

Article

The Collisional Atomic Processes of Rydberg Hydrogen and Helium Atoms: Astrophysical Relevance

Vladimir A. Srećković ¹, Milan S. Dimitrijević ^{2,3,*}, Ljubinko M. Ignjatović ¹, Nikolai N. Bezuglov ⁴ and Andrey N. Klyucharev ⁴

¹ Institute of Physics, Belgrade University, Pregrevica 118, 11080 Zemun, Belgrade, Serbia; vlada@ipb.ac.rs (V.A.S.); ljuba@ipb.ac.rs (L.M.I.)

² Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia

³ LERMA, Observatoire de Paris, UMR CNRS 8112, UPMC, 92195 Meudon CEDEX, France

⁴ Saint Petersburg State University, 7/9 Universitetskaya nab., St. Petersburg 199034, Russia; bezuglov50@mail.ru (N.N.B.); anklyuch@gmail.com (A.N.K.)

* Correspondence: mdimitrijevic@aob.rs

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Abstract: Elementary processes in astrophysical environments traditionally attract researchers' attention. 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 atmosphere layers. The first type of processes are collisional ionisation (chemi-ionization) processes, and the second ones are excitation and de-excitation (i.e., $(n - n')$ -mixing processes). We give the rate coefficients of the aforementioned processes for the conditions that exist in the solar photosphere, the atmosphere of DB white dwarfs, M-type red dwarfs, etc.

Keywords: atomic data; molecular data; atomic and molecular databases

1. Introduction

Many fields in astrophysics, especially the modelling of various stellar atmospheres and the kinetics of stellar and other astrophysical plasmas, depend on data for atomic and molecular collisions [1–6]. Modern codes for stellar atmosphere modelling (e.g., [7,8]) require knowledge of atomic data, so the accuracy of these data becomes very important. Among these data there are atomic and molecular processes and spectral regions that even today are poorly investigated. Therefore, there is a need for further investigation and development of methods for improving the existing ones [9–11]. Recently, the research community has become aware of the need for better atomic data which could be important in modelling of AGN BLR clouds [12].

In this paper we analyze the current state of research on ionisation (chemi-ionization) processes and excitation and de-excitation ($(n - n')$ -mixing) processes in collisional reaction $A^*(n) + A$ involving hydrogen and helium atoms.

Since these processes have already been treated for a long time on the basis of the so-called dipole resonant mechanism (DRM), we will briefly describe its main features. In this description of collisional ionisation and excitation events, it is envisaged that processes are induced by the dipole part of the electrostatic interaction between the outer Rydberg electron and the inner ion-atom system. Figure 1 schematically illustrates the chemi-ionization/recombination and $(n - n')$ -mixing processes. A detailed description of the mechanism can be found in [13].

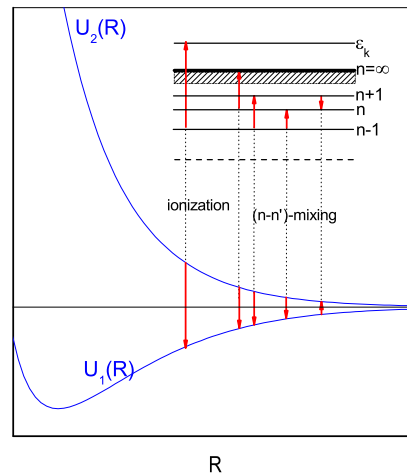


Figure 1. The graph of schematic illustration of the resonant transitions which cause the processes of chemi-ionization/recombination and $(n - n')$ -mixing processes in the $A^*(n) + A$ collision.

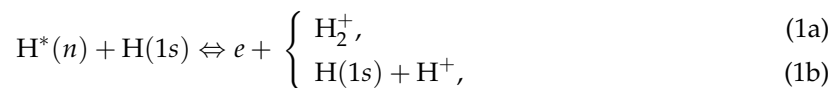
2. Hydrogen

The inelastic collisions of hydrogen atoms is an important factor in the modelling of stellar atmospheres [9,14]. This kind of calculation requires accurate atomic data (e.g., hydrogen collisional excitation/ionization cross-sections and rate coefficients) [11,15]. The reason is that even if the cross-sections for such collisions are quite small, their abundance is large (number of neutral hydrogen atoms are a few orders of magnitude higher than electrons in the atmospheres of solar-type stars).

