

# Time Dependent Wave Packet Study of the $H^- + H_2$ Nonreactive Scattering

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## Abstract

Time dependent wave packet calculations have been performed for the  $H^- + H_2$  nonreactive scattering, summed of elastic and inelastic probabilities, on the recent reported potential energy surface of the  $H_3^-$  systems. The total probabilities for total angular momentum  $J$  up to 35 have been calculated to get the converged integral cross sections over collision energy range of 0.20 - 1.42 eV. Integral cross-sections and rate constants have been calculated from the wave packet transition probabilities for the initial states ( $v = 0, j = 0$ ) by means of J-shifting method and uniform J-shifting method for  $J > 0$ .

**Keywords:** Reaction Dynamics, Non-Reactive Scattering

## 1. Introduction

The quantum wave packet method is especially useful and transparent for studying the dynamics of elementary chemical processes, because it allows the direct calculation of the observables and shows the possible elementary mechanisms. Over the past years, several wave packet methods were suggested and become very popular, and significant progress in this method has been done in order to solve better the time dependent Schrödinger equation (*i.e.*, more efficient iterative method, the use of better representations) [1-9].

The ion-molecule reactions are of interest in understanding the collision processes in interstellar media, the plasma, and high-energy physic studies [10-24]. However, there have been a number of experimental and theoretical studies on the reaction cross sections of  $H^- + H_2$  reactions and its isotopic variants [10-16]. Experimentally, Michels and Paulson [15] measured the reaction cross sections for the collisions of  $H^-$  and  $D^-$  with  $H_2$ ,  $D_2$ , and HD using the tandem mass spectrometer (TMS). Muller *et al.* [17] performed crossed beam measurement of rotationally inelastic scattering of  $H_2$  from  $H^-$ . Haufler *et al.* [18] determined the integral cross sections for the  $H^- + D_2$  and  $D^- + H_2$  reactions and a pronounced isotope effect was found in the experiment.

Theoretically, an analytical *ab initio* Potential Energy Surface (PES) for the ground electronic state of  $H_3^-$  was reported by Starck and Meyer (SM) [19]. Gianturco

and Kumar [20] calculated the differential and integral cross sections for vibrationally in elastic processes in ( $H^-, H_2$ ) collisions over collision energy (107.69-922.4 kcal/mol) on SM PES. Recently, Panda and Sathya-murthy [21] have computed an *ab initio* PES of  $H_3^-$  systems using coupled cluster singles and doubles with nonperturbative triples method for a wide range of geometries. Subsequently, there are many theoretical studies about the title reactions using this global *ab initio* potential energy surface (PES) [10,21,22]. The pioneer work by Michels and Paulson [15] reported the biggest theoretical value of the cross section of this system (*i.e.*, 2.5 Angs squared). Panda and Sathya-murthy [21] used the time dependent quantum mechanics method within the centrifugal sudden approximation for computing the integral reaction cross section values for  $H^- + H_2$  reaction ( $v = 0, j = 0$ ) and its isotopic variants. Their results were also found to be in good agreement with the experimental results of Muller *et al.* [17] but larger than those of Haufler *et al.* [18]. Using SM PES, Morari and Jaquet [14] calculated the excitation function for the exchange reaction by including coriolis coupling and they found the results were in agreement with experimental results of Muller *et al.* [17] for all the range of energies studied and not with those of Haufler *et al.* [18]. Recently, using *ab initio* PES of Ref. 21 and time-dependent wave-packet quantum method, Yao *et al.* [10] calculated the cross sections for both the reaction  $D^- + H_2$  and the reaction  $H^- + D_2$  in the collision energy range of 0.2 -

2.4 eV. Their calculations showed that the Coriolis coupled method was more consistent with the experimental ones than the centrifugal sudden approximation, and a pronounced isotopic effect was also observed to compare the two reactive systems in their previous report [10]. Giri et al. have computed the differential and integral cross sections for elastic and two dimensional inelastic  $H^- + H_2$  ( $v = 0, j = 0, 1$ ) reactions at four different relative translational energies ( $E_{\text{trans}} = 1.66, 2.03, 2.40$  and  $2.79$  eV) by a time independent quantum mechanical approach [23]. To our knowledge, there are no experimental rate constant results of  $H^- + H_2$  nonreactive scattering to compare in all the energy ranges studied in this paper. So, up to now, theoretically, there are not any three-dimensional studies of  $H^- + H_2$  nonreactive scattering using time dependent quantum wave packet method to obtain cross sections and the reaction rates.

