SF2A 2014
J. Ballet, F. Bournaud, F. Martins, R. Monier and C. Reylé (eds)

NON-LTE MODELING OF COLD STELLAR ATMOSPHERES

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Abstract. Non-LTE modelisation of stellar atmospheres requires an accurate knowledge of collisional rate coefficients (mainly with H atoms) that compete with radiative rates to populate the atomic levels. In the framework of the SAM-GAIA project we carry out an interdisciplinary work combining quantum chemistry and collision physics.

Present studies concern collisional excitation of MgI, CaI and OI by H-atoms. Considering the Mg-H case, the resulting cross sections and rate coefficients point out the sensitivity of the results with the quantum chemistry data. The calculations show that the usual approximate Drawin formula leads to errors by factors up to 10^5. As was already found in Li+H and Na+H collisions, excitation processes were found of the same order of magnitude as charge transfer processes. However, unlike Li and Na, Mg has different spin terms, singlet and triplet, leading both to doublet molecular MgH electronic states. Collisional rates between spin-allowed and optically spin-forbidden atomic states are found to be of the same order of magnitude although optically spin-forbidden states are only collisionally coupled. Thus, we may expect consequences on non-LTE calculations.

Keywords: atomic data, line formation, stars: abundances

1 Introduction

Non-LTE modeling implies a competition between radiative and collisional processes. The radiative data are well known thanks to the Opacity and the Iron projects. The influence of inelastic hydrogen atom collisions dominant in cold atmospheres on non-LTE spectral line formation has been, and remains to be, a significant source of uncertainty for stellar abundance analyses, due to the difficulty in obtaining accurate data for such low-energy collisions, either experimentally or theoretically. For lack of a better alternative, the classical so-called Drawin formula (Drawin 1969) is often used. The question is : does the Drawin formula provide reasonable estimates of this process ? After a brief presentation of the different steps used to obtain accurate quantum calculations for collisions with H atoms (Section 2), the comparison with the approximate formulae is made in Section 3. Finally, preliminary conclusions on stellar abundance determination are drawn.

2 Molecular data

In the standard adiabatic approach, the theoretical treatment of atomic collisions requires two steps: (i) calculations of fixed-nuclei potential energies and non adiabatic radial and rotational couplings, (ii) an appropriate treatment of the nuclear motion based on the previous calculated molecular data leading to the wave function for the nuclear motion. This leads in the Jacobi coordinates system to the usual close-coupled equations. But, most of the non-adiabatic couplings are nonzero when the internuclear distance goes to infinity. This corresponds to the fact that the Jacobi system is not appropriate for the description of the collisions partners long before and after the collision. To remove this difficulty, Belyaev et al. (2001) proposed a way to connect the R-matrix calculated at some R_0 internuclear distance from close coupled equations in the Jacobi coordinates system to the asymptotic S-matrix allowing the calculation of cross sections.

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The first step concerns quantum chemistry and the main challenge is to build large basis sets adapted to the study of highly excited states. All the electronic states arising from Mg+H for energies up to the Mg 3s3d ^{3}D, 3s4p ^{1}P and 3s4p ^{3}P states were considered using large active spaces and basis sets (Guitou et al. 2010; Belyaev et al. 2012). The energies and related couplings were calculated using the 2009.1 version of the MOLPRO code (*). The potential energy functions (PEFs) of the $^2\Sigma^+$ and $^2\Pi$ states are represented on Figure 1 as function of the internuclear distance. The more striking feature of these potentials is the presence in the $^2\Sigma^+$ of a series of avoided crossings due to a strong mixing with the Mg^+-H^- ionic state. Those pseudo-crossings occur at larger and larger distances for the highest molecular states. This leads to ion-pair production and to the reverse reaction, mutual neutralization. This perturbation due to the Mg^+-H^- ionic configuration leads to large non-adiabatic radial coupling terms among consecutive states. The cross sections for the excitation and ion-pair production processes show large variations in amplitude for different transitions (Belyaev et al. 2012). We point out that cross sections for transitions between spin-allowed and spin-forbidden atomic states are of the same order of magnitude owing to relevant molecular mechanisms. The role of $^2\Pi$ states was found smaller than that of $^2\Sigma^+$ states, except for transitions between some excited states (Rodionov et al. 2014).

