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Data Descriptor

Data for Photodissociation of Some Small Molecular Ions Relevant for Astrochemistry and Laboratory Investigation

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Abstract: The calculated photodissociation data of some small molecular ions have been reported. The cross-sections and spectral rate coefficients data have been studied using a quantum mechanical method. The plasma parameters, i.e., conditions, cover temperatures from 1000 to 20,000 K and wavelengths in the EUV and UV region. The influence of temperature and wavelength on the spectral coefficients data of all of the investigated species have been discussed. Data could also be useful for plasma diagnostics in laboratory, astrophysics, and industrial plasmas for their modelling.

Dataset: Supplementary File.

Keywords: atomic and molecular data; photodissociation; small molecules; radiative processes; spectroscopy; astrochemistry; planetary chemistry; planetary geochemistry; modelling

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1. Summary

Atomic and molecular databases and data have become crucial for data interpretation, diagnostics, and the creation of models and simulations of intricate physical processes [1–4]. The importance of studying optical properties in different fields, especially when modelling those systems, is of particular interest [5–7]. If the required data, i.e., information, are available, we can simulate the spectral properties [8–11].

One can note the current importance of the investigation of optical properties of various small molecules and corresponding atomic and molecular data [12–17]. Here, we investigate the photodissociation processes that occur in non-symmetric systems that contain hydrogen and helium, and alkali atoms, ions, and molecular-ions. As noted in [18], the helium hydride ionic molecule has been discovered to be one of the primary constituents in He/H plasma sources, including synchrotron devices, high voltage glow discharges, inductively coupled plasma generators, capacitively coupled RF discharges, and magnetically confined plasmas, and plays a very special role in the advancement of thermonuclear fusion nowadays. The majority of alkali hydride species, both ionic and neutral, are highly important for comprehending how the molecular universe was created and developed [19]. Although they have a role in a number of astrophysical and astrochemical processes such as radiative transfer, their spectroscopy is mostly unknown in both theory and observation, especially when it comes to molecule ions [20]. In addition, one can note the potential importance of the aluminum monohydride cation in solar and in laboratory investigations [21,22].

Our aim is to obtain spectroscopic information, i.e., data, about such systems. We determined the spectral absorption rate coefficients and average cross-sections for molecular ions AlH^+, HeH^+, and HK^+. The outcomes, i.e., the data gathered, could be used

for various applications, such as plasma chemistry or experiments such as PLEIADES synchrotron [23–25], for modelling atmospheres of diverse environments such as the interstellar medium, planets, and dwarf stars, and also in the plasma fusion area [7,26–30].

2. Data Description

A dataset, i.e., new results for the average cross-section, as well as the spectral absorption rate coefficients for small molecular ions AlH^+, HeH^+, and HK^+ has been provided (see Tables S1–S9). In addition, the results are illustrated in this section by Figures 1 and 2 and also in Supplementary Materials.

