Charge-transfer processes in collisions of ground-state C^+ ions with H_2, D_2, CO, and CO_2 molecules in the energy range from 0.15 to 4.5 keV

Toshio Kusakabe, Kenji Hosomi, and Hiroshi Nakanishi
Department of Nuclear Engineering, Kinki University, Higashi-osaka, Osaka, Japan

Hiroyuki Tawara and Mamiko Sasao
National Institute for Fusion Science, Toki, Gifu, Japan

Yohta Nakai
Atomic Energy Research Institute, Kinki University, Higashi-osaka, Osaka, Japan

Mineo Kimura
School of Medicine, Yamaguchi University, Ube, Yamaguchi, Japan

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Charge-transfer processes in collisions of C^+ ions with H_2, D_2, CO, and CO_2 molecules have been studied based on joint experimental and theoretical approaches in the collision energy from 0.15 to 4.5 keV. In the present experiment, the ground-state $C^+(^2P)$ ion projectiles have been produced by carefully energy-controlled electron impact to minimize the influence of the metastable-state ions. The observed cross sections are compared with the present theoretical prediction, and while the theoretical results are somewhat smaller than the measurements, they are found to be in reasonable agreement for H_2, D_2, and CO above around 1 keV. The present experimental cross sections for CO and CO_2 are smaller by a factor of 2 to 3 than those of earlier measurements. We provide some remarks on the effect of the metastable-state ions. [S1050-2947(99)03907-4]

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I. INTRODUCTION

An understanding of charge-transfer processes at low-collision energies has become increasingly important in a number of applications such as plasma science [1] and material science [2] where low-temperature plasmas play a key role in determining characteristics of plasma behavior and of target materials. Although many investigations have been performed on charge transfer of various ions in collisions with various gas atoms and molecules, data are still limited and fragmentary, in particular at energies less than 10 keV. Furthermore, they often contradict each other.

Since the electron-capture processes at low energies are known to be strongly dependent upon the internal electronic state of ions, even a small fraction of the metastable excited-state ions present in the incident ion beam may significantly influence the cross sections observed for charge-transfer processes. Indeed in our previous measurement [3], the metastables in the C^+, N^+, and O^+ ion beams in collisions with H_2 molecules and He atoms in the energy range between 0.7 and 4.0 keV were found to significantly enhance the magnitude of the observed cross sections. A similar effect has been also noted by Moran and Wilcox [4] and Moran and Mathur [5]. Later, Kimura *et al.* [6] have shown theoretically that the metastable ion contribution to charge transfer in $O^+ + He$ collisions at a few keV increases the cross section more than a factor of two if the amount of the metastable-state ions exceeds 10%. This is consistent with the measurement by Kusakabe *et al.* [3].

Contrary to the relatively vast volume of experimental and theoretical studies for ion-atom collision systems, those investigations of slow ion-molecule collisions are scarce. Experiments have been limited to a few attempts [7]. Kimura *et al.* have theoretically investigated charge-transfer processes in collisions of H^+ ions with CH_4 and C_2H_2 molecules in the collision energy below 2 keV, and shown that charge transfer is extremely sensitive to the molecular orientation, i.e., a strong steric effect [8,9]. These separate attempts in the previous studies have suggested the more systematic and rigorous study presented here.

In the present paper, we have carried out a joint experimental and theoretical study for understanding collision dynamics for charge-transfer processes of the ground-state $C^+(^2P)$ ions, which are typical impurity ions in most laboratory plasmas. Charge-transfer cross sections have been determined over the kinetic energy of 0.15 to 4.5 keV in collisions with H_2, D_2, CO, and CO_2 molecules. The specific processes we have studied are collisions of the ground state $C^+(^2P)$ ion with the various molecules:

$$C^+(^2P) + H_2, D_2(v=0) \rightarrow C + H_2^+,\ D_2^+(v=0) - 4.166 \text{ eV}, \quad (1)$$

$$C^+(^2P) + CO(v=0) \rightarrow C + CO^+(v=0) - 2.754 \text{ eV}, \quad (2)$$

$$C^+(^2P) + CO_2(v=0) \rightarrow C + CO_2^+(v=0) - 2.513 \text{ eV}, \quad (3)$$

where v describes the vibrational quantum number.

