The role of HeH^+ in cool helium rich white dwarfs.

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ABSTRACT

HeH^+ is found to be the dominant positive ion over a wide range of temperatures and densities relevant to helium rich white dwarfs. The inclusion of HeH^+ in ionization equilibrium computations increases the abundance of free electrons by a significant factor. For temperatures below 8000 K, He^- free-free absorption is increased by up to a factor of 5, by the inclusion of HeH^+. Illustrative model atmospheres and spectral energy distributions are computed, which show that HeH^+ has a strong effect upon the density and pressure structure of helium rich white dwarfs with T_{eff}<8000 K. The inclusion of HeH^+ significantly reddens spectral energy distributions and broad band color indices for models with T_{eff}<5500 K. This has serious implications for existing model atmospheres, synthetic spectra and cooling curves for helium rich white dwarfs.

Subject headings: white dwarfs, equation of state, opacities, HeH^+, model atmospheres.

1. Introduction

Bergeron & Leggett (2002) analyzed the recently discovered white dwarfs SDSS J133739 +000142 and LHS 3250 (Harris *et al.* 1999, 2001), identifying both objects as extreme helium rich cool white dwarfs. However they encountered significant problems when attempting to fit the spectral energy distributions (SEDs). Bergeron & Leggett (2002) concluded that the reason for the discrepancy between their SEDs and the observed fluxes, lay in the physics used to calculate their model atmospheres. In this work we investigate the much neglected molecular ion HeH^+, as a possible part of the missing physics of helium rich white dwarfs.

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We demonstrate that the opacity of a helium rich white dwarfs photosphere is significantly affected by HeH^+. From the discussion of Fontaine *et al.* (2001), it follows that increased opacity arising from HeH^+, will lengthen the cooling time for helium rich white dwarfs with $T_{eff} < 8000$ K.

Gaur *et al.* (1988) have previously performed molecular dissociation equilibrium calculations which include HeH^+ and He_2^+, but neglect H_3^+. They first identified that HeH^+ exists in significant quantities in helium rich white dwarfs. In a later paper, Gaur *et al.* (1991) suggested a search for the infrared lines of HeH^+ within the spectra of a helium rich white dwarfs. To our knowledge no other attempts to study HeH^+ within the atmospheres of helium rich white dwarfs have been made.

In section 2 we present our modified version of the Luo (1997) non-ideal equation of state and demonstrate the effect of HeH^+ upon the ionization equilibrium. In section 3 we investigate the direct and indirect effect of HeH^+ on the opacity function. We discuss our model atmosphere code, computed model atmospheres and SEDs in section 4, and finally we conclude in section 5.

2. Equation of state

The equation of state is a vital component of any model atmospheres. Not only does the equation of state link state parameters such as temperature, pressure, density, and internal energy, it also calculates the relative abundance of each species within the gas. These relative abundances are essential for the accurate calculation of radiative opacity. The photospheres of cool extremely helium rich stars have densities which can reach upward of 1 g cm^{-3}, under such conditions the gas is highly non-ideal, requiring the use of a non-ideal equation of state.

In this work we have adapted the non-ideal hydrogen/helium equation of state of Luo (1997). This equation of state accounts for the non-ideal effects of electron degeneracy, Coulomb coupling and pressure ionization. The equation of state however lacks an accurate treatment of pressure dissociation, the abundance of molecular hydrogen is estimated using an equilibrium constant (K(T)) for the reaction: $H_2 \rightleftharpoons 2H$, so that molecular hydrogen pressure dissociates as hydrogen pressure ionizes.

