Effects of reagent's rotational and vibrational excitations on reaction $O(^3P) + H_2(\nu = 0, 3,\ j = 0, 3, 5, 7, 9, 12, 15) \rightarrow OH + H^*$

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To investigate the effect of reagent's rotational and vibrational excitations on the stereo-dynamics of reaction product, the title reaction is theoretically simulated using the quasi-classical trajectory (QCT) method on the $^3A''$ and $^3A'$ potential energy surfaces (PESs). The reaction cross section is considered as the only scalar property in this work at four different collision energies. Furthermore the vector properties including two polarization-dependent differential cross sections (PDDCSs), the angular distributions of product' rotational momentum are discussed at one fixed collision energy. Effects of reagents' rotational excitation on the reaction do exist regularly.

Keywords: chemical stereo-dynamics, quasi-classical trajectory calculation, vector correlation, rotational and vibrational excitations

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1. Introduction

In the past few decades, the three-atom reaction system A+BC[1−38] has been investigated worldwide both theoretically and experimentally in that it is one of the most fundamental chemical reactions. Especially with the development of the experimental and computer technologies, it is possible to obtain the vector properties of reactions of this type. The research results become more comprehensive owing to the combination of the scalar and vector properties. Vector properties, such as velocity and angular momentum, possess not only magnitudes that can be directly related to translational and rotational energies but also well defined directions.[1] At the end of last century, the chemical reactions of three-atom system with different reagent mass combinations on attractive, repulsive, and mixed potential energy surfaces (PESs), have been carefully investigated by Han and co-workers[1−3] with the purpose of studying the dependence of product's rotational alignment on collision energy. Currently, Wu[4] studied the reaction $H + FCl\,(\nu = 0, 1, \ldots, 5,\ j = 0, 3, 6, 9) \rightarrow HF + Cl$ and investigated the effect of collision energy on the integral cross section of reaction product as well as the effects of initial reagent's rotational and vibrational excitations on the product stereo-dynamics of the reaction using the QCT method on the ground potential energy surface of $1\ ^2A'$.

The reaction $O + H_2 \rightarrow OH + H$ together with its isotope reactions is one of the most important three-atom-system reactions and has been widely investigated both theoretically and experimentally during the past decades.[4−19,21−25] The quantum mechanical method and the quasi-classical trajectory (QCT) method are fundamental methods that are applied to study this reaction. In 2006, Martínez and his co-workers[5] investigated the ion-molecule reaction $O^+ + H_2(\nu = 0, j = 0) \rightarrow OH^+ + H$ using the close-coupling hyperspherical (CCH) quantum method and made a comparison with the results of QCT calculation. A very good accordance between both methods was obtained for the OH^+ vibrational distribution, and so were the OH^+ rotational distributions. They also found that the $\boldsymbol{k}$–$\boldsymbol{k}'$ angular distributions except the peak heights resulting from the two methods are the same, and the CCH integral cross sec-

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tion decreases with the collision energy E_T. Although the QCT results were generally similar to the CCH ones, they observed a significant deviation from the CCH data within the collision energy range of 0.2–0.6 eV, where the QCT method could not describe correctly the reaction probability, i.e., describe quantum-mechanical effects. However, these effects were proved to play a comparatively small role in the overall dynamics and kinetics of chemical reaction.[6] In recent years theoretical studies on the stereo-dynamics of the reaction $O + H_2 \rightarrow OH + H$ on different potential energy surfaces have attracted much interest.[19,21−25] In 2009, Chen *et al.*[19] studied the reaction $O(^1D) + H_2(\nu = 0, 1, 2, 3,\ j = 0)$ using the QCT method on the Dobbyn–Knowles (DK) PES. The obtained vector-correlation information demonstrated that the product alignment is sensitive to the reactant's vibrational quantum number v at the collision energy of 19 kcal/mol. By increasing the value of v backward scattering becomes weaker while forward scattering becomes stronger. In 2010, using Rogers *et al.*'s $^3A''$ PES[20] Wu[21] reported the stereo-dynamical behaviors in the reaction $O(^3P) + H_2 \rightarrow OH + H$ at the collision energies of 0.5, 0.75, and 1.0 eV via discussing the angular distributions (i.e., $P(\theta_r)$, $P(\phi_r)$, and $P(\theta_r, \phi_r)$) and PDDCSs. In the same year, Wei *et al.*[22] studied the stereo-dynamics of the $O(^3P) + H_2(\nu = 0, 1, 2, j = 0) \rightarrow OH + H$ reaction via the QCT method at the collision energy of 34.6 kcal/mol on BMS1 PES for the lowest $^3A''$ state. The results of cross section agree well with the quantum calculation. Their results also indicated that the vector properties are sensitively affected by vibrational excitation. Liu *et al*[23] investigated the PES of ground state $^3A''$ in the reaction $O(^3P) + H_2(\nu = 0, j = 0, 1, \ldots, 9)$ by the QCT method. They studied both scalar properties and vector properties. Especially they studied effects of the reagent rotational excitation on the reaction at the collision energy of 25 kcal/mol and found both scalar and vector properties are sensitive to the reagent rotational excitation.

