ATOM-RYDBERG ATOM PROCESSES IN THE STELLAR ATMOSPHERES: DWARF ATMOSPHERES, QUIET SUN AND SUNSPOTS

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A.N. Klyucharev, Bezuglov …, others from AOB…, Italy, Croatia… Now I present:

I will present the results from our recent papers:

Atom-Rydberg atom chemi-ionization processes in solar and DB white dwarf atmospheres in the presence of (n-n')-mixing channels

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CHEMI-IONIZATION IN SOLAR PHOTOSPHERE: INFLUENCE ON THE HYDROGEN ATOM EXCITED STATES POPULATION

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ABSTRACT

In this paper, the influence of chemi-ionization processes in $H^*(n \geqslant 2) + H(1s)$ collisions, as well as the influence of inverse chemi-recombination processes on hydrogen atom excited-state populations in solar photosphere, are compared with the influence of concurrent electron–atom and electron–ion ionization and recombination processes. It has been found that the considered chemi-ionization/recombination processes dominate over the relevant concurrent processes in almost the whole solar photosphere. Thus, it is shown that these processes and their importance for the non-local thermodynamic equilibrium modeling of the solar atmosphere should be investigated further.

Key words: atomic processes – Sun: atmosphere

THE INFLUENCE OF CHEMI-IONIZATION AND RECOMBINATION PROCESSES ON SPECTRAL LINE SHAPES IN STELLAR ATMOSPHERES

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and few more rec. papers …

<u>Outline</u>

> ➤ Present our investigation: of chemi-ionization processes, and influence on solar photosphere and WD atmospheres

> ➤ our investigation : of chemi-ionization + pre-ionization(mixing), and influence on solar photosphere

> ➤ investigation : chemi-ionization + pre-ionization(mixing), and influence on DB WD atmospheres

> ➤ Further invest. of chemi-ionization + pre-ionization(mixing), influence on sunspot atmospheres…

and

> ➤ few words about MOL-D Database

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.

Group of chemi-ionization atom collisional processes in weakly ionized layers of stellar atmospheres (ionization degree less than 10^{-3}) was studied. In order to demonstrate the significance of these processes it was necessary to compare their efficiency, from the aspect of their influence on the free electron and excited atom populations, with the efficiency of the known concurrent processes of electron–atom impact ionization and etc.
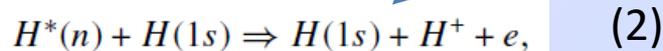
We study

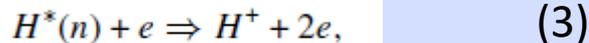$$H^*(n) + H(1s) \Rightarrow H_2^+ + e, \qquad (1)$$
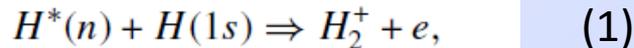
hydrogen in excited Rydberg state
in collision with hydrogen in ground state
we have asoc. ion.ization H_2^+ and e

Associative chemi-ion.

2 possible channels

$$H^*(n) + H(1s) \Rightarrow H(1s) + H^+ + e, \qquad (2)$$

Consequently, in this case the efficiency of the chemi-ionization processes has to be compared with the efficiency of the processes

$$H^*(n) + e \Rightarrow H^+ + 2e, \qquad (3)$$

Let us emphasize the fact that here as the starting point we focus on the hydrogen case, since our main aim is to draw attention of astronomers to the processes (1)–(2), and to show that the importance of these processes for non-local thermodynamic equilibrium (LTE) modeling of solar atmosphere should be investigated. For this purpose, it should be demonstrated that in the solar photosphere the efficiency of these processes is greater than, or at least comparable to, the efficiency of processes (3) within those ranges of values of $n \geq 2$ and temperature T which are relevant to the chosen solar atmosphere model.
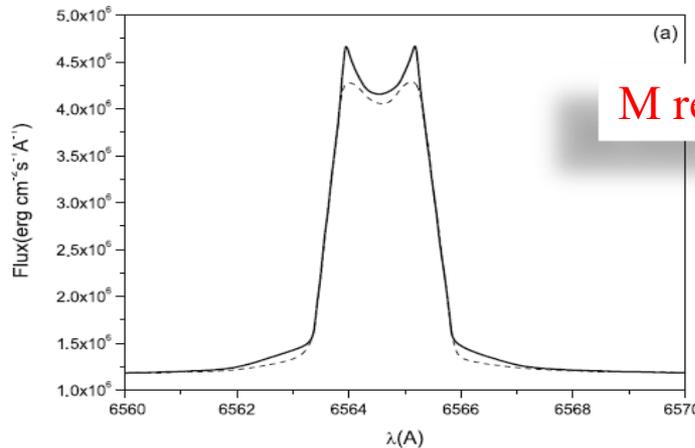
M red dwarf's

Fig. 6. Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for H_α line.
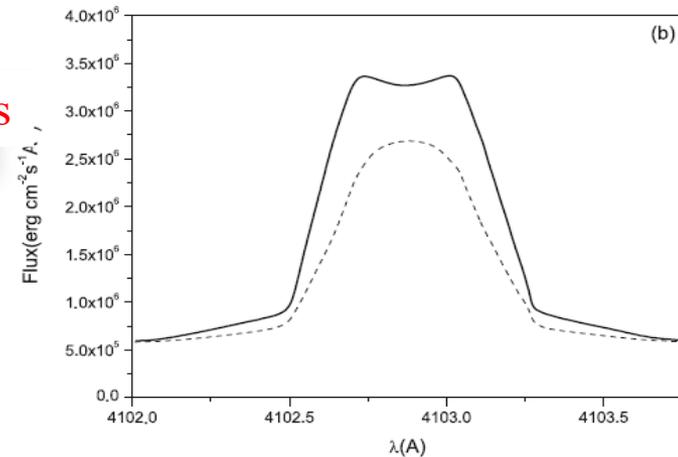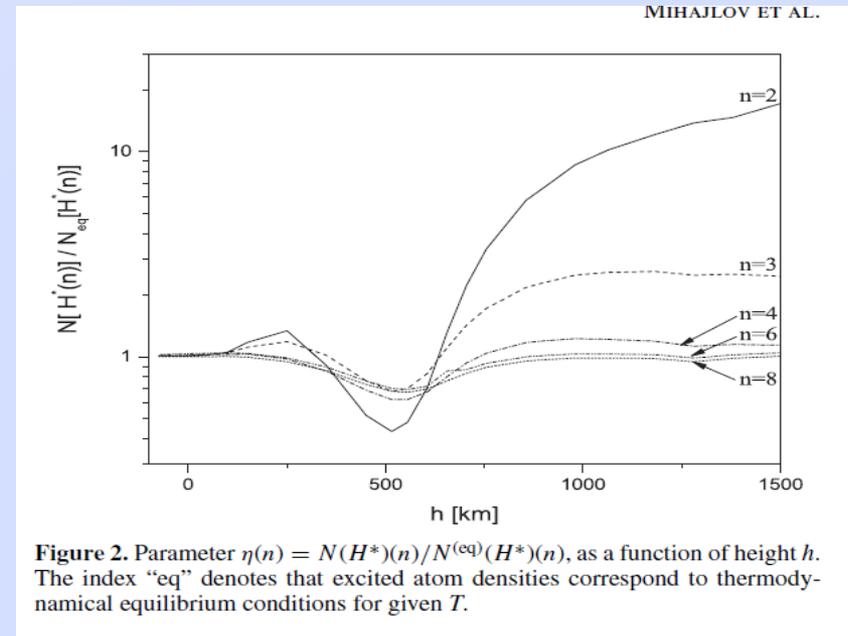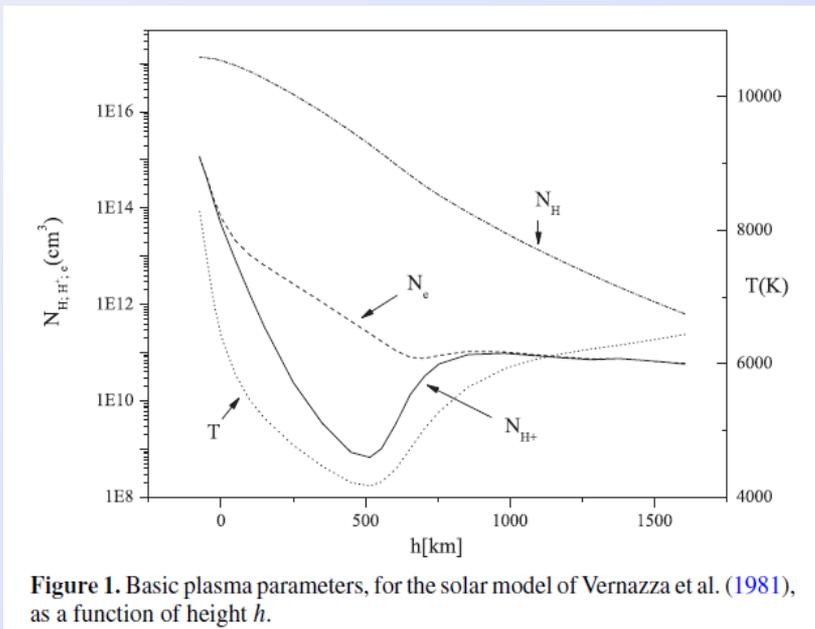
Fig. 7. Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for H_β line.

Important thing: Besides all that is mentioned above, the fact that the processes (1)–(2) could be very important for the solar photosphere is supported by the results obtained in Mihajlov et al. (2003a, 2007b), where these processes were included *ab initio* in a non-LTE modeling of an M red dwarf atmosphere with the effective temperature $T_{eff} = 3800$ K, using PHOENIX code (see Baron & Hauschildt 1998; Hauschildt et al. 1999; Short et al. 1999). A fact was established that including even the chemi-ionization/recombination only for $4 \leq n \leq 8$ generates significant changes (by up to 50%), at least in the populations of hydrogen-atom excited states with $2 \leq n \leq 20$, and if all these processes (with $n \geq 2$) are included, a significant change (somewhere up to 2–3 times) is also generated on the free electron density Ne, and, as one of further consequences, significant changes in hydrogen line profiles.

Idea: Keeping in mind that the compositions of the solar and the considered M red dwarf's photospheres are practically the same and the values of hydrogen-atom density, Ne, and T in these photospheres change within similar regions (Fontenla et al. 2007; Vernazza et al. 1981; Mihajlov et al. 2007b), one can expect that the influence of processes (1)–(2) on the hydrogen-atom excited states and free-electron populations in the solar atmosphere will be at least close to their influence in that of the M red dwarf, and that these processes will be very important for weakly ionized layers of the solar atmosphere.

