New line profiles of potassium perturbed by molecular hydrogen for very cool brown dwarfs

N.F. Allard [1,2], D. Homeier [3,4]
F. Spiegelman [5] and J.F. Kielkopf [6]

[1] Observatoire de Paris GEPI, UMR 8111, CNRS, 61, Avenue de l'Observatoire, F-75014 Paris, France
[2] Institut d'Astrophysique de Paris, UMR 7095, CNRS, Université Pierre et Marie Curie, 98^{bis} Boulevard Arago, F-75014 Paris, France
[3] ZAH/Landessternwarte, Königstuhl 12, 69117 Heidelberg, Germany
[4] CRAL, ENS de Lyon, UMR CNRS 5574, 46 allée d'Italie, 69363 Lyon cedex 07, France
[5] Laboratoire de Physique Quantique, UMR5626, CNRS, Université Paul Sabatier, 118 route de Narbonne, F-31400 Toulouse, France
[6] Department of Physics and Astronomy, University of Louisville, Louisville, Kentucky 40292 USA

Abstract

In this poster, we evaluate K-H_2 collisional profiles for temperatures and densities appropriate for modeling very cool brown dwarf atmospheres. Laboratory measurements are used to validate new *ab initio* molecular potentials which support the spectral line profile theory.

We also report the dependence of line parameters on temperature, and compare with previous calculations obtained from pseudo-potentials.

Density profiles

Figure 1 displays a plot of the perturber densities as a function of Rosseland optical depth for 5 atmosphere models: an early and a mid-T type brown dwarf corresponding to the two members of the ϵ Indi B system shown in Fig. 2, a late T, and early Y brown dwarf and an extreme low-mass Y dwarf or typical old, Jupiter-mass planet (in order of decreasing effective temperature).

With such extremely cool objects, the near IR and optical flux is emitted from very deep layers. The spectrum of the flux peak around 1-1.1 μm in these objects is formed at typical Rosseland optical depths $\tau_{\rm Ross}$ of 20-200. Because of the depletion of alkali metals in atmospheric regions cooler than ~ 800 K, the line formation region shifts to the deepest observable layers of the photosphere in the coolest brown dwarfs and in massive gas giants, where molecular hydrogen number density far exceeds $10^{19}\,{\rm cm}^{-3}$.

Unified theory is needed to model collisional broadening at such extreme densities. The line profiles covering that domain of densities and temperatures are shown in Figs 3-5.

