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The collisional atomic processes in geo-cosmical plasmas: data needed for spectroscopy

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Abstract. The rate coefficients for the chemi-ionization (CI) processes in $Na^*(n)$ + Na, $Li^*(n)$ + Na, $Li^*(n)$ + Li and $H^*(n)$ + Li collisions are calculated for wide region of temperatures and the principal quantum numbers. The presented values of the rate coefficients are very useful for the improvement of modelling and analysis of different layers of weakly ionized plasmas in atmospheres of various stars where these and other CI processes could be important and could change the optical characteristics. Also, the results are of interest in spectroscopy of low temperature laboratory plasma.

Key words: Atomic processes – Planets and satellites: general – Line: profiles – Plasmas– ISM: clouds

1. Introduction

Collisional processes which include atoms and molecules in geo-cosmical plasmas, constantly attract attention of scientists (see e.g. Chary et al., 1999; Klyucharev et al., 2007). Among these processes, those involving highly excited Rydberg atoms are of particular interest (Gnedin et al., 2009; O'Keeffe et al., 2012). Primarily this can be attributed to a group of chemi-ionization (CI) processes in Rydberg atom collisions with ground state parent atoms. In a series of papers (Mihajlov et al., 2008; Mihajlov et al., 2011a; Mihajlov et al., 2011b; Mihajlov et al., 2016; Srećković et al., 2018), the group of atom-Rydberg atom collisional processes involving hydrogen and helium have been studied from the point of view of their effect on the optical (spectral line shapes) and kinetic properties of weakly ionized laboratory and astrophysical plasmas.

In this contribution we investigate CI processes for astrophysical usage for the case of alkali metals and give results which enable modeling of geo-cosmic weakly ionized plasma for wide range of plasma parameters. The obtained CI

data are needed for modeling and research of cool stars, like white and brown dwarfs (Debes et al., 2012; Xu & Jura, 2014), lithium stars (Shavrina et al., 2001, 2003), sodium clouds around Io (Mendillo et al., 1990; Wilson et al., 2002), cometary tails (Cremonese et al., 2002, 1997), and primordial gas containing Li atoms and ions (Gnedin et al., 2009; Coppola et al., 2011), etc. Also, study of the CI collisional processes of alkali atoms are of basic interest for some laboratory spectroscopical investigation and technical applications (Vujčić et al., 2015; Efimov et al., 2017; Marinković et al., 2017; Pichler et al., 2017; Beuc et al., 2018a,b).

In Section 2 we describe the methods of calculation and then in Section 3 we give the results of the calculation. In Section 4 the conclusions are presented.

2. Theoretical remarks

2.1. The method of calculations

We will consider two types of CI processes: the symmetric processes

$$A^*(n) + A \Rightarrow e + \begin{cases} A_2^+, & \text{(1a)} \\ A + A^+, & \text{(1b)} \end{cases}$$

and the non-symmetric processes

$$A^*(n) + B \Rightarrow e + \begin{cases} AB^+, & \text{(2a)} \\ A + B^+, & \text{(2b)} \end{cases}$$

where A, B, A^+ and B^+ are atoms and ions in the ground states, $A^*(n)$ is highly excited atom i.e. Rydberg atom, A_2^+ and AB^+ are the molecular ions in the ground electronic states. In Eq. (2) B atoms ionization potential is less than A ionization potential. The CI processes (1) and (2) can be divided to the associative ionization channel (a) with formation of molecular ions A_2^+ or AB^+ and to the non-associative ionization channel (b).

These processes have already been treated on the basis of the so-called dipole resonant mechanism (DRM), so we will briefly describe its main features. In this description of collisional ionisation and excitation events, these processes are induced by the dipole part of the electrostatic interaction between the outer Rydberg electron and the inner ion-atom system (see Fig. 1). A detailed description of the mechanism can be found in Mihajlov et al. (2012).