Here, we report three dimensional time dependent quantum calculations of  $H^- + H_2(v, j) \rightarrow H^- + H_2(v', j')$  nonreactive scattering with  $v$  and  $j$  being the vibrational and rotational quantum numbers. We use the  $H_3^-$  potential energy surface of Panda and Sathyamurthy for all the calculations. For computational reasons, we restrict our calculations for total angular momentum  $J = 0$  and use the J-shifting approximation [25] and uniform J-shifting approximation [26] to evaluate cross sections and rate constants.

The paper is organized as follows. In Section 2 we give a brief description of methodology. The results of our calculations are presented in Section 3.

## 2. Theory

In this work, we employed Jacobi coordinates  $(R, r, \gamma)$ , which are ideally suited for the calculation of the nonreactive state-to state and total probabilities. The corresponding Hamiltonian operator for  $J = 0$  is expressed as

$$\hat{H} = -\frac{1}{2\mu_R} \frac{\partial^2}{\partial R^2} + \frac{1}{2\mu_r} \frac{\partial^2}{\partial r^2} + \left( \frac{1}{2\mu_R R^2} + \frac{1}{2\mu_r r^2} \right) \hat{j}^2 + V(R, r, \gamma) \quad (1)$$

where  $r$  and  $R$ , respectively, the diatomic (H-H) and atom-diatom ( $H^-H_2$ ) distances with  $\mu_R$  and  $\mu_r$  as their reduced masses.  $\gamma$  is the angle between  $R$  and  $r$ .  $\hat{j}$  denotes the diatomic rotational angular momentum,  $V(R, r, \gamma)$  is the potential energy function for atom-molecule reaction.

Using the Hamiltonian operator in the form given in Equation (1) makes it necessary to use a large number of grid points in both  $R$  and  $r$  and an imaginary damping potential in the end of each grid. Having added and subtracted  $V(R = \infty, r, \gamma = 180)$  to the Hamiltonian opera-

tor given by Equation (1), we get

$$\hat{H} = -\frac{\hbar^2}{2\mu_R} \frac{\partial^2}{\partial R^2} + \frac{\hbar^2 \hat{j}^2}{2\mu_r R^2} + U(R, r, \gamma) + \hat{H}_{BC}(r) \quad (2)$$

where  $H_{BC}(r)$  is the Hamiltonian operator for the diatomic molecule and  $U(R, r, \gamma) = V(R, r, \gamma) - V(R = \infty, r, \gamma = 180)$ .

Starting from the initial wave packet at  $t = 0$  which is constructed according to the initial system, the time-dependent Schrödinger equation is solved in terms of modified complex Chebichev polynomials [2],

$$\psi(R, r, \gamma, t) = e^{-\frac{i}{\hbar} \left[ \frac{\Delta E}{2} + V_{\min} \right] t} \sum_{n=0}^N (2 - \delta_{n0}) \times J_n \left[ \frac{\Delta E t}{2\hbar} \right] \Phi_n \quad (3)$$

where  $\Phi_n = C_n(-i\hat{H}_{norm})\psi(R, r, \gamma, t = 0)$  with  $\psi(R, r, \gamma, t = 0)$  is the initial wavefunction,  $C_n(x)$  are complex Chebichev polynomials (CP),  $J_n(x)$  is the Bessel functions and  $\Delta E$  is the magnitude of the entire energy spread of the spectrum of the unnormalized Hamiltonian operator  $\hat{H}$ . The propagation requires the operation of the  $C_n(-i\hat{H}_{norm})$  on  $\psi$ . This is performed by using a three-term recursion relation of the Chebichev polynomials

$$\Phi_{n+1} = -2i\hat{H}_{norm} \Phi_n + \Phi_{n-1} \quad (4)$$

where the recurrence is started by setting two initial values as  $\Phi_0 = \psi(R, r, \gamma, t = 0)$  and  $\Phi_1 = -i\hat{H}_{norm}\psi(R, r, \gamma, t = 0)$ .

