

REGULAR ARTICLE

Theoretical calculation of vector correlations for the reaction

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Abstract: The stereodynamics of the reaction $\text{H}(^2\text{S}) + \text{NH} (\nu = 0, 1, 2, 3; j = 0) \rightarrow \text{N}(^4\text{S}) + \text{H}_2$ are studied using the quasi-classical trajectory method on a double many-body expansion potential energy surface to understand the alignment and orientation of the product molecules in the collision energy range of 2–20 kcal·mol⁻¹. The vibrational-rotational quantum number of the NH molecules is specifically investigated for $\nu = 0, 1, 2$, and 3 and $j = 0$. The $P(\theta_r), P(\phi_r), P(\theta_r, \phi_r)$, differential cross section [DCS; $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$], and average rotational alignment factor $\langle P_2(\cos \theta_r) \rangle$ are calculated. The stereodynamics results indicate that the reagent vibrational quantum number and initial collision energy significantly affect the distributions of the $k-j', k-k'-j'$ and $k-k'$ vector correlations along with $\langle P_2(\cos \theta_r) \rangle$. In addition, while DCS is extremely sensitive to the collision energy, it is not significantly affected by the vibrational excitation of the reagents.

Keyword: quasi-classical trajectory method, stereodynamics, potential energy surface, vector correlation

1. Introduction

Reactions between nitrogen and hydrogen atoms have attracted the attention of experimental and theoretical chemists for the past 30 years. With the development of molecular beam and polarized laser light techniques, [1,2] elementary chemical reactions can now be easily studied. Much of the information about an elementary chemical reaction is summarized by its excitation function or rate constant. Morley[3] studied NO formation

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from nitrogen compounds in hydrogen flame using laser fluorescence and determined the rate constant for the reaction between NH and H atoms at 1790–2200 K. In 1990, Koshi and Yoshimura[4] measured the rate constant for the reaction between $N(^4S)$ and H_2 at high temperature (1950–2850 K). In addition, the rate constant for the reaction $N + H_2 \rightarrow NH + H$ was reported as $1.60 \times 10^{14} \exp(-12650/T) (\pm 35\%) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ from 1950 to 2850 K.[5] In 2005, Adam et al.[6] obtained a rate constant of $k = (1.9 \pm 0.5) \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction $NH + H \rightarrow N + H_2$ using quasi-static laser-flash photolysis at room temperature.

Poveda and Varandas [7] theoretically derived the repulsive double many-body expansion[8] (DMBE) potential energy surface (PES) for the triatomic fragment of the $NH_2(4A')$ reactive system at the MRCI/aug-cc-pVQZ level of theory.[9,10] For both the forward reaction $N(^4S) + H_2 \rightarrow H(^2S) + NH$ and reverse reaction $H(^2S) + NH \rightarrow N(^4S) + H_2$, their calculations agreed with the experimental results and the best-available theoretical estimates. Consequently, many dynamic studies of forward and reverse reactions followed [11–15] this successful derivation of the DMBE PES using high-level ab initio calculations. For example, Zhang et al.[11] investigated the effect of isotope substitution on the stereodynamics of forward reactions at a collision energy of $40 \text{ kcal} \cdot \text{mol}^{-1}$ and discussed the distributions $P(\theta_r)$, $P(\phi_r)$, and $P(\theta_r, \phi_r)$ of the vector correlations between products and reagents. Yu et al.[12] studied the rotational excitation and collision energy of the forward reaction $N(^4S) + H_2 (v=0, j=0, 2, 5, 10) \rightarrow NH(X^3\Sigma^-) + H$ using the quasi-classical trajectory (QCT) method. Using the same method, Xia et al.[13] investigated the effects of isotope substitution and collision energy on the stereodynamics of the forward reaction. Yu et al.[14] discussed the product polarization of the forward reaction $N(^4S) + H_2 (v=0-3, j=0) \rightarrow NH(X^3\Sigma^-) + H$ for collision energies from 25 to $140 \text{ kcal} \cdot \text{mol}^{-1}$ and calculated four polarization-dependent differential cross sections (PDDCSs) along with the distributions $P(\theta_r)$, $P(\phi_r)$, $P(\theta_r, \phi_r)$ and $\langle P_2(\cos \theta_r) \rangle$ for the rotational ground state and vibrational excited states of the reagent. For

