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

G. J. Harris, A. E. Lynas-Gray\(^1\), S. Miller and J. Tennyson\(^2\).

Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK.

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 \(T_{\text{eff}}\)<8000 K. The inclusion of HeH\(^+\) significantly reddens spectral energy distributions and broad band color indices for models with \(T_{\text{eff}}\)<5500 K. This has serious implications for existing model atmospheres, synthetic spectra and cooling curves for helium rich white dwarfs.

Subject headings: stars: white dwarfs, stars: atmospheres, equation of state.

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 discrepancy between their SEDs and the observed fluxes, is due to the physics used to calculate their model atmospheres. Here we investigate the molecular ion HeH\(^+\) as part of the missing physics of helium rich white dwarfs. We demonstrate that the opacity of a helium rich white dwarfs photosphere is significantly affected by HeH\(^+\). From the discussion

---

\(^1\)Permanent address: Department of Physics, University of Oxford, Keble Road, Oxford OX1 3RH, UK.

\(^2\)Corresponding Author: j.tennyson@ucl.ac.uk
of Fontaine et al. (2001), it follows that increased opacity arising from HeH$^+$, will lengthen the cooling time for helium rich white dwarfs with $T_{\text{eff}} < 8000$ K.

The only attempts to study HeH$^+$ in helium rich white dwarfs known to us was made by Gaur et al. (1988, 1991). They showed that HeH$^+$ exists in significant quantities in helium rich white dwarfs and suggested a search for the infrared lines of HeH$^+$.

2. Equation of state

The equation of state (EoS) is a vital component of any model atmosphere, it links the state parameters such as temperature, pressure, density, and internal energy. It also calculates the relative abundance of each species within the gas, which are essential to obtain accurate radiative opacities. The photospheres of cool extremely helium rich white dwarfs have densities which can reach upward of 1 g cm$^{-3}$, under such conditions the use of a non-ideal EoS is required.

We have adapted the non-ideal H/He EoS of Luo (1997). This EoS accounts for the non-ideal effects of electron degeneracy, Coulomb coupling and pressure ionization, but lacks an accurate treatment of pressure dissociation. The abundance of H$_2$ is estimated using an equilibrium constant for the reaction: H$_2 \rightleftharpoons 2$H, so that H$_2$ pressure dissociates as hydrogen pressure ionizes.

To 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

$$ y_{H^-} = \frac{L_{H^-}}{L_H} $$

$$ L_H = L_{HI} + L_{HII} + L_{H^-} $$

where $y_{H^-}$ is the ionization fraction of atomic and ionic hydrogen in the form of H$^-$, $L_{HI}$ and $L_{HII}$ 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

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

where $\lambda$ 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).

Under certain conditions, the trace ionic molecules H$_2^-$, H$_2^+$, H$_3^+$, HeH$^+$, and He$_2^+$ are responsible for nearly all the free electrons in a H/He gas. We calculate equilibrium constants
for the formation of \( \text{H}_2, \text{H}_2^-, \text{H}_3^+, \text{HeH}^+, \) and \( \text{He}_2^+ \) from atomic H and He, H\(^-\), and free electrons with the Saha equation. Subject to conservation of charge, and of H and He nuclei, the equilibrium constants and ionization fractions are used to construct 3 nonlinear 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 \( \lambda \). The internal partition functions we use are detailed in Harris et al. (2004), for HeH\(^+\) we use the partition function of Engel et al. (2005). A converged value of \( \lambda \) is found by iterating over a further conservation of charge equation:

\[
 C_e T^{3/2} F_{1/2}(\lambda - \epsilon_{CC}/kT) = N_{\text{H}^+} + N_{\text{He}^+} + 2 N_{\text{HeH}^+} - N_{\text{H}^-} + N_{\text{H}_2^+} - N_{\text{H}_2^-} \\
+ N_{\text{H}_3^+} + N_{\text{HeHe}^+} + N_{\text{He}_2^+}
\]  

