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RADIATIVE AND NONRADIATIVE CHARGE TRANSFER IN COLLISIONS OF H^+ WITH Li BELOW 1 keV

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ABSTRACT

Charge transfer resulting from collisions of H^+ with Li is studied from 1 keV u^{-1} down to 10^{-5} eV u^{-1}. Excitation to Li*(2*p*) and charge transfer to H($n = 2$) are found to be dominant above 10 eV. Below 10 eV, nonradiative charge transfer to H(1*s*) takes over, and at much lower energies radiative charge transfer/association becomes dominant. The rate coefficient for radiative charge transfer/association is on the order of 10^{-17} cm^3 s^{-1} with a slowly decreasing trend as the temperature increases, while that for non-radiative charge transfer varies drastically from 10^{-20} cm^3 s^{-1} at 100 K to 10^{-12} cm^3 s^{-1} at 10,000 K.

Subject heading: atomic processes

1. INTRODUCTION

The importance of charge transfer in astrophysics has been known for many years. For example, it is known to play a major role in understanding the galactic corona (Ferland & Shields 1985). Quantitative data of charge transfer cross sections are essential in modeling the solar and stellar structures and modeling their evolutions. In the universe, hydrogen atoms are the most abundant species, and most of them are ionized to form H^+ by X- and γ-rays and galactic cosmic rays. Lithium atoms are also abundant in the interstellar gas (Hobbs & Pilachowski 1988) and in some stars (Pallavicini, Randich, & Giampapa 1992; Randich, Gratton, & Pallavicini 1993), as well as in the solar photosphere (Turck-Chieze et al. 1991). In the domain where the gas density is low, such as the interstellar gas, charge transfer cross sections for the $H^+ + Li \rightarrow H + Li^+$ process are expected to be of importance practically. In the present work, we have calculated the radiative and nonradiative charge transfer cross sections for a collision of H^+ with Li in the collision energy range from 10^{-5} eV to 1 keV and the corresponding rate coefficients up to a temperature of 10,000 K. Processes (and corresponding asymptotic energy defects) studied are the following:

$$H^+ + Li(2s) \rightarrow \begin{cases} H(n=2) + Li^+ & \text{charge transfer} & -1.9 \text{ eV} & \text{(1a)} \\ H^+ + Li^*(2p) & \text{excitation} & -1.8 \text{ eV} & \text{(1b)} \\ H(1s) + Li^+ & \text{nonradiative charge transfer} & +8.2 \text{ eV} & \text{(1c)} \\ H(1s) + Li^+ + h\nu & \text{radiative charge transfer} & +8.2 \text{ eV} & \text{(1d)} \end{cases}$$

Unlike other (H-alkali atom)$^+$ systems (Kimura, Olson, & Pascale 1982; Sato & Kimura 1983), e.g., Na, K, Rb, and Cs, the excitation channels for Li (1b) are energetically closer to the initial channel than any of charge transfer channels. This difference makes the HLi^+ system unique and more complex, theoretically.

2. THEORETICAL MODEL

2.1. *Molecular States*

The configuration interaction method based on a linear combination of atomic orbitals representation was used to obtain molecular electronic states (MOs). The $(HLi)^+$ system was treated as a quasi–one-electron system, with the $Li^+(1s^2)$ core represented by a Gaussian-type pseudopotential (Sato & Kimura 1983). Slater-type orbitals were used as a basis set. All parameters used in the calculation can be found in previous reports (Kimura et al. 1982; Sato & Kimura 1983). The eigenenergies obtained were compared with spectroscopic data (Bashkin & Stoner 1975) and found to agree within 0.2%. At low collision energies, below ~ 1 eV, distant collisions are expected to be important; accordingly, we have modified the initial adiabatic potential by adding a long-range polarization term (Dutta, Lane, & Kimura 1992).

