J)
40 CONTINUE
A(I,J)=A(I,J)-SUM
50 CONTINUE
60 CONTINUE
DO 100 I=W,2,-1
DO 90 J=I-1,1,-1
SUM=0.
IF (J+1.EQ.I)GO TO 80
DO 70 K=J+1,I-1
SUM=SUM+A(I,K)*A(K,J)
70 CONTINUE
A(I,J)=-A(I,J)-SUM
80 CONTINUE
90 CONTINUE
100 CONTINUE
A(W,W)=1.0/A(W,W)
DO 140 I=W-1,1,-1
DIV=A(I,I)
DO 120 J=W,I+1,-1
SUM=0.
DO 110 K=I+1,J
SUM=SUM+A(I,K)*A(K,J)
110 CONTINUE
A(I,J)=-SUM/DIV
120 CONTINUE
A(I,I)=1.0/A(I,I)
140 CONTINUE
DO 200 I=1,W
DO 160 J=1,I-1
SUM=0.0
DO 150 K=I,W
SUM=SUM+A(I,K)*A(K,J)
150 CONTINUE
200 CONTINUE
```
150 CONTINUE
A(I,J)=SUM
160 CONTINUE
DO 180 J=I,N
  SUM=A(I,J)
  IF (J.EQ.1) GO TO 180
  DO 170 K=J+1,I
    SUM=SUM+A(I,K)*A(K,J)
  170 CONTINUE
180 A(I,J)=SUM
190 CONTINUE
RETURN
END

SUBROUTINE ROTFUNC(IL,XX,A,YMOD,DYDA,MA)
C Model function subroutine for MBQM2 used in rotation fit
C
C IMPLICIT REAL*8 (A-B,0-Z)
C Compiler parameters
C PARAMETER (M=12, MPIX=801)
C Parameters
C INTEGER IL, MA
DIMENSION A(MA), DYDA(MA)
C Main data COMMON block
C INTEGER DPIX(ML), MLS
REAL*8 DOSIG(MPIX,ML), DOI(MPIX,ML), DOY(MPIX,ML)
REAL*8 RTO000(MPIX,ML), RT0001(MPIX,ML), RT0010(MPIX,ML)
REAL*8 RT0011(MPIX,ML), RT0100(MPIX,ML), RT0101(MPIX,ML)
REAL*8 RT0110(MPIX,ML), RT0111(MPIX,ML), RT1000(MPIX,ML)
REAL*8 RT1001(MPIX,ML), RT1010(MPIX,ML), RT1011(MPIX,ML)
REAL*8 RT1100(MPIX,ML), RT1101(MPIX,ML), RT1110(MPIX,ML)
REAL*8 RT1111(MPIX,ML)
COMMON /MAI/DPII, ILIES, DOSIG, DOI, DOY, RTO000, RT0001,
: RT0010, RT0100, RT0101, RT0110, RT0111, RT1000,
: RT1001, RT1010, RT1100, RT1101, RT1110, RT1111
C Functions
C INTEGER DLOCATE
C Start of executable statements
C DO I=1,MA
  DYDA(I)=0.
ENDDO
I=XX-A(3+IL)
L=DLOCATE(DOI(I,IL),DPIX(ML),I)
L=Mil(DPII(IL)-2,Mil(2,L))
I1=DOI(L-1,IL)
I2=DOI(L,IL)
I3=DOI(L+1,IL)
I4=DOI(L+2,IL)
C Calculate interpolant for each mesh point.
C INF=RT0000(L-1,IL)
Y2=RT0000(L,IL)
Y3=RT0000(L+1,IL)
Y4=RT0000(L+2,IL)
Y0000=INF*(X-X3)*(X-X4)/(((X-X2)*(X-X3)*(X-X4))+
: Y2*(X-X1)*(X-X3)+(X-X4))/((X-X1)*(X-X2)*(X-X4))++
: Y3*(X-X1)*(X-X2)+(X-X3))/((X-X1)*(X-X2)*(X-X3))++
: Y4*(X-X1)+(X-X2)*(X-X3))/((X-X1)*(X-X2)*(X-X3))++)
DY0000D3=Y1*(X-X2)*(X-X3)*(X-X4)+(X-X2)+(X-X3))/
: ((X-X2)*(X-X3)*(X-X4))+
: -Y2*(X-X3)*(X-X4)+(X-X1)*(X-X3))/
: ((X-X1)*(X-X2)*(X-X4))+
: -Y3*(X-X2)*(X-X4)+(X-X1)*(X-X2))/
: ((X-X1)*(X-X2)*(X-X3))+
: -Y4*(X-X2)+(X-X3)+(X-X4)+(X-X1)*(X-X2))/
: ((X-X1)*(X-X2)*(X-X3))
```
Y1=RT0001(L-1,IL)
Y2=RT0001(L,IL)
Y3=RT0001(L+1,IL)
Y4=RT0001(L+2,IL)

