Proceedings of the 22nd International Conference on Gas Discharges and Their Applications

Novi Sad — Serbia
September, 2-7, 2018

Volume 2

Serbian Academy of
Sciences and Arts

PROCEEDINGS OF THE XXIIND INTERNATIONAL CONFERENCE ON GAS DISCHARGES AND THEIR APPLICATIONS

- VOLUME 2 -

2nd - 7th September 2018

Novi Sad, SERBIA

Serbian Academy of Sciences and Arts
&
Institute of Physics, University of Belgrade

Editors: Prof. Zoran Lj. Petrović
Dr. Nevena Puač
Dr. Saša Dujko
Dr. Nikola Škoro

THE RATE COEFFICIENTS OF THE SLOW ATOM-RYDBERG ATOM COLLISIONS: ALKALI CASE

V. A. SREĆKOVIĆ[1], M. S. DIMITRIJEVIĆ[2,3]*, LJ. M. IGNJATOVIĆ[1], N. N. BEZUGLOV[4], A. N. KLYUCHAREV[4]

[1] Institute of Physics, University of Belgrade, P.O. Box 57 11001, Belgrade, Serbia
[2] Astronomical Observatory, Volgina 7 11060, Belgrade 38, Serbia
[3] LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universites, UPMC (Univ. Pierre & Marie Curie) Paris 06, 5 Place Jules Janssen, 92190 Meudon, France
[4] Saint Petersburg State University, St. Petersburg State University, 7/9 Universitetskaya nab., St. Petersburg 199034 Russia
*mdimitrijevic@aob.rs

ABSTRACT

The chemi-ionization processes in slow-atom-Rydberg-atom collisions are investigated in this contribution. The method [1, 2] is applied to the cases of Li and Na collisions [3, 4], for the principal quantum numbers $n \geq 4$ and temperatures $500\,\text{K} \leq T \leq 1500$ K. The chemi-ionization processes in slow collisions of excited alkali atoms with atoms in ground and excited states were considered, with a particular accent to the applications for low temperature laboratory plasma research [5, 6] created in gas discharges, for example in microwave-induced discharges at atmospheric pressure, where plasma conditions [7] may be favorable for processes investigated here. Also, further development of research of the chemi-ionization processes involving alkali metals in different stellar atmospheres as the factors which influence their spectral characteristics is important [4]. The same refers to the role of the chemi-ionization processes in atmospheres of some planets (Io, for example). Presented results and preliminary model evaluations show that in the weakly ionized astrophysical formations of alkalis, specifically in volcanic gases on Io, chemi-ionization processes can provide effective channels for medium ionization.

The main aim of this work is to extend the investigation present in [8] for the wider region of principal quantum numbers and temperature and introduce the results of calculation of the rate coefficients of the corresponding associative ionization and Penning ionization channels of chemi-ionization processes in the tabulated form easy for further use in low temperature plasma research.

1. INTRODUCTION

In this paper we studied the non-symmetric chemi-ionization processes

$$A^*(n) + B \Longrightarrow e + AB^+, \qquad (1)$$

$$A^*(n) + B \Longrightarrow e + A^+ + B, \qquad (2)$$

where Rydberg atom $A = \text{Li}$ and $B = \text{Na}$, LiNa^+ is the molecular ion in the electronic ground state ($X^2\Sigma^+$). The resonant mechanism method is used for the calculations of the rate coefficients of the processes (1) and (2). The short description and basic theory is presented here (for details see paper [2]). The calculations of these rate coefficients are performed for the principal quantum number $4 \leq n \leq 25$ and temperatures $500\,\text{K} \leq T \leq 1500$ K. The obtained results of calculation, as well as the necessary discussion, are presented in Sec. 2.

