

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

Jia Liu, Meishan Wang*, Aihua Gao, Chuanlu Yang, Xiaolin Sui, and Zhenhua Gao

School of Physics and Optoelectronics Engineering, Ludong University, Yantai 264025, China

Received 2 April 2015; Accepted (in revised version) 16 May 2015
Published Online 6 June 2015

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 $C(^3P)+CH(X^2\Pi)$ ($v=0; j=0-6$) has been performed using the quasi-classical trajectories(QCT) method. The cross sections are calculated. The differential cross sections (DCSs) and the distributions of $P(\theta_r)$, $P(\phi_r)$ are presented in detail at the selected collision energy of 0.3 eV. The product rotational alignment parameter $\langle P_2(j' \cdot k) \rangle$ are also obtained as a function of the reagent rotational quantum number. The results show that the reagent rotational excitation plays an important role in the title reaction.

PACS: 02.70.Ns, 36.20.Kd, 31.50.Df

Key words: stereodynamics; QCT method; rotation excitation; rotational alignment; reaction mechanism.

1 Introduction

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's an important intermediate species of numerous combustion reactions [6,7]. It is also the simplest organic triatomic molecule involving a triple $C\equiv C$ bond and has a low-lying electronic state. What's more, C_2H plays an important role in the formation and the destruction of carbon chain molecules C_2H_n (with $n=2-6$)[8]. To shed more light on the details of the formation and destruction of C_2H , it is essential to study the relevant property of the molecular reaction dynamics.

*Corresponding author. *Email address:* mswang1971@163.com (M.-S. Wang)

In experiments, the researchers have done many spectroscopic studies of C_2H and its isotopic species using a variety of techniques, including Laser Magnetic Resonance (LMR) [9, 10], microwave and millimeter-wave spectroscopy [11-13], color center laser spectroscopy [14-16] and Fourier Transform Infrared Spectroscopy (FTIR) [17]. Meanwhile, these experimental studies have been accompanied by the extensive theoretical work and promoted the development of the understanding of the spectroscopy of C_2H [18-20]. However, the experimental work concerning the dynamics of the title reaction is very sparse. To our knowledge, only three estimated values of the rate constant can be found in the literature and databases [22-24]. Theoretically, a series of high-level *ab initio* studies of the X and A state of CCH by Peyerimhoff and co-workers have shown that two A' surface intersect at the C-C distance are near 2.5 bohrs [25, 26]. More recently, Boggio-Pasqua and co-workers [1] 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 . These three surfaces belong to the $^2A'$ or $^2A''$ symmetry species [1, 6, 27]. 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 [6, 27]. In 2010, Yang *et al.* studied the effect of initial rotational quantum number on the $1^2A'$ surface [28]. However, there are only four report on properties of its vector properties about this reaction on $1^2A''$ PES [29-32]. Zhang *et al.* found the cross sections and the value of $\langle P_2(j' \cdot k) \rangle$ of the title reaction decrease with the increase of collision energy [29]. 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 [30]. 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 [31]. Recently, Our team studied the effect of reagent vibrational excitation for this title reaction and it increased the total reaction probability and enhanced the forward scattering [32].

To gain more insight into the detailed dynamics of the title reactions, we have carried out quasiclassical trajectory for the $C(^3P)+CH(X^2\Pi)(v=0, j=0-6)\rightarrow C_2+H$ reaction at 0.3 eV based on the $1^2A''$ PES [1]. The paper is organized as follows: Section 2 provides a brief review of the theoretical methodologies. Section 3 discusses the results. Finally, the main conclusions are presented in Section 4.

2 Theory

2.1 Vector correlations

Fig. 1 illustrates the CM reference frame used in the present investigation. The reagent initial relative velocity vector k is parallel to the z-axis of the CM frame. The scattering plane (x-z plane) contains k and relative velocity vector k' of final product. The scattering angle θ_t is the angle between k and k' . θ_r and ϕ_r are the polar and azimuthal angles of the final rotational angular momentum j' , respectively.