THE ASTROPHYSICAL JOURNAL, 502:1006–1009, 1998 August 1

CHARGE TRANSFER IN COLLISIONS OF C^+ WITH H AND H^+ WITH C

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Received 1997 November 12; accepted 1998 March 6

ABSTRACT

Charge transfer rate coefficients for collisions of C^+ with H and H^+ with C are presented for temperatures from 30,000 to 10^7 K and from 10 to 10^7 K, respectively. The rate coefficients were calculated from recommended cross sections deduced in a recent theoretical and experimental investigation that took into account previous measurements. Nonadiabatic radial coupling is the dominant mechanism for both reactions above $\sim$50,000 K, but for lower temperatures the reaction of H^+ with C proceeds primarily by radiative charge transfer. Implications, due to the magnitude of the rate coefficients, for various astrophysical environments are discussed.

Subject headings: atomic processes — ISM: atoms — supernovae: individual (SN 1987A)

1. INTRODUCTION

In astrophysical and laboratory plasmas, the ionization structure of carbon is often predominantly established through a balance of photoionization with radiative and dielectronic recombination. However, the charge transfer process

$$C^+(^2P^o) + H \rightarrow C(^3P) + H^+ , \quad (1)$$

which is endothermic by 2.33 eV, and its reverse,

$$C(^3P) + H^+ \rightarrow C^+(^2P^o) + H , \quad (2)$$

may also be important if their rates are fast enough and if the neutral densities are high enough. In addition, an electron can be removed from a carbon atom via the radiative charge transfer reaction

$$C(^3P) + H^+ \rightarrow C^+(^2P^o) + H + h\nu , \quad (3)$$

so that this reaction should also be considered to describe the ionization structure, especially for low temperatures. The available data on reactions (1)–(3) is limited to an estimate of the rate coefficients at $T = 10{,}000$ K (Butler & Dalgarno 1980) and ion-beam measurements of reaction (1) for energies between $\sim$70 eV amu^{-1} and $\sim$150 keV amu^{-1} by Phaneuf, Meyer, & McKnight (1978), Nutt, McCullough, & Gilbody (1979), and Goffe, Shah, & Gilbody (1979). This paucity of data, which makes it difficult to model the ionization structure of carbon reliably, motivated us to investigate these processes.

In this paper, we present rate coefficients for processes (1)–(3), calculated from a critical synthesis of cross sections obtained from recent state-of-the-art theoretical and experimental approaches (Stancil et al. 1998) and the previous measurements. The theoretical and experimental methods are briefly discussed in §§ 2 and 3, respectively. The results are presented in § 4, while § 5 addresses their implications regarding planetary nebulae, interstellar clouds, and supernova ejecta.

2. THEORY

Since no present theoretical method is reliable (or applicable) over the entire energy range considered, processes (1) and (2) were investigated with a variety of theoretical approaches, each of which is appropriate over a segment of the overall energy range. For collision energies greater than $\sim$5 keV amu^{-1}, the cross sections were computed with the classical trajectory Monte Carlo (CTMC) method (Abrines & Percival 1966; Olson & Salop 1977). CTMC is a simulation of an atomic collision in which a large ensemble of projectile-target configurations is sampled, subject to the classical evolution of initial electronic orbits created to approximate the quantum-mechanical distributions. It has been shown to provide reliable results for a wide range of intermediate-energy ($v_{\rm projectile} \sim v_{\rm orbital}$) ion-atom collisions. At low energies this model yields essentially a classical over-the-barrier result and does not account for the existence of the reaction threshold.

Similarly, the maximum value of the cross section near 2 keV amu^{-1} was corroborated with the so-called quantal decay model (e.g., Janev, Presnyakov, & Shevelko 1984). The model accounts for decay of a quasi-stationary state in the field of a charged ion and describes charge transfer by tunneling of an electron through a barrier.

