Effect of reagent vibrational excitation and isotope substitution on the stereo-dynamics of the Ba + HF → BaF + H reaction

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Based on an extended London–Eyring–Polanyi–Sato (LEPS) potential energy surface (PES), the Ba+HF reaction has been studied by the quasi-classical trajectory (QCT) method. The reaction integral cross section as a function of collision energy for the Ba + HF → BaF + H reaction is presented and the influence of isotope substitution on the differential cross sections (DCSs) and alignments of the product's rotational angular momentum have also been studied. The results suggest that the integral cross sections increase with increasing collision energy, and the vibrational excitation of the reagent has great influence on the DCS. In addition, the product's rotational polarization is very strong as a result of heavy–heavy–light (HHL) mass combination, and the distinct effect of isotope substitution on the stereodynamics is also revealed.

Keywords: quasi-classical trajectory method, London–Eyring–Polanyi–Sato potential energy surface, vibrational excitation of the reagent, isotope substitution

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1. Introduction

In recent years, as a practical and effective measure, the quasi-classical trajectory (QCT) method has been widely used to study the dynamics of chemical reactions, especially for the reaction system with very large mass.[1−3] Later, Han *et al.* developed the stereodynamics QCT computational method, which makes it possible to compare the theoretical alignments of the product's rotational angular momentum with the experimental one.[2,3] So far, the product's rotational polarization of many chemical reactions[4−18] has been successfully studied with this method. Moreover, the reaction $M + \mathrm{H}X \rightarrow MX + \mathrm{H}$ ($M = \mathrm{Be, Mg, Ca, Sr, Ba}$; $X = \mathrm{F, Cl, Br, I}$)[19−34] shows interesting dynamical features, and many studies of this reaction family have been done, theoretically and experimentally. Using crossed molecular beams and a laser induced fluorescence method, Zare and his coworkers have done much experimental work,[21−24,27−34] and some theoretical simulations to investigate the very highly detailed dynamical features of these reactions have also been made. Han *et al.* and Stolte *et al.* have investigated the reactions between the alkaline earth atoms and halocarbon halide RX, $M + \mathrm{R}X \rightarrow MX + \mathrm{R}$ ($M = \mathrm{Be, Mg, Ca, Sr, Ba}$; $X = \mathrm{F, Cl, Br, I}$), and found many different properties and experimentally observable phenomena describing the dynamics of these reactions.[26,35−41]

For the reaction $M + \mathrm{H}X \rightarrow MX + \mathrm{H}$, there are usually two processes involved. One is direct abstraction and the other is insertion. These two reaction mechanisms often play different roles in different initial situations and different reactions. In addition, this reaction family belongs to the heavy–heavy–light (HHL) mass system, which makes the product rotation strongly aligned about the direction of the relative velocity of the reagent. Taking the reaction Ba + HF → BaF + H as an interesting example, Zhang *et al.* calculated the state distribution of the BaF product and described the reaction mechanism of Ba + HF based on the extended London–Eyring–Polanyi–Sato (LEPS) potential energy surface (PES).[42] In their studies, the QCT method was used, and the results agreed closely with the experimental ones. Later, Liu *et al.* employed symplectic integrators in the classical trajectory calculations of the Ba + HF reaction,[43] compared the total energy conservation of the Hamiltonian system between the traditional RK4-ADH4 integrator, and the symplectic integrators at fourth and sixth order. Their results indicate that the sixth-order symplectic integrator is the

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most suitable method for the quasiclassical trajectory calculation, since it consumes less computational expense and exhibited better energy conservation.

As far as we know, the existing work on the Ba + HF reaction mainly focuses on the study of the scalar property, while there are few reports about the stereodynamics and the isotope effects. In order to understand the dynamics of this reaction better, in this paper, we utilize the stereodynamics QCT program, which contains the sixth-order symplectic integrator,[44] to calculate the integral cross section and the effect of isotope substitution on the stereodynamics of the title reaction, expecting to make some discovery.

