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The characteristics of O+HD ($v = 0$, $j = 0$) reaction dynamics*

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The analytical potential energy function of HDO is constructed at first using the many-body expansion method. The reaction dynamics of O+HD ($v = 0$, $j = 0$) in five product channels are all studied by quasi-classical trajectory (QCT) method. The results show that the long-lived complex compound HDO is the dominant product at low collision energy. With increasing collision energy, O+HD → OH+D and O+HD → OD+H exchange reactions will occur with remarkable characteristics, such as near threshold energies, different reaction probabilities, and different reaction cross sections, implying the isotopic effect between H and D. With further increasing collision energy (e.g., up to 502.08 kJ/mol), O+HD → O+H+D will occur and induce the complete dissociation into single O, H, and D atoms.

Keywords: O+HD, molecular reaction dynamics, analytical potential energy function (APEF), quasi-classical trajectory (QCT) method

PACC: 3400, 3430, 8220T, 3450L

1. Introduction

Exchange reactions are the main methods to separate deuterium (D) out from deuterium-containing water at present, such as the methods of LPCE, CECE, etc.[1−4] In order to investigate the micromechanism of these exchange reactions to further improve the reaction efficiency, it is necessary to study the reaction dynamics of isotopic water molecules, including HDO.

There are many studies on molecular reaction dynamics related to H and O, such as H^-+D_2, O+HF, O+H_2, OH+H_2, etc.,[5−8] but few researches on that of the HDO system, except that Wang *et al*[9] have investigated the rate coefficients for the isotopic exchange reaction OH+D → OD+H, and Sierra *et al*[10] have researched the reaction dynamics of OH+D_2 → HOD+D. This paper focuses on the reaction dynamics characteristics of all product channels of collision O+HD ($v = 0, j = 0$) by using the quasi-classical trajectory (QCT) method, based on constructing the analytical potential energy function (APEF) of HDO by the many-body expansion (MBE) method, and solving the classical Hamilton motion equations with random initial conditions produced by Monte Carlo method.

2. Theories and calculations

2.1. Constructing the APEF of HDO ($\tilde{X}^1A_1$)

An accurate potential surface is a prerequisite for studying the reaction dynamics of O+HD, so the APEF of HDO must be constructed at first. The ground electronic state of HDO can be easily determined as $\tilde{X}^1A_1$ by *ab initio* calculation. Based on the exact dissociation limit of HDO ($\tilde{X}^1A_1$),[11] the APEF in the form of many-body expansion can be expressed as[12]

$$V_{\rm HDO} = V_{\rm O}^{(1)} + V_{\rm HO}^{(2)}(R_1) + V_{\rm OD}^{(2)}(R_2) + V_{\rm HD}^{(2)}(R_3) + V_{\rm HDO}^{(3)}(R_1, R_2, R_3), \quad (1)$$

where $V_{\rm O}^{(1)}$ is the excited energy of O atom from ground electronic state to excited state ^1D, whose experimental value is 1.97 eV.[13] $V_{\rm HO}^{(2)}(R_1)$, $V_{\rm OD}^{(2)}(R_2)$, and $V_{\rm HD}^{(2)}(R_3)$ are the two-body terms, i.e., the APEFs of OH($A^2\Sigma^+$), OD($A^2\Sigma^+$), and HD($X^1\Sigma^+$), respectively. These can be expressed by Murrell–Sorbie function as[14,15]

$$V = -D_{\rm e}(1 + a_1\rho + a_2\rho^2 + a_3\rho^3)\exp(-a_1\rho), \quad (2)$$

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where $\rho = R - R_e$, R and R_e are respectively the interatomic distance and equilibrium interatomic distance; a_1, a_2 and a_3 are the coefficients; D_e is the dissociation energy. Using the same method used in Ref.[16] and the spectra data taken from Ref.[17], the above parameters are calculated and listed in Table 1.

