

# ELECTRON CAPTURE CROSS SECTIONS IN COLLISIONS OF ${}^3\text{He}^{2+}$ IONS WITH CO MOLECULE

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**Abstract:** The single electron capture process in collisions of  ${}^3\text{He}^{2+}$  ions with CO molecule have been studied theoretically using semiclassical collision methods in which the adiabatic potentials and nonadiabatic couplings were obtained using the multireference single- and double-excitation configuration-interaction (MRDCI) approach. The partial and total single electron capture cross sections have been obtained for energies between 0.6 to 6 keV. The calculated cross sections depend very sensitively on the molecular configuration, thus revealing a strong steric effect. The calculated single electron capture cross sections are in good agreement with the experimental measurements of Kusakabe *et al.* [Phys. Rev. A 73, 022706 (2006)] and Čadež *et al.* [J. Phys. B: At. Mol. Opt. Phys. 35, 2515 (2002)]. The present study provides a theoretical basis for the experimental measurements by interpreting the detailed collision dynamics.

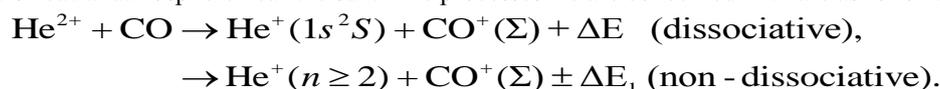
**Keywords:** electron capture cross section; MRDCI; radial and rotational coupling

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## 1. Introduction:

In last few decades there have been numerous important advances in the experimental and theoretical techniques which have significantly improved our understanding of various processes occurring in the astrophysical plasma [1]. The electron capture in collisions of slow multiply charged ion with atomic or molecular targets plays an important role in our understanding of mechanisms responsible for the emission of x-rays and extreme ultraviolet (EUV) photons from astrophysical plasmas [2, 3]. The emission lines of these multiply charged ions are used to provide direct information about the ionization structure of astrophysical objects. Protons and doubly ionized helium ( $\text{He}^{2+}$ ) i.e. the  $\alpha$  particle, are the primary ion constituents of cosmic rays and the solar-wind. The helium ion was observed in outer space by an EUV scanner on the Mars Orbiter Planet-B [4]. The EUV satellite has performed detailed spectroscopic studies of comets in the vacuum ultraviolet (VUV) spectral range [5, 6]. The lines observed in the spectra have confirmed that electron capture processes are present in the comets. Some spectral lines of helium appeared to be very bright, and well separated from other lines. They are the result of de-excitation subsequent to electron capture into excited states of singly charged or neutral helium. The luminosities of these lines have been determined from these observations. To interpret them, one needs to know the underlying electron capture and subsequent line emission cross sections.

Recently measured  $\text{He}^+$  emission lines from the comet Hyakutake [5] has led us to calculate total and partial cross sections for the collision of  $\text{He}^{2+}$  ion with the CO molecule, since the latter is one of the major constituents of the comet's neutral atmosphere near the sun. The processes we are concerned with are as follows [7]:



where  $n$  is the principal quantum number,  $\Delta E$  and  $\Delta E_1$  are the energy defects for individual product channels and  $\text{CO}^+(\Sigma)$  includes final bound or dissociative molecular states. The collision of  $\text{He}^{2+}$  ion with the CO molecule has been widely studied experimentally [7-12] but limited systematic theoretical work has been reported [8]. The agreement between the experimental measurements and theoretical calculations is not satisfactory and hence, so far no clear explanation for the observed results has been given [8].

Therefore, in the present study, the impact-parameter method [13] has been used to study the single electron capture (SEC) process. The adopted adiabatic potentials and nonadiabatic couplings were obtained with the multireference single- and double-excitation configuration interaction (MRDCI) approach [14-21]. In order to provide suitably accurate results, we have used an optimization method for the atomic basis sets used in the MRDCI calculation for multiply charged ions. The calculation of the ion-molecule collisions is based on the perturbed stationary state (PSS) model [22] in which the basis functions are constructed from the molecular orbitals.

The partial and total SEC cross sections have been calculated for collision energies lying between 0.6 to 6 keV, corresponding to a solar-wind ion velocity of about 3 keV at low heliographic latitudes [23]. The calculated electron capture cross sections have been compared with the available experimental data [7-9] and it has been shown that the impact parameter method provides cross sections which are in good agreement with experimental measurements [7-9] in the range of energy considered in the present work.