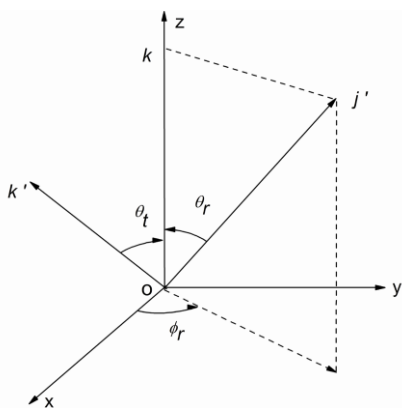


Figure 1: Center-of-mass coordinate system that describes the correlation between k , k' , and j' .

the reverse reaction $\text{H}(^2\text{S}) + \text{NH} \rightarrow \text{N}(^4\text{S}) + \text{H}_2$, Han et al.[15] applied the QCT and quantum mechanical methods to calculate the reaction probabilities at zero total angular momentum, the total reaction cross section, and the product rotational alignment for the ground rotational–vibrational state of the reverse reaction. To date, the stereodynamics of the reverse reactions and the effects of collision energy and vibrational quantum number on the DMBE PES have not been discussed. Thus, in this study, to evaluate the effects of collision energy and vibrational quantum number on the stereodynamics of reverse reactions, we performed QCT calculations of the DMBE PES. We calculated the three angular distributions [$P(\theta_r)$, $P(\phi_r)$, and $P(\theta_r, \phi_r)$], the DCSs, and the average rotational alignment factor $\langle P_2(\cos \theta_r) \rangle$ based on the DMBE PES for different vibrational excited states and the rotational ground state of the reagents. Moreover, we investigated the effects of collision energy and the vibrational excited states of the reagents on the stereodynamics. As mentioned above, many interesting dynamic results were reported in the $\text{NH}_2(4\text{A}')$ system, which motivated us to study the effects of vibrational excitation on the stereodynamics in the reaction $\text{H}(^2\text{S}) + \text{NH} (v = 0, 1, 2, 3; j = 0) \rightarrow \text{N}(^4\text{S}) + \text{H}_2^*$.

2. Theory

2.1 Rotational polarization of the products

The center of mass (CM; **Figure 1**) is the reference frame used in this work. The z-axis denotes the direction of the relative velocity vector $\mathbf{k}$ of the reactants. The scattering x–z-plane contains the relative velocity vectors $\mathbf{k}$ and $\mathbf{k}'$ of the reactants and products. The y-axis is perpendicular to the scattering plane; θ_r and ϕ_r are the azimuthal and polar angles of the product rotational angular momentum vector $\mathbf{j}'$, respectively, and θ_t is the scattering

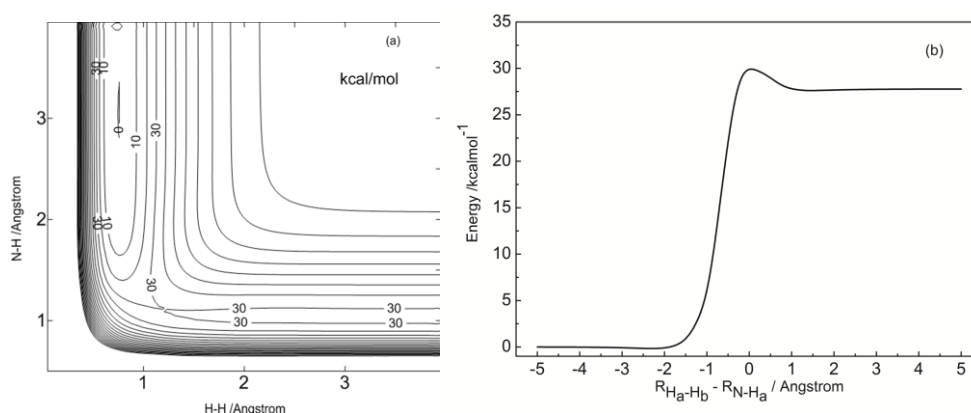


Figure 2: Potential energy surfaces showing (a) contours for the stretching of N–H–H in a linear configuration and (b) the reaction profile along the minimum-energy path from reactants to products on our chosen PES for the $\text{H} + \text{NH}$ reaction.

angle between k and k' .