Table 1. The parameters in Murrell–Sorbie APEFs of OH($A^2\Sigma^+$), OD($A^2\Sigma^+$), and HD($X^1\Sigma^+$).

	a_1/nm^{-1}	a_2/nm^{-2}	a_3/nm^{-3}	Re/nm	D_e/eV
OH($A^2\Sigma^+$)	39.726	266.05	1988.5	0.10121	3.3680
OD($A^2\Sigma^+$)	39.701	265.23	1984.9	0.10121	3.3693
HD($X^1\Sigma_g^+$)	39.430	399.00	3492.0	0.07414	4.7470

$V_{\rm HDO}^{(3)}(R_1,\ R_2,\ R_3)$ is the three-body term which can be expressed by a polynomial $P(R_i)$ and a range function $T(R_i)$ as [18]

$$V_{\rm HDO}^{(3)}(R_1,R_2,R_3) = P(R_i)T(R_i), \tag{3}$$

where R_i is interatomic distance, i.e., the internal coordinates of APEF. R_i is often transformed to symmetrical internal coordinates S_i for convenience of calculation. We can choose the equilibrium geometrical values of HDO ($\tilde{X}^1A_1$) as the reference frame for this transformation.[19] Then $P(R_i)$ and $T(R_i)$ can be expressed as functions of S_i[20]

$$\begin{aligned} P =\ & C_0 + C_1S_1 + C_2S_2 + C_3S_2^2 + C_4S_3^2 + C_5S_1S_2 \\ & + C_6S_3^4 + C_7S_1^2 + C_8S_1(S_2^2 + S_3^2) + C_9S_2S_3^2, \end{aligned} \tag{4}$$

$$\begin{aligned} T =\ & [1 - \tanh(\gamma_1S_1/2)] \cdot [1 - \tanh(\gamma_2S_2/2)] \\ & \cdot [1 - \tanh(\gamma_3S_3/2)], \end{aligned} \tag{5}$$

where the ten linear coefficients $C_0 - C_9$ can be solved from ten linear equations constructed based on ten known conditions, i.e., one dissociation energy D_e, three first-order force constants whose values are zero at equilibrium position, and six second-order force constants f_{R1R1}, f_{R2R2}, f_{R1R2}, $f_{\theta\theta}$, $f_{R1\theta}$, and $f_{R2\theta}$. Three parameters γ_1, γ_2, γ_3 can be obtained by optimizing the potential energy surface. Using the same method in Ref.[21], the calculated results are all listed in Table 2.

Table 2. The dissociation energy, equilibrium geometry, force constants, and parameters of three-body term in APEF of HDO ($\tilde{X}^1A_1$).

$D_e = 11.4133$eV	$R_{\rm HO} = R_{\rm OD} = 0.09621$nm	$R_{\rm HD} = 0.15272$nm	$\angle$HOD=105.06°		
$f_{R1R1} = 0.54335$a.u.	$f_{R2R2} = 0.54304$a.u.	$f_{R1R2} = -0.00713$a.u.	$f_{\theta\theta} = 0.16175$a.u.	$f_{R1\theta} = 0.03225$a.u.	$f_{R2\theta} = 0.03220$a.u.
$C_1 = 2.1594$	$C_2 = 1.8767$	$C_3 = -8.4050$	$C_4 = -7.3971$	$C_5 = 4.1677$	$C_6 = 6.8095$
$C_7 = 1.0293$	$C_8 = -7.5491$	$C_9 = -0.3695$	$C_0 = -0.4785$	$\gamma_1 = 1.65$	$\gamma_2 = 1.85$
$\gamma_3 = 3.25$					

So far, the APEF of HDO ($\tilde{X}^1A_1$) has been completely derived, and the potential surface of HDO ($\tilde{X}^1A_1$) constructed.

2.2. The quasi-classical trajectory (QCT) method

The main task in using the QCT method[22] to study the reaction dynamics for atom–diatom collision A+BC is to solve the classical Hamilton motion equations, so as to obtain the characteristics of the collision trajectory on the potential surface. Assuming the Cartesian coordinates of atoms A, B, and C are $A(q_1,\ q_2,\ q_3)$, $B(q_4,\ q_5,\ q_6)$, and $C(q_7,\ q_8,\ q_9)$, then the classical Hamilton equations of this collision system can be written as[23]

$$\begin{aligned} &\partial H/\partial p_i = \dot{q}_i, \quad \partial H/\partial q_i = -\dot{p}_i, \\ &(i = 1, 2, \ldots, 9). \end{aligned} \tag{6}$$