## 2. Theoretical models:

### 2.1. Molecular state:

The geometry for the collision of  $\text{He}^{2+}$  ion with CO molecule is shown in Fig. 1. The  $\text{He}^{2+} + \text{CO}$  system has been described by the internal Jacobi coordinates  $\{R, r, \alpha\}$  with the origin at the center of mass of the CO molecule. The *ab initio* calculations have been performed using the MRDCI method [14-21] for three different directions of approach of  $\text{He}^{2+}$  ion towards the CO molecule. In the linear conformation, the  $\text{He}^{2+}$  ion approaches the carbon and oxygen ends of CO molecule at an angle  $\alpha = 0$  and  $180^\circ$ , respectively. In these cases, the calculations are done in the  $C_{2v}$  subgroup (the highest Abelian subgroup) of the  $C_{\infty v}$  point group. In the perpendicular approach ( $\alpha = 90^\circ$ ),  $\text{He}^{2+}$  ion approaches the center of mass of CO vertically along the Z axis. The only symmetry plane for the system is the YZ plane ( $C_s$  point group) and the electronic states are classified according to the two irreducible representations  $A'$  and  $A''$  of the  $C_s$  point group. In this case the interactions are through radial couplings between  $A'$  states, the X component of the rotational couplings between the  $A'$  states, and the Y and Z components of the rotational couplings between the  $A'$  and  $A''$  states. Other interactions have been excluded due to symmetry constraints.

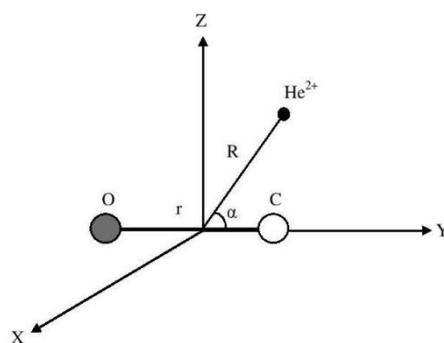
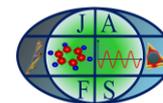


Figure 1: Internal coordinates for the  $[\text{HeCO}]^{2+}$  system.

In all three directions of approach, the origin of the scattering coordinates is located at the center of mass of the  $[\text{HeCO}]^{2+}$  system. In the collision energy range considered in the present work, the collision time is much shorter than the relaxation time of the target CO. Hence, the molecular state calculation has been performed with CO internuclear distance fixed at  $2.13222 a_0$  corresponding to the equilibrium geometry of the ground state of CO molecule.

The basis set employed in this work consists of contracted Cartesian Gaussian functions. For carbon the aug-cc-pVQZ [24] basis set  $[6s, 5p, 4d, 3f, 2g]$  is contracted to  $[6s, 5p, 4d, 3f]$  augmented with two diffuse  $s$  ( $\alpha_s = 0.0230000$  and  $0.0055000 a_0^{-2}$ ), two diffuse  $p$  ( $\alpha_p = 0.021000$  and  $0.0049000 a_0^{-2}$ ) and two diffuse  $d$  ( $\alpha_d = 0.0150000$  and  $0.0032000 a_0^{-2}$ ). For oxygen the aug-cc-pVQZ [24] basis set  $[6s, 5p, 4d, 3f, 2g]$  is contracted to  $[6s, 5p, 4d, 3f]$  augmented with two diffuse  $s$  ( $\alpha_s = 0.0320000$  and  $0.0022000 a_0^{-2}$ ) two diffuse  $p$  ( $\alpha_p = 0.0310000$  and  $0.0011000 a_0^{-2}$ ) and two diffuse  $d$  ( $\alpha_d = 0.0150000$  and  $0.0032000 a_0^{-2}$ ) are added into this contracted basis set. For helium optimized aug-cc-pVQZ [25] basis set  $[10s, 5p, 2d, 1f]$  is used.



A self-consistent field (SCF) calculation has been carried out for the lowest-energy  $^1A_1$  state at each internuclear distance considered for all the three directions of approach. The resulting molecular orbitals (MOs) form the orthonormal one-electron basis for the subsequent CI treatments.