These collision processes, which are all endothermic with appreciable energy defects (as shown above), are important to low-temperature edge plasmas such as those in the ther-

monuclear fusion devices with carbon-coated or graphite-lined walls as plasma facing material [1]. Also collisions of low-charged ions with the excited molecules are critical in understanding features in plasma-based material and thin-film production [2]. In addition, these collision systems are very important for understanding the dynamics for the cancer therapy [10], which employs accelerated ion beams, and also constitute an essential part of the interstellar cloud formation in astronomy [11].

In the present experiments, the ionizing electron energy in ion source is carefully controlled to avoid the production of the metastable-state ions so that the cross section values for the ground-state ions are more accurately determined. However, there is always a possibility that a small amount of metastables exists in the ion beam, therefore, it is important to assess the contribution from the $C^+*(^4P)$ metastable state to the total charge-transfer processes. We examine the effect both experimentally and theoretically.

II. EXPERIMENTAL AND THEORETICAL APPROACHES

A. Experiment

A detailed description of the present experimental apparatus and method has been previously given [3,12,13], and hence, only essential features will be briefly summarized here.

A carbon ion beam was extracted from a conventional electron-impact ion source where the electron accelerating voltage V_{ae} could be varied up to 50 V. The incident C^+ ion beam produced from CO molecules fed into the ion source was mass analyzed with a Wien filter and introduced into a 40-mm-long collision cell with a 0.5-mm-diam entrance and a 3.5-mm-diam exit apertures. The target gases of high purity ($>$99.95%) were introduced into the cell and the gas pressure was measured with a sensitive Pirani gauge [14], which was calibrated with a MKS-Baratron capacitance manometer. The front and main chambers were evacuated down to the base pressure less than about 6×10^{-6} Pa by a 500 l/s turbomolecular pump and a 6″ cryopump. The ions emerging from the cell after collisions were charge separated with a pair of the electrostatic parallel plates and sent into a position-sensitive detector (PSD) consisting of a microchannel plate (MCP) and a resistive anode (MCP-PSD). The output signals from both ends of its anode were converted to the position information in an analogue divider [15,16] and recorded on a pulse-height analyzer giving the charge distribution of ions after collisions. Peak areas corresponding to the singly charged primary ions and product energetic neutral particles were integrated. Relative detection efficiencies of MCP-PSD were assumed to be the same for both the singly charged ions and neutral particles as the front end of the MCP was grounded. After subtracting dark current noises of the MCP-PSD, the fractions of singly charged ions and of neutrals, F_1 and F_0, were determined as a function of the target gas thickness (length of the collision cell times density of target gas molecules). The charge-transfer cross sections were derived based upon the growth rate method by fitting the observed fractions F_0 to a quadratic function of the target gas thickness. During the present experiment the charge-transfer cross sections in He^+-He and H^+-H_2 collisions were also measured from time to time and found to be in good agreement with the previous data down to 0.2 keV.

The statistical uncertainties of the cross sections are a few % for most of the present work. Uncertainties due to those of the target thickness, the temperature of target gases, and so forth is estimated to be from 10.5% at high energies to 17.6% at low energies. Total experimental uncertainties of the absolute cross sections are given as the quadratic sum of these uncertainties involved.

The absolute (effective) energy E_e of the ionizing electrons in the ion source has been determined by measuring the threshold ionization energies of helium and neon atoms and the appearance potentials of C^+ reactant ions from CO, of N^+ ions from N_2, and of O^+ ions from CO_2. In order to obtain the purely ground state $C^+(^2P)$ ions, these ions were prepared from CO molecules colliding with the electrons at $E_e=25.3$ eV. The effects of ions in different electronic states were carefully investigated through measuring the variation of charge changed fraction F_0 as a function of the electron-impact energy E_e (see Sec. III A).

B. Theory

The semiclassical molecular orbital (MO) expansion method used here is standard and has been described in detail elsewhere [17]. Hence, only a brief summary is provided here.

1. Molecular states

The *ab initio* calculations are performed for two different molecular configurations for H_2 and D_2 (the incident ions come perpendicular to, and parallel to the molecular axis), while for CO molecule, the calculation is done for three different configurations (perpendicular to, and parallel to the molecular axis from two ends). In the perpendicular case, C^+ ion vertically approaches the center of mass of the molecule. The molecule is located along the *y* axis. The only symmetry plane for the system is the *yz* plane. In the parallel case, the C^+ ion approaches H_2, D_2, and CO collinearly. The molecule lies along the collision trajectory. For the CO case, the C^+ approaches either toward the C or O atom. In all three cases, the origin of the scattering coordinates is located at the center of mass of the C-CO^+ system. Considering the present collision energy region, the collision time is much shorter than the relaxation time of the target molecule, which is in the order of 10^{-14} sec. Based on this argument, the CO distance is always fixed at the equilibrium geometry of the ground state of CO during the calculation. In the present *ab initio* calculations for the C^+-CO system, we use Dunning's cc-pVTZ basis sets for H, C, and O atoms [18]. The potential curves are obtained by the configuration-interaction (CI) method, with configuration selection and energy extrapolation using the Table CI algorithm [19]. In the CI calculations, the two lowest MOs are always kept doubly occupied, whereas the two highest ones are discarded. The radial coupling matrix elements are obtained using the calculated molecular wave functions by a finite-difference method [20].