Using Legendre polynomials, the distribution function $P(\theta_r)$ describing the $k-j'$ correlation can be expanded as [16-18]

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

In this study, $P(\theta_r)$ is expanded to $k = 18$ to ensure convergence, and

$$a_0^{(k)} = \int_0^\pi P(\theta_r) P_k(\cos \theta_r) \sin \theta_r d\theta_r = \langle P_k(\cos \theta_r) \rangle, \quad (2)$$

The expansion coefficient $a_0^{(k)}$ is either the orientation parameter (when k is odd) or the alignment parameter (when k is even). In particular, for $k = 2$, $a_0^{(k)}$ represents the product rotational alignment and is expressed as

$$a_0^{(2)} = \langle P_2(\cos \theta_r) \rangle = \langle P_2(j' \cdot k) \rangle = \frac{1}{2} \langle 3 \cos^2 \theta_r - 1 \rangle, \quad (3)$$

Since the rotational alignment of the products is measured in most experiments, we only calculate the average rotational alignment factor $P(\theta_r)$.

Using a Fourier series, the dihedral angle distribution function $P(\phi_r)$ for the $k-k'-j'$ correlation is expanded as

$$P(\phi_r) = \frac{1}{2\pi} \left(1 + \sum_{\text{even}, n \geq 2} a_n \cos n\phi_r + \sum_{\text{odd}, n \geq 1} b_n \sin n\phi_r \right), \quad (4)$$

where $a_n = 2\langle \cos n\phi_r \rangle$, and $b_n = 2\langle \sin n\phi_r \rangle$. To achieve convergence, $P(\phi_r)$ is expanded to $n = 24$.

In the CM frame of reference, the direction of j' depends on θ_r and ϕ_r , and the spatial distribution function $P(\theta_r, \phi_r)$ of the product rotational angular momentum j' is given by

$$P(\theta_r, \phi_r) = \frac{1}{4\pi} \sum_k \sum_{q \geq 0} [a_{q\mp}^k \cos(q\phi_r) - a_{q\mp}^k \sin(q\phi_r)] C_{kq}(\theta, 0), \quad (5)$$

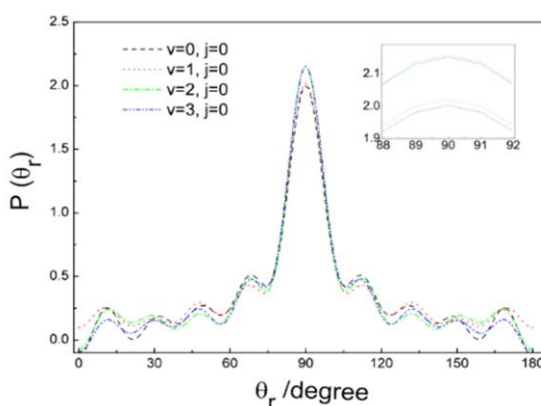


Figure 3: The $P(\theta_r)$ distribution for the title reaction calculated on the DMBE PES at a collision energy of 10 kcal·mol⁻¹.

where $C_{kq}(\theta_r, \phi_r)$ denotes the modified spherical harmonics, which are expressed as $a_{q\mp}^k = 2\langle C_{k|q|}(\theta, 0) \cos(q\phi_r) \rangle$ when k is odd and $a_{q\mp}^k = 2i\langle C_{k|q|}(\theta, 0) \sin(q\phi_r) \rangle$ when k is even. In this study, $P(\theta_r, \phi_r)$ is expanded to $k = 7$ to ensure convergence.

The full three-dimensional angular distribution function $P(\omega_t, \omega_r)$ for the $k-k'-j'$ correlation is

$$P(\omega_t, \omega_r) = \sum_{kq} \frac{2k+1}{4\pi} \frac{1}{\sigma} \frac{d\sigma_{kq}}{d\omega_t} C_{kq}(\theta_r, \phi_r)^*, \quad (6)$$

where the angles $\omega_r = \theta_r, \phi_r$ and $\omega_t = \theta_t, \phi_r$ refer to the coordinates of the unit vectors k' and j' along the directions of the product's relative velocity and angular momentum vectors in the CM frame of reference, respectively; $C_{kq}(\omega_r)$ denotes the modified spherical harmonics; σ represents the integral cross section; and $(1/\sigma)(d\sigma_{kq}/d\omega_t)$ denotes the PDDCSs and is expressed as