The Considered Model of the Solar Photosphere

In accordance with the aim of this work, we consider here model C of solar atmosphere from Vernazza et al. (1981) and Fontenla et al. (2007). Namely, this is a non-LTE model which is still actual (see Stix 2002), and it is only for this model that all the quantities necessary for our calculations are available in tabular form as functions of height (h) in solar photosphere. In Figure 1, plasma parameters for this model are shown. More significant Fig 2. In Figure 2 are illustrated deviations of non-LTE populations of excited hydrogen atom states with $2 \leq n \leq 8$ in solar photosphere within the C model of Vernazza et al. (1981). One can see that these deviations are particularly exist for $n = 2$. Around $h = 500$ km $N\,(H^*(n = 2))$ is one-half of the corresponding equilibrium density, and for h larger than 1000 km it is around 10 times greater. These deviations rapidly decrease with an increase of n. However, even for $n = 8$ this deviation is around 40% around $h = 500$ km, illustrating the importance of taking into account the considered processes *ab initio* in the modeling of solar atmosphere

Figure 1. Basic plasma parameters, for the solar model of Vernazza et al. (1981), as a function of height h.

Figure 2. Parameter $\eta(n) = N(H^*)(n)/N^{(eq)}(H^*)(n)$, as a function of height h. The index "eq" denotes that excited atom densities correspond to thermodynamical equilibrium conditions for given T.

All <u>theoretical data</u> which are needed <u>given in next part:</u>

when one of the processes <u>(1) and (2)</u> is occurred, <u>the ionization probabilities</u> are obtained in the form

$$P_{ci}^{(a,b)}(n, \rho, E) = \frac{1}{2}\left(1 - e^{-2\int_{R_0}^{R_n} \frac{W_n(R)dR}{v_{rad}}}\right),$$

$$H^*(n) + H(1s) \Rightarrow H_2^+ + e,$$

$$H^*(n) + H(1s) \Rightarrow H(1s) + H^+ + e,$$
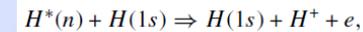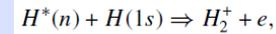
partial cross sections

$$\sigma_{ci}^{(a,b)}(n, E) = 2\pi \int_0^{\rho_{max}^{(a,b)}(E)} P_{ci}^{(a,b)}(n, \rho, E)\rho d\rho,$$

partial rate coefficients for the chemi-ionization processes (1) and (2)

Schematic, steps.

$$K_{ci}^{(a,b)}(n, T) = \int_{E_{min}^{(a,b)}(n)}^{E_{max}} v\sigma_{ci}^{(a,b)}(n, E)f(v; T)dv,$$

using partial rate coefficients for each channel we will determine the **total** one

Finally, using partial rate coefficients $K_{ci}^{(a,b)}(n, T)$, we will determine the total one, namely,

$$K_{ci}(n, T) = K_{ci}^{(a)}(n, T) + K_{ci}^{(b)}(n, T), \qquad (19)$$

The values of the total chemi-ionization rate coefficients obtained in the described way, are presented in Table 1 . This table cover the regions $2 \leq n \leq 8$ and $4000\ \text{K} \leq T \leq 10000\ \text{K}$. we can analyze importance of ch.ion. for solar photosphere (see Fig. Vernazza)

n →

T ↓

Table 1
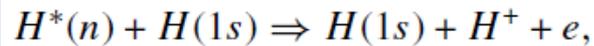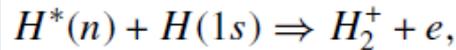Calculated Values of Coefficient K_{ci} (cm^3 s^{-1}) as a Function of n and T

T (K)	n						
	2	3	4	5	6	7	8
4000	0.150E−11	0.619E−09	0.126E−08	0.576E−09	0.554E−09	0.463E−09	0.366E−09
4250	0.202E−11	0.549E−09	0.106E−08	0.617E−09	0.583E−09	0.482E−09	0.378E−09
4500	0.260E−11	0.501E−09	0.900E−09	0.656E−09	0.611E−09	0.500E−09	0.389E−09
4750	0.324E−11	0.488E−09	0.833E−09	0.694E−09	0.637E−09	0.517E−09	0.400E−09
5000	0.403E−11	0.495E−09	0.815E−09	0.730E−09	0.662E−09	0.533E−09	0.410E−09
5250	0.504E−11	0.501E−09	0.800E−09	0.765E−09	0.686E−09	0.548E−09	0.420E−09
5500	0.623E−11	0.500E−09	0.782E−09	0.799E−09	0.709E−09	0.563E−09	0.428E−09
5750	0.756E−11	0.493E−09	0.764E−09	0.832E−09	0.731E−09	0.576E−09	0.437E−09
6000	0.909E−11	0.490E−09	0.757E−09	0.864E−09	0.752E−09	0.589E−09	0.445E−09
6250	0.108E−10	0.502E−09	0.766E−09	0.895E−09	0.772E−09	0.602E−09	0.453E−09
6500	0.128E−10	0.519E−09	0.783E−09	0.924E−09	0.791E−09	0.613E−09	0.460E−09
7000	0.175E−10	0.540E−09	0.808E−09	0.981E−09	0.827E−09	0.635E−09	0.473E−09
7500	0.232E−10	0.574E−09	0.848E−09	0.103E−08	0.860E−09	0.655E−09	0.485E−09
8000	0.300E−10	0.609E−09	0.891E−09	0.108E−08	0.892E−09	0.674E−09	0.497E−09
8500	0.380E−10	0.650E−09	0.939E−09	0.113E−08	0.920E−09	0.691E−09	0.507E−09
9000	0.470E−10	0.688E−09	0.986E−09	0.118E−08	0.948E−09	0.707E−09	0.516E−09
9500	0.574E−10	0.733E−09	0.104E−08	0.122E−08	0.973E−09	0.722E−09	0.525E−09
10000	0.689E−10	0.787E−09	0.109E−08	0.126E−08	0.997E−09	0.736E−09	0.533E−09

Relative contribution of partial chemi-ionization processes for given n and T with respect to the ch.-ion. total one are characterized by the corresponding branch coefficients

$$X_{ci}^{(a,b)}(n, T) = \frac{K_{ci}^{(a,b)}(n, T)}{K_{ci}(n, T)},$$

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

relative contributions of the associative ionization

$$H^*(n) + H(1s) \Rightarrow H_2^+ + e,$$

$$H^*(n) + H(1s) \Rightarrow H(1s) + H^+ + e,$$

when T increases X decreases i.e. rate coefficient for asoc. ion. (1) is smaller comparing to process (2) as is expected.

Table 3
Calculated Values of Coefficient $X^{(a)} \equiv K_{ci}^{(a)}/K_{ci} = K_{cr}^{(a)}/K_{cr}$ as a Function of n and T

T (K)	n						
	2	3	4	5	6	7	8
4000	0.998	0.955	0.877	0.507	0.408	0.335	0.281
4250	0.969	0.934	0.827	0.484	0.388	0.318	0.266
4500	0.924	0.907	0.765	0.463	0.371	0.303	0.254
4750	0.872	0.881	0.709	0.443	0.354	0.289	0.242
5000	0.819	0.857	0.664	0.425	0.339	0.277	0.231
5250	0.769	0.831	0.619	0.408	0.325	0.265	0.221
5500	0.721	0.800	0.568	0.393	0.312	0.254	0.212
5750	0.673	0.764	0.515	0.378	0.300	0.244	0.203
6000	0.627	0.728	0.466	0.364	0.288	0.235	0.196
6250	0.585	0.699	0.430	0.351	0.278	0.226	0.188
6500	0.546	0.672	0.399	0.339	0.268	0.218	0.182
7000	0.474	0.610	0.336	0.317	0.250	0.204	0.169
7500	0.414	0.558	0.289	0.297	0.235	0.190	0.158
8000	0.363	0.510	0.250	0.280	0.221	0.179	0.149
8500	0.321	0.469	0.220	0.264	0.208	0.169	0.141
9000	0.287	0.429	0.193	0.250	0.197	0.160	0.133
9500	0.258	0.398	0.174	0.237	0.187	0.151	0.126
10000	0.234	0.376	0.160	0.225	0.177	0.144	0.120

Comparison of Fluxes of the Considered Processes and concurrent

$I_{ci}(n, T)$ is the total flux caused by the chemi-ionization processes (1, 2)

$$I_{ci}(n, T) = K_{ci}(n, T) \cdot N_n N_1,$$

$$H^*(n) + H(1s) \Rightarrow H(1s) + H^+ + e,$$

$$H^*(n) + H(1s) \Rightarrow H_2^+ + e,$$
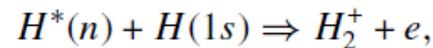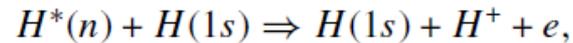
where N_1, N_n, N_i, and N_e are, respectively, the densities of the ground and excited states of a hydrogen atom, of ion H^+, and of free electron in the considered plasma with given T.

and $I_{i;ea}(n, T)$, be the fluxes caused by the concurrent ionization processes
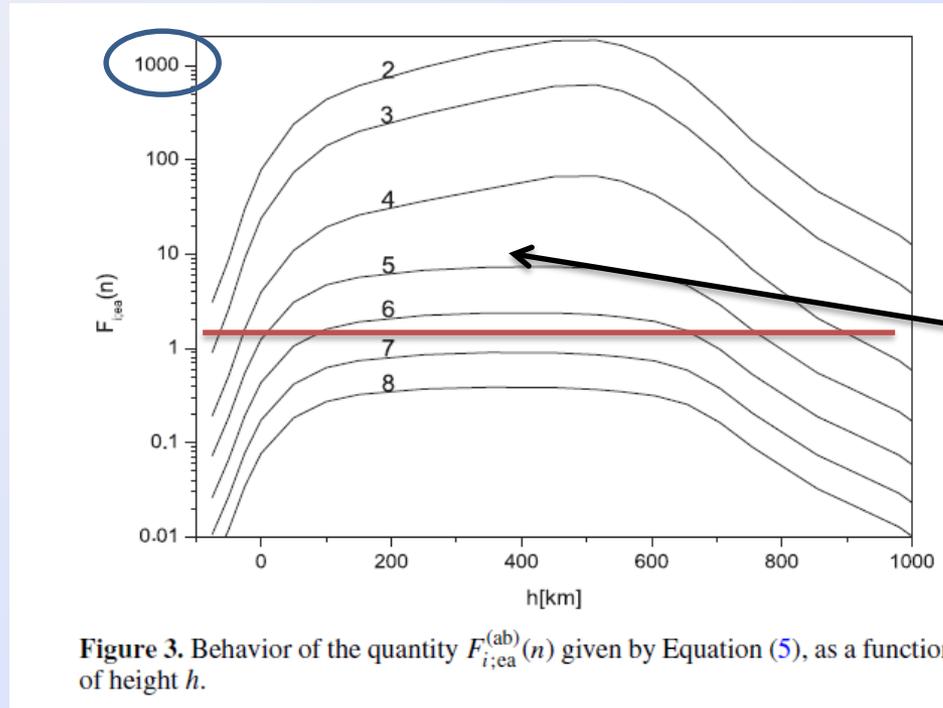
$$I_{i;ea}(n, T) = K_{ea}(n, T) \cdot N_n N_e,$$

$$H^*(n) + e \Rightarrow H^+ + 2e,$$
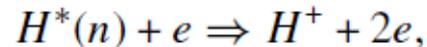
Using these expressions, we first calculate quantities *Fi (n, T)* which characterize the relative efficiency of **partial** chemi-ionization processes (1, 2) together and the impact electron–atom ionization (3) in the considered plasma.

