Stereodynamics of the Ca+HCl-CaCl+H reaction imposed by the reagent rotational-excited states

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Abstract

The influences of the initial states of HCl on the stereodynamics properties of the Ca+HCl reaction are investigated by utilizing the method based on the quasi-classical trajectory (QCT) theory and the analytical potential energy surface (APES). The orientation and alignment behaviors for the rotational angular momentum of the product, along with the generalized differential cross-section (PDDCS) dependent polarization, are employed to explore the stereodynamics properties. The initial rotational states of the HCl molecule impose a remarkable affection on the vector correlation distributions, regardless of the orientation, alignment, or PDDCS. The obvious forward or backward scattering, as well as the weak sideway scattering phenomena, are found for the different initial rotational states of the HCl molecule. The initial higher rotational-excited state of j=3 results in more obvious stereodynamics effects.

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