Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Theoretical Studies of Dissociative Recombination of Electrons with SH^+ Ions[1] D. O. KASHINSKI[2], US Military Academy, A. P. HICKMAN, Lehigh University, J. ZS. MEZEI, ATOMKI, I. F. SCHNEIDER, Université du Havre, D. TALBI, Université Montpellier — We are investigating the dissociative recombination (DR) of electrons with the molecular ion SH^+, i.e. $e^- + SH^+ \rightarrow S + H$. SH^+ is found in the interstellar medium, and understanding its loss through DR will lead to more accurate astrophysical models. Recently we addressed the $^2\Pi$ potential energy curves (PECs) of SH as a DR pathway[3]. We have extended this work to investigate alternate DR pathways. Early results suggest that direct-mechanism DR through a $^4\Pi$ pathway may resolve the low-energy ($< 10\,\text{meV}$) discrepancy between experimentally determined rate coefficients and those determined through the indirect mechanism DR $^2\Pi$ pathway. PECs are obtained by performing large active space multi-reference configuration interaction (MRCI) electronic structure calculations for several values of SH separation. Rydberg-valence coupling has proven to be important. The block diagonalization method is used to disentangle interacting states forming a diabatic representation of the PECs. The status of this ongoing work will be presented at the conference.

[1]work supported by the French CNRS, the NSF, the XSEDE, and USMA
[2]travel supported by DoD-HPCMP
[3]Kashinski *et al.*, J. Chem. Phys. **146**, 204109 (2017)

David Kashinski
US Military Academy

Date submitted: 31 Jan 2020 Electronic form version 1.4