# Theoretical analysis of the Mg(3 $^3$P)-Mg(4$^3$S) line shape in cool DZ white dwarfs

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## Abstract

Traces of heavy metal in cool DZ white dwarfs are now attributed to the accretion of circumstellar dust. This dust is thought to originate from the tidal disruption of some rocky material. They provide a unique opportunity to study the composition of extra-solar planetary systems.
The determinations of precise atmospheric parameters and abundances require accurate description of the line profiles of the identified features.

In this poster we will present a determination of the Mg(3 $^3$P)-Mg(4 $^3$S) collisional line profiles using very recent *ab initio* potential energies. Results are reported for the conditions prevailing in cool DZ white dwarf atmospheres.



## Potentials

The *ab initio* computation of the adiabatic potential energy curves of MgHe have been carried out using a large core pseudopotential* for Mg complemented by operatorial Core Polarisation Potential (CPP), with the MOLPRO package. For Mg, we have build a large basis set inspired from the standard (pseudopotential) basis set† and the one used in rather high Rydberg calculations‡ leading to a 10s9p6d3f3g basis set. For He, the huge 30s17p10d6f3g basis set of Deguilhem and coworkers§ State specific orbitals were obtained from CASSCF calculations, where the active space consisted of 4 electrons distributed in all orbitals up to the 4s of Mg. These orbitals were then used in subsequent MRCI calculations to obtain the potential energy curves as well as static and transition dipole moments for all allowed transitions. For this 4 electrons system, this leads to almost full CI quality calculations.
The *ab initio* energy curves for the 3$p$-4$s$ line are shown in Figure 1.

*P. Fuentealba et al. J. Phys. B 16, L323 (1983)
†P. Fuentealba et al. Chem. Phys. Lett. 89, 418 (1982)
‡N. Khemini et al. J. Phys. Chem.
§B. Deguilhem et al. J. Phys. B 42 015102 (2009)



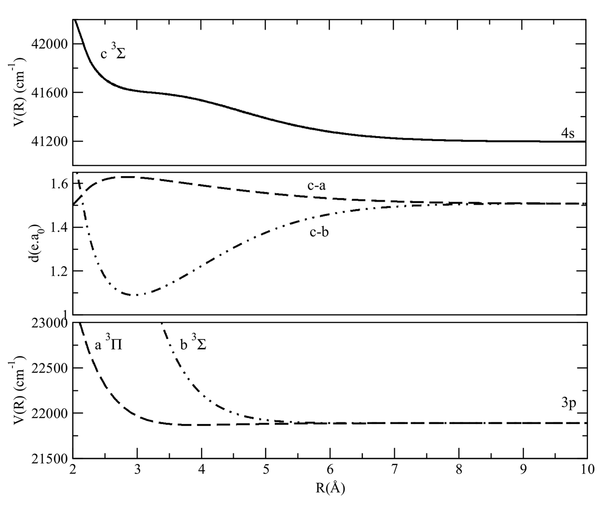

Figure 1
*Ab initio* potential energies for the triplet 4$s$ and 3$p$ states of the Mg–He molecule.



## Line profile

In radiative collision transitions it is the difference potential between the final and initial states that determines the frequency and the energy emitted or absorbed by a single photon. The unified theory of Anderson (Phys. Rev. **86**, 809, 1952) predicts that there will be satellites centered periodically at frequencies corresponding to the extrema of the difference potential between the upper and lower states.

There are 2 transitions which contribute to the line $3p\ ^3P \rightarrow 4s\ ^3S$

- $3p\,^3\Sigma \rightarrow 4s\,^3\Sigma$ (b-c)
- $3p\,^3\Pi \rightarrow 4S\,^3\Sigma$ (a-c)



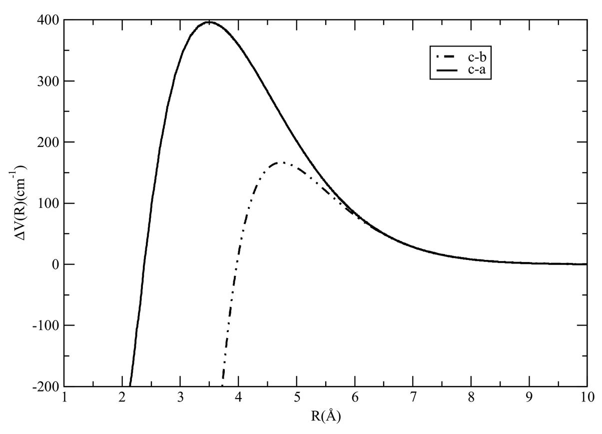

Figure 2
$\Delta V$ for the two transitions contributing to $3p \rightarrow 4s$ line.