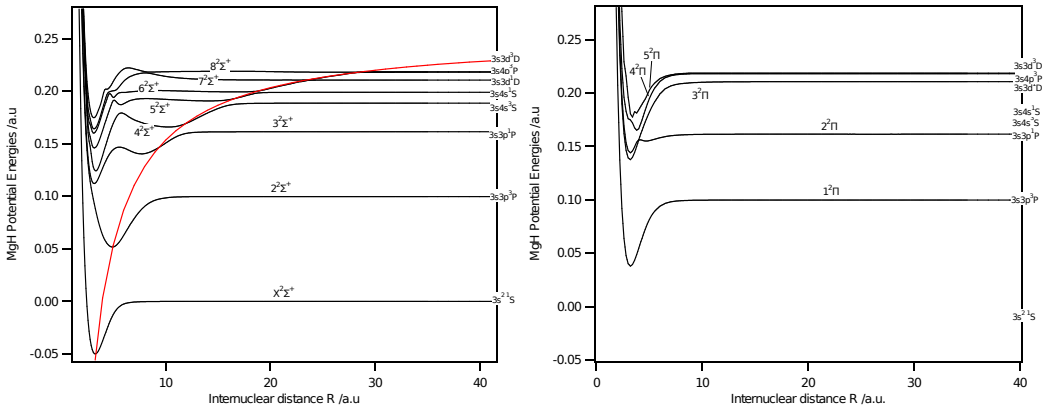

Fig. 1. Lowest interaction potentials **Left**: $^2\Sigma^+$ states (In red is the ionic interaction). **Right:** $^2\Pi$ states (Guitou et al. 2011).

3 Rate coefficients - Comparison with approximate formulae

From the cross sections, one can obtain the corresponding thermal rate coefficients at temperature T by an average over a Maxwellian velocity distribution. Rate coefficients at 4000 K for excitation and de-excitation processes :

$$\mathrm{Mg}(3s\ nl\ ^{2S+1}L) + \mathrm{H}(1s) \rightleftharpoons \mathrm{Mg}(3s\ n'l'\ ^{2S'+1}L') + \mathrm{H}(1s)$$

and for the charge transfer processes, ion-pair production and mutual neutralisation :

$$\mathrm{Mg}(3s\ nl\ ^{2S+1}L) + \mathrm{H}(1s) \rightleftharpoons \mathrm{Mg}^+(3s\ ^2S) + \mathrm{H}^-$$

were calculated among the $^2\Sigma^+$ states, including all the coupling tems. They are displayed in table 1. As expected, the rate coefficients follow the same trends as cross sections, i.e. large rate coefficients for ion-pair production/mutual neutralisation and large rates even for optically spin-forbidden transitions.

The ratio (Drawin/quantum) rate coefficients (expressed in terms of effective collision strengths†) are displayed in figure 2 vs the quantum results. The Drawin formula, which is an extension of the classical formula for ionisation of atoms by electron impact (Drawin 1969), cannot represent the physics of the quasi molecular interactions underlying the mechanisms of excitation by H atom collisions. This formula has only two parameters, ΔE and the f-value of the atomic transition. The most remarkable aspect of the Drawin formula results is that

* `http://www.molpro.net`

†For convenience, the collisional rate coefficients R_{ij} are expressed in terms of dimensionless collisional strengths $\gamma_{ij} = \gamma_{ji} = 4.96510^6 g_i \sqrt{T} R_{ji}$ where R_{ji} are the downward rate coefficients in unit of $\mathrm{cm}^3\mathrm{s}^{-1}$.