$$F_i(n, T) = \frac{I_{ci}(n, T)}{I_{i;ea}(n, T)} = \frac{K_{ci}(n, T)}{K_{ea}(n, T)} \cdot N_1 / N_e, \qquad \text{RATIO}$$

impact ionization rate coefficients $K_{ea}(n, T)$ are taken from Vriens & Smeets (1980).

$$F_i(n, T) = \frac{I_{ci}(n, T)}{I_{i;ea}(n, T)} = \frac{K_{ci}(n, T)}{K_{ea}(n, T)} \cdot N_1/N_e,$$
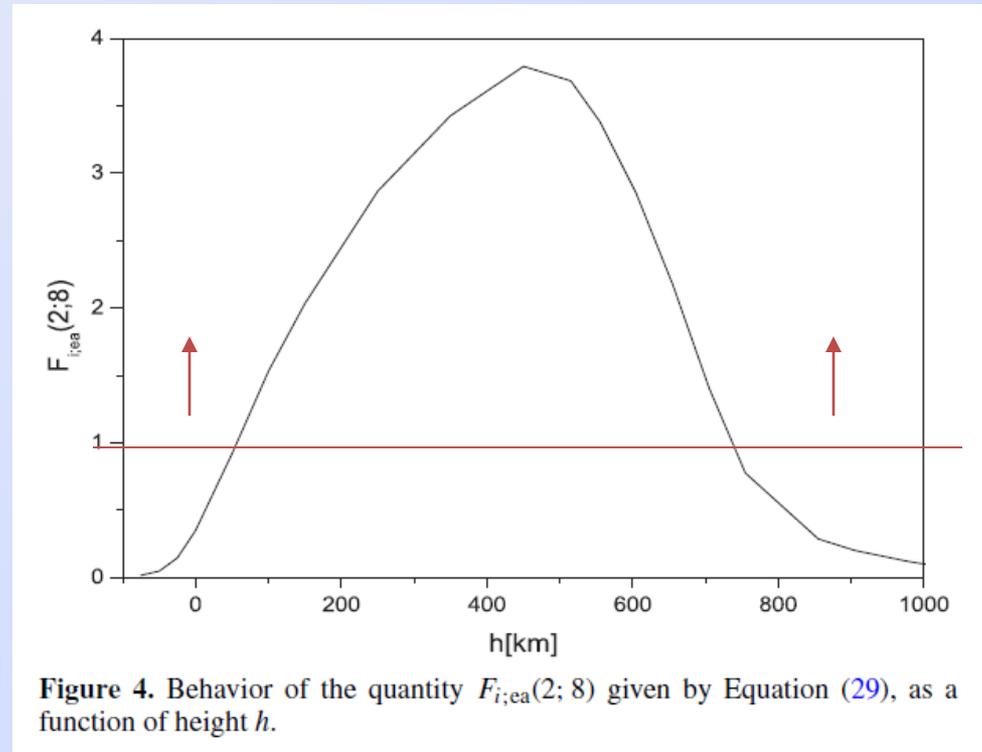
Partial i.e. for every n

Figure 3. Behavior of the quantity $F_{i;ea}^{(ab)}(n)$ given by Equation (5), as a function of height h.

In Figure 3, the behavior of the quantities $F_{i,ea}(n, T)$ for $2 \leq n \leq 8$ as functions of height h is shown, according to the data (N_1 ground state dency, N_e, and T) from Vernazza et al. (1981) for solar photosphere. One can see that the efficiency of the considered chemi-ionization processes in comparison with the electron–atom impact ionization is dominant for $2 \leq n \leq 6$ and becomes comparable for $n = 7$ and 8.

in order to compare the relative influence of the chemi-ionization processes (1) and (2) together to that of the impact electron–atom ionization process (5) on the whole block of the excited hydrogen atom states with $2 \leq n \leq 8$, we will calculate quantity $F_{i,ea;2-8}(T)$, given by

summing

$$F_{i,\mathrm{ea};2-8}(T) = \frac{\sum_{n=2}^{8} I_{\mathrm{ci}}(n, T)}{\sum_{n=2}^{8} I_{i;\mathrm{ea}}(n, T)}$$
$$= \frac{\sum_{n=2}^{8} K_{\mathrm{ci}}(n, T) \cdot N_n}{\sum_{n=2}^{8} K_{\mathrm{ea}}(n, T) \cdot N_n} \cdot N_i/N_e,$$

Figure 4. Behavior of the quantity $F_{i;\mathrm{ea}}(2; 8)$ given by Equation (29), as a function of height h.

In Figure 4, the behavior of the quantity $F_{i,\mathrm{ea};2-8}(T)$ as functions of height h is shown according to the same data from Vernazza et al. (1981). As one can see, the real influence of the chemi-ionization processes on the total populations of states with $2 \leq n \leq 8$ remains dominant with respect to the concurrent electron–atom impact ionization processes almost in the whole photosphere (50 km $\leq h \leq$ 750 km). This means that the chemi-ionization processes influence the radiative properties of the whole solar atmosphere in the optical region.

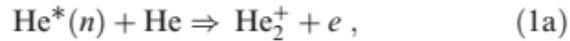## Main result. From ApJS few years ago 2011

The obtained results demonstrate the fact that the considered chemi-ionization processes have a very significant influence on the optical properties of the solar photosphere in comparison with the concurrent electron–atom impact ionization processes.

Thus, it is shown that the importance of these processes for non-LTE modeling of solar atmosphere should be necessarily investigated.

End of the first part for solar atmospheres

Present the investigation of symmetrical chemi-ionization processes of the helium atom in weakly ionized layers of helium-rich DB white dwarfs.

$$\text{He}^*(n) + \text{He} \Rightarrow \text{He}_2^+ + e \,, \qquad (1a)$$

$$\text{He}^*(n) + \text{He} \Rightarrow \text{He} + \text{He}^+ + e \,, \qquad (1b)$$

symmetrical chemi-ionization processes have been considered in domains of principal quantum numbers $n \geq 3$ and temperatures $12\,000\,\text{K} \leq T_{eff} \leq 30\,000\,\text{K}$

Results showed that these processes can be dominant ionization mechanisms in helium-rich DB white dwarf atmosphere layers for log g = 7 and 8 and T_{eff} ≤ 20000 K and have to be implemented in relevant models of weakly ionized helium plasmas

The influence of examined processes is determined by comparison with other relevant ionization processes, electron-Rydberg atom impact ionization

$$\text{He}^*(n) + e \Rightarrow \text{He}^+ + e + e \,, \qquad (2)$$
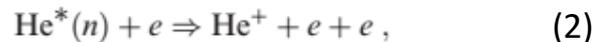
$$\boxed{\text{Theory}}$$

total chemi-ionization rate coefficients as sum of partial (1a) and (1b).

$$K_i^{(ab)}(n;\ T) = K_i^{(a)}(n;\ T) + K_i^{(b)}(n;\ T)\ ,$$

$I_i^{(a;b)}$ denote part. fluxes due to processes (1a)–(2b), respectively.

$$I_i^{(a)}(n;\ T) = K_i^{(a)}(n, T) \cdot N(\text{He}) \cdot N(\text{He}^*(n))\ ,$$
$$I_i^{(b)}(n;\ T) = K_i^{(b)}(n, T) \cdot N(\text{He}) \cdot N(\text{He}^*(n))\ ,$$

where $N(\text{He})$ and $N(\text{He}^*(n))$ denote He($1s^2$) atom and He*(n) Rydberg atom ($n \geq 3$) densities, and $K_i^a(n;\ T)$ and $K_i^b(n;\ T)$ denote rate coefficients of processes (1a) and (1b).

We have the total chemi-ionization fluxes $I_i^{(ab)}$

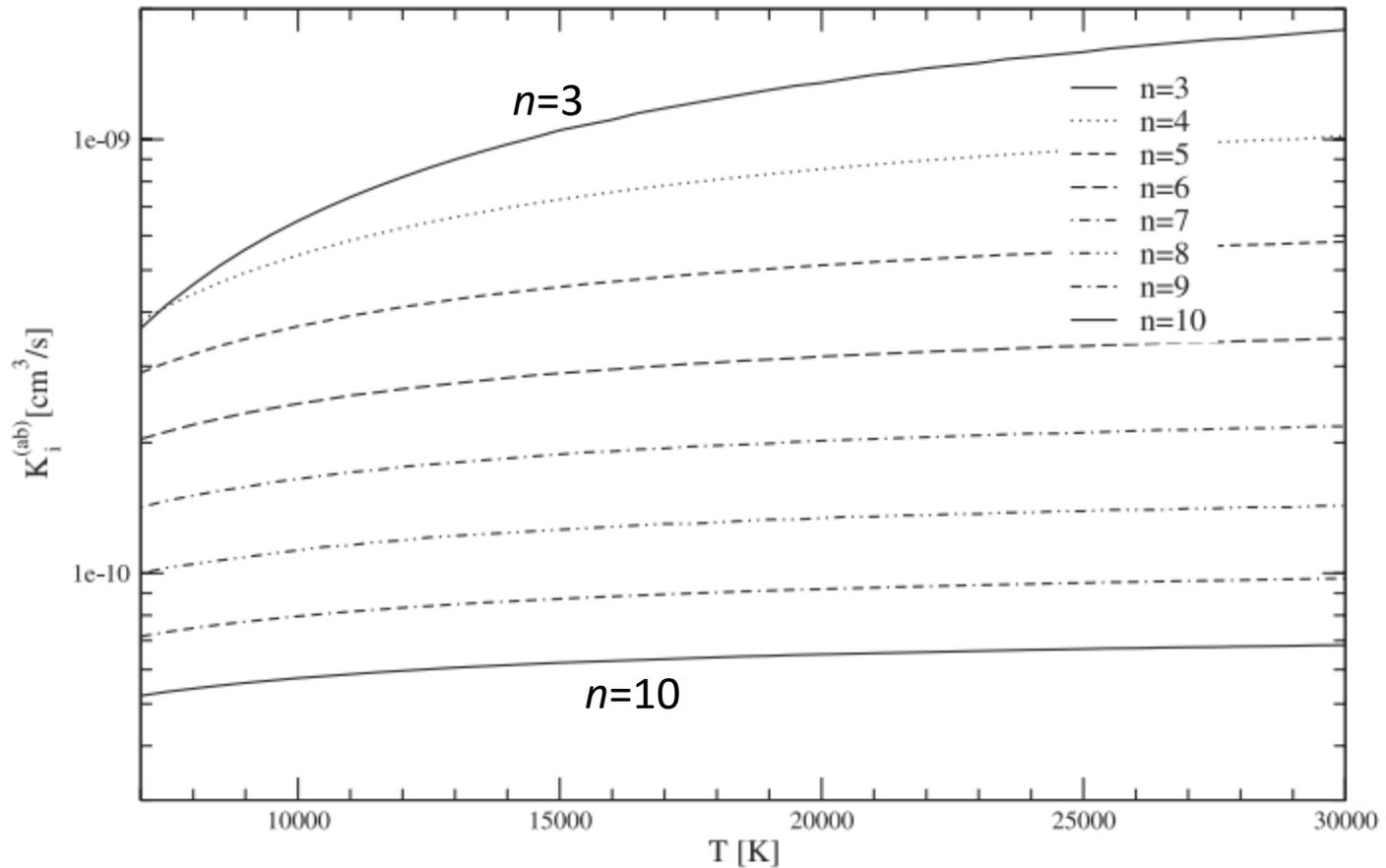$$I_i^{(ab)}(n;\ T) = I_i^{(a)}(n;\ T) + I_i^{(b)}(n;\ T)\ ,$$