2. Theory

2.1. LEPS potential energy surface

The extended LEPS PES employed in this calculation is as follows,

$$V(r_1, r_2, r_3) = Q_1 + Q_2 + Q_3 - (J_1^2 + J_2^2 + J_3^2 - J_1J_2 - J_2J_3 - J_1J_3)^{1/2}, \quad (1)$$

where

$$Q_i = \frac{1}{2}({}^1E_i + {}^3E_i), \quad (2)$$

$$J_i = \frac{1}{2}({}^1E_i - {}^3E_i), \quad (3)$$

in Eqs. (2) and (3) ${}^1E_i$ is defined as the diatomic Morse potential, and ${}^3E_i$ stands for the anti-Morse function

$${}^1E_i = D_i(\{1 - \exp[-\beta_i(r_i - r_{0i})]\}^2 - 1), \quad (4)$$

$${}^3E_i = {}^3D_i(\{1 + \exp[-\beta_i(r_i - r_{0i})]\}^2 - 1), \quad (5)$$

where

$${}^3D_i = \frac{D_i(1 - S_i)}{2(1 + S_i)}, \quad (6)$$

S_i is an adjustable parameter (so-called Sato parameter), D_i, β_i and r_i represent the Morse parameters of the diatom, subscript $i = 1,\ 2,\ 3$ indicates HF, BaF and BaH, respectively.

Table 1. Parameters for the LEPS PES for the Ba + HF reaction, 1 Å=0.1 nm.

	BaF	HF	BaF
D_i/eV	6.050	5.869	1.950
β_i/Å^{-1}	1.058	2.269	1.136
R_{0i}/Å	2.162	0.917	2.232
S_i	0.178	0.160	0.300

The parameters D_i, β_i and r_{0i} for potential energy surface are referred to Ref. [42] for the reaction Ba+HF. The potential energy surface by adjusting S_i ($i = 1,\ 2,\ 3$) is constructed, and all of the parameters are presented in Table 1.

2.2. QCT calculations

The calculation method of the QCT is the same as the one used in Refs. [44]–[49]. The classical Hamilton's equations are numerically integrated in three dimensions. In the present work, 20000 trajectories are run for each reaction, the initial distance from the Ba atom to the centre of mass of HF is 15.0 Å and the integration step size in the trajectories is chosen to be 0.1 fs, which can guarantee the conservation of the total energy and total angular momentum. The impact parameter, $b_{\max}$, is computed by calculating 20000 trajectories at a fixed value of the impact parameter b and systematically increasing the value of b until no reactive trajectories are obtained. The reaction cross section is defined as $\sigma = \pi b_{\max}^2(N_{\rm r}/N)$ ($N_{\rm r}$, the number of reactive trajectories; N, the total number of trajectories). The sampling error is defined as $\varepsilon = \sqrt{(N - N_{\rm r})/NN_{\rm r}} \times 100\%$, and the reaction cross section error in our calculation is defined as $\sigma_{{\rm r}\varepsilon} = \varepsilon\sigma_{\rm r}$.

The general theory of the product's rotational polarization has been developed perfectly, and the reader is referred to the relevant articles[44−53] and to the references therein.

3. Results and discussion

Figure 1 shows the dependence of the integral reaction cross section on the collision energy. As can be seen in this figure, the integral cross section increases rapidly with the relative translational energy increasing from 0.025 kcal/mol to 20 kcal/mol, and then slowly increases when the collision energy is larger than 20 kcal/mol. In addition, there is almost no threshold for the title reaction. This is ascribed to the property of the LEPS PES, which has almost no potential well but a barrier whose height is about 16.7 kJ/mol appearing on the exit valley (see Fig. 2), that is to say, the barrier is late for this exothermic reaction, and the PES is repulsive. Generally, for one reaction with the repulsive PES, the vibrational excitation of the reagent has a great effect on the integral reaction cross section. Considering our reaction, this

conclusion has been confirmed by the data in Table 2. Seen in Table 2, at the same collision energy, the higher the vibrational energy of the reagent, the larger the value of the reaction cross section. In addition, the differential cross sections (DCS) for the reaction Ba + HF at different vibrational quantum numbers ($v = 0, 2, 4;\ j = 0$) are shown in Fig. 3. From this figure, it is clear that the influence of the vibrational excitation on the DCS is large. The reaction Ba + HF ($v = 0,\ j = 0$) is mainly dominated by backward scattering and there is no distinct scattering direction for Ba + HF ($v = 2,\ j = 0$) reaction, while the reaction Ba + HF ($v = 4,\ j = 0$) is governed by strong forward scattering. Therefore, one can conclude that the tendency of forward scattering is enhanced with the increase in vibrational quantum number of the reagent.

