Abstract Submitted
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Theoretical Studies of Dissociative Recombination of Electrons with N_2H^+ Ions[1] D.O. KASHINSKI, R.F. MALENDA, A.P. HICKMAN, Lehigh University, D. TALBI, F. GATTI, Université Montpellier II — We are currently investigating the dissociative recombination (DR) of electrons with the molecular ion N_2H^+. The ion exists 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 $e^- + N_2H^+ \rightarrow N_2 + H$. The work is based on using the block diagonalization method to determine diabatic potential surfaces. The dissociating surface that governs DR is then is identified, and off-diagonal coupling terms can be used to determine the autoionization width Γ that is essential for a dynamics calculation. The surface has been calculated for several different values of the NH distance and the NN–H bond angle. Dynamics calculations using the Multi-Configuration Time-Dependent Hartree (MCTDH) method are also underway. The status of these calculations will be presented at the conference.

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