In this work, we focus our main attention on the stereo-dynamics of the reaction $O(^3P) + H_2(\nu = 0, 3, j = 0, 3, 5, 7, 9, 12, 15) \rightarrow OH + H$ adopting the QCT method. We also compare our results about the $^3A'$ PES with those of Rogers *et al.*[20] Products' scalar and vector properties such as reaction cross section, product alignment and orientation, scattering directions and the polarization-dependent differential cross sections (PDDCSs) are presented. Meanwhile, effects of the vibrational and rotational excitations on these properties are discussed in detail.

2. Theoretical methods

2.1. Products rotational polarization

The center-of-mass (CM) reference frame[21−25] is used to describe the distributions of the vectors $\boldsymbol{k}$, $\boldsymbol{k}'$ and $\boldsymbol{j}'$. The reagent's initial relative velocity vector $\boldsymbol{k}$ is parallel to the z axis. The y axis is perpendicular to the x–z plane which contains the initial velocity vector $\boldsymbol{k}$ and final product's relative velocity vector $\boldsymbol{k}'$. The θ_t is the angle between $\boldsymbol{k}$ and $\boldsymbol{k}'$ (called scattering angle). The ϕ_r and θ_r are the polar and azimuthal angles of the final rotational angular momentum $\boldsymbol{j}'$. The PDDCSs are used to describe the fully correlated angular distributions of $\boldsymbol{k}$, $\boldsymbol{k}'$, and $\boldsymbol{j}'$ in the CM frame.

The fully correlated angular distribution can be written as[1,3,11]

$$P(\omega_t, \omega_r) = \sum_{kq} \frac{[k]}{4\pi} \frac{1}{\sigma} \frac{d\sigma_{kq}}{d\omega_t} C_{kq}(\theta_r, \phi_r)^*, \qquad (1)$$

where $[k] = 2k + 1$, $\sigma^{-1} d\sigma_{kq}/d\omega_t$ is a generalized polarization dependent differential cross section, and $C_{kq}(\theta_r, \phi_r)$ is the modified spherical harmonics. In this work, we only calculate four PDDCSs: $(2\pi\sigma^{-1})d\sigma_{00}/d\omega_t$, $(2\pi\sigma^{-1})d\sigma_{20}/d\omega_t$, $(2\pi\sigma^{-1})d\sigma_{22+}/d\omega_t$, and $(2\pi\sigma^{-1})d\sigma_{21-}/d\omega_t$, which are denoted as $P_{00}(\omega_t)$, $P_{20}(\omega_t)$, $P_{22+}(\omega_t)$, and $P_{21-}(\omega_t)$.

The dihedral angle distribution function $P(\phi_r)$ describing $\boldsymbol{k}'$–$\boldsymbol{k}$–$\boldsymbol{j}'$ correlation can be expanded in terms of Fourier series as[1−3,11]

$$P(\phi_r) = \frac{1}{2\pi}\left(1 + \sum_{n=2m} a_n \cos n\phi_r + \sum_{n=2m-1} b_n \sin n\phi_r\right), \quad m = 1, 2, \ldots \qquad (2)$$

The distribution function $P(\theta_r)$ describing $\boldsymbol{kj}'$ correlation can be expanded into a series of Legendre polynomials as[1−3,11]

$$P(\theta_r) = \frac{1}{2} \sum_k (2k + 1) a_0^{(k)} P_k(\cos\theta_r). \qquad (3)$$

Generally, θ_r and ϕ_r are used to define the direction of $\boldsymbol{j}'$, and the distribution of product rotational momentum $P(\theta_r, \phi_r)$ can be expanded as

follows:[1−3,11]

$$P(\theta_{\rm r},\phi_{\rm r}) = \frac{1}{4\pi}\sum_{kq}[k]a_q^k C_{kq}(\theta_{\rm r},\phi_{\rm r})^* = \frac{1}{4\pi}\sum_k\sum_{q\geq 0}[a_{q\pm}^k\cos q\phi_{\rm r} - {\rm i}a_{q\mp}^k\sin q\phi_{\rm r}]C_{kq}(\theta_{\rm r},0). \quad (4)$$

The details of the product rotational polarization theory are already discussed in our previous work.[21−25]

2.2. Potential energy surfaces and quasi-classical trajectory calculations

The PES adopted in this work is the Rogers *et al.*'s PES of $^3{\rm A}''$ state,[20] which has a saddle point. It is one of the two triplet states which were generated from *ab initio* configuration interaction calculation, and its properties can be found in Refs. [24] and [25]. Details of the QCT method can be also found in Refs. [24] and [25]. The collision energies are 17.5, 20.0, 22.5, and 25.0 kcal/mol. The reagent's vibrational quantum number v is set to be 0 and 3, and the rotational quantum number j is set to be 0, 3, 5, 7, 9, 12, and 15. A group of 10000 trajectories are run for each collision energy and the integration step is chosen to be 0.1 fs. We adopted the same method used by Cao *et al.*[26] and Wang *et al.*[27] to determine the optimization of the impact parameter $b_{\rm max}$. The basic steps of the method are given as follows: first, to calculate a small amount of trajectories at some fixed values of b, and systematically change the value of b until no reactive trajectories are obtained; then, use the obtained values of b as the initial values in calculating a large amount of trajectories; finally, to adjust the values of b several times with a small amount of trajectories, we can obtain $b_{\rm max}$ that ensures the convergence of the present QCT calculations. Moreover, Cao *et al.*[26] have studied both the $H + SiH_4$ abstraction and exchange reactions on the accurate global 12-dimensional *ab initio* PES. They investigated the excitation functions and product angular distributions in detail at various collision energies and provided insights into the underlying reaction mechanism. Wang *et al.*[27] have investigated the reaction $SiH_4 + H \rightarrow SiH_3 + H_2$ on the 12-dimensional *ab initio* Wang–Sun–Bian surface. In their work, various dynamical quantities are obtained and reaction mechanisms are analyzed. Both calculations adopted the QCT method and considered the quantum-mechanical zero-point energy (ZPE) with a non-active method, which follows the genuine QCT approach but discards all of the reactive trajectories that fulfill one of the following conditions: (i) the initial total energy is lower than the sum of the classical energy and harmonic ZPE of the saddle point; (ii) the vibrational energy of the products is lower than the sum of their ZPEs.[26,27] In our present study, we also take ZPE correction into account in the QCT calculation.

