Dynamics of reaction of O with H_2 and its isotopic variants in different rotational excited states*

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Scalar properties and vector correlations of the reactions O+H_2 →OH+H, O+HD→OH+D, O+DH→OD+H, and O+D_2 →OD+D at collision energies of 25 and 34.6 kcal/mole have been studied via quasi-classical-trajectory (QCT) method based on a BMS1 potential energy surface (PES). Generalized polarization-dependent differential cross section and the distributions of the dihedral angle at the collision energy of 34.6 kacl/mole are presented. The calculated results indicate that both reagent rotational angular momentum and the mass factor have a significant influence on the scalar properties and vector correlations of the title reactions.

Keywords: quasi-classical-trajectory calculation, rotational excited state, isotopic effect, vector correlation

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1. Introduction

Reactions of O(^{3}P) with H_2 and its isotopic variants have always attracted attention from researchers due to its importance in atmospheric chemistry, ozone depletion mechanism, combustion reaction, and interstellar chemistry.[1−3] Recently, there have been numerous studies reported on scalar properties,[4−10] dynamics,[11−17] and potential energy surface (PES).[18−20] Title reactions involving oxygen atom and prototype are regarded as the simplest chemical reactions to test theoretical and experimental studies.

For the title reactions, Rogers *et al.*[19] constructed a potential energy surface, which was applied by Weck *et al.*[21] and named BWS1. Based on this potential energy surface, Wei *et al.*[22] have reported their theoretical study on the stereo dynamics of the title reaction O(^{3}P)+H_2 with different vibration quantum numbers (v =0,1,2). Han *et al.*[16] have reported their study on the intersystem crossing effects on the reactions for the first time. They found that the vector properties of reaction O(^{3}P)+H_2 are sensitively affected by the vibrational excitation. Liu *et al.*[14] have studied the effects of the reagent rotational quantum numbers on both the scalar and dynamic properties of the title reactions based on the PES obtained through the generalized London–Eyring–Polanyi–Sato double polynomial (GLDP) method.[19] They found that the two kinds of properties are sensitive to the reagent rotational excitation. Garton *et al.*[2] presented the measurements of the relative excitation function for the title reaction, where a crossed molecular beam apparatus in conjunction with a high-energy laser-detonation source of O atom were applied.

Regarding the reaction O(^{3}P)+D_2, Xu *et al.*[23] have studied the product polarization behaviors and found that the isotope mass factor differs on two different potential energy surfaces. Presser *et al.*[24] reported the kinetic isotopic effect in the reactions of O(^{3}P) with H_2, D_2, and HD based on the flash photolysis-resonance fluorescence method. Schatz[25] has carried out a couple-state-distorted-wave study on the O(^{3}P)+H_2(D_2, HD, DH) reactions. Wei *et al.*[13] have published their study on the intermolecular isotopic effect in the reaction O(^{3}P)+H_2/HD and their calculated results indicate that the product polarization is very sensitive to the mass factor. Recently, reaction cross section, vector properties, and the mass factor of reactions O+H_2/D_2 have been studied by Liu *et al.*[26]

However, most previous studies mainly deal with the scalar properties and the studies on the mass factor consider only one vibrational or rotational quan-

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tum number. As the vector correlation between reagents and products can describe extremely rich information about atomic and molecular reactions,[33,34] it is important to study the vector properties of atomic and molecular reactions more extensively. Furthermore, it is necessary to study the isotopic effect with different vibration or rotational states. To obtain more information of the reaction of O(^{3}P) with H_2 and its isotopic variants, we not only investigate the scalar properties and the vector correlation, but also discuss the mass factor with different rotational quantum numbers ($j = 0, 1, \ldots, 9$; $v = 0$).