It can be seen from Reference [9] that there exists a difference in collision rate data. In view of the present large uncertainties in the data for excitation/ionization by collisions with hydrogen atoms, it is important to further investigate the $H(n) + H(1s)$ system, especially for higher values of n where uncertainties are very noticeable.

2.1. Collisional Ionization

The collisional ionisation (chemi-ionization) includes two possible channels: the associative ionisation and the non-associative one:



where $H^*(n)$ is the hydrogen atom in the excited state with the principal quantum number n , H_2^+ is the molecular ion in the ground electronic state, and e is a free electron.

The values of the total chemi-ionization and recombination rate coefficients $K_{ci}(n, T)$ and $K_{cr}(n, T)$ are presented in Figures 2 and 3, respectively. These figures cover the regions $2 \leq n \leq 10$ and $4000 \text{ K} \leq T \leq 10,000 \text{ K}$, which are relevant for the solar photosphere [1,16], some atmospheres of late type (M) stars [7], etc. The values for $2 \leq n \leq 8$ and $4000 \text{ K} \leq T \leq 8000 \text{ K}$ are from [17]. By analyzing the partial rate coefficients of both possible channels of chemi-ionization, we conclude that the associative channel (1a) is dominant for lower n and T . This gives important information about the presence of the molecular ion H_2^+ . The importance of the associative channel (1a) decreases with temperature increase when the non-associative channel (1b) takes the dominant place.

A review of rate coefficient data from the existing literature and the current stage of development has been analyzed in [9,14].

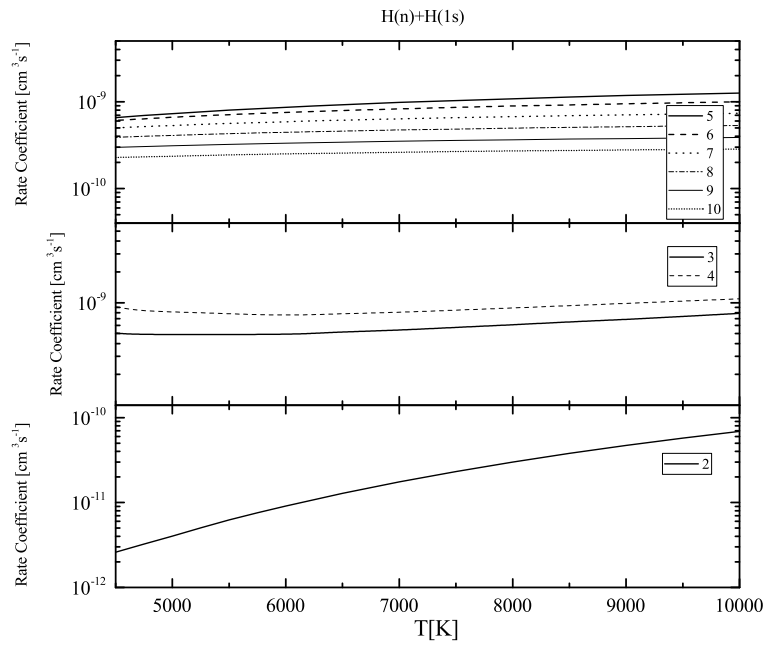


Figure 2. Plot of the rate coefficients for collisional ionisation $H^*(n) + H(1s)$ (i.e., for chemi-ionization processes (1)) as a function of n and T .