where \( N_x \) is the number density of species \( x \), \( \epsilon_{CC} \) is the free electron Coulomb coupling energy (Luo 1997), \( F_{1/2} \) is a Fermi-Dirac integral, \( T \) is temperature and a constant \( C_e = (2^{1/2}/\pi^2)(km_e/h^2)^{3/2} \). 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 number fraction of the species within our EoS, as a function of H to He number ratio, density, and temperature. At 5000 K and density of 0.2 g cm\(^{-3}\) \( \text{H}_2^+ \) is the dominant positive ion for the hydrogen rich case. \( \text{HeH}^+ \) is the dominant positive ion for the helium rich range \(-10 < \log_{10}(N_{\text{H}}/N_{\text{He}}) < -2.5 \) and \( \text{He}_2^+ \) becomes the dominant positive ion for \( \log_{10}(N_{\text{H}}/N_{\text{He}}) < -10 \). Figure 1 indicates that \( \text{HeH}^+ \) continues to be the dominant positive ion over a range of densities and temperatures. Lenzuni et al. (1991) present an EoS and mean opacities for a H/He gas of 72% hydrogen by mass, they correctly state that the opacity coefficient of \( \text{HeH}^+ \) is wholly irrelevant. However, as illustrated below, for a helium rich mix \( \text{HeH}^+ \) strongly affects the opacity and cannot be neglected.

### 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 \( \text{H}_2\)-He collision induced and \( \text{He}^- \) free-free absorption, and \( \text{He\text{I}} \) Rayleigh scattering (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 \( \text{H}_2 \). The sources of opacity data that we use is discussed in Harris et al. (2004).

The monochromatic absorption coefficient at \( \rho = 0.5 \text{ g cm}^{-3}, \log_{10}(N_{\text{H}}/N_{\text{He}}) = -5 \), over a
range of temperatures, computed both including and neglecting HeH$^+$ from our EoS, is shown in figure 2. It is evident that if HeH$^+$ is neglected the gas opacity can be underestimated by as much as a factor of 5, over a significant range of temperatures. The dominant opacity, across the frequency range shown in figure 2 and for temperatures upward of 5000 K, is He$^-$ free-free absorption. At lower temperatures collision induced absorption, in the infrared, and He I Rayleigh scattering, in the visible/ultra-violet, become important and eventually take over from He$^-$ free-free.

To determine if HeH$^+$ rotation-vibration lines would be observable in a helium rich white dwarf we have employed the recent publicly available HeH$^+$ linelist of Engel et al. (2005). We find that the absorption lines of HeH$^+$ are too weak to overcome the continuous opacity, under the temperatures and densities found in helium rich white dwarfs. Therefore HeH$^+$ lines will not be visible in the spectra of helium rich white dwarfs. For a discussion of HeH$^+$ line opacity and some of the temperatures densities in which it is important see Engel et al. (2005).

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 EoS subroutines, discussed in section 2, and the new continuous opacity subroutines, discussed in section 3. The new EoS and opacity function subroutines are fast enough to be run in real time.

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 H/He 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 $T_{\text{eff}} \leq 5000$ 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 ($\nabla$) is very close to the adiabatic gradient ($\nabla_{\text{ad}}$), so that $(\nabla - \nabla_{\text{ad}})/\nabla \sim 10^{-3}$ in the convective zone. In the cool highly non-ideal regions, numerical noise in the value of $\nabla_{\text{ad}}$ calculated within our EoS is of this order, resulting in convergence problems with the convective flux. We have therefore not been able to obtain converged models below $T_{\text{eff}} = 4500$ K.

We have computed a set of model atmospheres for $\log g = 8$, $\log_{10}(N_H/N_{\text{He}}) = 10^{-5}$, 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 \(T_{\text{eff}}\) 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 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 \(\sim 5000\) K 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. These colors were computed by using the bandpasses given by Bessell & Brett (1988); Bessell (1990) and calibrating using a spectrum of Vega. There are significant differences, at \(T_{\text{eff}}=5500\) 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. In general all our colors are redder than the colors of Bergeron & Leggett (2002).

5. Conclusion

A non-ideal H/He equation of state (EoS) 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 EoS, 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. (2005), 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 H/He plasmas must be improved.

Our EoS 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 of the model atmospheres is reduced by up to a factor of five by the inclusion of HeH$^+$. Furthermore, HeH$^+$ significantly reddens the SEDs and color indices, for models below $T_{\text{eff}} = 5500$ K. The importance of HeH$^+$ should prompt a review of all current model atmospheres, synthetic spectra and cooling curves for cool helium rich white dwarfs.