2.2. *Collision Dynamics*

2.2.1. *Nonradiative Process*

Nonradiative charge transfer is treated by (*a*) a semiclassical impact parameter method and (*b*) a quantum mechanical approach, both based on the MO expansion. Atomic-type electron translation factors (ETFs) were properly included (Kimura & Lane 1989). For the semiclassical approach, the total wave function is expanded in products of MOs and ETF. Substitution of the total wave function into the time-dependent Schrödinger equation yields first-order coupled equations for the expansion coefficients. For the quantum approach, the total wave function is expanded in products of MOs, ETFs, and nuclear wave functions. Substitution of the

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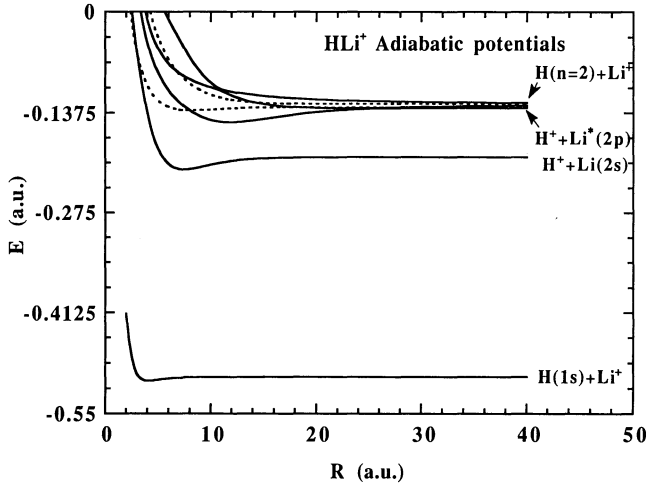

FIG. 1.—Adiabatic potentials for the HLi^+ system

total wave function into the time-independent Schrödinger equation leads to a second-order coupled equation for the nuclear wave function. Both sets of coupled equation are solved numerically to obtain a scattering amplitude for the semiclassical approach and a scattering S-matrix for the quantal approach. By a standard procedure, one can easily relate these quantities to transition probabilities and cross sections (Kimura & Lane 1989).

2.2.2. *Radiative Process*

The optical potential method (Cohen & Bardsley 1978) is used for radiative charge transfer. In this model, the total transition probability per unit time for radiative charge transfer and association from the $A\Sigma$ state to the $X\Sigma$ state is described by a complex potential, the imaginary part of which is the spontaneous radiative transition probability at a particular internuclear distance: the Einstein A-coefficient. The coupled equations are solved by using a partial wave decomposition of the amplitude. The partial wave solution has complex phase shifts, the imaginary part of which contains information about the loss of flux by photon emission from the initial channel, hence radiative charge transfer and association.

3. RESULTS

Figure 1 illustrates the adiabatic potential curves for the HLi^+ system. Above 1.8 eV one notes a set of excitation channels (1b) that have a strong avoided crossings, with charge transfer channels (1a) around $R = 25\ a_0$. These charge transfer channels, which lie about 0.1 eV (asymptotically) above the excitation channels, are known to be dominant in charge transfer at high energies (Sato & Kimura 1983). Nonradiative and radiative H(1s) charge transfer channels are located about 8 eV below the initial channel. As previous studies have shown (Zygelman et al. 1989), the radiative charge transfer process is not expected to become important unless energy is less than a few eV. The relevant nonadiabatic coupling matrix elements were presented previously (Sato & Kimura 1983). Figure 2 shows the Einstein coefficient for the $H^+ + Li(2s): A\,^2\Sigma \rightarrow H(1s) + Li^+: X\,^2\Sigma$ transition. Figure 3 presents the charge