$$\frac{1}{\sigma} \frac{d\sigma_{kq\mp}}{d\omega_t} = \sum_{k_1} \frac{2k_1+1}{4\pi} S_{kq\mp}^k C_{k,q}(\theta_t, 0), \quad (7)$$

where $k_1 > q$, and

$$S_{kq\mp}^{k_1} = \langle C_{k_1q}(\theta_t, 0) C_{kq}(\theta_r, 0) \times [(-1)^q e^{iq\phi_r} \mp e^{-iq\phi_r}] \rangle, \quad (8)$$

The items in the angle brackets in Eq. (8) are averages.

Most previous studies involving double-molecular experiments have focused on the polarization components $k = 0$ and $k = 2$. For the case of $k = 0$, Eq. (7) reduces to $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$. This can be simply interpreted as a differential reaction cross section and reflects the molecular scattering direction of the product. To ensure good convergence, the generalized differential polarization reaction cross section is expanded to $k_1 = 7$.

2.2 PES properties

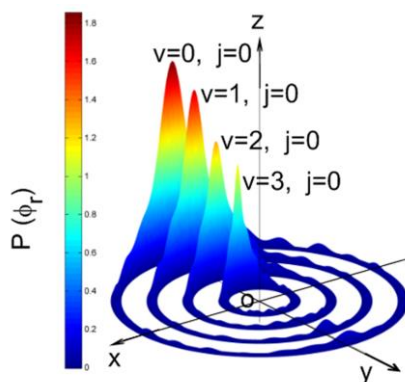


Figure 4: The $P(\phi_r)$ distribution for the title reaction calculated on the DMBE PES at a collision energy of 10 kcal·mol⁻¹.

The contours of the DMBE PES for the linear arrangement are highlighted in **Figure 2(a)**. The contours are equally spaced at $10 \text{ kcal}\cdot\text{mol}^{-1}$. The PES was analytically expressed based on a new switch function and the DMBE, which is highly efficient for calculating the QCT. In addition, the PES has a saddle point with coordinates $(1.17 \text{ \AA}, 1.12 \text{ \AA})$. **Figure 2(b)** shows the reaction profile along the minimum energy path from reactants to products on the selected PES. The forward barrier height of the reaction $\text{N} + \text{H}_2 \rightarrow \text{H} + \text{NH}$ is approximately $29.2 \text{ kcal}\cdot\text{mol}^{-1}$, which agrees well with the experimental results[4,5] and indicates that the reaction is endothermic. Conversely, the reverse reaction $\text{N} + \text{NH} \rightarrow \text{N} + \text{H}_2$ has a lower barrier; thus, the threshold of the reverse reaction is lower.

2.3 QCT calculations

The most rigorous theoretical calculation of the integral cross section of the gas-phase triatomic reaction is obtained using quantum dynamics based on scattering theory. If the quantum effect is negligible, the QCT approach yields reasonably reliable results. The standard QCT method is described in Refs. 19–21. In this study, we adopt an adiabatic approach and do not consider the non-adiabatic effects reported in Ref. 22. The QCT method is applied to calculate stereodynamic properties in Refs. 23–28. In this study, the vibrational and rotational levels of the reactant molecules are $v = 0, 1, 2$, and 3 and $j = 0$, respectively. The