For the transitions $a \rightarrow c$ and $b \rightarrow c$ the difference potential maxima are respectively 400 and 165 cm$^{-1}$ which lead to distinct wide shoulder at about 240 cm$^{-1}$ (5120 Å). The other maximum at $\Delta V$= 165 cm$^{-1}$ leads to a blue asymmetry without any distinct feature (Fig. 3).



The unified profile is asymetrical and contributes in the blue part.

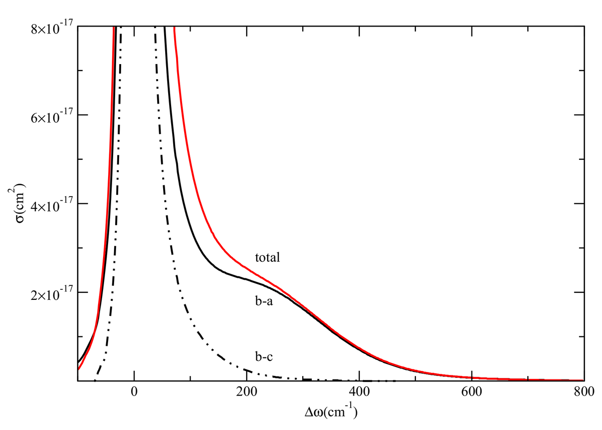

Figure 3
Individual components of the line compared to the total profile. (T=6000 K and $n_{\rm He}$= $10^{20}$ atoms cm$^{-3}$).



## Density dependence

Figures 4 and 5 reveal that the development of the blue wing leads to the overwhelming of the line by the satellite,

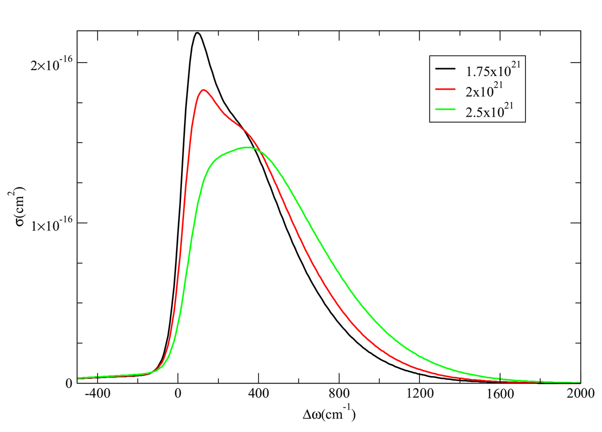

Figure 4
Evolution of the unified profiles with increasing helium density from
$n_{\rm He}$ = 1.75× $10^{21}$ to 2.5× $10^{21}$ cm$^{-3}$.



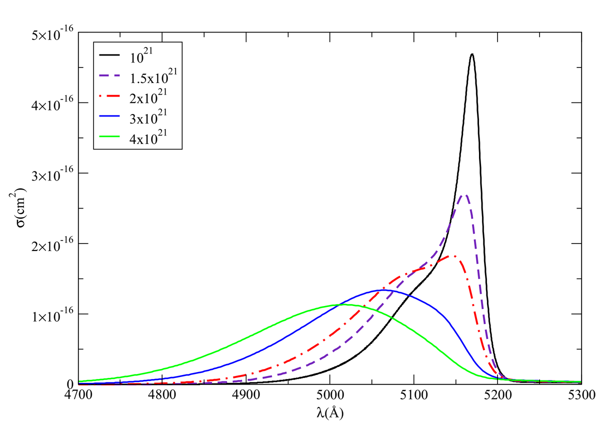

Figure 5
Evolution of the unified profiles with increasing helium density from
$n_{\rm He}$ =1× $10^{21}$ to 4× $10^{21}$ cm$^{-3}$.

When $n_{\rm He}$ = 4× $10^{21}$ cm$^{-3}$ the main line has totally disappeared.