Y0001+Y1=(X-X2)+(X-X3)+(X-X4)/(X1-X2)*(X1-X3)*(X1-X4)+
    Y2=(X-X1)*(X-X4)+(X-X3)*(X-X4)+
    Y3=(X-X1)+Y2*(X-X3)+Y4*(X-X3)+
    Y4=(X-X1)+Y3*(X-X2)+Y4*(X-X2)+

DY0001D3=-(X-X1)+Y2*(X-X3)+Y4*(X-X3)+
    Y3=(X-X1)+Y2*(X-X3)+Y4*(X-X3)+
    Y4=(X-X1)+Y2*(X-X3)+Y4*(X-X3)+

Y1=RT0010(L-1,IL)
Y2=RT0010(L,IL)
Y3=RT0010(L+1,IL)
Y4=RT0010(L+2,IL)

Y0010+Y1=(X-X2)*(X-X3)+(X-X4)/(X1-X2)*(X1-X3)*(X1-X4)+
    Y2=(X-X1)+(X-X3)*(X-X4)+
    Y3=(X-X1)+(X-X3)*(X-X4)+
    Y4=(X-X1)+(X-X3)*(X-X4)+

DY0010D3=-(X-X1)+(X-X3)*(X-X4)+
    Y2=(X-X1)+(X-X3)*(X-X4)+
    Y3=(X-X1)+(X-X3)*(X-X4)+
    Y4=(X-X1)+(X-X3)*(X-X4)+

Y1=RT0100(L-1,IL)
Y2=RT0100(L,IL)
Y3=RT0100(L+1,IL)
Y4=RT0100(L+2,IL)

Y0100+Y1=(X-X2)*(X-X3)+(X-X4)/(X1-X2)*(X1-X3)*(X1-X4)+
    Y2=(X-X1)*(X-X4)+(X-X3)*(X-X4)+
    Y3=(X-X1)*(X-X4)+(X-X3)*(X-X4)+
    Y4=(X-X1)*(X-X4)+(X-X3)*(X-X4)+

DY0100D3=-(X-X1)+(X-X3)*(X-X4)+
    Y2=(X-X1)+(X-X3)*(X-X4)+
    Y3=(X-X1)+(X-X3)*(X-X4)+
    Y4=(X-X1)+(X-X3)*(X-X4)+

Y1=RT0101(L-1,IL)
Y2=RT0101(L,IL)
Y3=RT0101(L+1,IL)
Y4=RT0101(L+2,IL)
Y1 = RT0110(L-1, IL)
Y2 = RT0110(L, IL)
Y3 = RT0110(L+1, IL)
Y4 = RT0110(L+2, IL)

Y2 = Y2(X-1)(X-3)(X-4)/(X-2)(X-3)(X-4)
Y3 = Y3(X-1)(X-2)(X-4)/(X-1)(X-2)(X-4)


Y1 = RT0111(L-1, IL)
Y2 = RT0111(L, IL)
Y3 = RT0111(L+1, IL)
Y4 = RT0111(L+2, IL)