2. Theoretical methods

2.1. Correlations between $\boldsymbol{k}$, $\boldsymbol{k}'$, and $\boldsymbol{j}'$

Details of the classical description of product polarization has been reported.[27−29] Here we introduce the part relevant to our present work in brief. The center-of-mass (CM) frame is shown in Fig. 1. The reagent relative velocity vector $\boldsymbol{k}$ is parallel to the z axis. The scattering plane containing the initial and final relative velocity vectors ($\boldsymbol{k}$ and $\boldsymbol{k}'$) is x–z plane. The scattering angle θ_t is the angle between the reagent relative velocity and product relative velocity. The θ_r and φ_r are the polar and azimuthal angles of the final rotational momentum $\boldsymbol{j}'$, respectively. The distribution function $P(\theta_r)$, describing the $\boldsymbol{k}$–$\boldsymbol{j}'$ correlation, can be expanded into a series of Legendre polynomial[27,30]

$$P(\theta_r) = \sum_l a_l P_l(\cos\theta_r),$$

where l=2 indicates the product rotational alignment, a_l is the alignment parameter, and

$$a_2 = 5\langle P_2(\cos\theta_r)\rangle = 5\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle,$$

and

$$\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle = \frac{1}{2}\langle 3\cos^2\theta_r - 1\rangle = \frac{1}{2}(3\langle\cos\theta_r\rangle^2 - 1),$$

where the angular bracket represents an average over all the reactive trajectories. The dihedral angle distribution function $P(\phi_r)$ describing the $\boldsymbol{k}$–$\boldsymbol{k}'$–$\boldsymbol{j}'$ correlation can be expanded into a Fourier series[31,32]

$$P(\phi_r) = \frac{1}{2\pi}\Big[1 + \sum_{n=2i} a_n\cos(n\phi_r) + \sum_{n=2i-1} b_n\sin(n\phi_r)\Big], \quad i = 1, 2, \ldots$$

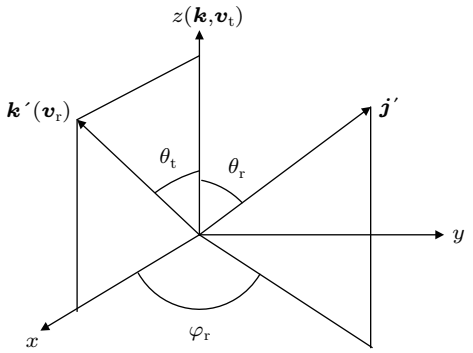


Fig. 1. Center-of-mass coordinate system used to describe the $\boldsymbol{k}$–$\boldsymbol{k}'$–$\boldsymbol{j}'$ correlation.

2.2. Coefficients in the calculation

In our calculation, the BWS1 potential energy surface is chosen and the standard quasi-classical-trajectory calculation is employed. The same coefficients as Ref. [14] are chosen in order to compare the calculated results obtained using different potential energy surfaces. To study the effect of isotope on the title reactions, we set the collision energy as 34.6 kcal/mole (about 1.5 eV), the rotational quantum number j is from 0 to 9, and the vibrational quantum number v is set to be 0. We use 50000 trajectories in total to run for each rotational state and the integral step size is set to be 0.1 fs. The initial distance between O atom and the mass centre of H_2, HD, DH, or D_2 molecule is 10 Å for each trajectory. N_{r1} and N_{r2} are respectively the react trajectory numbers of Channels 1 and 2, and the total react trajectory number N_r is equal to the sum of N_{r1} and N_{r2}. The react probability is defined as N_r/N, where $N = 50000$ is the total number of trajectory. The cross section is expressed as: $\sigma_r = \pi b_{max}^2(N_r/N)$, where b_{max} is the maximum impact parameter.

3. Results and discussion

Liu *et al.*[14] have studied both scalar and vector properties of the reaction O(^{3}P)+H_2. The PES is derived using generalized London–Eyring–Polanyi–Stato double polynomial at a collision energy of 25 kcal/mole. We make a comparison between our results with those in Ref. [14] (see Table 1 and Figs. 2–5). Figures 2–5 shows the results of reaction probability, cross section, $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$, and distribution function $P(\theta_r)$ obtained through our calculation and from Ref. [14], respectively.

