Integral cross sections of He^+/He and He_2^+/He interaction systems for optimization of low temperature plasma sources for biomedical uses

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We present interaction potentials, collision cross sections and transport coefficients of both He^+/He and He_2^+/He systems. Elastic and inelastic momentum charge tranfer cross sections are determined from both semi classical and quantum approaches using DIM or ab-initio interaction potentials. The corresponding sets of cross sections are then used in an optimized Monte Carlo code to calculate the ion transport coefficients over a wide range of reduced electric field E/N. Such ion transport data will be used in electro-hydrodynamic and chemical kinetic models of the low temperature plasma jet to quantify and to tune the active species production for a better use in biomedical applications.

The ion transport data (ion mobility and diffusion coefficients) in weakly ionized gases under the action of an external electric field are closely related to the ion–neutral interaction potentials and the corresponding collision cross sections. In this work, the ion transport data are calculated from optimized Monte Carlo simulation [1]. In the case of electrical discharges using helium carrier gas at atmospheric pressure, the diatomic ion He_2^+ which is the most abundant ion can significantly affect the physical and chemical properties of the low temperature plasma jet used in biomedical field [2].

In this work, elastic and inelastic cross sections have been calculated for He^+/He and He_2^+/He interaction systems by using both a semi classical Jeffreys-Wentzel-Kramers-Brillouin (JWKB) [3] and exact quantum methods (EQM), which is a direct numerical integration of the Schrödinger equation without approximation [4]. We used the scattering amplitudes for u *(ungerade)* and g *(gerade)* states and integrate the differential cross section over angles. Assuming distinguishable particles, the integral elastic (Q_{el}) and charge exchange (Q_{CT}) cross sections are obtained as:

$$Q_{el} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left[sin^2\left(\delta_l^g+\delta_l^u\right)+4\,sin^2\left(\delta_l^g\right)sin^2\left(\delta_l^u\right)\right] \tag{1}$$

$$Q_{CT} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)sin^2(\delta_l^g-\delta_l^u) \tag{2}$$

where l and k are respectively the angular momentum and the relative wavevector.
In the He^+/He case, the two helium nuclei are undistinguishable bosons, elastic and charge transfer processes interfere, thus providing a single collision cross-section including both processes.

In the case of JWKB approximation [3], the phase shifts δ_l^g and δ_l^u were obtained respectively with the *gerade* $V^g(r)$ and *ungerade* $V^u(r)$ interaction potentials as the following:

$$\delta_l^{g,u} = \left(l+\frac{1}{2}\right)\frac{\pi}{2} - kr_0^{g,u} + \int_{r_0^{g,u}}^{\infty}\left(\sqrt{k^2-\frac{2\mu V^{g,u}(r)}{\hbar^2}-\frac{(l+\frac{1}{2})^2}{r^2}}-k\right)dr \tag{3}$$

where r is the internuclear distance, μ the reduced mass, $\hbar$ the reduced Planck constant and $r_0^{g,u}$ represents the distance of closest approach for both potentials $V^g(r)$ *and* $V^u(r)$.

The ion–molecule interaction is described by an analytical potential for He^+/He which is adapted to the ab-initio potential given by Gadea [5]. The He_2^+/He interaction system is described by DIM (Diatomic In Molecules) potentials and couplings [6].

The Infinite Order Approximation is made for the He_2^+/He collision [7]. This amounts to freezing the vibrational and rotational motions of the diatomic, and taking into account the anisotropy of the atome-molecule interaction by a simple average over the approach angle.

Figure 1 shows the interaction potential curves for He^+/He interaction system obtained from *ab-initio* calculation [5]. The corresponding elastic and inelastic cross sections are shown in figure 2 while the calculated reduced ion mobility is shown in figure 3 and compared to experimental literature data [9]. Present EQM collision cross sections agree well with computed results from ref. [8].