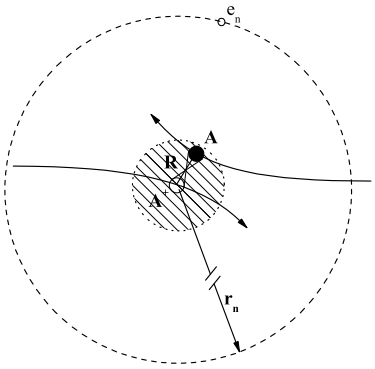


Figure 1. Schematic illustration of RA + A collision. Here R is the internuclear distance in the collision system, $r_n \sim n^2$ is the characteristic radius of Rydberg's atom A^*, e_n is outer electron and A and A^+ are atoms and their positive ions.

2.2. The CI rate coefficients

In accordance with the CI theory the partial rate coefficients $K^{(a)}(n,T)$ and the total ones $K^{(ab)}(n,T)$ can be presented with relations

$$K^{(a)}(n,T) = \int_0^{E_m^{(a)}(n)} v\sigma^{(a)}(n,E) f(v;T) dv, \quad K^{(ab)}(n,T) = \int_0^{\infty} v\sigma^{(ab)}(n,E) f(v;T) dv, \tag{3}$$

where the cross-sections $\sigma^{(a,ab)}(n,E)$ are given in Mihajlov et al. (2012), $E_m^{(a)}(n)$ is the upper limit of E relevant for the associative ionization process (1a) or (2a), and $f(v;T) = f_{cell}(v;T)$ is Maxwell distribution function. The rate coefficient $K^{(b)}(n,T)$ for the process (b) is obtained from $K^{(ab)}(n,T) = K^{(a)}(n,T) + K^{(b)}(n,T)$.

For understanding plasma chemistry and improvement of modelling and analysis of different layers of weakly ionized plasmas in atmospheres of various stars the cross sections and rate coefficients for reactions are needed (Mihajlov et al., 2011c; Srećković et al., 2017, 2018). In this contribution we investigate CI processes for astrophysical usage and give results which enable modeling of geo-cosmic weakly ionized plasma.

3. Results and Applications

3.1. The calculated quantities

In accordance with the described method, we calculate the rate coefficients $K^{(ab)}(n,T)$ for the extended range of principal quantum numbers $n \leq 25$ and temperatures 500 K $\leq T \leq$ 1500 K for the CI processes in $Li^*(n) + Na$, $Na^*(n) + Na$ collisions, and 500 K $\leq T \leq$ 4000 K for $Li^*(n) + Li$ and $H^*(n) + Li$ collisions in order to use in modelling and analysis of different layers of weakly ionized plasmas in atmospheres of various stars. We have extended the range of temperatures up to 4 000 K for lithium to enable the possible inclusion of CI processes in modelling of cool stars with low effective temperatures and enormous high Li abundances.

We note that the rate coefficient $K^{(ab)}(n,T)$ (for $Li^*(n) + Li$, $Li^*(n) + Na$, and $Na^*(n) + Na$) has the maximum between $n = 6$ and $n = 10$. The maximum position depend on temperature and moves to lower values of n with the increase of the temperature. A different behavior of $K^{(ab)}(n,T)$ is for the case of $H^*(n) + Li$ where the rate coefficient decreases with the increase of n, with different dependence on temperature. In the regions of lower T the process of associative CI, i.e. creation of molecular ions, in (1a) or (2a) collisions dominate in comparison with the non-associative CI channel except for the case of $H^*(n) + Li$ collisions where the associative channel is totally negligible for the analyzed conditions.

3.2. Fitting formula

In astrophysics, especially for the modeling of stellar atmospheres, fitting formula and coefficients as functions of temperature are needed, since such fitting coefficients are easier to be imported to the codes for stellar atmosphere modeling than tabulated data for a set of temperatures. To enable easy and more adequate use in laboratory as well as to allow a faster computation in stellar atmospheres modeling we construct a fitting formula. The results are in the form of a simple fitting formula:

$$\log(K^{(ab)}(n;T)) = k_1(n) + k_2(n) \cdot \log(T) + k_3(n) \cdot (\log(T))^2. \qquad (4)$$

In Tabs. 1 and 2 the selected fits for $4 \leq n \leq 25$ are listed for the total rate coefficients of CI processes (1) and (2). It should be noted that fits in Tab. 1 are valid within the temperature range 500 K $\leq T \leq$ 1500 K for $Li^*(n) + Na$, $Na^*(n) + Na$ collisions and in Tab. 2 are valid within the temperature range 500 K $\leq T \leq$ 4000 K for $Li^*(n) + Li$ and $H^*(n) + Li$ collisions.

