

REGULAR ARTICLE

Quasi-Classical Trajectory Study of the Effects of Reactant Ro-Vibrational Excitation on the $\text{H} + \text{LiH}^+ \rightarrow \text{Li}^+ + \text{H}_2$ Reaction

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Abstract: Theoretical studies of the dynamics of the $\text{H} + \text{LiH}^+ \rightarrow \text{Li}^+ + \text{H}_2$ reaction have been performed using quasiclassical trajectory (QCT) method via a three-dimensional potential energy surface (PES) structured by Martinazzo et al. [J. Chem. Phys., 119 (2003), 11241]. The differential cross section (DCS) and reaction probability branching ratio between dissociation channel and the title channel are strongly affected by the vibrational excitation and translational energy. There is a Vander Waals well about 0.286eV in the product valley of the PES, which is too shallow to form a long-lived complex in the transition state, and the lifetime of the LiH_2^+ complex becomes shorter with collision energy increasing. The calculation of stereodynamics indicates that rotational angular momentum (j') polarization of the product molecule is sensitive to both rotational and vibrational excitations at the collision energy 0.03eV. With the increasing vibrational energy of reactant, the j' polarization increases and the molecular rotation of the products prefers an in-plane reaction mechanism rather than the out-of-plane mechanism. However, the opposite conclusion has been drawn for rotation excitation.

AMS subject classifications: 68U05, 74F25, 81v55

Key words: Quasiclassical trajectory theory, Stereodynamics, Differential cross section

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1 Introduction

Recently, the title reaction has attracted a lot of attentions because of the importance of LiH molecule and related reactions in the early universe [1-6]. According to the standard Big Bang model, the primordial universe is full of radiation at a quite high temperature. During this time, the universe is opaque [7], and a majority of moleculars are ionized including the LiH⁺ ion [8-9]. Generally, the LiH molecule and its ionic variant are thought to be a coolant because they can absorb thermal energy by internal ro-vibrational excitations and release it through emission of photons [10]. When the temperature of the galaxy is reduced, the universe gets transparent. The time is called recombination epoch, during which the lithium chemistry has played a vital role [11]. That is why people focus on the LiH molecule and its ionic related reaction.

In order to get an accurate three-dimensional potential energy surface (PES) of LiH₂⁺ system, Bodo and co-workers have made a significant progress in past decade [10, 12-17]. Ro-vibrational levels of the ground electronic state LiH₂⁺ have also been studied [18-20]. Haxton et al have reviewed the indirect dissociative recombination of LiH₂⁺, they showed that LiH⁺ complex is weakly bounded with dissociation energy of 0.112 eV, therefore this ion is easily broken up [21]. Much work has been done in LiH molecule related reaction recently [22-24], and this work has been performed on accurate three-dimensional potential energy surfaces which allowed reactions within the two lowest-lying electronic states of the LiH₂⁺ system [17]. The ground-state H+LiH⁺→Li⁺+H₂ reaction is a barrierless, exoergic process. The exoergicity of the title reaction is 4.365(4.609) eV with (without) the zero-point energy corrections. For this reaction, the first quantum mechanical (QM) calculations were implemented for the collinear geometries by Bodo and coworkers [25]. They argued that a direct reactive dynamics should be expected. Afterwards, Pino and coworkers studied the thermal rate constants and integral cross sections of different ro-vibrational states for three channels by QCT method [26]. They found that this reaction was well described by the classical capture model, and the break-up channel at energies of a few tenths of eV should be considered. The influence of the low energy collision induced dissociation (CID) channel has been discussed by Roy and coworkers using a time-dependent wave packet approach [27].

As mentioned above, much effort has been made in the title reaction. However, most of the work is concerning the scalar properties, in order to get a whole dynamics of a reaction, the vector properties should also be taken into account. Stereodynamics of the title reaction had been carried out by our previous work [28]. We stressed that the reaction mainly behaves as an exoergic reaction rather than an insertion mechanism because of a shallow Vander Waals well about 0.286eV. We also calculated the changes of j' polarization with

different collision energy. Li and coworkers had also done much work on the title reaction [29, 30]. In this paper, the influence of different ro-vibrational excitation states of reagent LiH^+ ion has been studied. In Section 2 we give a short introduction of the theory of stereodynamics. Then the calculated results and discussions are presented in Section 3. Finally, conclusions are given in Section 4.