To properly account for the pressure ionization of H^- we have added a term to the hydrogen ionization equilibrium, given by eq. (22) and (23) in Luo (1997), so that

$$\begin{aligned} y_{H^-} &= L_{H^-}/L_H \\ L_H &= L_{HI} + L_{HII} + L_{H^-} \end{aligned} \tag{1}$$

where y_{H^-} is the ionization fraction of atomic and ionic hydrogen in the form of H^-, $L_{\rm HI}$ and $L_{\rm HII}$ are the grand partition functions of atomic hydrogen and a proton (see Luo (1997) eq. 23). The grand partition function of H^- is given by

$$L_{H^-} = W_{H^-} \exp(2\lambda - E_{H^-}/kT) \tag{2}$$

where λ is the electron degeneracy, E_{H^-} is the sum of the ionization potential of hydrogen and H^- (14.352 eV), and W_{H^-} is given by eq. (11)-(16) in Luo (1997) using a characteristic radius for H^- of 1.15 Å (Lenzuni & Saumon 1992).

The trace ionic molecules H_2^-, H_2^+, H_3^+, HeH^+, and He_2^+ have little or no effect on the temperature, pressure, and density, but under certain conditions can be responsible for nearly all the free electrons in a hydrogen helium gas. We calculate equilibrium constants for the formation of H_2, H_2^-, H_2^+, H_3^+, HeH^+, and He_2^+ from atomic H and He, H^-, and free electrons with the Saha equation. Subject to the conservation of charge, and of H and He nuclei, the equilibrium constants and ionization fractions are used to construct 3 non-linear simultaneous equations. These 3 equations are solved using a multi-variable Newton-Raphson technique. In this way the number densities for each species can be calculated for any given temperature, pressure, hydrogen fraction and value of λ. The sources of the internal partition functions which we use are detailed in Harris *et al.* (2004), we have also used the recent HeH^+ partition function of Engel *et al.* (2004). A converged value of λ is found by iterating over a further conservation of charge equation:

$$\begin{aligned} C_e T^{3/2} F_{1/2}(\lambda - \epsilon_{CC}/kT) &= N_{\rm HII} + N_{\rm HeII} + 2N_{\rm HeIII} - N_{\rm H^-} + N_{\rm H_2^+} - N_{\rm H_2^-} \\ &\quad + N_{\rm H_3^+} + N_{\rm HeH^+} + N_{\rm He_2^+} \end{aligned} \tag{3}$$

where N_x is the number density of species x, ϵ_{CC} is the free electron Coulomb coupling energy (Luo 1997), $F_{1/2}$ is a Fermi-Dirac integral, T is temperature and a constant $C_e = (2^{1/2}/\pi^2)(km_e/\hbar^2)^{3/2}$. The left hand side of eq 3 is the number density of free electrons (see Luo (1994, 1997)) and the right hand side counts the charge on all ions.

Figure 1 shows the abundance fraction by number of the various species within our equation of state, as a function of hydrogen to helium number ratio, density, and temperature. At a temperature of 5000 K and density of 0.2 g cm^{-3} H_3^+ is the dominant positive ion for the hydrogen rich case. HeH^+ is the dominant positive ion for the helium rich range $-10 < \log_{10}(N_H/N_{He}) < -2.5$ and He_2^+ becomes the dominant positive ion for $\log_{10}(N_H/N_{He}) < -10$. Figure 1 indicates that HeH^+ continues to be the dominant positive ion over a range of densities and temperatures. This is in contrast to the findings of Malo *et al.* (1999) who neglected HeH^+ and so believed that He_2^+ is the dominant positive ion in the photosphere of helium rich white dwarfs with $\log_{10}(N_H/N_{He}) < -7$ and of $T_{\rm eff}$=6000 K. Furthermore HeH^+

appears to have been neglected from all other theoretical studies of hydrogen-helium mix, cool white dwarfs (Bergeron *et al.* 1995; Bergeron & Leggett 2002; Rohrmann *et al.* 2002).

3. Opacity function

The opacity of a gas under the extreme pressures found in the photospheres of helium rich white dwarfs remains in question (Iglesias *et al.* 2002; Bergeron & Leggett 2002). The opacity of a cool helium rich atmosphere is dominated by H_2-He collision induced absorption, He^- free-free opacity and Rayleigh scattering from helium (Malo *et al.* 1999; Iglesias *et al.* 2002; Rohrmann *et al.* 2002). As such the opacity is strongly dependent upon the abundance of free electrons and molecular hydrogen.

