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Atom-Rydberg Atom Collisions in Hydrogen Plasmas: Cross Sections and Rate Coefficients

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Abstract.
Non-LTE modelling requires accurate atomic data e.g. collisional excitation and ionization cross-sections and rate coefficients. In order to improve the modeling of the solar photosphere, as well as to model atmospheres of other similar and cooler stars where the main constituent is also hydrogen, it is necessary to take into account the influence of all the relevant collisional processes on the excited-atom populations in weakly ionized hydrogen plasmas. In this context we present the data needed for the inclusion of the specific atomic collisional processes in the investigation of the optical and kinetic properties of weakly ionized stellar atmospheres layers. The ionization processes in collisions of excited hydrogen atoms with atoms in ground states were considered for the principal quantum numbers $2 \le n \le 20$ and temperatures $4000\ \mathrm{K} \le T \le 20000\ \mathrm{K}$.

1. Introduction

The interpretation of laboratory and interstellar line spectra with radiative transfer calculations requires different kinds of atomic/molecular input data such as energy levels, statistical weights, transition probabilities, collision data etc. [1, 2]. The main aim of this short contribution is to present the investigation of the hydrogen collisional excitation and ionization processes which are important for accurate non-LTE modeling [3, 4]. The role of an inelastic collision with hydrogen atoms is important even if the cross-sections for that collisions are small because their abundance is very large and dominant in such environments [5, 6]. The values of the corresponding rate coefficients are very useful for the modelling and analysis of the photospheres of Sun and solar like stars and as similar layers which exist in very dense weakly ionised domains in clouds in BLR and NLR regions of AGN.

2. Theory

This investigation is a continuation of our research of atomic processes and optical and kinetic properties of weakly ionized stellar atmospheres layers [7, 8, 9, 10]. As presented in [11, 12] when an electron is excited into a high lying Rydberg state, with large principal quantum number, even inelastic thermal collisions can be sufficiently energetic to lead to ionization reactions. These

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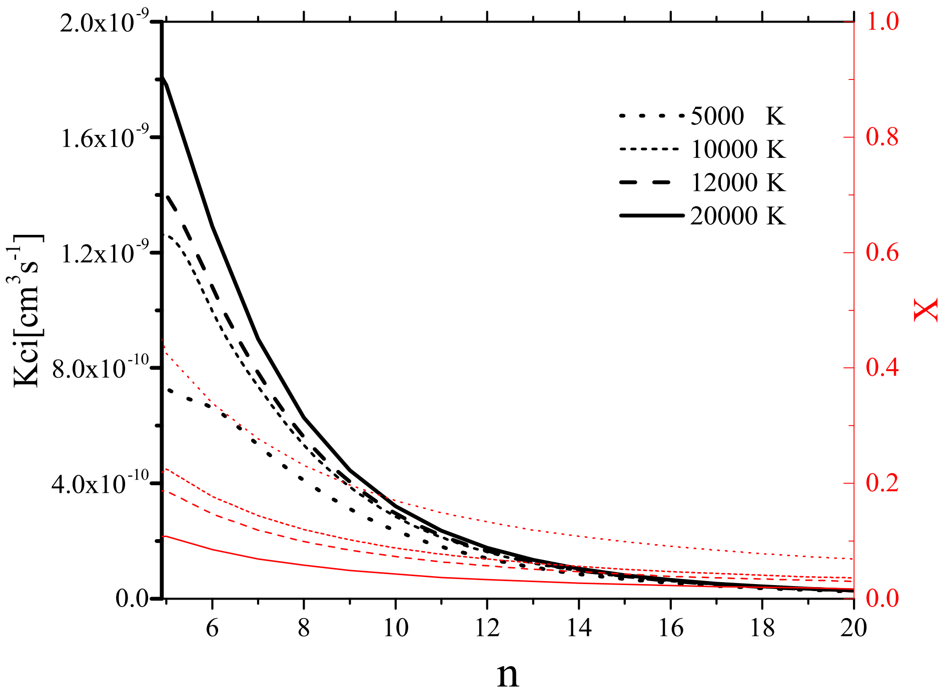

Figure 1. Behavior of collisional ionisation (1) and (2) total rate coefficient $K_{ci}(n, T)$ for selected temperatures and excited states.

types of reactions/collisions can be classified under the chemi-ionization reactions [13, 14] with possible channels

$$H^*(n) + H \Rightarrow H_2^+ + e, \tag{1}$$

of associative ionization and the non-associative ionization

$$H^*(n) + H \Rightarrow H + H^+ + e, \tag{2}$$

where H is hydrogen atom in ground state.

In this contribution we present the results of calculation of the cross sections and rate coefficients of the corresponding ionization processes (1) and (2) using methods introduced in [15, 16].