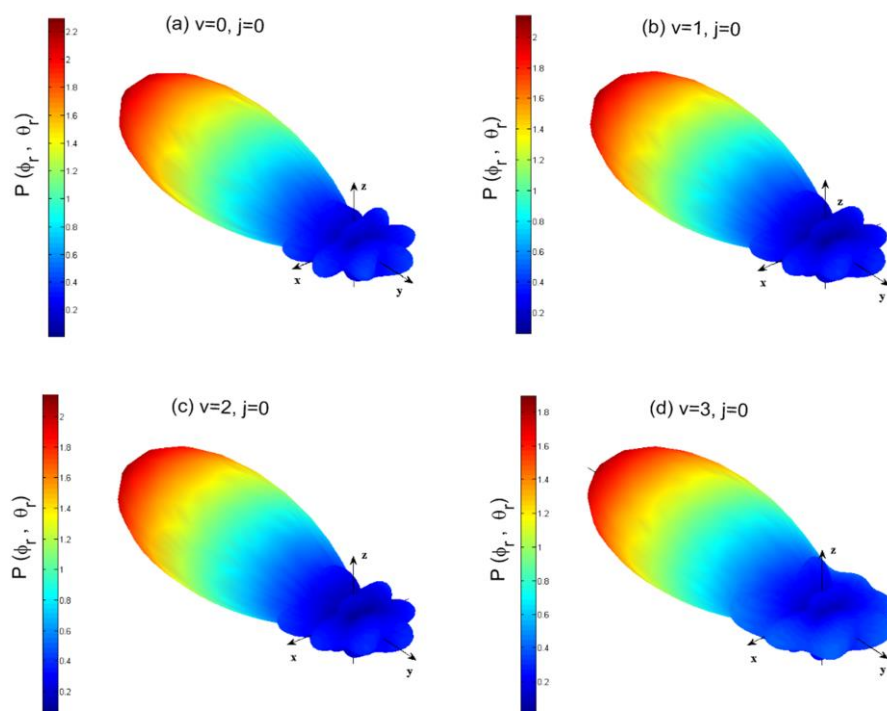


Figure 5: The $P(\theta_r, \phi_r)$ distribution for the title reaction calculated on the DMBE PES at a collision energy of $10 \text{ kcal}\cdot\text{mol}^{-1}$: (a) $v = 0, j = 0$; (b) $v = 1, j = 0$; (c) $v = 2, j = 0$; and (d) $v = 3, j = 0$.

collision energy (E_c) for the reaction ranges from 2 to 20 kcal·mol⁻¹ in steps of 2 kcal·mol⁻¹. In the calculations, batches of 100,000 trajectories are run for each reaction, and the integration step size is 0.1 fs to conserve the total energy and total angular momentum. The initial azimuthal and polar angles of the reagent molecule's internuclear axis are randomly sampled using the Monte Carlo method, and the trajectories begin with an initial distance of 15 Å between the H atom and the CM of NH.

3. Results and discussion

3.1 Reagent vibrational excitation and stereodynamics

Figure 3 shows the calculated $P(\theta_r)$ distribution of the product H₂ produced by the reaction H(²S) + NH ($v = 0, 1, 2, 3; j = 0$) → N(⁴S) + H₂ at a collision energy of 10 kcal·mol⁻¹ on the DMBE PES, which describes the k - j' correlation. The distribution $P(\theta_r)$ has an apparent maximum and is symmetric about $\theta_r = 90^\circ$ because of the planar symmetry of the system. The calculation results suggest that the excitation of the initial NH vibration hardly affects the stereodynamics. The maxima of $P(\theta_r)$ are located at angles θ_r close to 90° for $v = 0, 1, 2$, and 3, suggesting that the product rotational angular momentum vector is strongly aligned perpendicular to the relative velocity direction.

The distribution $P(\phi_r)$ at the collision energy of 10 kcal·mol⁻¹ on the DMBE PES is shown in **Figure 4**. In **Figure 4**, $P(\phi_r)$ represents the dihedral angle distribution of j' with respect to the k - k' plane, where the k - k' scattering plane is at an angle ϕ_r of approximately 180° . $P(\phi_r)$ tends to be asymmetric about $\phi_r = 180^\circ$, reflecting the strong polarization of the angular momentum. The maximum value of $P(\phi_r)$ at angle ϕ_r close to 270° suggests that the rotational angular momentum vector j' of the product is mainly oriented along the

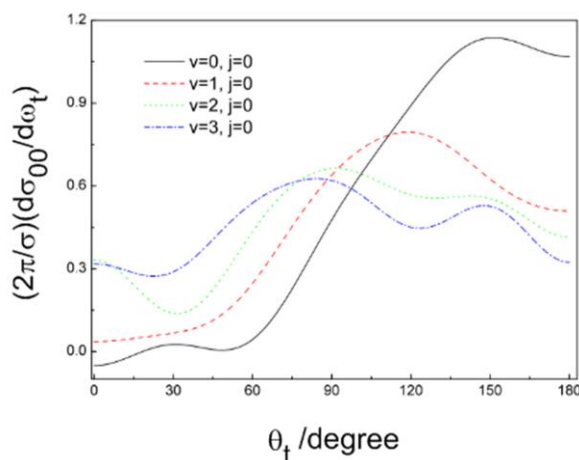


Figure 6: The PDDCS $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$ as a function of θ_t at a collision energy of 10 kcal·mol⁻¹.

negative direction of the y-axis in the CM frame. Moreover, further information obtained from the peak positions of $P(\phi_r)$ with different vibrational quantum numbers suggests that increasing the vibrational quantum number causes the peak of $P(\phi_r)$ to decrease rapidly. These results suggest that the orientation of the dihedral angle distribution of j' depends on the vibrational quantum number.

