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Theoretical study on stereodynamics of H + NeH^+ (v=0, j=0) → NeH^+ +H reaction

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Abstract. The stereodynamics of reaction H + NeH^+ (v=0, j=0) → H + NeH^+ is studied on a new potential energy surface (PES) constructed by Lü *et al.*, using the quasi-classical trajectory (QCT) method. The influence of collision energy for the reaction H + NeH^+ (v=0, j=0) → H + NeH^+ has been studied. The distributions of $P(\theta_r)$, $P(\phi_r)$ and PDDCSs have been calculated at four different collision energies. It can be found that the product rotational angular momentum j' aligned along the y-axis. Moreover, the product rotational angular momentum vector j' is preferentially oriented along the positive direction of y-axis at low collision energy, but preferentially oriented along the negative direction of y-axis at high collision energy. The results indicate the collision energy plays an important part in the stereodynamics of the title reaction.

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Key words: vector correlation; QCT method; polarization; alignment; exchange reaction.

1 Introduction

In order to understand those interesting phenomenons that include the interstellar processes, planetary ionospheres, and electric discharges, the ion-molecules reactions containing rare gas atoms are very necessary to investigate. Therefore, the proton scattering of rare gas atoms had offered a good research object in the past decades. In 1993, Pendergast *et al.* [1] employed the coupled-electron method to establish an accurate potential energy surface (PHHJ3) of the ground state of the NeH_2^+ system. Shortly after, the state-to-state reaction probabilities were reported by Kress *et al.* [2] with an approximate quantum dynamics calculation. Gilibert and co-workers [3-4] applied the coupled-states approximation to calculate the state selected integral cross sections as a function of collision

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energy. In 2008, Mayneris *et al.* [5] calculated the reaction probabilities and cross sections of the Ne + H_2^+/Ne + HD^+/Ne + HT^+ in a wide range of collision energy by using a time dependent real packet quantum method on the PHHJ3 PES. In order to study the influence of vibrational excitation, Mayneris-Perxachs *et al.* [6] applied the time-dependent quantum dynamics method at the centrifugal sudden level (CS-RWP method) to study the reaction probabilities and cross sections of the Ne + H_2^+ (v=0-9, j=0) and D_2^+ (v=0-12, j=0) proton transfer reactions. In 2010, Lü *et al.* [7] constructed the ground state ($1^2A'$) analytical potential energy surface (LZHH PES) that was fitted using 7000 energy points. Based on the LZHH PES, some theoretical researches about the reaction Ne + $H_2^+ \rightarrow H_2^+$ + Ne have been done. In 2011, Xiao *et al.* [8-10] investigated the isotopic effects and influences of the collision energies to vector correlations between reagents and products by using quasi-classical trajectory (QCT) method. Wang *et al.* [11] investigated dynamics of Ne + H_2^+ by QCT method, which reagent molecules are in different collision energy or vibrational States. The results showed that the reagent vibrational excitation had greater influence on the polarization of the product rotational angular momentum vectors j' than the collision energy. Ge *et al.* [12] calculated the dynamics of the Ne+H_2^+ using QCT method, which indicated that the reaction is dominated by forward-scattering and the NeH^+ product showed rotationally hot and vibrationally cold distributions. The product polarizations in the reactions H + NeH^+/NeD^+/NeT^+ $\rightarrow$ H_2^+/HD^+/HT^+ + Ne were studied by Zou *et al.* [13] using the QCT method. Moreover, the effects of the potential well on stereodynamics of the above reactions were discussed in their work. Yin *et al.* [14, 15] investigated the effects of collision energy, vibrational and rotational excitation of reagent molecules on the dynamic of the H + NeH^+ by QCT method. The results demonstrated that the title reaction was a typical barrierless atom (ion)–ion (molecule) reaction and was mainly dominated by the direct reaction mechanism.

From the above, most of the studies have focused on the reaction Ne + H_2^+, its reverse reaction H + NeH^+ and those isotopic effects. However, the exchange reaction H + NeH^+ $\rightarrow$ NeH^+ + H has seldom been studied to date. We will adopt a QCT calculation on the new LZHH PES in this paper to shed more light on this exchange reaction.

2 Theory

The standard quasiclassical trajectory (QCT) method is employed to investigate the stereodynamics of the title reaction in this paper. Details of the QCT method can be found in Refs [19-22], and only the most important details are described here.

2.1 QCT calculation

The classical Hamilton's equations are integrated in three dimensions numerically. Four collision energies (20, 40, 60, 80 kcal/mol) were chosen for the title reaction. The rotational and vibrational levels of NeH^+ were taken as j=0 and v=0, respectively. Batches of