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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 molecular ions such as N_2H^+ and $C_3H_3^+$. Both these ions exist in the interstellar medium, and accurate DR rate constants are needed for astrophysical models. Elaborate electronic structure calculations of potential surfaces for $e^- + N_2H^+ \rightarrow N_2 + H$ have been carried out in the linear geometry [D. Talbi, Chem. Phys. **332** 289–303 (2007)]. Additional work is necessary to determine the autoionization width Γ, which is essential for a dynamics calculation. We are using the block diagonalization method to determine both diabatic potential curves and Γ; the status of the calculations will be presented at the conference. In addition, preliminary work on the $C_3H_3^+$ molecular ion has investigated the normal modes of the motion. 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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