A COMPARISON OF LABORATORY SPECTRA WITH A NEW THEORETICAL STUDY OF POTASSIUM RESONANCE LINES PERTURBED BY HELIUM

J.F. Kielkopf1, N.F. Allard2,3 and J. Babb4

Abstract. The optical spectra of L- and T-type dwarfs exhibit a continuum dominated by the far wings of the absorption profiles of the Na 3s-3p and K 4s-4p doublets perturbed by molecular hydrogen and helium. We examine the K resonance line wing and core with a unified line profile theory and compare to laboratory experiments and observations of the cool brown dwarf $\epsilon$ Indi Ba,b.

1 Introduction

As shown in the work of Allard et al. (2007a), the temperature of the H$_2$–He atmosphere of cool brown dwarf stars is so low that elements other than the two abundant alkalis, Na and K, have condensed and precipitated out. The resonance lines of both Na and K are optically thick, and the wings of the lines determine the observed visible and near-infrared spectrum. The construction of model atmospheres and synthetic spectra for cool brown dwarfs and extrasolar giant planets is necessary to derive reliable atmospheric parameters and the surface chemical composition for these objects. Conventional laboratory absorption spectroscopy can be used to examine the line wings and test the line shape theories and molecular potentials. We report calculations based on the potential energy surfaces of the K–H$_2$ and K–He systems that predict line satellites that are observed in both laboratory and stellar spectra. This establishes the accuracy of the interaction potentials, which are difficult to compute a priori. Moreover the laboratory results also confirm the identification of a brown dwarf spectral feature previously interpreted as CaH absorption bands as due to line satellites of potassium perturbed by H$_2$ and He.

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Fig. 1. Potential curves for the $B^2\Sigma$, $A^2\Pi$ and $X^2\Sigma$ states of the K-He molecule of P83 (dashed curves) compared to SK05 (full line).

Fig. 2. Theoretical absorption K-He collisional profiles. The dashed line indicates the profile using P83 potentials compared to SK05 (full line). ($T = 1000$ K, $n_{\text{He}} = 1 \times 10^{19}$ cm$^{-3}$.)

2 Potentials and line shapes

In previous work, molecular potentials for K–H$_2$ were computed using a valence pseudopotential with Gaussian orbitals on potassium for an H$_2$ molecule assumed
to be in its ground state. The potentials were input data for a unified spectral line shape evaluation of the complete K resonance line profiles (Allard et al. 1999, 2007b). When included in the stellar atmosphere program PHOENIX, the profiles predicted a K–H\textsubscript{2} absorption feature at 6950 Å nearly matching the position of the observed feature (Allard et al. 2007a). Although the theoretical satellite did not extend enough to the red to reproduce the shape of the observed feature, we have found that there is an additional contribution from K–He opacity that improves the agreement. The K-He potentials of Pascale (1983) (P83) and Santra et al. (2005), Zhu et al. (2006) (SK05) are shown in Figure 1. We have computed profiles using these potentials and the same semiclassical unified theory. Table 1

Table 1. Half-widths at half maximum ($10^{-20} \text{ cm}^{-1}/\text{cm}^{-3}$) of K resonance lines perturbed by He.

<table>
<thead>
<tr>
<th>Transition</th>
<th>Potential</th>
<th>400 K</th>
<th>500 K</th>
<th>1000 K</th>
<th>2000 K</th>
<th>3000 K</th>
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<tr>
<td>$4s^2S_{1/2}-4p^2P_{1/2}$</td>
<td>P83</td>
<td>0.94</td>
<td>1.22</td>
<td>1.62</td>
<td>1.9</td>
<td></td>
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<tr>
<td></td>
<td>SK05</td>
<td>1.00</td>
<td>1.26</td>
<td>1.57</td>
<td>1.84</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CC</td>
<td>0.99</td>
<td>1.35</td>
<td>1.9</td>
<td>2.37</td>
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<tr>
<td></td>
<td>EXP</td>
<td>0.823</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$4s^2S_{1/2}-4p^2P_{3/2}$</td>
<td>P83</td>
<td>1.52</td>
<td>2.03</td>
<td>2.69</td>
<td>3.07</td>
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<tr>
<td></td>
<td>SK05</td>
<td>1.47</td>
<td>1.97</td>
<td>2.52</td>
<td>3.04</td>
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<tr>
<td></td>
<td>CC</td>
<td>1.37</td>
<td>1.86</td>
<td>2.46</td>
<td>2.95</td>
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<tr>
<td></td>
<td>vDW</td>
<td>1.12</td>
<td>1.38</td>
<td>1.70</td>
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<tr>
<td></td>
<td>EXP</td>
<td>1.09</td>
<td></td>
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</table>

Fig. 3. Satellites due to H\textsubscript{2} and He predicted by theoretical absorption coefficients are seen in $\epsilon$Indi Ba and laboratory measurements.
compares the width of the doublet components in a close coupling calculation by Mullamphy et al. (2007) (CC), a conventional van der Waals potential, and the well-regarded experimental measurement at 400 K by Lwin (1978). Laboratory measurements for the wing are shown in Figure 3. Together, these results point to a need to explore both experimentally and theoretically the transition from the line core to the far wing, and the discrepant broadening in the two components of the doublet.

References

Santra, R., & Kirby, K., 2005, J. Chem. Phys., 123, 214309