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M. S. Dimitrijević

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Photoionization of the alkali molecular ions in geo-cosmical plasmas

Lj.M. Ignjatović¹, V.A. Srećković¹ and M.S. Dimitrijević^{2,3}

¹ *Institute of Physics Belgrade, BU, Pregrevica 118, 11080 Belgrade, Serbia
(E-mail: vlada@ipb.ac.rs)*

² *Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia (E-mail:
mdimitrijevic@aob.rs)*

³ *Sorbonne Université, Observatoire de Paris, Université PSL, CNRS,
LERMA, F-92190, Meudon, France*

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Abstract. Opacities of the solar and stellar atmospheres are caused by a large number of radiative processes. Within development of more sophisticated stellar atmosphere models, we can further investigate known processes and include all processes not considered before. We calculate the average cross-section and rate coefficients for the photodissociation of the alkali molecular ions Li_2^+ , Na_2^+ and LiNa^+ ready for further use with a particular accent to the applications for astro plasma research and low temperature laboratory plasma research.

Key words: Atomic processes – Line: profiles – Plasmas – ISM: clouds

1. Introduction

The influence of some hydrogen and helium radiative processes on the optical characteristics of the stellar atmospheres was already established (see e.g. Fontenla et al., 2006; Ignjatović et al., 2009). Here we keep in mind such symmetric and non-symmetric radiative processes as photoabsorption/emission described in Srećković et al. (2017) and Marinković et al. (2017)

Recently, in the papers Mihajlov et al. (2007); Ignjatović et al. (2014); Srećković et al. (2014); Babb (2015); Heays et al. (2017) has been pointed out that the photodissociation of the diatomic molecular ion in the symmetric and non-symmetric cases, are of astrophysical relevance and could be important in modeling of specific stellar atmosphere layers and they should be included in some chemical models. In the symmetric case, it was considered the processes of molecular ion photodissociation and inverse photoassociation:



where A and A^+ are atom and ion in their ground states, and A_2^+ is molecular-ion in the ground electronic state. In the non-symmetric case, the similar processes of photodissociation/ photoassociation are:



where B is an atom whose ionization potential is less than the corresponding value for atom A . AB^+ is also molecular-ion in the ground electronic state.

For the solar atmosphere, A designates atom H(1s) and B one of the relevant metal atoms Si, Ca, Na, Mg. Also there are cases where $A=He$, and $B=H$, Mg, Si, Na, Ca (Mihajlov *et al.*, 2007; Ignjatović *et al.*, 2014; Srećković *et al.*, 2014). For the helium-rich white dwarf atmospheres A designate He(1s²) and B H(1s), and eventually oxygen or carbon (Ignjatović *et al.*, 2009; Mihajlov *et al.*, 2013). Recently, Srećković *et al.* (2017, 2018) show the importance of including the symmetric processes (1) with $A = H(1s)$ in the solar atmosphere models like Fontenla *et al.* (2006). Also, for modeling the DB white dwarf atmospheres results for case $A = He(1s^2)$ have been used (Koester, 2010).

It is well known (Puy *et al.*, 2007) that the chemical composition of the primordial gas consists of electrons and species such as: helium - He, He⁺, He²⁺ and HeH⁺; hydrogen - H, H⁻, H⁺, H₂⁺ and H₂; deuterium - D, D⁺, HD, HD⁺ and HD⁻; lithium - Li, Li⁺, Li⁻, LiH⁻ and LiH⁺. One can see that among them are species like molecular ions A₂⁺ and AB⁺ whose role in the primordial star formation is important (see also Coppola *et al.*, 2011; Glover *et al.*, 2014).

The average cross-section for the photodissociation and the corresponding spectral absorption coefficients of the alkali molecular ions Li₂⁺, Na₂⁺ and LiNa⁺ are calculated for the wide region of temperatures and wavelengths. The presented results are ready for further use with a particular accent to the applications for astro plasma research and low temperature laboratory plasma research created in gas discharges, where plasma conditions may be favorable for processes investigated here (Pichler *et al.*, 2017; Beuc *et al.*, 2018).

We describe in Section 2 the methods of calculation and then in Section 3 the results of the calculation. The conclusions are presented in Section 4.

2. The methods of calculation

In accordance with the Ignjatović *et al.* (2014) the mean thermal photodissociation cross section, is

$$\sigma^{(phd)}(\lambda, T) = \frac{\sum_{J,v} (2J+1) e^{-\frac{E_{J,v}}{kT}} \cdot \sigma_{J,v}(\lambda)}{\sum_{J,v} (2J+1) e^{-\frac{E_{J,v}}{kT}}}, \quad (3)$$

and $\sigma_{J,v}(\lambda)$ is the partial photodissociation cross-section for the ro-vibrational states with given quantum numbers J and v , and $E_{J,v}$ - the energies of these states with the respect to the ground ro-vibrational states. Here $E_{J,v} = E_{dis} + \epsilon_{J,v}$, where E_{dis} is the dissociative energy of the molecular ion, and the energies $\epsilon_{J,v} < 0$ are determined as in Srećković *et al.* (2014); Srećković *et al.* (2017) together with the wave functions of the considered ro-vibrational states. Within

