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The radiative processes involving some non-symmetric systems relevant for astrochemistry: data needed for modeling

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Abstract. The photo-association, charge-exchange, and photo-dissociation absorption processes in non-symmetric systems including hydrogen and calcium atoms, ions, molecules, and molecular-ions are investigated in this paper. For the current computation, we have calculated the data for molecules and molecular state characterizations. We obtained the cross-sections and corresponding spectral absorption rate coefficients - as the functions of wavelengths, and temperatures. The collected data has the potential for an impact on vast additional applications, such as modeling of laboratory plasmas and numerous astrophysical objects.

Key words: atomic and molecular data – astrophysical plasma – optical characteristics – absorption

1. Introduction

Due to the complexity of electron dynamics in molecules and the sophistication of most experimental setups used in this context, atomic and molecular (A&M) data and databases are an indispensable ingredient in new experimental approaches and accurate theoretical support (Hauschildt & Baron, 2010; Albert et al., 2020; Epée Epée et al., 2022; Srećković et al., 2021). Furthermore, one can observe the present importance of investigating the optical properties of numerous small molecules as well as the associated A&M data (Sansone et al., 2010; Djuissi et al., 2020; Iacob et al., 2019; Srećković et al., 2022; Mihajlov et al., 2011). Precision spectroscopy of molecular ions has applications in astrochemistry, quantum state controlled chemical reactions, and measurements of fundamental constants (Vázquez-Carson et al., 2022; Iacob, 2020; Brown et al., 2016; Ignjatović et al., 2020; Pop et al., 2021). Such precise spectroscopy measurements open the path for search for astrophysical presence of those small molecules like CaH^+, etc. (Khanyile et al., 2013).

Our aim is to obtain spectroscopic information, i.e., data, about such systems involving hydrogen and calcium atoms, ions, molecules and molecular-ions. For example, CaH^+ molecular ions are of great scientific interest due to possible applications to astrophysics and fundamental physics, similar to other alkaline earth hydride ions (Monteiro et al., 1988; Dutta et al., 2006; Kimura et al., 2011). Interstellar medium (ISM) and comets are believed to contain these hydrides. For such systems, we calculated spectral absorption rate coefficients and average cross-sections. These parameters cover a wide range of temperatures and EUV and UV region of wavelengths.

The outcomes, i.e. the obtained datasets, may be applied to important tasks, such as modelling or in PLEIADES SOLEIL synchrotron (Giuliani et al., 2014). Also, the collected data have the potential to have a high impact and vast applications, such as lasers, ultra-short lasers and laser physics, modeling of laboratory plasmas and numerous astrophysical objects (Canuto et al., 1993; Barklem & O'Mara, 1998; Brown et al., 2016). Also, for quality modelling accurate data is needed, which makes the research relevant and up to date.

Brief theory and calculated quantities are presented in section 2; section 3 describes and discusses the results. Finally, the section 4 is devoted to conclusions and future directions of research.

2. Theory

2.1. Processes

In this study, radiative processes are investigated in terms of their impact on the optical properties of weakly ionized astrophysical and laboratory plasmas. In particular, in the case of strongly non-symmetric systems, the processes of photo-association i.e. free-bound (fb), absorption charge-exchange i.e. free-free (ff) and photo-dissociation i.e. bound-free (bf) are investigated.

We shall investigate the processes that can be described as non-symmetric

$$\varepsilon_\lambda + AB^+ \Rightarrow A^+ + B, \tag{1}$$

$$\varepsilon_\lambda + A + B^+ \Rightarrow A^+ + B. \tag{2}$$

$$\varepsilon_\lambda + A + B^+ \Rightarrow (AB^+)^* \tag{3}$$

Here, B represents a calcium atom (Ca), and A=H. Molecular-ion in the ground electronic state HCa^+ is represented by the symbol AB^+, and molecular-ion in the first excited electronic state is represented by the symbol $(AB^+)^*$.

2.2. The spectral characteristics

As stated in Srećković et al. (2014), the free-free spectral rate coefficients $K_{(ff)}(\lambda, T)$ which described the processes (2) can be presented by relation:

$$K_{(ff)}(\lambda, T) = \int_0^\infty \left(\frac{2E}{\mu}\right)^{\frac{1}{2}} \sigma_{(ff)}(\lambda, E) f(E) dE \tag{4}$$

Here quantity $\sigma_{(ff)}(\lambda, E)$ denotes the cross section and $f(E)$ is the Maxwell energy distribution function

$$f(E) = \frac{2}{\pi^{1/2}(kT)^{3/2}} e^{-\frac{E}{k_B T}} E^{1/2} dE, \tag{5}$$

where μ is the reduced mass of the considered system.

