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The stereodynamics study on the isotopic substitution $C+SH(D,T) \rightarrow H(D,T)+CS$ reactions on the new $HCS(X^2A')$ potential energy surface

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The quasi-classical trajectory (QCT) calculations are carried out to investigate the isotopic substitution effect on title reactions based on the recently developed, accurate potential energy surface (PES) of the $HCS(X^2A')$ (Song & Zhang et al. *Sci. Rep.* 2016, 6, 37734). The total integral cross sections (ICSs) and vibrational state resolved ICSs are obtained for $C+SH(D, T) \rightarrow H(D, T)+CS$ reactions. In addition, differential cross sections (DCS) and two angle distribution functions $P(\theta_r)$, $P(\phi_r)$ at different collision energies are investigated. It is found that the peaks of $P(\theta_r)$ and $P(\phi_r)$ become lower with the reagent molecule SH turning into SD and ST.

1. Introduction

Among many ways to study the properties of $A+BC \rightarrow AB+C$ system, the quasi-classical trajectory (QCT) method is an effective one to investigate the molecular reaction dynamics.¹⁻⁶ In recent decades, the $HCS(X^2A')$ system has received a great deal of attention both from theorists and experimentalists.⁷⁻²³ As a fundamental reaction intermediate in combustion processes,¹² it plays an important role in molecular formation processes of interstellar clouds.¹¹ Stoecklin *et al.*⁷⁻⁹ investigated two analytic models of the lowest

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potential energy surface (PES) based on the *ab initio* calculations and the related thermodynamical, spectroscopic and empirical data. Then with the PES, they calculated the rate constant of $C(^3P) + SH(X^2\Pi) \rightarrow H(^2S) + CS(X^1\Sigma^+)$ reaction at 300K using QCT method. In 2004, Voronin¹⁰ reported a global PES for the lowest adiabatic X^2A' state of HCS using the high-quality *ab initio* calculations (aug-cc-pVTZ basis set) at the MRCI level. By employing the PES, the integral cross section (ICS) and rate constants of the $C(^3P) + SH(X^2\Pi) \rightarrow H(^2S) + CS(X^1\Sigma^+)$ reaction have been calculated using the QCT method. Recently, our group reported an accurate global adiabatic PES for the ground state of HCS, in building which both aug-cc-pVQZ (AVQZ) and aug-cc-pV5Z (AV5Z) atomic basis sets have been employed.²⁴ In order to improve the accuracy of PES, such obtained *ab initio* energies are then extrapolated to the complete basis set. Based on the PES, the ICS, differential cross section (DCS) and rate constants of reaction $C + SH$ were calculated using the QCT method, which agree well with other theoretical results.⁷⁻¹⁰

Among the vast breadth of theoretical work related to the $HCS(X^2A')$ system, there have been several reports on the accurate PES. In 1983, Goddard²⁵ firstly predicted the equilibrium geometries of the lowest $^2A'$ and $^2A''$ electronic states of HCS using the single-double configuration interaction (SDCI) method with a double-zeta basis. For the $^2A'$, the calculated equilibrium geometries are: $R_{CH}=1.086\text{\AA}$, $R_{CS}=1.570\text{\AA}$, and $\alpha_{HCS}=132.8^\circ$, for the $^2A''$, $R_{CH}=1.066\text{\AA}$, $R_{CS}=1.556\text{\AA}$, and $\alpha_{HCS}=180^\circ$, respectively. Senekowitsch *et al.*²⁶ calculated the potential energy, electric dipole and transition moment functions for the X^2A' and A^2A'' electronic states of the HCS radical at the multiconfiguration self-consistent field (MCSCF) CI level. They also reported that in linear geometry the two lowest X^2A' and A^2A'' states become degenerate components of the $^2\Pi$ state and exhibit a strong Renner-Teller coupling effect. In 1999, Chen *et al.*¹⁸ presented the hyperfine structures of the HCS and isovalent HCO, HSiS and HSiO radicals using the density functional theory (DFT) and multi-reference single and double excitation configuration interaction (MRSDCI) methods. Mitrushchenkov *et al.*¹⁹ performed theoretical studies on HC_nS ($n = 1 - 12$) radicals in the $^2\Pi$ electronic ground state using the Hartree Fock (HF), complete active space self-consistent field (CASSCF) and MRCI methods with different

basis sets. In experiment, Habara *et al.*^{20–23} detected microwave transition of the HCS, HSC, H¹³CS and HS¹³C radicals in the X²A' ground electronic state.

