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COLLISIONAL LINE PROFILES OF SODIUM PERTURBED BY H_2 FROM THE OPTICAL TO THE INFRARED SPECTRAL RANGE

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Abstract. Our aim is to present new unified line profiles of sodium perturbed by H_2 from the optical to the infrared spectral range. We compare the specific results obtained for the 3s-3p transition to laboratory spectra.

1 Introduction

In Allard *et al.* (2003) and Tinetti *et al.* (2007) we presented the first applications of semi-classical profiles of sodium and potassium perturbed by molecular hydrogen to the modeling of brown dwarfs and extra-solar planets. The resonance line profiles were calculated using the Rossi & Pascale (1985) pseudo-potentials (hereafter labeled RP85). We now extend this work to excited states. Na–H_2 *ab initio* potentials (hereafter labeled S11) were recently computed allowing a more accurate determination of the far wings. Preliminary results for the 3s-3p transition are reported and compared to laboratory spectra.

2 Theoretical spectra

A unified treatment of the shape of a pressure-broadened alkali absorption line from near resonance to the far wing is obtained using autocorrelation formalism. Complete details and the derivation of the theory are given by Allard *et al.* (1999).

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Table 1. Half-width (10^{-20} cm^{-1}/cm^{-3}) of Na 3s-3p and 3p-4s lines.

Transitions	500 K	650 K	1000 K	1500 K	2000 K	3000 K
3s $^2S_{1/2}$-3p $^2P_{1/2}$	1.46	1.6	1.86	2.16	2.42	2.8
3s $^2S_{1/2}$-3p $^2P_{3/2}$	1.96	2.16	2.49	2.94	3.24	3.87
3p $^2P_{1/2}$-4s $^2S_{1/2}$	4.43	5.07	5.71	6.67	7.87	8.89
3p $^2P_{3/2}$-4s $^2S_{1/2}$	4.34	5.43	5.58	7.17	7.6	9.35

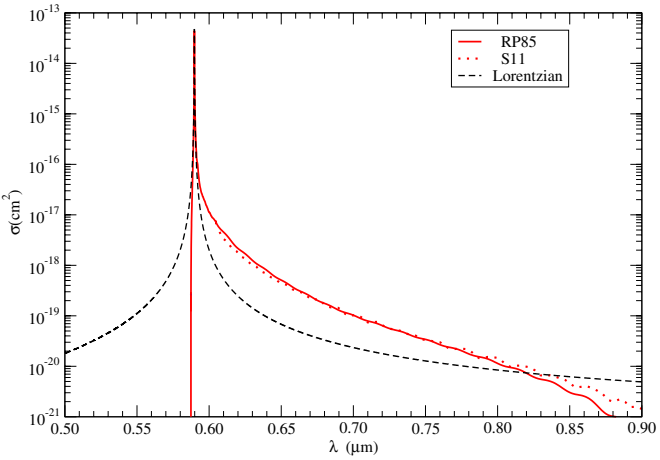

Fig. 1. Absorption cross sections of the 3s-3p D1 line component of NaH_2, taking into account the two symmetries C_{2v} and $C_{\infty v}$ using RP85 (full line) compared to S11 (dotted lines) compared to the corresponding Lorentzian profile. The density of perturbers is $n_{H_2} = 10^{20}$ cm^{-3}. The temperature is 1000 K.

This treatment includes the finite duration of collision. It is well known that the impact approximation, which assumes that collisions occur instantaneously, causes the Lorentz theory to fail not too far from the line center. Consequently, it is not correct to use Lorentzian profiles in the far wings, as is the standard practice for most stellar atmosphere work (Désert *et al.* 2008). Figures 1 and 2 emphasize the non-Lorentzian behavior of the two components of the Na–H_2 resonance line. Figure 9 of Allard *et al.* (2007) presents the potential energy surfaces of Na-H_2 with spin-orbit coupling in the C_{2v} and $C_{\infty v}$ symmetries. We present in Figure 3 the absorption cross section of the resonance line of Na compared to those of the first excited states. The Lorentzian profiles are calculated using the line widths presented in Table 1. Calculations have been done for the $D1$ and $D2$ lines