If transforming Cartesian coordinates q_i into centroidal coordinates Q_i, then the above 18 Hamilton equations can be reduced to 12 equations, i.e.,

$$\begin{aligned} &\partial H_{\rm rel}/\partial P_i = \dot{Q}_i, \quad \partial H_{\rm rel}/\partial Q_i = -\dot{P}_i, \\ &(i = 1, 2, \ldots, 6), \end{aligned} \tag{7}$$

where

$$\begin{aligned} H_{\rm rel} =\ & \frac{1}{2\mu_{\rm BC}}\sum_{i=1}^{3} P_i^2 + \frac{1}{2\mu_{\rm A,BC}}\sum_{i=4}^{6} P_i^2 \\ & + U(Q_1, Q_2, ..., Q_6), \end{aligned}$$

$$1/\mu_{\mathrm{BC}} = 1/m_{\mathrm{B}} + 1/m_{\mathrm{C}},$$
$$1/\mu_{\mathrm{A,BC}} = 1/m_{\mathrm{A}} + 1/(m_{\mathrm{B}} + m_{\mathrm{C}});$$

m_{A}, m_{B}, and m_{C} are the masses of atoms A, B, and C, respectively; $U(Q_1, Q_2, ..., Q_6)$ is the APEF of ABC molecules, which can be further transformed to a function of internal coordinates R_{AB}, R_{BC}, and R_{CA} in a form of $V(R_{\mathrm{AB}}, R_{\mathrm{BC}}, R_{\mathrm{CA}})$, where R_{AB}, R_{BC}, R_{CA} are the distances between every two atoms.

After solving the 12 differential equations by using Runge–Kutta–Gill method combining with the Adams–Moulton method,[24] the collision trajectories can be found. Then, the reaction probability, reaction cross section, energy distribution, and scattering angle distribution of reaction products can be calculated based on the statistics of the trajectories. For example, the reaction cross section σ_{r} can be calculated by using

$$\sigma_{\mathrm{r}}(E_{\mathrm{t}}, v, j) = 2\pi \int_0^{b_{\max}} P(E_{\mathrm{t}}, v, j, b) b \mathrm{d}b = \pi b_{\max}^2 \lim_{N\to\infty} \frac{N_{\mathrm{r}}(E_{\mathrm{t}}, v, j)}{N(E_{\mathrm{t}}, v, j)}, \quad (8)$$

where N is the total number of trajectories and N_{r} is the number of specified trajectories in a product channel; $b_{\max}$ is the maximum collision parameter; E_{t} is the initial relative translation energy; v and j are respectively the initial quantum numbers for vibration and rotation of diatomic BC. N should be large enough to match the allowable calculation error, for example, N is chosen to be 20000 in this paper, while $b_{\max}$ can be determined as follows: a series of calculations are performed using a series of test b at certain E_{t}, then the only one which brings the collision to the critical state between elastic and inelastic collision is the $b_{\max}$. Except for E_{t}, v, j, and $b_{\max}$, the other initial conditions are all produced randomly by Monte Carlo method so as to respond to the requirement of statistics.

3. Results and discussion

3.1. Product distributions

There are five product channels for collision O+HD ($v = 0$, $j = 0$), i.e.,

$$\mathrm{O} + \mathrm{HD}(v = 0, j = 0) \rightarrow \begin{cases} \mathrm{OH}(v', j') + \mathrm{D} & \text{channel 1,} \\ \mathrm{O} + \mathrm{HD}(v', j') & \text{channel 2,} \\ \mathrm{OD}(v', j') + \mathrm{H} & \text{channel 3,} \\ \mathrm{HDO}(v', j') & \text{channel 4,} \\ \mathrm{O} + \mathrm{H} + \mathrm{D} & \text{channel 5.} \end{cases} \quad (9)$$

With the initial quantum numbers $v = 0$, $j = 0$ of HD, and with the initial relative translation energy $E_{\mathrm{t}} = 2.092 - 1673.600\,\mathrm{kJ/mol}$, the distribution numbers of collision products in all channels are calculated and listed in Table 3.

Table 3. The product distributions of collision O+HD ($v = 0$, $j = 0$).