Table 1. The fits to the rate coefficient. The fits were made to the results over the range 500 K $\leq T \leq$ 1500 K.

	$Li^*(n) + Na$			$Na^*(n) + Na$		
n	k1	k2	k3	k1	k2	k3
4	-41.35531	18.67062	-2.69225	-46.51493	21.4718	-3.10971
5	-16.97267	4.48624	-0.58834	-29.28982	11.44201	-1.62003
10	-14.06446	2.72686	-0.34263	-11.58289	1.24937	-0.11571
15	-15.367	3.08165	-0.40038	-9.68059	0.23985	0.00292
20	-15.80875	2.96859	-0.38137	-9.50371	0.07705	0.00612
22	-15.8578	2.86113	-0.36295	-9.31387	-0.10334	0.03144
25	-16.2462	2.93717	-0.37582	-9.38528	-0.14156	0.03217

Table 2. Same as in Tab.1 but over the temperature range 500 K $\leq T \leq$ 4000 K.

	$Li^*(n) + Li$			$H^*(n) + Li$		
n	k1	k2	k3	k1	k2	k3
4	-35.12844	14.13288	-1.89755	-5.79278	-1.1651	0.13442
5	-23.31012	7.66745	-0.99756	-6.22763	-1.12647	0.12474
10	-11.29713	1.25562	-0.12888	-7.78576	-1.05661	0.11177
15	-9.71227	0.36138	-0.0305	-8.67836	-1.04816	0.11043
20	-9.45545	0.06564	0.00121	-9.23865	-1.08876	0.11676
22	-9.46101	0.00324	0.00775	-9.46812	-1.07506	0.11468
25	-9.5051	-0.07041	0.01609	-9.75651	-1.06821	0.11363

3.3. Astrophysical Targets

3.3.1. Li-rich stars

Study of CI processes may be of interest for the investigation and modelling of plasma in cold lithium stars (see North et al., 1998; Shavrina et al., 2001, 2003). Recently Li et al. (2018) found high-lithium abundance in newly discovered 12 low-mass, metal-poor, main-sequence stars, and in red giant stars in the Milky Way halo. Collisional processes including CI could be of interest for studying of lithium-rich stellar atmospheres as an additional canal for the creation of Li I atoms. The considered CI processes influence as well the ionization level and atom excited-state populations, so that they could affect the optical properties of the weakly ionized regions of alkali rich plasmas.

As it is known lithium is easily ionized and in the spectra of cool stars the Li I resonance line 6707.8 Å is commonly observed. The lithium abundance data in such stars are mostly acquired from the spectral analysis of this particular line. The investigated CI processes, which influence atom excited-state populations and the ionization level, influence the optical properties and could be important

for the lithium spectra. Consequently the CI processes could be important for atmospheres of lithium-rich stars as an supplementary channel for the creation of the lithium atoms and RA atom populations. We give the data for extended range of temperatures for the calculation for lithium (see Tab. 2) to enable the possible inclusion of CI processes in $Li^*(n) + Li$ and $H^*(n) + Li$ collisions in modeling of cool stars with low effective temperatures ($T_{\rm eff} \leq 6000$ K) and enormous high Li abundances (Li et al., 2018).