The free-free absorption cross section $\sigma_{(ff)}(\lambda, E)$ for radiative charge exchange processes can be represented as

$$\sigma_{(ff)}(\lambda, E) = \frac{g_1 g_2}{g_{1'} g_{2'}} \frac{8\pi^4 \hbar^2 \varepsilon_\lambda}{3c2\mu E} \cdot \left[(J+1) \cdot |D_{J,E;J+1,E'_{imp}}|^2 + J \cdot |D_{J,E;J-1,E'_{imp}}|^2\right], \tag{6}$$

where $D_{J,E;J\pm1,E'_{imp}} =< in, J, E; R|D_{in,fin}(R)|fin, J \pm 1, E' > .$ $D_{in;fin}(R) =< in; R|\mathbf{D}(R)|fin; R >$ is the electronic dipole matrix element and $\mathbf{D}$ is the operator of the dipole moment of the investigated system. Detailed theory and definitions of all quantities can be found in Srećković et al. (2014).

The rate coefficient $K_{(fb)}(\lambda, T)$ for the free-bound processes (3) can be presented as in Ignjatović et al. (2014) by:

$$K_{(fb)}(\lambda, T) = \frac{(2\pi)^3}{3\hbar\lambda} \left(\frac{2\pi\hbar^2}{\mu kT}\right)^{3/2} \sum_{J',v'} \left(\frac{\mu}{2E}\right)^{1/2} e^{-\frac{E}{kT}} \cdot S_{J',v'}, \tag{7}$$

where

$$S_{J',v'} = \frac{g_{12}}{g_1 g_2} \cdot [J'|D_{J'-1,E;J',v'}|^2 + (J'+1)|D_{J'+1,E;J',v'}|^2]. \tag{8}$$

Here $D_{J'\pm1,E;J',v'} =< in, J' \pm 1, E; R|D_{in,fin}(R)|fin, J', v' > .$ Detailed definitions of all quantities and theory can be found in papers Srećković et al. (2014); Ignjatović et al. (2014).

The (bf) i.e. photo-dissociation spectral rate coefficient for processes (1) can be presented by

$$K_{(bf)}(\lambda, T) = X^{-1}(T) \cdot \sigma_{(bf)}(\lambda, T). \tag{9}$$

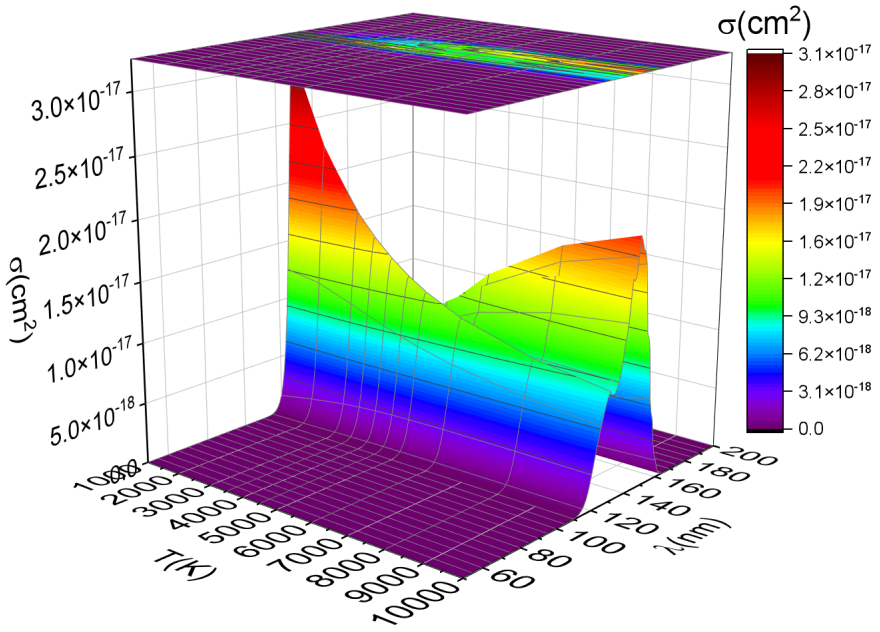

Figure 1. 3D plot of the mean thermal photo-dissociation cross- section for molecular-ion CaH+.

