

COMMUNICATION

Effects of the reagent vibrational excitation on the stereodynamics of the reaction $C(^3P)+CH(X^2\Pi)\rightarrow C_2+H$

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Abstract: Based on the $1^2A''$ global three-dimensional adiabatic potential energy surface [Boggio- Pasqua et al., Phys Chem. Chem. Phys 2:1693 2000], a theoretical study of the stereodynamics of the reaction $C(^3P) + CH(X^2\Pi)(v = 0 - 6, j = 0)$ has been performed using the quasi-classical trajectories (QCT) method. The cross sections as a function of the reagent vibrational quantum number are presented. The differential cross sections (DCSs) and the distributions of $P(\theta_r)$, $P(\phi_r)$ at the selected collision energy of 0.3eV are discussed in detail. Through the study of reaction trajectories, the change of reaction mechanism is revealed. The product rotational alignment parameter $\langle P_2(j \cdot k) \rangle$ are also obtained as a function of the reagent vibrational quantum number. The calculated results show that the reagent vibrational excitation plays an important role in the title reaction.

AMS subject classifications: 81U10, 81V45

Keywords: Stereodynamics; QCT method; Vibration excitation; Rotational alignment; Reaction mechanism

The ethanol radical C_2H is one of the most abundant polyatomic species in carbon-rich stars and interstellar clouds [1, 2]. C_2H is believed to be the major source of C_2 in comets and interstellar media [3-6]. It is also the simplest organic triatomic molecule involving a triple $C \equiv C$ bond and has a low-lying electronic state. Moreover, C_2H plays an important role in the formation and the destruction of carbon chain molecules C_2H_n (with $n=2-6$) [7]. The C_2H radical is not only the product of some reactions like $C_2 + CH_4$ [8], $H_2 + CH_4$ [9] and the photo dissociation of acetylene [10], but also an important intermediate species of numerous

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combustion reactions [3, 11].

More recently, Boggio-Pasqua and co-workers [2] build an analytical representation of the three lowest adiabatic potential energy surfaces which correspond to the states $X^2\Sigma^+$ and $A^2\Pi$ of C_2H [11,12]. These three surfaces belong to the $2^2A'$ or $2^2A''$ symmetry species [2, 11, 12]. In 2001, Tang et al. calculated the dynamics of the title reaction by using a quantum time-dependent wave packet method on the $1^2A'$ and $2^2A'$ surface [2, 11]. In 2010, Yang et al. studied the effect of initial rotational quantum number on the $1^2A'$ surface [13]. As far as we know, the most theoretical studies are based on the $1^2A'$ and $2^2A'$ PES and the calculated results conform the accuracy of these PES [11-18]. However, there are only three reports on properties of its vector properties about this reaction on $1^2A''$ PES [19-21]. Zhang et al. found the cross sections and the value of $\langle P_2(j',k) \rangle$ of the title reaction decrease with the increase of collision energy [19]. Liu et al. reported the product C_2 is mainly backward-forward scattering and the orientation of the product rotational angular momentum tends to point to the negative direction of the y -axis at $E_{col}=0.1eV$ on the $1^2A''$ PES [20]. Wu et al. discovered that the title reaction performed a preference of forward scattering and a weak of product rotation alignment considering isotopic effect of CH [21]. To shed more light on the dynamics of this reaction, we apply the QCT method [22-26] to study the effects of reagent vibrational excitation on the stereodynamics of the $C(^3P) + CH(X^2\Pi)(v = 0 - 6, j = 0) \rightarrow C_2 + H$ reaction based on the $1^2A''$ PES [2].

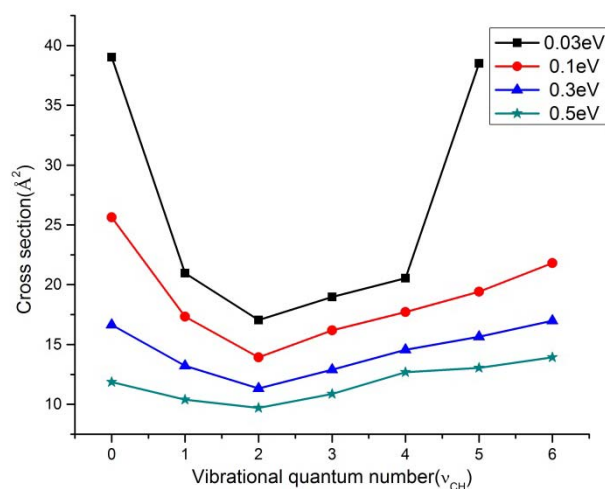


Figure 1: Total reaction cross section for $C(^3P) + CH(X^2\Pi)(v = 0 - 6, j = 0) \rightarrow C_2 + H$ as a function of v at different collision energies.

Figure 1 shows the influence of the initial reagent vibrational excitation on the reaction cross sections for $C(^3P) + CH(X^2\Pi)(v = 0 - 6, j = 0)$ at the relative collision energies $E_{col} =$