Although there have been a lot of reports about C + SH reaction, the investigation about isotope substitution effect on this reaction is rare. So in the present work, the QCT method is adopted to study the isotopic effect for the C+SH(D, T) → H(D, T)+CS reactions based on the new global PES.²⁴ The selected collision energies are from 0.01 to 1.20 eV, and the vibrational and rotational levels of SH(D, T) are taken as $v = 0$ and $j = 0$, respectively. The paper is organized as follows. In Section 2, we briefly describe the main details of the theoretical methodologies. In Section 3, the detailed results and discussion of the QCT simulations are accounted. Finally, the conclusions are summarized in Section 4.

2. Theory

2.1. PES and QCT calculations The PES was obtained by our group using a wealth of *ab initio* energies calculated at the multi-reference configuration interaction method with AVQZ and AV5Z atomic basis sets. In order to improve the accuracy of PES, such obtained *ab initio* energies are then extrapolated to the complete basis set limit. We have shown that the reaction $C(^3P) + SH(X^2\Pi) \rightarrow H(^2S) + CS(X^1\Sigma^+)$ is highly exothermic, with the exothermicity being ~ 84.3 kcal mol⁻¹.²⁴

The QCT calculation method used in this paper is similar to that used in other previous literatures.^{27–34} In the present calculation, the classical Hamilton equations are integrated numerically in three dimensions. Because the reaction is highly exothermic which can occur at the lower collision energy, and when the collision energy is greater than a value, the ICS of the reaction may be changing very little, so when we study the effect of isotope substitution C+SH(D,T) ($v = 0$, $j = 0$) reactions on stereodynamics at the different collision energy, the collision energy is chosen from 0.01 to 1.20 eV. In this paper, for each reaction, a batch of 10 0000 trajectories are run, the integration step size in the trajectories is chosen to be 0.1 fs, and the initial distance from the C atom to the

center of mass of SH is set to be 20 Å, which can guarantee conservation of the total energy and angular momentum. The assignment of the product CS rotational quantum numbers is carried out by equating the classical rotational angular momentum to the value of $\sqrt{j'(j'+1)}\hbar$. Subsequently, the usual histogram binning (HB) method is used to assign the final product states in which the classical vibrational quantum numbers were rounded to their nearest integers.

2.2. Product rotational polarizations To describe product rotational polarizations, we will use the standard product rotational polarization theory,^{27–31,35–43} but for the sake of simplicity, here we only summarize the details relevant to the present work. The angle relationship between the initial relative velocity and the final relative velocity vectors is described in the center-of-mass (CM) reference frame. The z axis is parallel to the initial relative velocity vector $\mathbf{k}$, and the y axis is perpendicular to the $x-z$ plane containing the initial and final relative velocity vectors $\mathbf{k}$ and $\mathbf{k}'$. The angle θ_t between $\mathbf{k}$ and $\mathbf{k}'$ is so-called scattering angle. θ_r and ϕ_r are the dihedral and the azimuthal angles of the final rotational angular momentum $\mathbf{j}'$.

