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COLLISION RATES AND THE DETERMINATION OF ATMOSPHERIC PARAMETERS

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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, with colleagues from Uppsala, St. Petersburg and Nice, an interdisciplinary work combining quantum chemistry, collision physics and astrophysical modeling. Present studies concern collisional excitation of Mg and O by H-atoms. In the particular case of Mg, 15 electronic states of the MgH molecule as well as the associated couplings that mix the states during the collision were calculated. The resulting cross sections and rate coefficients point out the sensitivity of the results with the quantum chemistry data. Our detailed calculations show that the usual approximate formulae (Drawin, Kaulakys) lead to errors by factors up to 10^6. Consequences on atmospheric parameters are analyzed.

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 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 Quantum mechanical calculations

There are two steps to compute collisional rate coefficients : the first one is the calculation of the interaction potentials between the studied atom and H atom and the determination of the couplings between these potentials which allow collisional transitions. This concerns quantum chemistry, and the main difficulty is to build large basis sets adapted to the study of high excited states : it is a real challenge for quantum chemistry. Dynamics using these molecular data constitutes the second step. Accurate collisional cross sections and rate coefficients are obtained using the quantum close-coupling approach. In order to account for the so-called electron translation effect, the coupled-channel equations are solved by means of the reprojection method (Belyaev 2010). Calculations were recently done for Li (Belyaev & Barklem 2003) and Na (Belyaev et al. 2010). Mg-H collisions and molecular interactions between O and H atoms are under study. Future work will be devoted to study H-collisions for atomic Ca, Ca^+ ion and possibly iron.
When the two colliding atoms come close together, they form temporarily a molecule whose electronic symmetry

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and spin multiplicity depend on the electronic states of the two partners. In the case of magnesium we have considered all states up to the ^{1}D and now ^{3}D states. This gives more than twenty molecular states to be calculated. Fig. 1 displays the corresponding $^2\Sigma^+$ potentials as function of the interatomic distance R. The more interesting aspect for these potentials is the existence for the $^2\Sigma^+$ states of a strong mixing with the Mg^+-H^- ionic state . This leads to an ion-pair production channel for Mg in collision with H atoms and to the reverse reaction. For the Π and Δ states, no such perturbation occurs. This perturbation may lead to large coupling terms among the $^2\Sigma^+$ states , mainly at large R distances between high excited states (Guitou et al. 2010). So large cross sections and rate coefficients between Mg excited states are expected (Guitou et al. 2011), as well as Mg^+ formation through ion-pair production (Barklem et al. 2011). Preliminary results* show that the dominant rates are those between the closest final states, large rates between atomic levels of different spin symmetry and an important contribution of ion-pair production are found.

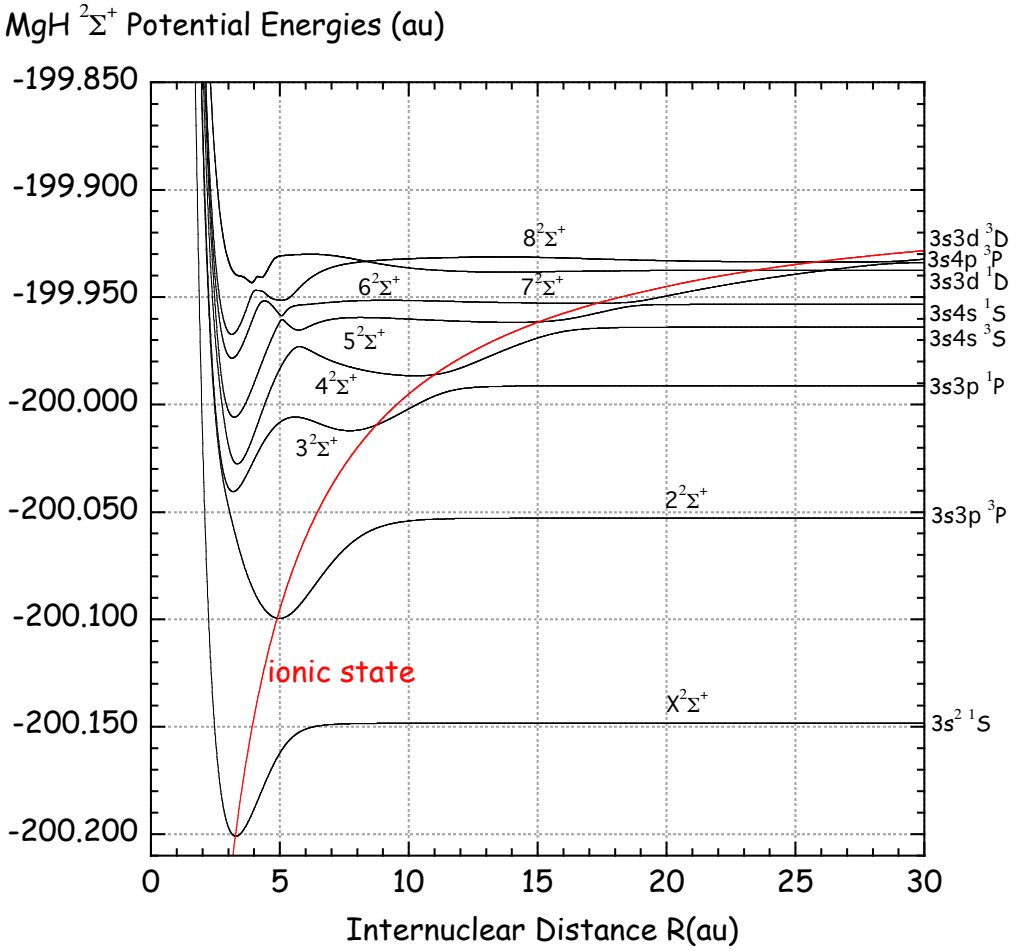

Fig. 1. $^2\Sigma^+$ electronic states as function of the internuclear distance. In red is displayed the ionic state

