

## TOTAL SINGLE ELECTRON CAPTURE CROSS SECTIONS FOR SLOW He<sup>2+</sup>-Ne and He<sup>2+</sup> - H<sub>2</sub> COLLISIONS

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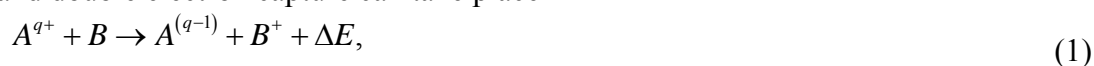
### Abstract

Total cross sections for single electron capture in He<sup>2+</sup>-Ne collisions have been measured in the impact energy range of 260 – 2000 eV. Such data are not yet available in the literature. Our results were interpreted with a simple two state Landau-Zener theory. From the Landau-Zener formula with an empirical transition matrix element the maximum cross section is predicted at ion impact energy of 36.5 eV. The experimental cross section values follow the expected trend with impact energy, suggesting that they are in an energy range above the location of the maximum cross section. Using these measured total single electron capture cross sections for He<sup>2+</sup>-Ne, a calibration for total single electron capture cross sections for He<sup>2+</sup>-H<sub>2</sub> collisions could be carried out. We note, e.g., that at an impact energy of 600 eV the single electron capture cross section for He<sup>2+</sup>-H<sub>2</sub> collisions is only about 2 % of the one for Ne, i.e. of the order of  $4 \times 10^{-18}$  cm<sup>2</sup> and therefore rather small.

### INTRODUCTION

Electron capture by multicharged ions (MCI) is relevant from both fundamental and practical points of view. Cross sections for such reactions provide useful input data for the study of astrophysical plasmas and diagnostics in controlled thermonuclear fusion research [1]. Ion-atom collisions involve many different inelastic processes that can end in different final channels. Some of these processes are single ionization, double ionization, electron capture (single or double capture) and transfer ionization. In general, single and double ionization are dominant at high projectile energy, while electron capture becomes dominant at low projectile energy. Transfer ionization consists of ionization accompanied by single electron capture. At low projectile energy, it may involve double electron capture followed by autoionization [2]. In general, the interaction between collision partners is of a dynamic nature where the particles carry with them a cloud of electrons moving about the nucleus. When two atoms collide, their electronic charge distributions change continuously. If the motion of the centres is slow, the electrons can adapt to this

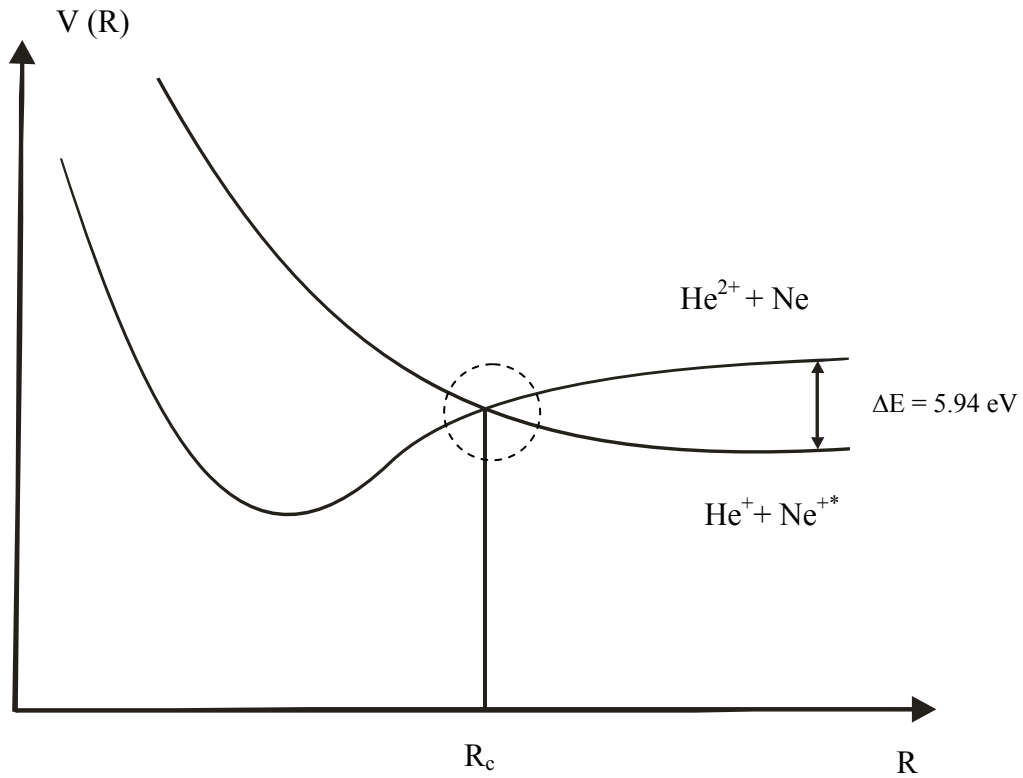
motion and after the collision return to their initial configuration (adiabatic process) where the electrons did not gain or lose energy. Fast collisions are given if the relative velocity of the particles is much larger than the average velocity of the bound electrons ( $v \gg v_e$ ), where  $v_e = 2.18 \times 10^6$  m/sec. For slow collisions the relative velocity of the particles is smaller than the average velocity of the bound electrons ( $v < v_e$ ). The relative motion of the atoms is slow enough so that their electronic motion during transition can adjust itself to small changes in the inter-nuclear distances. When multicharged ions (MCI) collide with neutral atoms or molecules, different kinds of processes may take place. The atom may be excited and lose one or more electrons either by direct ionization or in a charge transfer process. The ion may capture or lose electrons, and it may go into an excited state and then deexcite by emitting photons or electrons. When MCI  $A^{q+}$  collides with a neutral particle (atom, molecule) B, e.g., single and double electron capture can take place