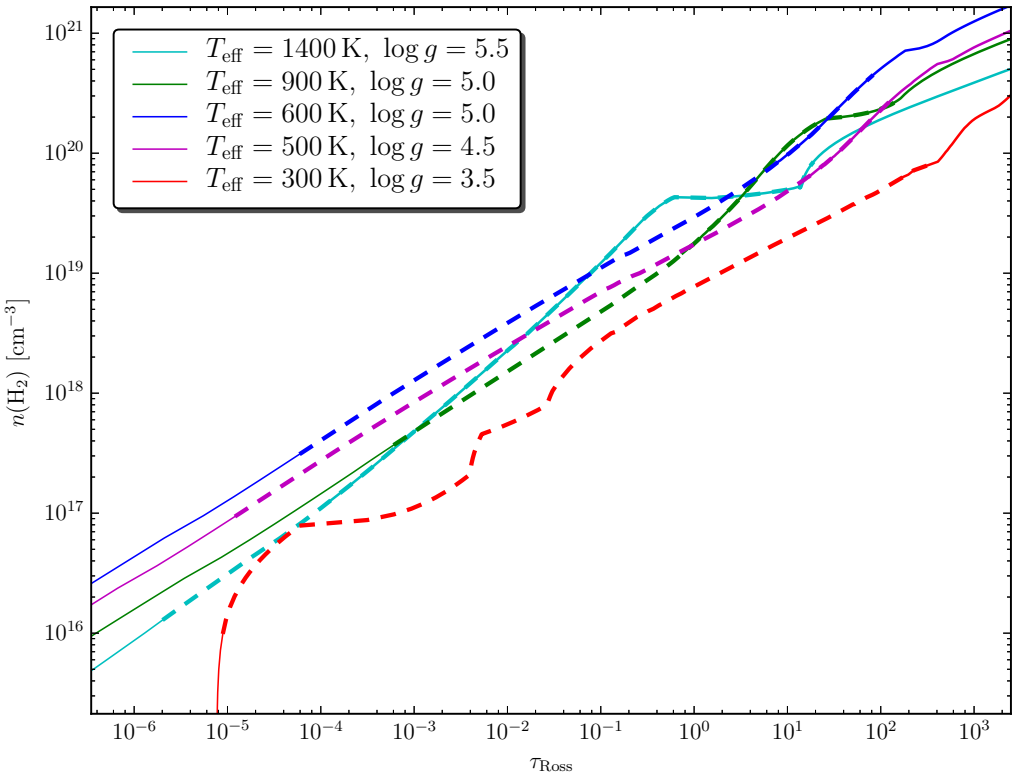

Figure 1
Number density of molecular hydrogen for 5 models of brown dwarf and planetary atmospheres.
The ranges where the optical and near infrared spectra form are indicated by thick dashes, extending to very deep layers in the coolest objects. The thicker solid lines show the region where potassium is left in the gas phase, while the thin lines indicate where it is depleted higher up in the atmosphere due to the condensation effects discussed in Fig. 2.

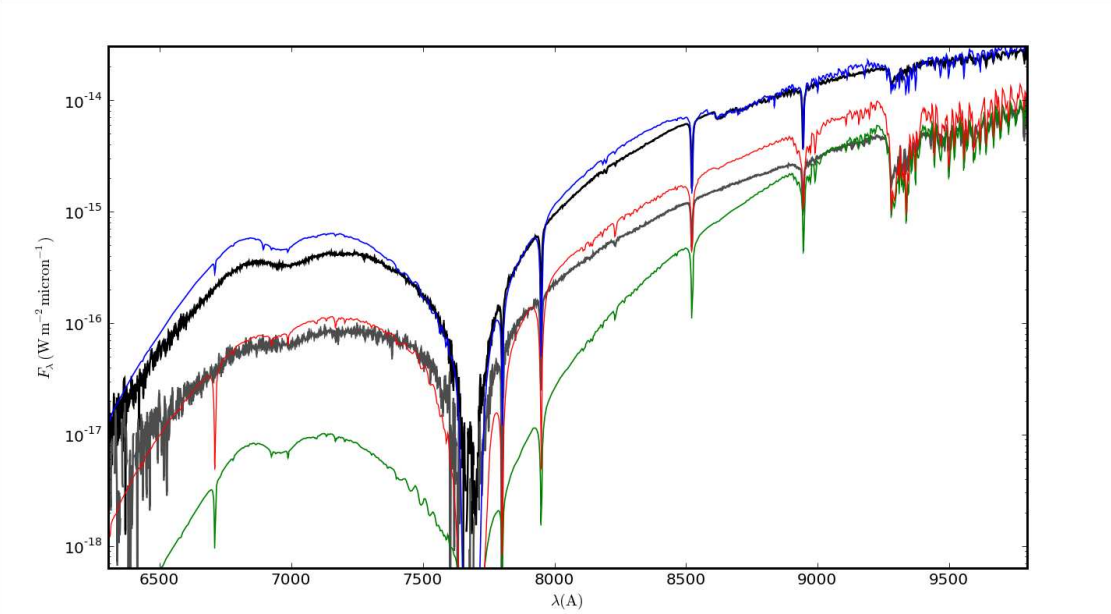

Figure 2
Observed spectra of the T1+T6 binary ϵ Indi B (King et al. 2010) compared to synthetic spectra. The potassium line dominates the red optical spectra well into the IR (Y band). In the T6 dwarf ϵ Indi Bb (lower spectrum) the alkali metals show the effects of depletion into low-temperature condensates (Homeier et al. 2007), starting with the formation of Na_2S and later NaCl and KCl, which removes most of the sodium and also potassium from the upper atmosphere (red model). Without this effect, the absorption in the line core would be far stronger (green model).