The associative ionization cross section $\sigma_{ci}^{(a)}(n, E)$ for channel (1) and the total chemi-ionization cross-section $\sigma_{ci}^{(ab)}(n, E)$ for channels (1) and (2) can be presented in the form

$$\sigma_{ci}^{(a,ab)}(n, E) = 2\pi \int_0^{\rho_{max}^{(a,ab)}(E)} P_{ci}^{(a,ab)}(n, \rho, E)\rho d\rho. \qquad (3)$$

Here $P_{ci}^{(a,ab)}(n, \rho, E)$ is chemi-ionization probability which characterize the processes (1) and (2) separately and together, ρ is the impact parameter, $\rho_{max}^{(ab)}(E)$ is the absolute upper limit of values

ρ for a given E, and $\rho_{max}^{(a)}(E)$ is the upper limit of values ρ for the associative ionization channel only (see [1, 8]). The partial and the total rate coefficients which characterize the processes (1) and (2) separately and together can be represented by $K_{ci}^{(a)}(n,T)$, $K_{ci}^{(b)}(n,T)$ and $K_{ci}^{(ab)}(n,T)$, where

$$K_{ci}^{(ab)}(n,T) = K_{ci}^{(a)}(n,T) + K_{ci}^{(b)}(n,T). \quad (4)$$

By definition, rate coefficients $K_{ci}^{(ab)}(n,T)$ and $K_{ci}^{(a)}(n,T)$ are given by relations

$$K_{ci}^{(ab)}(n,T) = \int_0^\infty v\sigma_{ci}^{(ab)}(n,E)f(v;T)dv, \quad (5)$$

$$K_{ci}^{(a)}(n,T) = \int_0^{E_{max}^{(a)}(n)} v\sigma_{ci}^{(a)}(n,E)f(v;T)dv \quad (6)$$

where the cross-sections $\sigma_{ci}^{(a,ab)}(n,E)$ are determined by Eq. (3), $E_{max}^{(a)}(n)$ is the upper limit of the region of E relevant for the associative ionization process (1) (see [1, 2]), and $f(v;T) = f_{cell}(v;T)$ is Maxwell distribution function

$$f(v;T) = \frac{4}{\sqrt{\pi}}\frac{1}{v_x}x^2e^{-x^2}, \quad (7)$$

where $x = v/v_x$, $v_x = \sqrt{2kT/M_{red}}$. Here M_{red} is the reduced mass of $A^+ + B$ subsystem. The rate coefficient $K_{ci}^{(b)}(n,T)$ for the process (2) is determined from the Eq. (4). The potential curves of several lowest Σ states of the molecular ion $LiNa^+$, the square of dipole matrix element for the transition between $X^2\Sigma^+$- and $A^2\Sigma^+$-states, as well as other needed parameters can be found in [8].

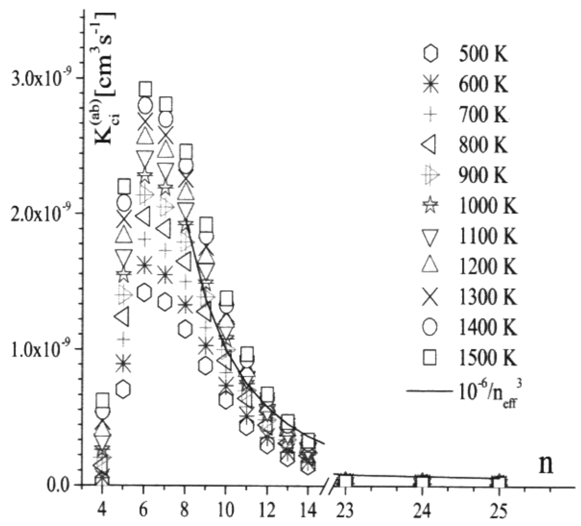

Fig. 1: The total rate coefficient $K_{ci}^{(ab)}(n,T)$, Eq. (5) for chemi-ionization processes (1) and (2) in $Li^*(n) + Na$ collisions.

2. RESULTS AND DISCUSSION

In this paper we calculate the values of the partial $K_{ci}^{(a)}(n,T)$, $K_{ci}^{(b)}(n,T)$ and total chemi-ionization rate coefficients $K_{ci}^{(ab)}(n,T)$, for the extended regions of principal quantum numbers $n \geq 4$ and temperatures 500 K $\leq T \leq$ 1500 K. The results of calculations of rate coefficients $K_{ci}^{(a)}(n,T)$ and $K_{ci}^{(b)}(n,T)$ of both channels are presented in Tabs. 1 and 2.

