CHARGE EXCHANGE PROCESSES FROM THE COLLISIONS OF ALPHA PARTICLES WITH WATER MOLECULES

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Collisions of multiply charged solar wind ions with cometary molecules lead to infrared and far ultraviolet photon emissions [1]. As it was shown in previous work by [2-4] the resulting spectra of the emission yields have astrophysical implications and can be used for testing such properties of the solar wind as velocity, density, and chemical composition. In present work experimental data for the state selective electron capture by He^{2+} ions from water molecules are presented. Three complimentary experimental techniques: Translational Energy Spectroscopy, Photon Emission Spectroscopy and Fragment Ion Spectroscopy were used for measuring state selective electron capture cross sections [5]. Experimental data are compared to the theoretical calculations. Theoretical calculations were carried out using basis approach which is proven to provide a good agreement with the experimental measurements.

PACS: 31.10.+z, 34.70.+e

1. INTRODUCTION

Experimental and theoretical data of the collisional processes between solar wind ions and cometary molecules are needed for investigating comets by detecting the resulting solar wind ions that underwent collision with cometary molecules. In present work experimental data for the state selective electron capture by He^{2+} ions from water molecules are presented. Three complimentary experimental techniques: Translational Energy Spectroscopy, Photon Emission Spectroscopy and Fragment Ion Spectroscopy were used for measuring state selective electron capture cross sections [5]. Electron capture cross sections obtained using each of the above mentioned experimental techniques are in a good agreement with one another. We used basis approach which takes into account all possible reaction channels from the collision of ions with complex molecules. The system of coupled differential equations is obtained that determine the amplitudes and cross sections of all the possible reaction channels (eleastic and inelastic scattering, electron capture into different quantum states, impact ionization).

2. RESULTS ON He^{2+} - H_2O COLLISION

Three experimental techniques of Translational Energy Spectroscopy (TES), Photon Emission Spectroscopy (PES) and Fragment Ion Spectroscopy (FIS) were used to measure state selective electron capture cross sections by He^{2+} ions from H_2O molecules. Those techniques are described in detail in [5]. Each of the three above mentioned techniques has its advantages and drawbacks. All together they are complimentary and form a well comprehensive picture of the charge transfer process. Fig. 1 shows dependence of the cross sections of the electron capture into various states of $He^+(n,l)$ on the energy of the impact.

It is experimentally shown that at low collision energies (less than 500 eV/amu) the following process dominates:

$$He^{2+} + H_2O = He^+(n = 1) + H_2O^{2+} + e^-. \quad (1)$$

At higher collision energies: formation of $He^+(n = 2)$ is the dominant one. A quasi classical theoretical approaches, which treat nuclear motion classically and electrons quantum mechanically, were used here to estimate the cross sections. Our model calculations show that $He^+(n = 2)$ formation proceeds via a single-electron process governed by the nucleus-electron interaction. In contrast, the $He^+(1s)$ formation mechanism involves an exothermic two-electron process driven by the electron-electron interaction, where the potential energy released by the electron capture is used to create H_2O^{2+} with a further fragmentation.

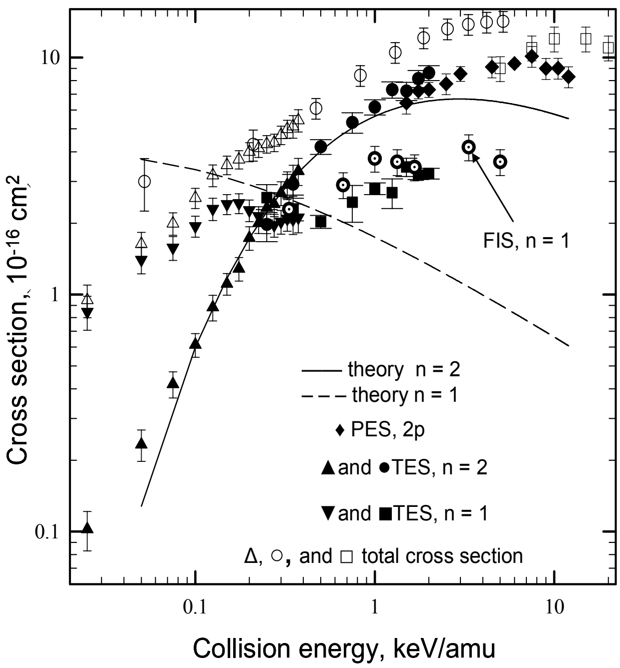

Fig.1. State selective electron capture cross sections measured using 3 independent experimental techniques along with quasi-classical models of Landau-Zener and Demkov

