

Abstract Submitted
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Theoretical Studies of Dissociative Recombination of Electrons with N_2H^+ Ions R.F. MALEND A, Lehigh University, D.O. KASHINSKI, U. S. Military Academy, D. TALBI, F. GATTI, Université Montpellier II, A.P. HICKMAN, Lehigh University — We are investigating the dissociative recombination (DR) of electrons with the molecular ion N_2H^+ . (The process is $e^- + \text{N}_2\text{H}^+ \rightarrow \text{N}_2 + \text{H}$.) N_2H^+ is found in the interstellar medium, and a better understanding of the DR process will aid the development of astrophysical models. We have performed large scale electronic structure calculations of several excited-state diabatic potential surfaces of N_2H involved in DR. Additional calculations used the multiconfiguration time-dependent Hartree (MCTDH) method to propagate quantum mechanical wave packets on the potential surfaces involved in the direct DR process. For these calculations, R_{NN} is fixed at its equilibrium value, and the angular dependence in the Jacobi coordinate system is fit with a Legendre polynomial expansion. The cross section for the direct method has been found to be small for low energies. Rydberg potentials are being calculated for use in investigation of the indirect method. The current status of the work will be reported at the conference.

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