Table 1. Comparison between our calculated results and those from Ref. [14].

j	N_r		b_{max}		N_r/N		$\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$		σ_r	
	Ref. [14]	This work	Ref. [14]	This work	Ref. [14]	This work	Ref. [14]	This work	Ref. [14]	This work
0	13225	13626	1.418	1.42	0.2645	0.27252	−0.36347	−0.42679	1.67081	1.72633
1	17552	13464	1.28	1.44	0.35104	0.26928	−0.40487	−0.42492	1.80687	1.7542
2	15690	14466	1.448	1.46	0.3138	0.28932	−0.31328	−0.41752	2.0670	1.93747
3	17084	16171	1.462	1.49	0.34168	0.32342	−0.3434	−0.41131	2.29437	2.25574
4	18852	18489	1.4628	1.50	0.37704	0.36978	−0.2472	−0.39376	2.53459	2.61382
5	20369	20253	1.479	1.53	0.40738	0.40506	−0.2804	−0.37672	2.79954	2.97887
6	21231	20283	1.514	1.57	0.42462	0.40566	−0.2906	−0.3485	3.05775	3.14131
7	22056	22932	1.5526	1.58	0.4413	0.45864	−0.14000	−0.32286	3.34197	3.59696
8	24083	23831	1.556	1.60	0.48166	0.47662	−0.08038	−0.29932	3.66361	3.83321
9	25721	25101	1.59	1.62	0.50542	0.50202	−0.20349	−0.27027	4.01418	4.13905

As can be seen in Fig. 2, two calculated cross sections are similar. Figure 3 indicates that the results of reaction probability are similar at highly-excited rotational states, and there is only a small difference for $j < 4$. We attribute this difference to the distinction of the potential energy surface. The distribution $P(\theta_r)$ we obtain is the same as Ref. [14], as shown in Fig. 4. The value of the peak decreases monotonously with the increase in the rotational quantum number. This means that the alignment of product rotation becomes weaker. By contrast, figure 5 shows a different result of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ from Ref. [14]. It is obvious that the values of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ in Ref. [14] oscillate with the increase in the rotational quantum number, but our values increase monotonously as the rotational quantum number increases. The minimum value of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ which reflects the product rotational alignment approaches −0.5. The alignment of the product rotation will become weak as $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ increases.[32] From Fig. 4, it is obviously seen that our calculated results are better consistent with the distribution of $P(\theta_r)$ than Ref. [14].

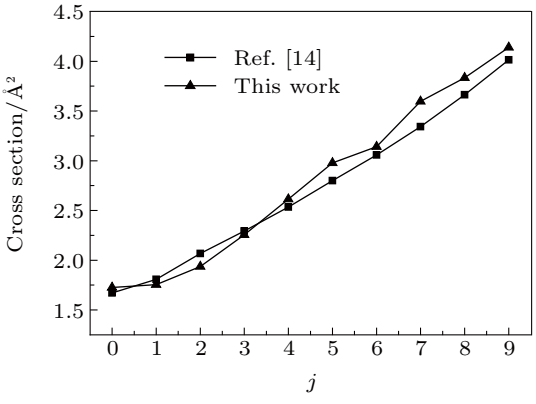


Fig. 2. Calculated results of cross section based on two different PESs.

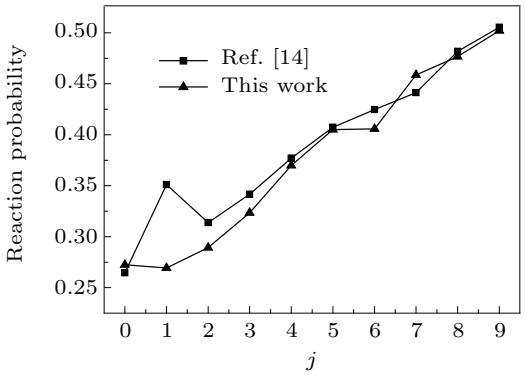


Fig. 3. Calculated results of reaction probability based on two different PESs.

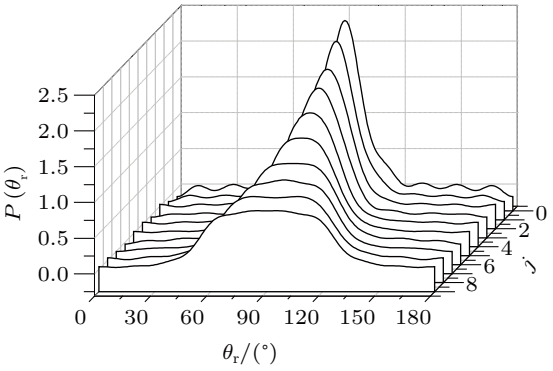


Fig. 4. Distribution function $P(\theta_r)$ at a collision energy of 25 kcal/mole based on the potential energy of BMS1.

