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Photodissociation data for small molecular ions of astrochemical interest

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Abstract. This study examines radiative processes, with a focus on photodissociation, in non-symmetric hydrogen–silicon molecular systems. for the wide range of parameters. The results provide essential input for photochemical modeling in both laboratory plasmas and astrophysical contexts.

Key words: atomic and molecular datasets – laboratory and astrophysical plasma – optical characteristics – absorption – photodissociation – non-symmetric systems – modeling

1. Introduction

Atomic and molecular (A&M) data are vital for advancing spectroscopy, supporting theoretical models, and guiding experiments in molecular physics and astrochemistry (Hauschildt & Baron, 2010; Ferland et al., 2017; Albert et al., 2020; Mihajlov et al., 2011; Srećković et al., 2017; Srećković et al., 2021). Optical properties of small molecules, particularly molecular ions, remain of high interest for applications in astrochemistry, precision spectroscopy, and searches for interstellar species (Ignjatović et al., 2014; Vázquez-Carson et al., 2022; Mihajlov et al., 2011; Iacob, 2020; Srećković et al., 2022; Quitián-Lara et al., 2024).

Photodissociation governs molecular fragmentation in interstellar clouds and must be accurately modeled to predict abundances across environments such as protoplanetary disks, stellar envelopes, and galactic molecular clouds (Heays et al., 2017; Öberg, 2016). Among these, silicon-bearing molecules are notable, representing nearly 10% of known interstellar species (McCarthy et al., 2003). SiH and SiH^+, in particular, have astrophysical importance as components of interstellar clouds and stellar atmospheres (Singh & Vanlandingham, 1978; Stancil et al., 1997; van der Tak et al., 2020). Recent experiments confirmed SiH^+ production and provided benchmark data for astrochemical modeling (Mosnier et al., 2016).

Photodissociation cross-sections can be incorporated into astrophysical modeling tools such as CLOUDY, PDR Toolbox, or UCL-PDR to simulate the chemical and thermal balance of interstellar and circumstellar environments (see e.g. Ferland et al., 1998). These cross-sections are used to calculate wavelength-dependent photodissociation rates, which determine the destruction efficiencies of molecules under varying radiation fields. By integrating the cross-section data into the chemical reaction networks, the models can more accurately predict molecular abundances, emission features, and the evolution of photodissociation regions (PDRs) exposed to ultraviolet or X-ray radiation.

Here, we focus on spectroscopic properties of hydrogen–silicon systems, with emphasis on SiH^+ molecular ions, which are relevant to both astrophysical and fundamental studies (Yang et al., 2025). We present calculated absorption coefficients e.g. cross-sections in the EUV and UV ranges, applicable to synchrotron experiments and broader areas such as plasma modeling, ultrafast laser research, and astrophysical simulations (Mosnier et al., 2016; Doménech et al., 2017). Section 2 outlines the theoretical framework, Section 3 discusses findings in laboratory and astrophysical contexts, and Section 4 concludes with perspectives for future work.

2. Theory

This work examines how radiative processes influence the optical behavior of weakly ionized plasmas in both laboratory and astrophysical environments, with emphasis on bound–free photodissociation in strongly non-symmetric systems.

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

$$\varepsilon_\lambda + AM^+ \Rightarrow A^+ + M. \tag{1}$$

M is a silicon atom (Si), and A=H. Molecular-ion in the ground electronic state SiH^+ is represented by the symbol AM^+.

For the species under investigation, the mean thermal photodissociation cross-section $\sigma^{(bf)}(\lambda, T)$ can be represented in the form given by Srećković et al. (2017); Srećković et al. (2021)

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

Here, $\sigma^{(bf)}_{J,v}(\lambda)$ represents the partial photodissociation cross-section for the ro-vibrational states characterized by the quantum numbers v and J, while $E_{J,v}$ denotes the energies of these states relative to the ground ro-vibrational state. In the given expression, $E_{J,v} = E_{dis} + \epsilon_{J,v}$, where E_{dis} is the dissociation energy of the molecular ion, and the energies $\epsilon_{J,v} < 0$ are determined as described in Srećković et al. (2017). Under the dipole approximation, the partial cross-sections $\sigma_{J,v}^{(bf)}(\lambda)$ can be defined by the expression from (Srećković et al., 2021)