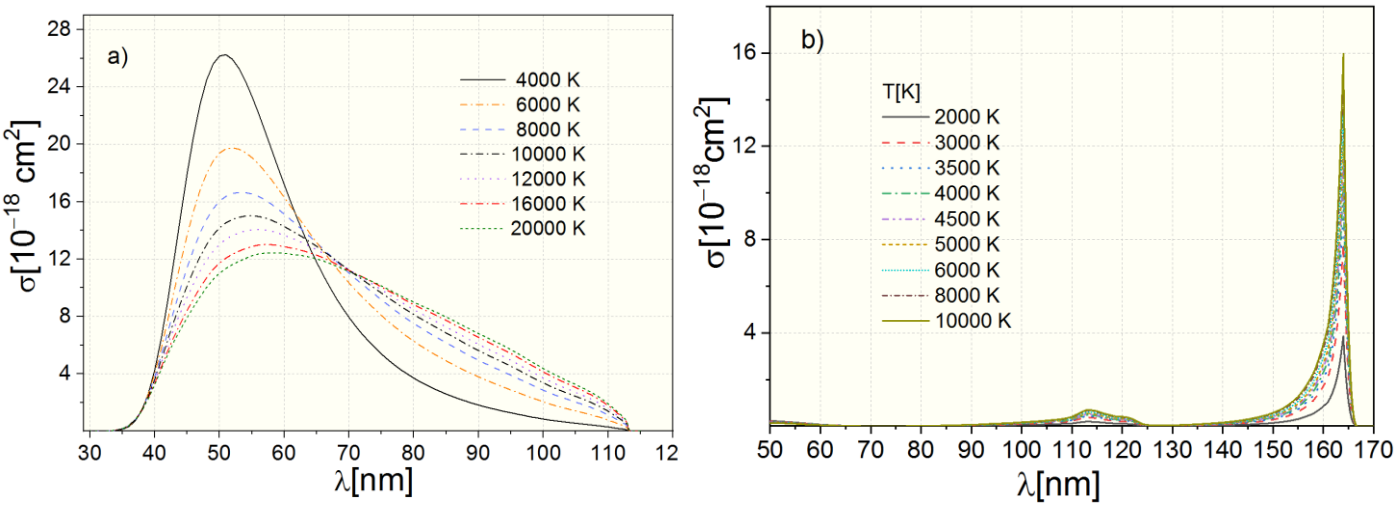

Figure 1. Examples of the averaged cross-section for photodissociation for some small molecular ions for the wide region of temperatures in EUV and VUV spectral region. (**a**) The averaged cross-section for photodissociation of the HeH^+ molecular-ion, as a function of wavelength and temperature. (**b**) The averaged cross-section for photodissociation of the AlH+ molecular-ion, as a function of wavelength and temperature.

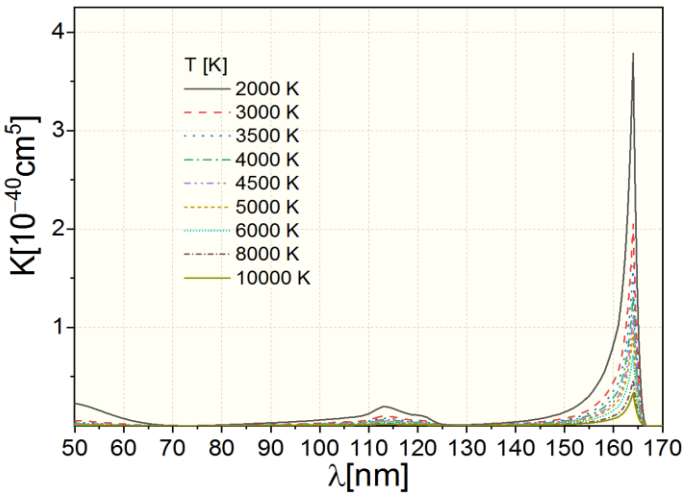

Figure 2. The photodissociation spectral rate coefficients K(λ, T) for the case of AlH^+ molecular ions as a function of wavelength and temperature.

The averaged cross-section for photodissociation for some small molecular ions for the wide region of temperatures in EUV and VUV spectral region are depicted in Figure 1a,b.

Figure 1a,b demonstrates that the temperature dependence of the mean thermal photoionization cross-section differs considerably for those species. In addition, the maxima of the cross section for those molecular ions are located at different wavelengths and with different behaviors (with slow and faster changes). Looking at Figure 1a,b and the data in the tables, it can be seen that cross-section maxima for HeH^+ are located around 50 nm. It is very wide (several tens of nm), i.e., cross-section slowly increases and also slowly decreases. The opposite behavior is shown by the KH^+ cross-section. The maxima are very sharp and at a wavelength of about 125 nm. In addition, AlH^+ has sharp maxima, but is located at higher wavelengths. All average cross-section data for photodissociation are presented in the Supplementary Material.

As an example, the behavior of the aluminum hydride cation photodissociation rate coefficient K(λ, T) data is graphically shown in Figure 2 as a function of wavelength and temperature. A similar behavior, i.e., shape can be observed as its average cross section. All of the data are organized into tables in the Supplementary Material for all of the analyzed species.