Here the X factor is given by

$$X(T) = \left(\frac{\mu kT}{2\pi\hbar^2}\right)^{\frac{3}{2}} \frac{g_1 g_2}{g_{12}} \cdot \frac{1}{\sum\limits_{J,v}(2J+1)e^{\frac{E_{dis}-E_{J,v}}{kT}}}. \tag{10}$$

The average thermal photo-dissociation cross section $\sigma_{(bf)}(\lambda, T)$ is:

$$\sigma_{(bf)}(\lambda, T) = \frac{\sum\limits_{J,v}(2J+1)e^{\frac{-E_{J,v}}{kT}} \cdot \sigma_{J,v}^{(bf)}(\lambda)}{\sum\limits_{J,v}(2J+1)e^{\frac{-E_{J,v}}{kT}}}. \tag{11}$$

The partial cross-sections $\sigma_{J,v}^{(bf)}(\lambda)$ can be presented with the expression:

$$\sigma_{J,v}^{(bf)}(\lambda) = \frac{8\pi^3}{3\lambda}\left[\frac{J+1}{2J+1}|D_{J,v;J+1,E'_{imp}}|^2 + \frac{J}{2J+1}|D_{J,v;J-1,E'_{imp}}|^2\right]. \tag{12}$$

All needed quantities and relations are given in detail in e.g. papers of Srećković et al. (2014); Srećković et al. (2021); Ignjatović et al. (2014).

3. Results and Discussion

The dataset i.e. results have been provided in tabulated form by Tabs. 1 - 3. In addition, the results are also illustrated in this section by Figure 1. The data cover the region 50 nm $\leq \lambda \leq$ 200 nm and 1000 K $\leq T \leq$ 10000 K. Data could be beneficial for laboratory plasma diagnostics, astrophysics and industrial plasma modeling.

Table 1. The spectral absorption coefficient $K_{(bf)}(\lambda, T)$ [cm^5] which characterizes absorption processes (1) for calcium hydride molecular ion as a function of wavelength λ [nm] and temperature T [K].

lambda/T	1000	2000	3000	4000	6000	8000	10000
50	1.16E-36	1.40E-41	6.05E-43	1.44E-43	3.43E-44	1.57E-44	9.26E-45
60	2.29E-36	6.82E-41	2.52E-42	4.91E-43	9.14E-44	3.68E-44	2.02E-44
70	2.40E-36	7.81E-41	3.15E-42	6.87E-43	1.52E-43	6.76E-44	3.94E-44
80	4.62E-36	1.60E-40	7.97E-42	1.97E-42	4.95E-43	2.35E-43	1.43E-43
90	9.37E-36	3.35E-40	1.73E-41	4.66E-42	1.31E-42	6.56E-43	4.10E-43
100	1.73E-35	4.02E-40	2.47E-41	7.67E-42	2.45E-42	1.29E-42	8.30E-43
110	2.40E-34	7.96E-39	4.49E-40	1.25E-40	3.57E-41	1.78E-41	1.11E-41
120	4.12E-31	4.04E-36	1.05E-37	1.79E-38	3.07E-39	1.21E-39	6.62E-40
130	8.04E-30	4.61E-35	7.87E-37	1.01E-37	1.24E-38	4.13E-39	2.04E-39
140	1.05E-32	3.32E-36	2.17E-37	5.40E-38	1.24E-38	5.45E-39	3.14E-39
150	4.71E-35	4.50E-37	8.59E-38	3.46E-38	1.22E-38	6.44E-39	4.10E-39
160	4.13E-38	6.29E-39	2.67E-39	1.54E-39	7.51E-40	4.62E-40	3.20E-40
165	5.80E-42	2.02E-42	1.10E-42	7.11E-43	3.86E-43	2.51E-43	1.79E-43

Table 2. The spectral absorption coefficient $K_{(ff)}(\lambda, T)$ [cm^5] which characterizes absorption processes (2) as a function of wavelength λ [nm] and temperature T [K].