Line profile

The theory of spectral line shapes, especially the unified approach we have developed, makes possible accurate models of stellar spectra that account both for the centers of spectral lines and their extreme wings in one consistent treatment. Complete details and the derivation of the theory are given by Allard et al (1999).

Blue satellite bands in alkali-He/H_2 profiles are correlated with maxima in the excited B state potentials and can be predicted from the maxima in the difference potentials ΔV for the B-X transition.

Details on the properties of the K-H_2 quasi-molecular line satellite have been reported in Allard et al (2003) and Allard et al (2007a). *Ab initio* calculations of the potentials of K–H_2 reported in Allard et al (2007a) allowed a better agreement with the observations. The main difference between our previous work reported in Allard et al (2003) was to predict a K–H_2 quasi-molecular line satellite closely matching the position and shape of an observed feature in the spectrum of the T1 dwarf ε Indi Ba (Allard et al (2007b)).

Density dependence

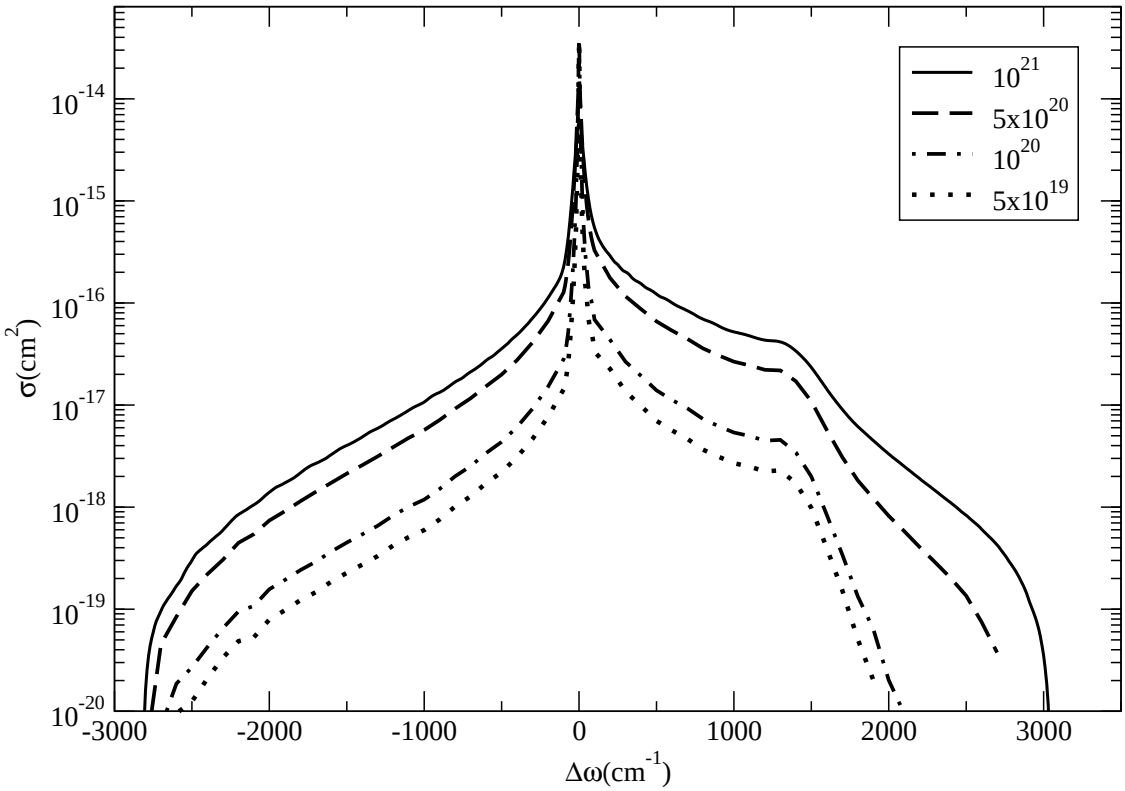

Figure 3
Evolution of the unified profiles with increasing helium density from
$n_{\mathrm{He}} = 5\times\ 10^{19}$ to 10^{21} cm^{-3}.