For energies less than $\sim$1 keV amu^{-1}, we utilized the most reliable theoretical method, the quantal molecular-orbital close-coupling (MOCC) approach (e.g., Zygelman et al. 1992). The adiabatic potentials and coupling matrix elements (Kimura et al. 1997a) were obtained with the

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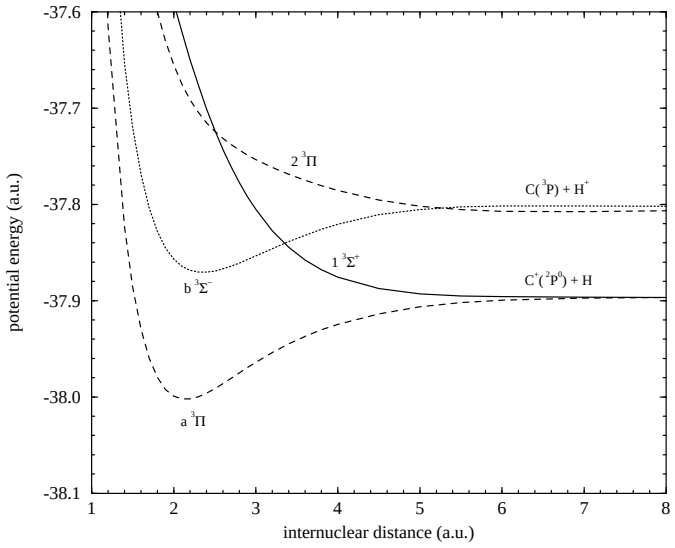

FIG. 1.—Adiabatic potential energies of the four lowest triplet states of CH^+.

multi-reference single- and double-excitation configuration-interaction method (Buenker & Peyerimhoff 1974a,1974b; Buenker & Phillips 1985). Two six-channel scattering calculations, one each for the singlet and triplet multiplicities, were performed including all radial and rotational couplings. The triplet adiabatic potentials, the dominant collision channels, are displayed in Figure 1.

To provide greater substantiation for the low-energy behavior of the MOCC results, we have also applied the multielectron hidden-crossing theory (Krstić, Bent, & Schultz 1996; Bent, Krstić, & Schultz 1997) for energies less than ~ 1 keV amu^{-1}. It was applied only for the $a\ ^3\Pi$ and $2\ ^3\Pi$ states, the dominant channels were indicated by the MOCC analysis, for which a branch point at the complex internuclear distance $R = (3.8, 0.9)\ a_0$ was located. It results in a cross section that is in good agreement with the MOCC calculations.

Reaction (3), radiative charge transfer, was investigated with a fully quantum-mechanical approach (e.g., Zygelman et al. 1989) for collision energies less than ~ 10 eV amu^{-1}. In many instances when a collision system lacks favorable avoided crossings, radiative charge transfer can be the dominant process at low energies (Butler, Guberman, & Dalgarno 1977). Further details on the calculations can be found in Stancil et al. (1998).

3. EXPERIMENT

Previous measurements of reaction (1) charge transfer cross section (Nutt et al. 1979) indicated a plateau of the cross section at low energy ($\sim$70–300 eV amu^{-1}), whereas one would expect that the cross section would quickly drop in this range owing to the endoergic nature of the reaction. Therefore, new measurements were performed with the Oak Ridge National Laboratory (ORNL) ion-atom merged-beams apparatus (Havener 1997). Ions in the range of 8–22 keV C^+ from the ORNL electron cyclotron resonance (ECR) ion source were electrostatically merged with a 5–9 keV ground-state D beam. In order to perform these measurements with the current merged-beams apparatus, D was used (Havener 1997) instead of H. However, the cross section is not expected to be isotope-dependent at these energies (Stancil & Zygelman 1995). The ground-state D beam was produced by photodetachment of D^-. Both the C^+ and D beams interacted along a field-free region of 47 cm, after which the primary beams and the product D^+ ions were separated magnetically. The neutral beam was monitored by measuring secondary emission from a stainless steel plate, and the intensity of the C^+ beam was measured using a Faraday cup. The product signal D^+ ions were detected by a channel electron multiplier. The absolute charge transfer cross section is obtained from directly measurable parameters, including the beam intensities, beam velocities, beam-beam signal rate, and the beam-beam overlap integral.