The initial wavepacket is located in the asymptotic region of entrance channel and propagated on the potential energy surface toward the strong interaction region. We wish to compute state-to-state nonreactive scattering probabilities and we have to follow the development of the wavepacket being reflected from the interaction region. The flux that goes into reactive channel is absorbed and not analyzed. In order to extract the cross section and other observable quantities from the wavepacket dynamics, the wavepacket is analyzed at each time step by taking cuts through at a fixed value of the scattering coordinate  $R = R_\infty$ .

$$C_{v'j'}(t) = \int_{r=0}^{\infty} \left( \sum_k \psi(R_\infty, r, \gamma_k, t) P_{j'}(\gamma_k) w_k \right) \varphi_{v'j'}(r) dr \quad (5)$$

where  $\psi(R_\infty, r, \gamma_k, t)$  is initial wave function,  $P_{j'}(\gamma_k)$  is an angular wave function for a rotational state  $j$ ,  $\varphi_{v'j'}(r)$  is vibrational wave function of  $H_2$  molecule,  $w_k$  are the weights in Gauss quadrature formula. The transition probabilities for the production of specific final vibrational-rotational states from a specified initial reactant level are given by [26-28].

$$P_{vj', v'j'}^{J=0}(E) = \frac{\hbar^2}{\mu_R \mu_r} k_{vj'} k_{v'j'} \left| \frac{A_{v'j'}(E)}{f(-|k_v|)} \right|^2 \quad (6)$$

where  $A_{vj}(E)$  is the Fourier transform of time-dependent coefficients ( $C_{vj}(t)$ ).  $k_{vj}$  and  $k_{v'j'}$  are the wave vectors for initial and final channels.  $f(-|k_v|)$  is the Fourier transform of initial Gaussian.

When using a time-dependent quantum method for scattering problems one is always faced with numerical difficulties associated with the reflection of the wave function from the end of the grid. Therefore, in order to avoid such a reflection, an imaginary potential is used to damp the wave packet at the edges of the grid. The absorbing potential parameters are optimized as instructed by Vibok and Balint-Kurti [29]. At present calculations, a negative complex damping potential with a quadratic form has been used at both edges of the grid.

Usually, it is not possible to obtain the integral cross sections and the thermal rate constants by nonreactive probabilities calculated for  $J = 0$ . Because, all important  $J$  values must be used to calculate the cross sections, and for high  $J$  values each calculation becomes very difficult. This problem is often handled approximately by the J-shifting method [25]. In general, J-shifting method, which relies on the identification of ‘‘bottleneck’’ geometry, such as a transition state, works very well when the reaction proceeds through an energy barrier, as is the case for present system. The changes in rotational energy of the system, when fixed at this geometry, provide an energy shift  $E_{shift}^{J,K}$ , which is used in estimating the nonreactive probabilities and depends on the  $J$  and  $K$  quantum numbers. When  $K = 0$ , there is no component on angular momentum and the relationship is

$$P_{v'j',vj}^J = P_{v'j',vj}^{J=0} (E - E_{shift}^J) \quad (7)$$

where  $P_{v'j',vj}^{J=0}(E)$  is the accurately computed nonreactive probability for  $J = 0$ , at the total energy  $E$ , and  $P_{v'j',vj}^J(E)$  is the estimated nonreactive probability for another value of  $J$ .

