Theoretical Studies of Dissociative Recombination of Electrons with $\text{N}_2\text{H}^+$ Ions

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— We are investigating the dissociative recombination (DR) of electrons with the molecular ion $\text{N}_2\text{H}^+$. (The process is $e^- + \text{N}_2\text{H}^+ \rightarrow \text{N}_2 + \text{H}$.) $\text{N}_2\text{H}^+$ is found in the interstellar medium, and a better understanding of the DR process will aid the development of astrophysical models. For a quantitative DR study of $\text{N}_2\text{H}^+$, an even-handed treatment of the excited valence and Rydberg surfaces of $\text{N}_2\text{H}$ is required. We are currently performing large scale multi-reference configuration interaction (MRCI) electronic structure calculations to obtain these highly excited-state surfaces of $\text{N}_2\text{H}$. The effects of strong Rydberg-valence mixing in excited $\text{N}_2\text{H}$ are then disentangled to identify the primary dissociating surface that governs the DR process. This work is based on using the block diagonalization method to determine diabatic potential surfaces. The surfaces have been calculated at several different values of the NH distance and the NN–H bond angle. Preliminary results indicate that the direct method cross section is small at low energies which suggests the indirect method (or Renner-Teller effect) may play a role in the DR process. The current status of this work will be presented at the conference.

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