

# RATE COEFFICIENTS FOR CHARGE TRANSFER OF $\text{He}^+$ WITH C

M. KIMURA<sup>1</sup> AND A. DALGARNO

Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138

AND

L. CHANTRANUPONG, Y. LI, G. HIRSCH, AND R. J. BUENKER

Theoretische Chemie, Bergische Universität-Gesamthochschule Wuppertal, Gauss str. 20, D-5600 Wuppertal 1, Germany

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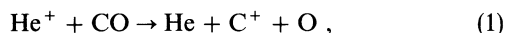
## ABSTRACT

Rate coefficients for nonradiative charge transfer in collisions of  $\text{He}^+$  with C are calculated for temperatures up to 10,000 K. The rate coefficients increase from  $2.8 \times 10^{-15} \text{ cm}^3 \text{ s}^{-1}$  at 100 K to  $6.8 \times 10^{-13} \text{ cm}^2 \text{ s}^{-1}$  at 10,000 K.

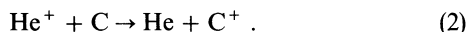
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## 1. INTRODUCTION

The ionization in the ejecta of supernova 1987a is initially driven by the  $\gamma$ -rays released in the decay of  $^{56}\text{Co}$  and later  $^{57}\text{Co}$  and  $^{44}\text{Ti}$ . The  $\gamma$ -rays lose energy in Compton collisions with electrons and are degraded into X-rays. The elements are multiply ionized by Compton and X-ray ionization. They recombine by dielectric and radiative recombination and, once neutral material is formed, by charge transfer, which rapidly reduces the ions to the singly ionized state. The fate of the singly charged ions is uncertain. Of particular significance for the abundance of the molecules CO and SiO is the ion  $\text{He}^+$  (Lepp, Dalgarno, & McCray 1990). Because of the destructive effect of the reaction



it has been argued that only limited microscopic mixing of the light and heavy elements can occur if the observed abundances of CO and SiO are to be explained (Liu, Lepp, & Dalgarno 1992). However, these authors pointed out that the conclusion would be modified if the  $\text{He}^+$  ions were removed preferentially by reaction with neutral atoms. One such possibility is the charge transfer process:



We present here a calculation of the potential energy curves of  $\text{CHe}^+$  and identify the quasi-molecular states of  $\text{CHe}^+$  that control the charge transfer at low velocities. We conclude that the rotational coupling of the  $D^2\Sigma^-$  and  $B^2\Pi$  states drives the low-energy charge transfer, and we calculate the rate coefficient as a function of temperature.

## 2. THEORY

The electronic states of  $\text{HeC}^+$  were described by the multi-reference single- and double-excitation configuration interaction (MRD-CI) method (Buenker & Peyerimhoff 1974;

Buenker 1981; Buenker & Phillips 1985; Knowles et al. 1990). The carbon atom basis set is a double-zeta polarization type  $(9s5p1d)/[4s2p1d]$  (Dunning 1970), supplemented by the Rydberg functions of 3s, 3p, and 3d with exponents  $\alpha_s = 0.023$ ,  $\alpha_p = 0.021$ , and  $\alpha_d = 0.015$ . This basis set for the carbon atom may be characterized as  $(10s6p2d)/[5s3p2d]$ . The helium atom basis set is  $(7s)/[5s]$  (Huzinaga 1965), and we added a set of polarization functions consisting of two s ( $\alpha_s = 0.08, 0.02$ ), three p ( $\alpha_p = 1.0, 0.2, 0.08$ ), and one d ( $\alpha_d = 0.8$ ) functions onto the helium atom. This basis set for the helium atom is characterized as  $(9s3p1d)/[7s3p1d]$ . For the  $\text{HeC}^+$  system, the initial and charge transfer channels correspond to the  $[\text{He}^+(^2S) + \text{C}(^3P)]$  ( $1\sigma^2 2\sigma^2 3\sigma 1\pi^2$ ) and  $[\text{He}(^1S) + \text{C}^+(^2D)]$  ( $1\sigma^2 2\sigma^2 3\sigma 4\sigma 1\pi$ ) states, respectively. The calculated potential energy curves suggest that in low-energy collisions the charge transfer is driven by the rotational coupling of an initial  $^2\Sigma^-$  state and a final  $^2\Pi$  state. Figure 1 illustrates the adiabatic CI potentials for the  $D^2\Sigma^-$  initial state and the  $B^2\Pi$  charge transfer state. The calculated dissociation energy of the initial state is 3.0 eV.