The opacity data that we use is discussed in our earlier paper (Harris *et al.* 2004). To determine if HeH^+ rotation-vibration lines would be observable in a helium rich white dwarf we have used the recent HeH^+ linelist of Engel *et al.* (2004). Figure 2 shows the monochromatic absorption coefficient at $\rho = 0.5$ g cm^{-3}, $\log_{10}(N_{\rm H}/N_{\rm He})$=–5, at temperatures of 9000, 7000, 5000, 4000 and 3500 K, computed both including and neglecting HeH^+ from our equation of state. It is evident that if HeH^+ is neglected from the equation of state the gas opacity can be underestimated by as much as a factor of 5, over a significant range of temperatures, in this case 3500 to 9000 K.

The dominant opacity, across the frequency range shown in figure 2 and for temperatures upward of 5000 K, is He^- free-free absorption, also visible are H I lines. At lower temperatures collision induced absorption, in the infrared, and He Rayleigh scattering, in the visible/ultra-violet, become important and eventually take over from He^- free-free. At the densities found in the photospheres of helium rich white dwarfs, we find that the absorption lines of HeH^+ are too weak to overcome absorption by H_2-He collisions and free-free opacity from He^-. This contradicts the findings of Gaur *et al.* (1991). However, HeH^+ lines do make a contribution to opacity at densities below 3×10^{-3} g cm^{-3} and T$\sim$3500 K, if helium rich, very metal poor, objects exist with such temperatures and densities in their photospheres then HeH^+ lines should be observable.

4. Model atmospheres & spectral energy distributions.

We use the plane parallel model atmosphere code MARCS (Gustafsson *et al.* 1975), modified for the new non-ideal equation of state subroutines, discussed in section 2, and the new continuous opacity subroutines, discussed in section 3. The new equation of state and opacity function subroutines are fast enough to be run in real time. For all calculations reported here we use convection mixing length of 1.5 pressure scale heights.

As discussed in Saumon *et al.* (1994) and Bergeron *et al.* (1995), in the optically thin regions the unusual opacity function of a metal free hydrogen helium gas results in multiple roots in the equation of radiative equilibrium. The high temperature solution to radiative equilibrium in the optically thin regions is preferentially found in our models. Such a solution is not physically realistic, rendering our models of T_{eff}≤5000 K below $\log \tau_R = -2$ unreliable. However, as this only occurs at very small optical depths the emergent flux is unaffected.

We also experienced a problem with convergence of the convective flux at temperatures of 5000 K and below. The pressure-temperature gradient (∇) is very close to the adiabatic gradient (∇_{ad}), so that $(\nabla - \nabla_{ad})/\nabla \sim 10^{-3}$ in the convective zone. In the cool highly non-ideal regions, numerical noise on the value of ∇_{ad} calculated within our equation of state is of this order, resulting in convergence problems with the convective flux. We have therefore not been able to obtain converged models below T_{eff}=4500 K.

We have computed a set of model atmospheres for $\log g = 8$, $\log_{10}(N_{\rm H}/N_{\rm He}) = 10^{-5}$, and between effective temperatures of 4500 and 8000 K, including and neglecting HeH^+. Figure 3 shows optical depth verses temperature and density for model atmospheres of 4500, 5000, 6000, 7000 and 8000 K. Although the temperatures remain relatively unperturbed by the inclusion of HeH^+, there is a very strong affect upon the density and pressure. If HeH^+ is neglected then the density and pressure can be overestimated by up to a factor 5, similarly the electron pressure significantly underestimated. For T_{eff} of $\geq$ 8000 K there are significant electrons released from H II and He II, which reduces the importance of HeH^+.

