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Dissociative recombination (DR) and associative ionization (AI), $N_2^++e^- = N+N$, cross section calculations for atmospheric entry modeling EWA PAPAJAK, WINIFRED M. HUO, DAVID W. SCHWENKE, RICHARD L. JAFFE, NASA Ames Research Center — In order to maintain desired safety margins during atmospheric entry of a space vehicle, reaction models need to accurately account for processes leading to excited species that contribute to radiative heating of the vehicle. These reactions include ionization and electron-molecule processes that ionization enables. In particular, N + N AI is one of the mechanisms that can initiate production of free electrons during Earth entry. While experimental data on some of the total cross sections are available, few experiments address the need for the accurate AI cross sections starting from higher-lying atomic states and for 1,000-40,000K temperature range. In this work, theoretical cross sections and branching ratios for AI are calculated for a range of atomic states of N. We first calculate DR cross sections and then obtain AI cross sections and rate coefficients using detailed balance. For the DR calculations, we use state-of-the-art MRCI potential energy curves. The adiabatic potential curves are transformed to a diabatic representation, which is used in time-dependent wave packet calculations to describe the nuclear motion of the dissociating cation. The electron-scattering resonance widths are calculated by the R-matrix method. Based on the state distribution profiles in time, these calculations provide DR cross sections including recombination into high energy atomic states. The DR and AI rate coefficients and branching ratios are calculated and compared with the available experimental data.

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