Y2 = Y2(X-1)(X-3)(X-4)/(X-2)(X-3)(X-4)
Y3 = Y3(X-1)(X-2)(X-4)/(X-1)(X-2)(X-4)


Y1 = RT1000(L-1, IL)
Y2 = RT1000(L, IL)
Y3 = RT1000(L+1, IL)
Y4 = RT1000(L+2, IL)

Y2 = Y2(X-1)(X-3)(X-4)/(X-2)(X-3)(X-4)
Y3 = Y3(X-1)(X-2)(X-4)/(X-1)(X-2)(X-4)

DY1000D3 = Y2(X-1)(X-3)(X-4)/(X-2)(X-3)(X-4)
DY1000D3 = Y3(X-1)(X-2)(X-4)/(X-1)(X-2)(X-4)

Y1 = RT1001(L-1, IL)
Y2 = RT1001(L, IL)
Y3 = RT1001(L+1, IL)
Y4 = RT1001(L+2, IL)

Y2 = Y2(X-1)(X-3)(X-4)/(X-2)(X-3)(X-4)
Y3 = Y3(X-1)(X-2)(X-4)/(X-1)(X-2)(X-4)


Y1 = RT1010(L-1, IL)
Y2 = RT1010(L, IL)
Y3 = RT1010(L+1, IL)
Y4 = RT1010(L+2, IL)

Y2 = Y2(X-1)(X-3)(X-4)/(X-2)(X-3)(X-4)
Y3 = Y3(X-1)(X-2)(X-4)/(X-1)(X-2)(X-4)
\[
Y_1 = R_{T1101}(L-1, IL)
\]
\[
Y_2 = R_{T1101}(L, IL)
\]
\[
Y_3 = R_{T1101}(L+1, IL)
\]
\[
Y_4 = R_{T1101}(L+2, IL)
\]

\[
Y_{1101} = Y_1 \cdot (I-I_2) \cdot (I-I_3) \cdot (I-I_4) \cdot (I_1-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4)
\]
\[
Y_{1102} = Y_2 \cdot (I-I_1) \cdot (I-I_3) \cdot (I-I_4) \cdot (I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)
\]
\[
Y_{1103} = Y_3 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_4) \cdot (I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)
\]
\[
Y_{1104} = Y_4 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_3) \cdot (I_4-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3)
\]

\[
DY_{1101} = Y_1 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4) \cdot (I_1-I_2)
\]
\[
DY_{1102} = Y_2 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4) \cdot (I_2-I_1)
\]
\[
DY_{1103} = Y_3 \cdot (I-I_2) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4) \cdot (I_3-I_1)
\]
\[
DY_{1104} = Y_4 \cdot (I-I_2) \cdot (I-I_3) \cdot (I-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3) \cdot (I_4-I_1)
\]

\[
Y_1 = R_{T1100}(L-1, IL)
\]
\[
Y_2 = R_{T1100}(L, IL)
\]
\[
Y_3 = R_{T1100}(L+1, IL)
\]
\[
Y_4 = R_{T1100}(L+2, IL)
\]

\[
Y_{1100} = Y_1 \cdot (I-I_3) \cdot (X-I_4) \cdot (X-I_1) \cdot (X-I_4) \cdot (X-I_1) \cdot (X-I_3)
\]
\[
Y_{1102} = Y_2 \cdot (I-I_1) \cdot (I-I_3) \cdot (I-I_4) \cdot (I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)
\]
\[
Y_{1103} = Y_3 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_4) \cdot (I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)
\]
\[
Y_{1104} = Y_4 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_3) \cdot (I_4-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3)
\]

\[
DY_{1100} = Y_1 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4) \cdot (I_1-I_2)
\]
\[
DY_{1102} = Y_2 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4) \cdot (I_2-I_1)
\]
\[
DY_{1103} = Y_3 \cdot (I-I_2) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4) \cdot (I_3-I_1)
\]
\[
DY_{1104} = Y_4 \cdot (I-I_2) \cdot (I-I_3) \cdot (I-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3) \cdot (I_4-I_1)
\]