The calculation of total cross sections requires having the transition probabilities for all available  $J$  values:

$$\sigma_{v'j'}(E_{col}) = \frac{\pi}{k_{v'j'}^2} \sum_{J=0}^{\infty} (2J+1) P_{vj}^J(E) \quad (8)$$

where  $E_{col} = E - \varepsilon_{vj}$  is the collision energy and  $\varepsilon_{vj}$  is the initial rovibrational energy of the diatomic molecule,  $P_{vj}^J(E)$  is the energy-dependent total reaction probability for a given initial state

The state-to-state rate constant can be calculated by Boltzmann averaging of the integral cross section over collision energy

$$k_{vj}(T) = \left( \frac{8}{\pi \mu_R k_B^3 T^3} \right)^{1/2} \int_0^{\infty} dE_{col} E_{col} e^{-E_{col}/k_B T} \sigma_{vj}(E_{col}) \quad (9)$$

where  $k_B$  is the Boltzmann constant,  $T$  is temperature [30].

Another very appealing method for evaluating nonreactive rate constants is the Uniform J-Shifting approach developed by Zhang and Zhang [26]. In this approach, the optimized value of rotational constant ( $B$ ) at a given temperature ( $T$ ) for a range ( $J_i$  and  $J_{i+1}$ ) of  $J$  value is extracted from these accurate probability functions,

$$B_i(T) = \frac{k_B T}{J_{i+1}(J_{i+1}+1) - J_i(J_i+1)} \ln \left( \frac{Q^{J_i}}{Q^{J_{i+1}}} \right) \quad (i=1,2) \quad (10)$$

where  $Q^{J_i}$  and  $Q^{J_{i+1}}$  are partition like functions for  $J_i$  and  $J_{i+1}$  reference angular momentum and can be written in a simple form

$$Q^{J_i}(T) = \int P^{J_i}(E_{col}) e^{-E_{col}/k_B T} dE_{col} \quad (11)$$

$$\text{and} \quad Q^{J_{i+1}}(T) = \int P^{J_{i+1}}(E_{col}) e^{-E_{col}/k_B T} dE_{col} \quad (12)$$

In result, the rate constant is given by

$$k(T) = \left( \frac{2\pi}{\mu^3 k_B^3 T^3} \right)^{1/2} Q^0(T) \sum_J (2J+1) e^{-B_i(T)J(J+1)/k_B T} \quad (13)$$

### 3. Results and Discussions

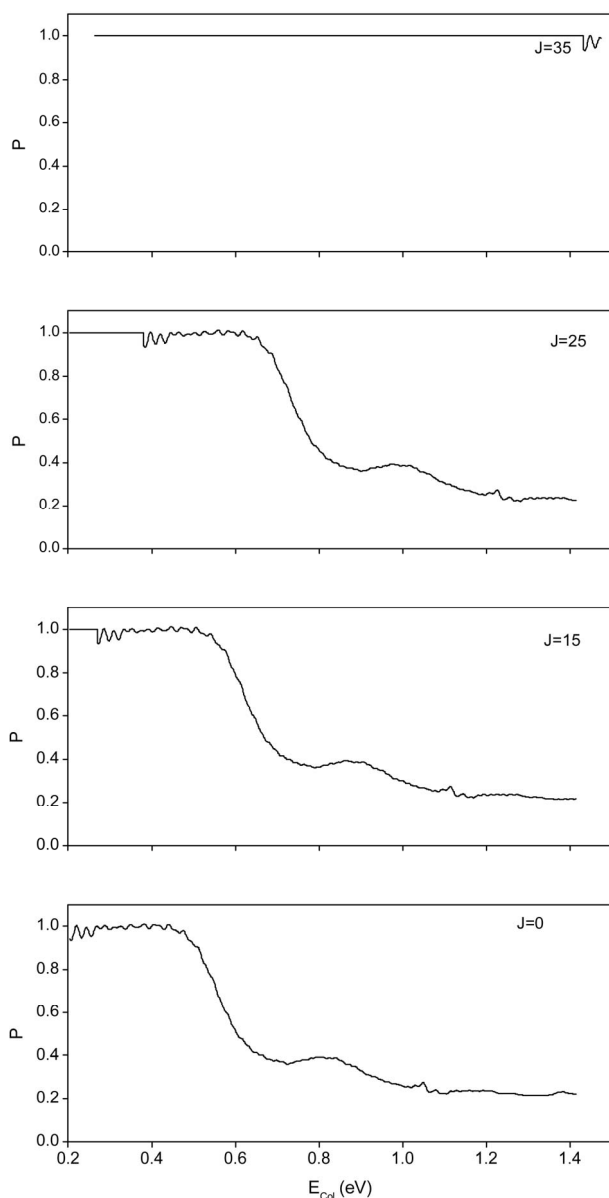
We have calculated the rovibrational nonreactive probabilities at  $J = 0$  for  $\nu = 0, j = 0, 1, 2$  propagating of initial wave packet in Jacobi coordinates  $R, r$ , and  $\gamma$ , using the parameters of **Table 1**. The calculation required 40000 iterations steps to converge. The potential energy surface of Ref. [21] has been used in this paper. It has in the following features: 1) Barrier height (0.47 eV) of proposed potential energy surface found to be a minimum for the collinear geometry, with the saddle point located at  $1.999a_0$ . 2) A van der Waals minimum was also found for the collinear geometry at  $r = 1.419a_0$  and  $R = 5.915a_0$  ( $a_0$  is Bohr radius) with a well of depth 0.0475 eV. 3) This potential has been constructed by fitting an analytical function to the ab initio potential energy values computed using coupled cluster singles and doubles.