The density effect on the shape of the blue wing is very significant when the H_2 density gets larger than 10^{20} cm^{-3}. Because of multiple perturber effects we can notice in Fig. 3 a first line satellite at 1300 cm^{-1} and a second one due to K-$(H_2)_2$ which appears as a shoulder about 2700 cm^{-1} from line center.

Temperature dependence

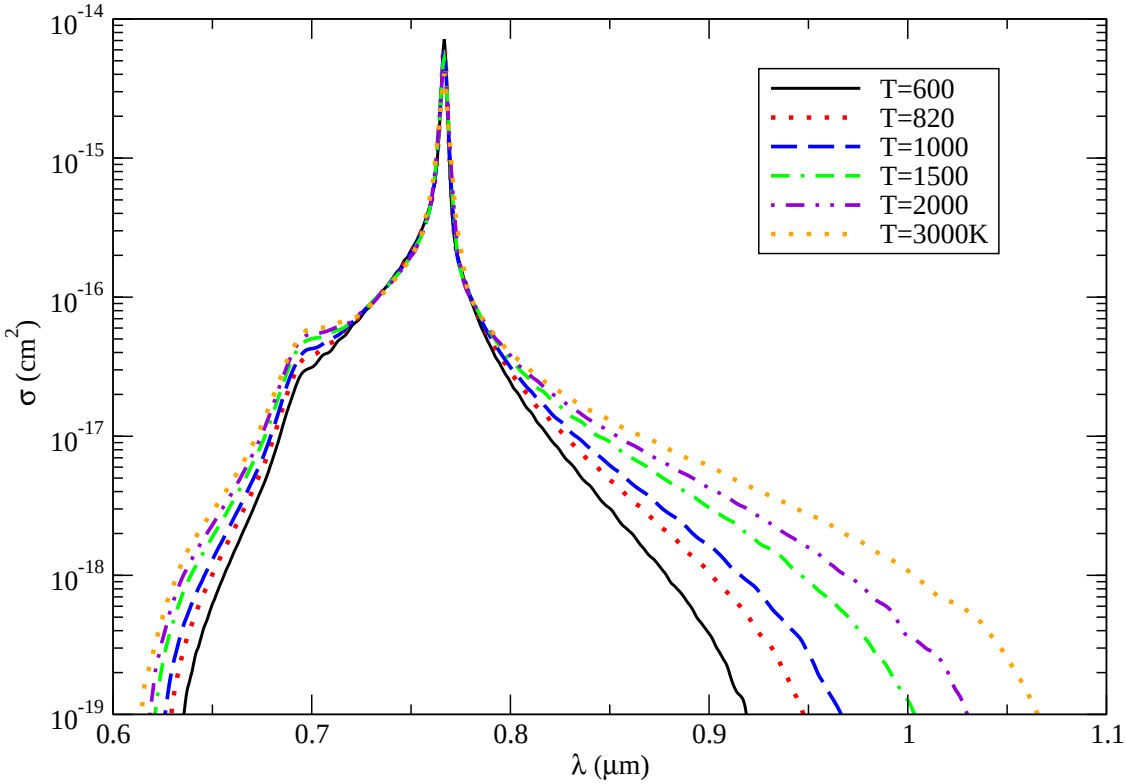

Figure 4
Variation with temperature of the $D2$ component of the K I resonance doublet perturbed by H_2. The density of perturbers is n_{H_2}=10^{21} cm^{-3}.