where  $\Delta E$ ,  $\Delta E'$  are the energy defects of these reactions. For single electron capture, a projectile ion captures one electron from the atom or molecule while for a double electron capture process the projectile ion captures two electrons. The potential curve of the incoming channel,  $A^{q+} + B$ , is principally flat at large inter-nuclear distances, decreases somewhat at intermediate inter-nuclear distances due to the polarization of the target atom or molecule by the ion, and rises sharply at small inter-nuclear distances as the nuclear Coulomb potential starts to dominate. Once an electron has been captured by a projectile ion, both the projectile and the target are positively charged. Then the outgoing channel will be repulsive due to the mutual Coulomb interaction. After electron capture has occurred, the energy defect  $\Delta E$  will be converted into kinetic energy between the target and the projectile ion. Fully quantum-mechanical or semi-classical models can be used for theoretical treatments of charge transfer in slow MCI-atom collisions. The main difference between the semi-classical and the quantum-mechanical model is that in the first case the nuclear motion is described classically and only the electron motion is treated in a quantum-mechanical way. Theoretical description of charge transfer collisions at low and intermediate energies are usually treated by fully quantum-mechanical or at least semi-classical models. In this paper, the Landau-Zener-model was used for the calculation of SEC cross sections for  $\text{He}^{2+}$  - Ne collisions at impact energies up to 2000 eV. In this work, total cross sections for single electron capture in  $\text{He}^{2+}$ -Ne collisions have been measured in the impact energy range of 260 – 2000 eV.

### **CALCULATED CROSS SECTION FOR $\text{He}^{2+}$ -Ne COLLISIONS USING LANDAU-ZENER MODEL**

Inelastic transitions in slow atomic collisions are strongly favoured near crossings of potential energy curves [3]. These crossings occur for, e.g., collisions of doubly charged ions with neutral atoms, where the potential energy curve of the final quasi-molecular state is dominated by Coulomb repulsion (Fig.1).



**Fig. 1** Adiabatic potential energy curves for the ( $\text{He}^{2+}$ -Ne) collision system with a crossing at atomic inter-nuclear distance  $R_c$ .

The Landau-Zener model [4, 5, 6] provides the probability for transition between two states for single electron charge transfer reactions. Later, this model was extended to multi-state transition systems [7]. It is applicable in the adiabatic velocity region ( $v \ll v_0$ ). In such reactions, the incoming channel will be dominated by the polarization attraction force, while the outgoing channel (reaction products) shows Coulombic repulsion. Single electron transfer can be described as a transition at avoided crossings at the inter-atomic distances  $R_c$ :

$$R_c = \frac{27.21(q-1)}{\Delta E}, \quad (3)$$

where  $q$  is the initial charge state of the multicharged ion and  $\Delta E$  is the respective exothermic energy defect between the two states at infinite separation of the colliding particles. At smaller inter-atomic distances, the transition at the avoided crossing with inter-atomic distance  $R_c$  is determined as following:

$$\frac{q-1}{R_c} + \frac{\alpha_p q^2}{2R_c^4} \cong \Delta E, \quad (4)$$

where  $\alpha_p$  is the target polarizability. The transition probability between  $V_1$  and  $V_2$  at the distance  $R_c$  of the avoided crossing is given by [8]:

$$P = \exp(-\delta(b)), \quad (5)$$

with 
$$\delta(b) = \frac{2\pi H_{12}^2(R_c)}{\hbar v_r(b) \left| \frac{d}{dr}(V_1 - V_2) \right|_{r=R_c}}, \quad (6)$$

where  $V_1(r)$  and  $V_2(r)$  are the potential curves for the incoming and the outgoing channel, respectively,  $r$  is the inter-atomic distance and  $b$  is the impact parameter.  $H_{12}$  is the transition

matrix element that corresponds to the separation energy between the adiabatic state-representative curves at the avoided crossing, and  $v_r$  is the relative collision velocity ( $v_r < 2.18 \times 10^6$  m/sec). The transition is assumed to take place only in a narrow region around the crossing point. The cross section can be derived by noting that the probability of remaining on  $V_2$  as:

$$P = 2P(1 - P). \quad (7)$$

By integrating over all impact parameters, the cross section is given by:

$$\sigma_{LZ} = 4\pi R_c^2 I(\eta), \quad (8)$$

with 
$$\eta = \frac{2\pi H_{12}^2(R_c)}{\hbar v \left| \frac{d}{dr}(V_1 - V_2) \right|_{R_c}}, \quad (9)$$

where  $v$  is the projectile velocity, and

$$I(\eta) = \int_1^\infty \exp(-\eta x)(1 - \exp(-\eta x))x^{-3} dx, \quad (10)$$

where 
$$\left| \frac{d}{dr}(V_1 - V_2) \right|_{R_c} = \frac{q-1}{R_c^2}, \quad (11)$$

if the polarization of the target particle is neglected. The transition matrix element can be estimated according to:

$$H_{12} = H_{12}^* I_1^{1/2} I_2^{1/2}, \quad (12)$$

with 
$$H_{12}^* = R_c^* \exp(-0.86 R_c^*), \quad (13)$$

and  $R_c^*$  given by the empirical formula [9]:

$$R_c^* = \frac{I_1^{1/2} + I_2^{1/2}}{2^{1/2}} R_c, \quad (14)$$

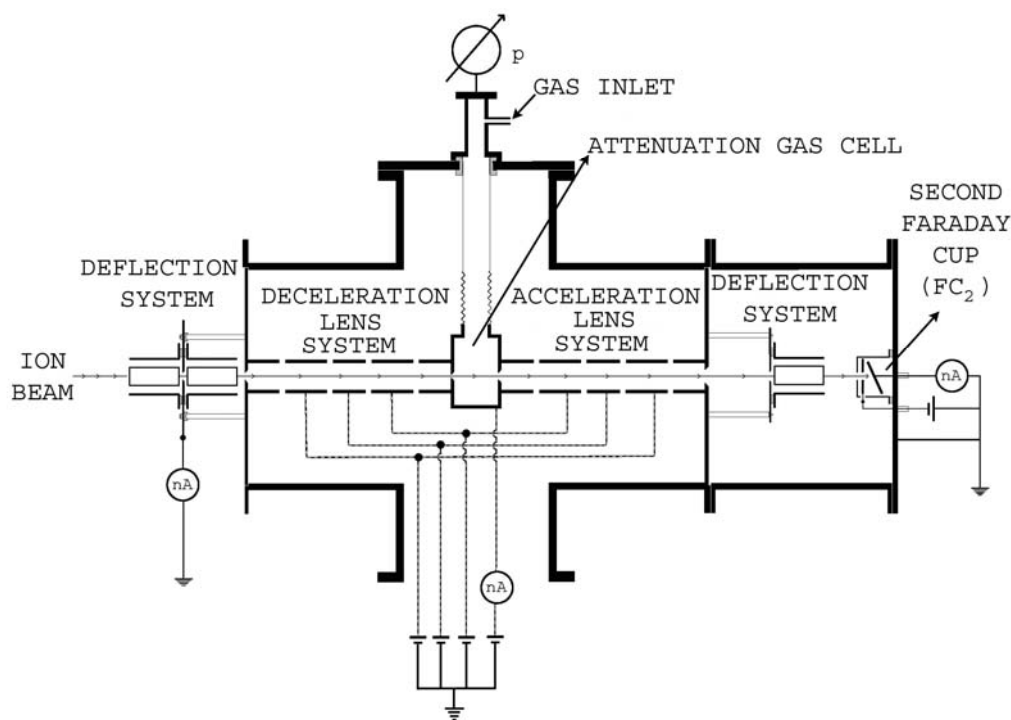
where  $I_1$  and  $I_2$  are the initial and final ionization potentials of the transferred active electron, respectively. Then, the cross section for single electron transfer at the transition of the avoided crossing with inter-atomic distance  $R_c$  can be calculated using equ. 3.