3. Results and discussion

The cross section as a function of the reagent's rotational quantum number is shown in Fig. 1, where four collision energies of 17.5, 20.0, 22.5, and 25.0 kcal/mol and two vibrational quantum numbers are considered in order to investigate the effect of the rotational excitation on the cross section. For $v = 0$, as shown in Fig. 1(a), the cross section increases monotonically with increasing rotational quantum number, which indicates that the effect of the collision energy on the cross section is regular. The curve at the collision energy of 25.0 kcal/mol is in good agreement with the result of Liu *et al.*[23] who used 50000 trajectories. These phenomena reveal that the reagent's rotational excitation has a positive influence on the cross section, and indirectly reflect that for the same value of rotational quantum number the collision energy plays an increasing role on the cross section. At a higher value of rotational quantum number the values of the cross section at different collision energies are close to each other, which means that at high values of rotational quantum number the effect of the collision energy on the cross section becomes weak. In Fig. 1(b), the reagent's vibrational quantum number is chosen to be 3. From this figure, similar conclusion can be obtained that the reagent's rotational excitation has a positive effect on the cross section. It is noteworthy that in Fig. 1(a) the initial value is 0.8, while in Fig. 1(b) the initial value is 6.5. Furthermore, the cross section on the $^3{\rm A}'$ PES is plotted in Figs. 1(c) and 1(d), which is similar to that on the $^3{\rm A}''$ PES because the way in which the cross section on the $^3{\rm A}'$ PES changes with increasing vibrational quantum number does not show any difference with that for $^3{\rm A}''$ PES. Thus, the features of these two PESs almost do not affect the relation between the cross section and the vibrational quantum number. The reason for all the above results could be that at the high value of rotational quantum number the ratio of the reaction $O + H_2 \rightarrow O + H + H$ becomes higher, leading to the

reduction of the cross section with the increase of the collision energy. This means that for a large rotational quantum number, the effect of the collision energy on the cross section becomes weak. Furthermore the vibrational excitation also has a positive effect on the cross section In addition we make an error analysis on the effect of the random seed on the cross section. For each couple of collision energy, rotational quantum number and vibrational quantum number, we run 10000 trajectories at 10 different random seeds and the average number and standard deviation are obtained. The ratio of the standard deviation and average number is less than 1.5%. Thus, the error bar does not appear in Fig. 1 as the error is small.

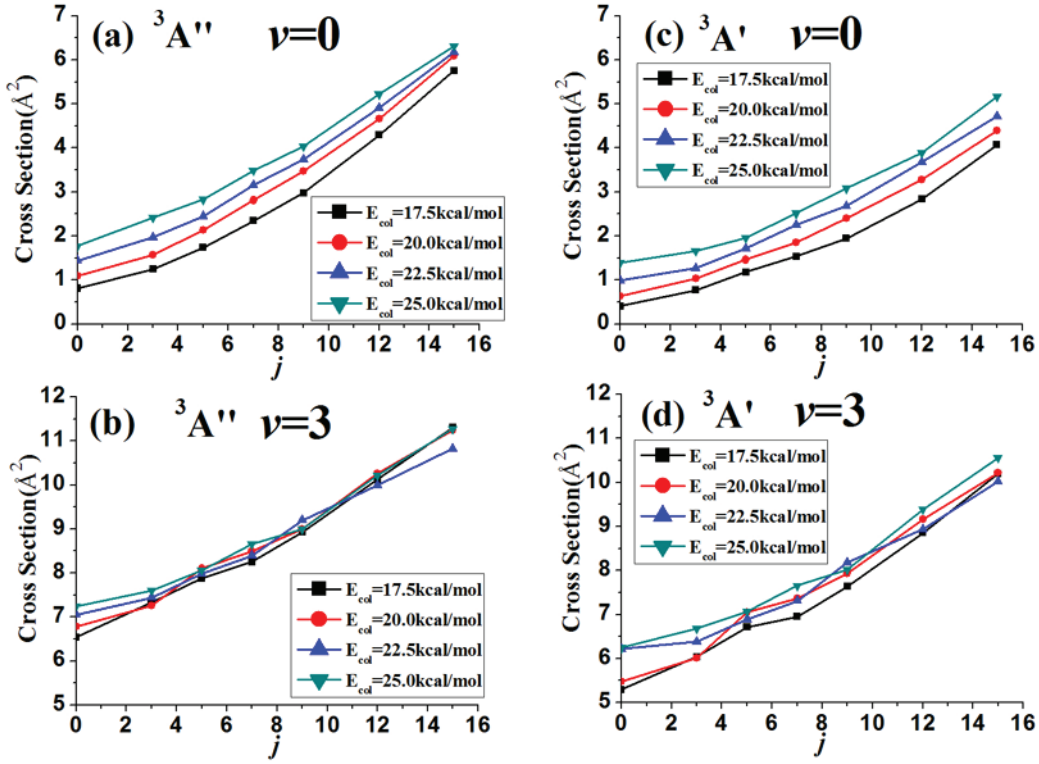


Fig. 1. (colour online) Cross section for the title reaction at four collision energies ($E_{\rm col}$) as a function of j For ^{3}A$''$ PES: (a) $v = 0$; (b) $v = 3$. For ^{3}A$'$ PES: (c) $v = 0$; (d) $v = 3$.