The adiabatic MRDCI energies have been calculated at 173 internuclear separations in the range  $1.5 \leq R \leq 50.0 a_0$  ( $R$  being the distance of  $He^{2+}$  from the center of CO. The MRDCI method is employed with configuration selection and perturbative energy corrections [14-21]. A set of reference configurations is chosen based on a preliminary scan of the wave functions of the lowest roots of a given symmetry at representative internuclear distances.

A selection threshold of  $T = 1.0 \times 10^{-6}$  hartree is employed to divide the generated configurations into two sets based on their ability to lower the total energy of a given root relative to that obtained in the small reference secular equations. The details regarding the numbers of reference configurations, roots selected and the corresponding sizes of the generated and selected CI spaces are given in Table I. The calculations are carried out in the  $C_{2v}$  subgroup of the  $C_{\infty v}$  point group, but the MOs themselves transform according to the irreducible representations of  $D_{\infty h}$  linear symmetry, making identification of the resulting CI eigenfunctions straightforward.

The configuration interaction (CI) treatment has been carried out by employing the Table CI method [19-21] for efficient treatment of the various open-shell cases which arise because of the single and double substitutions relative to the reference configurations. Sums of squared coefficients of reference configurations  $\sum_p c_p^2$  for each of the lowest roots are also given in Table I. This quantity is an indication of the quality of the choice of the reference species in each case. Typically values of 0.929–0.914 are found, which is a satisfactory range for CI treatments with only ten active electrons (the carbon  $1s$  shell and oxygen  $1s$  shell are always doubly occupied). The  $\sum_p c_p^2$  values are also employed in the multireference analog to the Davidson correction [26, 27] to the energy of each root in order to estimate the effect of higher excitations and therefore to obtain the corresponding full CI energy to a good approximation.

Table 1: Number of reference configurations  $N_{ref}$  and number of roots  $N_{root}$  treated in each irreducible representation and the corresponding number of generated ( $N_{tot}$ ) and selected ( $N_{sel}$ ) symmetry-adapted functions with analog of Davidson-Langhoff correction for a threshold of  $1.0 \times 10^{-6}$  hartree. Note that  $R$  is the distance between  $He^{2+}$  ion and CO center of mass.

State	$N_{ref}$	$N_{tot}$	$N_{sel}$	$N_{root}$	$\sum_p c_p^2$
carbon end	$R = 2.1 a_0$				
$^1A_1$	117	25107571	152860	8	0.91925
$^1B_1$	131	36530868	130437	5	0.91400
$^1A_2$	58	19913451	100128	4	0.91925
$^3A_1$	122	56874767	132811	6	0.91783
$^3B_1$	131	66373749	123435	5	0.91880
$^3A_2$	58	36315855	100829	4	0.91825
oxygen end	$R = 2.7 a_0$				
$^1A_1$	108	24130542	159236	8	0.92560
$^1B_1$	72	19081874	141719	5	0.92100
$^1A_2$	41	12479242	114371	4	0.91875
$^3A_1$	113	54168588	128649	6	0.92980
$^3B_1$	124	65232445	150152	5	0.92960
$^3A_2$	70	46421304	119775	4	0.92790
center of mass	$R = 3.5 a_0$				
$^1A'$	214	76191198	193952	10	0.92620
$^1A''$	127	60828104	160514	6	0.92050
$^3A'$	217	149263062	201955	10	0.92740
$^3A''$	154	134429332	149371	6	0.92616

The calculated first ionization potential of CO molecule, giving rise to  $\text{CO}^+$  ( ${}^2\Sigma^+$ ), is 13.6692 eV, which agrees well with the experimental value of 13.99 eV determined from photoelectron spectroscopy [28]. The calculated energy differences between the single electron capture channel,  $\text{He}^+$  ( $1s\ {}^2S$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ ) and the entry channel,  $\text{He}^{2+}$  +  $\text{CO}$  ( $X\ {}^1\Sigma^+$ ) at  $R = 50\ a_0$  are 2.20786 and 2.24599 eV for  $\text{He}^{2+}$  ion approaching the carbon and oxygen ends, respectively. For the triplet manifold the calculated energy differences for the single electron capture channel,  $\text{He}^+$  ( $1s\ {}^2S$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ ) and the entry channel,  $\text{He}^{2+}$  +  $\text{CO}$  ( $X\ {}^3\Sigma^+$ ) are 9.2834 and 9.2913 eV for  $\text{He}^{2+}$  ion approaching the carbon and oxygen ends, respectively. For the perpendicular approach, the asymptotic energy difference could not be calculated as the entry channel lies much above the calculated adiabatic potentials.