The ICS is then calculated by

$$\sigma = \pi b_{\max}^2 \frac{N_r}{N}, \quad (1)$$

where N_r is the number of reactive trajectories in a total number of N , and $b_{\max}$ is the maximal value of the impact parameters. The distribution function $P(\theta_r)$, which describes the $\mathbf{k} - \mathbf{j}'$ correlation with $\mathbf{j}' \cdot \mathbf{k} = \cos\theta_r$, is expanded in a series of Legendre polynomials,

$$P(\theta_r) = \frac{1}{2} \sum_k (2k+1) a_0^{(k)} p_k(\cos\theta_r), \quad (2)$$

in which the expanding coefficients $a_0^{(k)}$, described by $a_0^{(k)} = \int_0^\pi p(\theta_r) p_k(\cos\theta_r) \sin\theta_r d\theta_r = \langle p_k(\cos\theta_r) \rangle$ are orientation parameter (k is odd) or alignment parameter (k is even), and k is integer to ensure the convergent results of $P(\theta_r)$. The dihedral angle distribution function $P(\phi_r)$ describing the $\mathbf{k} - \mathbf{k}' - \mathbf{j}'$ correlation can be expanded in a Fourier series as

$$P(\phi_r) = \frac{1}{2\pi} \left(1 + \sum_{\text{even}, n \geq 2} a_n \cos n\phi_r + \sum_{\text{odd}, n \geq 1} b_n \sin n\phi_r \right), \quad (3)$$

where

$$a_n = 2\langle \cos n\phi_r \rangle, b_n = 2\langle \sin n\phi_r \rangle, \quad (4)$$

In the present calculations, $P(\theta_r)$, $P(\phi_r)$ are expanded up to $k = 18$ and $n = 24$, respectively, which acquires a good convergence.

3. Results and discussion

The reaction ICSs computed using Eq. (1) are displayed in Figure 1. As can be seen in this figure, the value of ICS is very large at the low collision energies, and rapidly decreases with increase of relative translational energy, which is very similar to other exothermic reactions.^{44–48} In order to further investigate the isotopic effect of $C + SH(D, T) \rightarrow H(D, T) + CS$ reactions, we also plotted the ICSs of $C + SH(D, T)$ reactions in Figure 1. As the mass increases, the ICSs for the D(T) are all smaller than that of the H, and the larger the mass, the smaller the related ICSs, especially at lower collision energy. The reason for these results may be that at the lower collision energy, the ICS is probably attributable to the insertion mechanism, and when the mass of target molecule becomes much bigger, the reaction becomes more difficult. At the higher collision energy, the reactant velocity is very fast, the reaction is mainly controlled by abstraction mechanism. However because of the mass impact of target molecule being very small, the difference among the three reactions is small. Therefore, according to the Eq. (1), the probability and the biggest impact parameter b_{max}^2 at different collision energies for the reaction $C + SH(D, T)$ reactions are plotted and shown in Figure 2. An obvious decline is seen in Figure 2(b) with increasing collision energy, which is ascribed to the deep well and barrierless aspect of the PES. As expected for barrierless PES, it is clear that the value of b_{max}^2 is large and rapidly decreases when the collision energy < 0.2 eV, but is small and decreases very slowly when the collision energy > 0.2 eV. From these figures it can be seen that the shape of ICSs is mainly influenced by the b_{max}^2 dependence for these three reactions.

The DCSs offer an excellent opportunity to study the most familiar vector correlation

between the reagent and product relative velocity $k - k'$. Figure 3 represents the DCSs, which reflect the angular distribution for the reactions $C + SH(D, T) \rightarrow H(D, T) + CS$ at the collision energy of 0.1 eV, and 0.8 eV. It is clear that at different collision energies, the $C + SH(D, T)$ reactions are dominated by strongly forward - backward scattering, which is consistent with the complex-forming mechanism for this reaction, and is similar to other exothermic reactions.⁴⁹⁻⁵² In order to gain more insight into the collision energy effect on the DCSs for the $C + SH(D, T)$ forming channel, the opacity function $P(b)$, the reaction probability as a function of the impact parameter b , is often used. The opacity function $P(b)$ for title reaction at the collision energy of 0.1 and 0.8 eV is shown in Figure 4. At the low collision energy, it is clear from left panel that the forward - backward scattering is mainly due to the reactions with big impact parameters. This behavior corresponds to a simple indirect reaction mechanism. While at the higher collision energy, impact parameters become little, the forward and backward scattering becomes strong and the products tend to forward - backward symmetrical scattering. The reason for these results may be due to the deep well in PES and the title reaction's being mainly controlled by an indirect reaction mechanism. The increase in collision energy can speed up the complex rotation, which makes the products tend to forward - backward symmetrical scattering. At the same collision energy, when the target molecule SH is substituted by SD and ST, one can find the same forward - backward distribution. As the collision energy increases, it is obvious that the relative velocity of the product molecule of the $C + SD(T) \rightarrow D(T) + CS$ reactions are higher than that of $C + SH \rightarrow H + CS$, which may make forward - backward scattering stronger.