3. RESULTS ON H^+ - H THEORY

According to the basis approach the wave function is formed as a direct product of the wave functions from 3 different subsets:

$$\{\varphi_\sigma(\vec{r})\} = \{\phi_i(\vec{r})\} \oplus \{\phi_j(\vec{r}-\vec{R})\} \oplus \{\varphi_{\vec{k}}(\vec{r})\}, \quad (2)$$

where $\phi_i\left(\vec{r}\right)$ are wave functions of the electron in the H^+ target; $\phi_j\left(\vec{r}-\vec{R}\right)$ electronic wave functions of the atom that captured the electron; and $\varphi_{\vec{k}}(\vec{r})$ orthogonal waves that describe free unbound electron. Then the total wave function of the system is:

$$\Psi\left(\vec{r},\vec{R}\right) = \sum_\sigma F_\sigma\left(\vec{R}\right)\varphi_\sigma\left(\vec{r}\right) = \sum_i \phi_i(\vec{r})F_i(\vec{R}) + \sum_j \phi_j(\vec{r}-\vec{R})F_j(\vec{R}) + \sum_k \varphi_{\vec{k}}(\vec{r})F_k(\vec{R}), \quad (3)$$

where $F_\sigma(\vec{R})$ are the functions that take into account the formation of the bound states in H_2^+ which is an intermediate product. First approximation of $F_\sigma(\vec{R})$ is a harmonic oscillator of the electron in the field of two protons. The wave function of this oscillator was taken as follows:

$$F_0(\vec{R}) = \sqrt{\frac{\sqrt{\pi a}}{3}} \cdot \exp\left\{-\frac{9}{2}\left(\frac{R-R_0}{a}\right)\right\},$$

where a – Bohr radius, R_0 – internuclear distance with a minimum potential energy of H_2^+. Equation (3) contains all the possible reaction channels: first summand – elastic and inelastic scattering without charge exchange; second summand – charge exchange; third summand – impact ionization. The electron capture cross section is as follows:

$$\sigma = 2\pi\int_0^\pi \left|f_j(\theta)\right|^2 \cdot \sin\theta \cdot d\theta, \quad (4)$$

where $f_j(\theta)$ is the amplitude of the matrix element of the effective interaction potential $V^{eff}(R)$, which is the electrostatic potential avaraged on the initial and final state wave functions. $f_j(\theta)$ can be written as follows:

$$f_j(\theta) = -\frac{M}{2\pi\hbar^2}\cdot\left\{\alpha_j^0 - \alpha_j^1 - \alpha_j^2\right\}, \ \textit{where}$$

$$\alpha_j^0 = \int d\vec{R}V^{eff}(\vec{R})\exp\left\{i\left(\vec{k}_0\vec{R}\right) - ik_0\left(\vec{e}\vec{R}\right)\right\},$$

$$\alpha_j^1 = \left\{\int d\vec{R}V^{eff}(\vec{R})F_0^*(\vec{R})\exp\left(i(\vec{k}_0,\vec{R})\right)\right\}F_0^*\left(\vec{k}_0\right),$$

$$\alpha_j^2 = \left\{\int d\vec{R}V^{eff}(\vec{R})F_0^*(\vec{R})\exp\left(-ik_0(\vec{e},\vec{R})\right)\right\}F_0\left(\vec{k}_0\right).$$

The main contribution α_j^0 is proportional to the matrix element of the interaction potential of the incoming proton with the target proton screened by the electron. α_j^1 and α_j^2 are adjustments that take into account formation of bound states in H_2^+. Fig. 2 shows results of the theoretical calculations along with the experimental values. It is shown that theory and experiment are in a good agreement.

