



Research paper

Accurate integral cross sections for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ reactionPeng Sun^{a,b}, Jun Chen^c, Shu Liu^{a,*}, Dong H. Zhang^{a,*}^a State Key Laboratory of Molecular Reaction Dynamics and Center for Theoretical Computational Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, PR China^b University of Chinese Academy of Sciences, Beijing 100049, PR China^c Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, PR China

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ABSTRACT

A full-dimensional quantum dynamics calculation has been carried out to yield the coupled-channel reaction probabilities with total angular momentum J up to 60 for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ reaction on the PIP-NN PES potential energy surface. Well converged integral cross section (ICSSs) for collision energy up to 2.4 eV were obtained for the ground initial state. As compared with previous study, it is found that the CS approximation substantially underestimated ICSSs, which is inadequate for the title reaction. In addition, the agreement between QM and QCT ICSSs is quite satisfactory, indicating that the QCT method is rather accurate on describing dynamics of this complex-forming reaction.

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1. Introduction

The endothermic reaction $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$, and its reverse, play vital roles in atmospheric [1], combustion [2], and interstellar chemistry [3,4]. They represent a prototype for complex-forming four-atom reactions as $\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$ for direct four-atom reactions. Over the years, many experimental studies have been devoted to the title reaction for dynamical and kinetic properties [5–12]. Theoretically, extensive studies have been carried out for the HOCO system [13,14]. Following the first global analytic potential energy surface (PES) (denoted as SFH), a few more PESs had been constructed and widely used for dynamics studies [15–20], but the accuracy of the PESs were still not ideal. The situation has been greatly improved, thanks to new PESs [21–23] based on large numbers of high-level *ab initio* points and more accurate permutation invariant polynomial (PIP) [24], neural network (NN) [25], and PIP-NN [26,27] fitting methods. Recently, good agreement was achieved between state-resolved results from experiment and quasi-classical trajectory (QCT) calculation on the PIP-NN PES of the $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ reaction, leading to the conclusion that this PES is the most accurate so far for the HOCO system [28]. Schatz and co-workers performed pioneering QCT calculations for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ reaction on various PESs [15,17,29]. In 2012, QCT calculations on the PIP PES [21] reproduce for the first time the monotonically increasing integral cross section (ICSSs) with collision energy, consistent with experimental

observations. The influence of initial excitations of CO_2 and product final state distributions were also investigated [30]. Subsequently, Valero and coworkers carried out a QCT study of the title reaction on a new interpolated PES based on the M06-2X density functional. They found the calculated cross sections were in quantitative agreement with experiment in the whole range of relative translational energies 1.2–2.5 eV [31].

The HOCO system presents a huge challenge to quantum dynamics. The combination of a relatively long-lived collision complex and three heavy atoms in the reaction makes the rigorous quantum scattering calculations extremely difficult. Extensive quantum mechanical (QM) studies were carried out for the total reaction probabilities and rate constants on different PESs for the $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ reaction [32–36,23]. Since 2012, we performed full-dimensional state-to-state quantum dynamics calculations for total angular momentum $J = 0$ on LTSH and PIP-NN PESs for the $\text{OH} + \text{CO}$ reaction [37,38], representing the first state-to-state quantum study of a complex forming four-atom reaction. Recently, we carried out the first QM calculation in full dimensions for the title reaction on the PIP-NN PES, and compared the total reaction probabilities from the ground and some vibrationally excited initial states for the total angular momentum $J = 0$ [39]. The total reaction probabilities for some $J > 0$ states were also computed under the centrifugal sudden (CS) approximation for the ground initial state. The resulting CS ICSSs increase monotonically with the collision energy, but are substantially smaller in the whole energy range than the experimental measurements [8], and previous QCT results on the LTSH and CCSD-3/d PES [29,30]. The CS approximation, which assumes that K -block (the projection of the total angular momentum on the body-fixed axis) is a good quantum

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number, has been widely used in time-dependent wave packet (TDWP) calculations. It has been found that the approximation works rather well for most direct reactions, but is less ideal for some atom-polyatom reactions, such as $\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$ and $\text{H} + \text{CHD}_3 \rightarrow \text{H}_2 + \text{CD}_3$ [40,41]. We suspect the CS approximation is the main reason for the huge discrepancy between QM ICSS and the experiment. Although the quantum wave packet methods have been developed to compute differential cross sections (DCS) for some direct four-atom reactions, such as the $\text{HD} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{D}$ and $\text{H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{OH}$ [42–47], it is still not feasible at present to compute final state resolved cross sections for complex-forming four-atom reactions due to the long wave packet propagation time and huge basis sets required. Therefore, it is also important to test the validity of the QCT method to describe chemical reaction dynamics for the title reaction.