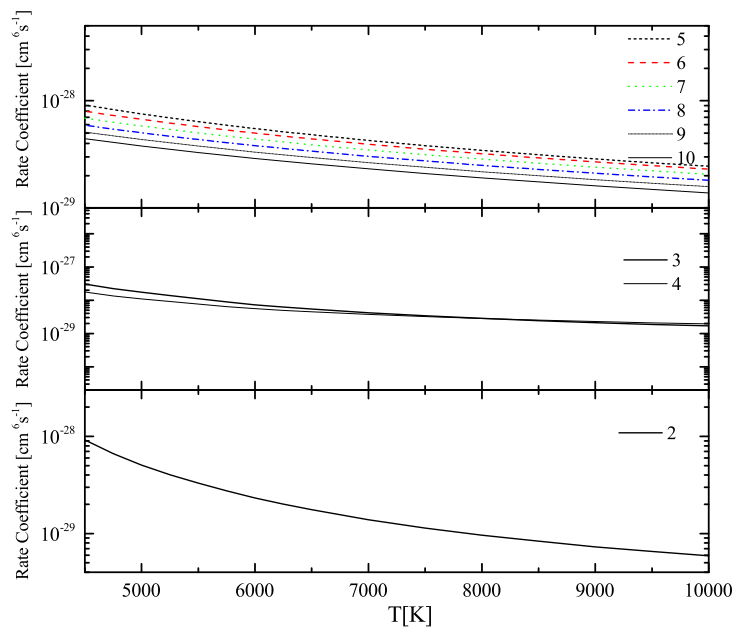


Figure 3. Same as in Figure 2 but for inverse process (i.e., recombination processes).

2.2. Collisional Excitation and De-Excitation

Collisional excitation process by hydrogen atoms includes two possible channels—the direct excitation process and the excitation process involving excitation transfer:

$$H^*(n) + H(1s) = \begin{cases} H^*(n' = n + p) + H(1s), \\ H(1s) + H^*(n' = n + p), \end{cases} \quad p \geq 1, n \geq 4. \quad (2)$$

The inverse de-excitation processes are:

$$H^*(n) + H(1s) = \begin{cases} H^*(n' = n - p) + H(1s), \\ H(1s) + H^*(n' = n - p), \end{cases} \quad n - p \geq 4, \quad (3)$$

where $H^*(n)$ is a Rydberg state hydrogen atom with principal quantum number $n \geq 4$ and e is a free electron.

The processes (2) and (3) are characterized by the excitation and de-excitation rate coefficients $K_{n;n+p}(T)$ and $K_{n;n-p}(T)$, where T is the local temperature of the atomic particles. The values of excitation rate coefficients for $3000 \text{ K} \leq T \leq 7000 \text{ K}$ are from [18]. In the extended region of temperature coefficients are determined here using the semi-classical approach similar to that described in [19] or [20]. The de-excitation rate coefficients $K_{n;n-p}(T)$ are determined according to the principle of thermodynamical balance. All necessary expressions are given and explained in Mihajlov et al. [20].

The selected results for excitation rate coefficients $K_{n;n+p}(T)$ with $4 \leq n \leq 10$, $1 \leq p \leq 5$ and $3000 \text{ K} \leq T \leq 10,000 \text{ K}$ are presented in Figure 4. As in the case of collisional ionization, the review of rate coefficients data for excitation from the existing literature and current stage of development can be found in [9,14].