## THE CHARGE EXCHANGE EXPERIMENTAL SETUP

The charge exchange experiment consists, as shown in fig. 2, of a first beam deflection system, a deceleration lens system, the collision chamber itself (gas cell), an acceleration lens system, a final deflection system and a Faraday cup for measuring the ion currents without and with attenuation. The deceleration and acceleration lens systems are symmetrical and consist of 10 electrodes made of stainless steel. The gap between each electrode is 1 mm. The deceleration-and acceleration lens systems are electrically connected internally and the potential difference applied to the lens elements was previously calculated using the SIMION program [10] to ensure a well collimated beam (see below). Collisions of slow doubly ( $\text{He}^{2+}$ ) charged ions with target atoms (Ne) take place in the collision cell which is connected to a gas inlet system controlled with a UHV dosing valve.

The attenuation gas pressure inside the collision chamber has to be low enough to assure single collision conditions. The collision chamber has a cylindrical shape with 2.5 cm length, a 1 mm diameter aperture at the entrance-and a 2 mm diameter aperture at the exit end.

Consequently, the acceptance angle for the scattered ions in this system is  $\pm 1.15^\circ$ . In this case, the product ion is recoiled nearly perpendicular to the impact momentum vector, but the scattering angle of the projectile is small. The region outside of the collision cell near the entrance and exit apertures is at a pressure much lower than inside the collision chamber. To this purpose, holes in the deceleration/acceleration electrodes permit rapid decrease of the gas pressure outside the collision cell. The collision cell is electrically insulated for making ion deceleration possible. A Baratron capacitance manometer permits precise pressure measurements for typical target gas pressures between  $10^{-4}$  and  $10^{-3}$  mbar.



**Fig. 2** Schematic view of the collision chamber containing the charge exchange experimental setup.

## DETERMINATION OF SINGLE ELECTRON CAPTURE CROSS SECTIONS

The attenuation method has been used for determination of total single electron capture cross sections for impact of doubly charged ions ( $\text{He}^{2+}$ ) colliding with neutral atoms (Ne). When the primary ion beam passes through the target gas of a certain density ( $n$ ) and length ( $L$ ), it is attenuated depending on the target gas density. The factor  $nL$  is called the target thickness ( $\pi$ ) and is obtained from:

$$\pi = nL = \frac{pL}{k_B T}, \quad (15)$$

where  $p$  is the target gas pressure,  $k_B$  is the Boltzmann's constant and  $T$  the absolute temperature in K at room temperature ( $20^\circ\text{C}$ ). The target thickness was thus calculated as:

$$\pi[\text{cm}^{-2}] = 6.55 \times 10^{16} p[\text{mbar}]. \quad (16)$$

where  $p$  has been measured with a Baratron capacitance manometer in mbar.

The effective length of the collision chamber ( $L = 2.65$  cm) was calculated as:

$$L = L_1 + \left( \frac{d_1 + d_2}{2} \right), \quad (17)$$

where  $L_1$  is the length of the collision chamber = 2.5 cm,  $d_1$  (diameter aperture at the entrance) = 0.1 cm, and  $d_2$  (diameter aperture at the exit end) = 0.2 cm.

By using the LabVIEW program for data taking, the total cross section for single electron capture in  $\text{He}^{2+}$ -Ne collisions has been calculated with equ. 19.