To further investigate the effect of vibrational excitation on the reaction and validate the angular momentum polarization, we calculate the spatial distribution function $P(\theta_r, \phi_r)$ of the rotational angular momentum j' of the product molecule. The results are shown in the form of polar plots of θ_r and ϕ_r averaged over all scattering angles at collision energy $E_c = 10 \text{ kcal}\cdot\text{mol}^{-1}$ (**Figure 5**). The distribution $P(\theta_r, \phi_r)$ at 90° and 270° clearly agrees with the distributions $P(\theta_r)$ and $P(\phi_r)$ at $E_c = 10 \text{ kcal}\cdot\text{mol}^{-1}$. The distribution $P(\theta_r, \phi_r)$ shows that j' is preferentially oriented along the negative direction of the y-axis in the vibrational ground state and all excited states. Therefore, the distribution $P(\theta_r, \phi_r)$ suggests that the product H_2 is strongly polarized perpendicular to the scattering plane and mainly rotates in the plane parallel to the scattering plane.

The DCS provides detailed information about the reaction stereodynamics and describes the $k - k'$ correlation or the scattering direction of the product. The DCS for the

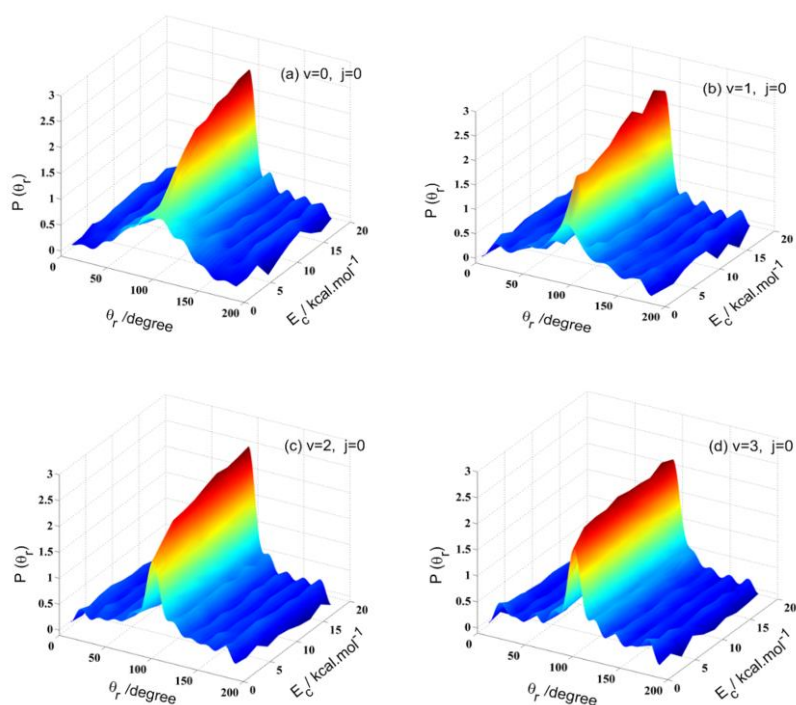


Figure 7: The $P(\theta_r)$ distribution as a function of polar angle θ_r and collision energy for the title reaction: (a) $v=0, j=0$; (b) $v=1, j=0$; (c) $v=2, j=0$; and (d) $v=3, j=0$.

reaction $\text{H}(^2\text{S}) + \text{NH} (v = 0, 1, 2, \text{ and } 3; j = 0) \rightarrow \text{N}(^4\text{S}) + \text{H}_2$ at $E_c = 10 \text{ kcal}\cdot\text{mol}^{-1}$ is shown in **Figure 6** as a function of the scattering angle. The reaction $\text{H} + \text{NH} (v = 0; j = 0)$ is clearly dominated by strong backward scattering, whereas the reaction $\text{H} + \text{NH} (v = 1, 2, 3; j = 0)$ is governed by lateral scattering. Lateral scattering becomes more likely to occur as the vibration state of the reactants increases; this is because the ratio between the reduced mass of product H_2 and the mass of N affects the scattering direction of H_2 , which is less affected by the initial dynamics of the reactant NH .