Theoretical cross sections $\sigma_{ci}^{(a,b)}(n; E)$ and the partial rate coefficients of the chemi-ionization processes (1) and (2) are obtained here as in Ref. [15]. The corresponding partial rate coefficients are denoted here with $K_{ci}^{(a,b)}(n; T)$, where T is the temperature of the considered plasma. Using these partial rate coefficients we will determine the total one, namely,

$$K_{ci}(n, T) = K_{ci}^{(a)}(n, T) + K_{ci}^{(b)}(n, T), \tag{3}$$

which characterizes the efficiency of the considered chemi-ionization processes together (for details see [11]).

3. Results and discussion

We considered chemi-ionization processes (1) and (2) for the principal quantum numbers $2 \leq n \leq 20$ and temperatures $4000\ \mathrm{K} \leq T \leq 20000\ \mathrm{K}$. The values of the partial cross sections

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$\sigma_{ci}^{(a,b)}(n;E)$ of the chemi-ionization processes (1) and (2) are calculated for $2 \le n \le 20$ and energies E up to 20 eV. Here we present only a fraction of these data, and we will show only chemi-ionization rate coefficients. Also in this research we examined the inverse processes of chemi-recombination, but this is not the topic of this contribution.

In Fig.1 the values of the total chemi-ionization rate coefficients $K_{ci}(n,T)$ Eq. (3) and of the branching coefficient $X^{(a)}(n,T) = K_{ci}^{(a,b)}(n,T)/K_{ci}(n,T)$ are presented for wide range of principal quantum numbers, and temperatures. The results of the total chemi-ionization rate coefficients $K_{ci}(n,T)$ (left y axis) show the expected behavior i.e. decreasing with the quantum number increasing and temperature dependence. As can bee seen from Fig. 1 by analyzing $X^{(a)}(n,T)$ values (right y axis) the associative channel (1) is dominant for lower n and T. This gives important information about presence of molecular ion H_2^+. The importance of associative channel (1) decreases with temperature increase when non-associative channel (2) take dominant place. We compare the efficiency of chemi-ionizatiom processes (1) and (2) with the efficiency of the concurrent impact electron-atom ionization for the considered plasma conditions and we report the domination of chemi-ionizatiom processes especially in the lower temperature region.

We conclude that this topic is very important because improved calculations data are needed for excitation/ionisation of hydrogen atoms due to existence of uncertainties on the rate coefficients in hydrogen collisions [3] in order to be properly included in modern codes and simulations like [17].

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References
[1] Przybilla N and Butler K 2004 *Astrophys. J.* **609** 1181
[2] Marinković B P, Vujčić V, Sushko G, Vudragović D, Marinković D B, Djordjević S, Ivanović S, Nešić M, Jevremović D, Solov'yov A V *et al.* 2015 *Nucl. Instr. Meth. Phys. Res. B* **354** 90–95
[3] Barklem P S 2007 *Astron. Astrophys.* **466** 327–337
[4] Fontenla J M, Avrett E, Thuillier G and Harder J 2006 *Astrophys. J.* **639** 441–458
[5] Mashonkina L 2009 *Phys. Scr. Vol. T* **134** 014004
[6] Barklem P S 2008 *Phys. Scr.* **2008** 014023
[7] Ignjatović L M, Mihajlov A A, Srećković V A and Dimitrijević M S 2014 *Mon. Notices Royal Astron. Soc.* **441** 1504–1512
[8] Ignjatović L M, Mihajlov A A, Srećković V A and Dimitrijević M S 2014 *Mon. Notices Royal Astron. Soc.* **439** 2342–2350
[9] Srećković V A, Mihajlov A A, Ignjatović L M and Dimitrijević M S 2014 *Adv. Space Res.* **54** 1264–1271
[10] Srećković V A, Mihajlov A A, Ignjatović L M and Dimitrijević M S 2013 *Astron. Astrophys.* **552** A33
[11] Mihajlov A A, Srećković V A, Ignjatović L M and Klyucharev A N 2012 *J. Clust. Sci.* **23** 47–75
[12] Gnedin Y N, Mihajlov A A, Ignjatović L M, Sakan N M, Srećković V A, Zakharov M Y, Bezuglov N N and Klycharev A N 2009 *New.Astr.Rev.* **53** 259–265
[13] Bezuglov N, Borodin V, Klyucharev A and Matveev A 2002 *Russ. J. Phys. Chem.* **76** S27–S42
[14] O'Keeffe P, Bolognesi P, Avaldi L, Moise A, Richter R, Mihajlov A A, Srećković V A and Ignjatović L M 2012 *Phys.Rev.A* **85** 052705
[15] Mihajlov A A, Ignjatović L M, Srećković V A and Dimitrijević M S 2011 *Astrophys. J., Suppl. Ser.* **193** 2
[16] Mihajlov A A, Srećković V A, Ignjatović L M and Dimitrijević M S 2016 *Mon. Notices Royal Astron. Soc.* **458** 2215–2220
[17] Hauschildt P H and Baron E 2010 *Astron. Astrophys.* **509** A36