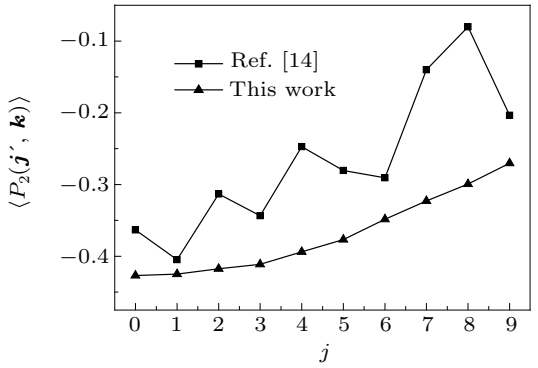


Fig. 5. Calculated results of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ based on two different PESs.

The scattering direction of the product molecule OH and the $\boldsymbol{k}$–$\boldsymbol{k}'$–$\boldsymbol{j}'$ correlation are described by polarization-dependent generalized differential cross sections (PDDCSs). We only discuss the PDDCS $(2\pi/\sigma)(\mathrm{d}\sigma_{00}/\mathrm{d}\omega_\mathrm{t})$ (σ denotes the cross section), which describes the scattering direction of the product or the $\boldsymbol{k}$–$\boldsymbol{k}'$ correlation and has nothing to do with the orientation and alignment of the product rotational angular momentum $\boldsymbol{j}'$. The product distributions of $P(\theta_\mathrm{t})$ for $\mathrm{O}(^3\mathrm{P})+\mathrm{H_2} \rightarrow \mathrm{OH+H}$, $\mathrm{O}(^3\mathrm{P})+\mathrm{HD} \rightarrow \mathrm{OH+D}$, $\mathrm{O}(^3\mathrm{P})+\mathrm{DH} \rightarrow \mathrm{OD+H}$, and $\mathrm{O}(^3\mathrm{P})+\mathrm{D_2} \rightarrow \mathrm{OD+D}$ are shown in Fig. 6. Evidently, the reagent rotational excitation states almost have no influence on the $\boldsymbol{k}$–$\boldsymbol{k}'$ correlation for each reaction. As shown in Fig. 6, the scattering direction of product OH is highly sideways for the reaction $\mathrm{O}(^3\mathrm{P})+\mathrm{H_2}$in all rotational levels, and the scattering direction of product OH for the reaction $\mathrm{O}(^3\mathrm{P})+\mathrm{HD}$ is similar to that for $\mathrm{O}(^3\mathrm{P})+\mathrm{H_2}$. However, the peaks of distribution of $P(\theta_\mathrm{t})$ for $\mathrm{O}(^3\mathrm{P})+\mathrm{HD}$ moves forward compared with that for $\mathrm{O}(^3\mathrm{P})+\mathrm{H_2}$. Regarding the reaction O+DH, most of the products are scattered sideways and the rest are scattered backward, but the peaks move backward (see Fig. 6). The products are scattered strongly sideways again for the reaction $\mathrm{O+D_2}$, and the $P(\theta_\mathrm{t})$ distributions are similar to that of the reaction $\mathrm{O+H_2}$. Obviously, $(2\pi/\sigma)(\mathrm{d}\sigma_{00}/\mathrm{d}\omega_\mathrm{t})$ is sensitive to the mass factor of the reaction of $\mathrm{O}(^3\mathrm{P})$ with $\mathrm{H_2}$ and its isotopic variants.