Figure 4 shows the spectral energy distributions (SEDs) of our 4500, 5000 and 6000 K models, with and without HeH^+. The 4500 and 5000 K SEDs show a significant changes if HeH^+ is included in the ionization equilibrium, but the effect is only small for the 6000 K model. The reason for this is that above ∼5000 K HeH^+ He^- free-free is the only significant source of opacity, so although the total opacity is increased the shape of the absorption function and hence SED is unchanged. For temperatures below 5500 K, He Rayleigh scattering and He-H_2 collision induced absorption contribute to opacity. As these opacity sources are unaffected by the increased abundance of electrons from HeH^+, the increase in He^- free-free opacity changes the shape of the total opacity function and SED. These differences are reflected in the broadband color indexes given in tables 1 and 2. There are significant differences, at T_{eff}=5500 K and below, between colors computed whilst including and neglecting HeH^+. The large increase in the V–K magnitude, and most of the other color indices indicates that the models calculated with HeH^+ are significantly redder than the models calculated without HeH^+, this is also apparent in the SEDs. The new colors presented here illustrate that the currently accepted bluer colors of cool helium rich white dwarfs (Serenelli *et al.* 2001; Bergeron *et al.* 1995) are in need of revision. The broadband color indices were computed by using the bandpasses given by Bessell & Brett (1988); Bessell (1990) and calibrating using a spectrum of Vega.

5. Conclusion

A non-ideal hydrogen-helium equation of state which includes the molecular ion HeH^+ within the ionization equilibrium, has been presented. It has been demonstrated, that under helium rich conditions and over a range of temperatures and densities relevant to helium rich white dwarfs, HeH^+ is the dominant positive ion. Using the equation of state, we have computed a set of continuous opacities which illustrate that HeH^+ can indirectly increase the opacity of a helium rich gas by up to a factor of 5. Using the recent HeH^+ linelist of Engel *et al.* (2004), we have found that HeH^+ line opacity does not significantly contribute to the opacity at the densities found in helium rich white dwarfs.

From a physical point of view one of the most interesting reasons for studying helium rich white dwarfs is that the densities of their photospheres access regions in which the gas is strongly non-ideal. Saumon & Chabrier (1991); Saumon *et al.* (1995) have studied the pressure dissociation of H_2 in a pure hydrogen environment. However, one of the shortcomings of our, and all other equations of state known to us is that there has been no study of the pressure dissociation of the important molecular ions, H_3^+. HeH^+, and He_2^+. Before we can fully understand helium rich white dwarfs, our understanding of the physics of cool dense hydrogen-helium plasmas must be improved.

Our equation of state and opacity function have been incorporated into a version of MARCS (Gustafsson *et al.* 1975). Using this code we have computed model atmospheres, spectral energy distributions and broad band color indices for an illustrative range of helium rich white dwarfs. We find that in all models below 8000 K the pressure and density structure of the model atmospheres is significantly affected by HeH^+ and by as much as a factor of 5 in the lower temperature models. Furthermore, HeH^+ also has a strong effect on the spectral energy distributions and color indices of models below 5500 K. These SEDs and color indices are significantly reddened upon the inclusion of HeH^+. The importance of HeH^+ should prompt a review of all current model atmospheres, synthetic spectra and cooling curves for cool helium rich white dwarfs.

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Table 1: Color indices for models calculated whilst neglecting HeH^+. $\log g = 8$ and $\log_{10}(N_{\rm H}/N_{\rm He})$=$10^{-5}$.

T_{eff}	B–V	V–R	V–K	R–I	I–J	J–H	H–K
4500	0.85	0.52	0.58	0.48	0.30	–0.54	–0.17
5000	0.72	0.44	0.81	0.42	0.35	–0.18	–0.22
5500	0.60	0.38	1.14	0.36	0.32	0.12	–0.04
6000	0.50	0.32	0.98	0.30	0.24	0.12	–0.01
6500	0.42	0.27	0.77	0.25	0.18	0.09	–0.03
7000	0.36	0.23	0.59	0.21	0.12	0.07	–0.05
7500	0.30	0.20	0.43	0.17	0.07	0.05	–0.06
8000	0.25	0.17	0.30	0.14	0.03	0.03	–0.08

Table 2: Color indices, for models calculated with HeH^+. $\log g = 8$ and $\log_{10}(N_{\rm H}/N_{\rm He})$=$10^{-5}$.