E_{t}/(kJ·mol^{-1})	Ch.1	Ch.2	Ch.3	Ch.4	Ch.5	total
2.092		7860		11752		19612
12.552		8459		11140		19599
20.920		9577		10048		19625
29.288		10972		8665		19637
41.840		13211		6504		19715
83.680		18774		1133		19907
167.360	1594	17442	959			19995
251.040	3820	14859	1316			19995
334.720	5247	13523	1225			19995
502.080	5819	13015	396		769	19999
669.440	5524	12253	212		1999	19988
836.800	4369	12755	67		2802	19993
1673.60	2336	12013	52		5596	19997

It can be seen that a number of products are distributed in channel 2 all the time, indicating that the elastic collision O+HD ($v = 0$, $j = 0$) and the inelastic collision O+HD (v', j') always appear easily. At low E_{t}, the collision products are dominantly distributed in channel 4 to form the complex compound HDO.

With increasing E_t, for example, to 167.360 kJ/mol, no complex HDO is formed again; instead, exchange reaction products OH+D in channel 1 and OD+H in channel 3 begin to occur. When E_t further increases, for example, to 502.080 kJ/mol, the complete scattering products in channel 5 appear. This trend indicates that low collision energy is favourable to form complex HDO, however, with increasing collision energy the exchange reactions will occur, and finally the collision system will be scattered as single atoms H, D, and O at high collision energy.

It is remarkable that the product distributions in channels 1 and 3 are asymmetrical but with large probability to produce OH+D and with small probability to produce OD+H; furthermore, the greater the E_t, the more different the probabilities. This phenomenon just represents the isotopic effect between H and D, which can be well explained as follows by using the spectator model.[25] When O atom impacts HD with a considerable relative velocity, it will seize fast the H (or D) to form OH (or OD), while D (or H) maintains its initial state as a spectator. In the centroid coordinate system, if the masses of O, H, D and their combinations are denoted as m_O, m_H, and m_D the initial relative velocity is V, and the initial relative translational energy as E_t, then the available translational energies of OH and OD after collision are different from each other, i.e.,

$$E_t = \frac{1}{2}\frac{m_O(m_H+m_D)}{m_O+m_H+m_D}V^2,$$

$$\begin{aligned} E_{OH}^t &= \frac{1}{2}\frac{m_O m_H}{m_O+m_H}V^2 \\ &= \frac{m_H(m_O+m_H+m_D)}{(m_O+m_H)(m_H+m_D)}E_t \approx 0.37E_t, \\ E_{OD}^t &= \frac{1}{2}\frac{m_O m_D}{m_O+m_D}V^2 \\ &= \frac{m_D(m_O+m_H+m_D)}{(m_O+m_D)(m_D+m_H)}E_t \approx 0.70E_t, \end{aligned}$$

where E_{OH}^t is remarkably smaller than E_{OD}^t. This means that the translational energy of OH after collision is about 37% of E_t, and the rest of 63% can be used for dissociation of HD, while with the OD only about 30% of E_t can be used for dissociation of HD. Obviously, that O impacts H is more beneficial to the dissociation of HD to form OH than that O impacts D to form OD. Therefore, even if the probabilities of O impacting H and D are the same, the probability to from OH is larger than that to form OD.

3.2. Reaction cross sections

In the collision system O+HD ($v = 0$, $j = 0$), only channels 1, 3, and 4 are the reaction channels, whose reaction cross sections σ_r can be calculated by formula (8), and the calculated results are listed in Table 4.

According to these results, a graph is plotted in Fig.1, which illustrates the relation between reaction cross sections σ_r and initial relative translation energy E_t.

Table 4. Reaction cross sections in channels 1, 3, and 4.

$E_t/(\mathrm{kJ\cdot mol^{-1}})$	b_{max}/nm	σ_{Ch1}/nm^2	σ_{Ch3}/nm^2	σ_{Ch4}/nm^2
2.0920	0.5535	0	0	0.5767
12.5520	0.4981	0	0	0.4430
20.9200	0.4783	0	0	0.3680
29.2880	0.4681	0	0	0.3038
41.8400	0.4529	0	0	0.2126
83.6800	0.4239	0	0	0.0321
167.3600	0.3626	0.0329	0.0198	0
251.0400	0.3423	0.0703	0.0242	0
334.7200	0.3152	0.0819	0.0191	0
502.0800	0.2911	0.0775	0.0053	0
669.4400	0.2663	0.0616	0.0024	0
836.8000	0.2582	0.0458	0.0007	0
1673.6000	0.2313	0.0196	0.0004	0