Figure 2 shows the $P(\theta_{\rm r})$ distributions which describe the correlation between the $\boldsymbol{k}$–$\boldsymbol{j}'$ vectors. Though at different vibrational quantum numbers and rotational quantum numbers, all peaks of $P(\theta_{\rm r})$ distributions are at $\theta_{\rm r} = 90°$ and well symmetric with respect to $\theta_{\rm r} = 90°$ which indicates that the product rotational angular momentum $\boldsymbol{j}'$ strongly aligns in the direction perpendicular to the reagent's initial relative velocity vector $\boldsymbol{k}$. As shown clearly in the figure, the conclusion is very easy to acquire owing to evident and regular results. Firstly, the peaks get much lower and wider with the increase of reagent's rotational quantum number. Though at different collision energies, the result of the distribution in this work agrees well with that of Liu *et al.*[23] Secondly, the height changes of the peaks are greater at small values of rotational quantum number especially at $j = 0$, 3, 5. These phenomena reveal that the alignment of the product rotational angular momentum $\boldsymbol{j}'$ becomes weaker and weaker with the increase of rotational quantum number and the effect is stronger at small rotational quantum number. It is abnormal that, at $j = 0$, the distribution oscillates at the angles which do not correspond to the peaks, but does not oscillate at other values of rotational quantum number. In addition, as shown in Fig. 2(a), there exists the interchange of the peaks between adjacent values of rotational quantum number. Therefore, the rotational excitation has a negative effect on the alignment of the product rotational angular momentum $\boldsymbol{j}'$. In Figs. 2(c) and 2(d), the $P(\theta_{\rm r})$ distributions on the ^{3}A$'$ PES are also provided. Through comparing these results on the two PESs, not much

difference can be found. In addition the effect of the vibrational quantum number on the distribution on the $^3A'$ PES is almost the same as that on the $^3A''$ PES since they both have similar trend with the increase of quantum vibrational number.

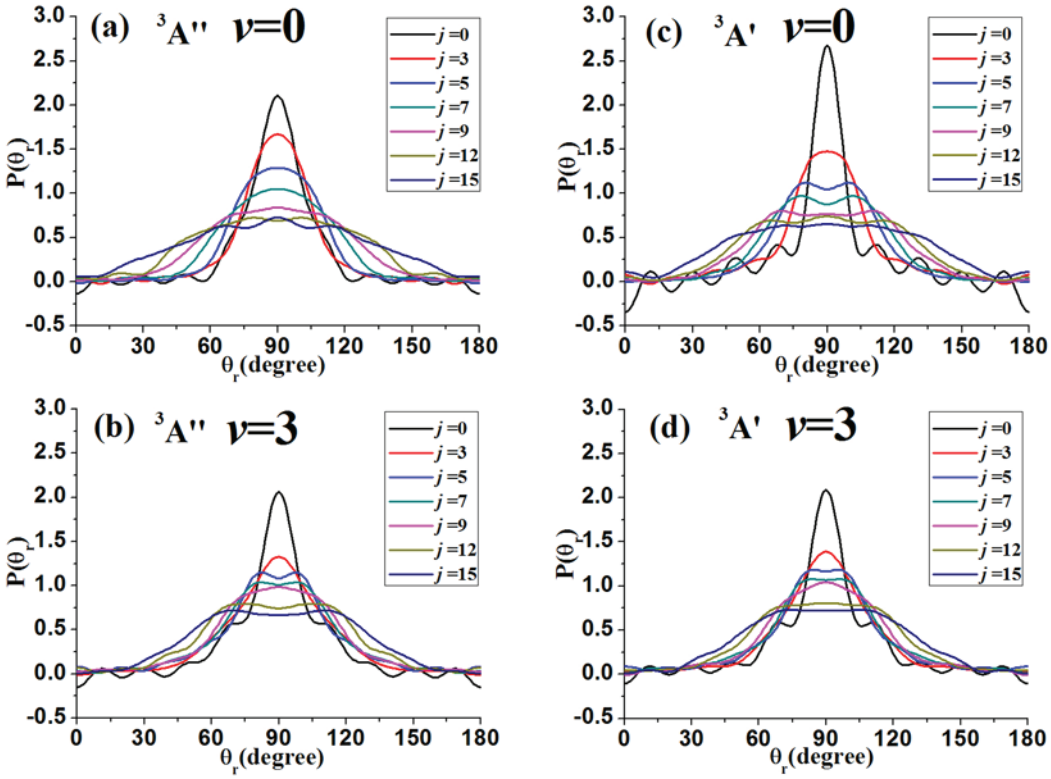


Fig. 2. (colour online) $P(\theta_r)$ distributions for the title reaction at a collision energy of 22.5 kcal/mol with $j = 0$, 3, 5, 7, 9, 12, and 15. For $^3A''$ PES: (a) $v = 0$; (b) $v = 3$. For $^3A'$ PES: (c) $v = 0$; (d) $v = 3$.

