Abstract Submitted
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Theoretical Studies of Dissociative Recombination[1] D.O. KASHINSKI, R.F. MALENDA, A.P. HICKMAN, Lehigh University, D. TALBI, Université Montpellier II — We are currently investigating the dissociative recombination (DR) of electrons with the molecular ions N_2H^+ and and $C_3H_3^+$. These ions exist in the interstellar medium, and accurate DR rate constants are needed for astrophysical models. We are performing large scale electronic structure calculations of the excited-state potential surfaces of N_2H necessary to treat the process $e^- + N_2H^+ \rightarrow N_2 + H$ or $N + NH$. The work is based on using the block diagonalization method to determine diabatic potential curves. The dissociating curve that governs DR is then easily identified, and off-diagonal coupling terms can be used to determine the autoionization width Γ that is essential for a dynamics calculation. The status of the calculations will be presented at the conference. We have also investigated the normal modes of the molecular ion $C_3H_3^+$. We expect that energy flow into and out of the vibration of a single CH bond may influence the overall DR dynamics, and we account for this effect using an appropriate quantum mechanical wave function for the initial state.

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