3.3.2. Primordial gas

It is known that in the early Universe the chemical composition of the primordial gas contained lithium, and during the cooling of Universe there is an epoch when conditions for presently investigated RA collisional processes were favorable (Gnedin et al., 2009; Puy et al., 2007). Collisional recombination, ionization and Rydberg states can play important role for the early Universe chemistry (Coppola et al., 2011). As concluded in (Coppola et al., 2011; Puy et al., 2007) LiH^+ represents the most abundant molecular species containing lithium at low redshift. Consequently, data on rate coefficients for CI processes in atom - Rydberg atom collisions of Li atoms presented in Tab. 2, may be of interest for the early Universe chemistry. We therefore computed the necessary quantities.

3.3.3. Io atmosphere

In Brown & Chaffee (1974) the first neutral sodium cloud near Jovian satellite Io has been detected (see also paper Brown, 1974; Fegley & Zolotov, 2000). Since the investigation of these sodium clouds are necessary to better understand the interaction between Io's atmosphere and Jovian magnetosphere and the processes in the Jovian surroundings (Mendillo et al., 1990; Wilson et al., 2002), the data on CI processes during alkali RA collisions may be of interest. In a recent paper Schaefer & Fegley (2005), authors estimated and expected abundance of lithium at Io.

The obtained CI rate coefficient $K^{(ab)}(n, T)$ (see Tab. 1) are calculated for a wide range of plasma parameter important for the models of Io's atmospheres (Strobel et al., 1994). CI processes may be important and could be used for accurately modelling and computer simulations. The investigation of these processes is needed for better understanding of the interaction between the Io's atmosphere and Jovian magnetosphere and of the processes in the Jovian environment. In Fig 2 the density and temperature altitude profiles for moderate-density (on panel a) left), and high-density (on panel a) right) of Io model atmospheres (Strobel et al., 1994; Moses et al., 2002) are presented. The Fig. 2 (panels b), c), d)) shows the total rate coefficient $K_{ci}^{(ab)}(n, T)$ for CI processes in $Li^*(n) + Na$, $Li^*(n) + Li$ and $Na^*(n) + Na$ collisions for modeled atmospheres of Io (Strobel et al., 1994; Moses et al., 2002). For both models it can be observed the growth of coefficients at higher altitudes. Also, one can see that the rate