The $P(\phi_r)$ distributions which describe the $\boldsymbol{k}'$–$\boldsymbol{k}$–$\boldsymbol{j}'$ vector correlations are illustrated in Fig. 3. It can be seen that all the $P(\phi_r)$ distributions have a peak at the angle around $\phi_r = 270°$, implying a preference for the left-hand product rotation in the planes parallel to the scattering plane. It indicates that all the products have a strong orientation along the direction of the negative y axis, namely a strong polarization of the product rotational angular momentum. The situation that the product molecules prefer a left-hand rotation in the planes parallel to the scattering plane will be called "in plane" situation. By contrast, the term "out of plane" refers to the situation that the product molecules prefer to rotate in planes perpendicular to the scattering plane at the same time. Even at different values of vibrational quantum number, the peak of $P(\phi_r)$ distribution decreases monotonically and becomes a little wider with increasing rotational quantum number. This reflects that the polarization of the product's rotational angular momentum is reduced with the increase of reagent's rotational quantum number. Hence, the reagent's rotational excitation has a negative influence on the polarization of the product rotational angular momentum. However, by comparing the results of the two PESs, it can be found that at the same rotational quantum number, the peaks of the $^3A'$ PES are higher than those of the $^3A''$ PES. This is especially obvious under small values of the vibrational quantum number. This phenomenon could be due to different characters of the two PESs. In the above discuss, the $P(\theta_r)$ distribution is symmetric with respect to $\theta_r = 90°$ while the $P(\phi_r)$ distribution is asymmetric with respect to the $\boldsymbol{k}$–$\boldsymbol{k}'$ scattering plane. These phenomena can be explained by the impulsive model.[28] For the reaction of this type A + BC → AB + C, the product's rotational angular momentum can be written as

$$\boldsymbol{j}' = \boldsymbol{L}\sin^2\beta + \boldsymbol{J}\cos^2\beta + \boldsymbol{J}_1 m_B/m_{AB}, \qquad (5)$$

where $\boldsymbol{L}$ and $\boldsymbol{J}$ are the reactant's orbital angular mo-

mentum and rotational angular momentum, respectively. In addition,

$$\boldsymbol{J}_1 = \sqrt{\mu_{\rm BC}\boldsymbol{R}}(r_{\rm AB} \times r_{\rm CB}), \quad (6)$$

$$\cos^2\beta = m_{\rm A}m_{\rm C}/(m_{\rm A}+m_{\rm B})(m_{\rm B}+m_{\rm C}), \quad (7)$$

where $\mu_{\rm BC}$ is the reduced mass of BC molecule, $\boldsymbol{R}$ is the repulsive energy, $r_{\rm AB}$ and $r_{\rm CB}$ are unit vectors with B pointing to A and C, and $\cos^2\beta$ is the mass factor. During the chemical-bond forming and breaking processes in the reaction, the term $\boldsymbol{L}\sin^2\beta + \boldsymbol{J}\cos^2\beta$ in Eq. (5) is symmetric, but the term $\boldsymbol{J}_1 m_{\rm B}/m_{\rm AB}$ has a preference for the direction influenced by the repulsive energy R, which will lead to the preferred orientation of the product's angular momentum.