Table 1. Mg+H rate coefficients (in cm^3/s) at 4000 K.

Initial/Final states	3s ^{1}S	3p ^{3}P$_0$	3p ^{1}P$_0$	4s ^{3}S	4s ^{1}S	3d ^{1}D	ionic
3s ^{1}S	—	1.67 e-17	9.32 e-20	5.37 e-20	2.14 e-20	6.31 e-21	5.05 e-22
3p ^{3}P$_0$	4.87 e-15	—	2.76 e-13	7.95 e-14	2.07 e-14	4.35 e-15	1.47 e-16
3p ^{1}P$_0$	1.05 e-14	1.07 e-10	—	5.21 e-11	7.88 e-12	9.96 e-13	1.84 e-13
4s ^{3}S	5.26 e-14	2.67 e-10	4.52 e-10	—	1.38 e-10	1.18 e-11	9.14 e-12
4s ^{1}S	1.46 e-13	4.83 e-10	4.75 e-10	9.56 e-10	—	1.42 e-09	8.64 e-10
3d ^{1}D	2.23 e-14	5.28 e-11	3.12 e-11	4.28 e-11	7.41 e-10	—	1.73 e-10
ionic	2.42 e-13	2.42 e-10	7.84 e-10	4.48 e-09	6.10 e-08	2.35 e-09	—

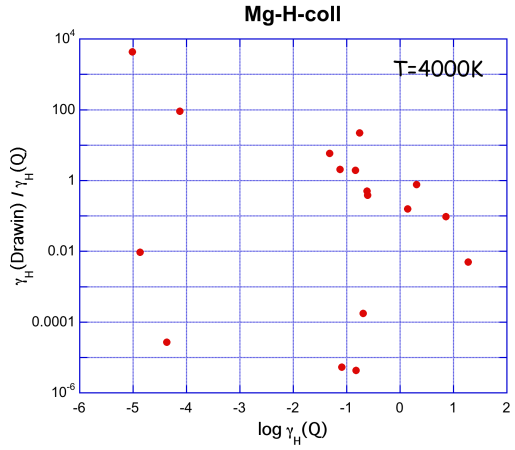

Fig. 2. Ratio γ_{Drawin}/γ_Q between the Drawin rates and the calculated quantum rates as function of the quantum rates.

among the 21 excitation transitions considered, only 5 transitions are optically allowed and could be calculated according to the Drawin formula. For the optically allowed transitions, the Drawin results are generally larger than the quantum results by a few orders of magnitude (Barklem et al. 2012). The same trend has been already found for Li and Na atoms (Barklem et al. 2011) in collision with H (Merle et al. 2013).

4 Conclusion and perspectives

As found previously in calculations for Li and Na, collisional excitation rate coefficients are smaller than rate coefficients for charge transfer. A comparison with the results found for Li and Na show that Mg-rate coefficients for excitation from the ground to the first excited states are roughly an order of magnitude larger (Barklem et al. 2012). Moreover, contrarily to Li and Na atoms, Mg has two spin symmetries and large collisional rates are found between singlet and triplet states which are only weakly radiatively coupled. This fact, together with the high rates lead one to expect that H-collisional processes could be important for non-LTE modeling.

However, the theoretical approaches used in the present work could not be easily generalized to more complex atoms, such as iron, or to very high electronic states. Our objective is then to develop approximate but realistic methods. Such work, in collaboration with Pr. A. K. Belyaev, is under progress (Belyaev 2013).

This work was partly supported by the French CNRS-PNPS (Programme National de Physique Stellaire), the GAIA program of Paris Observatory and by the Russian Fondation for Basic Research (grant N^o 13-03-00163-A). Part of the ab initio quantum chemistry calculations were performed using HPC resources from GENCI-[TGCC/CINES/IDRIS] (grant N^{o}2010040883) and on work stations at the Centre Informatique of Paris Observatory and at MSME laboratory (University of Paris-Est).

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