FIG. 1.—Total chemi-ionization rate coefficients, $K_i^{(ab)}(n, T)$, with $7000\ \text{K} \leq T \leq 30{,}000\ \text{K}$ and for principal quantum numbers $n = 3$–10

Rate coefficient as a function of temp.

Parameter X which describe the relative importance of the particular channel ("a" and "b") of the considered processes.

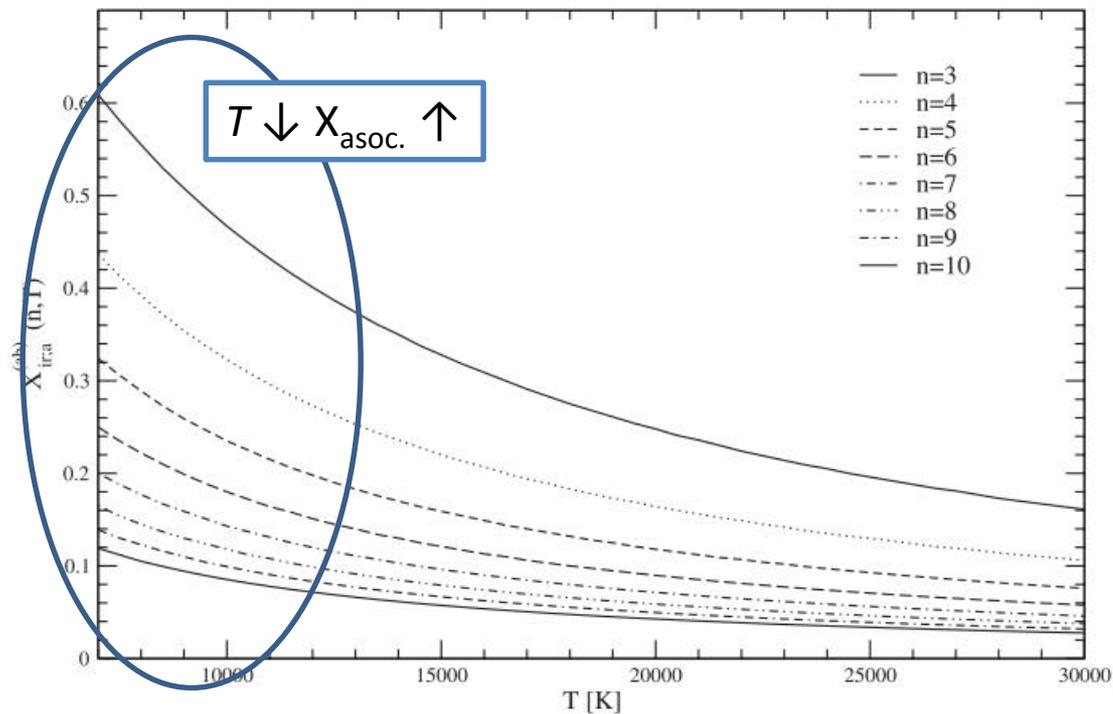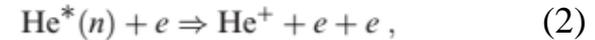$$X_{ir;a,b}^{(ab)}(n, T) = \frac{I_i^{(a,b)}(n, T)}{I_i^{(ab)}(n, T)}$$

FIG. 3.—Same as in Fig. 1 but for the parameter $X_{ir;a}^{(ab)}(n, T)$, characterizing the relative importance of the particular channel ("a" and "b") for the chemi-ionization and chemi-recombination processes.

Other, concurrent ionization processes

electron-excited atom impact ionization (eq. [2])

$$\mathrm{He}^*(n) + e \Rightarrow \mathrm{He}^+ + e + e \,, \qquad (2)$$

flux

$$I_i^{(ea)}(n, T) = \alpha_i^{(ea)}(n, T) \cdot N(\mathrm{He}^*(n)) \cdot N(e) \,,$$

$\alpha_i^{(ea)}(n, T)$ the ionization and rate coefficients determined by semiempirical expressions from Vriens & Smeets (1980).

The relative importance of chemi-ionization (eqs. [1a]– [1b]) processes in comparison with electron-excited atom impact ionization (eq. [3]), processes is characterized by parameters $F_{ir}^{(ab)}$ defined as ratios of the corresponding fluxes:

where η_e^a denotes He atom and free electron densities ratio

$$F_{ir}^{(ab)}(n, T) = \frac{I_i^{(ab)}(n, T)}{I_i^{(ea)}(n, T)}$$

$$F_{ir}^{(ab)}(n, T) = \frac{K_i^{(ab)}(n, T)}{\alpha_i^{(ea)}(n, T)} \cdot \eta_e^a$$
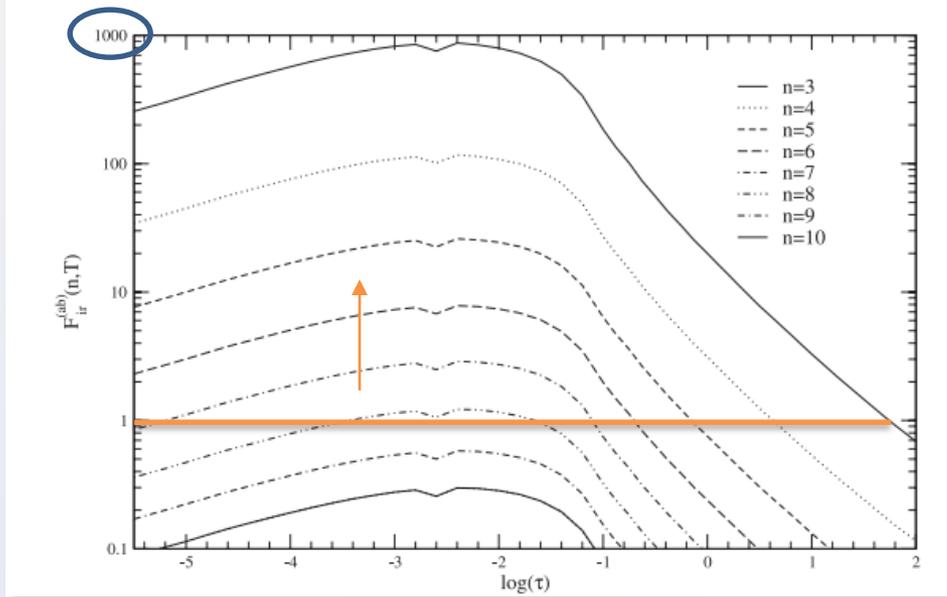
$$\eta_e^a = \frac{N(\mathrm{He})}{N(e)} \,.$$

Fig. 4.—Parameter $F_b^{(ab)}(n, T)$ as a function of the logarithm of Rosseland optical depth $\log \tau$, for principal quantum numbers $n = 3$–10, with $T_{eff} = 12{,}000$ K and $\log g = 8$.
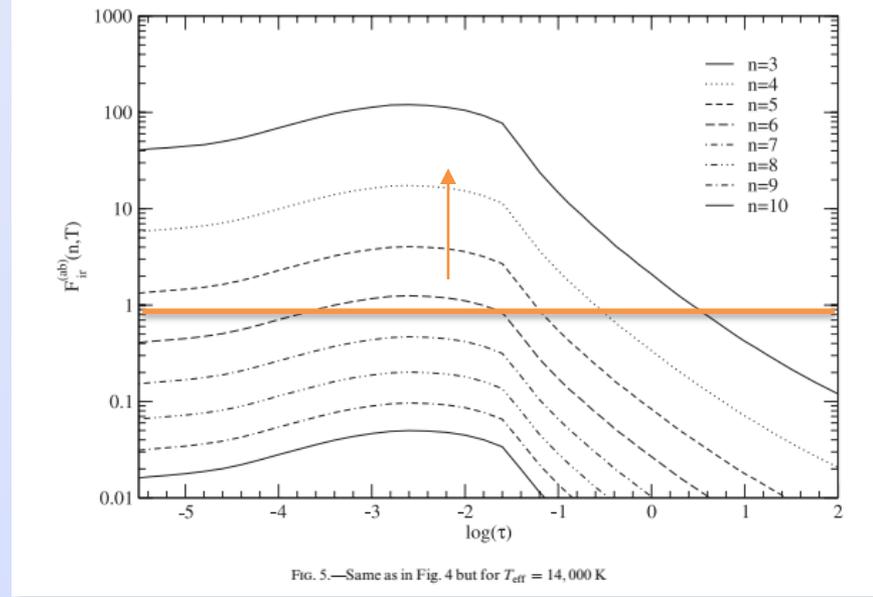
Fig. 5.—Same as in Fig. 4 but for $T_{eff} = 14{,}000$ K