T_{eff}	B–V	V–R	V–K	R–I	I–J	J–H	H–K
4500	0.84	0.52	1.32	0.51	0.49	–0.03	–0.18
5000	0.70	0.44	1.44	0.43	0.42	0.16	–0.01
5500	0.59	0.37	1.23	0.36	0.32	0.16	0.02
6000	0.50	0.32	0.98	0.30	0.24	0.13	0.00
6500	0.42	0.27	0.80	0.25	0.18	0.10	–0.03
7000	0.35	0.23	0.59	0.21	0.12	0.07	–0.04
7500	0.30	0.20	0.43	0.17	0.07	0.05	–0.06
8000	0.25	0.17	0.29	0.14	0.03	0.03	–0.08

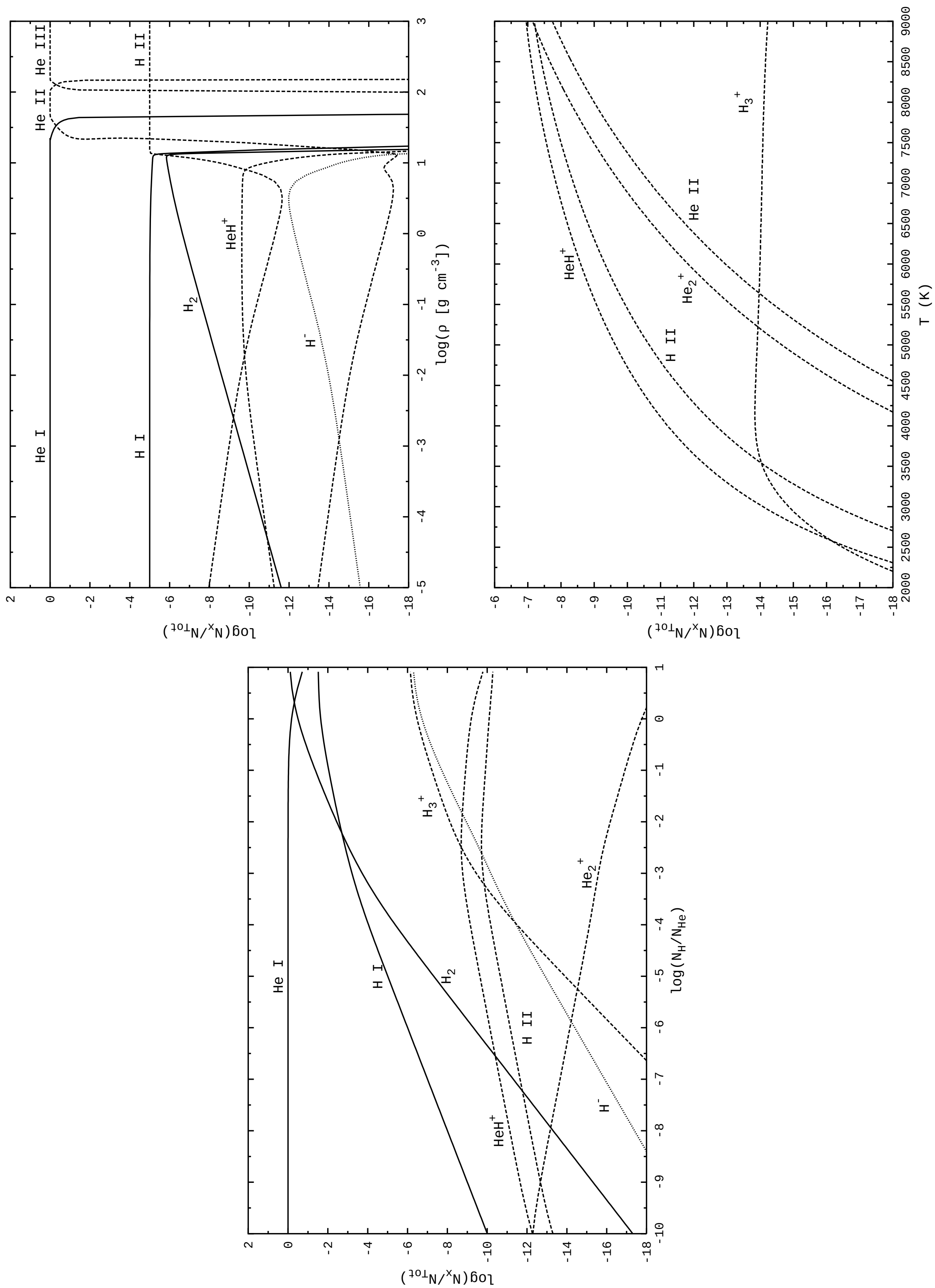

Fig. 1.— Chemical and ionization equilibrium as a function of $\log_{10}(N_{\rm H}/N_{\rm He})$, density and