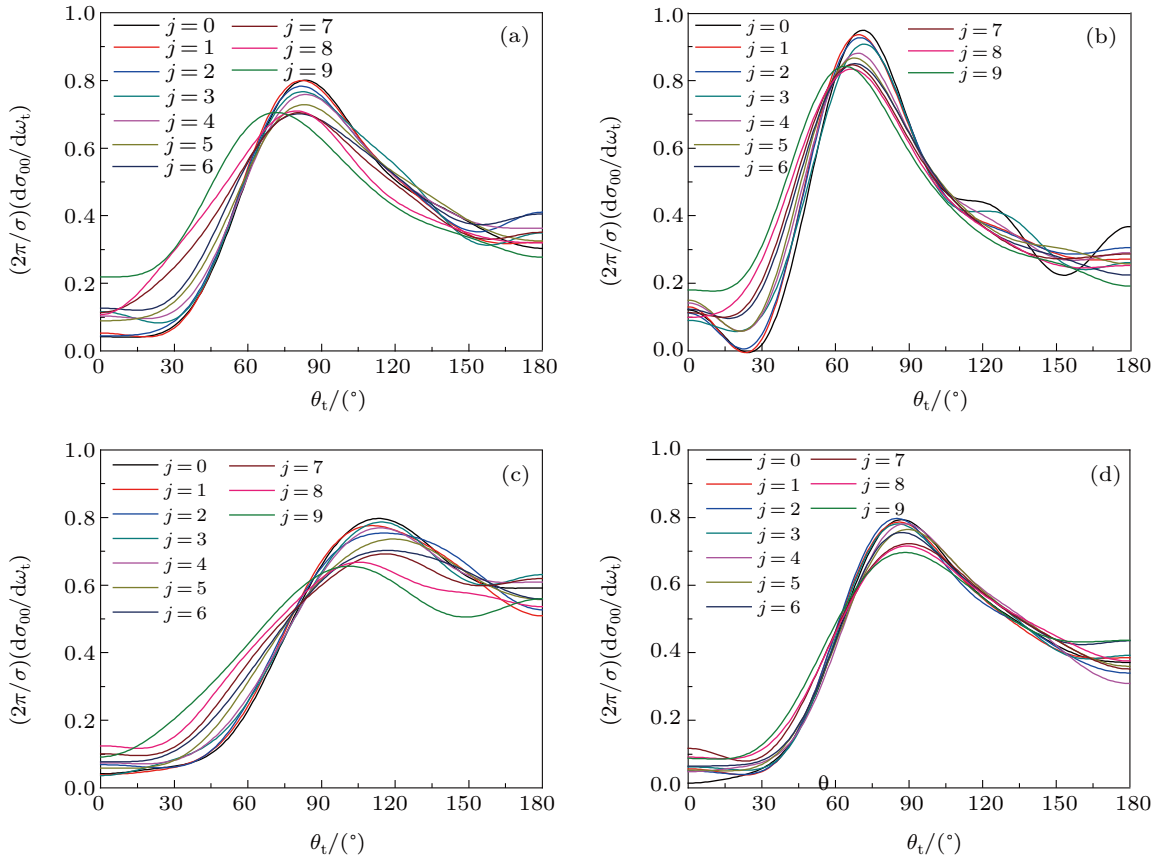


Fig. 6. (colour online) Distribution of $P(\theta_\mathrm{t})$ at a collision energy of 34.6 kcal/mole for reactions (a) $\mathrm{O+H_2}$, (b) O+HD, (c) O+DH, and (d) $\mathrm{O+D_2}$.

The distribution function $P(\theta_\mathrm{r})$, which describes the $\boldsymbol{k}$–$\boldsymbol{j}'$ correlation is illustrated in Fig. 7. The peaks of $P(\theta_\mathrm{r})$ take place at $\theta_\mathrm{r} = 90^\circ$ and are symmetric with respect to $\theta_\mathrm{r} = 90^\circ$ for every reaction, implying that the product rotational angular momentum $\boldsymbol{j}'$ of the reactions is strongly aligned and perpendicular to the line of centers. It is clear that the peaks of the distributions of $P(\theta_\mathrm{r})$ become lower and broader with the increase in the rotational quantum number for the reactions $\mathrm{O+H_2}$, O+HD, O+DH, and $\mathrm{O+D_2}$ ($v = 0$, $j = 0, 1, \ldots, 9$), which confirms the variation of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ as shown in Fig. 8, indicating that the alignment effect of the product rotational angular momentum become weaker as the value of j increases.

