IOP Conf. Series: Journal of Physics: Conf. Series **810** (2017) 012023 doi:10.1088/1742-6596/810/1/012023

Blue line wings of resonance lines of potassium and sodium perturbed by molecular hydrogen and rare gases

J F Kielkopf [1], N F Allard [2,3], V A Alekseev [4], F Spiegelman [5], G Guillon [6] and H Berriche [7,8]

[1] University of Louisville, Louisville, Kentucky 40292 USA [2] Observatoire de Paris GEPI, F-75014 Paris, France [3] Institut d'Astrophysique de Paris, Université Pierre et Marie Curie, F-75014 Paris, France [4] St.Petersburg State University, St. Petersburg 199034, Russia [5] Laboratoire de Physique Quantique, Université Paul Sabatier, F-31400 Toulouse, France [6] Université de Bourgogne, 21078 Dijon Cedex, France [7] Faculty of Science, University of Monastir, Monastir, Tunisia [8] American University of Ras Al Khaimah, Ras Al Khaimah, UAE

E-mail: [1] john.kielkopf@louisville.edu [2] nicole.allard@obspm.fr

Abstract. We report on work in progress that compares unified line shape calculations based on *a priori* potentials with experiments to determine the wings of the sodium and potassium resonance lines broadened by H_2, He, and other rare gases.

1. Line profiles in an astrophysical context

The spectra of ultra-cool brown dwarf stars, such as the type T1 ϵ Indi Bab, and inflated hot-Jupiter exoplanets such as HD209458b, show absorption due to neutral Na and K. The strength and shape of these resonance lines is diagnostic of their atmospheric conditions, chemistry, and history. In the coolest and densest of such atmospheres, radiative transfer in the visible and near-IR spectrum may be dominated by far wings of the lines broadened by collisions with neutral H_2 and He. Similarly, DZ class white dwarfs are low temperature Earth-sized degenerate stars of solar mass lacking atomic H lines but showing heavier elements. Detected through recent observations with the Spitzer and Hubble Space Telescopes, these surprising key spectral signatures are attributed to accreted material and inform us about the star's planetary environment when accurate pressure broadened profiles are incorporated into spectral models. The theory of spectral line shapes, especially the unified approach we have developed and refined, makes possible models of stellar spectra that account for the centers of spectral lines and their extreme wings in one consistent treatment. Complete details and the derivation of the theory are given elsewhere. [1]

2. *Ab initio* molecular potentials

Our unified approach to calculating the spectral line profile requires molecular potentials of high accuracy because the shift and shape of the line are very sensitive to the details of the molecular potential curves. New calculations of the potentials of Na/K-H_2 by F. Spiegelman have been

reported by Allard et al [2, 3]. We also use here Na-He potentials of Dell'Angelo et al [4], K-He potentials of Santra & Kirby [5], and *ab initio* Na/K-Ar, Ne, Kr, and Xe of V. Alekseev computed using MOLCAS 7.6 [6]. These potential curves are shown in Fig. 1 and 2.

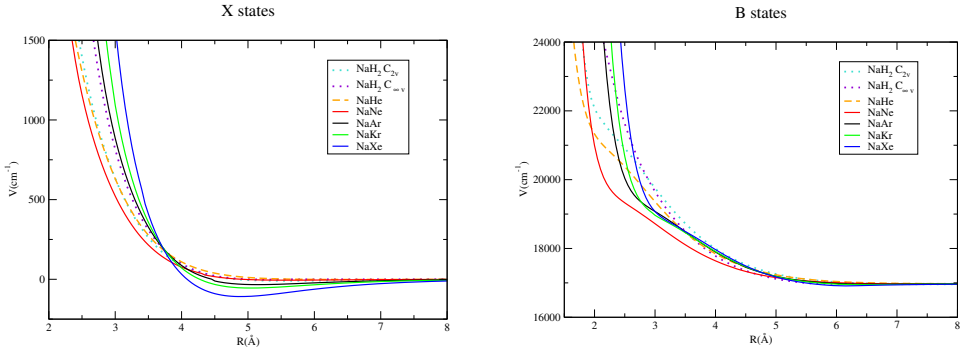

Figure 1. Potential curves for the X and B states of the Na-H_2/rare gas molecules.

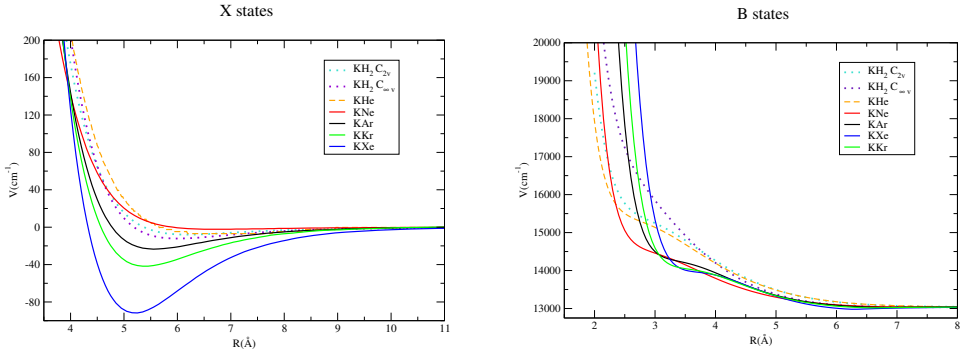

Figure 2. Potential curves for the X and B states of the K-H_2/rare gas molecules.

