Comparative Study of Emission Spectra of He(3S)-He(2P) at 706 and 728 nm Due to the Triplet and Singlet Transitions.

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Abstract. This study of the self-broadening of the 728 nm He line is performed in order to establish similarities and differences to the self-broadening of the triplet 3s-2p line at 706 nm. In a previous work we presented the first calculations of He-He collisional profiles at 706 nm due to the triplet 3s-2p transition in a unified line shape semi-classical theory using ab-initio molecular potentials. The excellent agreement between experimental and theoretical determinations of the near wing of the line profiles established the accuracy of the interaction potentials. New ab-initio potentials for the singlet 3s-2p transitions allow us to extend our previous study to the line at 728 nm.

1. Potentials
The interatomic interactions are the main physical quantities needed for a good understanding of collisional processes. The ab initio computation of the adiabatic potential energy curves of He\textsubscript{2} have been carried out using the MOLPRO 2009 package \textsuperscript{1}. A huge MultiReference Configuration Interaction (MRCI) has been performed starting from a very large Multi Configuration Self Consistent Field (MCSCF). The accuracy of the approach is below the wavenumber compared to full CI approaches \cite{1}, as we have checked for the quintet states. Moreover errors due to BSSE are also far below the wavenumber thanks to the huge basis set involved. Therefore an accuracy about the wavenumber is expected. However, non adiabatic and relativistic corrections have been ignored. The ab initio energy curves for the He\textsubscript{2} line at 728 nm are shown in figure 1. They are input data for a unified spectral line shape evaluation of the complete He-He collisional line profiles \cite{2}.

2. Line profile
In radiative collision transitions it is the difference potential \(\Delta V\) between the final and initial states that determines the frequency and the energy emitted or absorbed by a single photon.

\textsuperscript{1} http://www.molpro.net
The difference potential maxima (figures 2 and 3) lead to blue satellite bands in proximity to the atomic lines. Figure 4 shows the asymmetrical shape of the singlet and triplet lines in agreement with experimental spectra reported in [3, 4]. The blue asymmetry is due to a blend of four quasi-molecular satellites. Because of the blending, the line profile can be accurately described only with a unified spectral line shape theory that is valid from the center to the far wing.

The emission spectrum produced at 300 K in dense plasmas of helium excited by a corona discharge shows an asymmetric atomic line at 706nm. Theoretical calculations of the line profiles have been performed for the experimental physical conditions, T=300 K and $n_{He} = n_{He}(T,P)$ for the triplet line. The agreement for a pressure of 1 and 1.6 MPa is remarkable [4]. We emphasize that no free potential parameters are used to readily fit the measured line shape. Such an agreement has only been possible because of the accuracy of the ab initio potentials.

Line shapes show a strong pressure dependence. Important features of the 728 nm line is the development of blue satellites already observed in the 706 nm line. Increasing the He density results in a shift of the whole profile towards the position of the satellite band (figure 6). When the He density reaches $10^{21}$ cm$^{-3}$ the satellite band is more intense than the main line for the singlet line. Whereas it has to $1.2 \times 10^{21}$ cm$^{-3}$ for the triplet line as the line satellite is farther in the wing [4]. We can, then, predict that the dependence in perturber density on the line parameters of the singlet line, as done in [5, 6], will show a greater slope, as the associated line satellites are closer to the parent line.
Figure 4. Unified profiles for singlet (dashed lines) and triplet (full line). T=300 K and \(n_{\text{He}}=10^{19} \text{ cm}^{-3}\).

Figure 5. Unified profiles for singlet (dashed lines) and triplet (full line). T=300 K and \(n_{\text{He}}=7\times10^{20} \text{ cm}^{-3}\).

Figure 6. Unified profiles for singlet (dashed lines) and triplet (full line). T=300 K and \(n_{\text{He}}=10^{21} \text{ cm}^{-3}\).

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