Having used the optimized basis, the radial coupling matrix elements between all pairs of states of same symmetry have been calculated by applying a finite-difference method [29]

$$A_{ij} = \langle \psi_i | \frac{\partial}{\partial R} | \psi_j \rangle = \lim_{\Delta R \rightarrow 0} \frac{1}{\Delta R} \langle \psi_i(R) | \psi_j(R + \Delta R) \rangle,$$

with a step size of  $0.0002\ a_0$  and the electronic coordinate origin at the center of mass of the  $[\text{HeCO}]^{2+}$  system. The rotational couplings between states of angular momentum  $\Delta J = \pm 1$  have been calculated from the angular momentum tensor using a standard procedure [30].

## 2.2. Scattering calculation:

The scattering calculation has been performed in the keV region, where it has been found that the straight-line trajectories are satisfactory [31] and semiclassical approaches have been applied with good accuracy [32]. The computations have been performed using the EIKONX program [13] based on an efficient propagator method [33].

For  $\text{He}^{2+}$  ions of keV energy, the collision times are approximately of the order of  $10^{-16}$  s, whereas the molecular rotation and vibration times are typically of the order of  $10^{-11}$  and  $10^{-14}$  s, respectively [34]. Hence, the internuclear distance between the C and O atoms can be assumed to remain fixed during the collision, i.e. the Franck–Condon (FC) principle can be applied as the molecular rotation and vibration time are longer than the collision time. Cross sections corresponding to purely electronic transitions are thus determined by solving the impact parameter equation as in the usual ion-atom approach, considering the internuclear distance of the molecular target fixed in a given geometry.

The electronic transitions between the molecular states are mainly governed by the nonadiabatic radial and rotational coupling matrix elements. Hence, the coupled equations have been solved taking account of all the relevant radial and rotational couplings. In the present study, electron translation factors (ETFs), which are often used to ensure that the cross sections are independent of the origin of coordinates, have been used. The ETFs have been evaluated in the approximation of common translation factors (CTFs) [35]. The influence of ETFs is expected to be very low in the energy range considered in the present work, but their inclusion ensures that the correct scattering boundary conditions are satisfied.

The influence of spin-orbit couplings is expected to be low in the range of energy considered in the present work. Hence, singlet and triplet states have been considered separately. Singlet states included in the dynamical calculations are: the entry channel  $2\ {}^1\Sigma^+$  [ $\text{He}^{2+}$  +  $\text{CO}$  ( $X\ {}^1\Sigma^+$ )] and SEC channels:  $1\ {}^1\Sigma^+$  [ $\text{He}^+$  ( $1s\ {}^2S$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ )],  $3\ {}^1\Sigma^+$  [ $\text{He}^+$  ( $n=2$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ )],  $4\ {}^1\Sigma^+$  [ $\text{He}^+$  ( $n=3$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ )],  $5\ {}^1\Sigma^+$  [ $\text{He}^+$  ( $n=3$ ) +  $\text{CO}^+$  ( $A\ {}^2\Sigma^+$ )],  $1\ {}^1\Pi$  [ $\text{He}^+$  ( $n=2$ ) +  $\text{CO}^+$  ( $A\ {}^2\Pi$ )],  $2\ {}^1\Pi$  [ $\text{He}^+$  ( $n=3$ ) +  $\text{CO}^+$  ( $A\ {}^2\Pi$ )]. Triplet states included in the dynamical calculations are: the entry channel  $5\ {}^3\Sigma^+$  [ $\text{He}^{2+}$  +  $\text{CO}$  ( $X\ {}^3\Sigma^+$ )] and SEC channels:  $1\ {}^3\Sigma^+$  [ $\text{He}^+$  ( $1s\ {}^2S$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ )],  $2\ {}^3\Sigma^+$  [ $\text{He}^+$  ( $1s\ {}^2S$ ) +  $\text{CO}^+$  ( $A\ {}^2\Sigma^+$ )],  $3\ {}^3\Sigma^+$  [ $\text{He}^+$  ( $n=2$ ) +  $\text{CO}^+$  ( $X\ {}^2\Sigma^+$ )],  $4\ {}^3\Sigma^+$  [ $\text{He}^+$  ( $n=2$ ) +  $\text{CO}^+$  ( $A\ {}^2\Sigma^+$ )],  $1\ {}^3\Pi$  [ $\text{He}^+$  ( $1s\ {}^2S$ ) +  $\text{CO}^+$  ( $A\ {}^2\Pi$ )],  $2\ {}^3\Pi$  [ $\text{He}^+$  ( $n=2$ ) +  $\text{CO}^+$  ( $A\ {}^2\Pi$ )].