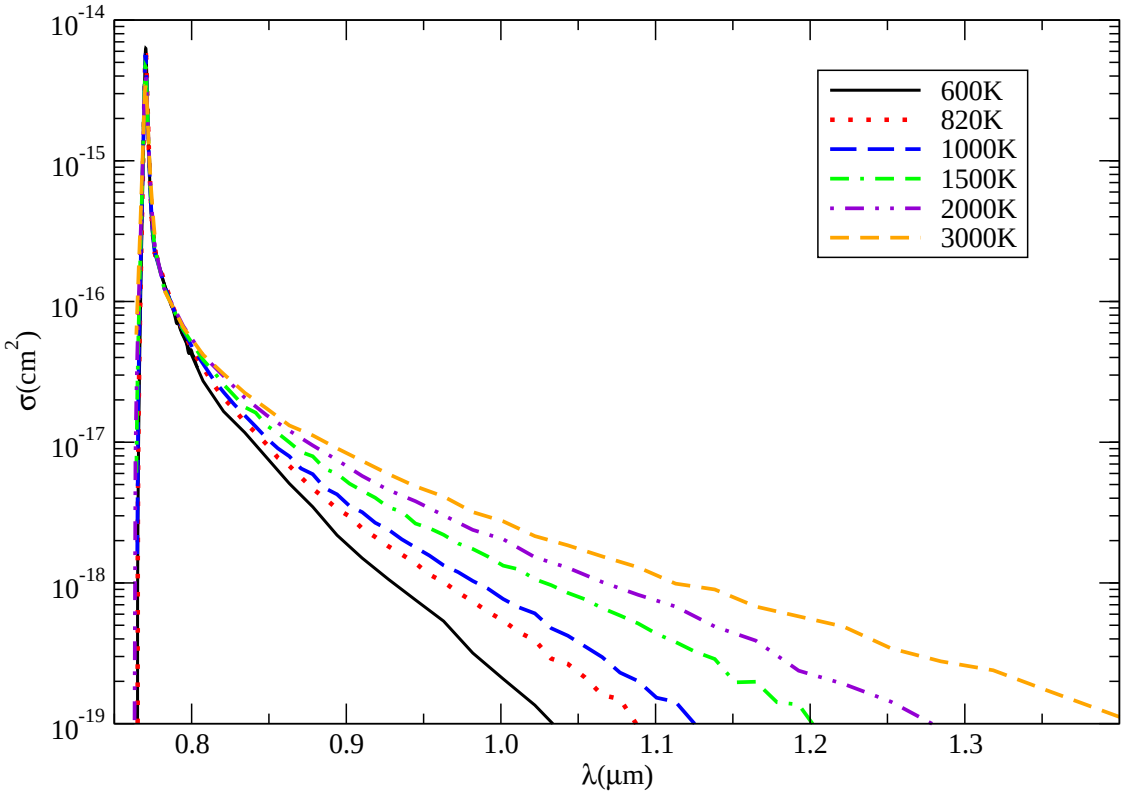

Figure 5
Variation with temperature of the $D1$ component of the K I resonance doublet perturbed by H_2. The density of perturbers is n_{H_2}=10^{21} cm^{-3}.

Laboratory spectra

The broadening produced by H_2 in brown dwarf atmospheres at an effective temperature of about 1000 K can be effectively studied with laboratory absorption spectroscopy. We measured the absorption coefficient of the $D2$ component at a spectral resolution of approximately 20 cm^{-1} from the line center into the regime of the K_2 molecular bands. We also measured broadening by rare gases, and used those spectra to remove the common K_2 absorption in the regions of interest [6, 8].

Figure 6 shows an exceptionally good match between the experimental spectrum and the model from the unified line shape theory with the new potentials. While laboratory conditions cannot fully duplicate those in brown dwarf or stellar atmospheres, test comparisons such this confirm the validity of the potentials and the accuracy of the line shape theory.