temperature. Values of temperature of 5000 K, density of 0.2 g cm^{-3}, and $\log_{10}(N_{\rm H}/N_{\rm He})$=–5 are used. Neutral species are given solid lines, positively charged species dashed lines, and negatively charged species dotted lines.

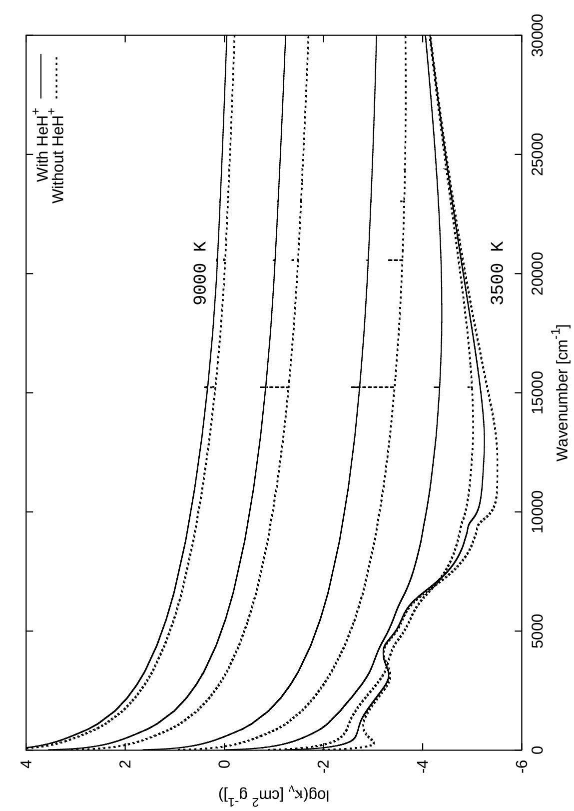

Fig. 2.— The continuous opacity function as a function of wavenumber at constant values of $\rho = 0.5$ g cm^{-3} and $\log_{10}(N_{\rm H}/N_{\rm He})$=-5, calculated at temperatures of 9000, 7000, 5000, 4000, and 3500 K.