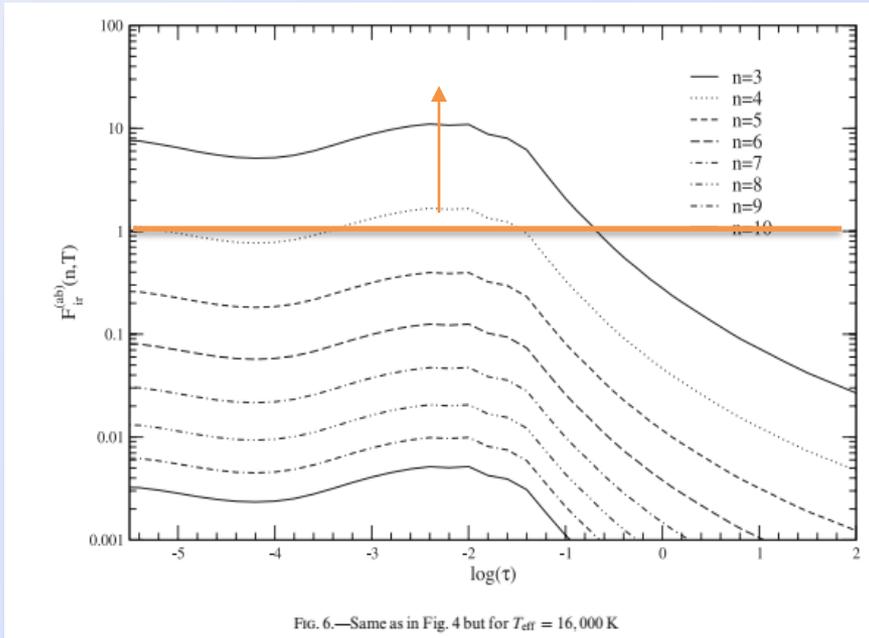$$T_{eff} \uparrow F \downarrow$$

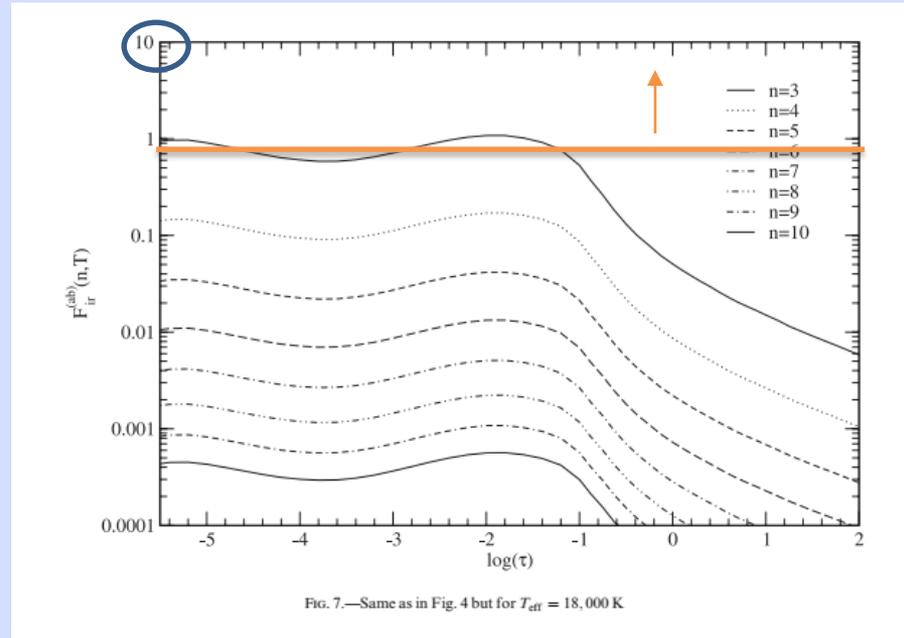Fig. 6.—Same as in Fig. 4 but for $T_{eff} = 16{,}000$ K

Fig. 7.—Same as in Fig. 4 but for $T_{eff} = 18{,}000$ K

Conclusion

from the papers we published few years ago
in ApJS and Baltic Astr. 2011 is

The influence of the chemi-ionization (eqs. [1a]–[1b]) processes must be taken into account for the *ab initio* modeling of helium-rich DB white dwarf atmospheres, for log g = 7 and 8 and $T_{eff} \leq 20\ 000$ K, since they would influence the basic structure of the atmosphere model. These results and similar ones for hydrogen solar plasma clearly proved the importance of the symmetrical chemi-ionization processes in weakly ionized layers of stellar atmospheres.

End of the first part for WD atmospheres

In our previous research has been notice that such inelastic processes in atom Rydberg-atom collisions, as chemi-ionization and (n-n') mixing, should be considered together.

In this context will be considered the **influence** of the (n-n')-mixing during a symmetric atom Rydberg-atom collision processes **on the intensity** of chemi-ionization process. It will be taken into account $A + A^*(n,l)$ collisional systems, where the principal quantum number n >> 1, where A=H or He

$$A^*(n,l) + A \rightarrow A + A^*(n',l'),$$
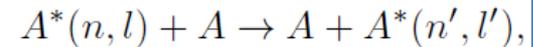
For the first time theoretically to describe together with 1 rate coeff.
Real influence of atom-Rydberg atom processes (chi+mix) in stellar atm.

It will be demonstrated that the inclusion of (n-n') mixing in the calculation, influences significantly on the values of chemi-ionization rate coefficients (reducing it), particularly in the lower part of the block of the Rydberg states.

Two groups of inelastic processes in slow atom- Rydberg atom collisions, namely: chemi-ionization processes, including the processes of associative ionization and the processes of so called (n-n')-mixing, were for a longer time examined and discussed in literature. Let us note that concerning the processes of chemi-ionization, symmetrical as well as non-symmetrical atom-Rydberg atom collisions have been considered, while the (n-n')- mixing processes have been considered only in the case of symmetrical collisions.

We note that several unsolved problems remained concerning the mentioned processes, connected with the fact that theoretical investigations and interpretation of existing experimental results have been based on the semi-classical approximation. However, as the principal problem we see the fact that the processes of chemi-ionization and (n-n')-mixing in symmetrical atom-Rydberg atom collisions have been up to now considered independently, in spite that one considers that as the ones as well the others are conditioned by the same mechanism[2]. We have in view here the so called dipole resonant mechanism, described several times in literature and discussed in details in Mihajlov et al. (2012).

chemi-ionization processes

$$A^*(n,l) + A \rightarrow A + A^+ + \vec{e} \qquad \text{(1a)}$$

$$A^*(n,l) + A \rightarrow A_2^+ + \vec{e} \qquad \text{(1b)}$$
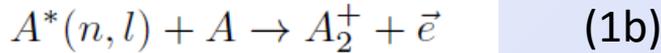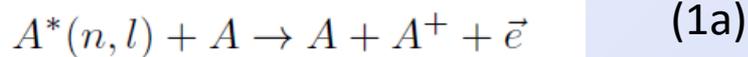
and (n-n')-mixing processes, i.e. excitation-deexcitation processes

$$A^*(n,l) + A \rightarrow A + A^*(n',l'), \qquad \text{(2)}$$
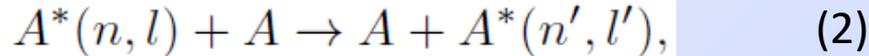
where A and $A^*(n,l)$ denote atoms in the ground and in a highly excited (Rydberg) state with the given principal and otrbital quantum numbers n and l, A^+ and $\vec{e}$ - atomic ion in the ground state and free electron, and A_2^+ molecular ion in the ground state. These processes are illustrated in Fig 1a and Fig 1b.

In this work we will investigate the influence of processes (2) on the processes of chemi-ionization (1a) and (1b).

Here, **as first** is described for this purpose, the way of inclusion of process (2) in the procedure of calculation of rate coefficients of the chemi-ionization processes (1a,b).
Their values are determined under the conditions characteristic for the Solar photosphere in the case $A = H(1s)$ and $A = He(1s^2)$ in the case of atmosphere of DB white dwarfs.
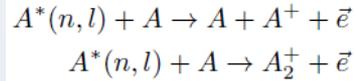
Than, the determined here values of these rate coefficients, are compared with the rate coefficients of the same chemi-ionization processes, determined also for the Solar photosphere and DB WD atm. in the previous articles Mihajlov et al. (2003, 2011a, 2011b), but without inclusion of (n-n')-mixing processes. We draw attention that, as a difference from this previous article, chemi-ionization rate coefficients are here without the simplification of the expression for Gaunt factor,

Expressions now without simplification comparing to Mihajlov et al. (2003;2011) and with averaging

Besides, here, as a difference from Mihajlov et al. (2003; 2011a; 2011b), the average chemi-ionization rate coefficient for a given n is obtained as a result of the corresponding averaging of partial chemi-ionization rate coefficients for every l where $0 \leq l \leq n$-1. l orbital quantum number and n principal q.n
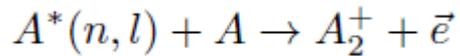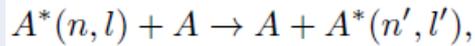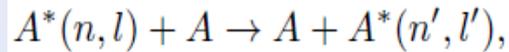
2. THE THEORY

2.1. General formulas

$$A^*(n,l) + A \rightarrow A + A^+ + \vec{e}$$
$$A^*(n,l) + A \rightarrow A_2^+ + \vec{e}$$

A)

+ pre-ionization

$$A^*(n,l) + A \rightarrow A + A^*(n',l'),$$

$$A^*(n,l) + A \rightarrow A_2^+ + \vec{e}$$

B)

+ pre-ionization

$$A^*(n,l) + A \rightarrow A + A^*(n',l'),$$

$K_{1a}(n; l; T)$ and $K_{1b}(n; l; T)$ are <u>partial rate coefficients</u> of processes (1a) and (1b) (+pre-ionization), separately determined for given n, l and T, where T is temperature of the considered plasma,

$K_1(n; l; T)$ is the <u>partial rate</u> coefficient of processes (1a) and (1b)(+ pre-ionization) together, namely $K_1(n; l; T) = K_{1a}(n; l; T) + K_{1b}(n; l; T)$ for given n, l and T.