2 Theory

2.1 Theory of stereodynamics

The stereodynamics of the title reaction has been calculated by QCT method. The distribution $P(\theta_r)$ can be written as

$$P(\theta_r) = \frac{1}{2} \sum_k (2k+1) a_0^{(k)} P_k(\cos \theta_r) \quad (2.1)$$

Where

$$a_0^{(k)} = \int_0^\pi P(\theta_r) P_k(\cos \theta_r) \sin \theta_r d\theta_r = \langle P_k(\cos \theta_r) \rangle \quad (2.2)$$

The coefficients $a_0^{(k)}$ are called orientation (k is odd) or alignment (k is even) parameters. k=2 indicate the product rotational alignment:

$$a_0^2 = \langle P_2(\cos \theta_r) \rangle = \langle P_2(\mathbf{j}' \cdot \mathbf{k}) \rangle = \frac{1}{2} \langle 3 \cos^2 \theta_r - 1 \rangle \quad (2.3)$$

Where P_2 is the second Legendre moment and the brackets indicate an average over the distribution of \mathbf{j}' about \mathbf{k} . In this work, we only calculate the rotational alignment parameter of the product.

The dihedral angle distribution function $P(\phi_r)$ describing k-k'-j' correlation can be expanded in Fourier series as

$$P(\phi_r) = \frac{1}{2\pi} \left(1 + \sum_{\text{even}, n>2} a_n \cos n\phi_r + \sum_{\text{odd}, n \geq 1} b_n \sin n\phi_r \right) \quad (2.4)$$

Where

$$a_n = 2 \langle \cos n\phi_r \rangle \quad \text{and}$$

$$b_n = 2 \langle \sin n\phi_r \rangle$$

The detailed theory can be found in others' work [31-40], and the differential cross-section(DCS) is given by

$$\frac{\partial\sigma}{\partial\theta} = \pi b_{\max}^2 \frac{N_R(\theta)}{N} \quad (2.5)$$

Where b_{\max} is impact parameter, $N_R(\theta)$ is the number of reactive trajectories which product scatters at the angle of θ , and the N is the total number of trajectories.

2.2 Potential energy surface and QCT calculation

The ab initio PES used in this paper was obtained from Martinazzo et al [17]. The ground and the first excited state of the PESs are separated in energy throughout the reactive regions. The reaction of the ground surface had been studied, which has a barrierless, exoergic process. The minimum energy reaction path of the title reaction is shown in **Figure 1**. There is a shallow Vander Waals well of about 0.286eV at the exit channel, which has a deep influence on the title reaction. Although the well is too shallow to form a long-lived complex in the transition state, short-lived complex exists in low collision energy. For this work, batches of 50,000 trajectories were sampled for each reaction, and the integration step size is chosen as 0.1fs. The trajectories are started at an initial distance of 30Å between the H atom and the center of mass of the LiH⁺ ion.

3 Results and discussion

3.1 Products of Li⁺+H+H/ Li⁺+H₂ reaction probability branching ratio

It is important that LiH⁺ ion has a low dissociation energy ($D_0=0.112\text{eV}$). Consequently, the CID channel $\text{LiH}^+\text{+H} \rightarrow \text{Li}^+\text{+H+H}$ become dominant at high energy. The reaction probability branching ratio between CID channel and the title channel had been calculated at different energies. The results are shown in **Table 1** and **Figure 2**, which indicate that the reaction probability branching ratio increase obviously by vibration exciting and collision energy increases. Compared with that, the reaction probability branching ratio is almost invariant with different rotation states. Time-dependent wave packet approach used by Roy and coworkers indicated the same phenomenon that CID channel made primary contribution in this reaction [27]. In order to reduce the impact of CID channel, the collision energy was kept

at 0.03 eV for further study.

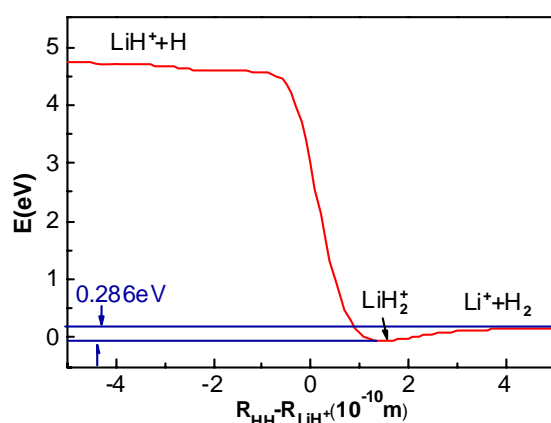


Figure 1: The minimum energy path of the title reaction.

