§8. Theoretical Study of Elementary Collision Processes Related to Vibrationally Excited Molecules: A Case Study of Isotope Effect on Dynamics of a Collinear Collision of He with H_2^+ (v_i)

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In gas divertor plasmas, it is estimated that gas temperature is in the range of several eV and number density of particles is in the order of $10^{21} \sim 10^{22}$ m^{-3}. Hydrogen atoms in these relatively high density regions are easily recombined into molecular form on divertor plates. Newly formed hydrogen molecules can be in rotationally and vibrationally excited states, and are predominantly abundant in number density over any other molecules. Since hydrogen molecules and its molecular ions have no permanent electric dipole moment, radiative lifetime of rotationally and vibrationally excited states is known to be $10^5 \sim 10^6$ s. Hydrogen molecules with different mass combinations are considered to be a heteronuclear molecule having very small permanent electric dipole moment in the order of $10^{-(4 \sim 5)}$D (1 debye(D) = 10^{-18}e.s.u.). Although radiative lifetime of them becomes shorter, it is highly probable that H_2 molecules and its molecular ions in vibrationally excited states collide with other atoms, molecules, or their ions in the divertor chamber.

The Schrödinger equation[1] describing collision processes between an atom and diatomic molecule has been numerically solved with quantum mechanically sufficient accuracy. We have applied our method to a collinear collision of He with $H_2^+(v_i)$ and specifically aimed at investigating chemical reaction and dissociation of the target molecule in this collision system by employing the reliable potential energy surface provided by Joseph and Sathyamurthy. The energy dependence of the dissociation and atom exchange reaction probabilities has been studied at the total energy up to 10 eV, and interesting numerical results have been obtained.[2] The dissociation energy of this collision system is 2.787 eV measured from the lowest minimum of the diatomic well. In this report, the mass of a ^1H atom is 1.008 u (1 u being 1 universal atomic mass unit = one twelfth the mass of a ^{12}C atom) and that of He is 4.003 u as the normal mass, respectively. The normal mass of He is employed throughout this report. In order to investigate isotope effect on dynamics of this collinear He + H_2^+ collision, we have studied He + $HD^+(v_i)(0 \leq v_i \leq 20)$, $HT^+(v_i)(0 \leq v_i \leq 21)$, $DH^+(v_i)(0 \leq v_i \leq 20)$, and $TH^+(v_i)(0 \leq v_i \leq 21)$ collisions at the total energy from 4 to 10 eV by considering all of the vibrational bound states as an initial state. We mention that a collinear collision of A + BC is different from that of A + CB. The former arrangement produces AB as a reaction product, and the latter does AC.

Representative results of isotope effect are briefly mentioned on He + HD^+ collision. The non-reactive vibrational transitions dominate over the atom exchange reaction and dissociation processes for $0 \leq v_i \leq 3$ and $12 \leq v_i \leq 19$ at $4 \leq E_{tot} \leq 10$ eV.

Atom exchange reactions become the major processes for $4 \leq v_i \leq 11$ at the total energy $4 \leq E_{tot} \leq 6$ eV, and the magnitude of these probabilities is about 0.4 - 0.6. The reaction probability appreciably decreases as the increase of the total energy at $4 \leq E_{tot} \leq 6$ eV for $v_i \leq 14$, but becomes almost independent of E_{tot} for $v_i \geq 16$.

The dissociation probability becomes larger as the total energy is increased from 4 to 10 eV, but dissociation in this collision system is more or less suppressed, and the values of these probabilities are less than 0.3 except for the highest vibrational state $v_i = 20$. The internal energy stored in the vibrational mode is effective to enhance the dissociation process for $3 \leq v_i \leq 12$ at $4 \leq E_{tot} \leq 10$ eV. Both the reaction and dissociation probabilities are comparable in magnitude to each other for the vibrational states of $12 \leq v_i \leq 19$ at the total energy of $4 \leq E_{tot} \leq 6$ eV, and are undulatory as a function of E_{tot}.

These results[3,4] are appreciably different from those of the collinear He + $H_2^+(v_i)$ collisions. Different characteristics are observed for this collision system with different mass combinations. Thus, it is important to emphasize that the detailed studies for different isotopes are necessary to understand the present collinear collision dynamics as no simple interpolation or extrapolation seems work.

References

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