In this letter, we perform a further quantum dynamics calculation of the title reaction with 3 K -blocks included to provide coupled-channel (CC) reaction probabilities for total angular momentum J up to 60 on the PIP-NN PES. The computational effort increases by up to a factor of 7 compared to that with the CS approximation, making the calculation extremely time-consuming. Well converged ICSSs for the ground initial state with collision energy up to 2.4 eV were obtained from the CC probabilities, and compared with the CS and QCT ones on the same PES. This paper is organized as follows: Section 2 outlines the method used in current calculation. We present the results of our calculation in Section 3, and examine the accuracy of the CS approximation and QCT method for the ground initial state, followed by the conclusion in Section 4.

2. Theory

We outline the theory of the TDWP method for calculating the initial state selected total reaction probability for a atom-triatom reaction $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ in full dimensions. For details, please refer to our early works [48]. The Hamiltonian expressed in the reactant Jacobi coordinates shown in Fig. 1 for a given total angular momentum J can be written as

$$H = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial R^2} + h_1(r_1) + h_2(r_2) + \frac{(\mathbf{J} - \mathbf{j}_{12})^2}{2\mu R^2} + \frac{\mathbf{j}_1^2}{2\mu_1 r_1^2} + \frac{\mathbf{j}_2^2}{2\mu_2 r_2^2} + (V(R, r_1, r_2, \theta_1, \theta_2, \varphi) - V_1(r_1) - V_2(r_2)), \quad (1)$$

where μ is the reduced mass between the center-of-mass of H and CO_2 , \mathbf{J} is the total angular momentum operator of the system, \mathbf{j}_{12} is the total angular momentum operator of CO_2 , \mathbf{j}_2 is the rotational angular momentum operator of CO, and $\mathbf{j}_1 = \mathbf{j}_{12} - \mathbf{j}_2$ is the orbital angular momentum of CO_2 . The diatomic reference Hamiltonian $h_i(r_i)$ ($i = 1, 2$) is defined as

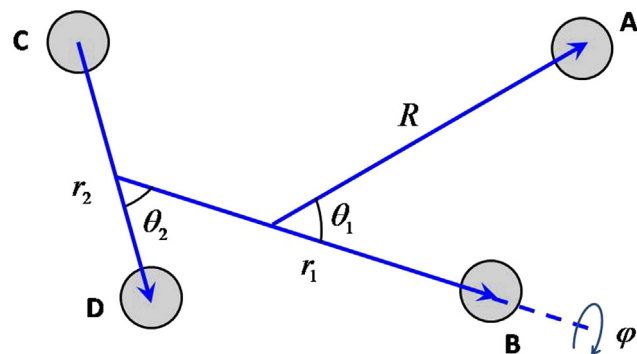


Fig. 1. The reagent Jacobi coordinates ($R, r_1, r_2, \theta_1, \theta_2, \varphi$) for the $\text{H} + \text{CO}_2$ atom-triatom reaction.

$$h_i(r_i) = -\frac{\hbar^2}{2\mu_i} \frac{\partial^2}{\partial r_i^2} + V_i(r_i). \quad (2)$$

The time-dependent wave function can be expanded in terms of the translational basis of R , the vibrational basis $\phi_{v_i}(r_i)$, and the body-fixed (BF) rovibrational eigenfunction as

$$\Psi_{v_{0j_0K_0}}^{JM\epsilon}(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, t) = \sum_{n, v, j, K} F_{n, v, j, K, v_{0j_0K_0}}^{JM\epsilon}(t) u_n^{v_1}(R) \phi_{v_1}(r_1) \phi_{v_2}(r_2) \mathcal{Y}_{jK}^{JM\epsilon}(\hat{R}, \hat{r}_1, \hat{r}_2). \quad (3)$$