Tables show that in the considered regions of n and T the process of associative chemi-ionization (1) dominate in comparison with the non-associative chemi-ionization channel (2). Also, one can see that the $K^{(b)}(n,T)$ has the maximum at $n = 6$.

Fig. 1 present the total chemi-ionization rate coefficient $K_{ci}^{(ab)}(n,T)$ for all mentioned conditions. One can see that the rate coefficient $K_{ci}^{(ab)}(n,T)$ has the maximum at $n = 6$. From Fig. 1 evidently the total chemi-ionization rate coefficient can be approximated by the function of n i.e. $\sim 10^{-6}/n^3$ valid for the higher values of n and which does not depend on temperature. Unlike the symmetric case, in the non-symmetric one associative channel changes non-monotonically with a maximum displaced to the region of small values of n.

Table 1: The rate coefficient $K_{ci}^{(a)}(n,T)$ in [cm^3s^{-1}] for chemi-ionization associative channel (1).

n/T	500 [K]	600 [K]	700 [K]	800 [K]	900 [K]	1000 [K]	1100 [K]	1300 [K]	1500 [K]
4	2.61E-11	5.52E-11	9.53E-11	1.44E-10	1.98E-10	2.56E-10	3.16E-10	4.33E-10	5.40E-10
5	6.98E-10	8.70E-10	1.02E-09	1.14E-09	1.23E-09	1.30E-09	1.35E-09	1.41E-09	1.43E-09
6	1.39E-09	1.55E-09	1.66E-09	1.74E-09	1.79E-09	1.82E-09	1.83E-09	1.82E-09	1.77E-09
7	1.32E-09	1.49E-09	1.62E-09	1.73E-09	1.80E-09	1.86E-09	1.89E-09	1.93E-09	1.93E-09
8	1.14E-09	1.30E-09	1.43E-09	1.53E-09	1.61E-09	1.67E-09	1.72E-09	1.78E-09	1.81E-09
9	8.72E-10	1.00E-09	1.11E-09	1.19E-09	1.26E-09	1.32E-09	1.36E-09	1.42E-09	1.45E-09
10	6.24E-10	7.19E-10	7.98E-10	8.63E-10	9.15E-10	9.57E-10	9.89E-10	1.03E-09	1.06E-09
11	4.34E-10	5.01E-10	5.57E-10	6.03E-10	6.41E-10	6.71E-10	6.94E-10	7.26E-10	7.43E-10
12	3.00E-10	3.48E-10	3.87E-10	4.20E-10	4.46E-10	4.67E-10	4.83E-10	5.06E-10	5.18E-10
13	2.10E-10	2.43E-10	2.71E-10	2.94E-10	3.12E-10	3.27E-10	3.39E-10	3.55E-10	3.64E-10
14	1.49E-10	1.73E-10	1.92E-10	2.09E-10	2.22E-10	2.33E-10	2.41E-10	2.52E-10	2.59E-10
15	1.07E-10	1.25E-10	1.39E-10	1.51E-10	1.60E-10	1.68E-10	1.74E-10	1.82E-10	1.87E-10
16	7.87E-11	9.13E-11	1.02E-10	1.10E-10	1.18E-10	1.23E-10	1.28E-10	1.34E-10	1.37E-10
17	5.86E-11	6.80E-11	7.58E-11	8.23E-11	8.75E-11	9.17E-11	9.50E-11	9.96E-11	1.02E-10
18	4.43E-11	5.14E-11	5.73E-11	6.22E-11	6.62E-11	6.94E-11	7.19E-11	7.53E-11	7.72E-11
19	3.39E-11	3.94E-11	4.39E-11	4.77E-11	5.07E-11	5.32E-11	5.51E-11	5.77E-11	5.91E-11
20	2.63E-11	3.06E-11	3.41E-11	3.70E-11	3.94E-11	4.13E-11	4.28E-11	4.48E-11	4.59E-11
21	2.07E-11	2.40E-11	2.68E-11	2.91E-11	3.09E-11	3.24E-11	3.36E-11	3.52E-11	3.61E-11
22	1.64E-11	1.91E-11	2.13E-11	2.31E-11	2.46E-11	2.57E-11	2.67E-11	2.79E-11	2.86E-11
23	1.32E-11	1.53E-11	1.70E-11	1.85E-11	1.97E-11	2.06E-11	2.14E-11	2.24E-11	2.30E-11
24	1.06E-11	1.24E-11	1.38E-11	1.50E-11	1.59E-11	1.67E-11	1.73E-11	1.81E-11	1.86E-11
25	8.69E-12	1.01E-11	1.13E-11	1.22E-11	1.30E-11	1.36E-11	1.41E-11	1.48E-11	1.52E-11