The single electron capture cross section  $\sigma_{sc}$  for  $\text{He}^{2+}$ -Ne was determined as follows:

$$I = I_0 \exp(-\sigma_{sc}\pi) + \frac{I_0}{2} [1 - \exp(-\sigma_{sc}\pi)] \approx \frac{I_0}{2} [2 - \sigma_{sc}\pi] \quad (\text{for } \pi\sigma_{sc} \ll 1), \quad (18)$$

$$\frac{I}{I_0} = 1 - \frac{\pi\sigma_{sc}}{2},$$

we finally obtain the relation

$$\sigma_{sc} = \frac{2}{\pi} \left[ 1 - \frac{I}{I_0} \right], \quad (19)$$

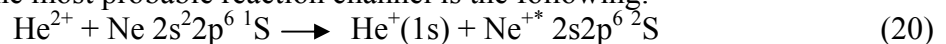
where  $I$  is the attenuated current normalized to the current in the first Faraday cup ( $I_{FC1}$ ), and  $I_0$  the same current measured at the second Faraday cup with no target gas and also normalized to  $I_{FC1}$ . It was found that the current measured at the gas cell ( $I_{GC}$ ) increases with gas pressure, and therefore we normalised the data by dividing  $I_{FC2}$  by  $I_{FC1}$ .

The ion beam in the first Faraday cup placed before the collision chamber was firstly monitored in order to normalize the current measured in the second Faraday cup to the incoming current. The ions were guided into the second Faraday cup by means of deflection plate sets behind the gas attenuation cell. The applied neon target gases were 99.9 % pure. In order to assure single collision conditions, the attenuation current was only reduced by up to 15 % of its initial value. For small target thickness (single collision conditions), the fitting can be made to a linear function because the exponential function for small arguments can be approximated by a linear function.

The attenuation process was carried out in the following way. The singly or doubly charged ions were extracted from the 14.5 GHz ECR ion source [11], focused, separated and passed to the charge exchange experiment. With the UHV dosing valve connected to the collision chamber, the gas was injected inside the attenuation chamber. Using the LabVIEW program, input data as gas pressure, ion current measured at the second Faraday cup ( $I_{FC2}$ ) with and without attenuation were stored. Also, the ion currents measured at the gas cell ( $I_{GC}$ ) and at the first Faraday cup ( $I_{FC1}$ ) were stored. The attenuation currents were normalized to the currents in the first Faraday cup.

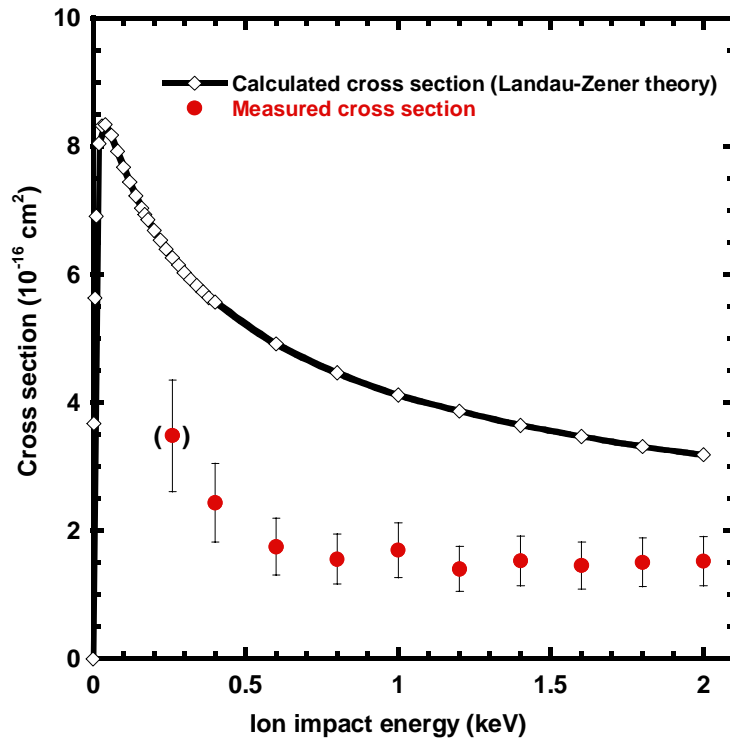
### **TOTAL SINGLE ELECTRON CAPTURE CROSS SECTIONS FOR $\text{He}^{2+}$ -Ne COLLISIONS**

Cross sections for single electron capture in slow collisions between  $\text{He}^{2+}$  and Ne have been determined by observing the incident  $\text{He}^{2+}$  ion current attenuation as a function of the Ne target gas density in the attenuation cell, in the impact energy range of 260 to 2000 eV. The lowest achievable energy was 260 eV where a still sufficiently large and stable ion current could be obtained. The most probable reaction channel is the following:



with an exothermic energy defect of  $\Delta E = 5.94$  eV.