Adiabatic potential curves for three target systems are rather smooth without much structure and strong avoided crossing because a polarization potential arising from a singly charged ion-neutral molecule interaction dominates. There are, however, some avoided crossings among the ex-

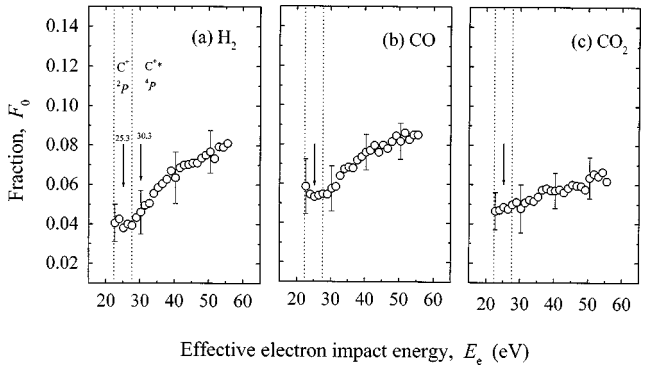

FIG. 1. Typical variations of neutral particle fractions F_0 produced in the 0.8-keV C^+ ions colliding with (a) H_2, (b) CO, and (c) CO_2 molecules against the effective impact-electron energy E_e. Note that the two dotted vertical lines represent threshold energies for the ground $C^+(^2P)$ state and excited $C^{+*}(^4P)$ state from the lower side, respectively.

cited states considered. Because of the weak-coupling feature described above, the dynamical-coupling scheme is typical Demkov-type mechanism. Hence, the relevant and primary radial coupling matrix elements are found to be all weak except for those in the excited states.

2. Semiclassical approach

A semiclassical molecular-orbital expansion method [17] with a straight-line trajectory is employed to study the dynamics for these collisions above 100 eV. Transitions are driven by nonadiabatic couplings. The total scattering wave function was expanded in terms of products of a molecular electronic state and atomic-type electron translation factors (ETFs). Substituting the total wave function into the time-dependent Schrödinger equation and retaining the ETF correction up to the first order of relative velocity yields a set of the first-order coupled equations. By solving the coupled equations numerically, we obtain the scattering amplitudes for transitions: the square of the amplitude gives the transition probability, and integration of the probability over impact parameter gives the cross section. Two sets of the dynamical calculations have been carried out and molecular states included in the calculations are the initial state $[C^+ + X]$ both for the ground and metastable states, and two to three charge-transfer states corresponding to $[C + X^+]$ where $X = H_2$, D_2, and CO.

III. RESULTS

A. Production of primary carbon ions

Figure 1 shows typical variations of fractions F_0 of neutral particles produced in the 0.8-keV C^+ ions colliding with H_2, CO, and CO_2 molecules against the effective impact electron energy E_e. The threshold electron energies for producing the ground-state $C^+(^2P)$ ions and the metastable state $C^{+*}(^4P)$ ions from the ground-state CO molecules in the following processes,

$$e + CO \rightarrow 2e + C^+(^2P) + O(^3P), \quad (4)$$

$$\rightarrow 2e + C^{+*}(^4P) + O(^3P), \quad (5)$$

TABLE I. Charge-transfer cross sections (in units of 10^{-16} cm^2) for C^+ ions in collisions with H_2 and D_2 molecules.

Energy (keV)	Target molecules	
	H_2	D_2
0.15	0.309±0.055	
0.2	0.329±0.062	0.456±0.081
0.3	0.416±0.077	
0.4	0.461±0.082	
0.45		0.679±0.120
0.65	0.630±0.114	
1.0	0.770±0.089	0.892±0.158
1.6	0.930±0.098	
2.0		1.19 ±0.16
2.5	1.09 ±0.12	
3.5	1.25 ±0.13	
4.0		1.62 ±0.22
4.5	1.35 ±0.14	

are known [21] to be 22.4 and 27.7 eV, respectively. Although the fluctuations indicated with the error bars are relatively large, the constant fraction F_0 from the threshold up to 27.7 eV is due to the process (4), while above 27.7 eV, the sharp increase with increasing electron-impact energy can be attributable to the formation of neutral particles from the metastable $C^{+*}(^4P)$ ions [the process (5)] produced by electrons with the impact energy above 27.7 eV. It is noted that similar results were observed for D_2 target, too.