**Figure 1** shows nonreactive transition probabilities in  $\nu = 0, j = 0$  at total angular momentum  $J = 0, 15, 25, 35$  obtained from Equation (7) as a function of the collision energy. Transition probabilities show no threshold and decrease with increasing collision energy as expected for a nonreactive scattering with a small barrier to the reactive channel. That is, after barrier height for  $J = 0$ , the nonreactive probability decreases slowly in the energy interval considered. Therefore, it can be seen nonreactive probabilities rapidly shift towards higher energies on increasing  $J$  values. Probabilities are very small

**Table 1. Parameters of the calculations.**

Translational energy center of the initial WP	0.4 eV
$R$ center and width of the initial WP	13.32 and 5
$R$ range and no. of grid points	1.18 - 29.5 and 512
$r$ range and no. of grid points	0.56 - 8.5 and 64
No. of Legendre polynomials and of $\gamma$ points	40
$R$ and $r$ absorption start at	22 and 6.52
$R$ and $r$ absorption strength	0.01
Analysis at $R$	17

Values in a.u



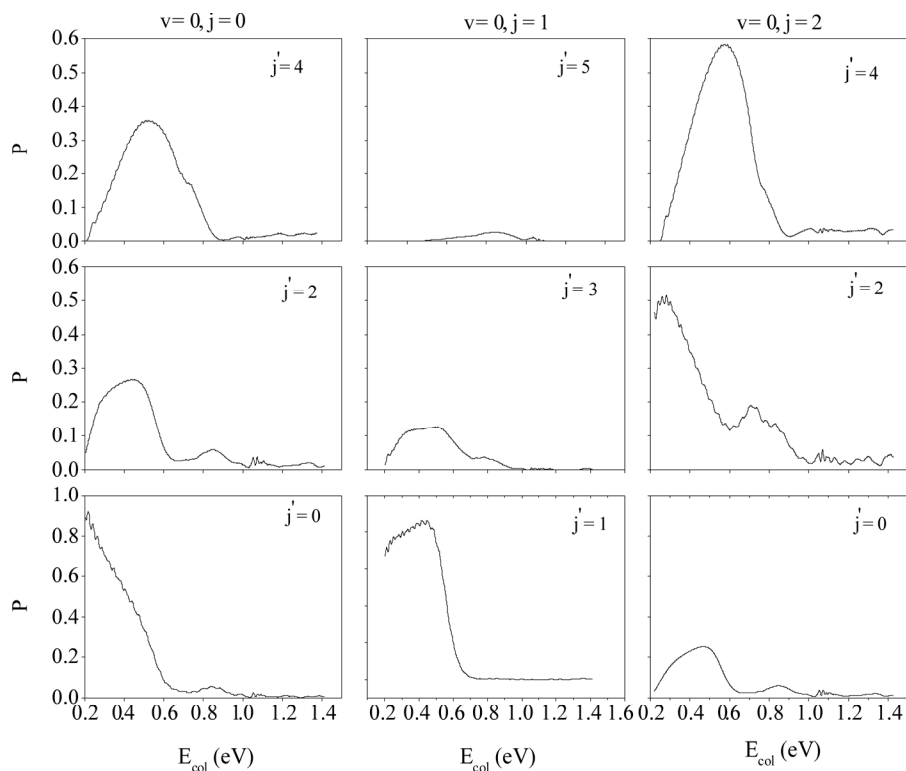
**Figure 1. Nonreactive transition probabilities for  $H^- + H_2$  ( $\nu=0, j=0$ )  $\rightarrow$   $H^- + H_2$  ( $\nu'=0, j'=0$ ) summed over all final ro-vibrational states as a function of collision energy for different  $J$  values.**

