Modelling Alkali Line Absorption and Molecular Bands in Cool DAZs

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**Abstract.** Two peculiar stars showing an apparent extremely broadened and strong Na I D absorption have been discovered in surveys for cool white dwarfs by Oppenheimer et al. (2001) and Harris et al. (SDSS, 2003). We discuss the nature of these objects using PHOENIX atmosphere models for metal-poor brown dwarfs/very low mass stars, and new white dwarf LTE and NLTE models for hydrogen- and helium-dominated atmospheres with metals. These include complete molecular formation in chemical equilibrium and a model for the alkali resonance line broadening based on the damping profiles of Allard et al. (2003), as well as new molecular line opacities for metal hydrides. First results of our calculations indicate good agreement with a hydrogen-dominated WD atmosphere with a Na abundance roughly consistent with a state of high accretion. We analyse deviations of the abundances of Na, K, Mg and Ca from the cosmic pattern and comment on implications of these results for standard accretion scenarios.
1. Introduction

WD2356–209 is an apparent cool white dwarf identified in the high proper motion-survey for halo white dwarf candidates of Oppenheimer et al. (2001), with a spectrum showing very unusual wide and deep absorption at 5000–6000 Å. Its exotic properties have been confirmed by Salim et al. (2004), who found a combination of blue $B-V$ and extremely red $V-I$ colours putting this star far outside of observed and theoretical sequences of both hydrogen-and helium-atmosphere white dwarfs. Meanwhile, another star with a similar spectroscopic and photometric appearance had been identified in Data Release 2 of the Sloan Digital Sky Survey (Harris et al. 2003; Kleinman et al. 2004): SDSS J133001.13+643523.8 (hereafter SDSS J1330+6435), which is also showing high proper motion of $0''.193/yr$. The prominent flux depression in $V$ in these stars has been suggested to be due to a strong and heavily broadened Na I D doublet. Similar features have been observed in the coolest brown dwarfs of spectral type T and identified with the resonance lines of the alkali metals Na and K, broadened by van der Waals interaction with both H$_2$ and He (Tsuji et al. 1999; Burrows et al. 2000). These observations made clear that at line widths of more than some 10 Å the standard impact theory of line broadening, leading to a classical Lorentz profile of the far wings, could no longer adequately reproduce the observed line shapes. More detailed quantum-mechanical calculations of the interaction between alkali atoms and H$_2$ and He perturbers (Burrows & Volobuyev 2003; Allard et al. 2003) have shown that the Lorentzian line profile underestimates the absorption cross section at distances beyond 2–3 FWHM from the line centre, out to $\sim$2000 Å, while at very large detuning it significantly overestimates it. In this paper we are exploring theoretical spectra for a number of different stellar models, using our latest calculations of alkali line profiles, and evaluate their capability to explain the observed features of WD2356–209 and SDSS J1330+6435.

2. Model Atmospheres

We have calculated models using the general stellar atmosphere code PHOENIX v. 13.6 (Hauschildt & Baron 1999). PHOENIX has been continuously developed to model the atmospheres of the coolest stars, brown dwarfs and gas giant planets, incorporating an equation of state (EOS) that treats over 600 molecular species in chemical equilibrium (CE) and includes the formation of liquid and solid condensates (Allard et al. 2001). We are using the unified theory of Allard et al. (2003) to predict the complete spectrum of the resonance lines of the alkali metals Li, Na, K, Rb and Cs from the centre to the extreme wings, however with normal abundance patterns only Na and K are found to have widths beyond some tens of Å, and only for these perturbations due to both neutral He and H$_2$ in two interaction geometries are available at this time. These models have been successfully applied to the highly transparent and dense atmospheres of cool T dwarfs, the only astrophysical objects in which such lines have been observed prior to the two stars that are the topic of this paper (Allard et al. 2003, 2004). The colours of WD2356–209 and the blue spectrum of SDSS J1330+6435 suggest that the $\lambda$4227 Å Ca I line is also an important absorber, but for this earth alkali metal no detailed calculations of the line spectrum are available yet. We
have tried to simulate the broadening of this line by using the Na I data, but multiplying the damping constant with $60^{0.4}$ to account for its non-hydrogenic configuration.