Since the effective energy of the ionizing electrons in the ion source was set to be 25.3 eV during measurements, we believe that the present cross sections reported should be due to the ground-state $C^+(^2P)$ ions. However, there can be some possibilities of the mixing from a small but non-negligible amount of the metastable-state ions. We examine this possibility later in conjunction with theoretical results.

B. Cross sections for H_2 and D_2 targets

The present data for the cross sections of charge transfer of C^+ ions from H_2 and D_2 molecules are given in Table I. The cross sections for H_2 molecules are shown in Fig. 2 together with those previously published [3,4,22–27].

As the collision energy decreases, the present charge-transfer cross sections for the ground-state ions decrease monotonously. Our previous data [3] are slightly larger by 10–15% than the present measurements of the ground-state $C^+(^2P)$ ions, but they agree with each other within the experimental uncertainties. The present data are also in fairly good agreement with those of Moran and Wilcox [4] at the energy region overlapped, and those of Xu, Moran, and Thomas [25] at energies below 0.5 keV. The present results appear to tie well with those of Phaneuf, Meyer, and McKnight [23] at energies above 9 keV, while the data by Unterreiter, Aumayr, and Winter [26] are found to be rather small and show a slightly different energy dependence. On the other hand, the data of Itoh *et al.* [22] are much larger, suggesting that their beam might have a contamination of the metastable-state ions. This speculation seems to be supported by the fact that their data agree well with, and can be connected with those of Nutt, McCullough, and Gilbody [28], Moran and Wilcox [4], Lockwood, Miller, and Hoffman,

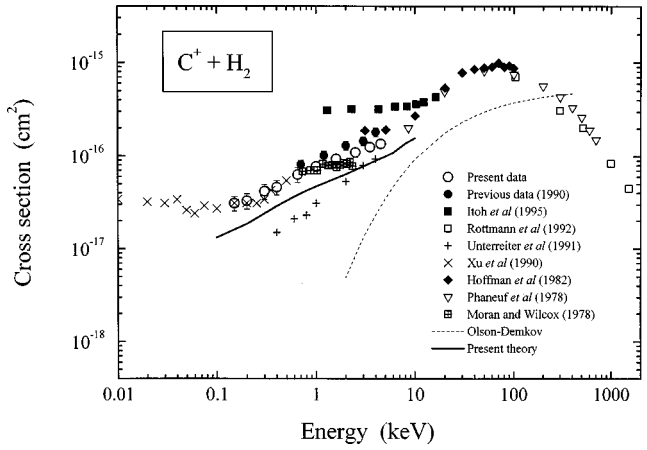

FIG. 2. Charge-transfer cross sections for C^+-H_2 collisions. ○, the present data; ●, the previous data [3]; ■, Itoh *et al.* [22]; □, Rottmann *et al.* [27]; +, Unterreiter, Aumayr, and Winter [26]; ×, Xu, Moran, and Thomas [25]; ◆, Hoffman, Miller, and Lockwood [24]; ▽, Phaneuf, Meyer, and McKnight [23]; ⊞, Moran and Wilcox [4]. The solid line is the present theory, and the dashed line is based on the Olson-Demkov model.

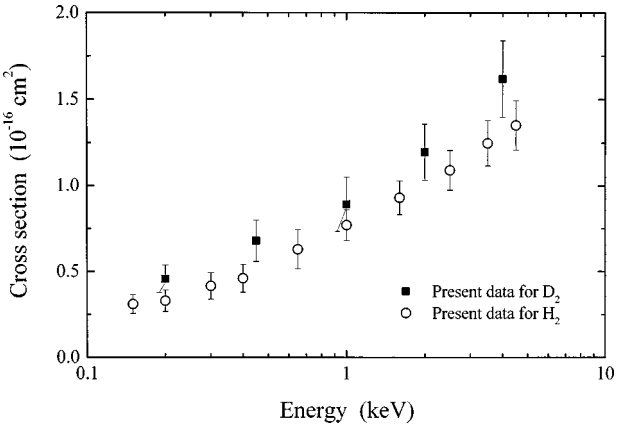

FIG. 3. Comparison of the present charge-transfer cross sections for C^+-hydrogen molecular isotopes collisions. ○, H_2; ■, D_2.