at high collision energy  $E_{col}$  and their resonances become less sharp.

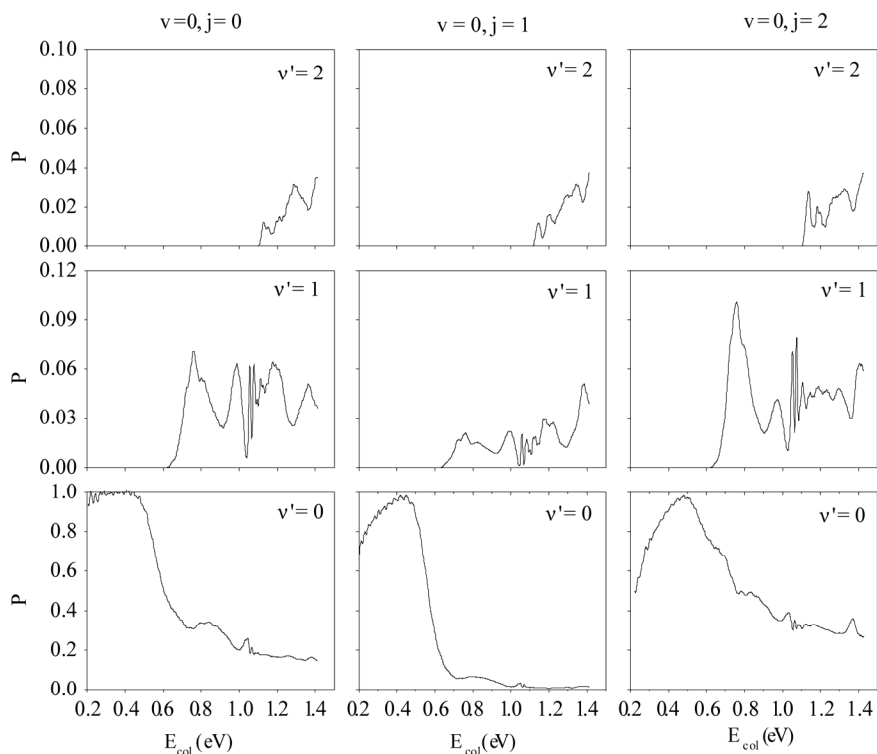
The nonreactive transition probabilities for  $H^- + H_2(\nu=0, j) \rightarrow H^- + H_2(\nu'=0, j')$  covering a collision energy range of 0.20 - 1.42 eV with  $\nu=0$  and  $j=0,1,2$  are shown in **Figure 2**. All the transition probabilities show the same structure with many resonances especially located in the low energy region. These resonances at the threshold region correspond to the metastable excited vibrational levels of the  $H_3^-$ . The general trend of the probabilities is to decrease with increasing energy, and they clearly show the tendency for even-odd alternation according to the parity selection rule. That is, there is no transition between the odd and even quantum states. The reason for the decrease in the probabilities with increasing collision energy is that the potential shows a small barrier to the reactive channel.