<u>average tot.</u> rate coefficient for 1a and 1b

$$K_{1;n}(T) = \frac{1}{n^2} \cdot \sum_{l=0}^{n-1} (2l+1) \cdot K_1(n,l;T),$$

<u>average rate coefficient</u> for <u>associative</u> ionization

$$K_{1b;n}(T) = \frac{1}{n^2} \cdot \sum_{l=0}^{n-1} (2l+1) \cdot K_{1b}(n,l;T).$$

<u>Partial rate coefficients</u> $K_1(n; l; T)$ and $K_{1b}(n; l; T)$ are determined on the basis of standard expressions

$$K_1(n,l;T) = \int_{E_{n;i}}^{\infty} \sigma_1(n,l;E) \left(\frac{2E}{\mu_{red}}\right) f_T(E)dE,$$

$$K_{1b}(n,l;T) = \int_{E_{n;i}}^{\infty} \sigma_{1b}(n,l;E) \left(\frac{2E}{\mu_{red}}\right) f_T(E)dE,$$

$\sigma_1(n,l;E)$ and $\sigma_{1b}(n,l;E)$ are the corresponding cross sections

$$\sigma_1(n,l;E) = 2\pi \int_0^{\rho_{1;max}} P_1(n,l;\rho;E)\rho d\rho,$$

$$\sigma_{1b}(n,l;E) = 2\pi \int_0^{\rho_{1b;max}} P_{1b}(n,l;\rho;E)\rho d\rho$$

mix.　　　　　chemi-ion. 1a+1b

$$P_1(n, l; \rho; E) = \frac{1}{2} \cdot p_{keep}(n, l; \rho; E) \cdot p_{i;1}(n, l; \rho; E),$$

for A) probabil. for process. (1a+1b)+pre-ioniz.

$$P_{1b}(n, l; \rho; E) = \frac{1}{2} \cdot p_{keep}(n, l; \rho; E) \cdot p_{i;1b}(n, l; \rho; E)$$

for B) probabil. for process. (1b)+pre-ioniz.

chemi-ion. 1b

Probability of ionization decay

Due to the chemi-ionization

$$p_{i;1}(n, l; \rho; E) = 1.0 - \exp(-2q_{i;1}),$$

$$p_{i;1b}(n, l; \rho; E) = \exp(-q_{i;2}) \cdot [1.0 - \exp(-2q_{i;as})],$$

where the quantities $q_{i;1}$, $q_{i;2}$ and $q_{i;as}$ are given as

$$q_{i;as} = q_{i;1} - q_{i;2}, \quad q_{i;1} = \int_{R_0}^{R_{n;i}} \frac{W_i(n, l; R)}{v_{rad}(E, \rho; R)} dR,$$

$$q_{i;2} = \int_{R_{1b;max}}^{R_{n;i}} \frac{W_i(n, l; R)}{v_{rad}(E, \rho; R)} dR,$$

Due to the mixing process.

one can notice that the basic difference, in comparison with previous papers, represents direct taking into account of the effect of decay of the initial electronic state of the considered atom-Rydberg atom system, due to the possibility of execution of excitation processes (2) with $n' > n$.

Partial pre-ionization probability

$$p_{keep}(n, l; \rho; E) = \prod_{p=1}^{5} p_{p;keep}(n, l; \rho; E),$$

$$p_{p;keep}(n, l; \rho; E) = \exp(-x_p),$$

$$x_p = \int_{R_{n;n+p+1-\delta_n}}^{R_p} \frac{w_{n;n+p}(n, l : R)}{v_{rad}(E, \rho, R)},$$

Results:

Total values of the rate coefficients of chemi-ionization processes (+pre-ionozation) $K_1(n;T)$ within the range $3 \leq n \leq 14$ are presented in Tab. 1. Bearing in mind the main application, of here obtained results, on the photosphere and lower chromosphere of the Sun, calculations of these rate coefficients were performed here for temperatures $4000\text{ K} \leq T \leq 10000\text{ K}$.

$n \longrightarrow$

Hydrogen

$T \downarrow$

Table 1
Calculated Values of Coefficient $K_{1;n}(T)\ (\text{cm}^3\ \text{s}^{-1})$ as a function of n and T.

T	3	4	5	6	7	8	9	10	11	12	13	14
4000	7.17E-12	1.54E-10	3.58E-10	4.28E-10	3.98E-10	3.30E-10	2.61E-10	2.06E-10	1.63E-10	1.28E-10	1.02E-10	8.14E-11
4250	9.01E-12	1.63E-10	3.88E-10	4.52E-10	4.15E-10	3.42E-10	2.69E-10	2.11E-10	1.66E-10	1.31E-10	1.04E-10	8.28E-11
4500	1.11E-11	1.72E-10	4.16E-10	4.76E-10	4.32E-10	3.53E-10	2.76E-10	2.16E-10	1.70E-10	1.33E-10	1.06E-10	8.40E-11
4750	1.33E-11	1.83E-10	4.43E-10	4.98E-10	4.48E-10	3.63E-10	2.83E-10	2.20E-10	1.73E-10	1.35E-10	1.07E-10	8.51E-11
5000	1.53E-11	1.96E-10	4.71E-10	5.20E-10	4.63E-10	3.72E-10	2.89E-10	2.24E-10	1.76E-10	1.38E-10	1.09E-10	8.62E-11
5250	1.73E-11	2.12E-10	4.98E-10	5.42E-10	4.77E-10	3.81E-10	2.95E-10	2.28E-10	1.78E-10	1.40E-10	1.10E-10	8.73E-11
5500	1.96E-11	2.31E-10	5.26E-10	5.63E-10	4.90E-10	3.89E-10	3.01E-10	2.31E-10	1.80E-10	1.41E-10	1.11E-10	8.84E-11
5750	2.30E-11	2.51E-10	5.53E-10	5.83E-10	5.03E-10	3.96E-10	3.06E-10	2.35E-10	1.82E-10	1.43E-10	1.13E-10	8.94E-11
6000	2.81E-11	2.71E-10	5.79E-10	6.03E-10	5.15E-10	4.04E-10	3.11E-10	2.38E-10	1.84E-10	1.44E-10	1.14E-10	9.03E-11
6250	3.53E-11	2.91E-10	6.03E-10	6.21E-10	5.26E-10	4.11E-10	3.16E-10	2.41E-10	1.86E-10	1.46E-10	1.15E-10	9.12E-11
6500	4.37E-11	3.11E-10	6.26E-10	6.39E-10	5.37E-10	4.17E-10	3.20E-10	2.44E-10	1.88E-10	1.47E-10	1.16E-10	9.19E-11
7000	6.01E-11	3.50E-10	6.70E-10	6.72E-10	5.59E-10	4.30E-10	3.28E-10	2.50E-10	1.92E-10	1.49E-10	1.18E-10	9.33E-11
7500	7.08E-11	3.90E-10	7.13E-10	7.03E-10	5.80E-10	4.43E-10	3.36E-10	2.55E-10	1.95E-10	1.51E-10	1.20E-10	9.46E-11
8000	7.91E-11	4.31E-10	7.54E-10	7.31E-10	5.99E-10	4.55E-10	3.44E-10	2.60E-10	1.98E-10	1.54E-10	1.21E-10	9.57E-11
8500	8.91E-11	4.71E-10	7.93E-10	7.57E-10	6.14E-10	4.65E-10	3.51E-10	2.64E-10	2.01E-10	1.56E-10	1.22E-10	9.66E-11
9000	9.91E-11	5.13E-10	8.27E-10	7.82E-10	6.27E-10	4.74E-10	3.56E-10	2.68E-10	2.04E-10	1.58E-10	1.23E-10	9.74E-11
9500	1.06E-10	5.56E-10	8.57E-10	8.06E-10	6.40E-10	4.82E-10	3.61E-10	2.72E-10	2.06E-10	1.59E-10	1.25E-10	9.82E-11
10000	1.07E-10	6.03E-10	8.82E-10	8.30E-10	6.55E-10	4.90E-10	3.66E-10	2.75E-10	2.08E-10	1.61E-10	1.26E-10	9.91E-11

The processes (1b) are characterized in this paper via the corresponding branch coefficient $X_{1b;n}(T)$ given as

Table 2
Calculated Values of The Branch Coefficient $X_{1b;n}$ as a function of n and T.

T	3	4	5	6	7	8	9	10	11	12	13	14	15
4000	0.684	0.608	0.458	0.365	0.306	0.243	0.218	0.208	0.201	0.186	0.169	0.154	0.137
4250	0.607	0.563	0.437	0.346	0.284	0.232	0.211	0.202	0.195	0.178	0.160	0.143	0.129
4500	0.543	0.519	0.421	0.329	0.265	0.222	0.206	0.198	0.189	0.170	0.152	0.132	0.122
4750	0.497	0.475	0.407	0.314	0.248	0.213	0.201	0.194	0.184	0.162	0.144	0.122	0.114
5000	0.467	0.431	0.395	0.301	0.232	0.205	0.197	0.190	0.180	0.155	0.137	0.112	0.108
5250	0.473	0.427	0.370	0.284	0.223	0.201	0.193	0.185	0.172	0.146	0.130	0.109	0.104
5500	0.467	0.419	0.347	0.269	0.215	0.197	0.189	0.181	0.164	0.137	0.123	0.107	0.101
5750	0.442	0.411	0.328	0.254	0.208	0.193	0.186	0.177	0.157	0.128	0.116	0.104	0.098
6000	0.397	0.403	0.310	0.242	0.201	0.190	0.183	0.173	0.150	0.119	0.110	0.101	0.095
6250	0.349	0.380	0.294	0.229	0.197	0.187	0.179	0.166	0.142	0.116	0.107	0.099	0.092
6500	0.308	0.360	0.279	0.218	0.194	0.184	0.175	0.159	0.134	0.113	0.104	0.096	0.089
7000	0.263	0.327	0.254	0.198	0.187	0.178	0.169	0.146	0.118	0.106	0.098	0.092	0.083
7500	0.223	0.292	0.234	0.190	0.180	0.172	0.157	0.133	0.112	0.101	0.093	0.086	0.078
8000	0.199	0.263	0.216	0.183	0.173	0.167	0.146	0.120	0.105	0.096	0.087	0.081	0.073
8500	0.198	0.243	0.194	0.178	0.169	0.161	0.134	0.112	0.100	0.092	0.083	0.075	0.070
9000	0.198	0.225	0.175	0.173	0.165	0.156	0.123	0.105	0.095	0.087	0.080	0.069	0.067
9500	0.201	0.210	0.164	0.167	0.161	0.142	0.116	0.099	0.091	0.084	0.075	0.067	0.065
10000	0.218	0.196	0.155	0.161	0.156	0.129	0.109	0.095	0.087	0.081	0.071	0.066	0.063

when T increases X decreases i.e. rate coefficient for asoc. ion. (1) is smaller comparing to process (2) as is expected.

In accordance with the above said rate coefficients are determined here by adding on of the probability of the decay of the initial state of the collisional system in pre-ionization zone with Rydberg electron transitions from state $\lvert n >$ to state $\lvert n+p >$, where $1 \leq p \leq 5$.

Helium

n →

T ↓

Table 3
Calculated Values of Coefficient $K_{1;n}(T)(\text{cm}^3\ \text{s}^{-1})$ as a function of n and T. Helium case.

