Theoretical Studies of Dissociative Recombination of Electrons with \( \text{SH}^+ \) Ions

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We are investigating the dissociative recombination (DR) of electrons with the molecular ion \( \text{SH}^+ \), i.e. \( e^- + \text{SH}^+ \rightarrow S + H \). \( \text{SH}^+ \) is found in the interstellar medium (ISM), and its chemistry is still not fully understood. Understanding the role of DR of electrons with \( \text{SH}^+ \) will lead to more accurate astrophysical models. Recently we addressed the \( ^2 \Pi \) potential energy curves (PECs) of \( \text{SH} \) as a DR pathway \(^3\). We are extending this work to investigate the ground and excited \( ^4 \Pi \) PECs of \( \text{SH} \) as an alternate DR pathway. Large active-space multi-reference configuration interaction (MRCI) electronic structure calculations were performed using the GAMESS code to obtain the PECs for several values of \( \text{SH} \) separation. Rydberg-valence coupling has proven to be important. The block diagonalization method was used to disentangle interacting states and form a diabatic representation of the PECs. The status of this ongoing work will be presented at the conference.

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