## 3. Results:

### 3.1. Adiabatic potentials and nonadiabatic couplings:

Rotational couplings are considered relative to the entry channel symmetries ( ${}^1\Sigma^+$  and  ${}^3\Sigma^+$ ), and thus  ${}^1\Pi$  and  ${}^3\Pi$  states have also been included in the collision dynamics. The adiabatic potential energy curves for  $\text{He}^{2+}$  ion approaching the oxygen ( $\alpha = 180^\circ$ ) end of the CO molecule (singlet states) are shown in Fig. 2. The  $2\ {}^1\Sigma^+$  state

corresponds to the entry  $\text{He}^{2+}/\text{CO}$  channel whereas all the remaining states correspond to  $\text{He}^+/\text{CO}^+$  single electron capture channels.

The  $1^1\Sigma^+$  and  $2^1\Sigma^+$  states show an avoided crossing lying between  $R = 8$  to  $9 a_0$  for  $\text{He}^{2+}$  ion approaching the oxygen end of the CO molecule, whereas for the carbon ( $\alpha = 0^\circ$ ) end the avoided crossings are observed beyond  $R = 9.5 a_0$ . The  $2^1\Sigma^+$  and  $3^1\Sigma^+$  states show an avoided crossing near  $R = 2.2 a_0$  for the carbon end, whereas there is very weak (or no) avoided crossing between these states for the oxygen end of the CO molecule. For both termini the  $4^1\Sigma^+$  and  $5^1\Sigma^+$  states exhibit multiple avoided crossings and they are expected to play a significant role in the SEC process in the high-energy collisions. The curve crossings between the entry channel  $2^1\Sigma^+$  and SEC channel  $1^1\Pi$  suggest that there is a significant contribution from the  $1^1\Pi$  state in the SEC process, whereas the curve crossing between the  $2^1\Pi$  state and high-lying  $4^1\Sigma^+$  and  $5^1\Sigma^+$  states contributes to the flux redistribution in high-energy collisions.

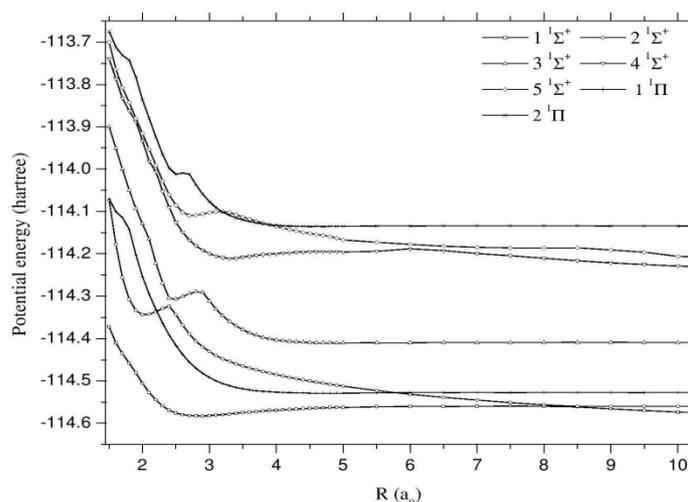


Figure 2: Adiabatic potential energy curves for the  $1^1\Sigma^+$  and  $1^1\Pi$  (singlet) states of the  $[\text{HeCO}]^{2+}$  system at equilibrium,  $\alpha = 180^\circ$ .