T	3	4	5	6	7	8	9	10	11	12	13	14	15
7000	1.54E-11	8.33E-11	1.53E-10	1.43E-10	1.15E-10	8.78E-11	6.59E-11	4.95E-11	3.78E-11	2.92E-11	2.27E-11	1.81E-11	1.45E-11
8000	2.10E-11	1.11E-10	1.70E-10	1.59E-10	1.23E-10	9.25E-11	6.90E-11	5.13E-11	3.93E-11	3.03E-11	2.34E-11	1.85E-11	1.48E-11
10000	3.36E-11	1.75E-10	2.06E-10	1.76E-10	1.35E-10	1.00E-10	7.33E-11	5.45E-11	4.11E-11	3.16E-11	2.44E-11	1.92E-11	1.53E-11
12000	4.74E-11	2.11E-10	2.41E-10	1.93E-10	1.45E-10	1.06E-10	7.69E-11	5.68E-11	4.26E-11	3.26E-11	2.51E-11	1.98E-11	1.57E-11
14000	6.75E-11	2.44E-10	2.64E-10	2.08E-10	1.53E-10	1.11E-10	7.99E-11	5.87E-11	4.39E-11	3.34E-11	2.57E-11	2.02E-11	1.60E-11
16000	8.57E-11	2.71E-10	2.87E-10	2.19E-10	1.59E-10	1.14E-10	8.23E-11	6.03E-11	4.47E-11	3.42E-11	2.61E-11	2.06E-11	1.63E-11
18000	9.83E-11	2.89E-10	3.05E-10	2.30E-10	1.65E-10	1.17E-10	8.42E-11	6.15E-11	4.57E-11	3.46E-11	2.66E-11	2.08E-11	1.65E-11
20000	1.13E-10	3.02E-10	3.21E-10	2.39E-10	1.70E-10	1.20E-10	8.62E-11	6.24E-11	4.64E-11	3.52E-11	2.69E-11	2.11E-11	1.67E-11
22000	1.29E-10	3.17E-10	3.30E-10	2.47E-10	1.74E-10	1.23E-10	8.77E-11	6.34E-11	4.71E-11	3.56E-11	2.72E-11	2.13E-11	1.69E-11
24000	1.49E-10	3.33E-10	3.36E-10	2.54E-10	1.78E-10	1.25E-10	8.87E-11	6.42E-11	4.76E-11	3.60E-11	2.75E-11	2.15E-11	1.70E-11

Table 4
Calculated Values of The Branch Coefficient $X_{1b;n}$ as a function of n and T. Helium case.

T	3	4	5	6	7	8	9	10	11	12	13	14	15
7000	0.472	0.379	0.304	0.250	0.216	0.193	0.173	0.154	0.132	0.116	0.103	0.097	0.089
8000	0.424	0.342	0.273	0.226	0.195	0.175	0.155	0.138	0.118	0.104	0.093	0.087	0.080
10000	0.338	0.276	0.221	0.186	0.161	0.144	0.127	0.112	0.096	0.085	0.077	0.072	0.066
12000	0.269	0.221	0.181	0.156	0.135	0.120	0.106	0.093	0.081	0.072	0.066	0.061	0.057
14000	0.215	0.179	0.151	0.133	0.116	0.102	0.090	0.079	0.070	0.063	0.058	0.054	0.050
16000	0.176	0.149	0.129	0.115	0.100	0.088	0.078	0.069	0.062	0.056	0.051	0.048	0.045
18000	0.150	0.129	0.113	0.101	0.088	0.078	0.068	0.061	0.055	0.050	0.046	0.043	0.040
20000	0.132	0.115	0.101	0.090	0.078	0.070	0.061	0.056	0.050	0.045	0.041	0.039	0.036
22000	0.119	0.105	0.092	0.082	0.071	0.064	0.055	0.051	0.045	0.041	0.037	0.035	0.032
24000	0.107	0.095	0.084	0.075	0.066	0.058	0.051	0.046	0.041	0.037	0.034	0.031	0.029

As expected

To make it possible to estimate the significance of the changes, introduced here, of this method of determining the rate coefficients of the considered chemi-ionization processes in relation to the method from Mihajlov et al. (2011), here are determined not only values of summary rate coefficient $K_{i;n}(T)$, but also the values of rate coefficient $K_{i;n}^*(T)$ which one obtains if one takes that $p_{keep}(n,l;\rho;E) = 0$, where $p_{keep}(n,l;\rho;E)$ is the totals probability of the preionization decay is given with Eqs. (13) - (15). All mentioned quantities are presented in Fig 2 for the case of $T = 5000$ K. Lets draw attention that in relation to the previous work of Mihajlov et al. (2011) in this figure are presented not only the summary rate coefficients, determined on the basis of dipole resonance mechanism for $3 \leq n \leq 8$ but also and rate coefficients determined there on the basis of data from Janev et al. (1987) for $n = 3$ and 4, from Urbain et al. (1991) for $n = 2$. One can notice from this figure that there are noticeable differences between the values of the rate coefficients determined in Mihajlov et al. (2011) and values $K_{i;n}^*(T)$, while the differences in relation to the rate coefficients $K_{i;n}(T)$ are very large for $n \leq 6$ and decrease

quickly with the increase n in the area $n > 6$.

Figure 2. Uporedjivanje naih konstanti brzine hemi-jonizacionih procesa sa vrednostima iz Mihajlov et al. (2011).

With simplif.(mih11)

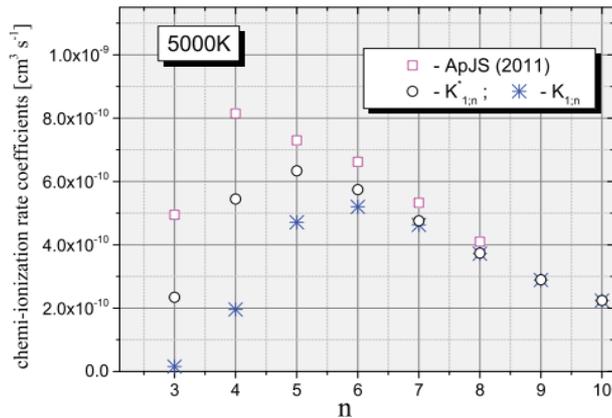Without simplif.(mih11)

+ pre-ionization

Figure 3. Comparison of the calculated values of rate coefficients of the chemi-ionization processes (1a) and (1b) with the data from Mihajlov et al. (2011a).
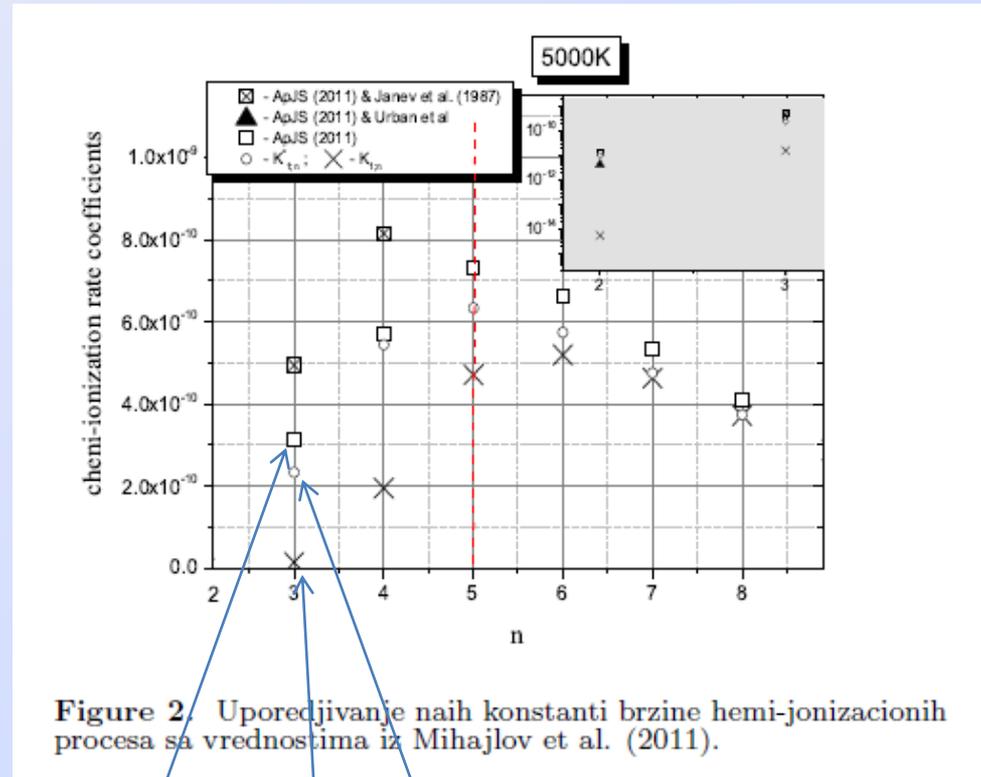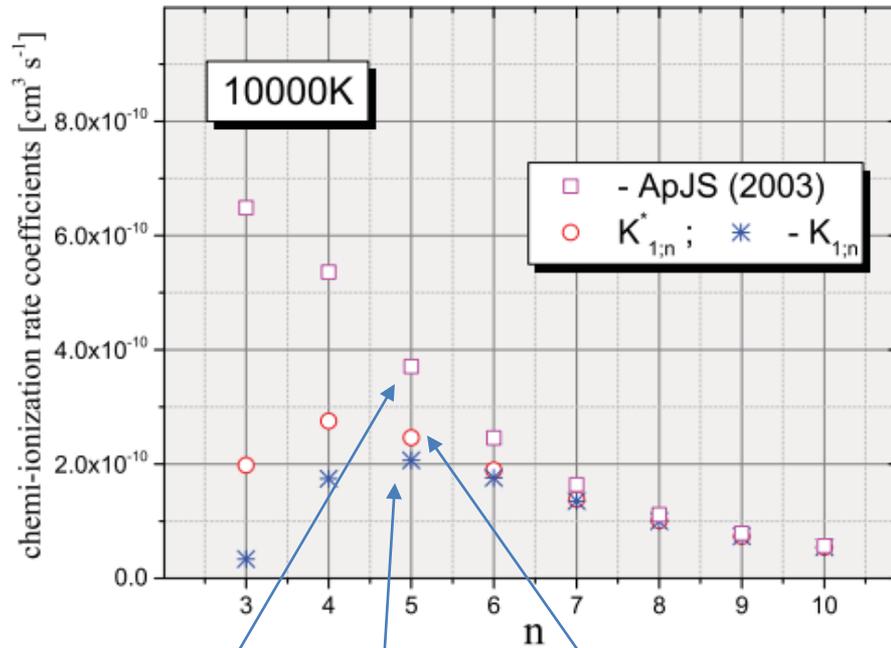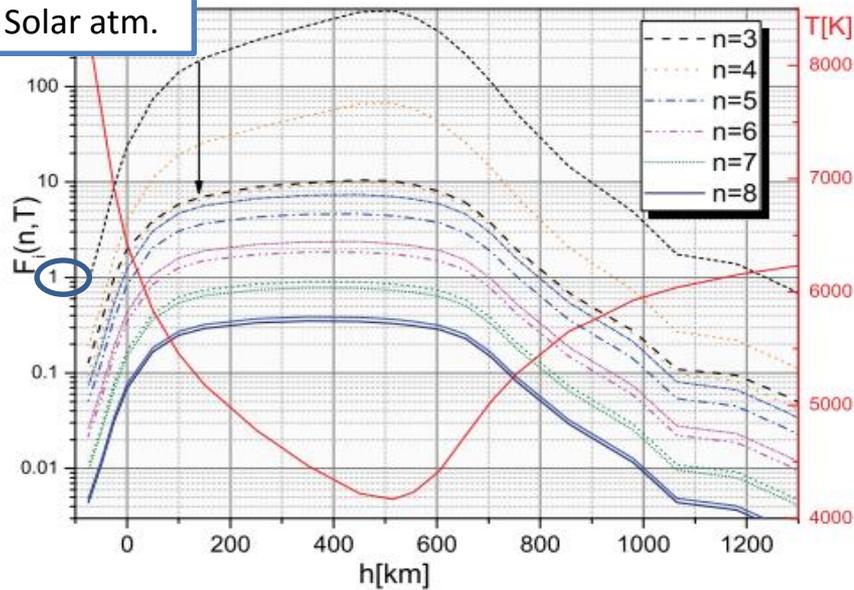
Figure 4. Comparison of the calculated values of rate coefficients of the chemi-ionization processes (1a) and (1b) with the data from Mihajlov et al. (2003a).