3.2 Collision energy and reaction stereodynamics

Figures 7(a)–(d) show the distributions $P(\theta_r)$ for four different vibrational quantum states and the rotational ground state on the PES with collision energy in the range of 2–20 $\text{kcal}\cdot\text{mol}^{-1}$. The results shown in **Figure 7** validate the abovementioned ordering. For a constant vibrational quantum state and rotational ground state on the PES, high collision energies are associated with high $P(\theta_r)$ distributions. This suggests that the rotational angular momentum of the product is strongly affected by the orientation, and that the degree of orientation increases with increasing collision energy.

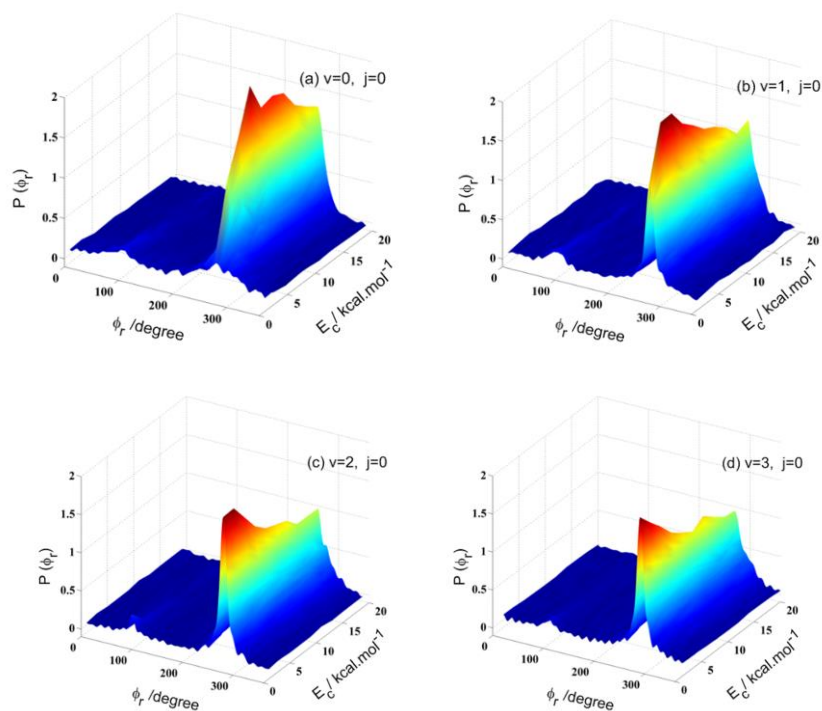


Figure 8: The $P(\phi_r)$ distribution as a function of polar angle ϕ_r and collision energy for the title reaction: (a) $v = 0, j = 0$; (b) $v = 1, j = 0$; (c) $v = 2, j = 0$; and (d) $v = 3, j = 0$.

Figures 8(a)–8(d) show the dependences of the distribution $P(\theta_r)$ on collision energy for four different vibrational quantum states and the rotational ground state on the PES for collision energy in the range of 2–20 kcal·mol⁻¹. $P(\theta_r)$ is asymmetric about $\phi_r = 180^\circ$, reflecting the strong polarization of the angular momentum. Each surface has only one clear peak at ϕ_r close to 270° ; this implies that the product H₂ exhibits left-handed rotation in the planes parallel to the scattering plane ($\mathbf{k}$ – $\mathbf{k}'$), and that the rotational angular momentum vector of the product is oriented along the negative y-axis. For all reactant rotational states, the peak values of $P(\theta_r)$ decrease with increasing collision energy.