Figure 1 shows the different characteristics of reaction cross sections in channels 1, 3, and 4. In channel 4, the reaction cross section σ_{HDO} reduces so fast with increasing E_{t} that it decreases to zero when E_{t} is only up to 167.36 kJ/mol, indicating that this reaction only occurs under low collision energy without threshold energy. In channels 1 and 3, $\sigma_{\mathrm{OH+D}}$ and $\sigma_{\mathrm{OD+H}}$ both rise at first and then drop with increasing E_{t}, showing that the reaction cross sections both have maximum values and the reactions both proceed with a threshold energy. However, there are obvious differences between $\sigma_{\mathrm{OH+D}}$ and $\sigma_{\mathrm{OD+H}}$, indicating that O+ HD→OH+D occurs more easily than O+ HD→OD+H, and the latter only occurs in a narrow range of E_{t}. The isotopic effect between H and D is shown here again. Figure 1 also shows the general selectivity of channels according to E_{t}, i.e., channel 4 is chosen to form complex compound at low E_{t}, channels 1 and 3 are chosen to carry out the exchange reactions at moderate E_{t}, and channel 5 is chosen gradually instead of channels 1, and 3 to make complete dissociation at high E_{t}.

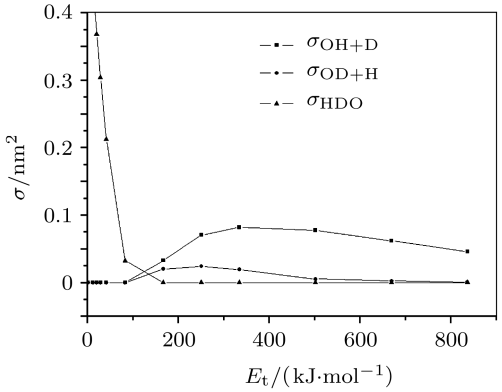


Fig.1. The relation between reaction cross sections σ_{r} and initial relative translation energy E_{t} in channels 1, 3, and 4.

3.3. Collision trajectories

The reaction dynamics characteristics in product channels 1, 3, and 4 can be further interpreted by trajectory graphs before and after collision. Figure 2 illustrates the course of collision among atoms H, D, and O in channels 1 and 3 at the same initial relative translation energy $E_{\mathrm{t}} = 251.04$ kJ/mol. It can be seen that the reaction dynamics characteristics of the two channels are generally similar, but the product OH in channel 1 moves more smoothly while the product OD in channel 3 vibrates and rotates more evidently after collision, the reason of which is mainly that the mass of D is heavier than that of H.

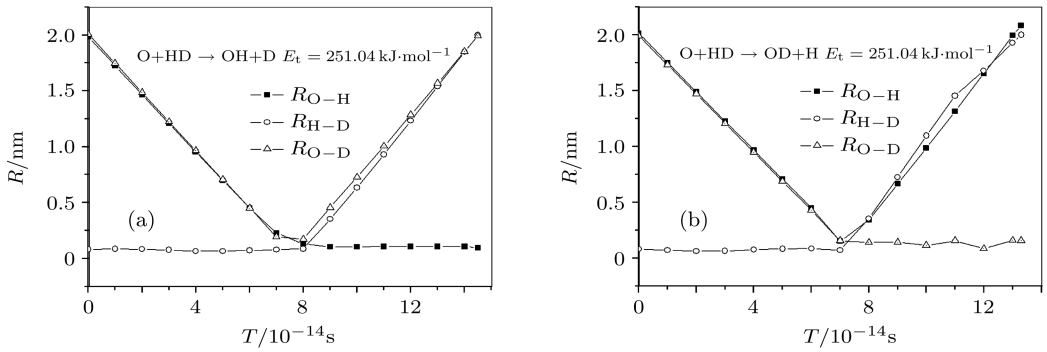


Fig.2. The trajectories of collisions O+HD → OH+D (a) and O+HD → OD+H (b).