Critical to a meaningful comparison to the theoretical studies that consider the C^+ to be in the ground state is the determination of the metastable fraction present in the C^+ beam. Thus, the C^+ beam was directed into the ORNL electron-crossed beams apparatus (Bannister 1996), where electron impact ionization was measured. No cross section was detected below the threshold for ionization of the C^+ ground state, indicating the absence ($<2\%$) of metastables in the C^+ beam produced by the ECR ion source.

4. RESULTS AND DISCUSSION

Figure 2 presents our best estimates of recommended cross sections for process (1) and the sum of reactions (2) and (3) over the very large energy range 0.1 meV amu^{-1} to 2000 keV amu^{-1}. Comparison of the individual recommended cross sections with all available theoretical and experimental data is given in Stancil et al. (1998). For reaction (1), the experimental and theoretical cross sections are generally in accord. However, between 0.07 and 100 keV amu^{-1}, the recommended cross section is primarily based on the current measurements (0.07–2 keV amu^{-1}; Stancil et al. 1998) and the previous experiments of Phaneuf et al. (1978) and Goffe et al. (1979). At higher and lower energies the current theoretical values are adopted. As noted above, the previous measurements of Nutt et al. (1979) appear to overestimate the cross section between 0.07 and 0.3 keV amu^{-1}, particularly in the light of the 2.5 eV amu^{-1} threshold for this reaction.

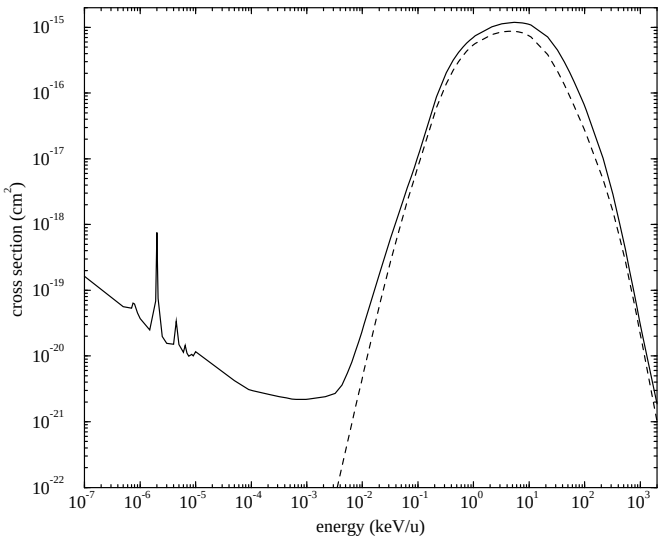

FIG. 2.—Cross sections recommended in this work for reaction (1) (*dashed line*) and the sum of reactions (2) and (3) (*solid line*).

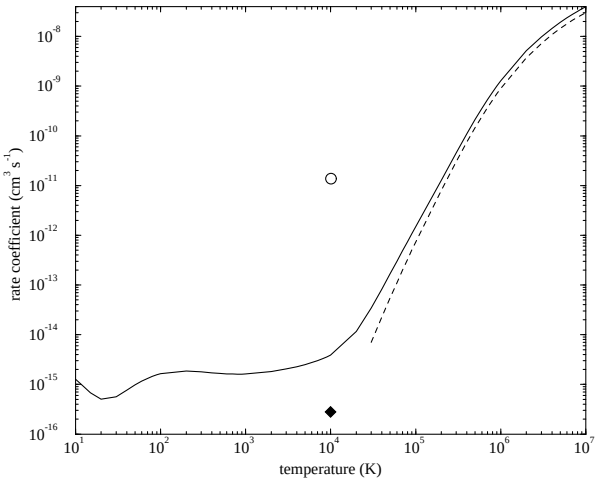

FIG. 3.—Rate coefficients: reaction (1), this work (*dashed line*); reaction (2), Butler & Dalgarno (1980) (*filled diamond*) and Péquignot et al. (1978) (*circle*); sum of reactions (2) and (3), this work (*solid line*).