[29] and Hoffman, Miller, and Lockwood [24], who all used an ion beam apparently mixed with the metastable state $C^+*(^4P)$ ions. Since Itoh *et al.* employed the so-called ''recoil ion source'' technique to produce a singly charged carbon-ion beam by impacting 1.7 MeV O^+ ions on CO_2, they indeed concluded that the incident beam might include as large as 30% of the metastable-state ions in their primary ion beams.

In Fig. 2, the present theoretical results are also included. The theory is in reasonable accord with the energy dependence of the present measurement above 0.3 keV, but the agreement becomes less satisfactory at lower energies. The present theoretical magnitude is found to be somewhat smaller. For the sake of the comparison, the result based on the Olson-Demkov model [30] is included in Fig. 2. This model was originally developed for study of atomic targets, and hence may not offer accurate results for molecular targets by a simple modification applicable for molecules. Nevertheless, the method is helpful in providing the general trend of cross sections for various systems. The result based on the Olson-Demkov theory underestimates the cross section at low energies substantially, and also its decrease of the cross section with decreasing the collision energy is too sharp, which is not in accord with the present experimental and theoretical findings.

The present theoretical result lies between the present measurement and those of Unterreiter, Aumayr, and Winter below 2 keV, and predicts a cross section that decreases faster than the experimental data below 0.2 keV. The present model is believed to be valid to 1 keV or so, but may begin to fail below this energy. Since the process (1) is endothermic with the appreciable threshold energy, the cross section is expected to decrease toward lower energies. In order to understand the discrepancy, we have analyzed our earlier investigation [3] on charge transfer from vibrationally excited molecules. The energy defect between $v=0$ and $v=1$ of H_2 molecules is approximately 0.516 eV, which is expected to influence charge transfer. Our preliminary study indicates that charge-transfer cross section from the vibrationally excited ($v=1$) molecule is found to be larger by a factor of two or three than that for the vibrationally ground ($v=0$) molecule at 0.1 keV, and the effect of vibrationally excited state increases as the collision energy decreases and indeed is not negligible at low energies. Under the present experimental condition of the gas temperature of about 300 K, however, only a small amount of $v=1$ H_2 molecules may be present (due to a filament of the Pirani gauge used). However, we have carried out the additional test to check the effect with and without the gauge, and have found very little difference. Hence, the contribution from vibrationally excited molecule thus formed is too small to explain the discrepancy. It is possible that the target molecule is vibrationally excited on the incoming part of the collision, and some fractions of vibrationally excited molecules are produced before they really undergo the charge-transfer collision event. Another source of the discrepancy may be the possible presence of a small fraction of the metastable-state ions in the present ion beam. We have examined the effect of the metastable-state ion for charge transfer by performing a small scale theoretical calculation with the initial metastable-state ion. The result thus obtained suggests that charge-transfer cross sections for the metastable-state ion colliding with H_2 molecule are larger by nearly an order of magnitude even at as low as 0.1 keV and is rather energy independent. However, as described above, we strongly believe that the contamination of the metastable-state ions should be less than a few %, and hence, it is highly unlikely that the present level of the contamination causes such a sizable difference in the cross section. On the theoretical side, there are two apparent weaknesses, i.e., the precision of molecular states and the fixed nuclei approximation used, of which may cause a serious problem as the incident energy becomes lower. Therefore, both experimental and theoretical approaches need to be further improved for attaining better agreement. Based on the above consideration, the experimental results of Xu, Moran, and Thomas below 0.5 keV are also believed to be somewhat in overestimation.

In Fig. 3, the present cross sections of charge transfer of C^+ ions from D_2 molecules are compared with those of H_2 molecules. The cross sections of D_2 molecules agree with those of H_2 molecules within the experimental uncertainties. Since the difference of the electron binding energy between

TABLE II. Charge-transfer cross sections (in units of $10^{-16}\,cm^2$) for C^+ ions in collisions with CO and CO_2 molecules.