The scattering calculation was carried out by using a fully quantum mechanical representation. In this representation, the coupled equations have the form (Kimura & Lane 1989)

$$\left[ \left\{ \frac{d^2}{dR^2} + \left[ 2\mu(E - \epsilon_n) + \frac{\ell(\ell+1)}{R^2} \right] \right\} I + \frac{\sqrt{2\ell(\ell+1)}}{R^2} L_{mn} \right] F_\ell(R) = 0, \quad (3)$$

where  $F_\ell(R)$  and  $I$  describe the radial wavefunction of the  $\ell$ th partial wave and a unit matrix in the vector representation,  $\mu$  and  $\epsilon_n$  represent the reduced mass and electronic energy of  $n$ th state, and  $L_{mn}$  is the rotational coupling matrix with the form

$$L_{mn} = \langle \phi_m | iL_y | \phi_n \rangle \delta_{m,n\pm 1}, \quad (4)$$

where  $L_y$  is the component of the electronic angular momentum perpendicular to the classical collision plane and  $\phi_i$  is the  $i$ th molecular wavefunction. We solved the coupled equation (1) numerically to obtain the scattering matrix  $S_\ell(E)$  corresponding to the orbital angular quantum number  $\ell$  and deter-

<sup>1</sup> Permanent address: Argonne National Laboratory, Argonne, IL 60439; also Department of Physics, Rice University, Houston, TX 77251.

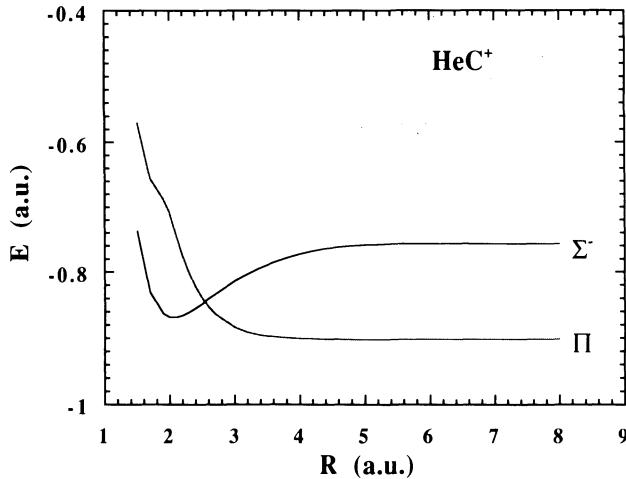


FIG. 1.—Adiabatic potential energy curves for the  $D^2\Sigma^-$  and  $B^2\Pi$  states of the  $\text{HeC}^+$  system.

mined the cross section for charge transfer according to the standard expression

$$\sigma(E) = g \frac{\pi}{2k^2} \sum_{\ell} (2\ell + 1) |S_{\ell}|^2, \quad (5)$$

where  $g = \frac{1}{9}$  is the probability of approach along the initial  $^2\Sigma^-$  state, and the energy  $E$  and the momentum  $k$  are related by  $k^2 = 2\mu E/\hbar^2$ . These procedures were applied to calculate total cross sections for the charge transfer process (2).

### 3. RESULTS

The calculated charge transfer cross sections for collision energies between  $10^{-5}$  and 10 eV are presented in Figure 2. The cross sections increase with increasing energy, reaching a plateau of about  $2 \times 10^{-19} \text{ cm}^2$  at 1.0 eV. Partial charge transfer cross sections at  $E = 1 \times 10^{-1} \text{ eV}$  and  $1 \times 10^{-2} \text{ eV}$  are shown in Figure 3 as a function of partial wave  $\ell$ . As the energy increases, the dominant contribution shifts to larger  $\ell$ . Above 20 eV,  $\Pi$ - $\Pi$  radial coupling connecting an initial  $D'^2\Pi$  channel and a final  $B^2\Pi$  channel becomes important, and a multi-channel close-coupling calculation is necessary to accurately