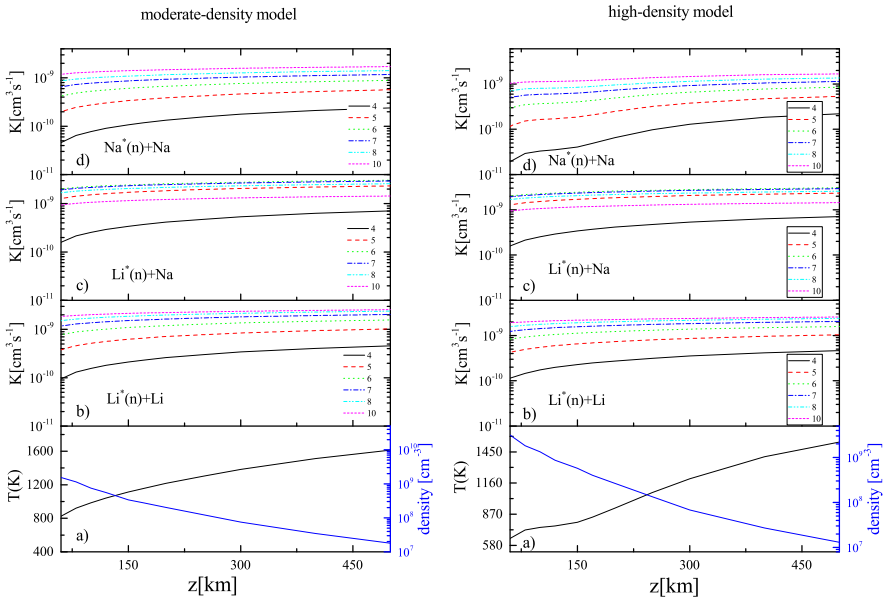


Figure 2. (left) Moderate-density model atmosphere of Io: the total rate coefficient $K_{ci}^{(ab)}(n,T)$ for CI processes in $\mathrm{Li}^*(n) + \mathrm{Na}$, $\mathrm{Li}^*(n) + \mathrm{Li}$ and $\mathrm{Na}^*(n) + \mathrm{Na}$ altitude profiles (panels b,c,d) for the corresponding model (a) (Strobel et al., 1994); (right) High-density model atmosphere of Io: the total rate coefficient $K_{ci}^{(ab)}(n,T)$ for CI processes in $\mathrm{Li}^*(n) + \mathrm{Na}$, $\mathrm{Li}^*(n) + \mathrm{Li}$ and $\mathrm{Na}^*(n) + \mathrm{Na}$ altitude profiles (panels b,c,d) for the corresponding model (a) (Strobel et al., 1994).

coefficients increase with the increase of the principal quantum number n and that they are the largest for the non-symmetric collisions.

3.3.4. Interstellar gas chemistry

The CI processes i.e. its associative channel (1(a) and 2(a)), are responsible for the formation of molecular ions and potentially important for molecular formations in interstellar gas (Dalgarno & Black, 1976). For knowing interstellar gas chemistry and for models of interstellar clouds the cross sections and rate coefficients for reactions (Srećković et al., 2018) are needed. The data for molecular ions LiNa^+, LiH^+ Li_2^+ and Na_2^+ are given and analysed in this contribution. The relative contribution (probability) of the associative channels (i.e. creation of molecular ions) are presented in Fig. 3 on the example of $\mathrm{Na}^*(n)$+Na, $\mathrm{Li}^*(n) + \mathrm{Na}$, $\mathrm{Li}^*(n) + \mathrm{Li}$ collisions. As expected the probability for the creation of molecular ions as CI product is noticeable and higher at lower temperatures

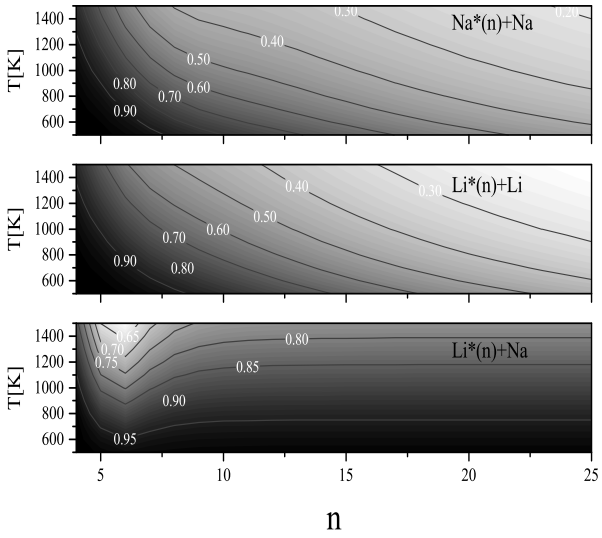


Figure 3. The surface plot of the quantity $K^{(a)}(n,T)/K^{(ab)}(n,T)$ i.e. probability of creation of molecular ions A_2^+ and AB^+ in CI collisions.

and n (see Fig. 3). Unlike presented cases in $H^*(n) + Li$ collisions the associative channel is totally negligible for the analyse conditions and consequently this channel could not be the main source of the LiH^+ molecular ion creation.

4. Summary

In this paper the rate coefficients for the CI processes in $Li^*(n)+Na$, $Li^*(n)+Li$, $H^*(n) + Li$ and $Na^*(n) + Na$ collisions were calculated. In order to enable the better and more adequate use of data, we present the results for the rate coefficients with a simple and accurate fitting formula. The calculated data have been applied to the models of atmosphere of Io. Also, the obtained rate coefficients could be very useful for the upgrading of modelling of different weakly ionized layers in atmospheres of various stars (solar like stars, lithium stars, etc) and low temperature laboratory plasmas. Note that the presented results indicate that considered CI processes are factors which influence on the ionization degree and atom excited-state populations in weakly ionized layers of atmospheres of various stars and must have a very significant influence on the optical properties of investigated atmospheres.

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