Energy (keV)	Target molecules	
	CO	CO_2
0.15	1.23±0.22	0.952±0.169
0.2	1.18±0.21	1.01 ±0.18
0.3	1.28±0.22	0.939±0.169
0.4	1.42±0.25	1.07 ±0.19
0.5	1.43±0.27	0.941±0.178
0.7	1.61±0.17	1.06 ±0.11
1.2	1.80±0.19	1.38 ±0.15
2.0	2.23±0.23	1.98 ±0.21
2.7	2.45±0.26	2.68 ±0.28
3.0	2.41±0.25	
3.5	2.68±0.28	3.60 ±0.38
4.5	3.07±0.36	4.74 ±0.50

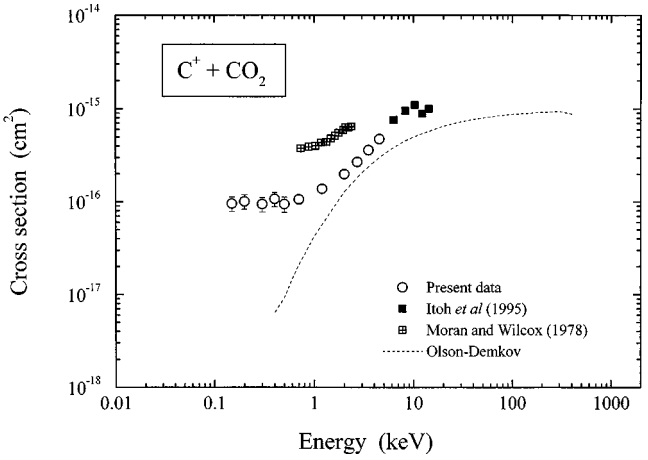

FIG. 5. Charge-transfer cross sections for C^+-CO_2 collisions. ○, the present data; ■, Itoh *et al.* [22]; ⊞, Moran and Wilcox [4]. The dashed line corresponds to the Olson-Demkov model.

H_2 and D_2 is merely 0.0015 eV, the isotope effect does not show up in the present collision energy region investigated, and is not significant for application. However, the different population for the different vibrational level for H_2 and D_2 may be responsible for a small difference seen in the figure.

C. Cross sections for CO and CO_2 targets

The present cross sections of charge transfer of the ground-state $C^+(^2P)$ ions in collisions with CO and CO_2 molecules are also listed in Table II and are shown in Figs. 4 and 5, respectively. We discuss the CO case first, then follow with the CO_2 case.

CO: The cross sections for CO decrease with the decreasing collision energy and become nearly a constant at the lowest energies below ~0.5 keV. For this collision system, only a very limited number of studies has been reported, and those are the measurements by Moran and Wilcox [4] for lower energies, and by Rottmann *et al.* [27] for higher energies, both of which are included in Fig. 4. The values obtained by Moran and Wilcox [4] are found to be larger by a factor of two or three over ours in the overlapping energy region, but their energy dependence is in good accord to ours. Approximate extrapolation of the present measurement appears to join reasonably well with that of Rottmann *et al.* above 100 keV. The present theoretical result is also shown in Fig. 4. Similar to the H_2 case, the present theoretical result is in reasonable accord with the present measurement although the theoretical magnitude is somewhat smaller. The theory drops somewhat faster at lower energies. This collision system is also endothermic, and the cross section is expected to drop as the collision energy decreases toward the threshold. The result based on the Olson-Demkov model shows the sharp decreasing trend with the decreasing collision energy, although its degree of decrease appears to be too fast and the magnitude of the predicted cross section too small. The present theoretical result shows significantly better agreement with the measurement.

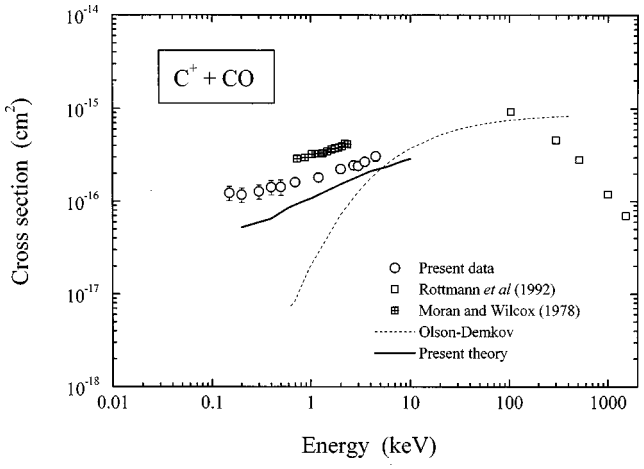

FIG. 4. Charge-transfer cross sections for C^+-CO collisions. ○, the present data; □, Rottmann *et al.* [27]; ⊞, Moran and Wilcox [4]. The solid line corresponds to the present theory, and the dashed line corresponds to the Olson-Demkov model.

