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RATE COEFFICIENTS FOR MOMENTUM TRANSFER, CHARGE TRANSFER, AND RADIATIVE ASSOCIATION PROCESSES IN COLLISIONS OF H^+ WITH He BELOW 10^5 K[1]

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ABSTRACT

The charge-transfer and momentum-transfer cross sections for protons in collisions with helium are calculated at relative energies up to 5 keV. Rate coefficients are presented for temperatures up to 10^5 K. Charge transfer is more rapid than radiative association at temperatures above 7500 K.

Subject headings: atomic processes — molecular processes

1. INTRODUCTION

Collisions of protons and helium atoms are significant in diverse astrophysical and atmospheric environments. At high energies, protons traversing helium gas undergo charge transfer and produce fast hydrogen atoms. At lower energies the cross section for charge transfer must decrease, and protons penetrate without being neutralized, losing energy primarily by momentum transfer in elastic collisions. At thermal energies in a nearly neutral gas, protons may be removed by radiative association to form HeH^+ molecular ions, which then undergo dissociative recombination. We extend previous calculations carried out at high energies down to the threshold region, and we compare the thermal rate coefficients with those for radiative association.

2. THEORY

The theory was described in detail by Kimura & Lane (1989). Adiabatic potentials were obtained for the initial state, $H^+ + He(1\,^1S)$, $X\,^1\Sigma^+$, and charge transferred state, $H(1s) + He^+(1s)$, $A\,^1\Sigma^+$. Full configuration interaction calculations were carried out, and the nuclear momentum coupling matrix element and the transition dipole moment were determined (Kimura 1985). The asymptotic energy defect is ~ 0.4 au (or 11 eV), which is the threshold energy of the process (Kimura 1985). The cross section for charge transfer at energy ϵ is given in terms of the off-diagonal elements of the scattering matrix $S_l(\epsilon)$ corresponding to the orbital angular quantum number l by

$$\sigma(\epsilon) = \frac{\pi}{2k^2} \sum_l (2l + 1)\,|S_l|^2\,, \qquad (1)$$

where k is the wavenumber of relative heavy particle motion. The energy ϵ and the momentum k are related by $k^2 = 2\mu\epsilon/\hbar^2$, where μ is the reduced mass. The S-matrix can be extracted from the set of radial wave functions $X(R)$, expressed as a matrix, by imposing the appropriate outgoing boundary conditions in the limit of large internuclear distances R. If E is the total energy, the radial wave functions $X(R)$ satisfy the coupled equations (Heil, Butler, & Dalgarno 1981),

$$\frac{-1}{2\mu}\,[\{\boldsymbol{I}\nabla_R - i(\boldsymbol{P} + \boldsymbol{A})\}^2 + \boldsymbol{V}]X(R) = EX(R)\,, \qquad (2)$$

where $\boldsymbol{P}$, $\boldsymbol{A}$, and $\boldsymbol{V}$, describe, respectively, the nonadiabatic (nuclear momentum) coupling, its correction (to first order in relative velocity) arising from electron translation factors, and the diagonal potential energy matrix with elements consisting of the electronic energies of the molecular states and the nuclear repulsion term (Zygelman et al. 1989). The molecular electron translation factors were determined by the optimization procedure (Kimura & Lane 1989) that minimizes the nonphysical radial coupling with states corresponding to the He($1s$, $n = 3$) manifold. The diabatic representation was used to solve equation (2) (Heil et al. 1981).

These procedures yielded differential and total cross sections for charge transfer

$$H^+ + He \rightarrow H + He^+ \qquad (3)$$

and elastic scattering

$$H^+ + He \rightarrow H^+ + He \qquad (4)$$

at energies between 0.5 and 5 keV in close agreement with experiment (Johnson et al. 1989) and should remain valid at lower energies.

The radiative association process

$$H^+ + He \rightarrow HeH^+ + h\nu \qquad (5)$$

is dominated by shape resonances (Dabrowski & Herzberg 1978; Roberge & Dalgarno 1982), and the rate coefficient at temperature T is given by the Breit-Wigner expression (Bain & Bardsley 1972)

$$k_r(T) = \left(\frac{2\pi}{\mu kT}\right)^{3/2} \sum_{v,J} \frac{(2J + 1)}{\tau^r_{vJ} + \tau^p_{vJ}} \exp\left(\frac{-E_{vJ}}{kT}\right), \qquad (6)$$

where τ^r and τ^p are the radiative and predissociative lifetimes, respectively, of the resonance with vibrational and rotational quantum numbers vJ, and E_{vJ} is the resonance energy measured from the dissociation limit of the $X\,^1\Sigma^+$ state.