\[
Y_1 = R_{T1110}(L-1, IL)
\]
\[
Y_2 = R_{T1110}(L, IL)
\]
\[
Y_3 = R_{T1110}(L+1, IL)
\]
\[
Y_4 = R_{T1110}(L+2, IL)
\]

\[
Y_{1110} = Y_1 \cdot (I-I_3) \cdot (X-I_4) \cdot (X-I_1) \cdot (X-I_4) \cdot (X-I_1) \cdot (X-I_3)
\]
\[
Y_{1112} = Y_2 \cdot (I-I_1) \cdot (I-I_3) \cdot (I-I_4) \cdot (I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)
\]
\[
Y_{1113} = Y_3 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_4) \cdot (I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)
\]
\[
Y_{1114} = Y_4 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_3) \cdot (I_4-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3)
\]

\[
DY_{1110} = Y_1 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4) \cdot (I_1-I_2)
\]
\[
DY_{1112} = Y_2 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4) \cdot (I_2-I_1)
\]
\[
DY_{1113} = Y_3 \cdot (I-I_2) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4) \cdot (I_3-I_1)
\]
\[
DY_{1114} = Y_4 \cdot (I-I_2) \cdot (I-I_3) \cdot (I-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3) \cdot (I_4-I_1)
\]

\[
Y_1 = R_{T1111}(L-1, IL)
\]
\[
Y_2 = R_{T1111}(L, IL)
\]
\[
Y_3 = R_{T1111}(L+1, IL)
\]
\[
Y_4 = R_{T1111}(L+2, IL)
\]

\[
Y_{1111} = Y_1 \cdot (I-I_3) \cdot (X-I_4) \cdot (X-I_1) \cdot (X-I_4) \cdot (X-I_1) \cdot (X-I_3)
\]
\[
Y_{1112} = Y_2 \cdot (I-I_1) \cdot (I-I_3) \cdot (I-I_4) \cdot (I_2-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4)
\]
\[
Y_{1113} = Y_3 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_4) \cdot (I_3-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4)
\]
\[
Y_{1114} = Y_4 \cdot (I-I_1) \cdot (I-I_2) \cdot (I-I_3) \cdot (I_4-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3)
\]

\[
DY_{1111} = Y_1 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_2) \cdot (I_1-I_3) \cdot (I_1-I_4) \cdot (I_1-I_2)
\]
\[
DY_{1112} = Y_2 \cdot (I-I_3) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_2-I_3) \cdot (I_2-I_4) \cdot (I_2-I_1)
\]
\[
DY_{1113} = Y_3 \cdot (I-I_2) \cdot (I-I_4) \cdot (I-I_1) \cdot (I_3-I_2) \cdot (I_3-I_4) \cdot (I_3-I_1)
\]
\[
DY_{1114} = Y_4 \cdot (I-I_2) \cdot (I-I_3) \cdot (I-I_1) \cdot (I_4-I_2) \cdot (I_4-I_3) \cdot (I_4-I_1)
\]
How calculate YFIT

Rotation interpolant

I=3*NLINES+4
A1=1.-A(I)
A2=A(I)
Y000=A1*Y000+A2*Y001
DYOO0D3=A1*DYOO0D3+A2*DY0001D3
DYOO0D5=A1*DYOO0D5+A2*DY0001D5
Y011=A1*Y010+A2*Y011
DY011D5=A1*DY011D5+A2*DY011D5
Y100=A1*Y100+A2*Y101
DY100D3=A1*DY100D3+A2*DY010D3
DY100D5=A1*DY100D5+A2*DY010D5
Y101=A1*Y101+A2*Y1011
Y110=A1*Y110+A2*Y111
Y111=A1*Y111+A2*Y1111
DY111D3=A1*DY111D3+A2*DY111D3
DY111D5=A1*DY111D5+A2*DY111D5