Figures 5 presents the product vibrational state resolved ICS at the collision energy of 0.1 and 0.8 eV for $C + SH(D, T)$. It is easy to figure out that the vibrational excitation of the product is quite strong, with the most probable population appearing at a high vibration number, which has been predicted by Stoecklin *et al.*⁷⁻⁹ and means that more translational energy can be converted into the excited vibrational states of products, and the shapes of the ICSs for each reaction are found to resemble each other. At lower collision energy (0.1 eV), the $v' = 17, 15$, and 15 are the most populated vibrational states

for C+SH, C+SD, and C+ST, respectively. The results demonstrate that if C+SD(T) reactions are expected to generate the most populated vibrational states at $v' = 17$, the C+SD(T) needs more energy. So at the same collision energy, the most populated vibrational state v' of C+SH $\rightarrow$ H+CS is higher than that of C+SD(T) $\rightarrow$ D(T)+CS. One can also find that the range of v' is expanded with the increasing collision energy, which means that more translational energy can be converted to vibrational energy. Another feature is that the CS products are inclined to distribute in lower vibrational states at higher collision energy. At lower collision energy, the target molecule SH rotates slowly, then the product molecules are easy to generate a higher level of vibration, while at higher collision energy, the reaction of C+SH is prone to the abstraction reaction.

Above statements give the investigation about the isotopic effects on the scalar properties of the title reaction. To consider isotopic effect fully, the isotopic effect on vector properties are also studied, such as $P(\theta_r)$ and $P(\phi_r)$ shown in Figure 6 and Figure 7, which describe the relative alignment of the $\mathbf{k}$ and $\mathbf{j}'$ vectors and the relative orientation of the $\mathbf{k}$, $\mathbf{k}'$ and $\mathbf{j}'$ vectors. In Figure 6, it is clear that the corresponding maximum of $P(\theta_r)$ for the product molecule is at 90° and the $P(\theta_r)$ distribution is symmetric with respect to 90° . Since the product rotational angular momentum vector is strongly aligned along a direction at right angles to the relative velocity direction, one can conclude that the three reactions are mainly governed by the “out plane” mechanism. Furthermore, the peaks of $P(\theta_r)$ display that the degree of the rotational alignment of the product decreases when the target molecule SH is substituted by SD and ST. The peak of the $P(\theta_r)$ distribution for C + SH reaction is the strongest, while for C + ST reaction it is the weakest both at lower collision energy and higher collision energy. The reason of this difference can be attributed to the mass factor, which has been illustrated by many other studies.^{31,53} Obviously because of the values of mass factor (ξ) for the C + SH(D, T) reactions being 0.00826, 0.0160, 0.0233, respectively, according to $\xi = \frac{m_A m_C}{(m_A + m_B)(m_B + m_C)}$, the $P(\theta_r)$ distribution for C + SH reaction is the strongest. From Figure 6, it is clear that no matter at lower or at higher collision energy, the isotope effect on $P(\theta_r)$ distribution is regular, and the larger the mass factor, the weaker the product molecular alignment. It can be

concluded that the enhancement of the mass factor of the reactants will weaken the degree of the rotational alignment. Moreover, the overall trends of the $P(\theta_r)$ distributions slowly increase as the collision energy increases from 0.01 eV – 1.20 eV. This means that the degree of the rotational alignment of the product becomes stronger with the increase of the collision energy. As is well known, the distribution of $P(\theta_r)$ is correlated to the rotational alignment parameter factor $\langle P_2(\mathbf{j}' \cdot \mathbf{k}) \rangle$, which also provides information about the product rotational alignment.