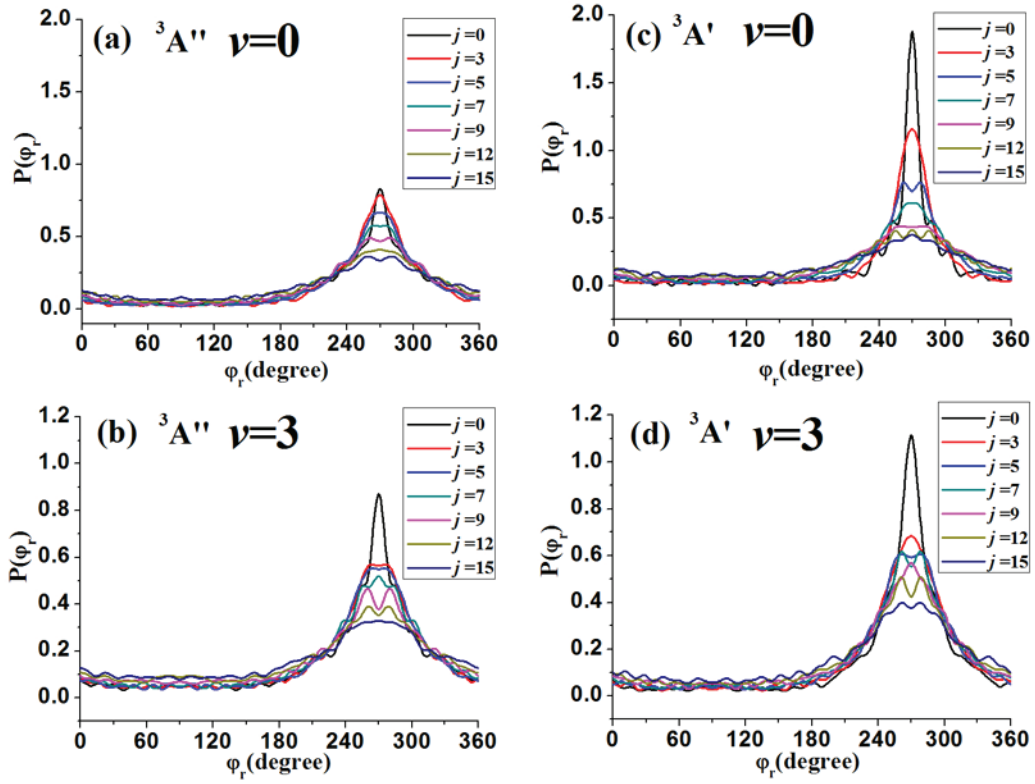


Fig. 3. (colour online) $P(\phi_{\rm r})$ distributions for the title reaction at a collision energy of 22.5 kcal/mol with j = 0, 3, 5, 7, 9, 12, 15. For ^{3}A$''$ PES: (a) v = 0; (b) v = 3. For ^{3}A$'$ PES: (c) v = 0; (d) v = 3.

In order to further understand the effect of the rotational excitation on the product polarization, the $P(\theta_{\rm r}, \phi_{\rm r})$ distribution is also plotted in Fig. 4. In this figure the collision energy is 22.5 kcal/mol, v = 3, and j are chose to be 0, 5, 9, and 12. It can clearly be seen that with the increase of the rotational quantum number, the single peak becomes much lower and wider. The phenomenon indicates that higher rotational excitation has a negative effect on both the product rotational angular momentum alignment and product polarization, which is in good accordance with the $P(\theta_{\rm r})$ and $P(\phi_{\rm r})$ distributions.

The QCT PDDCSs that describe the $\boldsymbol{k}'$–$\boldsymbol{k}$–$\boldsymbol{j}'$ correlation and the scattering direction of the OH product molecule for the title reaction are shown in Fig. 5. In this work, only parts of the PDDCSs are given, namely the $P_{00}(\omega_{\rm t})$ distribution and $P_{22+}(\omega_{\rm t})$ distribution at v = 0, 3 and j = 0, 5, 9, 12. The PDDCS $P_{00}(\omega_{\rm t})$ is indeed a simple differential cross section and describes the scattering direction of products. In Fig. 5(a), peaks of $P_{00}(\omega_{\rm t})$ distributions are moving far away gradually from $\theta_{\rm t}$ = 135° to $\theta_{\rm t}$ = 90° with increasing reagent rotational quantum number. In this situation, the product's scattering presents a change from backward scattering into strong sideways scattering which agrees well with the results of Liu *et al.*[23] On the contrary, as shown in Fig. 5(b), the $P_{00}(\omega_{\rm t})$ distribution exists a high peak at $\theta_{\rm t}$ = 0° at j = 0, then the peak decreases at j = 5, and finally the peak moves to around $\theta_{\rm t}$ = 35° at j = 9, 12. This indicates the initial strong forward scattering gets weak and turns slowly into sideways scattering with increasing rotational quantum number. Similar phenomenon can be found on the ^{3}A$'$ PES in Figs. 5(c) and 5(d). In Fig. 5(c), with the increase of the vibrational quantum number, the peaks become lower and move gradually

from $\theta_t = 180°$ to $\theta_t = 90°$, which indicates that product's scattering changes from backward scattering to sideways scattering. However, in Fig. 5(d), product's scattering changes from forward scattering into sideways scattering with the increase of the vibrational quantum number. Hence, the increase of reagent's rotational quantum number makes the products scatter sideways on both PESs. Thus, the effect of the vibrational excitation on the $P_{00}(\omega_t)$ distributions lies in that it changes the product's scattering direction from backward into forward with the increase of vibrational quantum number.