This demonstrates that the product rotational alignment is sensitively affected by the rotational excitation. It is simple to find that there are obvious differences in the product rotational alignment among the four reactions O+H_2, O+HD, O+DH, and O+D_2. The peaks of the $P(\theta_r)$ distribution of the reaction O+H_2 are lower and broader than that of the reaction O+D_2, and the peaks of the $P(\theta_r)$ distribution of the reaction O+HD are lower and broader than that of both reactions of O+H_2 and O+D_2. However, the product rotational alignment of the reaction O+DH is the strongest since its peaks of the $P(\theta_r)$ distribution are higher and narrower than that of the reactions O+H_2 and O+D_2, as shown in Fig. 7. This means that the isotope has great effect on the product rotational alignment of the reactions O+H_2, O+HD, O+DH, and O+D_2. The values of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ for the title reactions describing the rotational alignment are also calculated. As can be seen in Fig. 8, the variations of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ conforms to the distribution of $P(\theta_r)$, which proves that our calculated results are reliable.

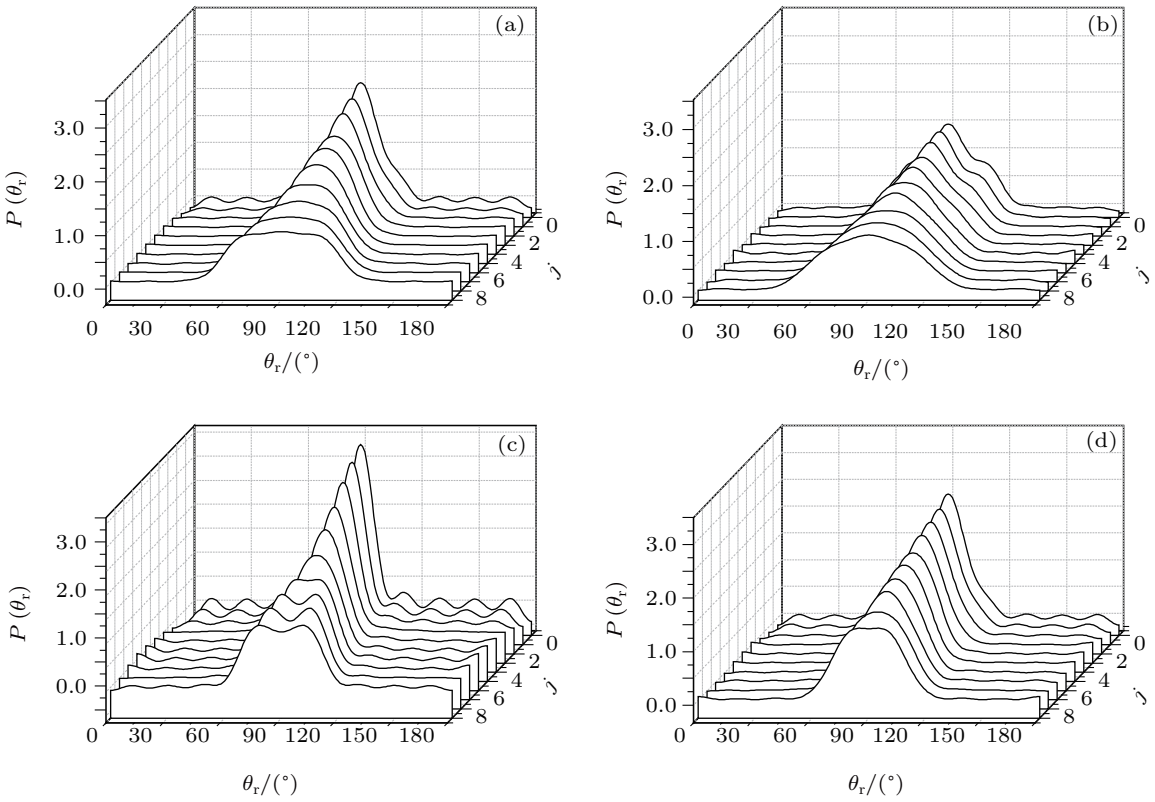


Fig. 7. Distribution of $P(\theta_r)$ indicating the $\boldsymbol{k}$–$\boldsymbol{j}'$ correlations of reactions (a) O+H_2, (b) O+HD, (c) O+DH, and (d) O+D_2 at a collision energy of 34.6 kcal/mole for reagent rotational excitation.