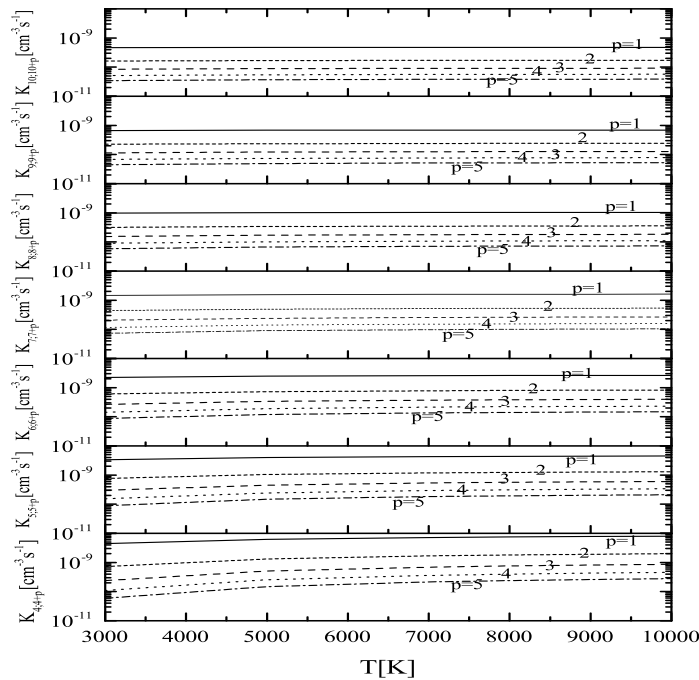


Figure 4. Collisional $H^*(n) + H(1s)$ excitation rate coefficients $K_{n;n+p}(T)$ for the transitions between the states with $4 \leq n \leq 10$, $1 \leq n' - n \leq 5$ as a function of n and T . Here $p = n' - n$.

2.3. Astrophysical Targets

Solar atmosphere modelling: The influence of collision processes $H^*(n \geq 2) + H(1s)$ and the corresponding $(n - n')$ -mixing processes on hydrogen atom excited-state populations in the solar photosphere has been examined. It has been concluded that the considered collision processes dominate over the relevant concurrent electron–atom and electron–ion processes in almost the entire solar photosphere [17,21]. It is shown that these processes are important for the non-local thermodynamic equilibrium modelling.

Atmospheres of late type (M) stars: In [22] it is shown that the examined processes influence the populations of all hydrogen atom excited states. This suggests that the examined processes, due to their influence on the excited state populations and the free electron density, should also influence the atomic spectral line shapes. Figure 5 (from [23]) shows the line profiles of H_α , H_δ , H_ϵ Pa ϵ with and without the inclusion of (1a) and (1b) processes. Profiles are synthesized with PHOENIX code [8] with Stark broadening contribution. The presented results suggest that the processes (1) influence the atomic spectral line shapes. Line shape changes, especially in the wings, show the influence of the electron density change having a direct influence on the Stark broadening of hydrogen lines in the atmospheres of late type (M) stars (see also [24]).

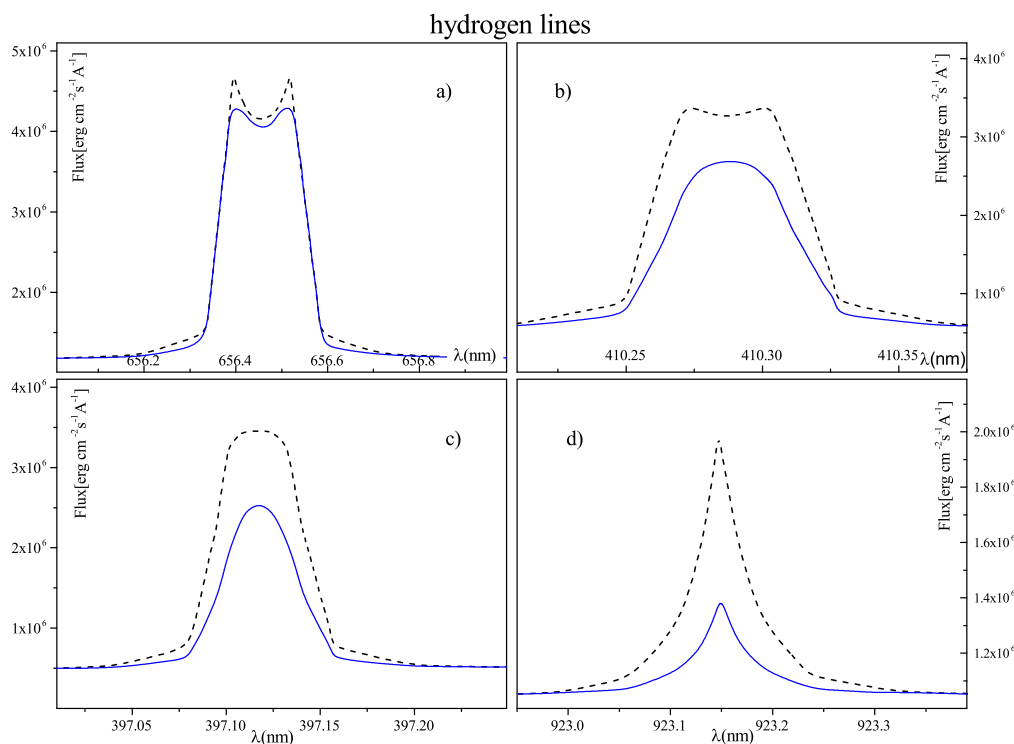


Figure 5. The hydrogen line profiles ((a) H_α ; (b) H_δ ; (c) H_ϵ ; (d) Pa ϵ) in the late type (M) stars' atmospheres. Dotted black and full blue curves denote lines without and with the inclusion of chemi-ionization and chemi-recombination processes (1), respectively.