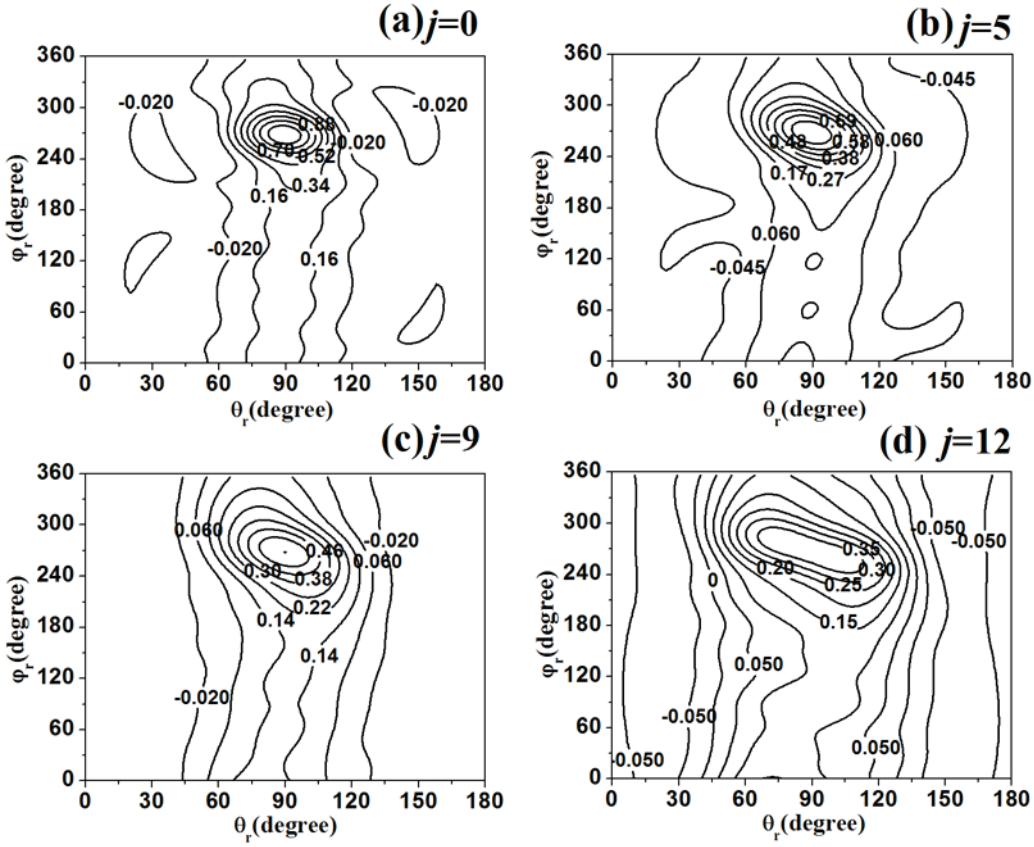


Fig. 4. $P(\theta_r\phi_r)$ distributions at $v = 3$ and (a), $j = 0$, (b) 5, (c) 9, (d) 12 and a collision energy of 22.5 kcal/mol only on the $^3A''$ PES

The negative value of PDDCS $P_{22+}(\omega_t)$ indicates the product alignment along the y axis, while the positive value indicates the product alignment along the x axis. The larger the absolute value is, the higher the degree of the product alignment is. In Fig. 6(a), there are positive values for $j = 0$ and $j = 5$ in the scattering angle ranges of 3°–40° and 7°–30°, respectively, which indicates that the products align along the x axis at corresponding scattering angles. However, no positive value can be observed at $j = 9$, 12. An interesting phenomenon is that the values at $j = 9$, 12 fluctuate so little in the range of 0°–130°. Even not in this range, the values are smaller than those at $j = 0$, 5. Thus, it can be concluded that a bigger rotational quantum number leads to a higher degree of product's scattering isotropy. While in Fig. 6(b) where the vibrational quantum number is 3, the value is very close to the extreme value of -0.612 at $j = 0$ and $\theta_t = 34°$. Then, with the increase of rotational quantum number, the negative extreme values of $P_{22+}(\omega_t)$ distribution are far from -0.612. It reveals that at $\theta_t = 34°$ the product's rotational angular momentum aligns along the y axis at the corresponding direction of $(\theta_r, \phi_r) = (45°, 90°)$. As for the scattering angles larger than about 60°, the fluctuations of the distributions gradually become weak with the increase of the rotational quantum number, which means that the scattering isotropy of products in this range is pretty good. In Figs. 6(c) and 6(d), the peak value approaches or exceeds the negative extreme value of -0.612 for both situations on the $^3A'$ PES: one is at the scattering angle of around 15° at $v = 0$ and $j = 0$, and the other is at the scattering angle of around 35° at $v = 3$ and $j = 0$. This means that at these scatter-

ing angles, the product's rotational angular momentum aligns along the y axis at the corresponding direction of $(\theta_r, \phi_r) = (45°, 90°)$.