Because no experimental data exist for process (2), except for the measurements of Rødbro et al. (1979; $E > 100$ keV amu^{-1}), we have estimated its cross section by applying detailed balance to the experimental data of process (1). This makes the assumption that the measured cross sections are dominated by captured to ground-state C as opposed to excited C, which is validated by our MOCC calculations (Stancil et al. 1998). Explicit calculations were performed to extend that result to higher and lower energies. While reaction (2) is exoergic, lacking a threshold, its low-energy cross section is small compared with radiative charge transfer, reaction (3), which dominates below ~ 1 eV amu^{-1}. For energies less than 1 eV amu^{-1}, we adopt the currently calculated radiative charge transfer cross sections. The resonant-like structures below 10 meV amu^{-1} are due to quasibound rovibrational levels of the initial 2 $^3\Pi$ state.

TABLE 1

CHARGE TRANSFER RATE COEFFICIENTS α (cm^3 s^{-1})

$T(K)$	Reaction (1)	Reactions (2) + (3)
10	...	1.27(−15)
20	...	5.03(−16)
50	...	9.75(−16)
100	...	1.64(−15)
200	...	1.86(−15)
500	...	1.66(−15)
1000	...	1.62(−15)
2000	...	1.81(−15)
5000	...	2.51(−15)
10000	...	3.90(−15)
20000	...	1.16(−14)
50000	5.45(14)	1.67(−13)
100000	7.38(13)	1.50(−12)
200000	8.03(12)	1.27(−11)
500000	1.46(10)	2.13(−10)
1×10^6	8.98(10)	1.29(−9)
2×10^6	3.72(9)	5.14(−9)
5×10^6	1.44(8)	1.92(−8)
1×10^7	2.99(8)	3.95(−8)
a_1	6.08(14)	2.80(−15)
b_1	1.96	2.13(−1)
c_1	1.7(5)	0.0
a_2	...	1.28(−15)
b_2	...	3.08
c_2	...	2.19(6)

NOTE.—The notation $A(B)$ corresponds to $A \times 10^B$.

Figure 3 presents rate coefficients obtained by averaging the recommended cross sections over a Maxwellian velocity distribution. The rates are fitted to the form

$$\alpha(T) = \sum_i a_i \left(\frac{T}{10{,}000\ \mathrm{K}}\right)^{b_i} \exp\left(\frac{-c_i}{T}\right), \quad (4)$$

with the parameters a_i (cm^3 s^{-1}), b_i, and c_i (K) given in Table 1 along with $\alpha(T)$ for several values of T. The fits are reliable to within $\sim 50\%$. However, the cross sections are generally reliable to within 25% for $E > 1$ keV amu^{-1} but may be uncertain to within a factor of 2–3 for lower energies. The rate coefficient is small and nearly constant at $\sim 2 \times 10^{-15}$ cm^3 s^{-1} for $T \lesssim 10^4$ K, where charge transfer is dominated by the radiative process. For higher temperatures, the rate coefficients for reactions (1) and (2) increase with temperature.