With simplif.(Mih. 2003)

Without simplif.(Mih. 2003)

+ pre-ionization

Solar atm.

Figure 5. Parameter $F_i[n, T; H^*(n)]$ as a function of the height h, for principal quantum numbers $n = 3$–8, for a model of the solar photosphere (Vernazza, Avrett & Loeser 1981); the wider bold lines denote present calculations, and the fainter lines denote calculations from Mihajlov et al. (2003a).

WD atm.

Figure 6. Parameter $F_i[n, T; He^*(n)]$ as a function of the logarithm of Rosseland optical depth $\log(\tau)$, for principal quantum numbers $n = 3$–10, with $T_{eff} = 12\,000$ K and $\log g = 8$; the wider bold lines denote present calculations, and the fainter lines denote calculation from Mihajlov et al. (2011a).

$$H^*(n) + e \rightarrow H^+ + e + e,$$
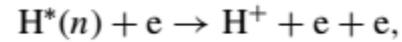
in the hydrogen case and

$$He^*(n) + e \rightarrow He^+ + e + e,$$
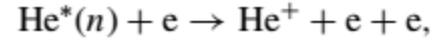
Fluxes generated in atom–Rydberg-atom and electron–excited-atom impact ionization are denoted by $I_A^{aa}(T; A^*)$ and $I_A^{ea}(T; A^*)$ and given by the expressions

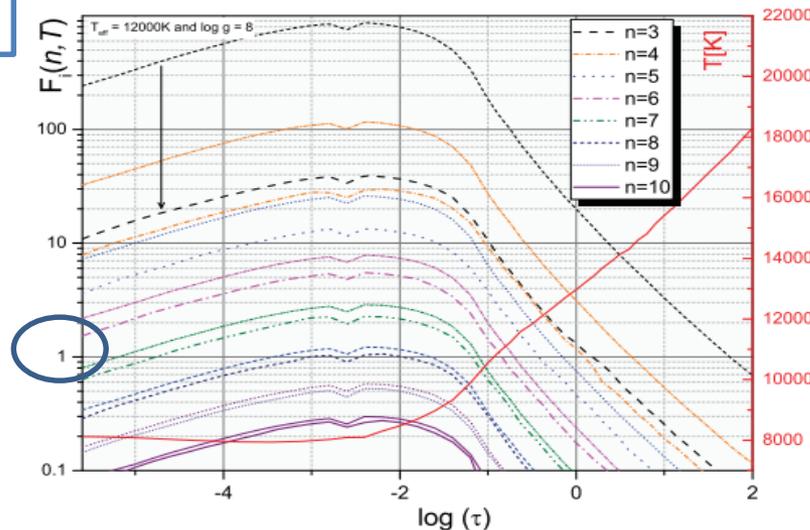$$I_A^{aa}(T; A^*) = K_A(n, T; A^*)N(A^*)N(A), \quad (26)$$

$$I_A^{ea}(T; A^*) = \alpha_A^{ea}(n, T; A^*)N(A^*)N(e), \quad (27)$$

where $A^* = H^*(n)$ or $He^*(n)$, the rate coefficient $K_A(n, T; A^*)$ is given by equation (10) and the ionization rate coefficient $\alpha_A^{ea}(n, T; A^*)$ is determined by means of semi-empirical expressions from Vriens & Smeets (1980).

The relative importance of the chemi-ionization processes in comparison with electron–excited-atom impact ionization can be characterized by parameters $F_A(n, T)$ defined as $F_A(n, T) = I_A^{aa}(T; A^*)/I_A^{ea}(T; A^*)$. According to equations (26) and (27) we have

$$F_A(n, T; A^*) = \frac{K_A(n, T; A^*)}{\alpha_A^{ea}(n, T; A^*)} \frac{N(A)}{N(e)}. \quad (28)$$

CONCLUSIONS   MNRAS paper 2016

From the presented material, it is shown that the processes of (n −n')-mixing (2) have considerable influence on the rates of chemi-ionization processes (1).

Direct calculations have been performed, which show this influence on the quantitative level. The results obtained here are presented in tabular form, where the values of total constants for rates of the processes (1), and also just the rates for the process of associative ionization (1b) for the hydrogen and helium cases are presented. Tables cover the range of values of principal quantum numbers of the Rydberg states of hydrogen and helium atoms from n = 3 to n = 15 and the temperature range from T = 4000 K to T = 10 000 K and T = 7000 K to T = 24 000 K respectively, so that they can be directly applied in connection with the modelling of the photosphere and the lower chromosphere of the Sun and the atmosphere of DB white dwarfs.

➢ The obtained results (Figs. with F) show that the efficiency of the chemi-ionization processes, in spite of the influence of (n − n')-mixing processes (2) with n'>n in most parts of the photosphere of the Sun and most parts of white-dwarf atmospheres, remains dominant or at least comparable to the efficiency of the concurrent processes.

To calculate efficiency of chemi-ionization with pre-ionization in respect to concurrent process for the sunspot atmosphere model.

To calculate for M red dwarfs atmosphere model with pre-ionization
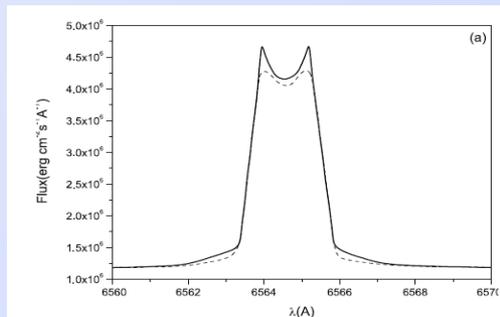

Fig. 6. Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for H_α line.
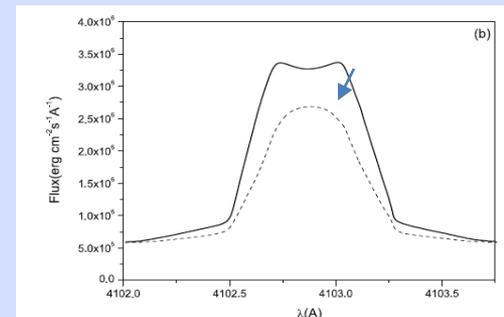
Fig. 7. Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for H_β line.

To get something like this

MOL-D

- The data presented here, soon can bee also access through http://servo.aob.rs as web service and database http://servo.aob.rs/mold.

- MOL-D database is a collection of cross-sections and rate coefficients for specific collisional processes and a web service within the Serbian Virtual Observatory (SerVO) and the Virtual Atomic and Molecular Data Center (VAMDC)

- Jevremovic, Vujcic, Sreckovic, Mihajlov, Dimitrijevic...

- Data needed for modeling stellar atmospheres, Early universe chemistry …

screenshot

Technical characteristics

MOL-D is services compatible with VAMDC standards and act as a VAMDC "nodes . They can be accessed by tools, applications or libraries which comply to VAMDC interoperability requirements, such as VAMDC portal query, Astrogrid VODesktop etc. VAMDC - compliant tools allow for distributed queries across multiple VAMDC nodes via SOAP protocol for web services, along with standardized VAMDC-TAP data access protocol and XSAMS XML schema for data serialization and representation.
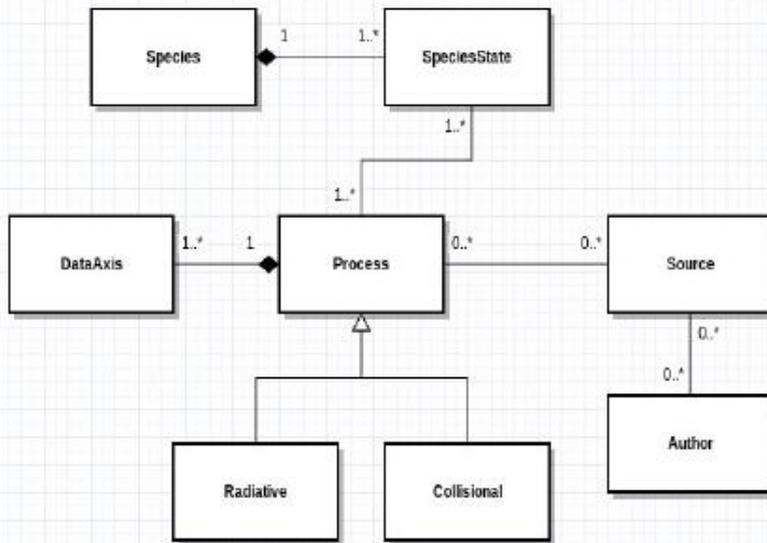

Figure 4. UML static diagram with high level of abstraction for MOL-D and BEAMDB nodes

MOL-D are implemented on top of VAMDC NodeSoftware in Django, a Python framework for web application development. They apply custom-built data models which fit their specfic datasets. All-encompasing VAMDC model would not offer optimal performance and would be more complicated to maintain. In the process of a node development, custom "dictionaries" (which map VAMDC reserved keywords to local models' attributes) are defined as well as query translator

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Thank you