Repeated measurements were made on different days for each impact energy to assure sufficiently accurate values of total electron capture cross sections. The experimental errors for these measurements are about 20 %.

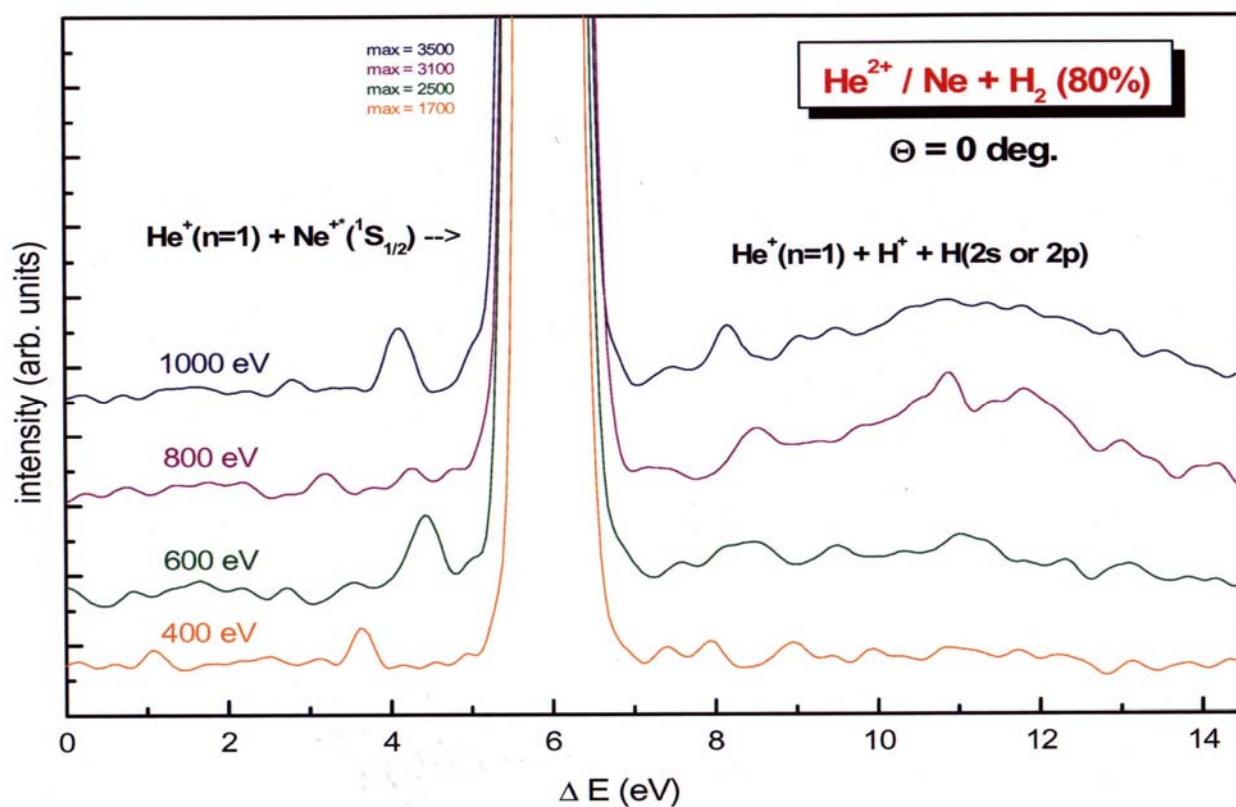


**Fig. 3** Measured and calculated single electron capture cross sections for  $\text{He}^{2+}$ -Ne collisions for impact energies up to 2000 eV. Full symbols show measured cross sections. Full line with open symbols shows calculated cross sections using the Landau-Zener formula. The data points at 260 eV impact energy (put between brackets) were probably subject to a larger systematic error due to extensive beam scattering.