Similarly, Figure 7 shows the dihedral angle distributions $P(\phi_r)$ describing the $\mathbf{k}-\mathbf{k}'-\mathbf{j}'$ correlations. It can be clear that the $P(\phi_r)$ distribution tends to be asymmetric with respect to the $\mathbf{k}-\mathbf{k}'$ scattering plane. Seen from this three panels, the main peaks of $P(\phi_r)$ distributions all appear at $\phi_r = 90^\circ$ and $\phi_r = 270^\circ$, and the peaks of $P(\phi_r)$ at $\phi_r = 90^\circ$ are slightly higher than the ones at $\phi_r = 270^\circ$, which indicates that the rotational angular momentum vector of the product molecule is not only aligned, but also slightly oriented along the positive y-axis, i.e., the isotope effect on $P(\phi_r)$ distribution is also noticeable for the same collision energy. What is more, it can be seen that the product molecule orientation becomes weaker after H is substituted by D and T, and that the orientation of the T + CS is the weakest. Another feature is that the peaks of $P(\phi_r)$ increase with the collision energy increasing no matter at $\phi_r = 90^\circ$ or at $\phi_r = 270^\circ$ for the $\text{C} + \text{SH}(\text{D}, \text{T}) \rightarrow \text{H}(\text{D}, \text{T}) + \text{CS}$. As stated previously, the isotope effect on $P(\phi_r)$ distribution is also regular.

4. Conclusion

This paper investigated the isotopic substitution effect on $\text{C} + \text{SH}(\text{D}, \text{T}) \rightarrow \text{H}(\text{D}, \text{T}) + \text{CS}$ reactions with different collision energy by using the QCT method. Because of the deep potential well existed in the used PES, the calculated cross sections show decreasing trends as the collision energy increasing. And when the target molecule SH is substituted by SD and ST, the cross sections for the D(T) are all smaller than that of the H, especially at lower collision energy. The reason for these results may be that at the

lower collision energy, the reaction is probably attributable to the insertion mechanism. The calculated DCS shows that the degree of the forward - backward scattering increases with the increase of reactant molecular mass. The production vibrational state resolved ICS obtained shows that the vibrational excitation of the product is quite strong, with the most probable population appearing at high vibration level. With the collision energy increasing, the range of v' is expanded, which means that more translational energy can be converted to vibrational energy. Meanwhile, the peak of the $P(\theta_r)$ and $P(\phi_r)$ distribution for C + SH reaction is the strongest, while for C + ST reaction it is the weakest both at lower and at higher collision energy. And we also found that the product rotation prefers an out-of-plane mechanism rather than an in-plane reaction mechanism with increasing collision energy.

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Figure 1: Calculated integral cross sections as a function of collision energy for the C + SH(D, T).

Figure 2: Reaction probability and $b_{\max}^2$ for the C + SH(D, T) at the collision energy of 0.01-1.20 eV.

Figure 3: Differential cross section for $C + SH(D, T) \rightarrow H(D, T) + CS$ with fixed collision energies (0.1 eV, 0.8 eV).

Figure 4: Reaction probability as a function of the impact parameter (opacity function) for $\text{C} + \text{SH}(\text{D}, \text{T})$ with fixed collision energies (0.1 eV, 0.8 eV).

Figure 5: Integral cross sections for the $\text{C} + \text{SH}(\text{D}, \text{T})(v = 0, j = 0) \rightarrow \text{H}(\text{D}, \text{T}) + \text{CS}(v', j')$ at $E_{\text{col}} = 0.1$ and 0.8 eV.

Figure 6: The distribution of $P(\theta_r)$ for the product molecule from reactions $\text{C} + \text{SH}(\text{D}, \text{T}) \rightarrow \text{H}(\text{D}, \text{T}) + \text{CS}$.

Figure 7: The distribution of $P(\phi_r)$ for the product molecule from reactions $\text{C} + \text{SH}(\text{D}, \text{T}) \rightarrow \text{H}(\text{D}, \text{T}) + \text{CS}$.