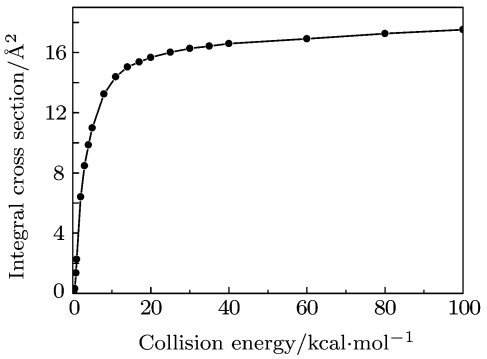


Fig. 1. The QCT-computed reaction cross section as a function of collision energy.

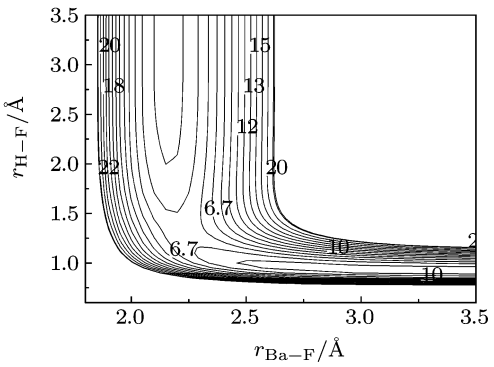


Fig. 2. The contour plots of the three-dimensional LEPS PES for the Ba–H–F linear direction.

Table 2. The integral reaction cross section values under the different vibrational quantum numbers of the reagent.

E_C/kcal·mol^{-1}	20	20	40	40	80	80
HF (v, j)	(0,0)	(1,0)	(0,0)	(1,0)	(0,0)	(1,0)
σ/Å^2	15.67	23.95	16.59	21.77	17.25	20.66

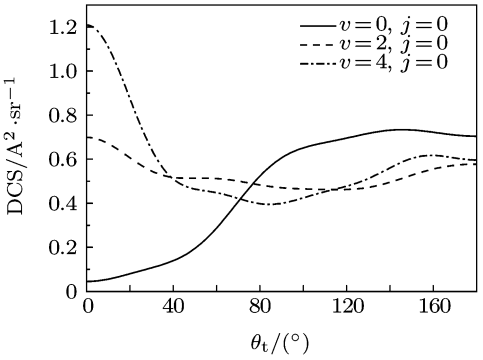


Fig. 3. The angular distributions for Ba + HF ($v = 0, 2, 4;\ j = 0$) reactions at $E_C = 14$ kcal/mol. Solid line for $v = 0$; dashed line for $v = 2$; and short dashed line for $v = 4$.

In order to obtain much more dynamics information, we investigated the isotope effect on the stereodynamics of the title reaction. Figure 4 represents the DCSs for the reactions Ba+HF/DF/TF ($v = 0,\ j = 0$) at a collision energy of 14 kcal/mol. As seen in Fig. 4, these three reactions are mainly dominated by backward scattering, and the tendency of forward scattering is enhanced while the mass of the target molecule increases. As discussed in Ref. [42], when the collision energy and vibrational energy of the reagent are low, the abstraction pathway dominates the reaction. Therefore, the product molecules from the reactions Ba + HF/DF/TF ($v = 0,\ j = 0$) are obviously backward scattered. According to the previous theoretical study of the impulsive model of the atom and molecule reaction for the reaction A + BC → AB + C,[54] the repulsion energy of the BC molecular becomes larger after H is substituted by D/T, which leads to the stronger forward scattering of the product molecule from Ba + DF/TF ($v = 0,\ j = 0$) reactions.