As stated above for measurements with H_2, a few sources are expected to contribute to the discrepancy: a small amount of the contamination of (i) the metastable-state C^+ ions in the ion beam, (ii) vibrationally excited molecular targets, and (iii) a lack of accuracy in the calculations for the theory.

CO_2: The present cross sections for CO_2 targets are displayed in Fig. 5 along with those of Itoh *et al.* [22] and Moran and Wilcox [4]. The present data appear to join with the recent high-energy measurement by Itoh *et al.* [22]. The data by Moran and Wilcox are larger by a factor of 2 to 3 at all energies, but their energy dependence seems similar. Itoh *et al.* acknowledged the presence of the metastable-state ions in their ion beam and estimated its amount approximately 30%. We believe that the amount of the metastable-state ions in our beam is only a small fraction, perhaps, less than a few %. Moran and Wilcox assessed the effect of the metastable-state ion by comparing their result for the ground-state ion and that for the mixed ions. The rough estimation of the cross section based on the Olson-Demkov model suggests that the cross section decreases with decreasing energy due to the endothermicity of the process. The agreement of the prediction based on the Olson-Demkov model with the present measurement is reasonably good above the collision

energy of 2 keV. However, a discrepancy exists below this energy. Possible sources of the discrepancy are the same as described for H_2 ands CO. More rigorous theoretical study based on the quantum chemistry calculation for adiabatic potentials and the close-coupling calculation for collision dynamics is highly desirable.

We briefly discuss the similarity and difference of the charge-transfer cross sections for these three-target systems. Because of the difference of ionization potentials for these molecules (H_2, 15.426 eV; CO, 14.014 eV; CO_2, 13.773 eV; and C, 11.260 eV), the magnitude of the charge-transfer cross sections is in the order of $CO_2 > CO > H_2$ at above 3.5 keV. Obviously their energy dependence is slightly different. As the incident energy increases above a few 10 keV, the difference in the ionization potentials would make only a small effect for charge transfer within the present molecular systems. However, the geometrical size of the molecule would then influence charge transfer more significantly.

IV. CONCLUSION

We have carried out a joint experimental and theoretical study on charge-transfer processes in collisions of C^+ ions with H_2, D_2, CO, and CO_2 molecules in the energy region from 0.15 to 4.5 keV. The measured and theoretical results agree reasonably well above 1 keV, while a discrepancy begins to show up at lower energies. The present experimental cross sections for charge transfer by the ground-state C^+ ion impact on H_2, D_2, CO, and CO_2 targets at 2 keV are approximately $1\times10^{-16}\,\mathrm{cm}^2$, $2.2\times10^{-16}\,\mathrm{cm}^2$, and $2.0\times10^{-16}\,\mathrm{cm}^2$, respectively. The observed cross sections decrease rather slowly with the decreasing collision energy, in disagreement with the present theoretical trend, which predicts a much more significant decrease. These results are significant for application in fusion research. For CO and CO_2, the present results are significantly smaller than those earlier measurements. There is no sizable difference found in the cross sections between H_2 and D_2 targets. These processes are important for the better understanding of the plasma diagnostics at the divertor edge. Though we have carefully chosen the ionizing electron energy far below the production threshold of the metastable C^+ ions, there is a slight chance that the present ion beam may not be completely free from the metastable ions. To some degree, vibrational excited molecules may contribute to the experimental overestimation of all the cross sections at lower energies. Further experiments employing high-purity electronic ground-state ions and vibrational ground-state molecular targets would be highly desirable to verify our results.

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[1] R. K. Janev, in *Proceedings of the International Symposium on Atomic Molecular Processes in Fusion Plasmas (NIFS-DATA-39)*, edited by H. Tawara (National Institute for Fusion Science, Nagoya, 1997), p. 1.

[2] *Proceedings for the International Workshop on Basic Aspects of Nonequilibrium Plasmas Interacting with Surfaces*, edited by S. Fujishiro, A. Garscadden, and T. Makabe (American Vacuum Society, New York, 1998).

[3] T. Kusakabe, Y. Mizumoto, K. Katsurayama, and H. Tawara, J. Phys. Soc. Jpn. **59**, 1987 (1990).

[4] T. F. Moran and J. B. Wilcox, J. Chem. Phys. **68**, 2855 (1978).

[5] T. F. Moran and B. P. Mathur, Phys. Rev. A **21**, 1051 (1980).

[6] M. Kimura, J. P. Gu, Y. Li, G. Hirsch, and R. J. Buenker, Phys. Rev. A **49**, 3131 (1994).

