

Abstract Submitted
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Theoretical Studies of Dissociative Recombination of Electrons with SH^+ Ions¹ D.O. KASHINSKI, O.E. DI NALLO, United States Military Academy, A.P. HICKMAN, Lehigh University, D. TALBI, Université Montpellier II — We are investigating the dissociative recombination (DR) of electrons with the molecular ion SH^+ . (The process is $e^- + \text{SH}^+ \rightarrow \text{S} + \text{H}$.) SH^+ is found in the interstellar medium (ISM), and little is known concerning its interstellar chemistry. The abundance of SH^+ in the ISM suggests that destruction processes, like DR, are inefficient. Understanding the role of DR as a destruction pathway for SH^+ will lead to more accurate astrophysical models. We are currently performing large scale multi-reference configuration interaction (MRCI) electronic structure calculations to obtain excited-state potential energy curves (PECs) of SH. PECs have been calculated at several different values of the SH separation. This preliminary work shows that low Rydberg states strongly interact with excited valence states and suggests that highly excited Rydberg states might be critically important. Currently we are expanding the active space of the MRCI calculations in order to assess the importance of these excited Rydberg states. The block diagonalization method will be used to disentangle interacting states forming a diabatic representation of the PECs. The current status of the work will be presented at the conference.

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