AGN BLR clouds: The possibility that the atom–Rydberg atom collisions (i.e., chemi-ionization processes as well as the inverse chemi-recombination processes) may be useful for the diagnostics, modelling, and confirmation of the existence or non-existence of very dense weakly ionised domains in clouds in BLR and NLR regions of AGN has been investigated recently. The preliminary results are presented in [12]. The importance of $(n - n')$ -mixing processes in $H^*(n) + H(1s)$ collisions, for the principal quantum number $n \geq 4$, in AGN BLR clouds has been investigated as well. The preliminary results show that the corresponding processes must have an influence on the populations of hydrogen

highly excited atoms in moderately ionized layers of sufficiently dense parts of the BLR clouds, if such exist.

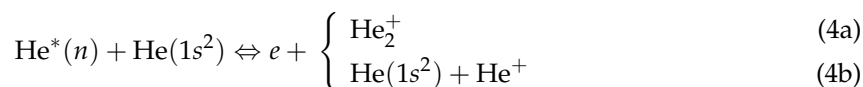
3. Helium

Non-LTE modelling, especially for helium plasma, needs accurate rate coefficients for all relevant elementary processes, including collisional ionization/recombination and excitation/de-excitation processes, because the great departure from LTE in laboratory conditions is more easily realized in helium than in hydrogen plasmas [25]. Such investigation of non-equilibrium helium plasmas is still current and of interest (see [26–30]).

Helium atoms play an important role in astrophysics [4,31,32]. Ionization processes of excited states of helium and their inverse recombination processes are significant for helium plasmas in the very low-density environment which exists in stellar atmospheres with weakly ionized layers [21]. Chemi-ionization/recombination and $(n - n')$ -mixing processes in low-temperature layers of white dwarf atmospheres are very important for the helium atom Rydberg states population where the gaseous mixture of hydrogen and helium exists.

The helium molecular ion He_2^+ is also present in stellar medium, as well as in the chemistry of the early universe [4,33,34]. Dissociative recombination (right side of Equation (4a)) is an inverse process occurring through the neutralization of the He_2^+ ion. It has been widely studied due to its importance in a relatively low-temperature system [35].

3.1. Collisional Ionization



The total chemi-ionization and chemi-recombination rate coefficients $K_{ci}(n, T)$ and $K_{cr}(n, T)$, in the temperature range $7000 \text{ K} \leq T \leq 30,000 \text{ K}$ and principal quantum numbers $3 \leq n \leq 10$, are shown in Figures 6 and 7. The data were calculated in [22]. The dependence of both coefficients $K_{ci}(n, T)$ and $K_{cr}(n, T)$ on the quantum number decreases with the increase of the temperature.

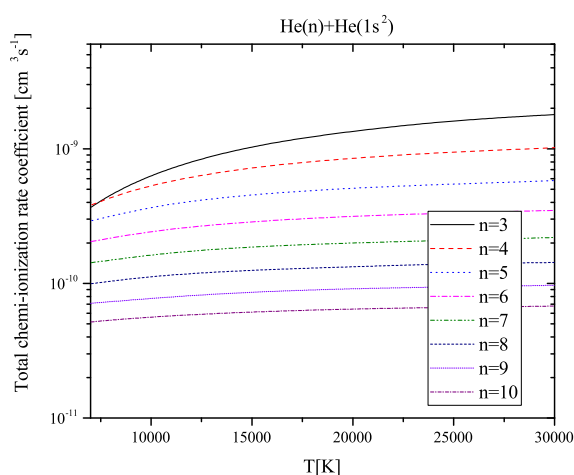


Figure 6. The plot of the $K_{ci}(n, T)$ and $K_{cr}(n, T)$ collisional ionisation $\text{He}^*(n) + \text{He}(1s^2)$ rate coefficients. That is, chemi-ionization processes (4) in the region $7000 \text{ K} \leq T \leq 30,000 \text{ K}$ and for principal quantum numbers $3 \leq n \leq 10$.