Figure 3 presents the collision process from O+HD to HDO at $E_{\mathrm{t}} = 83.68$ kJ/mol in channel 4, showing how the long-lived complex HDO is formed. Since a deep potential-well, whose value is 1101.27 kJ/mol, exists on the potential surface of HDO, the O atom cannot be disengaged from the deep well but is only engaged in vibration and rotation together with H and D to form the complex compound at low collision energy.

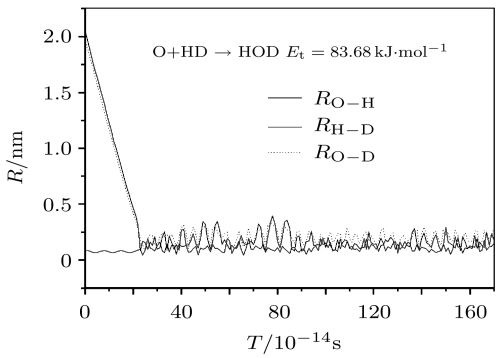


Fig.3. The trajectories of collision O+HD → HOD.

3.4. Distribution of scattering angle

The distributions of scattering angle in channels 1 and 3 are compared at $E_t = 502.08\,\mathrm{kJ/mol}$, as shown in Fig.4.

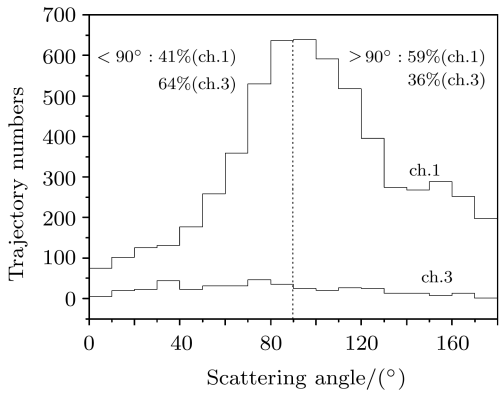


Fig.4. The distributions of scattering angle for channels 1 and 3 at $E_t = 502.08\,\mathrm{kJ/mol}$.

In channel 1, the forward scattering number is 2393, being 41% of total scattering while backward scattering number is 3242, being 59% of total scattering. In channel 3, the forward scattering number is 255 (64% of the total) while backward scattering number is 141 (36% of the total). The asymmetry of scattering angle distributions in the two channels implies that the collision types are both direct collision without a stage of long-lived complex. The forward scattering ratio of OH is larger than the backward scattering ratio, but that of OD in channel 3 is contrary to this, which shows the isotopic effect of H and D. This may be due to the fact that the translational energy of OH can only occupy 37% of E_t while that of OD can occupy 70%, as shown by the above calculation. The large translational energy is beneficial to the forward scattering; however, small translational energy is helpful to the backward scattering.

4. Conclusions

The APEF of HDO has been constructed by using the many-body expansion method. The reaction dynamics characteristics of collision O+HD ($v = 0$, $j = 0$) on the potential surface of HDO were studied via solving the classical Hamilton equations of the collision system, whose initial conditions were generated by Monte–Carlo method. The conclusions are summarized as follows:

(i) The complex HDO is the dominant collision product, and no OH+D and OD+H exchange reactions occur at low collision energy E_t (e.g., $E_t = 2.092 - 86.83\,\mathrm{kJ/mol}$).

(ii) For the moderate E_t (e.g., $E_t \geq 167.36\,\mathrm{kJ/mol}$), OH+D and OD+H exchange reactions appear in product channels 1 and 3 with an unsymmetrical product distribution, which displays the different reaction probabilities and indicates the isotopic effect between H and D. Furthermore, that the reaction cross sections $\sigma_{\mathrm{OH+D}}$, $\sigma_{\mathrm{OD+H}}$ both rise at first and then drop with increasing E_t shows the reactions both proceeding with a threshold energy. But the difference between $\sigma_{\mathrm{OH+D}}$ and $\sigma_{\mathrm{OD+H}}$ implies that O+HD → OH+D occurs more easily than O+HD → OD+H.

(iii) At a high collision energy (e.g., $E_t \geq 502.08\,\mathrm{kJ/mol}$), the non-reaction collision O+HD → O+H+D happens in channel 5, which induces complete dissociation to the single H, D, and O atoms.

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