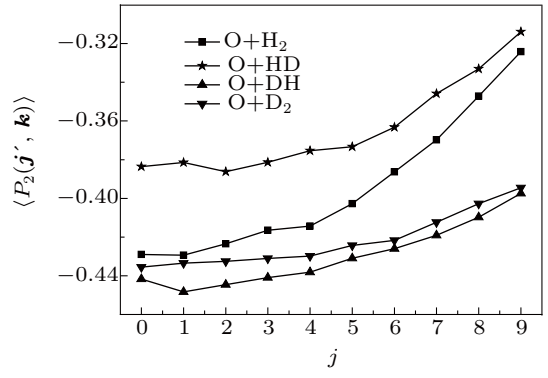


Fig. 8. Calculated results of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ for the reactions O+H_2, O+HD, H+DH, and O+D_2 based on $\boldsymbol{k}$–$\boldsymbol{k}'$ correlation at a collision energy of 34.6 kcal/mole.

To obtain a better graphical representation of the polarization of the products from the title reactions, the $P(\phi_r)$ distributions are plotted in Fig. 9 to describe the $\boldsymbol{k}$–$\boldsymbol{k}'$–$\boldsymbol{j}'$ correlation. It is clear that the product angular momenta of the four reactions having a strong polarization for the distributions of $P(\phi_r)$ tend to be asymmetrical with respect to the $\boldsymbol{k}$–$\boldsymbol{k}'$ scattering plane. The peaks of distribution $P(\phi_r)$ appear at 270° for all the reactions and rotational excited states, and almost disappear when $\phi_r < 90°$, indicating that the rotational angular momentum vectors are not only aligned mainly along y axis but also oriented preferentially towards the $-y$ direction. Figure 9 pre-

dicts that with the increase in the reagent rotational quantum number, the variations of the $P(\phi_r)$ distributions for the reactions O+H_2, O+HD, O+DH, and O+D_2 are obviously different from each other. As the reagent rotational quantum number increases, the peaks of the $P(\phi_r)$ distributions for the reaction O+H_2 oscillate quickly, while the values of the peaks change slightly. This is similar to the case of O+D_2. For the reaction O+HD, the peaks of the $P(\phi_r)$ distributions tend to become narrower and higher, indicating that the polarization of the product rotational angular momentum becomes stronger. The variations of the reaction O+DH show an opposite tendency and the change of the peaks is more obvious. Clearly, the polarization of the product rotational angular momentum for the reaction O+DH is the strongest due to the fact that the peaks of the $P(\phi_r)$ distributions are the highest and the polarization of the reaction O+HD is the weakest. In summary, the polarization of product rotational angular momentum is sensitive to the reagent rotational quantum numbers and the isotopic effect for the title reactions. The planar symmetry of the scattering process can always be seen in an atom–diatom (A+BC→AB+C) reaction, which makes a contribution to the reduction in the degree of freedom of the reagent. However, as can be seen in Fig. 9, the planar symmetry of the collision indicates that the distribution of the product angular momentum $\boldsymbol{j}'$ is not symmetric with respect to the scattering plane. Shafer-Ray *et al.*[30] owe this asymmetry to the chiral pathway of the reaction by arguing that it is a result of the fact that $\boldsymbol{j}' = \boldsymbol{r}' \times \boldsymbol{p}'$ is a vector that distinguishes right from left handedness, i.e., the case that $\boldsymbol{j}'$ is parallel to $\boldsymbol{r}' \times \boldsymbol{p}'$ is physically different from the case that $\boldsymbol{j}'$ is antiparallel to $\boldsymbol{r}' \times \boldsymbol{p}'$.