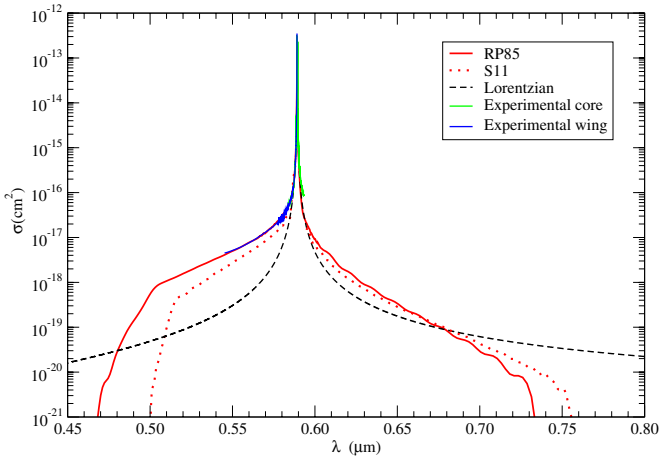

Fig. 2. Absorption cross sections of the 3s-3p D2 line component of NaH_2, taking into account the two symmetries C_{2v} and $C_{\infty v}$ using RP85 (full line) compared to S11 (dotted lines) compared to the corresponding Lorentzian profile. The density of perturbers is $n_{H_2} = 10^{20}$ cm^{-3}, the temperature is 1000 K.

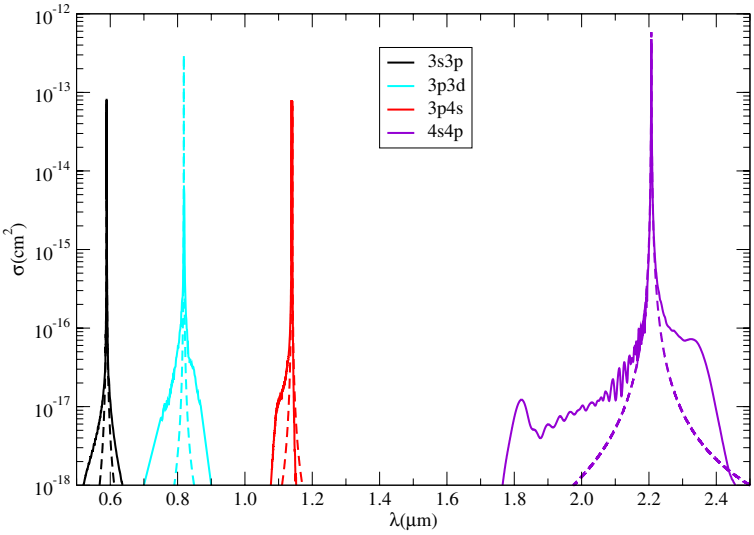

Fig. 3. Absorption cross section of the 3s-3p, 3p-3d, 3p-4s, 4s-4p lines (from the left to the right) Dashed curves represent the corresponding Lorentzians. (T = 1000 K, $n_{H_2} = 1 \times 10^{19}$ cm^{-3}).

from $T_{\rm eff}$ = 500 K to 3000 K with a step size of 500 K. Opacity tables of alkalies perturbed by He and H_2 can be obtained from an on-line database[1].

[1] http://mygepi.obspm.fr/~allard/

3 Far wing and quasi-molecular satellite of the 3s-3p transition

The line shape theory requires accurate atomic potentials and transition moments. Blue satellite bands in alkali-He/H_2 profiles can be predicted from the maxima in the difference potentials ΔV for the B-X transition. In calculations of Rossi & Pascale (1985), the alkali-H_2 complex was considered as a system with a single active electron. In Allard *et al.* (2012) we describe the new S11 calculations of the Na–H_2 potential energy surfaces in which the two electrons of H_2 and the valence electron of Na are explicitly treated. The major difference is that RP85 potentials are systematically less repulsive than those in S11. This difference affects the blue satellite position shown in Figure 2. The experimental absorption coefficients in Figure 2 have been scaled for comparison to the theoretical cross sections. On the blue side, the observed NaH_2 wing matches the profile from the RP85 potential. In this region the unified theory and experiment are approximately 100× a Lorentzian extrapolation of the line core.

References

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

Allard, N.F., Kielkopf, J.F., & Allard, F., 2007, EPJ D, 44, 507

Allard, N.F., Royer, A., Kielkopf, J.F., & Feautrier, N., 1999, Phys. Rev. A, 60, 1021

Allard, N.F., Spiegelman, F., Kielkopf, J.F., Tinetti, G., & Beaulieu, J.P., 2012, A&A, 543, A159

Désert, J.-M., Vidal-Madjar, A., Lecavelier Des Etangs, A., *et al.*, 2008, A&A, 492, 585

Rossi, F., & Pascale, J., 1985, Phys. Rev. A, 32, 2657

Tinetti, G., Vidal-Madjar, A., Liang, M.-C., *et al.*, 2007, Nature, 448, 169