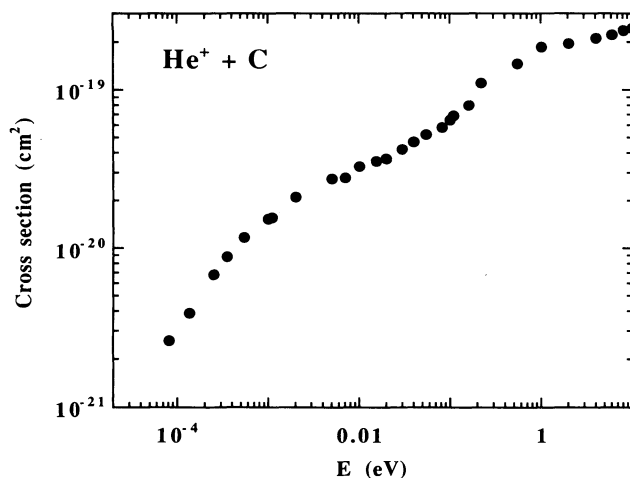


FIG. 2.—Charge transfer cross sections as a function of collision energy

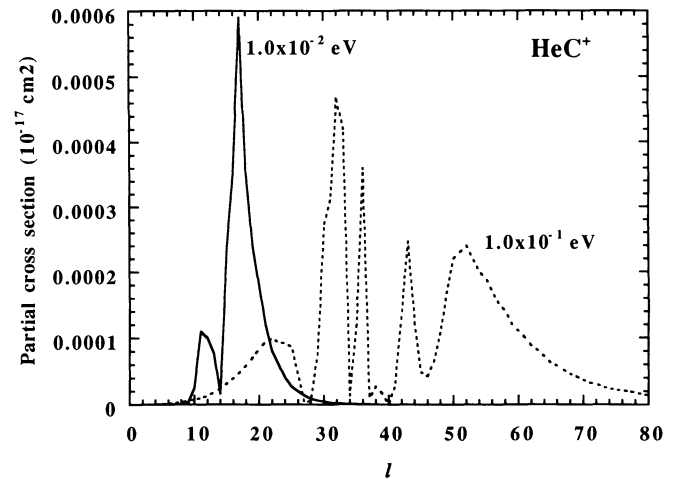


FIG. 3.—Partial charge transfer cross sections as a function of partial wave  $\ell$  at  $E = 1 \times 10^{-2}$  and  $1 \times 10^{-1} \text{ eV}$ .

determine the cross section. However, at lower energies our two-channel calculation should be valid.

The rate coefficients for the process (2) are summarized in Table 1 from 10 to 10,000 K. At 100 K the rate coefficient is  $2.8 \times 10^{-15} \text{ cm}^3 \text{ s}^{-1}$ , and it steadily increases with temperature, reaching  $6.8 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$  at  $10^4 \text{ K}$ .

The rate coefficient is small, and the conclusions of Liu et al. (1992) are unchanged. The process is similarly not important in the chemistry of carbon in interstellar clouds, but may exert a minor influence in shock-heated and photon-dominated regions.

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TABLE 1  
RATE COEFFICIENTS FOR CHARGE TRANSFER  
IN  $\text{He}^+ + \text{C}$  COLLISIONS

$T$ (K)	Rate Coefficient ( $\text{cm}^3 \text{ s}^{-1}$ )
10.....	$4.9 \times 10^{-16}$
20.....	$8.9 \times 10^{-16}$
40.....	$1.5 \times 10^{-15}$
60.....	$2.0 \times 10^{-15}$
80.....	$2.4 \times 10^{-15}$
100.....	$2.8 \times 10^{-15}$
200.....	$4.7 \times 10^{-15}$
400.....	$9.2 \times 10^{-15}$
600.....	$1.4 \times 10^{-14}$
800.....	$2.0 \times 10^{-14}$
1000.....	$2.6 \times 10^{-14}$
2000.....	$5.2 \times 10^{-14}$
4000.....	$1.3 \times 10^{-13}$
6000.....	$2.9 \times 10^{-13}$
8000.....	$4.8 \times 10^{-13}$
10000.....	$6.8 \times 10^{-13}$

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