Abundance interpolant

I=3*NLINES+3
A1=1.-A(I)
A2=A(I)
Y00=A1*Y000+A2*Y001
DY00D3=A1*DY000D3+A2*DY001D3
DY00D5=A1*DY000D5+A2*DY001D5
Y01=A1*Y010+A2*Y011
DY01D3=A1*DY010D3+A2*DY010D3
DY01D5=A1*DY010D5+A2*DY010D5
Y10=A1*Y100+A2*Y101
DY10D3=A1*DY100D3+A2*DY100D3
DY10D5=A1*DY100D5+A2*DY100D5
Y11=A1*Y110+A2*Y111

Gravity interpolant

I=3*NLINES+2
A1=1.-A(I)
A2=A(I)
Y0=A1*Y000+A2*Y01
DY0D3=A1*DY000D3+A2*DY01D3
DY0D5=A1*DY000D5+A2*DY01D5
Y1=A1*Y100+A2*Y11
DY1D3=A1*DY100D3+A2*DY101D3
DY1D5=A1*DY100D5+A2*DY101D5
Y11=A1*Y110+A2*Y111

Temperature interpolant

I=3*NLINES+1
A1=1.-A(I)
A2=A(I)
Y=A1*Y000+A2*Y1
DY0D3=A1*DY000D3+A2*DY01D3
DY0D5=A1*DY000D5+A2*DY01D5

Continuum fit

A1=(3*IL-2)
A2=(3*IL-1)
Y=1*Y+2
YM=1+YC
DYD(A3*IL-2)*X*Y
DYD(A3*IL-1)=Y
SUBROUTINE PLOTFUNC(XI, A, YFIT, DYDA, MA)

Generate continuum parameters for fit to line profiles.

IMPLICIT REAL*8(A-H,O-Z)
INTEGER PLM, PLI
DIMENSION A(S), DYDA(3), DIPLOT(801), DYFLOT(801)

Externals

INTEGER DLOCATE
EXTERNAL DLOCATE

PLOTFUNC common block

COMMON /PLOTFUNC/DIPLOT, DYFLOT, PLM

Start of executable statements

I=XI-1(3)
L=DLOCATE(DIPLOT, PLI, I)
I1=DIPLOT(L-1)
I2=DIPLOT(L)
I3=DIPLOT(L+1)
I4=DIPLOT(L+2)
Y1=DFLOT(L-1)
Y2=DFLOT(L)
Y3=DFLOT(L+1)
Y4=DFLOT(L+2)

YMOD=Y1*((I-I3)*(I-I4)+(I-I2)*(I-I4)+(I-I2)*(I-I3))/((I1-I2)*(I1-I3)*(I1-I4)) +
     Y2*((I-I3)*(I-I4)+(I-I1)*(I-I4)+(I-I1)*(I-I3))/((I2-I1)*(I2-I3)*(I2-I4)) +
     Y3*((I-I2)*(I-I4)+(I-I1)*(I-I4)+(I-I1)*(I-I2))/((I3-I1)*(I3-I2)*(I3-I4)) +
     Y4*((I-I2)*(I-I3)+(I-I1)*(I-I3)+(I-I1)*(I-I2))/((I4-I1)*(I4-I2)*(I4-I3))

DYMOD3=-Y1*((I-I3)*(I-I4)+(I-I2)*(I-I4)+(I-I2)*(I-I3))/((I1-I2)*(I1-I3)*(I1-I4)) +
     Y2*((I-I3)*(I-I4)+(I-I1)*(I-I4)+(I-I1)*(I-I3))/((I2-I1)*(I2-I3)*(I2-I4)) +
     Y3*((I-I2)*(I-I4)+(I-I1)*(I-I4)+(I-I1)*(I-I2))/((I3-I1)*(I3-I2)*(I3-I4)) +
     Y4*((I-I2)*(I-I3)+(I-I1)*(I-I3)+(I-I1)*(I-I2))/((I4-I1)*(I4-I2)*(I4-I3))

CONTA=A(1)*X*A(2)
YFIT=YMOD*CONTA
DYDA(1)=YMOD
DYDA(2)=YMOD
DYDA(3)=DYMOD3*CONTA
RETURN
END