In other respects though, T dwarf spectra disagree very strongly with the observed signatures of WD2356−209 and SDSS J1330+6435: they show equally prominent absorption from the K I λλ 7667,7701 Å resonance doublet as from Na, and they have extremely red optical-to-near IR spectra, with the optical flux almost completely quenched bluewards of the Na I D doublet. Objects this cool could therefore not account for the quite blue $B_V$ colours of WD2356−209. For any brown dwarf or very low mass-star of higher temperature ($T_{\text{eff}} \gtrsim 1400$ K) however the strength of alkali line absorption rapidly decreases, as the atmospheres become more opaque due to strong absorption from molecular bands and condensates. Keeping a strong signature of the resonance lines in atmospheres of higher temperature would require a metallicity significantly below the solar value. The thusly reduced amount of molecules and dust and would increase the transparency of the atmosphere, allowing the atomic lines to form again under conditions of high density and pressure. To explore this possibility we have therefore calculated a grid of dwarf atmosphere models at $T_{\text{eff}}$ up to 3000 K and [Fe/H] down to $-5$. For the main alternative explanation, these stars indeed being white dwarfs with a high abundance of photospheric metals, we computed models with $\log g$ of 7.0 – 8.5 and hydrogen- or helium-dominated atmospheres. For all models the partial pressures of all molecules in the EOS of Allard et al. (2001) have been calculated in full CE, although in the hydrogen-rich WD models chemistry is dominated by only a few hydrogen compounds, and in helium-rich ones of course not many molecules form at all. The models do not include, on the other hand, the effects of a non-ideal EOS that may become important in white dwarfs this cool and dense (cf. also Kowalski, Mazevet & Saumon, this vol.).

3. Comparison with Models

3.1. The Nature of the Dwarf(s)

Figure 1 shows a representative spectrum for an extremely metal-poor model in the L-dwarf temperature range, as might be conceived for a Population III star just above the hydrogen-burning limit. It is immediately apparent that, without the dust opacity dominating normal L-dwarf spectra, the alkali lines can be strong enough to qualitatively explain the observed absorption features. However the line profiles fail to reproduce the observed shapes in detail, and show still too red optical—near-IR colours. We conclude that a low mass-star or brown dwarf-type of model can be excluded for these two stars. This makes the most likely classification of these objects white dwarfs with traces of metal in an either helium- (DZ) or hydrogen-dominated atmosphere (we have denoted the latter as DAZ, in analogy to other hydrogen-rich white dwarfs showing metal absorption lines besides the Balmer series of hydrogen, although due to the extremely low temperatures in this case, Balmer lines would probably not be observable even at the highest resolutions).
3.2. White Dwarf Models

Hydrogen-dominated atmospheres A series of fits to WD2356−209 to hydrogen-LTE atmospheres is presented in Fig. 1b. The strong dependence of the alkali lines on temperature, becoming quickly weaker with increasing $T_{\text{eff}}$, is evident. Test models for solar abundance patterns predicted the formation of stronger molecular bands, chiefly due to MgH and CaH, than are present in the observations. Although the spectrum of WD2356−209 shows an apparent additional opacity source in the blue wing of the Na I doublet, its position does not quite agree with the modelled band, while SDSS J1330+6435 only shows a marginally detectable feature. In addition, CaH bands should be visible around 7000 Å if the elemental Ca abundance were in the same ratio to Na as in the Sun. The models shown here therefore have Na and K abundances set to −1.5 dex relative to solar, and all other metals to −3.5. As can be seen, even at $T_{\text{eff}} < 4000$ K quite high Na abundances are required to reproduce the strength of the D lines. In contrast the K I doublet, which is marginally if at all detectable in the observations, is predicted to be much stronger at that abundance. [K/H] therefore seems to have a lower abundance more similar to the other metals.