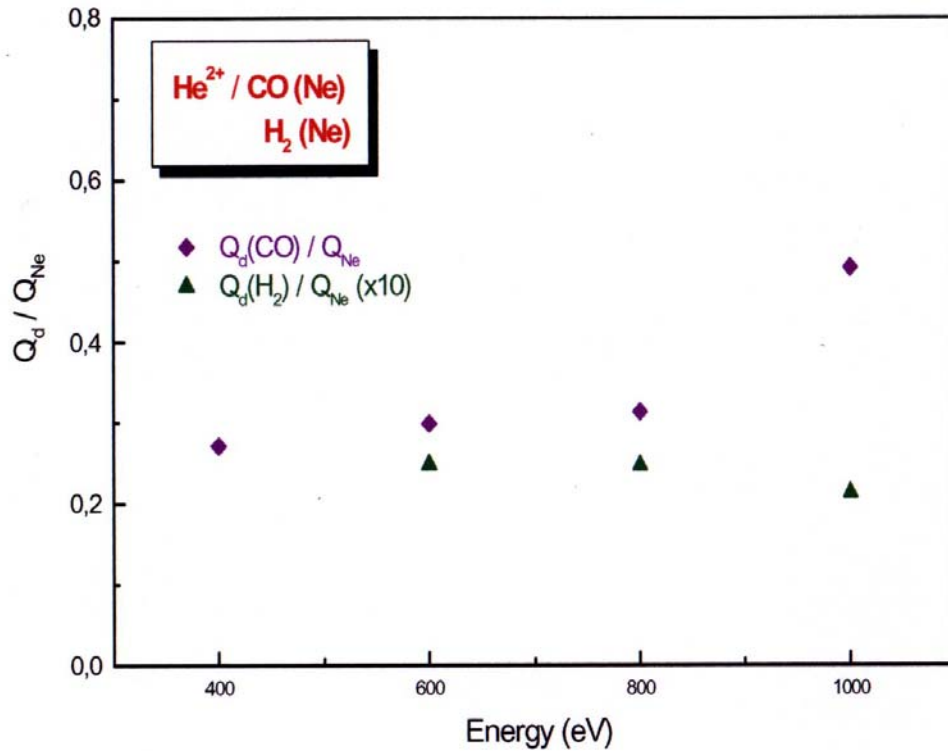
For discussion of the here for the first time measured cross sections for single electron capture in slow collisions between  $\text{He}^{2+}$  and Ne, theoretical cross sections were calculated by means of the semi-classical Landau-Zener formula. For a first estimate of these cross sections, only one Landau-Zener coupling between the two potential curves of the collision system (see equ. 20) has been taken into account. The application of the LZ-formula requires primarily appropriate values for the transition matrix element  $H_{12}$ . The latter can be obtained for the specific collision partners either by calculation of the adiabatic energy curves or from perturbation theory. In first approximation, it can be estimated according to the empirical relation given by equ. 14 where  $I_1$  and  $I_2$  are the ionisation potentials for the captured electron in its initial and final state, respectively. These ionisation potentials are  $I_1 = 1.78$  a.u. (48.5 eV) and  $I_2 = 2.0$  a.u. (54.4 eV) which, by substituting into equ. 10, results in a transition matrix element of  $H_{12} = 7.96 \times 10^{-3}$  a.u. A comparison of experimental and calculated cross sections is shown in fig.3. The Landau-Zener calculation predicts the maximum value for the cross section in a region not in compatible with our experimental data which could not be taken at impact energies below 260 eV. From the Landau-Zener formula with the empirical value for  $H_{12}$ , a maximum cross section of  $9.48 (\pi a_0^2)$  is derived at an impact velocity of 0.0191 a.u., which corresponds to an ion energy of 36.5 eV. The experimental cross section values follow this expected trend, suggesting that they are in an energy range still above the location of the maximum cross section.

## CALIBRATION OF SINGLE ELECTRON CAPTURE CROSS SECTIONS FOR $\text{He}^{2+}$ - $\text{H}_2$ COLLISIONS

The present measurements can be applied for determination of single electron capture cross section for  $\text{He}^{2+}$ - $\text{H}_2$  collisions in the same energy range, from earlier measured translational energy spectra for both collision systems ([2], figs. 4 and 5). From the relative data for single electron capture in  $\text{He}^{2+}$ - $\text{H}_2$  collisions as shown in fig.5 and the now available total cross sections for single electron capture in  $\text{He}^{2+}$ -Ne collisions as shown in fig.3, we can also derive for the first time absolute total single electron capture cross sections for  $\text{He}^{2+}$ - $\text{H}_2$  collisions.