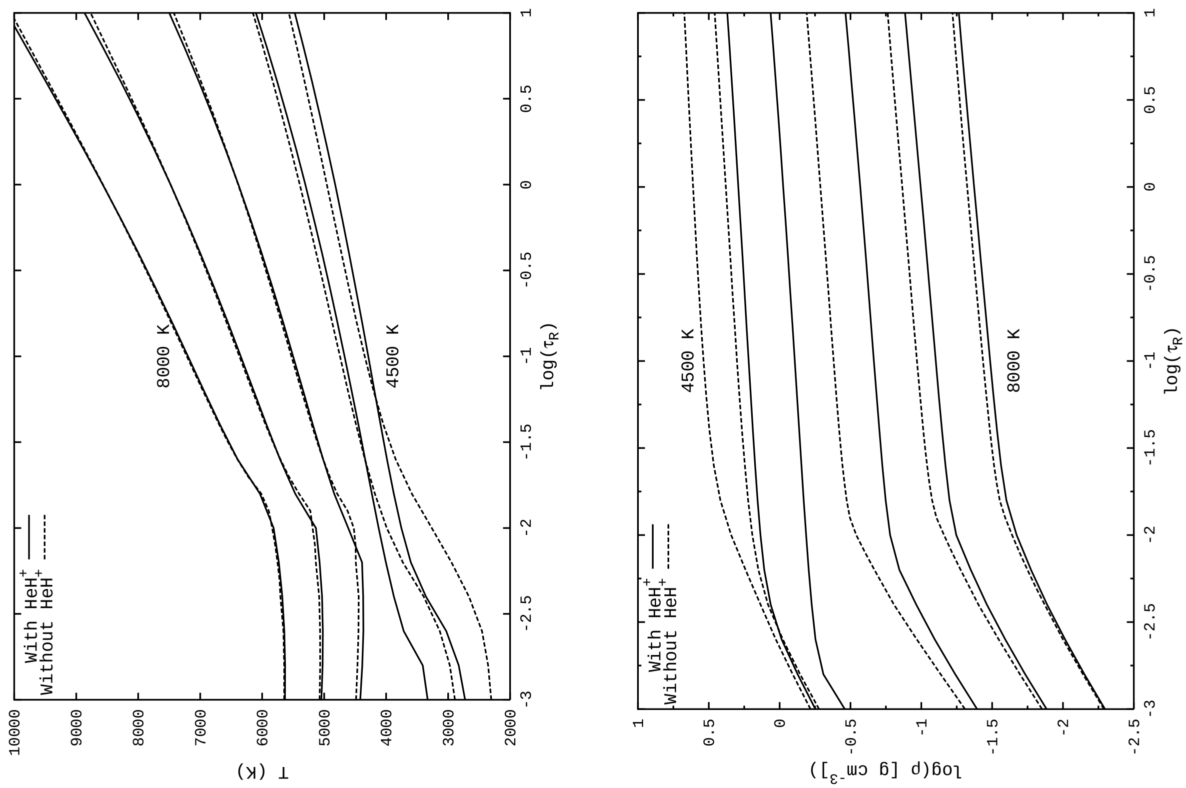

Fig. 3.— Optical depth verses temperature and density for models of 4500, 5000, 6000, 7000, and 8000 K, computed including and neglecting HeH^+ in the ionization equilibrium.

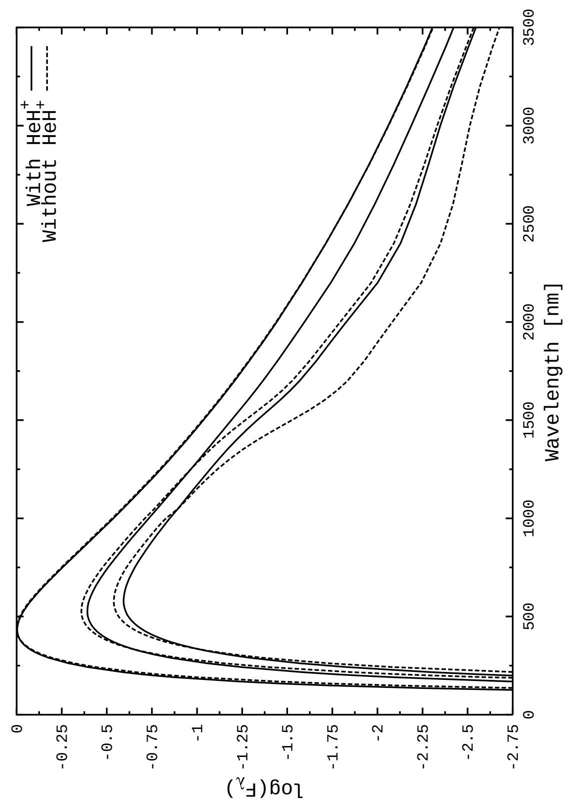

Fig. 4.— Spectral energy distributions for models of T_{eff}=4500, 5000, and 6000 K. The logarithm of the relative flux is given per unit wavelength interval.