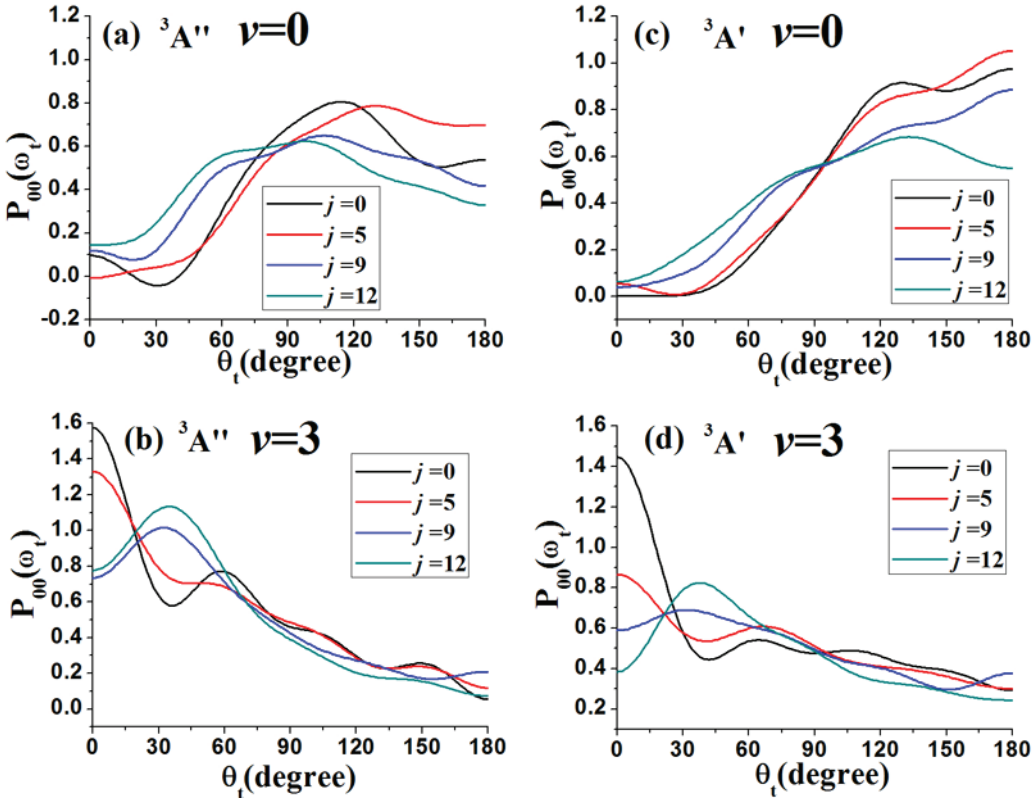


Fig. 5. (colour online) PDDCS $P_{00}(\omega_t)$ distributions with $j = 0$, 5, 9, 12 at a collision energy of 22.5 kcal/mol. For ^{3}A$''$ PES: (a) $v = 0$; (b) $v = 3$. For ^{3}A$'$ PES: (c) $v = 0$; (d) $v = 3$.

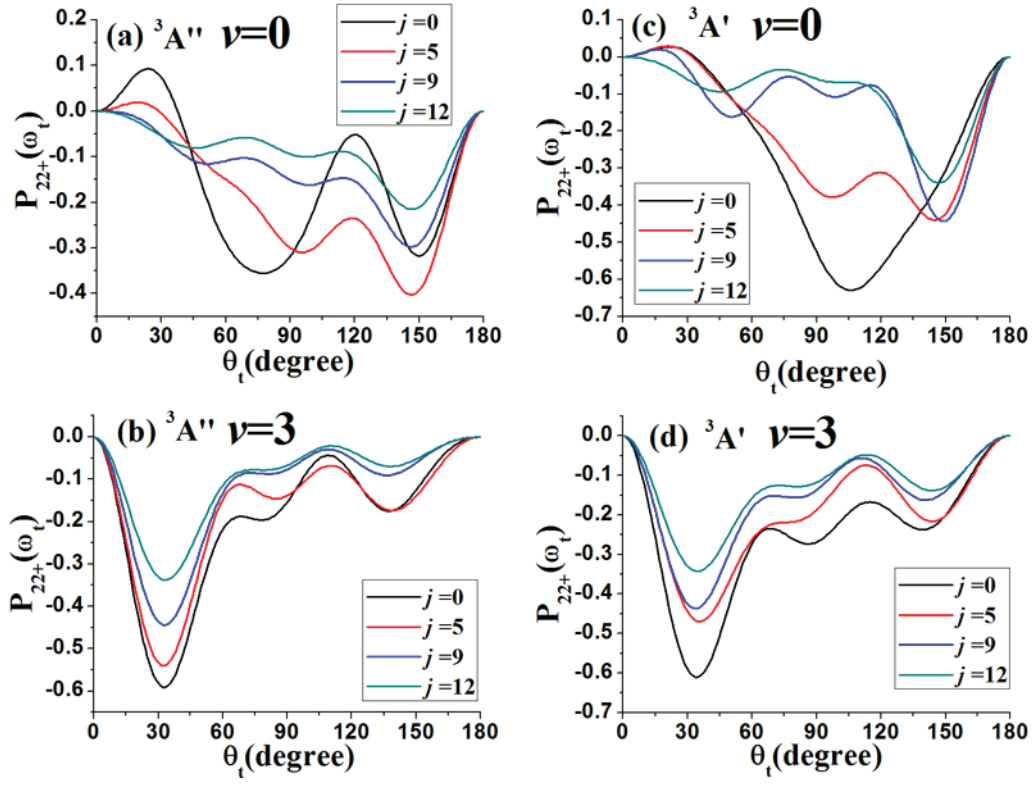


Fig. 6. (colour online) PDDCS $P_{20}(\omega_t)$ distributions with $j = 0$, 5, 9, 12 at a collision energy of 22.5 kcal/mol. For $^3A''$ PES: (a) $v = 0$; (b) $v = 3$. For $^3A'$ PES: (c) $v = 0$; (d) $v = 3$.

4. Conclusions

The calculations of the vector correlations between products and reagents for the title reaction have been performed on the $^3A''$ and $^3A'$ potential energy surfaces using the QCT method mainly at a collision energy of 22.5 kcal/mol. The initial vibrational quantum number of the reagent is chose to be 0 and 3, and the rotational quantum number is chose to be 0, 3, 5, 7, 9, 12, and 15, respectively. The main aim of our work is to investigate how the stereo-dynamics changes with the rotational excitation rather than vibrational excitation. The cross section, the only scalar property that is considered in this work, is very sensitive to the rotational excitation in that it increases monotonically with increasing rotational quantum number. The effects of reagent's rotational excitation on the $P(\theta_r)$ and $P(\phi_r)$ distributions are the same because both alignment and polarization of product's rotational angular momentum are reduced with increasing rotational quantum number. As for the PDDCSs, it can be simply seen that with the increase of vibrational quantum number, the product's scattering direction finally changes into forward, though it is backward or sideways at low vibrational quantum number. Thus, the vibrational excitation exactly plays a rather strong effect on the product's scattering direction compared with that on the above two distributions. The rotational excitation plays an important role to the PDDCSs. It changes the scattering direction from forward and backward into sideways gradually with increasing rotational quantum number. By comparing the results of the two PESs, the effects of vibrational excitation on both PESs are almost the same except the $P(\phi_r)$ and $P_{22+}(\omega_t)$ distribution. Hence, different characters of the two PESs do not have much influence on our investigation on how the vibrational excitation affects the title reaction.

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