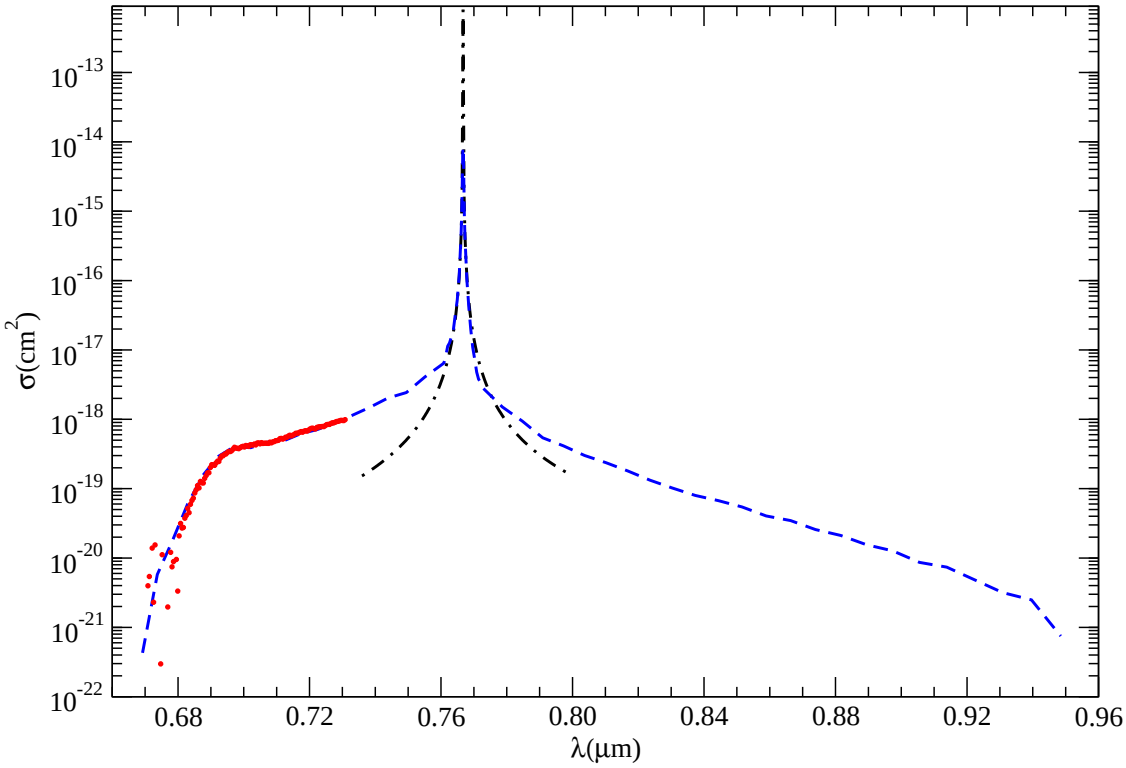

Figure 6
Comparison of the theoretical profile (dashed blue line) of the $D2$ component with the experimental absorption profile (dotted red line). Corresponding Lorentzian profile is overplotted (dashed dotted black line). The density of perturbers is n_{H_2}=10^{19} cm^{-3}, T=820 K.