The nonreactive transition probabilities for  $H^- + H_2$  ( $\nu=0, j$ )  $\rightarrow$   $H^- + H_2(\nu'=0, j')$  with  $\nu'=0,1,2$  summed over all final rotational  $j'$  states are displayed in **Figure 3**. It is seen from the figure that resonance structure is clearly changed as the vibrational quantum number  $\nu'$  is increased indicating vibrational state dependency of probabilities. Interestingly, the transition probabilities show threshold behavior for the first and second vibrational quantum states ( $\nu'=1,2$ ) of  $H_2$ . Threshold energy is about 0.61 eV for  $\nu'=1$  and is about at 1.1 eV for  $\nu'=2$ . As it is expected these energies correspond to the vibrational energies of  $\nu'=1$  and  $\nu'=2$  quantum states. An important feature that can be drawn from **Figures 2** and **3** is that the rotational states have no significant effect on transition probabilities.

The final state distributions at the fixed energies can also be of great utility in understanding the nonreactive scattering. The final rotational distributions for  $H_2$  initially in its ground and first two rotationally excited states are shown in **Figure 4** for 0.99, 1.18 and 1.37 eV collision energy values, respectively. The rotational distributions especially in the low collision energy show a structured shape and clear tendency for even-odd alternations according to parity selection rule as expected.



**Figure 2.** The nonreactive state to state transition probabilities for  $H^- + H_2 (\nu=0, j) \rightarrow H^- + H_2 (\nu' = 0, j')$  as a function of collision energy.



**Figure 3.** Vibrationally state resolved transition probabilities summed over all product rotational states plotted as a function of collision energy for  $H^- + H_2 (\nu=0, j) \rightarrow H^- + H_2 (\nu')$  with  $\nu' = 0, 1, 2$ .

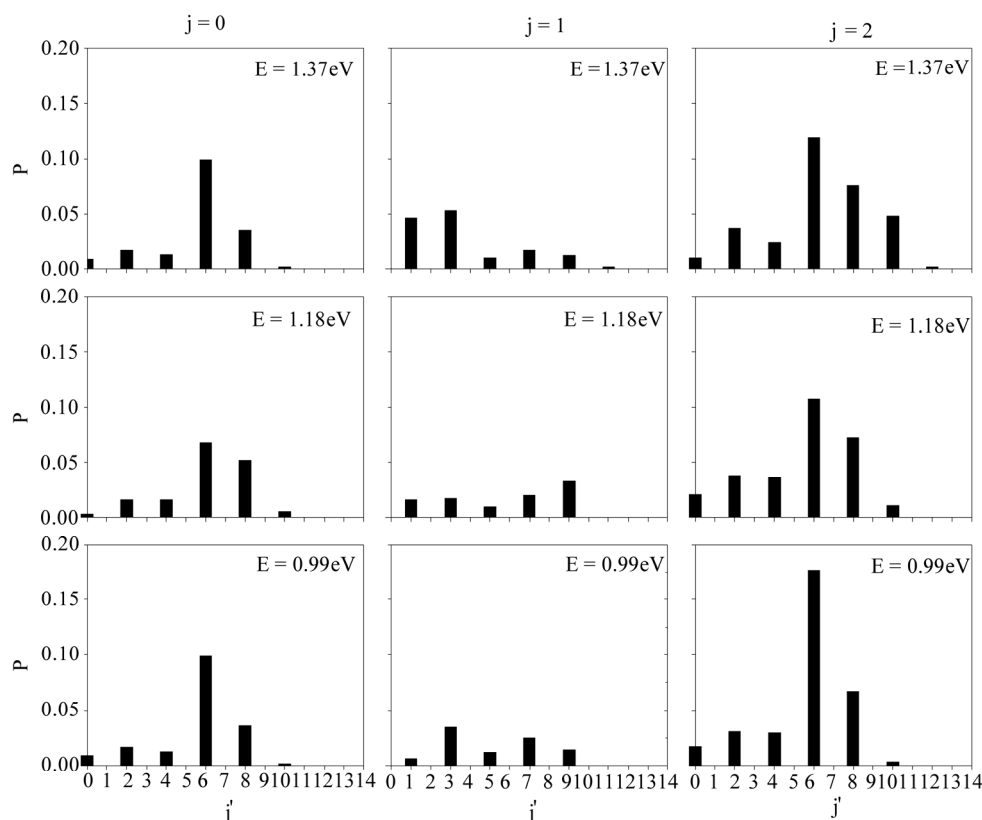


Figure 4. Product rotational distributions at fixed energy values.