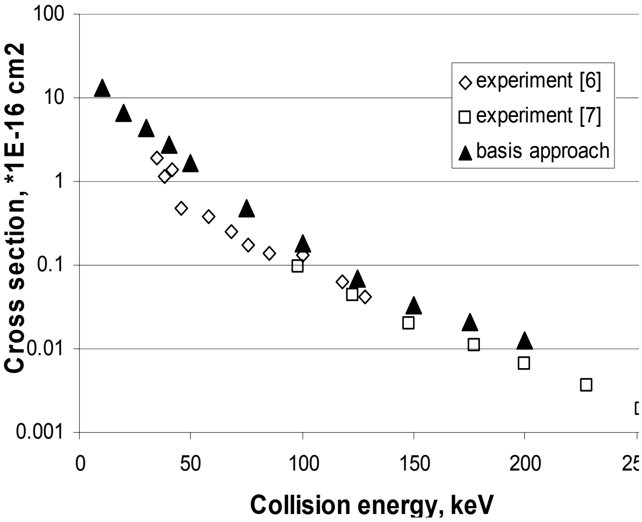

Fig.2. Electron capture cross sections for H^+ + H collision: experiment - capture into H(n,l); theory capture into H(1s)

CONCLUSIONS

TES, PES, and FIS experimental results for He^{2+} – H_2O collision are in a good agreement. Quasi classical theoretical treatment of He^{2+} – H_2O collision showed that He^+(n=2) formation proceeds via a single-electron process governed by the nucleus-electron interaction. In contrast He^+(1s) formation mechanism involves an exothermic two-electron process driven by the electron-electron interaction, where the potential energy released by the electron capture is used to create H_2O^{2+}. In this work we have tested quantum mechanical basis approach for calculating cross section of the electron capture of the following collision: H^+ + H(1s) = H(1s) + H^+. Experiment of [6] show that captures into states other than 1s are negligible so we compared H(1s) theoretical calculations with H(n,l) experimental values. Basis approach has shown a good agreement with the experimental data so it can be used for more complicated collision systems such as: He^{2+} – H_2O collision.

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Article received 22.09.08.

ПРОЦЕССЫ ПЕРЕЗАРЯДКИ ПРИ СТОЛКНОВЕНИЯХ АЛЬФА-ЧАСТИЦ С МОЛЕКУЛАМИ ВОДЫ

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Столкновения многократно заряженных ионов солнечного ветра с нейтральными частицами комет приводят к эмиссиям в рентгеновской и ультрафиолетовой областях [1]. Как было показано ранее [2–4], исходящий спектр перезаряженных ионов может быть использован для тестирования таких свойств солнечного ветра как скорость, концентрация и химический состав. Представлены экспериментальные данные для частичного захвата электрона при столкновениях альфа-частиц с молекулами воды. Для измерений сечений захвата электрона было использовано три независимые и взаимодополняющие методики – трансляционно-энергетической спектроскопии, фотонно-эмиссионной спектроскопии и фрагментарно-ионной спектроскопи [5]. Экспериментальные данные сравниваются с результатами теоретических расчетов. С этой целью нами предложен метод базисного подхода к описанию таких столкновений и показано, что используемый метод хорошо согласуется с экспериментальными данными.

ПРОЦЕСИ ПЕРЕЗАРЯДКИ ПРИ ЗІТКНЕННЯХ АЛЬФА-ЧАСТИНОК З МОЛЕКУЛАМИ ВОДИ

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Зіткнення багаторазово іонізованих зарядів сонячного вітру з нейтральними частинками комет призводять до емісій в рентгенівській і ультрафіолетовій областях [1]. Як було показано раніше [2–4], результуючий спектр перезаряджених іонів може бути використаний для тестування таких властивостей сонячного вітру як швидкість, концентрація частинок та хімічний склад. У роботі представлено експериментальні дані для вибіркового захоплення електрона при зіткненнях альфа-частинок з молекулами води. Для вимірювань поперечних перерізів захоплення електрона було використано три незалежні та взаємодоповнюючі методики – трансляційно-енергетична спектроскопія, фотонно-емісійна спектроскопія та фрагментарно-іонна спектроскопія [5]. Експериментальні дані порівнюються з результатами теоретичних розрахунків. З цією метою нами запропоновано метод базисного підходу до опису таких зіткнень і показано, що теоретичні розрахунки виконані з використанням цього методу добре узгоджуються з експериментальними даними.