**Fig. 4** Intensity dependence for  $\text{He}^{2+} / \text{Ne} + \text{H}_2$  (80%).

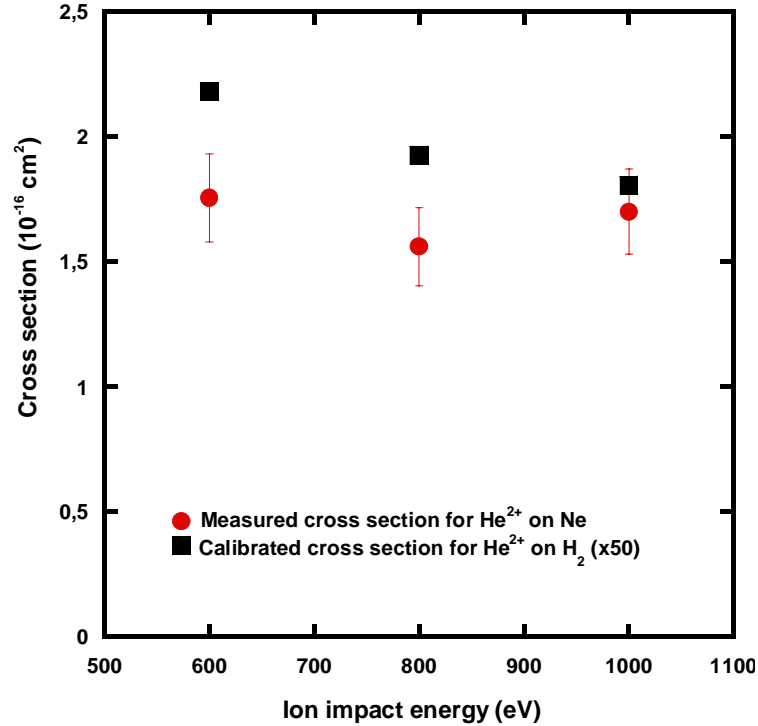


**Fig. 5** Ratio of single electron capture cross sections for impact of  $\text{He}^{2+}$  on  $\text{H}_2/\text{Ne}$  and  $\text{CO}/\text{Ne}$  gas mixtures, respectively [2]. Single electron capture cross sections for  $\text{He}^{2+}$ - $\text{H}_2$  collisions with respect to single electron capture data for  $\text{He}^{2+}$ - $\text{Ne}$  collisions at different impact energies are given in table 1.

**Table 1** Calibration of single electron capture cross sections for  $\text{He}^{2+}$  -  $\text{H}_2$  collisions from single electron capture data for  $\text{He}^{2+}$  -  $\text{Ne}$  collisions at impact energies of 0.6, 0.8 and 1 keV.

Impact energy (keV)	Calibrated cross section for $\text{He}^{2+}$ - $\text{H}_2$ ( $10^{-18} \text{ cm}^2$ )
0.6	4.4
0.8	3.9
1.0	3.6

Calibration of the single electron capture cross sections for  $\text{He}^{2+}$ - $\text{H}_2$  collisions from the single electron capture data for  $\text{He}^{2+}$  - $\text{Ne}$  collisions at impact energies of 0.6, 0.8 and 1 keV has thus been achieved. The SEC cross sections for  $\text{He}^{2+}$ - $\text{H}_2$  shown in fig. 5.6 were multiplied by a factor of 50 in order to fit them to the same scale as for the SEC cross sections for  $\text{He}^{2+}$ - $\text{Ne}$  collisions.



**Fig. 6** Comparison between the available SEC cross sections for He<sup>2+</sup> - Ne with SEC cross sections for He<sup>2+</sup>-H<sub>2</sub>.

## CONCLUSION

We note, e.g., that at the impact energy of 600 eV the single electron capture cross section for H<sub>2</sub> is only 2 % of the one for Ne, i.e. of the order of  $4 \times 10^{-18}$  cm<sup>2</sup> and therefore rather small. However, this derivation is still a matter of some concern, because of the following reason. In slow He<sup>2+</sup>-H<sub>2</sub> collisions, single electron capture is almost exclusively due to dissociative electron capture, which proceeds at relatively small inter-nuclear distance and thus gives rise to considerable projectile scattering out from the forward direction. TES measurements by Albu et al. 2004 involved a relatively small projectile acceptance angle of +/-0.5 degrees, under which conditions contribution for single electron capture from H<sub>2</sub> may have been suppressed in comparison to single electron capture from Ne. It is thus well possible that the total single electron capture cross section for He<sup>2+</sup>-H<sub>2</sub> collisions is actually by up to a factor of two larger than here derived.

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