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Abstract Submitted

for the DAMOP16 Meeting of
The American Physical Society

Theoretical Studies of Dissociative Recombination of Electrons with SH⁺ Ions¹ D. O. KASHINSKI², O. E. DI NALLO, United States Military Academy, A. P. HICKMAN, Lehigh University, J. ZS. MEZEI, F. COLBOC, I. F. SCHNEIDER, Université du Havre, K. CHAKRABARTI, University of Kolkatta, D. TALBI, Université Montpellier — We are investigating the dissociative recombination (DR) of electrons with the molecular ion SH⁺, i.e. $e^- + \text{SH}^+ \rightarrow \text{S} + \text{H}$. SH⁺ is found in the interstellar medium (ISM), and little is known concerning its chemistry. Understanding the role of DR of electrons with SH⁺ will lead to more accurate astrophysical models. Large active-space multi-reference configuration interaction (MRCI) electronic structure calculations were performed using the GAMESS code to obtain ground and excited ²Π state potential energy curves (PECs) for several values of SH separation. Core-excited Rydberg states have proven to be of huge importance. The block diagonalization method was used to disentangle interacting states and form a diabatic representation of the PECs. Currently we are performing dynamics calculations using Multichannel Quantum Defect Theory (MQDT) to obtain DR rates. The status of the work will be presented at the conference.

¹work supported by the French CNRS, the NSF, the XSEDE, and USMA

²travel supported by DoD-HPCMP

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Date submitted: 29 Jan 2016

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