For the triplet states the adiabatic potentials for  $\text{He}^{2+}$  ion approaching the oxygen end of the CO molecule are shown in Fig. 3. The entry channel ( $\text{He}^{2+}/\text{CO}$ ) is  $5^3\Sigma^+$ , whereas all other states correspond to SEC ( $\text{He}^+/\text{CO}^+$ ) channels. As in the case of singlet states, the adiabatic potentials for triplet states for both termini (carbon and oxygen) exhibit some distinctive characteristics. For the oxygen end, the  $5^3\Sigma^+$  and  $4^3\Sigma^+$  states show a strong avoided crossing near  $R = 2.8 a_0$  and other smoothly avoided crossings between  $R = 3.5 - 4 a_0$ ,  $4.5 - 5.5 a_0$  and beyond  $9 a_0$ . By contrast, for the carbon end ( $\alpha = 0^\circ$ ) these states show a smooth avoided crossing below  $R = 2 a_0$ , a very weak avoided crossing near  $R = 5.5 a_0$  and a weak avoided crossing around  $R = 10 a_0$ . The  $3^3\Sigma^+$  and  $4^3\Sigma^+$  states for the carbon-end approach show strong avoided crossings near  $R = 2.2, 4.1$  and  $7.5 a_0$ , whereas for the oxygen end these states ( $3^3\Sigma^+$  and  $4^3\Sigma^+$ ) undergo a smooth avoided crossing below  $R = 2.5 a_0$ , and a strong avoided crossing near  $R = 4.2, 6.0$  and  $6.5 a_0$ . For both ends, the  $3^3\Sigma^+$ ,  $2^3\Sigma^+$  and  $1^3\Sigma^+$  states exhibit very weak or no avoided crossings.

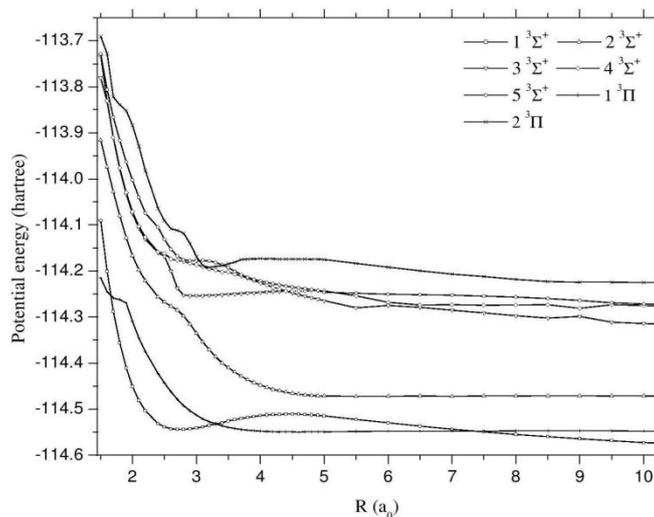


Figure 3: Adiabatic potential energy curves for the  $^3\Sigma^+$  and  $^3\Pi$  (triplet) states of the  $[\text{HeCO}]^{2+}$  system at equilibrium,  $\alpha = 180^\circ$ .

The curve crossings between the  $2\ ^3\Pi$  and  $5\ ^3\Sigma^+$  states suggest an important role played by the  $2\ ^3\Pi$  state in the SEC process, whereas the curve crossings between the  $1\ ^3\Pi$  and  $1\ ^3\Sigma^+$  states play a significant role in flux redistribution. For both singlet and triplet states the amount of mixing is comparatively weaker for  $\text{He}^{2+}$  ion approaching the carbon end than for the oxygen end of the CO molecule. Hence, a strong steric effect is expected to play an important role in the SEC process.

In the adiabatic potential energy curves for the  $\text{He}^{2+}$  ion approaching the center of mass ( $\alpha = 90^\circ$ ) of the CO molecule, the ground state entry channel ( $\text{He}^{2+}/\text{CO}$ ) lies much above the calculated potentials and hence it has not been included in the scattering calculation.

### 3.2. Cross sections:

The collision dynamics for the  $[\text{HeCO}]^{2+}$  system has been performed in the energy range of 0.6 to 6.0 keV. The spin-orbit effects have been neglected in the energy range of interest so triplet and singlet manifolds have been considered separately. According to the statistical weight, the triplet manifold accounts for 3/4 of the population of the ground state entry channel, against 1/4 for the singlet manifold. To understand the effect of molecular orientation on cross sections, the calculation has been performed for  $\text{He}^{2+}$  ion approaching both the carbon and oxygen termini of the CO molecule (Fig.4).