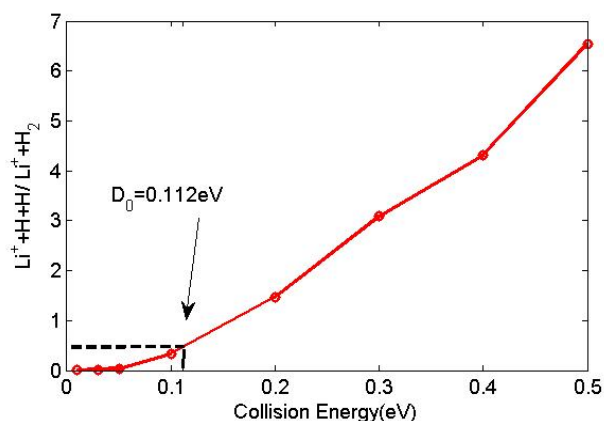


Figure 2: Products of $\text{Li}^+ + \text{H} + \text{H} / \text{Li}^+ + \text{H}_2$ reaction probability branching ratios at different collision energies.

Table 1: Products of $\text{Li}^+ + \text{H} + \text{H} / \text{Li}^+ + \text{H}_2$ with different ro-vibrational states at the collision energy 0.03 eV.

Different states of vibration with $j=0$	$v=0$	$v=1$	$v=2$
$\text{Li}^+ + \text{H} + \text{H} / \text{Li}^+ + \text{H}_2$	0.018	0.700	3.913
Different states of rotation with $v=0$	$j=0$	$j=5$	$j=10$
$\text{Li}^+ + \text{H} + \text{H} / \text{Li}^+ + \text{H}_2$	0.018	0.014	0.015

Generally, the main reason for the open of the dissociation channel is the energy of $\text{Li}-\text{H}$ bond exceeds the binding energy ($D_0=0.112\text{eV}$). The **Figure 1** indicates that the CID channel become more important when the collision energy surpasses 0.112eV. The vibrational excitation of reactant can bring more energy into the reaction system than rotational excitation, so that the vibrational excitation has a larger influence on the reaction probability branching ratio.

3.2 The differential cross sections (DCSs) at different ro-vibrational states

The DCSs of the title reaction at the collision energy 0.03eV (**Figure 3**) show an asymmetrical forward-backward scattering. It means that except for direct mechanism, indirect

mechanism also exists in this collision energy. With the increase of vibration quantum number, DCS ratios between extreme forward and backward scattering are 1.63, 2.11 and 2.67 respectively, which means that the title reaction prefers forward scattering when exciting the LiH⁺ bond. The DCS calculation results are similar as our prior studies [31]. It demonstrates that insert mechanism is weakened by vibration exciting clearly. It is because that a shallow Vander Waals well about 0.286eV at the exit channel has a great influence on the title reaction. Though the well is too shallow to form a long-lived complex in transition state, short-lived complex exists in low collision energy. In addition, the CID channel become dominant by vibration exciting, so that the title reaction cross section decrease with vibrational excitation, while the rotation excitation has little effects on DCS. The calculated DCS results are in good agreement with the reaction probability branching ratio results mentioned above.