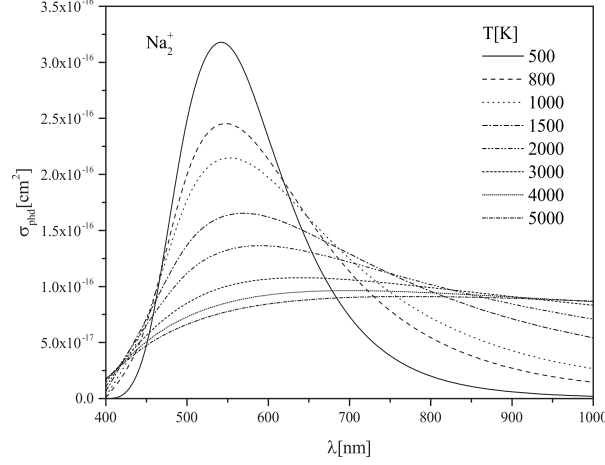


Figure 1. The behaviour of the averaged cross-section $\sigma_{phd}(\lambda, T)$ for photodissociation of the Na_2^+ molecular ion, as a function of λ and T .

the dipole approximation the partial cross-sections $\sigma_{J,v}(\lambda)$ are given by

$$\sigma_{J,v}(\lambda) = \frac{8\pi^3}{3\lambda} \left[\frac{J+1}{2J+1} |D_{J,v;J+1,E'_{imp}}|^2 + \frac{J}{2J+1} |D_{J,v;J-1,E'_{imp}}|^2 \right], \quad (4)$$

$$D_{J,v;J\pm 1,E'_{imp}} = \langle in, J, v; R | D_{in,fin}(R) | fin, J \pm 1, E' \rangle, \quad (5)$$

where $E' = \epsilon_{J,v} + \epsilon_\lambda$, E'_{imp} and E' and $D_{in,fin}(R)$ are given in Srećković et al. (2014). $D_{in;fin}(R)$ is the electronic dipole matrix element

$$D_{in;fin}(R) = \langle in; R | \mathbf{D}(R) | fin; R \rangle, \quad (6)$$

where \mathbf{D} is the operator of the dipole moment of the considered system.

The photodissociation spectral rate coefficient can be calculated using expression

$$K(\lambda, T) = \sigma^{(phd)}(\lambda, T) \cdot \chi^{-1}(T), \quad (7)$$

where the factor $\chi(T) = N(A)N(B^+)/N(AB^+)$ is given by the relation

$$\chi(T) = \frac{g_1 g_2}{g_{12}} \left(\frac{\mu k T}{2\pi \hbar^2} \right)^{\frac{3}{2}} \cdot \frac{1}{\sum_{J,v} (2J+1) e^{\frac{E_{dis} - E_{J,v}}{kT}}}, \quad (8)$$

where g_1 , g_2 and g_{12} are the electronic statistical weights of the species, A , B^+ and AB^+ respectively, and $\sigma^{(phd)}(\lambda, T)$ is given by Eqs. (3)-(5).

3. Results and discussion

The results for the average photodissociation cross-section $\sigma^{(phd)}(\lambda, T)$ on the example of the Na_2^+ molecular ion are illustrated by Fig. 1. The curves in this figure show the behavior of $\sigma^{(phd)}(\lambda, T)$ as a function of λ for a wide range of temperatures T , which are relevant for modeling geo-cosmical plasmas (Klyucharev *et al.*, 2007). The values of the Li_2^+ , Na_2^+ , LiNa^+ rate coefficient $K(\lambda, T)$, defined by Eq. (7), are presented in Fig. 2 for $500 \text{ K} \leq T \leq 5\,000 \text{ K}$ in order to enable easier use (interpolation) of this results (see e.g. Ignjatović *et al.*, 2019). This allows direct calculation of the spectral absorption coefficients during the process of applying an atmosphere model with the given parameters and composition of plasma.

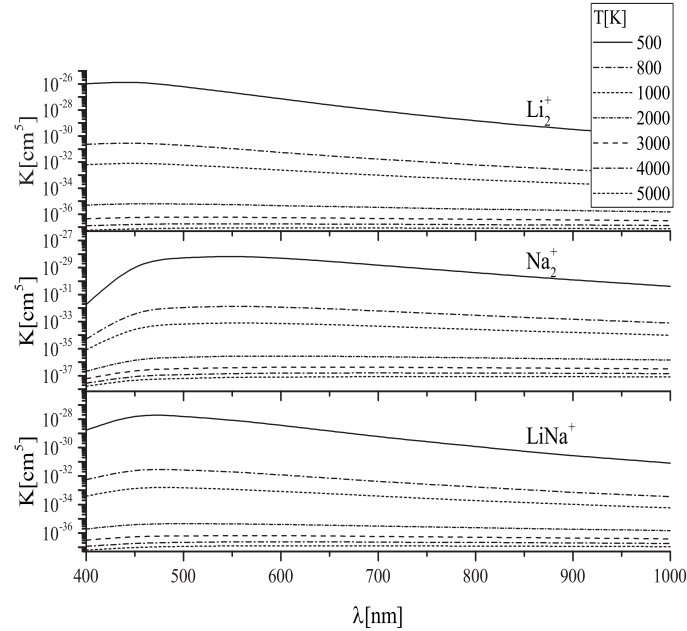


Figure 2. The plot of the spectral rate coefficients for photodissociation of the Li_2^+ , Na_2^+ , LiNa^+ , as a function of λ and T .

These figures show that exist a noticeable difference between temperature dependence of the mean thermal photo-ionization cross section and the corresponding spectral rate coefficient. The results obtained during this investigation will be implemented in the MolD database (Vujčić *et al.*, 2015; Marinković *et al.*, 2017, 2019).

4. Conclusions and Discussion

We determine the average cross-section for the photodissociation processes and the corresponding spectral rate coefficient of the alkali molecular ions Li_2^+ , Na_2^+ , LiNa^+ in the region $\lambda \leq 1000$ nm. The calculated data are useful for modelling and investigation of cool stars, especially brown and white dwarfs, lithium stars, Io's cloud of sodium atoms, and primordial gas containing Li atoms and ions. Also, the presented results are also important in theoretical and laboratory spectroscopic plasmas research.

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