As in the case of hydrogen, by analyzing the partial rate coefficients of both possible channels of chemi-ionization, we concluded that the associative channel (4a) is noticeable for lower n and T ($n \leq 6$ and $T \leq 10,000$ K). This gives important information about presence of the helium molecular ion He_2^+ . The importance of the associative channel (4a) decreases with temperature increase when the non-associative channel (i.e., dissociation (4b)) takes the dominant place.

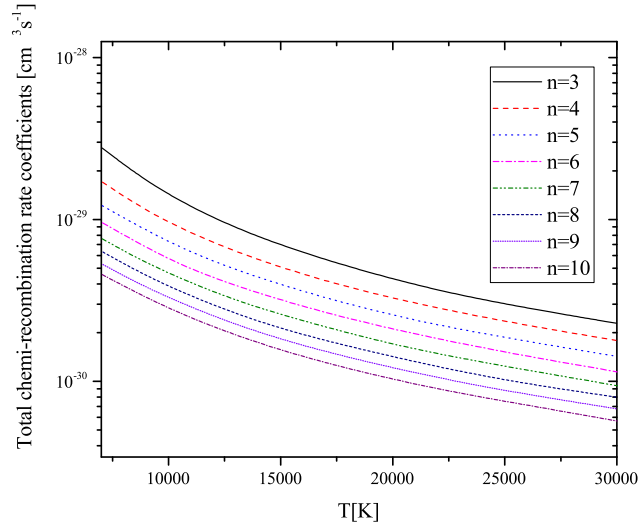


Figure 7. Same as in Figure 6, but for the inverse process (i.e., chemi-recombination).

3.2. Collisional Excitation and De-Excitation

$$\text{He}^*(n) + \text{He}(1s^2) = \begin{cases} \text{He}^*(n' = n + p) + \text{He}(1s^2), & p \geq 1, \\ \text{He}(1s^2) + \text{He}^*(n' = n + p), & \end{cases} \quad (5)$$

and the inverse de-excitation processes

$$\text{He}^*(n) + \text{He}(1s^2) = \begin{cases} \text{He}^*(n' = n - p) + \text{He}(1s^2), & 0 < p \leq n - 3, \\ \text{He}(1s^2) + \text{He}^*(n' = n - p), & \end{cases} \quad (6)$$

where $\text{He}^*(n)$ is a helium atom in the Rydberg states with the principal quantum number $n \gg 1$, $n + p$ and $n - p$ are the principal quantum numbers of the final Rydberg states, and $3 \leq n \leq 8$.

The results for collisional excitation helium rate coefficients $K_{n,n+p}(T)$ for $3 \leq n \leq 10$, $1 \leq n' - n \leq 5$, and $4000 \text{ K} \leq T \leq 20,000 \text{ K}$ are presented in Figure 8. The figure shows a monotonous decrease of rate coefficients with the increases of n and p , and a very slow increase as temperature increases, as concluded in [19,20].