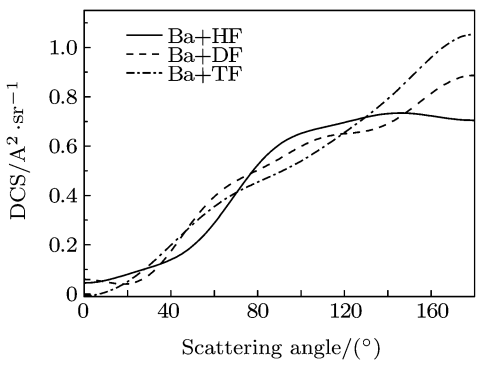


Fig. 4. The angular distributions for Ba + HF/DF/TF ($v = 0,\ j = 0$) → BaF + H/D/T reactions at $E_C = 14$ kcal/mol. Solid line for Ba + HF; dashed line for Ba + DF; and short dashed line for Ba + TF.

The polarization-dependent differential cross sections (PDDCSs) have also been calculated. $(2\pi/\sigma)(\mathrm{d}\sigma_{22+}/\mathrm{d}\omega_t)$ and $(2\pi/\sigma)(\mathrm{d}\sigma_{21-}/\mathrm{d}\omega_t)$ are depicted in Figs. 5 and 6, respectively. Figure 5 shows the $(2\pi/\sigma)(\mathrm{d}\sigma_{22+}/\mathrm{d}\omega_t)$ distribution. It is clear that the product's rotational angular momentum prefers to align along the y axis. It is necessary to pay attention to the fact that the products display a stronger polarization at about 150°, and the degree of the product's BaF polarization becomes stronger after H is substituted by D/T. Due to the late barrier in the PES, the product molecules from the Ba + HF/DF/TF ($v = 0$, $j = 0$) reaction are mainly backward scattering, moreover the reaction is controlled by an in-plane mechanism, and it is natural that the product rotational angular momentum displays a stronger polarization at about $\theta_\mathrm{t} = 150°$. When atom H is substituted by D/T,

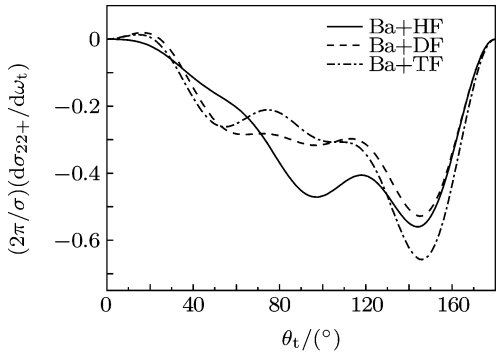


Fig. 5. The polarization-dependent generalized differential cross section $(2\pi/\sigma)(\mathrm{d}\sigma_{22+}/\mathrm{d}\omega_t)$ of the reaction Ba + HF/DF/TF. Solid line for Ba + HF; dashed line for Ba + DF; and short dashed line for Ba + TF.

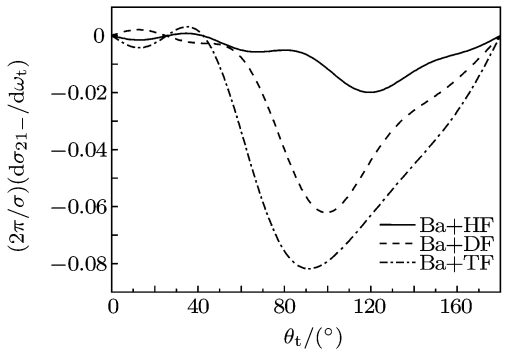


Fig. 6. The polarization-dependent generalized differential cross section $(2\pi/\sigma)(\mathrm{d}\sigma_{21-}/\mathrm{d}\omega_t)$ of the reaction Ba + HF/DF/TF. Solid line for Ba + HF; dashed line for Ba + DF; and short dashed line for Ba + TF.

the degree of the product BaF polarization has also changed, which indicates that the mass of the reaction system also impacts on the product polarization. The $(2\pi/\sigma)(\mathrm{d}\sigma_{21-}/\mathrm{d}\omega_t)$ distributions have been depicted. As shown in Fig. 6, there is significant difference among three $(2\pi/\sigma)(\mathrm{d}\sigma_{21-}/\mathrm{d}\omega_t)$ distributions. The alignment of product BaF is along the direction of the vector $\boldsymbol{x} + \boldsymbol{z}$ for the reactions Ba + HF/DF/TF ($v = 0$, $j = 0$). The strongest alignment is at the scattering angles about 120°, 100°, and 90°, respectively.

