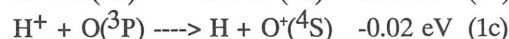
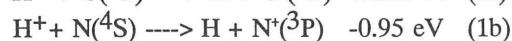
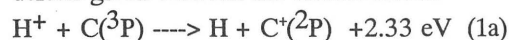


§4. Inelastic Processes in Collisions of H⁺ Ions with C, N and O Atoms below 1 keV

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Electron capture reactions resulting from collisions of protons with carbon, nitrogen and oxygen atoms are known to play an important role in earth's atmosphere, interstellar space, and astrophysical plasmas, and are fundamental for other relevant applied fields like fusion research¹⁾. Yet, accurate rates of these collision processes are rarely known except some crude and limited attempts for evaluation; certainly more reliable results are urgently needed. Rate coefficients for the [H⁺ + N] and [H⁺ + O] collision processes were theoretically evaluated by Steigman et al.⁵⁾ and Field and Steigman⁶⁾, respectively, based on an orbiting approximation with corresponding values of $2.5 \times 10^{-14} \text{ cm}^3/\text{s}$ and $7.4 \times 10^{-10} \text{ cm}^3/\text{s}$ at 10,000 K, respectively. Chambaud et al.⁷⁾ carried out a more rigorous study on electron capture in the [H⁺ + O] collisions using a molecular orbital method with the spin-orbit coupling as a driving force and determined the rate coefficient as $4.8 \times 10^{-10} \text{ cm}^3/\text{s}$ at 10,000 K. There is no large-scale theoretical study on the [H⁺ + C] and [H⁺ + N] collision systems except for an exploratory calculation by Butler and Dalgarno⁸⁾ for the [N⁺ + H] system.

In this paper, we attempt to investigate collision dynamics, and to evaluate electron capture cross sections and corresponding rate coefficients for the three (C,N,O) target atoms rigorously based on a molecular representation within a semiclassical framework for HC⁺, HN⁺ and HO⁺. The processes studied are as follows, with corresponding asymptotic energy defects given between the closest states:



The multireference single- and double-excitation (MRD-CI) configuration interaction method was employed⁹⁾. A semiclassical MO expansion method with a straight-line trajectory of the incident ion was employed to study the collision dynamics¹⁰⁾. Atomic-type electron translation factors (ETFs) were included. Substituting the total wave function into the time-dependent Schrödinger equation, we obtain a set of first-order coupled equations. By solving the coupled equations numerically, we obtain the scattering probabilities for transitions, and integration of this probability over the impact parameter gives the cross section. In adiabatic potentials

obtained, for the CH⁺ system, the ground [H⁺ + C(^3P)] channel lies above the dominant electron capture [H + C(^2P)] channel, whereas all the target-excitation [H⁺ + C(^1D, ^1S)] channels lie slightly above the ground state. For the NH⁺ system, the [H⁺ + N(^4S)] channel is the ground state with the electron capture [H + N(^3P)] channel nearby. Above this electron capture channel, a series of target excitation channels follows. For OH⁺ system, the [H⁺ + O(^3P)] channel is the lowest level similarly for the NH⁺ system and then, the electron capture [H + O(^4S)] channel and the target excitation [H⁺ + O(^1D)] channel follow. Because of a small asymptotic energy defect (near-resonant processes) between the initial and closest electron capture channels for almost all systems, the electron capture cross sections from the ground-state atoms are very large: approximately 10^{-16} – 10^{-15} cm^2 for all systems at above 100 eV. Corresponding rate coefficients are found to be much smaller than those previously reported for the NH⁺ and OH⁺ systems. The rate coefficients for the ground state atoms are found to increase with temperature (T) from less than $10^{-14} \text{ cm}^3/\text{s}$ to $2 \times 10^{-11} \text{ cm}^3/\text{s}$ for CH⁺, $3.5 \times 10^{-11} \text{ cm}^3/\text{s}$ to $2 \times 10^{-9} \text{ cm}^3/\text{s}$ for NH⁺ and $6.1 \times 10^{-11} \text{ cm}^3/\text{s}$ to $7 \times 10^{-9} \text{ cm}^3/\text{s}$ for OH⁺, when T is raised from 10,000 K to 100,000 K, respectively.

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