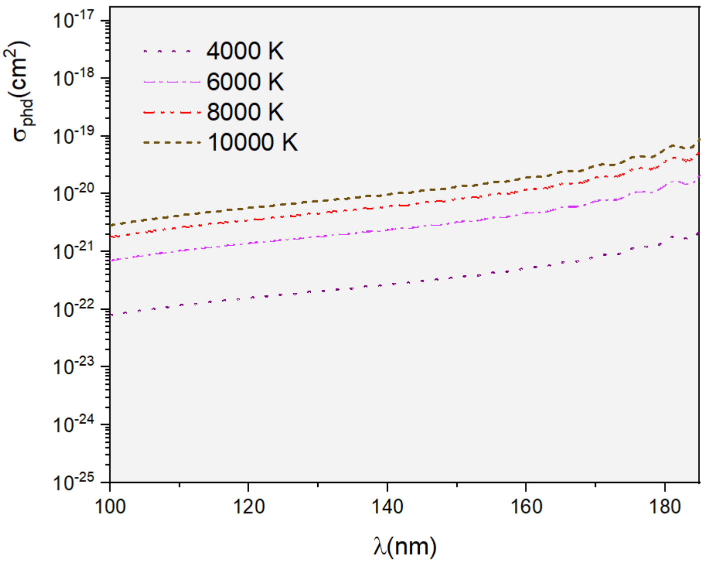

Figure 1. Calculated A&M data i.e. the mean thermal photodissociation cross-section for molecular-ion SiH^+.

3. Results and discussion

3.1. Astrophysical and laboratory relevance

Many astronomical software packages rely on photo-dissociation data (see e.g. Hauschildt & Baron, 2010, and references therein). In interstellar and circumstellar environments, UV photons strongly influence chemistry: atomic and molecular abundances in diffuse clouds are largely controlled by photodissociation and photoionization (Heays et al., 2017). In cometary comae, small molecules originate from UV-driven photodissociation of parent species (Irvine et al., 1998). These processes are essential for modeling diverse astrophysical regions, from dense star-forming clouds and protoplanetary disks to stellar envelopes and galactic molecular clouds (van Dishoeck et al., 2008). Such environments, where molecular destruction is dominated by photodissociation, are known as photon-dominated regions.

SiH^+, like other small molecular ions such as CH^+, OH^+, and NH^+, plays a important role in astrochemical networks and plasma environments, where its formation and destruction influence the chemistry of hydrogen- and silicon-bearing species. Comparable dissociation studies on ions such as BeT^+ and NS^+ highlight that accurate photodissociation data across diverse molecular systems are essential for reliably modeling molecular lifetimes and reaction pathways in both astrophysical and fusion plasmas (Hassaine et al., 2024; Iacob et al., 2022, 2020; Iacob, 2014, 2010).

Photodissociation of the SiH^+ ion is significant in plasma physics, spectroscopy, and semiconductor research (Zhao & Zeng, 2014). Silicon molecules occur in plasma environments such as etching and thin-film deposition, where understanding dissociation and ionization dynamics supports optimization of plasma-enhanced chemical vapor deposition (Gabriel et al., 2014). Laboratory measurements of photodissociation and photoionization cross-sections provide benchmark data for astrophysical and plasma modeling (Mosnier et al., 2016). Studies of VUV and EUV photon interactions with silicon ions further clarify bond strengths and reaction pathways.

3.2. The obtained quantities

The dataset spans the ultraviolet region and covers temperatures up to 10,000 K. These results are relevant for laboratory plasma diagnostics, astrophysical applications, and industrial plasma modeling.

Figure 1 shows the calculated average thermal photodissociation cross-section, $\sigma^{(bf)}_{SiH^+}(\lambda; T)$, of the silicon hydride ion over a wide temperature range (up tp 10,000 K) and wavelengths from 100 to 190 nm. The plot highlights a complex dependence on both variables, with pronounced maxima near 180–190 nm.

The calculated SiH^+ photodissociation cross-sections are generally consistent with previous theoretical data, including Stancil et al. (1997) and later MRCI studies (see e.g. McMillan et al., 2016), with minor resonance deviations. A conservative uncertainty is adopted, and these cross-sections are expected to refine SiH^+ photodissociation rates by up to an order of magnitude under typical interstellar and circumstellar radiation fields, improving predictions of silicon-bearing molecular abundances and emission. In the absence of experimental measurements, this semi-quantitative agreement with independent theoretical results supports the reliability of the present data.

4. Summary

This study investigates the photodissociation of non-symmetric molecular ions, focusing on the averaged cross-sections of SiH^+ across the EUV–UV range and temperatures up to 10,000 K. The resulting cross-sections enable more accurate modeling of SiH^+ destruction, directly influencing predicted silicon-bearing molecular abundances, emission features, and chemical evolution in UVirradiated interstellar and circumstellar environments. These findings are relevant for both laboratory and astrophysical applications, including spectroscopy, synchrotron-based experiments, and simulations of weakly ionized stellar and interstellar plasmas. SiH^+ plays a important role in interstellar chemistry, and its attosecond-scale photodynamics provide valuable insights for modeling space environments, laser-driven plasmas, and processes involving interstellar dust.

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