The simple DES $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$ describes the $\mathbf{k}$ – $\mathbf{k}'$ correlation and the scattering direction of the product. This DES is not associated with the orientation or alignment of the product rotational angular momentum vector $\mathbf{j}'$ in **Figure 9** and decomposes into the initial vibrational states of the reactant molecule NH with (a) $v = 0$ and $j = 0$, (b) $v = 1$ and $j = 0$, (c) $v = 2$ and $j = 0$, and (d) $v = 3$ and $j = 0$. Based on the results of $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$, we can conclude that the products are strongly scattered backward for the initial vibrational ground state of NH at low collision energy, and the increase of the collision energy reduces this. However, the DCS is significantly affected by the vibrational quantum number ($v = 0, 1, 2, 3$)

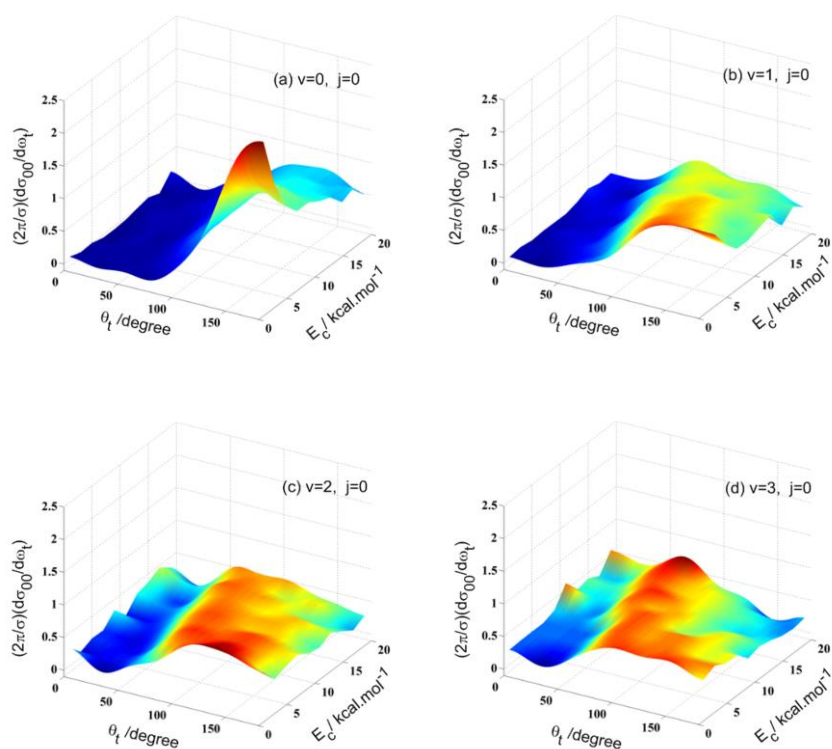


Figure 9: The DCS as a function of scattering angle θ_t and collision energy for the title reaction: (a) $v = 0, j = 0$; (b) $v = 1, j = 0$; (c) $v = 2, j = 0$; and (d) $v = 3, j = 0$.

of the reactants because of the contribution of the abstract reaction.

4. Conclusions

In this study, QCT dynamics were used to study the product polarizations in the reaction $\text{H}(\text{}^2\text{S}) + \text{NH}(v = 0, 1, 2, 3; j = 0) \rightarrow \text{N}(\text{}^4\text{S}) + \text{H}_2$ based on the DMBE PES. The distributions $P(\theta_r)$, $P(\phi_r)$, and $P(\theta_r, \phi_r)$ the DCS $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$ were calculated for collision energies ranging from 2 to 20 kcal·mol⁻¹ and four different vibrational excited states. The results suggest that the collision energy and vibrational excited states affect the rotational polarizations of the product in a variable manner. The distribution $P(\theta_r)$ suggests that the product vibrational alignment depends on the vibrational quantum number and collision energy, and the product rotational angular momentum vector j' of the product is strongly aligned in the vertical direction of the relative velocity k . The distributions $P(\phi_r)$ and $P(\theta_r, \phi_r)$ suggest that the product rotational angular momentum vector j' is oriented along the negative direction of the y-axis in the CM frame. In addition, the DES $(2\pi/\sigma)(d\sigma_{00}/d\omega_t)$ shows that the reaction $\text{H} + \text{NH}(v = 0; j = 0)$ is dominated by strong backward scattering, whereas the reaction $\text{H} + \text{NH}(v = 1, 2, 3; j = 0)$ is governed by lateral scattering, which is enhanced as the vibration state of the reactants increases.

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