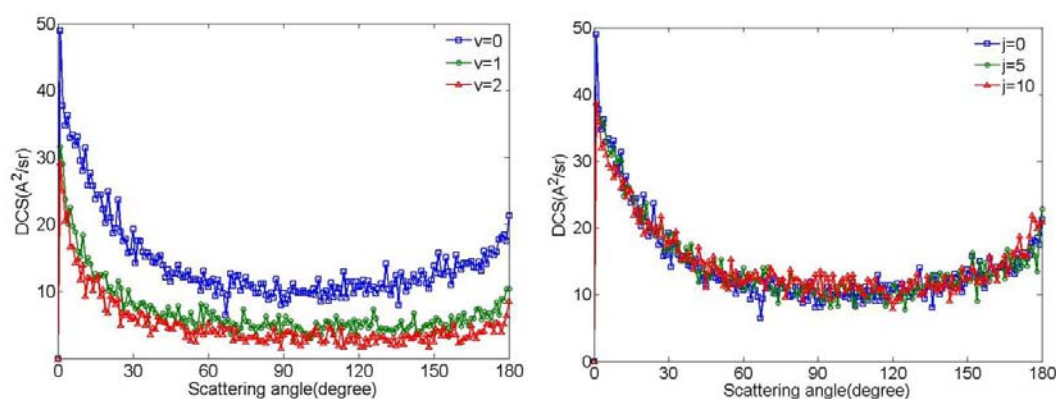


Figure 3: The DCS for different initial ro-vibrational states (v, j) of LiH⁺. Left panel for the chemical reaction $\text{H}+\text{LiH}^+(\text{E}_{\text{col}}=0.03\text{eV}, j=0) \rightarrow \text{Li}^{++}\text{H}_2$ reaction at different vibrational quantum number of $v=0$ (the blue line with squares), $v=1$ (the green one with circles), $v=2$ (the red one with triangles) and right panel for the chemical reaction $\text{H}+\text{LiH}^+(\text{E}_{\text{col}}=0.03\text{eV}, v=0) \rightarrow \text{Li}^{++}\text{H}_2$ reaction at different rotational quantum number of $j=0$ (the blue line with squares), $j=5$ (the green one with circles), $j=10$ (the red one with triangles).

3.3 Polarization of the Product with different ro-vibrational states

In order to get a whole dynamics of the reaction, we have calculated the distributions of $P(\theta_r)$ and $P(\varphi_r)$ for the reaction $\text{H}+\text{LiH}^+ \rightarrow \text{Li}^{++}\text{H}_2$ at different ro-vibrational states shown in **Figure 4** and **Figure 5**, respectively. The $P(\theta_r)$ distribution reflects the k - j' correlation and **Figure 4** shows the calculated results. The peak appears at $\theta_r=90^\circ$, and symmetric with

respect to 90° , which describes that j' is strongly aligned along the direction perpendicular to the reagent relative velocity vector k at the collision energy of 0.03eV. Obviously, with the vibrational excitation, the peak of $P(\theta_r)$ becomes sharper, which indicates that j' polarization is enhanced with the increase of vibrational quantum number. Conversely, the angular momentum polarization j' is receded with the advance of rotational quantum number.

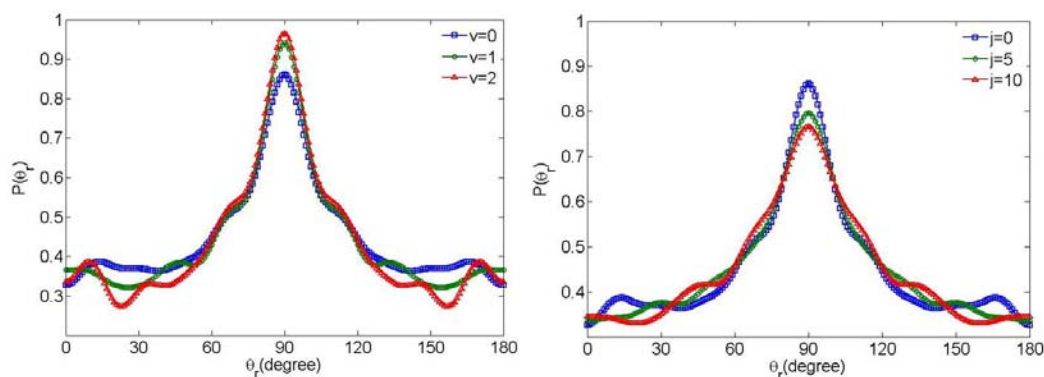


Figure 4: Polarization distribution of $P(\theta_r)$ for H_2 product of the $H+LiH^+(E_{col}=0.03eV, j=0) \rightarrow Li^+H_2$ reaction at different vibrational quantum number of 0(blue squares), 1(green circles), 2(red triangles)(left) and rotational quantum number of 0(blue squares), 5(green circles), 10(red triangles) with $v=0$ (right). The $P(\theta_r)$ distribution reflects the $k-j'$ correlation.

Figure 5 displays a similar phenomenon that j' polarization is stronger with the increase of vibrational quantum number but weaker with the rotational states exciting. As mentioned above, the dihedral angle distributions $P(\phi_r)$ reflects the $k-k'-j'$ correlation and the peak is located on 90° and 270° , moreover the peak of 90° is stronger than the other one. Obviously, it demonstrates the rotational angular momentum vector of the product molecule is mainly aligned along the y-axis of the center-of-mass (CM) frame, but is a little oriented along the positive direction of the y-axis. When the vibrational state is excited, j' orientation along the positive direction of the y-axis becomes stronger. Traditionally, when product molecule rotation in planes parallel to the scattering plane, the term 'in-plane' will be used to refer to it. So the reaction prefers the in-plane mechanism with the increase of vibration state excitation. However, it seems that the direction of product confused when the reactant has been rotational excited.

