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Chemi-recombination processes in astrophysical and low-temperature laboratory plasmas: the case of potassium

V.A. Srećković and L.M. Ignjatović

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

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Abstract. In this manuscript, the chemi-recombination (CR) processes i.e. electron driven collisions are examined. We obtained the rate coefficients for CR processes in potassium collisions for principal quantum numbers $n \geq 6$ and temperatures from 500 K to 5 000 K. The data presented here could help enhance the investigation and modeling of weakly ionized layers in various atmospheres and cosmic objects, including geocosmical ones.

Key words: atomic and molecular data – molecular ions – astrophysical plasma – spectroscopy – plasma diagnostics

1. Introduction

As referred over the recent years the collisional processes are of great interest to the scientists (Iacob et al., 2019; Ignjatović et al., 2019; Mihajlov et al., 2012). The reason for this is that they have an effect on the spectral properties of astrophysical and laboratory plasmas (see papers Tielens, 2013; Beuc et al., 2018a,b; Srećković et al., 2014; Ignjatović et al., 2020). Collisional processes involving various species including alkali atoms, ions, and small molecule ions can have an impact on the ionization level, atom excited-state populations, and optical properties (Mihajlov et al., 2011; Srećković et al., 2017). In low-temperature plasma astrophysics, collisional events are commonly acknowledged as an effective conduit for the creation/destruction of corresponding molecular ions (Iacob et al., 2019; Srećković et al., 2022; Pop et al., 2021; Epée Epée et al., 2022, and references therein).

It should be noted that potassium and its molecules are important in the study of cool brown dwarf atmospheres (see Allard et al., 2007). For instance, Allard et al. (2016) emphasize that for cool brown dwarfs, the wings of the alkali resonance lines—particularly the K I resonance doublet—dominate the opacity in the red optical to near-IR region. The corresponding data could be useful for modeling and investigation of potassium-containing chemical processes in Europa's atmosphere, as well as cometary gas tails and cool stars (see, e.g.

Fegley & Zolotov, 2000). Potassium atoms have been found in exospheres of Mercury and Moon, and also in circumstellar envelopes (see Valiev et al., 2020, and references therein) . Additionally, certain technological applications and laboratory tests involve the use of potassium collisional processes (Beuc et al., 2018b; Albert et al., 2020; Marinković et al., 2017; Srećković et al., 2021).

In this study, we obtained rate coefficients for potassium collisional symmetric chemi-recombination (CR) processes important for modeling planetary atmospheres, laboratory and geocosmic plasma. The collisional data are obtained for a wide range of temperatures 500 K $\leq T \leq$ 5 000 K and principal quantum numbers up to 20.

2. Theoretical remarks

2.1. Chemi-Recombination Processes

In this study, we investigated the electron driven collisional processes i.e. symmetric CR processes:

$$e + A_2^+ \Longrightarrow A^*(n) + A, \tag{1a}$$

$$e + A + A^+ \Longrightarrow A^*(n) + A, \tag{1b}$$

Here A denote potassium atoms in the ground states, $A^*(n)$ are corresponding Rydberg atoms, A_2^+ are the molecular ions in the ground electronic states. General symmetric CR processes (1) consist of two channels "a" (1a) and "b" (1a).

The calculations were carried out using the so-called dipole resonant mechanism (DRM), which is how the collisional reactions (1) were handled. The study in Mihajlov et al. (2003); Mihajlov et al. (2012) provides a complete and extensive overview. We offer a brief summary of the method together with the underlying theory in this section.

The DRM is used to calculate the rate coefficients for the principal quantum number $6 \leq n \leq 20$ with temperatures ranging from 500 K to 5000 K. Section 3 presents and discusses the data i.e. findings in depth.

2.2. Rate Coefficients

Rate coefficients $K_r^{(a,b)}(n,T)$ for the both channels "a" (1a) and "b" (1b) of CR processes (1) can be presented by

$$K_r^{(a,b)}(n,T) = Q_n(T) \cdot \int_{R_{min}}^{R_n} \exp\left[\frac{U_{12}(R)}{kT} - \frac{U_1(R)}{kT}\right] \cdot X^{(a,b)}(R,T) \cdot \frac{R^4 dR}{a_0^5} \tag{2}$$

using the theory from the papers (Mihajlov et al., 2003, 2011). $U_{12}(R) = U_2(R) - U_1(R)$, $U_1(R)$ and $U_2(R)$ are the ground and first excited electronic states of the system i.e. molecular ion, and R is the internuclear distance. Here R_n can

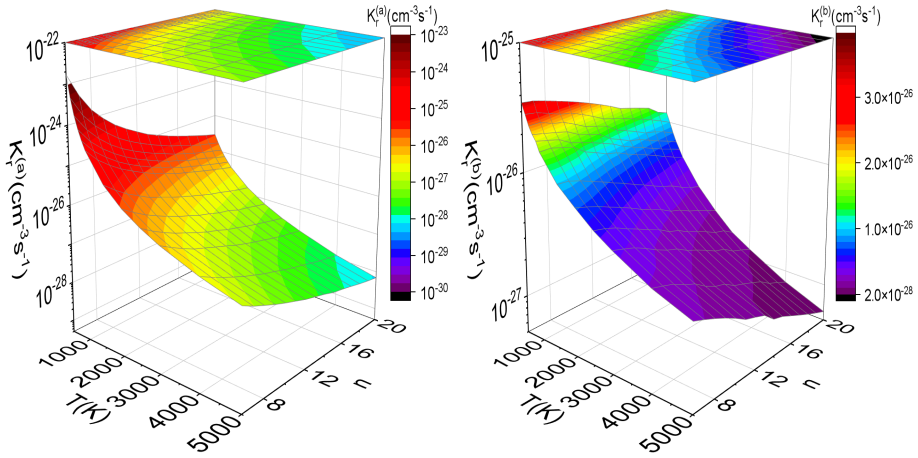

Figure 1. Left: Calculated values for rate coefficient $K_r^{(a)}$ (cm^3 s^{-1}) as a function of n and T for potassium case (A=K in Eq(1)); Right: Calculated values for rate coefficient $K_r^{(b)}$ (cm^3 s^{-1}) as a function of n and T for potassium case (A=K in Eq(1)).