As seen from the **Figure 5** that nonreactive cross section show threshold and firstly increases with increasing collision energy. Later, it decreases at collision energy higher than the reactive barrier. So, for even higher collision energies the nonreactive cross section will increase again, because the reaction probability will decrease. This is a characteristic of nonreactive and barrier reaction. It is our expectation that the cross section is large and not strongly dependent on the translational energy.

The initial rate constants multiplied by  $10^{10}$  for both J-shifting method and Uniform J-Shifting method are plotted in **Figure 6** for the  $H_2$  in ground state. The rate constant is sensitive to temperature and it shows threshold. This behavior may again be attributed to the well in the entrance channel. As can be seen, J-shifting approximation yields rate constants in good agreement with Uniform J-Shifting method. The rate constants for both methods increase monotonically with temperature as expected. Clearly, the rate constant data show a pronounced variation of rate constant with the temperature for the high temperature region. At 300 K, the rate constants are  $1126 \times 10^{-12}$  and  $1158 \times 10^{-12} \text{ cm}^3 \cdot \text{s}^{-1}$  for J-shifting approximation and Uniform J-Shifting method, respectively. So, J-Shift is only good at very low collision energies and the results between the both J-shift

method are comparable for the room temperature.

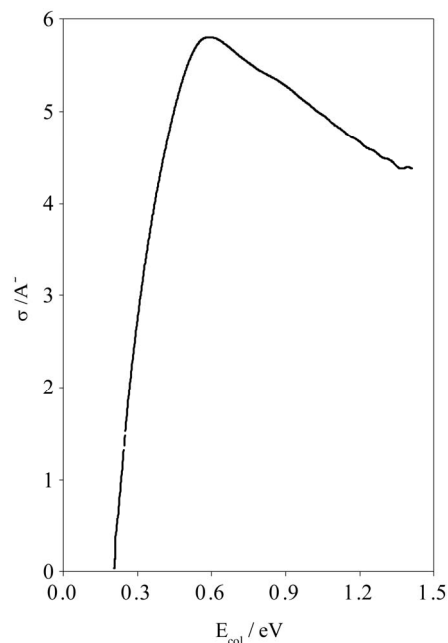
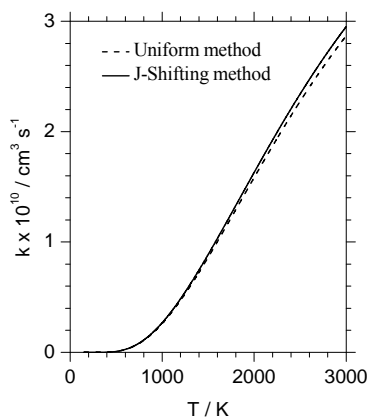


Figure 5. Initial state selected integral cross sections for  $H + H_2$  ( $v = 0, j = 0$ ) nonreactive scattering as a function collision energy for  $H_2$  in ground state.



**Figure 6.** Nonreactive rate constants depend on the initial quantum numbers for  $H^- + H_2(v = 0, j = 0)$  nonreactive scattering as a function of temperature.

#### 4. Conclusions

In this paper, we presented a time-dependent quantum wave packet calculation for the  $H^- + H_2$  nonreactive scattering and gave the dynamics information of nonreactive probability, cross section and rate constant. The  $H^- + H_2$  nonreactive system has an energy barrier height on potential energy surface. The nonreactive cross section has been obtained by summing up the nonreactive probabilities. The probability for  $J = 0$  was calculated while the probabilities for  $J > 0$  was estimated by means of two different J-shifting approximation. The calculations showed that the reaction cross section shows a threshold behavior and the initial state selected rate constant is significantly dependent on the temperature.

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