We thank Prof. Bengt Gustafsson for providing us with a version of marcs, Prof. Hugh Jones for providing a spectrum of Vega, and the UK Particle Physics and Astronomy Research Council (PPARC) for support.

REFERENCES

Bergeron, P., Saumon, D., and Wesemael, F., 1995, ApJ, 443, 764
Bergeron, P., Leggett, S. K., ApJ, 2002, 580, 1070
Bessel, M. S., Brett, J. M., 1988, Pub. Astron. Soc. Pacific, 100, 1134.
Bessel, M. S., 1990, Pub. Astron. Soc. Pacific, 102, 1181.
Engel, E. A., Doss, N., Harris, G. J., Tennyson, J., 2005, Mon. Not. R. Astron. Soc., SUBMITTED
Fontaine, G., Brassard, P., Bergeron, P., 2001, PASP 113, 409
Gaur, V. P., Tripathi, G. C., Joshi, G. C., Pande, M. C., 1988, Astrophysics & Space Science, 147, 107
Gaur, V. P., Joshi, G. C., Pande, M. C., 1991, Astrophysics & Space Science, 197, 57
Harris, G. J., Lynas-Gray, A. E., Miller, S., Tennyson, J., 2004, ApJ, 600, 1025
Harris, H. C., Dahn, C. C., Vrba, F. J., Henden, A. A., Liebert, J., Schmidt, G. D., Reid, I. N. 1999, ApJ, 524, 1000

Harris, H. C., et al., 2001, ApJ, 549, L109

Gustafsson, B., Bell, R. A., Eriksson, K., Nordlund, Å., 1975, A&A, 42, 407

Iglesias, C. A., Rogers, F. J., Saumon, D., 2002, ApJ, 569, L111

Lenzuni, P., Chernoff, D. F., Salpeter, E. E., 1991, ApJS, 76, 759

Lenzuni, P., Saumon, D., 1992, Rev. Mex. A. A., 23, 223

Luo, G. Q. 1994, A&A, 281, 460

Luo, G. Q. 1997, ApJ, 491, 366

Malo, A., Wesemael, F., Bergeron, P., 1999, ApJ, 517, 901

Saumon, D., Chabrier, G., 1991, Physical Review A, 44, 5122

Saumon, D., Bergeron, B., Lunine, J. I., Hubbard, W. B., Burrows, A., 1994, ApJ, 424, 333

Saumon, D., Chabrier, G., Van Horn, H. M, 1995, ApJS, 99, 713

Rohrmann, R. D., Serenelli, A. M., Althaus, L. G., Benvenuto, O. G., 1991, Mon. Not. R. Astron. Soc., 335, 499

This preprint was prepared with the AAS LaTeX macros v5.2.
Table 1: Color indices for models calculated whilst neglecting HeH$^+$. $\log g = 8$ and $\log_{10}(N_H/N_{He})=10^{-5}$.

| $T_{eff}$ | 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 $\log_{10}(N_H/N_{He})=10^{-5}$.

| $T_{eff}$ | 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|
are used. Neutral species are given solid lines, positively charged species dashed lines, and negatively charged species dotted lines.

Fig. 1.—Chemical and ionization equilibrium as a function of log $\log(N_H/N_{He})$, density, and temperature. Values of temperature of 5000 K, density of 0.2 g cm$^{-3}$, and log $\log(N_H/N_{He}) = -5$ 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 \( \rho = 0 \) and \( \log_{10}(N_{\text{He}}/N_{\text{H}})^{10} = -5 \), calculated at temperatures of 9000, 7000, 5000, 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, with $\log_{10}(N_{\text{He}}/N_{\text{H}}) = -2$. The graph shows the relationship between optical depth ($\tau_R$) and density ($\rho$) for different temperatures (T). The models are labeled with temperatures of 4500 K, 5000 K, 6000 K, 7000 K, and 8000 K, with and without HeH+ in the ionization equilibrium.
Fig. 4.— Spectral energy distributions for models of $T_{\text{eff}} = 4500, 5000,$ and 6000 K. The logarithm of the relative flux is given per unit wavelength interval.