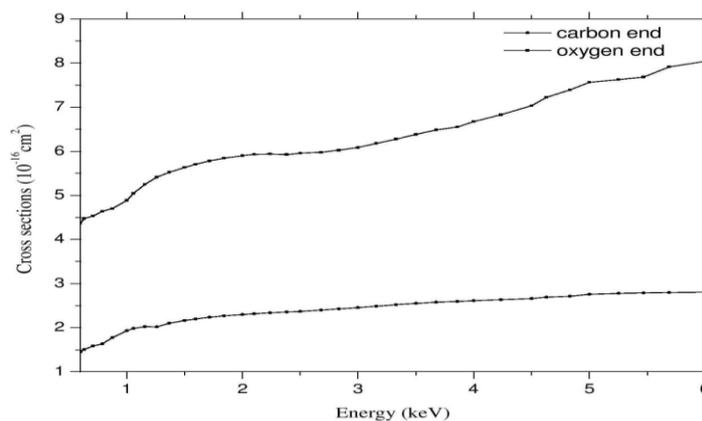


Figure 4. Total SEC cross sections for different orientations of the  $\text{He}^{2+}$  projectile towards CO molecule at equilibrium.

#### 1. Total cross sections:

Total SEC cross sections for  $\text{He}^{2+}$  ion approaching the carbon and the oxygen ends of CO molecule have been shown in Fig. 4. Total electron capture cross sections for the oxygen end increases with collision energy, whereas for the carbon end total electron capture cross sections increases slowly with collision energy. It is evident from the curves that the SEC process is favoured more towards the oxygen end. Thus, the calculated SEC cross sections are highly dependent on molecular orientation.

Finally, the computed total SEC cross sections averaged over two molecular orientations (carbon and oxygen termini) obtained in the present work and experimental measurements of Kusakabe *et al.* [8] and Čadež *et al.* [9] have been compared in the Fig. 5. In general, the overall agreement between the present calculations and the two experimental results is found to be good. In the range of energy considered in the present study, our calculated SEC cross sections increase with collision energy. The energy dependence of the calculated cross sections agrees both qualitatively and quantitatively with the experimental measurements. Previously reported theoretical results of Kusakabe *et al.* [8] were smaller by 50 % than their experimental measurements. Thus, the SEC cross sections obtained in the present study are a significant improvement over the previous theoretical calculations. The agreement between the theoretical and experimental results is expected to improve with the inclusion of SEC cross sections for the perpendicular approach of the  $\text{He}^{2+}$  ion towards the CO molecule.

### 3.3. Fragmentation:

Although in the present study no rigorous analysis of fragmentation of the CO molecule caused by  $\text{He}^{2+}$  ion impact was done, we briefly outline the possible mechanisms and consequences of fragmentation processes. For the collision of  $\text{He}^{2+}$  ion with CO molecule the energy difference between the entry channel  $\text{He}^{2+} + \text{CO}$  ( $X^1\Sigma^+$ ) and the SEC channel  $\text{He}^+(1s^2S) + \text{CO}^+$  [dissociative states] lies in the range of 0 to 20 eV [7]. The energy difference between the entry channel ( $\text{He}^{2+}/\text{CO}$ ) and the SEC channel,  $\text{He}^+(n=2) + \text{CO}^+$  ( $X^2\Sigma^+$ ) is small (-0.42 eV) [7]. Radial coupling matrix elements between the entry channel and single electron capture [ $\text{He}^+(1s^2S) + \text{CO}^+$ ] channels are sizable.