[7] See an extensive bibliography, H. Tawara *Electron Transfer Processes in Ion-Ion/Atom/Molecule Collisions (NIFS-DATA-42)* (National Institute for Fusion Science, Nagoya, 1997).

[8] M. Kimura, Y. Li, G. Hirsch, and R. J. Buenker, Phys. Rev. A **52**, 1196 (1995).

[9] M. Kimura, Y. Li, G. Hirsch, and R. J. Buenker, Phys. Rev. A **54**, 5019 (1996).

[10] *Proceedings of NIRS International Seminar on the Application of Heavy Ion Accelerator to Radiation Therapy of Cancer, NIRS-M-103/HIMAC-008*, edited by T. Kanai and E. Takada (NIRS, Chiba, Japan, 1994).

[11] *Molecular Astrophysics*, edited by T. W. Hartquist (Cambridge University, Press, Cambridge, England, 1990).

[12] T. Kusakabe, K. Kajiwara, K. Ohishi, K. Tsujimaru, K. Tominaga, K. Yamashita, T. Sugimoto, S. Hayashida, Y. Mizumoto, and K. Katsurayama, J. Faculty Sci. Technol., Kinki Univ. **24**, 257 (1998).

[13] T. Kusakabe, H. Yoneda, Y. Mizumoto, and K. Katsurayama, J. Phys. Soc. Jpn. **59**, 1218 (1990).

[14] T. Kusakabe, T. Horiuchi, Y. Nakai, and H. Tawara, Jpn. J. Appl. Phys., Part 1 **37**, 369 (1998).

[15] H. Hanaki, N. Nagai, T. Kusakabe, T. Horiuchi, and M. Sakisaka, Jpn. J. Appl. Phys., **22**, 748 (1983).

[16] T. Kusakabe, M. Ohmiya, and K. Wada, Jpn. J. Appl. Phys., Part 1 **31**, 4093 (1993).

[17] M. Kimura and N. F. Lane, in *Advances for Atomic, Molecular and Optical Physics*, edited by D. R. Bates and B. Bederson (Academic, New York, 1989), Vol. 26, p. 76.

[18] T. H. Dunning, Jr. and P. J. Hay, in *Methods of Electronic Structure Theory*, edited by H. F. Schaefer III (Plenum, New York, 1977).

[19] R. J. Buenker and S. D. Peyerimhoff, Theor. Chim. Acta **35**, 33 (1974); **39**, 217 (1975); R. J. Buenker, Int. J. Quantum Chem. **29**, 435 (1986).

[20] R. J. Buenker, in *Proceedings of the Workshop on Quantum Chemistry and Molecular Physics, Wollongong, Australia*, edited by P. G. Burton (University Press, Wollongong, 1980); in *Studies in Physical and Theoretical Chemistry, Current Aspects of Quantum Chemistry*, edited by R. Carbo (Elsevier, Amsterdam, 1981), Vol. 21, p. 17; R. J. Buenker and R. A. Phillips, J. Mol. Struct.: THEOCHEM **123**, 291 (1985).

[21] G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand Reinhold, New York, 1950).

[22] A. Itoh, N. Imanishi, F. Fukuzawa, N. Hamamoto, S. Hanawa, T. Tanaka, T. Ohdaira, M. Saito, Y. Haruyama, and T. Shirai, J. Phys. Soc. Jpn. **64**, 3255 (1995).

[23] R. A. Phaneuf, F. W. Meyer, and R. H. McKnight, Phys. Rev. A **17**, 534 (1978).

[24] J. M. Hoffman, G. H. Miller, and G. L. Lockwood, Phys. Rev. A **25**, 1930 (1982).

[25] Y. Xu, T. F. Moran, and E. W. Thomas, Phys. Rev. A **41**, 1408 (1990).

[26] E. Unterreiter, F. Aumayr, and H. Winter, Z. Phys. D **21**, S167 (1991).

[27] L. M. Rottmann, R. Bruch, P. Neill, C. Drexler, R. D. DuBois, and L. H. Toburen, Phys. Rev. A **46**, 3883 (1992).

[28] W. L. Nutt, R. W. McCullough, and H. B. Gilbody, J. Phys. B **12**, L157 (1979).

[29] G. J. Lockwood, G. H. Miller, and J. M. Hoffman, Phys. Rev. A **18**, 935 (1978).

[30] R. E. Olson, Phys. Rev. A **6**, 1822 (1972).