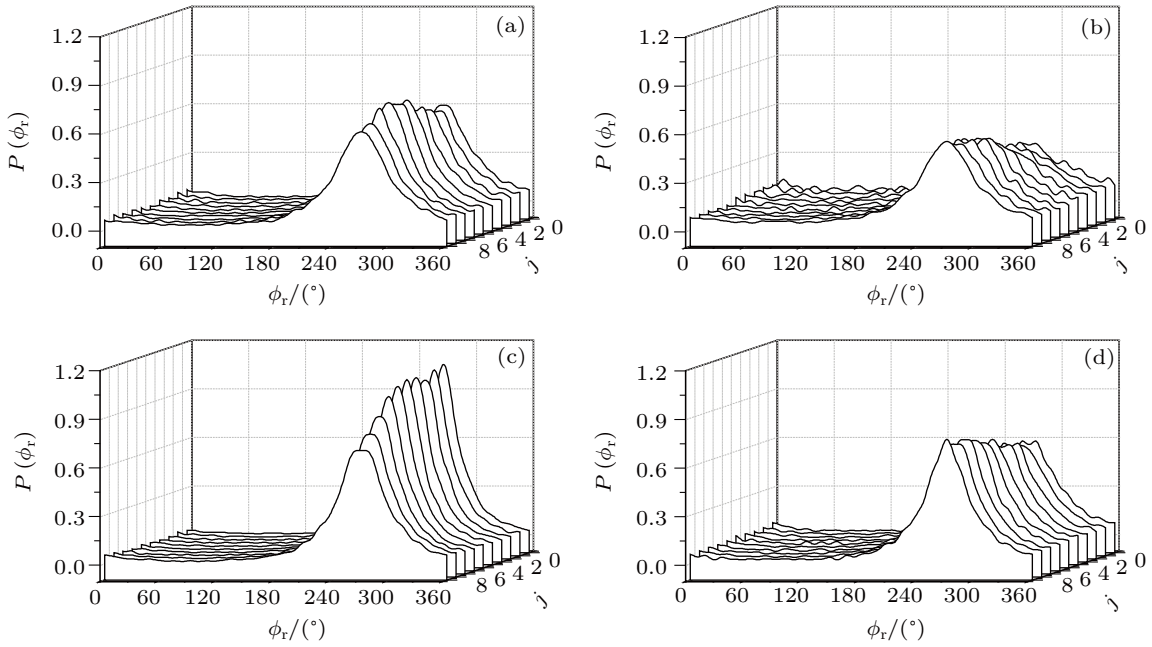


Fig. 9. Distributions of $P(\phi_r)$ at ten rotational states for the reactions (a) O+H_2, (b) O+HD, (c) O+DH, and (d) O+D_2 at a collision energy of 34.6 kcal/mole based on the BMS1 PES.

4. Conclusion

In this paper, the quasi-classical-trajectory calculations on the scalar and vector properties for the reactions O+H_2, O+HD, O+DH, and O+D_2 have been performed at the collision energies of 25 and 34.6 kcal/mole based on the BMS1 PES. The calculated results are compared with that in Ref. [14] at the energy of 25 kcal/mole and our calculation is more acceptable, because the values of $\langle P_2(\boldsymbol{j}', \boldsymbol{k})\rangle$ in our work conform with the $P(\theta_r)$ distribution better than that of Ref. [14]. We obtained the PDDCS $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$ of the reaction of an O atom with H_2 and its isotopic variants at the collision energy of 34.6 kacl/mole, which indicates the scattering distributions of the products. The $P(\theta_t)$ distribution does not vary obviously with the increase in the reagent rotational quantum number, but it is sensitive to the mass factor. The $P(\theta_r)$ and $P(\phi_r)$ distributions are also calculated, and the results indicate that the rota-

tional angular momentum vectors $\boldsymbol{j}'$ of the products from the title reactions are not only aligned, but also oriented. The reagent rotational quantum number has a negative influence on the alignment of the rotational angular momentum vectors $\boldsymbol{j}'$ for title reactions and the isotopic effect is distinct. When it comes to the $P(\phi_{\rm r})$ distributions, the mass factor has a great influence on the polarization of the product rotational angular momentum; the reagent rotational quantum number has a positive effect on the polarization of $\boldsymbol{j}'$ for the reaction O+HD, but it has a negative effect on the polarization of $\boldsymbol{j}'$ for the reaction O+DH.

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