Table 2: The rate coefficient $K_{ci}^{(b)}(n,T)$ in [cm^3s^{-1}] for chemi-ionization PI channel (2).

n/T	500 [K]	600 [K]	700 [K]	800 [K]	900 [K]	1000 [K]	1100 [K]	1300 [K]	1500 [K]
4	0.00E+00	0.00E+00	4.45E-15	9.04E-13	3.29E-12	7.80E-12	1.51E-11	4.05E-11	8.18E-11
5	7.52E-12	2.50E-11	5.72E-11	1.06E-10	1.70E-10	2.47E-10	3.37E-10	5.45E-10	7.71E-10
6	3.23E-11	7.87E-11	1.48E-10	2.38E-10	3.44E-10	4.64E-10	5.93E-10	8.64E-10	1.15E-09
7	2.13E-11	5.33E-11	1.02E-10	1.68E-10	2.47E-10	3.37E-10	4.37E-10	6.51E-10	8.79E-10
8	1.44E-11	3.68E-11	7.16E-11	1.19E-10	1.76E-10	2.43E-10	3.17E-10	4.80E-10	6.55E-10
9	9.94E-12	2.55E-11	5.00E-11	8.34E-11	1.25E-10	1.72E-10	2.26E-10	3.43E-10	4.71E-10
10	6.79E-12	1.75E-11	3.44E-11	5.75E-11	8.61E-11	1.19E-10	1.56E-10	2.38E-10	3.27E-10
11	4.63E-12	1.20E-11	2.35E-11	3.94E-11	5.89E-11	8.18E-11	1.07E-10	1.63E-10	2.25E-10
12	3.18E-12	8.21E-12	1.62E-11	2.71E-11	4.05E-11	5.63E-11	7.38E-11	1.12E-10	1.55E-10
13	2.21E-12	5.72E-12	1.13E-11	1.88E-11	2.82E-11	3.92E-11	5.14E-11	7.83E-11	1.08E-10
14	1.56E-12	4.04E-12	7.97E-12	1.33E-11	2.00E-11	2.77E-11	3.64E-11	5.54E-11	7.62E-11
15	1.13E-12	2.91E-12	5.74E-12	9.60E-12	1.44E-11	2.00E-11	2.62E-11	3.99E-11	5.48E-11
16	8.24E-13	2.13E-12	4.20E-12	7.03E-12	1.05E-11	1.46E-11	1.92E-11	2.92E-11	4.02E-11
17	6.13E-13	1.59E-12	3.13E-12	5.23E-12	7.84E-12	1.09E-11	1.43E-11	2.18E-11	2.99E-11
18	4.63E-13	1.20E-12	2.36E-12	3.95E-12	5.92E-12	8.22E-12	1.08E-11	1.64E-11	2.26E-11
19	3.55E-13	9.18E-13	1.81E-12	3.03E-12	4.54E-12	6.30E-12	8.26E-12	1.26E-11	1.73E-11
20	2.75E-13	7.12E-13	1.40E-12	2.35E-12	3.52E-12	4.89E-12	6.41E-12	9.77E-12	1.34E-11
21	2.16E-13	5.59E-13	1.10E-12	1.85E-12	2.77E-12	3.84E-12	5.03E-12	7.67E-12	1.05E-11
22	1.72E-13	4.44E-13	8.75E-13	1.46E-12	2.19E-12	3.05E-12	3.99E-12	6.09E-12	8.36E-12
23	1.38E-13	3.56E-13	7.02E-13	1.17E-12	1.76E-12	2.44E-12	3.20E-12	4.88E-12	6.71E-12
24	1.11E-13	2.88E-13	5.68E-13	9.50E-13	1.42E-12	1.98E-12	2.59E-12	3.95E-12	5.43E-12
25	9.08E-14	2.35E-13	4.63E-13	7.75E-13	1.16E-12	1.61E-12	2.11E-12	3.22E-12	4.43E-12