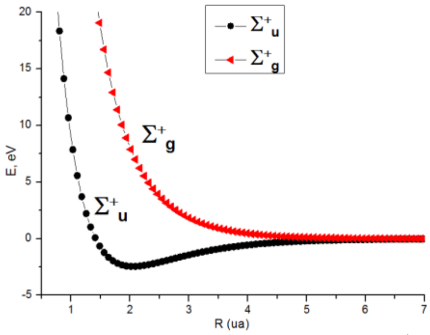

Fig. 1: Interaction potential curves for He^+/He system for the two lowest electronic states Σ_g^+ and Σ_u^+.

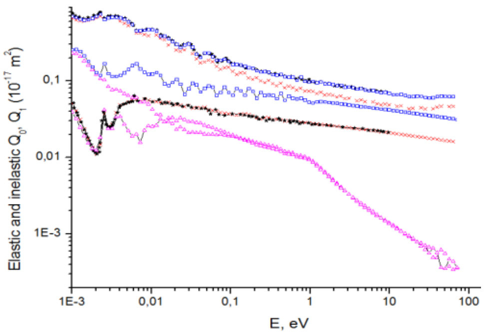

Fig. 2: EQM elastic Q_0 (×) and charge transfer Q_0 (–×–) cross-sections, EQM elastic Q_1 (△) and charge transfer Q_1 (–△–) momentum transfer cross-sections, assuming distinguishable particles. EQM Q_0 (□) and Q_1 (–□–) as well as JWKB elastic Q_0 (★) and charge transfer Q_0 (–★–) [8] or indistinguishable particles.

Figure 4 displays an overview on interaction potentials for He_2^+/He system versus internuclear distance between He and He_2^+ for a fixed distance (equilibrum one) between the two atoms of the diatomic ion, and also versus the angle between He^+-He internuclear axis and the axis between the He_2^+ center of mass and He atom.

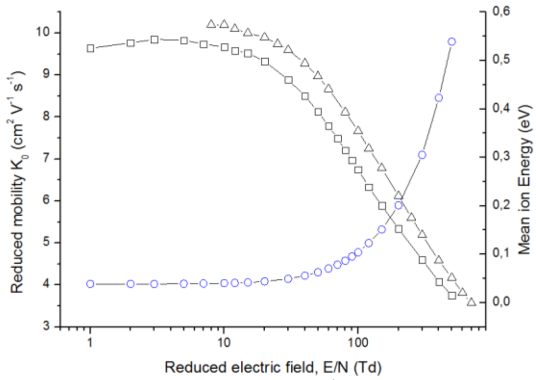

Fig. 3: Reduced ion mobility for He^+/He (-□-) and mean ion energy in the center of mass (-○-), obtained in this work with the Q_1 cross section for indistinguishable particles. These results are compared with the reduced ion mobility from experimental data (-△-) [9].

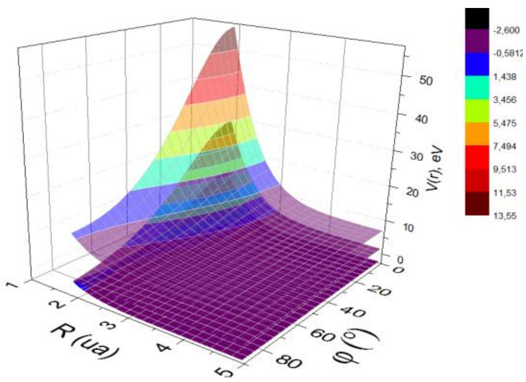

Fig. 4: Interaction potential for He_2^+/He for the three lowest electronic states.

In the case of He+/He system, it is noteworthy the quite good agreement (< 10%, i.e. coherent with the experimental errors) obtained (without any fitting) between experimental mobility data and the calculated one for indistinguishable particles. In the case of He_2^+/He interaction system, the cross-section calculations involve the 3 coupled potential energy surfaces displayed on figure 4. The corresponding He_2^+/He cross-sections and mobility data will be shown during the conference.

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