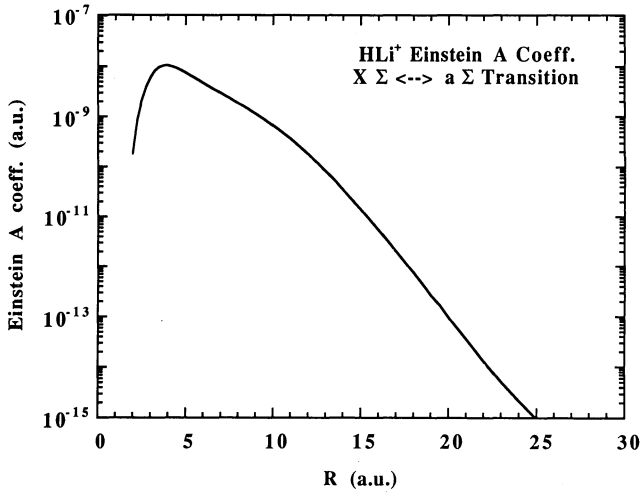

FIG. 2.—The Einstein coefficient

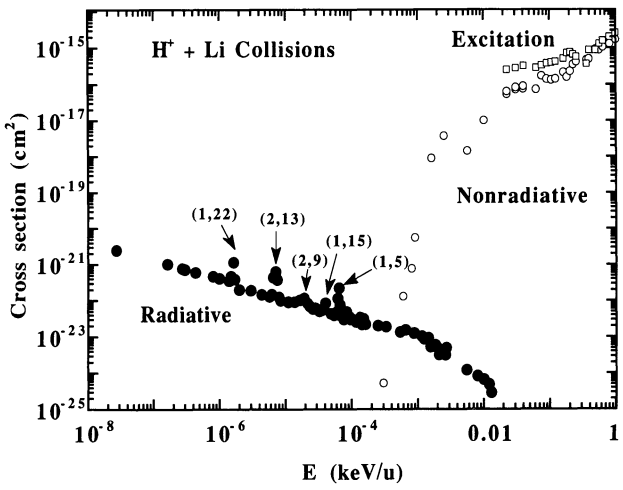

FIG. 3.—Nonradiative and radiative charge transfer cross sections above 10^{-5} eV u^{-1}. Some of the ro-vibrational (v, J) levels are accordingly labeled

TABLE 1

RATE COEFFICIENTS FOR RADIATIVE CHARGE TRANSFER/ASSOCIATION, NONRADIATIVE CHARGE TRANSFER, AND EXCITATION

TEMPERATURE (K)	RATE COEFFICIENTS ($cm^3\ s^{-1}$)		
	Radiative	Nonradiative	Excitation
100	2.0×10^{-17}	4.0×10^{-20}	...
200	1.8×10^{-17}	4.1×10^{-20}	...
400	1.7×10^{-17}	5.1×10^{-20}	...
600	1.6×10^{-17}	4.3×10^{-19}	1.6×10^{-27}
800	1.5×10^{-17}	5.5×10^{-18}	2.8×10^{-23}
1000	1.5×10^{-17}	4.8×10^{-17}	1.0×10^{-20}
2000	1.4×10^{-17}	9.3×10^{-15}	1.5×10^{-15}
4000	1.4×10^{-17}	2.5×10^{-13}	6.2×10^{-13}
6000	1.4×10^{-17}	9.2×10^{-13}	4.4×10^{-12}
8000	1.4×10^{-17}	1.8×10^{-12}	1.1×10^{-11}
10,000	1.3×10^{-17}	2.7×10^{-12}	3.5×10^{-11}

transfer and excitation cross sections. At 1 keV, the present calculation reproduces the theoretical value of the charge transfer cross section previously reported by Sato & Kimura (1983). Excitation is dominant below 200 eV because of the smaller energy defects with respect to the initial channel. However, charge transfer becomes comparable above 500 eV. Oscillatory structures seen in the excitation and charge-transfer cross sections, which are nearly out of phase with each other, are considered to be Rosenthal oscillations (Kimura & Lane 1989). The charge transfer cross section drops rather sharply toward threshold, while the excitation cross section decreases more slowly below 100 eV. This rapid drop of the charge transfer cross section is due to a sharply decreasing contribution from the charge transfer process (1*a*), i.e., H($n = 2$) formation, leaving the nonradiative charge transfer process (1*c*) the sole contributor. The cross section for the radiative charge transfer/association process is also included in Figure 3. Radiative charge transfer/association becomes dominant below 0.4 eV, while nonradiative charge transfer is comparable at that energy. The sharp, resonance-like structures seen in radiative charge-transfer are due to ro-vibrational bound states of the initial state. The (v, J) levels, where v and J represent vibrational and rotational quantum numbers, respectively, are labeled on some of peaks in the figure. Rate coefficients for the individual processes are given in Table 1.

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