lambda/T	1000	2000	3000	4000	6000	8000	10000
50	5.19E-45	1.49E-45	1.60E-45	1.67E-45	1.74E-45	1.90E-45	2.41E-45
60	2.04E-45	1.44E-45	1.89E-45	2.26E-45	2.89E-45	3.26E-45	3.93E-45
70	1.99E-44	1.74E-44	1.85E-44	1.96E-44	2.06E-44	2.34E-44	2.60E-44
80	1.94E-43	1.42E-43	1.54E-43	1.67E-43	1.91E-43	2.16E-43	2.37E-43
90	7.74E-43	6.30E-43	6.28E-43	6.37E-43	6.90E-43	7.40E-43	7.97E-43
100	1.94E-42	1.52E-42	1.51E-42	1.54E-42	1.64E-42	1.73E-42	1.85E-42
110	1.86E-41	1.07E-41	1.02E-41	9.63E-42	9.04E-42	8.54E-42	8.33E-42
120	2.58E-40	8.05E-41	8.53E-41	8.46E-41	7.65E-41	7.05E-41	7.81E-41
130	1.76E-40	6.19E-41	7.27E-41	8.04E-41	8.57E-41	8.81E-41	8.97E-41
140	2.92E-40	2.58E-40	2.86E-40	3.15E-40	3.52E-40	3.48E-40	4.39E-40
150	9.79E-40	6.34E-40	6.97E-40	7.46E-40	8.18E-40	8.52E-40	1.02E-39
160	5.08E-40	2.88E-40	3.16E-40	3.63E-40	3.86E-40	4.11E-40	5.01E-40
170	1.90E-41	7.52E-41	9.74E-41	1.10E-40	1.46E-40	1.63E-40	1.87E-40
180	1.34E-44	5.02E-43	1.74E-42	3.33E-42	7.45E-42	1.15E-41	1.68E-41
190	1.57E-48	4.58E-46	3.72E-45	9.59E-45	3.64E-44	8.86E-44	1.42E-43
200	2.01E-50	4.12E-47	4.71E-46	1.59E-45	5.19E-45	1.07E-44	1.62E-44

Figure 1 shows the results of calculations of the average thermal photo-dissociation cross-section $\sigma^{(bf)}_{CaH^+}(\lambda;T)$ for the calcium hydride molecular ion over a wide range of temperatures and wavelengths. The 3D plot shows a complex dependence on wavelength and temperature with noticeable maxima in the wavelength region 100 nm-160 nm.

The absorption coefficients as functions of wavelength and temperature, which involves hydrogen and calcium atoms, ions, molecules and molecular-ions, are given. The data of the bound-free $K_{(bf)}(\lambda,T)$, free-free $K_{(ff)}(\lambda,T)$ and free-bound $K_{(fb)}(\lambda,T)$ spectral rate coefficient are given by the Tabs. 1, 2 and 3. The tables cover the region 50 nm $\leq \lambda \leq$ 200 nm and 1000 K $\leq T \leq$ 10000 K which enables potential modeling. These tables show that the values of all rate coefficients have maxima depending on temperature and wavelength.

Table 3. The spectral absorption coefficient $K_{(fb)}(\lambda,T)$ [cm^5] which characterizes absorption processes (3) as a function of wavelength λ [nm] and temperature T [K].

lambda/T	1000	2000	3000	4000	6000	8000	10000
166	1.38E-41	5.54E-42	3.15E-42	2.09E-42	1.16E-42	7.64E-43	5.50E-43
170	1.06E-40	6.84E-41	4.64E-41	3.37E-41	2.06E-41	1.42E-41	1.05E-41
171	3.24E-40	2.39E-40	1.71E-40	1.28E-40	8.10E-41	5.67E-41	4.25E-41
175	2.06E-41	3.42E-41	3.29E-41	2.86E-41	2.10E-41	1.59E-41	1.25E-41
180	9.96E-45	3.93E-44	5.17E-44	5.29E-44	4.58E-44	3.76E-44	3.10E-44
185	5.57E-46	6.18E-45	1.12E-44	1.35E-44	1.37E-44	1.21E-44	1.05E-44
190	4.23E-47	1.42E-45	3.73E-45	5.38E-45	6.56E-45	6.39E-45	5.83E-45
195	4.13E-48	3.42E-46	1.22E-45	2.06E-45	2.94E-45	3.10E-45	2.97E-45
200	5.13E-49	9.99E-47	4.74E-46	9.20E-46	1.51E-45	1.71E-45	1.71E-45

4. Summary

In this contribution, we explored the absorption processes of photo-association, charge-exchange, and photo-dissociation for non-symmetric systems. We provide average cross-sections and also tabulated spectral rate coefficients for radiative processes involving calcium and hydrogen atoms, ions, molecules, and molecular ions in the wide region of temperatures in the EUV and VUV spectral region. The results have potential laboratory and astrophysical applications, such as in the spectroscopic investigation, synchrotron experiments, in the modeling of weakly ionized layers of the atmospheres of different stars and astronomical objects as well ISM.

The further step and our plan is to investigate absorption processes for other species in various environments. Also it would be very useful to include data in an A&M database. We plan to insert these datasets into a searchable A&M data provider - VAMDC (vamdc.eu), by extending one of the VAMDC nodes hosted by Serbian Virtual Observatory at servo.aob.rs.

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