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TABLE 1

MOMENTUM TRANSFER AND CHARGE TRANSFER CROSS SECTIONS

E (eV)	Momentum Transfer σ (cm^2)	Charge Transfer σ (cm^2)
0.01	8.7×10^{-15}	...
0.1	3.6×10^{-15}	...
1	7.4×10^{-16}	...
10	6.6×10^{-17}	...
20	3.9×10^{-17}	3.7×10^{-23}
50	2.0×10^{-17}	1.5×10^{-21}
100	1.1×10^{-17}	1.1×10^{-20}
500	5.4×10^{-18}	4.3×10^{-19}
1000	5.3×10^{-18}	1.4×10^{-18}
5000	5.1×10^{-18}	2.4×10^{-17}

3. RESULTS

The calculated charge-transfer cross sections between 20 eV and 5 keV are presented in Table 1 and are also shown in Figure 1. The cross sections decrease very rapidly with decreasing energy. Low-energy protons passing through helium will not be neutralized but will lose energy primarily through momentum-transfer in elastic collisions.

The cross sections for momentum transfer are also listed in Table 1. They decrease rather slowly with increasing energy, falling from 7.4×10^{-16} cm^2 at 1 eV to 5.1×10^{-18} cm^2 at 5 keV. At thermal energies, the rate coefficient for momentum transfer is related directly to the mobility of protons in helium gas. The calculated values of the rate coefficients, which agree with those of Dickinson (1968) within a few percent, are shown in Table 2. For temperatures below 1000 K, they are equal to the limiting value determined by the polarizability of helium (Radzig & Smirnov 1980). Above 10,000 K, the short-range forces contribute causing a slight enhancement.

The rate coefficients for charge transfer are listed in Table 3. They increase steeply from 7×10^{-19} cm^3 s^{-1} at 8000 K to 3.7×10^{-15} cm^3 s^{-1} at 40,000 K.

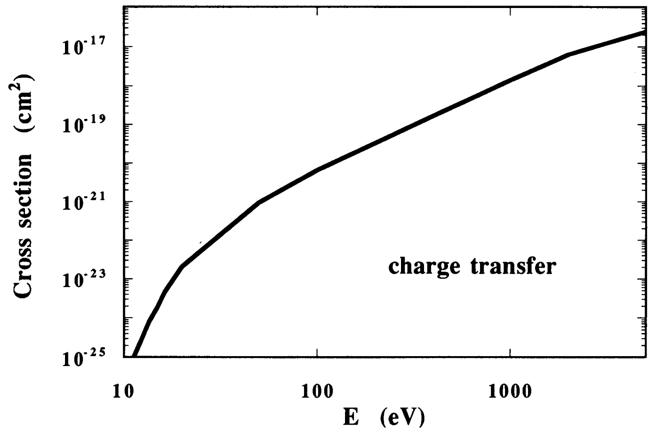

FIG. 1.—The cross section for He^+ ion formation as a function of collision energy.

Table 3 also includes the rate coefficients for radiative association. Below ~7500 K, radiative association proceeds more rapidly than direct charge transfer. However, radiative association is still very slow; other mechanisms such as radiative recombination with electrons will determine the proton neutralization rate in most plasmas at these temperatures.

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TABLE 2

RATE COEFFICIENTS FOR MOMENTUM TRANSFER

T (K)	Momentum Transfer k (cm^3 s^{-1})
50	1.05×10^{-9}
100	1.05×10^{-9}
500	1.05×10^{-9}
1000	1.05×10^{-9}
5000	1.06×10^{-9}
10000	1.17×10^{-9}
50000	1.44×10^{-9}
100000	1.83×10^{-9}

TABLE 3

RATE COEFFICIENTS FOR CHARGE TRANSFER AND RADIATIVE ASSOCIATION

T (K)	Charge Transfer k (cm^3 s^{-1})	Radiative Association k (cm^3 s^{-1})
6000	4.7×10^{-22}	2.7×10^{-20}
8000	7.4×10^{-19}	1.8×10^{-20}
10000	2.6×10^{-18}	1.3×10^{-20}
20000	2.7×10^{-16}	5.0×10^{-21}
40000	3.7×10^{-15}	1.5×10^{-21}
80000	4.5×10^{-14}	2.5×10^{-22}
100000	1.5×10^{-13}	1.2×10^{-22}

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