3. Laboratory spectra and comparisons to line shape theory

The laboratory spectra of both Na and K alkalis with H_2, He, and other rare gases are found to exhibit a systematic pattern of satellites in the blue wings shown in Fig. 3. [7] While Xe and Kr produce the strongest satellites that are closest to the parent line, H_2 and He produce weakly absorbing satellites farthest from the line. In that region the atomic wings of interest overlap alkali dimer absorption. When we use the far wings of Na and K broadened by Kr as a reference, the dimer contribution can be measured in those spectra and removed from the experimental absorption coefficient for the other gases.

Figure 3 shows an exceptionally good match between the K-H_2 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 as this confirm the validity of the potentials and the accuracy of the line shape theory. We have compared the line satellite positions for H_2, He and other rare gases in order to assess the accuracy of the potentials and ultimately to guide refinement of their computation. [8, 9, 10] The general properties of the full line profiles predicted by the unified line shape theory are confirmed by these comparisons, even where the specifics of the satellite positions set by the details of the potentials may differ between theory and experiment, especially for perturbers with many electrons.

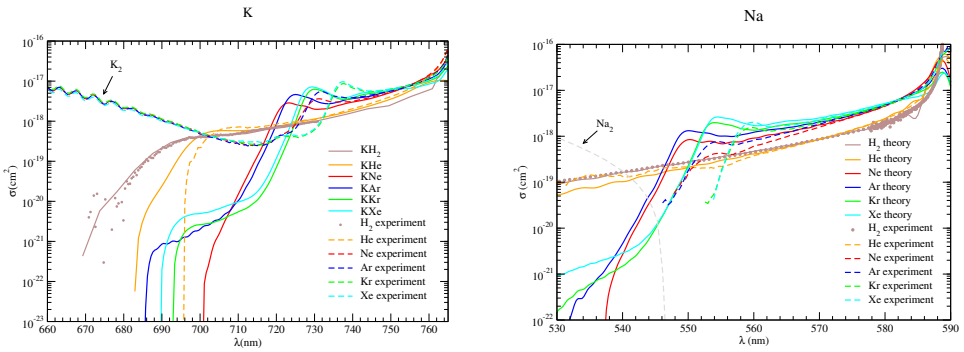

Figure 3. Comparison of the theoretical blue line wings of the resonance line of Na and K (full lines) with the experimental spectra (dashed lines). The density of perturbers is 10^{19} cm^{-3} at 800 K. The experimental spectra have been corrected for dimer absorption.

Pseudopotentials for K-Ar recently computed by H. Berriche improve on the earlier calculations of Li/Na/K-Ar by El Hadj Rhouma *et al* [11], and a comparison with the *ab initio* potentials is shown in Fig. 4. The new K-Ar pseudopotentials lead to a better agreement with the experimental position of the blue satellite.

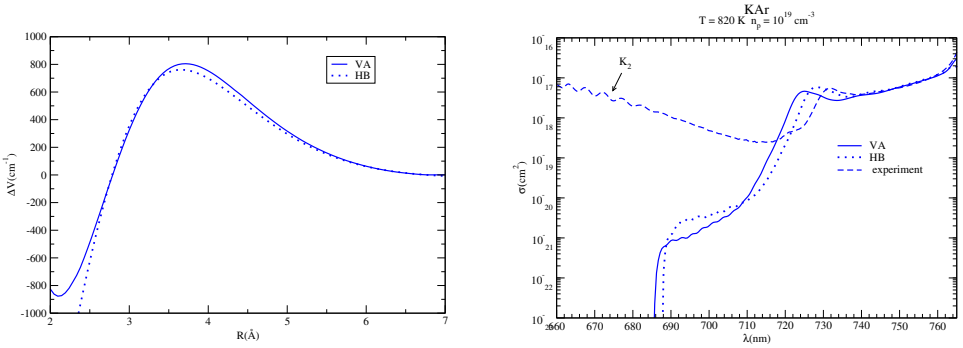

Figure 4. Comparison of difference potentials ΔV for the B-X transitions (left) and the experimental and theoretical blue line wings (right) of the resonance line of K-Ar based on *Ab initio* potentials of V. Alekseev (VA) and pseudopotentials of H. Berriche (HB).

References

[1] N.F. Allard, A. Royer, J.F. Kielkopf, N. Feautrier, Phys. Rev. A. **60**, 1021-1033 (1999)
[2] N. F. Allard, F. Spiegelman, J. F. Kielkopf, G. Tinetti and J. P. Beaulieu, A&A, 543, A159 (2012)
[3] N. F. Allard, F. Spiegelman and J. F. Kielkopf, A&A, 589, A21 (2016)
[4] D. Dell'Angelo, G. Guillon and A. Viel, J. Chem. Phys., 136, 114308 (2012)
[5] R. Santra and K. Kirby, J. Chem. Phys., 123, 214309 (2005)
[6] F. Aquilante, et al., MOLCAS 7: the next generation, Journal of Computational Chemistry, **31**, 224-247, (2010).
[7] J. F. Kielkopf and N. Allard, in preparation (2016).
[8] Allard, N. F., Allard, F., Hauschildt, P. H., Kielkopf, J. F., & Machin, L. 2003, A&A, 411, 473
[9] Allard, N. F., Spiegelman, F., & Kielkopf, J. F., A&A, 465, 1085 (2007)
[10] F. Allard, N. F. Allard, D. Homeier, J. Kielkopf, M. J. McCaughrean, and F. Spiegelman, K-H_2 quasi-molecular absorption detected in the T-dwarf ϵ Indi Ba . A&A 474, L21-L24 (2007)
[11] M.B. El Hadj Rhouma, H. Berriche, Z.B. Lakhdar and F. Spiegelman, J. Chem. Phys., **116**, 1839 (2002)