3. CONCLUSIONS AND PERSPECTIVES

The rate coefficients for the chemi-ionization processes in $\mathrm{Li}^*(n) + \mathrm{Na}$ collisions were calculated. The results of this work confirm the possibility of application of the resonant mechanism for the description of chemi-ionization collision processes, not only in the case, when the particles of the same type collide (symmetric case), but for the case of different type (non-symmetric) too. This provides extension of the class of atom-Rydberg atom collision systems from the aspect of the research of chemi-ionization processes.

We present the results of calculation of the rate coefficients of the corresponding chemi-ionization processes in the tabulated form easy for further use with a particular accent to the applications for low temperature laboratory plasma research created in gas discharges, for example in microwave-induced discharges at atmospheric pressure, where plasma conditions may be favorable for processes investigated here.

In the near future we aim to further investigate the chemi-ionization processes and develop completely quantum-mechanical methods of their description which could be applied in the cases of extremely low temperatures.

Acknowledgements: This work is partially supported by Ministry of Education, Science and Technological Development of the Republic of Serbia under the grants III 44002, and 176002.

REFERENCES

[1] Lj. M. Ignjatović and A. A. Mihajlov, "Rate coefficient for the chemi-ionization in slow Li*(n)+ Li and Na*(n)+ Na collisions.", Physical Review A, 72, 2, 022715 (2005)

[2] A. A. Mihajlov, V. A. Srećković, Lj. M. Ignjatović and A. N. Klyucharev, "The chemi-ionization processes in slow collisions of Rydberg atoms with ground state atoms: mechanism and applications", Journal of Cluster Science, 23, 1, 47-75 (2012)

[3] A. N. Klyucharev, N. N. Bezuglov, A. A. Matveev, A. A. Mihajlov, Lj. M. Ignjatović and M. S. Dimitrijević , "Rate coefficients for the chemi-ionization processes in sodium-and other alkali-metal geocosmical plasmas", New Astronomy Reviews, 51, 7, 547-562 (2007).

[4] Y. N. Gnedin, A. A. Mihajlov, Lj. M. Ignjatović, N. M. Sakan, V. A. Srećković, M. Y. Zakharov, N. N. Bezuglov and A. N. Klycharev, "Rydberg atoms in astrophysics", New astronomy reviews, 53, 7-10, 259-265 (2009)

[5] A. A. Mihajlov, V. A. Srećković, Lj. M. Ignjatović, Z. Simić and M. S. Dimitrijević, "Influence of Rydberg atom-atom collisional and (n-n')-mixing processes on optical properties of astrophysical and low-temperature laboratory plasmas", Journal of Physics: Conference Series, 810, 1, 012058 (2017)

[6] P. O'Keeffe, P. Bolognesi, L. Avaldi, A. Moise, R. Richter, A. A. Mihajlov, V. A. Srećković and Lj. M. Ignjatović, "Experimental and theoretical study of the chemi-ionization in thermal collisions of Ne Rydberg atoms", Physical Review A, 85, 5, 052705 (2012)

[7] C. Yubero, M. S. Dimitrijević, M. C. Garcia and M. D. Calzada, "Using the van der Waals broadening of the spectral atomic lines to measure the gas temperature of an argon microwave plasma at atmospheric pressure", Spectrochimica Acta B, 62, 2, 169-176 (2007)

[8] Lj. M. Ignjatović, A. A. Mihajlov, and A. N. Klyucharev. "The rate coefficients of the chemi-ionization processes in slow Li*(n)+ Na collisions." Journal of Physics B: Atomic, Molecular and Optical Physics 41, 2, 025203 (2008)