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Dissociative recombination (DR) and associative ionization (AI) cross section calculations for the NO^+ + e <—>N + O reaction for atmospheric entry modeling EWA PAPAJAK, WINIFRED M. HUO, DAVID W. SCHWENKE, RICHARD L. JAFFE, NASA Ames Research Center — AI of N + O is the main mechanism that initiates production of free electrons during the entry of a space vehicle into Earth atmosphere. Subsequent electron impact processes, such as excitation and dissociation, lead to excited species that contribute significantly to radiation. While experimental data on total AI cross sections is available, few experiments address the need for the accurate cross sections for metastable atomic states that are important in entry conditions. We present theoretical cross sections and branching ratios for AI calculated for atomic states which are crucial for non-equilibrium radiative heating. In this work, we calculate cross sections of DR, and determine AI cross sections and branching ratios using microscopic reversibility. First, we calculate and analyze state-of-the-art MRCI potential energy curves. Features of these curves, e.g., excited states of the neutral that cross the ion curve, location of avoided crossings, and the types of atomic states connected to the molecular states, determine the DR mechanism. Secondly, R-matrix calculations provide resonance widths for the electron-scattering. Thirdly, we use the potential curves along with the e-scattering data to carry out the time-dependent wave packet calculations to describe the nuclear motion of the molecular ion upon its collision with an electron. Based on the state distributions profiles in time, these calculations provide cross sections for DR including recombination into high energy atomic states.

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