Helium-rich models In addition to the degeneracy of solutions with respect to $T_{\text{eff}}$ and metal abundances, the main constituent in the atmosphere is also unknown. The effect of a varying H/He mixture is illustrated in Fig. 2a. We find a slight improvement of the line fit with moderate amounts of helium, e.g. 50–90%. Infrared flux is also more suppressed, due to the stronger $H_2$–He collision induced absorption (CIA), with increasing helium abundance even up to $H/\text{He} = 10^{-12}$. These models thus show rather blue synthetic IR colours of $V-H \lesssim 2.0$, as compared 3.0–3.5 for pure hydrogen models and an observed $V-H = 2.75$ for WD2356−209 (Bergeron et al., this vol.). The best fits seem to be obtained with H/He of order unity. We did not run any completely hydrogen-free models, which should eventually remove the CIA beyond 1 µm. Bergeron et al. report a good fit with such models, although they only use standard Lorentzian broadening for the Na I doublet.
NLTE Effects The line profiles particularly in our pure-hydrogen LTE models appear generally too deep in the near wings out to a few 100 Å, indicating that either the far wing is too weak compared to the core and near wing in our line profiles, or for some reason Na I absorption is overestimated in the upper atmosphere, where the inner parts of the lines form. NLTE effects could contribute to the latter. Departures from LTE are typically observed in white dwarfs of $T_{\text{eff}} \gtrsim 20,000$ K, and might seem unlikely in dwarfs this cool and dim. However, the highly neutral atmosphere of ultracool dwarfs leaves almost no free electrons as the main source of collisional deexcitation and could thus favour NLTE effects. Alkali line absorption under such circumstances has been studied by Barman et al. (2002) for the transit planet HD 209458b. Due to the extreme paucity of free electrons the dominant species, molecular hydrogen, will most likely become the driving force to restore LTE. This effect can not be precisely modelled, since no cross-sections for H$_2$–Na collisions are available yet. Barman et al. have discussed two limiting cases, including only $e^-$ collisions, and including H$_2$ collisions with the same cross-sections as for $e^-$. Theory suggests a much smaller H$_2$ cross-section, scaling with the inverse mass ratio. We have therefore also calculated NLTE models using 4000 and 40,000 times smaller cross-sections for H$_2$. The test models in Fig. 2, with $e^-$ only show very significant deviations from the LTE line shape, but even with the lowest estimate for H$_2$ collisional rates LTE is almost completely restored. NLTE effects are thus probably not the cause of the discrepancies between models and observation.

Limitations of the models Since LTE does seem to hold within the line-forming regions, actual depletion of elemental Na by gravitative diffusion could be another explanation for the missing opacity in the deep line cores. This is not an uncommon effect in white dwarf atmospheres, but a detailed calculation of it is beyond the scope of our current models. We also have to caution, however, that the calculations for the line spectra we used were designed to be used with perturber densities of up to $10^{19}$ cm$^{-3}$, whereas at the higher densities of white dwarf atmospheres the single-perturber approximation breaks down (Allard et al. 2003), leading to an underestimation of the far wing part of the line.
4. Conclusions

With the low resolution and $S/N$ of both observations and the uncertainties of our current models it is not possible to draw strong conclusions about the atmospheric conditions in these white dwarfs. E.g. the presence of hydride bands cannot be clearly established, which would allow a better determination of elemental abundance ratios, and confirm whether hydrogen is an important constituent of the atmosphere. The quite high Sodium abundance required in the DAZ scenario, which might be beyond what interstellar accretion could provide, is an obvious argument against such models. The apparent overabundance of Na relative to Ca, and perhaps also Mg and K, also disagrees with selective dust-accretion models, which predict rather lower abundances of the volatile Alkalis (Zuckerman et al. 2003). However, DZ models would face the same irregular abundance patterns, except that hydride bands are not expected. Also the problem of avoiding the accretion of hydrogen from the ISM is still unresolved. With the current knowledge, a model with He/H ratio of order unity might best reconcile both observed features and the problems with the extremely short diffusion timescales of pure hydrogen atmospheres.

Observations that could resolve molecular bands, and possibly lines from higher excitation and ionisation levels for better constraints on temperature, would be of great help in deciding between these different interpretations. New theoretical work on the behaviour of atomic lines at very high perturber densities should also both benefit from and aid in the study of these unusual white dwarfs.

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