

# Effects of reagent rotational excitation on the stereodynamics of the Ca+HCl-CaCl+H reaction

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## Abstract

The effects of HCl rotational excited states on the stereodynamics of the Ca+HCl reaction are explored based on quasi-classical trajectory (QCT) theory with potential energy surface (PES) [Verbockhave et al., J. Chem. Phys. 2005,122,204307]. Vibrational level  $v=0$  and rotational level  $j=0-3$  are considered. The polarization-dependent generalized differential cross sections (PDDCSs) and alignments of the product rotational angular momentum are used to demonstrate the stereodynamics effects. The rotational quantum number has a considerable influence on the distribution of vector correlation, including alignment, orientation, and PDDCSs. The product molecules are strongly forward and backward scattering and weakly sideways scattering because the reactant molecule HCl is in the rotational ground state and the lower rotational excited states. Strongly forward scattering is observed while the reactant is in high rotational excited states.

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