3 Comparison with approximate methods

It is important to compare accurate quantum rates with the results obtained using approximate formulae: the well known Drawin (1969) formula, which is an extension of the classical formula for ionization of atoms by electron impact, and the Kaulakys (1991) formula based on the free electron model applicable to Rydberg atoms. The Drawin formula gives rates proportional to the atomic oscillator strength (and thus equal to zero for spin

*Guitou, Belyaev, Barklem, Spielfiedel, Feautrier, unpublished 2011

forbidden transitions). In Fig. 2, which concerns collisions with Na atom (Lind et al. 2011), are plotted as function of the energy difference of the levels the ratio between Drawin and Kaulakys rates (right) and Drawin and quantum rates (left). Both approximate formulae give results far from the quantum one. This is expected as the detailed physics of the interactions is not at all introduced in the two models (Barklem et al. 2011). The same trends are found for collisions between H and Li and Mg atoms. The Drawin formula overestimates the rates by several orders of magnitude (up to 10^6). This is now well known, so in some modeling works the Drawin rates are multiplied by a corrective factor S_H ($0 \leq \mathrm{S}_H \leq 1$). Comparison with accurate quantum results shows that S_H is different for different processes.

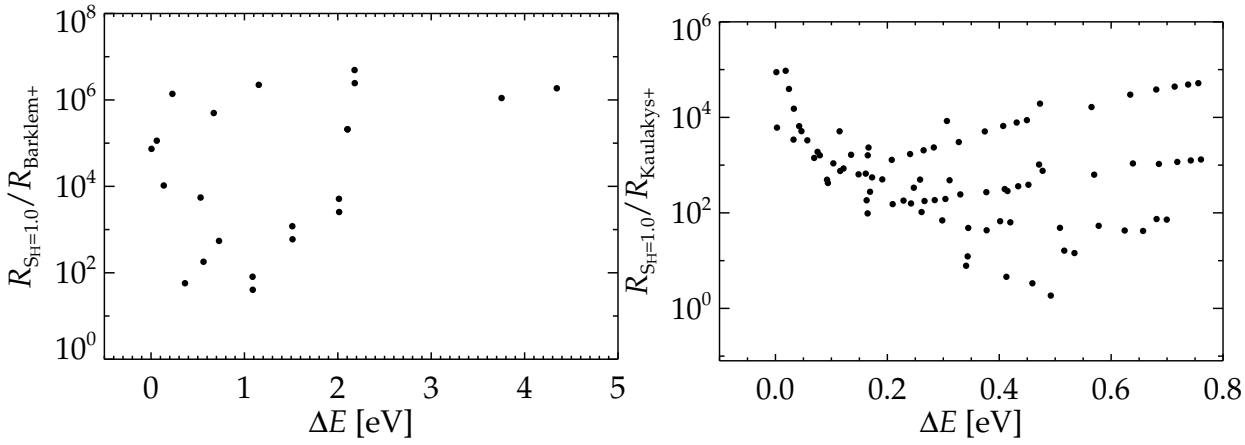

Fig. 2. Left: Drawin/quantum rates. **Right:** Drawin/Kaulakys rates.

4 Consequences on star atmosphere modeling

To date, no general conclusion on the effect of the new H-collisional rates seems possible as collisions compete with radiative processes for both excitation/deexcitation and ion-pair production of the species. As a consequence, the abundances depend non-linearly on many parameters: the physical conditions of the star atmosphere (temperature, gravity, metallicity), the number of atomic states included in the model, the radiative transfer and 1D or 3D modeling, the line considered for the diagnostics. However, some trends are available from recent studies on lithium, sodium, carbon and oxygen lines.

In a study relative to the Sun and to a sub giant metal-poor star, Barklem et al. (2003) show that H-collisions have a relatively small influence on the non-LTE predicted equivalent width of the resonance line for the Sun and larger effects for the metal-poor star. This is expected as collisional rate coefficients between the first atomic levels are very small and H atoms are not abundant in the Sun atmosphere. For a metal-poor star with low metallicity, the larger collisional effect is mainly due to mutual neutralisation with H^- which overpopulates the first levels. This last effect seems smaller for Na lines (Lind et al. 2011). In the absence of accurate H-collision rate coefficients for carbon and oxygen, Fabbian et al. (2006) and Fabbian et al. (2009) consider non-LTE abundance corrections using the Drawin formula with $\mathrm{S}_H = 0$ (no collisions) and $\mathrm{S}_H = 1$ (with H collisions). Both studies consider infra red lines, and large non-LTE effects (probably overestimated) are found for low metallicity stars.

5 Concluding remarks

H collisions play an important role for abundance determination of low metallicity stars when the diagnostics is obtained using lines between excited states. We note the importance of the 3D modeling. Preliminary results concerning lithium, sodium and magnesium show a large overestimation of the rate coefficients using the Drawin formula and the importance of ion-pair production by collisions with H atoms. These trends should be confirmed by studies on other atomic systems: work on oxygen is in progress and future work on neutral and ionized calcium is planned.

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