To get a better graphical representation of the polarization of the BaF products from the title reaction, we have plotted $P(\theta_\mathrm{r})$ and $P(\phi_\mathrm{r})$ distributions in Figs. 7 and 8, respectively. From the $P(\theta_\mathrm{r})$ distributions shown in Fig. 7, one can conclude that the product's rotational angular momentum vector is strongly aligned along the direction at right angles to the relative velocity direction. In addition, there is a discrepancy among the three $P(\theta_\mathrm{r})$ distributions. When the mass of the target molecule increases, the peak of $P(\theta_\mathrm{r})$ gets lower, and the corresponding values of the rotational alignment factor $\langle P_2(\boldsymbol{j}' \cdot \boldsymbol{k})\rangle$ are –0.4897, –0.4726 and –0.4536, respectively, which indicates that the degree of alignment of BaF becomes weaker. Due to the heavy–heavy–light (HHL) mass combination, the excessive translation energy will channel into rotational excitation, and the rotation momentum alignment is strong. In addition, according to Refs. [45] and [47], $P(\theta_\mathrm{r})$ is sensitive to two factors: one is the character of the PES, and the other is the mass factor (i.e., $\cos^2\beta = m_\mathrm{A}m_\mathrm{C}/(m_\mathrm{A}+m_\mathrm{B})(m_\mathrm{B}+m_\mathrm{C})$ for the reaction A + BC → AB + C). On the condition of adiabatic approximation, the influence of isotopic substitution on the PES is not considered here. Therefore, the difference in the $P(\theta_\mathrm{r})$ distribution is probably attributed to the difference in the mass factor among the reactions Ba + HF/DF/TF → BaF + H/D/T, the values of mass factor are 0.04426, 0.08417 and 0.1208,

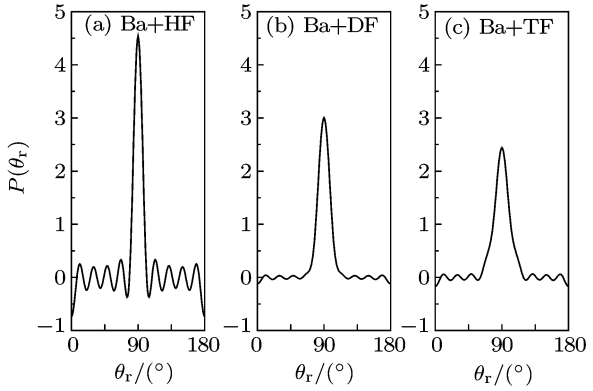


Fig. 7. The distribution of $P(\theta_\mathrm{r})$ for the product molecule from the reaction Ba + HF/DF/TF at $E_\mathrm{C} = 14$ kcal/mol. (a) Ba + HF, (b) Ba + DF, (c) Ba + TF.

respectively. Moreover, when D/T substitutes H, the reaction system deviates from the HHL mass combination, which can also make the alignment weaker.

Figure 8 shows the dihedral angle distributions $P(\phi_r)$ describing the $\boldsymbol{k}$–$\boldsymbol{k}'$–$\boldsymbol{j}'$ correlations. The $P(\phi_r)$ tends to be asymmetric with respect to the $\boldsymbol{k}$–$\boldsymbol{k}'$ scattering plane, directly reflecting the polarization of angular moment. As seen in the figure, for the Ba + HF → BaF + H reaction, there are two peaks at $\phi_r = 90°$ and 270°, respectively, and the peak at 90° is much higher than the one at 270°. While for Ba + DF → BaF + D, there is a sharp peak at 270° and slight concussion at about 90°, and for Ba + TF → BaF + T reaction, there is only one sharp peak at 270°. The above results indicate that the rotational angular momentum vectors of BaF are not only strongly aligned along the y axis but also oriented along the negative y axis for the three reactions, which is very consistent with the result reported in Ref. [47]. However, the orientation degree of the products is weaker when the mass of the target molecule increases. According to the discussion in Refs. [51] and [55], the difference in the orientation degree may be due to the different harmonic zero point energy (ZPE) of the reactant molecules HF (DF or TF), which induces the different effective potential barrier height for the Ba + HF/DF/TF → BaF + H/D/T reactions.