3. Methods

The spectral rate coefficients and average cross-sections were obtained using a quantum mechanical method in which the photodissociation process was studied as an outcome of radiative transitions among the ground state and the first excited adiabatic electronic state of the species, i.e., molecular-ion [5]. Here, in the dipole approximation, the transitions were caused by the electronic component of the ion-atom system interacting with the electromagnetic field. Within this theory, the mean thermal photodissociation cross-section can be given by:

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

where $E_{J,v}$ denotes the energies of the states with the respect to the ground rovibrational states. In the above equation, $\sigma_{J,v}(\lambda)$ is the partial cross-sections for the rovibrational states with specified quantum numbers J and v, given, e.g., in [5], with the dipole approximation. According to the processes' stated mechanism, the photon with energy ϵ_λ is absorbed close to the resonance point R = R_λ, where R_λ is the root of the equation $U_{12}(R) \equiv U_1(R) - U_2(R) = \epsilon_\lambda$. Here, the ground electronic state is represented by $U_1(R)$, while the first excited electronic state is represented by $U_2(R)$.

The photodissociation spectral rate coefficient can be presented using Equation (1) by the expression

$$K(\lambda, T) = \sigma(\lambda, T) \cdot \left(\frac{g_1 g_2}{g_{12}} \left(\frac{\mu k T}{2\pi\hbar^2} \right)^{\frac{3}{2}} \cdot \frac{1}{\sum\limits_{J,v} (2J+1) e^{\frac{E_{dest} - E_{J,v}}{kT}}} \right)^{-1} \quad (2)$$

In Equation (2) g_{12}, g_1, and g_2 denote the electronic statistical weights of the considered species, i.e., molecular ions, atoms, and ions, and E_{dest} is the molecular-ion dissociative energy. The theory, mechanism, and other needed quantities can be found in [5] in detail.

To prepare easier and more satisfying usage of calculated data in modelling as well as in an explanation of the experimental results in laboratories, we provide a simple fitting formula. We provide a simplified formula to prepare the calculated data for easier and more satisfactory employment in modelling and in the justification of experimental results in lab settings. Based on a least-square method, the photodissociation spectral rate coefficients for investigated small molecular ions can be presented as a logarithmic second-degree polynomial: $\log(K(\lambda, T)) = \sum\limits_{k=0}^{2} p_k(\lambda)(\log(T))^k$. In the Supplementary Tables coefficients,

$p_k(\lambda)$ for the selected fits and range of parameters for the aluminum hydride cation, helium hydride cation, and potassium hydride cation are given. We note that the simplified expression can be valid outside the range of defined plasma conditions, but their use should be taken with caution. In addition, we present Figure S1 in the Supplement Material, which simultaneously presents the photodissociation spectral rate coefficients data and simplified formula data on the example of HeH^+.

We note that both the cross-section and rate coefficient can be described by more sophisticated formulas. However, it is unclear how simple some of them are to use and whether they are appropriate when quick analysis and product delivery are crucial. The formula should be simple to use and allow for quick computations and practical analysis.

4. User Notes

A dataset with new results for photodissociation for corresponding molecular ion species is shown in Supplementary Material Tables S1–S9, which is appropriate for further use.

The presented data can be used in practice in different areas of science and in several possible ways:

- for laboratory research (spectroscopic investigation, synchrotron experiments, etc.)
- for industry and technology application
- for the advancement of chemistry and modelling of various layers of different atmospheres
- for potential astrophysical use (early universe chemistry and interstellar gas investigation)
- for various theoretical studies

Notably, the data and its analysis highlight interdisciplinary nature and usage, e.g., in physics, chemistry, astrophysics, astroinformatics, and astrobiology [24,31–35].

Supplementary Materials: The following supporting information are available online at https://www.mdpi.com/article/10.3390/data7090129/s1. Tables S1, S2, and S3 present data for average photodissociation cross-sections for molecular ions AlH^+, HeH^+, and KH^+. Tables S4, S5, and S6 the photodissociation spectral rate coefficients for investigated species. Tables S7, S8, and S9 present data for simplified formulas for photodissociation spectral rates. Figure S1 presents the simultaneous photodissociation spectral rate coefficients data and simplified formula data for the example of HeH^+.

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