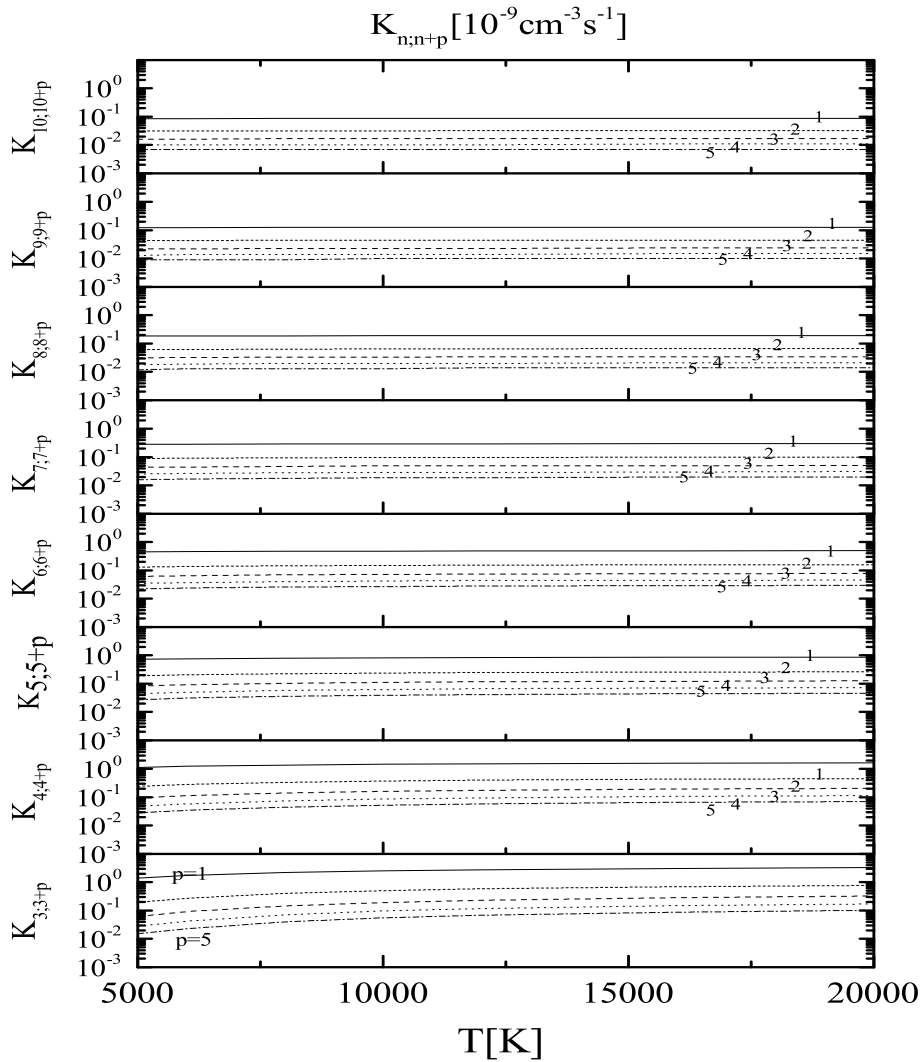


Figure 8. Collisional excitation helium rate coefficients $K_{n,n+p}(T)$ for the transitions between the states with $3 \leq n \leq 10$, $1 \leq n' - n \leq 5$ as a function of n and T . $p = n' - n$.

3.3. Astrophysical Targets

White dwarfs modelling: The influence of chemi-ionization processes (4) in reference to the other ionization processes was examined in the photospheres of the DB white dwarfs with $12,000 \text{ K} \leq T_{eff} \leq 20,000 \text{ K}$. On the basis of the data from Koester [2] it was established that in the parts of the considered photosphere (where $8000 \text{ K} \leq T \leq 20,000 \text{ K}$), these chemi-ionization processes dominate over the concurrent electron–Rydberg atom impact ionization processes. It is concluded that these processes should be included in the model atmospheres from the beginning in a consistent way.

It is shown that in significant parts of the DB white dwarf atmospheres (which contain weakly ionized layers (ionization degree $\leq 10^{-3}$)), the influence of the studied atom–Rydberg atom processes (5) and (6) on excited helium atom populations is dominant or at least comparable to the influence of the concurrent electron–He*(n)–atom processes.

4. Summary

In this paper it is shown that the collisional processes of atoms and molecules in ground and Rydberg states play an important role in the astrophysics. We present the results of two groups of collisional processes which are important for the optical and kinetic properties of weakly ionized stellar atmosphere layers. Quantitative estimations of the rate coefficients of the mentioned processes were made. These data are important for the modelling and interpretation of data provided by observations and laboratory measurements. These data are important and have a notable role in many fields in atmospheric physics, chemistry, industry, etc.

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Conflicts of Interest: The authors declare no conflict of interest.

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