

The effects of collision energy and isotope on stereodynamics for the reactions $O^+ + H_2/D_2/T_2$

Yanjie Wang, Xinguo Liu*, Hongzheng Li, Qi Li, Jiawu Chen, and Qinggang Zhang

School of Physics and Electronics, Shandong Normal University, Jinan 250014, the People's Republic of China

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Abstract. The vector correlations between products and reagents for the chemical reactions $O^+ + H_2/D_2/T_2$ at different collision energies (1.0eV-2.8eV) have been studied by means of the quasi-classical trajectory (QCT) method based on the RODRIGO potential energy surface(PES) [Rodrigo *et al* 2004]. *Chem. Phys.* 120 4705]. The four generalized polarization-dependent differential cross-sections (PDCCSs) $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$, $(2\pi/\sigma)(d\sigma_{20}/d\omega_t)$, $(2\pi/\sigma)(d\sigma_{22+}/d\omega_t)$ and $(2\pi/\sigma)(d\sigma_{21-}/d\omega_t)$ have also been calculated at seven different collision energies respectively. The isotope effect comparing with the effect of collision energies has been discussed further. The results indicate that the reaction is sensitive to the mass factors. Meanwhile the collision energies have a greater effect than the mass factors.

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Key words: Stereodynamics; Vector correlation; Quasi-classical trajectory method; Polarization-dependent differential cross-section; Isotope effect.

1 Introduction

The ion-molecule reaction has been of great importance recently [1-10]. The $O^+ + H_2$ reaction has played a great role in the development of ion-molecule reaction dynamics [1-5]. It has attracted extensive attention both experimentally and theoretically. The hydrogen atom transfer reaction $O^+ + H_2$ has served as a prototypic example for the study of the kinetics and dynamics of moderately exothermic ion-molecule systems. What's more interesting is that it presents a well for collinear OHH arrangements. It also plays an important role in interstellar chemistry and in the Earth's ionosphere [1-2, 6-8].

*Corresponding author. *Email address:* liuxinguo@sdsu.edu.cn (X.-G. Liu)

The most accurate PES for $O^+ + H_2$ reaction is constructed by Rodrigo *et al.* in 2004. Following, there are many theoretical and experimental works for the $O^+ + H_2$ reaction. For example, Rodrigo *et al.* reported rate constants and cross sections based on this PES using the quasi-classical trajectory method. Then he studied the reaction and its isotopic variants using the time dependent wave packet method [3]. Moreover, rate constant, cross section and angle-velocity distribution have also been studied experimentally. Experimental studies about the $O^+ + H_2$ reaction show that electronically nonadiabatic processes are only important at high relative translational energies [4, 5].

As is known, the vector properties of a chemical reaction can provide valuable information about stereodynamics of chemical reaction, so it is very important to study a reaction's vector properties. However, most studies in former work deal substantially with the scalar properties, which leads to much useful information missed. In order to get full information of the ion-molecule reaction, the scalar and vector properties should be considered together [11-19]. As far as we know, there are already some investigations about the $O^+ + H_2$ reaction and its isotopic variants, yet most of which are about their scalar characters, such as rate constant, cross section, reaction probability, etc. In order to obtain more information of this system, especially its vector characters and the effect of comparing the mass factors with collision energies, the title reactions are chosen for this paper.

2 Quasi-classical trajectory calculations

In our calculations, the RODRIGO PES [3] has been employed. The collision energy is chosen from 1.0 eV to 2.8 eV (the step is 0.3 eV) for the three title reactions. The vibrational and rotational numbers of the reactants molecule are all chosen as $v=0, j=0$. In the calculation method of QCT we use here is the same as that of references [20-22]. The initial azimuthal orientation angle and polar angle of the reagent molecule inter-nuclear axis are randomly sampled using Monte Carlo method, and the range of the angle θ_r and ϕ_r is from 0° to 180° and from 0° to 360° , respectively. In the calculation, batches of 20000 trajectories are run for each reaction and the integration step size is chosen as 0.1 fs which can leads to good results.

3 Results and discussion

The four commonly polarization-dependent differential cross-sections (PDDCSs) $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$, $(2\pi/\sigma)(d\sigma_{20}/d\omega_t)$, $(2\pi/\sigma)(d\sigma_{22+}/d\omega_t)$ and $(2\pi/\sigma)(d\sigma_{21-}/d\omega_t)$ as a func-

Table 1: The mass factor $\cos^2\beta$ calculated for different isotopic variants H_2 , D_2 and T_2 .

Reaction system	$O^+ + H_2$	$O^+ + D_2$	$O^+ + T_2$
$\cos^2\beta$	0.4704	0.4441	0.4206