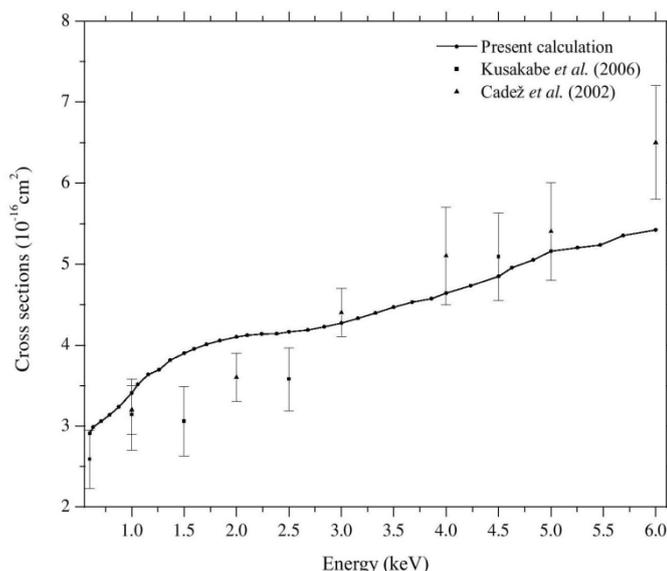


Figure 5: Total SEC cross sections averaged over two different orientations of the  $\text{He}^{2+}$  projectile towards CO molecule at equilibrium; filled circles with solid line, the present calculation; filled rectangles with error bars, the measurements of Kusakabe *et al.* [8]; filled triangles with error bars, the measurements of Čadež *et al.* [9].

Thus, the electron capture into the [ $\text{He}^+(1s^2S) + \text{CO}^+$ ] channel is very effective in low energy collisions. The final products of the electron capture process depend on the energy transfer to  $\text{CO}^+$  in the collision process. The lowest  $\text{CO}^+$  state has a binding energy of about 8.3 eV [36] and has a nearly identical equilibrium internuclear distance as that of the CO ground state. Therefore, in view of the FC principle, it is likely that most of the  $\text{CO}^+$  ions produced in the SEC into the  $\text{He}^+(n=2)$  will be into the low-lying bound states of  $\text{CO}^+$  which are quite stable. The SEC into the  $\text{He}^+(1s^2S)$  will result in an unstable  $\text{CO}^+$  ion, causing its dissociation. The  $\text{CO}^+$  ion formed in the single electron capture into the  $\text{He}^+(1s^2S)$  state will dissociate, leading to the formation of either  $\text{C}^+$  or  $\text{O}^+$  ion. According to Shah and Gilbody [37], in the collision of  $\text{He}^{2+}$  ion with CO molecule at 32 keV, the lowest energy they considered in their study, dissociative SEC channels account for a total cross section of

$5.05 \times 10^{-16} \text{ cm}^2$  compared with a total of  $11.9 \times 10^{-16} \text{ cm}^2$  from the non-dissociative SEC. They also found that the dissociative electron capture leads to the formation of  $\text{He}^+ + \text{C}^+ + \text{O}^+ + \text{e}^-$ ,  $\text{He}^+ + \text{C}^{2+} + \text{O} + \text{e}^-$ ,  $\text{He}^+ + \text{C}^{2+} + \text{O}^+ + 2\text{e}^-$  and  $\text{He}^+ + \text{C}^{2+} + \text{O}^{2+} + 3\text{e}^-$ . At 12 keV, Folkerts *et al.* [38] found that fragmentation channels account for about 46 % of total products of the ionization of CO.

#### 4. Conclusions:

The collision dynamics for the  $[\text{HeCO}]^{2+}$  system has been determined using the impact parameter method [13] in the energy range of 0.6 to 6.0 keV corresponding to a solar-wind ion velocity of about 3 keV at low heliographic latitudes [23]. Partial and total SEC cross sections have been calculated with respect to the statistical weights 1/4 and 3/4 for the singlet and triplet manifolds, respectively. To understand the effect of molecular orientation on calculated cross sections, the calculation has been performed for  $\text{He}^{2+}$  ion approaching the carbon and oxygen ends of CO molecule. The dominant contribution of the oxygen end in the electron capture process has been shown. The partial and total SEC cross sections averaged over the two molecular orientations (carbon and oxygen termini) considered in the present calculation have also been given.

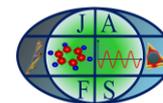
The calculated orientation-averaged total SEC cross sections have been compared with the available experimental measurements. It has been shown that the impact parameter method provides cross sections which are in good agreement with experimental measurements [8, 9] in the range of energy considered in the present work. The dominant contribution of the dissociative single electron capture in low-energy collisions has been shown. Single electron capture into  $\text{He}^+$  ( $1s\ ^2S$ ) states results in the formation of unstable  $\text{CO}^+$  ion and its subsequent fragmentation yielding multiply charged ions has been discussed. The calculated partial and total SEC cross sections illustrate the major role played by radial and rotational couplings compared to spin-orbit couplings. Their influence on processes in the cometary atmosphere leading to X-ray and the EUV photon emission has been demonstrated. The present SEC cross section data should be useful for a variety of applications.

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