In order to express the degree of polarization of j' with different ro-vibrational states, we have calculated the CM frame alignment parameters $\langle P_2(j' \cdot k) \rangle$. The results are shown in **Table 2**. The $\langle P_2(j' \cdot k) \rangle$ values of product molecule H_2 indicate that the alignment of the product rotational angular momentum j' is quite strong for the title reaction [28]. The

$\langle P_2(j' \cdot k) \rangle$ values are increased by vibration exciting, which clearly indicates that the product molecule rotational angular momentum polarization gets stronger with the increase of vibration excitation. Compared to that, the opposite results have been got for rotation excitation, which is consistent with the above study.

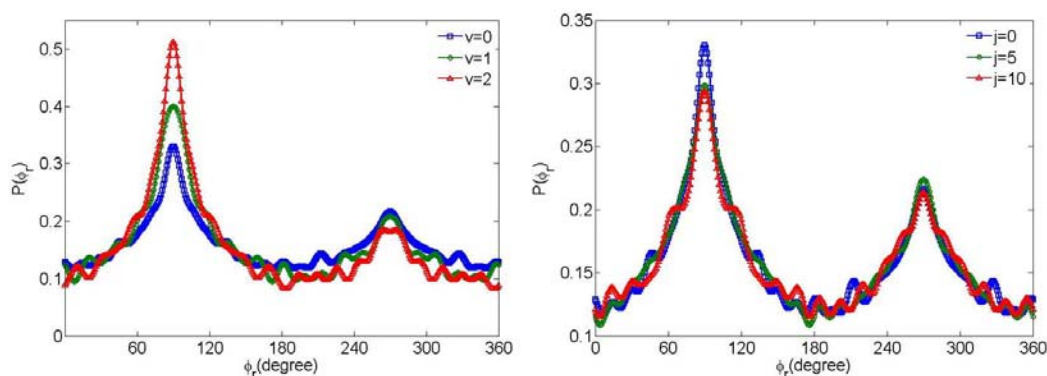


Figure 5: Polarization distribution of $P(\phi_r)$ for H₂ product of the H + LiH⁺ ($E_{\text{col}}=0.03$ eV, $j=0$) \rightarrow Li⁺+H₂ reaction at different vibrational quantum number of 0(blue squares), 1(green circles), 2(red triangles)(left) and rotational quantum number of 0(blue squares), 5(green circles), 10(red triangles) with $v=0$ (right). The $P(\phi_r)$ distribution reflects the $k-k'-j'$ correlation.

Table 2: The rotational alignment parameters $\langle P_2(j' \cdot k) \rangle$ for the reaction H+LiH⁺ ($v=0,1,2$, $j=0,5,10$) \rightarrow Li⁺ + H₂ at the collision energy 0.03eV.

$\langle P_2(j' \cdot k) \rangle (E_{\text{col}}=0.03\text{eV})$		
$v=0$	$v=1$	$v=2$
-0.105	-0.125	-0.140
$j=0$	$j=5$	$j=10$
-0.105	-0.102	-0.101

4 Conclusions

The effects of the reactant ro-vibrational excitation on the reaction H+LiH⁺ \rightarrow Li⁺+H₂ have been studied by QCT method in this work. The PES we used for this reaction has a shallow

Vander Waals well in the product valley, and the CID channel is facile open for the low dissociation energy of LiH^+ ion. The title reaction mainly undergoes a direct mechanism, but an insertion mechanism appears at low collision energy. Similar feature has been detected by increasing both vibrational and translational energies, which demonstrate that the CID channel changes to principal, and the title reaction prefers a direct mechanism rather than indirect one. However, the calculated results of the reaction probability branching ratio and DCS show little variation with rotational excitation. Consequently, the initial energy of the reaction leads a decisive role in the reaction probability branching ratio and DCS. The stereodynamics results indicate that rotational angular momentum (j') polarization of the product increases and the molecular rotation of the product prefer an in-plane reaction mechanism rather than the out-of-plane mechanism with the vibrational exciting. On the contrary, the direction of the product seems missed when the reactant has been rotational excited.

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