5. ASTROPHYSICAL APPLICATIONS

5.1. *Interstellar Medium*

Since the ionization potential of carbon (11.26 eV) is smaller than that of hydrogen, the abundance of C^+ is generally larger than that of C in photoionized gas. However, C I lines are observed in planetary nebulae and in the transition zone between H I and H II regions (for recent observations see, e.g., Baluteau et al. 1995). As the rate for formation of neutral C by radiative recombination

$$C^+ + e^- \rightarrow C + h\nu \quad (5)$$

is slow [$\sim 4.4 \times 10^{-12}(T/300\ \mathrm{K})^{-0.61}$ cm^3 s^{-1}], PN models underestimate the intensities of the C I lines. Péquignot, Aldrovandi, & Stasinska (1978) and Hippelein & Münch (1978) suggested that the charge transfer reaction (1) could neutralize the carbon. By matching observed and modeled line intensities, they inferred a rate coefficient of 7×10^{-13} cm^3 s^{-1} near 10,000 K (or 1.4×10^{-11} cm^3 s^{-1} for reverse process [2]). However, assuming that the $1\ ^+{}^3\Sigma - b\ ^3\Sigma$ spin-orbit coupling is the primary mechanism, Butler & Dalgarno (1980) calculated a rate coefficient of 1.4×10^{-17} cm^3 s^{-1} (2.8×10^{-16} cm^3 s^{-1} for the reverse process) at 10,000 K. These low rate coefficients suggest that neither reaction (1) nor reaction (2) play a role in the formation of PN C I lines. While the current rate coefficients are an order of magnitude larger than those obtained by Butler & Dalgarno (1980; see Fig. 3), charge transfer is still too weak to have an appreciable influence on PN C I lines.

Because reaction (1) is endothermic by $\sim 27{,}000$ K, it plays no role in interstellar clouds. Reactions (2) and (3) may contribute to the ionization of C in dark clouds where charge transfer can compete with photoionization.

5.2. *Supernovae*

The outer envelope of the ejecta of SN 1987A consists primarily of hydrogen and cosmic abundances of the other elements. Because of the low temperatures of the ejecta ($T \sim 2000$–6000 K), hydrogen is predominantly ionized by fast nonthermal electron impacts. However, Xu & McCray (1991) have suggested that if charge transfer reactions between protons and neutral metal atoms are considered, the hydrogen ionization fraction would be an order of magnitude less than what is inferred from observations of hydrogen recombination lines. They found that if only a

fraction ($\sim$10%) of the available metals were mixed with the hydrogen, the observed hydrogen ionization fraction could be reproduced.

It has generally been assumed that thermal charge transfer reactions between protons and metal atoms are fast if the process is exothermic. Consequently, numerous models of the supernova ejecta assume that metals with ionization potentials less than that of hydrogen will be primarily (or fully) singly ionized. The results of the current study show that the charge transfer of carbon (reactions [2] and [3]) is not fast and will have little effect on the hydrogen ionization fraction. The small rate coefficients also suggest that carbon may be primarily neutral, because photoionization is not very effective in the dense ejecta environment.

For other ejecta metals, we are only aware of robust calculations of charge transfer rate coefficients for Li (Kimura, Dutta, & Shimakura 1994, 1995; Stancil & Zygelman 1997), N (Kimura et al. 1997a), O (Chambaud et al. 1980; Kimura et al. 1997a), Na (Croft & Dickinson 1996), Mg (Allan et al. 1988), Si (Kimura et al. 1996), and S (Kimura et al. 1997b). Of these, only O and Si charge transfer rapidly with protons (see, e.g., Kingdon & Ferland 1996). Without reliable charge transfer rate coefficients for the remaining abundant metals, it is difficult to surmise their influence on the ejecta ionization structure.

The work of P. C. S., C. C. H., P. S. K., and D. R. S. was performed at Oak Ridge National Laboratory, which is managed by Lockheed Martin Energy Research Corp. for the US Department of Energy under contract DE-AC05-96OR22464. M. K. acknowledges the Science and Technology Agency of Japan. The Deutsche Forschungsgemeinschaft (grant Bu 450/7-1) supported the work of J. P. G., G. H., and R. J. B., and B. Z. acknowledges support from NSF Cooperative Agreement OSR-9353227.

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