be obtained by the equation $U_{12}(R) = I_n$ as the largest root, while R_{min} can be calculated as in Mihajlov et al. (2003). In (2) the needed quantity $Q_n(T)$ can be obtained by expression

$$Q_n(T) = \frac{(2\pi)^{5/2}}{3^{3/2}} \frac{(\hbar e a_0)^2}{(mkT)^{3/2}} n^{-3} \exp\left(\frac{I_n}{kT}\right), \tag{3}$$

where I_n is the excited atom ionization energy. $X^{(a)}$ parameter can be presented by:

$$X^{(a)}(R,T) = \begin{cases} \gamma\left(\frac{3}{2}; -\frac{U_1(R)}{kT}\right) / \Gamma\left(\frac{3}{2}\right) & U_1 < 0 \\ 0, & U_1 \geq 0 \end{cases} \tag{4}$$

Here γ and Γ are incomplete gamma functions. $X^{(b)}(R,T) = 1 - X^{(a)}(R,T)$. The total CR rate coefficient $K_r^{(ab)}(n,T)$ for the processes (2) is defined as

$$K_r^{(ab)}(n,T) = K_r^{(a)}(n,T) + K_r^{(b)}(n,T). \tag{5}$$

2.3. The Data

The rate coefficients are used as input parameters in many atmospheric models and spectrum synthesis software (Hauschildt & Baron, 2010). In order to be appropriately incorporated in codes and atomic and molecular (A&M) databases for modeling planetary atmospheres, early Universe chemistry, geocosmic plasma,

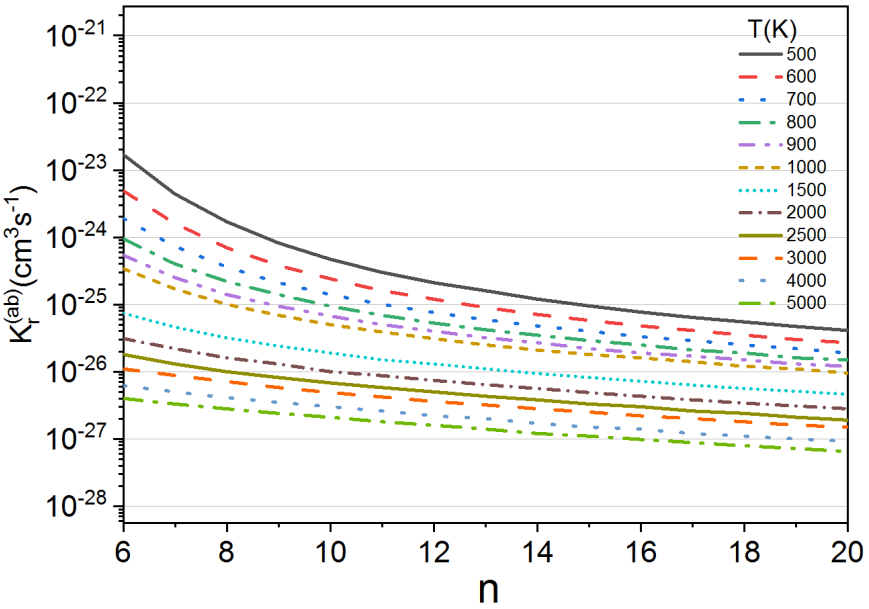

Figure 2. Calculated values for rate coefficient $K_r^{(ab)}$ (cm^3 s^{-1}) as a function of n and T for lithium case (A=K in Eq(1)).

etc., it is needed to establish good quality data (Albert et al., 2020; Marinković et al., 2017; Djuissi et al., 2020).

3. Results

The data i.e. the partial recombination rate coefficients $K_r^{(a,b)}(n,T)$, and total recombination rate coefficients $K_r^{(ab)}(n,T)$ obtained by Eqs. (2) and (5), for potassium are presented in figures 1 and 2.

The figs. 1a,b presents a 3D plot which covers the region $6 \leq n \leq 20$ and 500 K $\leq T \leq$ 5000 K. One can see that the probability for "a" channel of dissociative recombination is higher for lower n and lower temperature. Similar behavior is for the case of channel "b". Therefore, it appears that in the examined environment, these collisions form one of the primary processes for the production of Rydberg atoms.

Our future objective is to obtain and provide a straightforward approximative formula for the rate coefficients in order to facilitate the use of calculated data. It would also be extremely beneficial to include data in an A&M database. We intend to add these datasets to VAMDC (vamdc.eu), a searchable A&M data

provider, by extending one of the VAMDC nodes hosted by Serbian Virtual Observatory at servo.aob.rs (Jevremović et al., 2020).

4. Summary

For the electron-impact processes involving the potassium atoms, ions, molecular cations, we have calculated the rate coefficients for the chemi-recombination in domains of principal quantum numbers $n \geq 6$ and temperatures from 500 K to 5 000 K in this paper.

The numerical results demonstrate that the processes under investigation could have influence on the atom excited-state populations, and consequently on the optical characteristics in the weakly ionized layers of atmospheres of different stars which contain potassium. Additionally, the provided collisional data could be useful in interstellar chemistry as well as in geo-cosmical and cold plasma investigation.

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