Spectral line parameters

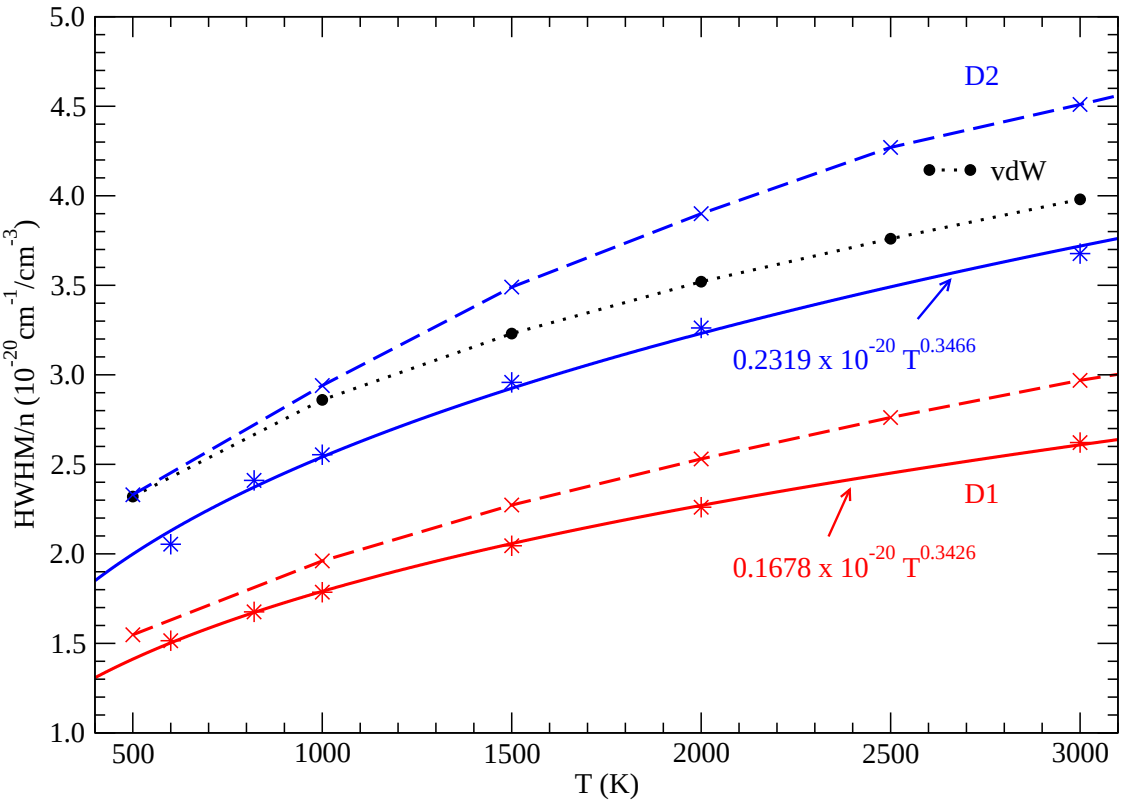

Figure 7
Variation with temperature of the half-width of the $D2$ (blue curves) and $D1$ (red curves) lines of K I perturbed by H_2 collisions.
We compare the results obtained using new *ab initio* potentials (full line) and pseudo-potentials of Rossi and Pascale (1985) (dashed lines) reported in Allard et al (2007c), van der Waals potential (black dotted lines).

References

1. N.F. Allard, A. Royer, J.F. Kielkopf, N. Feautrier, The effect of the variation of electric dipole moments on the shape of pressure broadened atomic spectral lines, Phys. Rev. A. **60**, 1021-1033 (1999)

2. Allard, N. F., Allard, F., Hauschildt, P. H., Kielkopf, J. F., & Machin, L. 2003, A&A, 411, 473

3. Allard, N. F., Spiegelman, F., & Kielkopf, J. F., A&A, 465, 1085 (2007a)

4. F. Allard, N. F. Allard, D. Homeier, J. Kielkopf, M. J. McCaughrean, and F. Spiegelman, 2007b. K-H_2 quasi-molecular absorption detected in the T-dwarf ϵIndi Ba . A&A 474, L21-L24

5. Allard, N. F., Kielkopf, J. F., & Allard, F. 2007c European Physical Journal D, 44, 507

6. N. F. Allard, F. Spiegelman, J. F. Kielkopf, G. Tinetti and J. P. Beaulieu 2012. Theoretical and laboratory spectra of sodium perturbed by molecular hydrogen. A&A, 543, A159

7. D. Homeier, N. F. Allard and F. Allard 2007, AIPS Conf. Series 938, 170

8. J. F. Kielkopf and N. F. Allard, Resonance line wings of Na and K broadened by He and other rare gases, in preparation (2015).

9. R. R. King, M. J. McCaughrean, D. Homeier, F. Allard, R.-D. Scholz and N. Lodieu 2010, ϵIndi Ba, Bb: a detailed study of the nearest brown dwarfs. A&A 510, A99

10. F. Rossi and J. Pascale, Pseudopotential molecular-structure calculations for alklali-metal-atom–H_2 systems, Phys. Rev. A **32**, 2657 (1985)