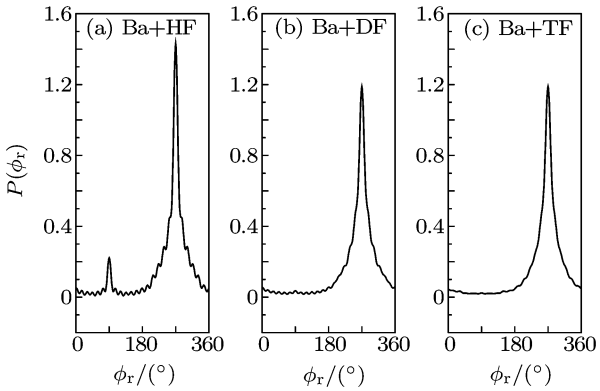


Fig. 8. The distributions of $P(\phi_r)$ for the product molecular from the reaction Ba + HF/DF/TF at E_C = 14 kcal/mol. (a) Ba + HF, (b) Ba + DF, and (c) Ba + TF.

In order to validate more information about the angular momentum polarization, we depict it in the form of polar plots θ_r and ϕ_r averaged over all scattering angles. As can be seen from Fig. 9, the three $P(\theta_r, \phi_r)$ all have a distinct peak at $\theta_r = 90°$ and $\phi_r = 270°$, and this peak becomes lower after H is substituted by D and T, which is in good agreement with the distribution of $P(\theta_r)$ and $P(\phi_r)$. Furthermore, one can also conclude from the distribution of $P(\theta_r, \phi_r)$ that the products are strongly polarized perpendicular to the scattering plane and the products of the reaction are mainly left-handed rotating in planes parallel to the scattering plane.

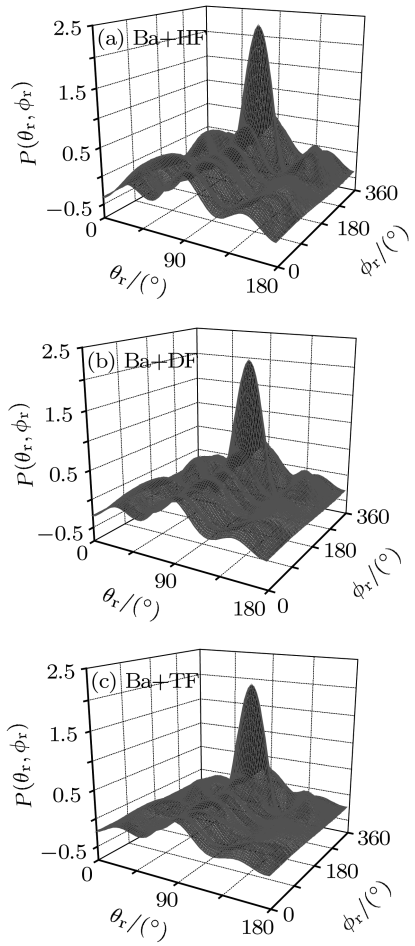


Fig. 9. Polar plots of $P(\theta_r, \phi_r)$ distributions of the reaction Ba + HF/DF/TF averaged over all scattering angles. (a) Ba + HF, (b) Ba + DF, and (c) Ba + TF.

4. Conclusion

In this paper, we have applied the QCT method to study the stereodynamics of the reaction Ba + HF ($v = 0, 2, 4$; $j = 0$) → BaF + H and its isotope substitution reaction based on the LEPS PES. Due to the barrier loaded on the exit valley of the PES, the integral cross section rapidly increases while the collision energy is increasing, and the vibrational excitation of the reagent has great influence on the integral cross section and the DCS; when the vibrational energy of the reagent becomes higher, the value of the reaction

cross section gets larger, and the angular distribution of products is from backward scattering to forward scattering. In addition, the product rotation strongly aligned about the direction of the reagent's relative velocity as the result of HHL mass combination, and the distinct effect of isotope substitution on the stereodynamics of Ba + HF/DF/TF ($v = 0$, $j = 0$) is also revealed.

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