The BF total angular momentum eigenfunctions can be written as,

$$\mathcal{Y}_{jK}^{JM\epsilon} = (1 + \delta_{K0})^{-1/2} \sqrt{\frac{2J+1}{8\pi}} [D_{K,M}^{J*} Y_{j_1 j_2}^{j_1 j_2 K} + \epsilon (-1)^{j_1 + j_2 + j_{12} + J} D_{-K, M}^{J*} Y_{j_1 j_2}^{j_1 j_2 -K}] \quad (4)$$

$$\equiv D_{K, M}^{J*} Y_{j_1 j_2}^{j_1 j_2 K} + \epsilon (-1)^j D_{-K, M}^{J*} Y_{j_1 j_2}^{j_1 j_2 -K} \quad (5)$$

where $D_{K, M}^J(\Theta\Phi\Psi)$ is the Wigner rotation matrix [49] with three Euler angles $(\Theta\Phi\Psi)$, ϵ is the parity of the system defined as $\epsilon = (-1)^{j_1 + j_2 + L}$ with $\mathbf{L} = \mathbf{J} - \mathbf{j}_{12}$ being the orbital angular momentum of H and CO_2 , and $Y_{j_1 j_2}^{j_1 j_2 K}$ is the angular momentum eigenfunction of \mathbf{j}_{12} defined as,

$$Y_{j_1 j_2}^{j_1 j_2 K} = \sum_m D_{K, m}^{j_1 j_2}(\chi, \theta_1, \varphi) \sqrt{\frac{2j_1 + 1}{4\pi}} \langle j_2 m j_1 0 | j_{12} m \rangle y_{j_2 m}(\theta_2, 0) \quad (6)$$

where y_{jm} are spherical harmonics. Note that in Eq. (4), the restriction $\epsilon(-1)^{j_1 + j_2 + j_{12} + J} = 1$ for $K = 0$ partitions the whole rotational basis set into even and odd parities. Thus a $K = 0$ initial state can only appear in one of these two parity blocks. For $K > 0$, however, there is no such restriction, the basis set is the same for even and odd parities. Hence a $K > 0$ initial state can appear in both parities.

We construct an initial wave packet $\psi_i(0)$ and propagate it using the split-operator method. The total reaction probability for that specific initial state i for a whole range of energies can be obtained by evaluating the reactive flux

$$P_i^R(E) = \frac{\hbar}{m_s} \text{Im} \left[\left\langle \psi_{iE}^+ \left| \delta(s - s_0) \frac{\partial}{\partial s} \right| \psi_{iE}^+ \right\rangle \right], \quad (7)$$

where s is the coordinate perpendicular to a dividing surface located at s_0 . ψ_{iE}^+ denotes the time-independent (TI) wavefunction, which can be obtained by performing a Fourier transform of the time-dependent wave function as

$$|\psi_{iE}^+\rangle = \frac{1}{a_i(E)} \int_{-\infty}^{\infty} e^{i(E-H)t} |\psi_i(0)\rangle dt. \quad (8)$$

The coefficient $a_i(E)$ is the overlap between the initial wave packet and the energy-normalized asymptotic scattering function, $a_i(E) = \langle \phi_{iE} | \psi_i(0) \rangle$.

The detailed numerical parameters for the wave packet propagation are listed in Table 1. In our present calculation, the number of K -blocks is up to 3 to obtain the converged results. The size of rotational basis functions was 1,825,090 for 3K calculation and even parity. Since there are two equivalent product channels in the reaction, we treat the OC' bond as a nonreactive bond in this work, which has been demonstrated to be a very good approximation in describing the $\text{H} + \text{H}_2\text{O}$ and the title abstraction reaction. The reaction probabilities should be multiplied by a factor of 2, if compared with experimental results.

The QCT calculations, as implemented in VENUS [50], were carried out at several collision energies. The propagation time step was selected to be 3 a.u., and exceptionally long trajectories were halted if the propagation time reached a pre-specified value (36 ps). The cutoff time 36 ps corresponds to 500,000 steps of propaga-

Table 1

Numerical parameters used for wave packet propagation. (Atomic units are used unless stated otherwise.)

Grid range and size	
R	$[1.5, 11.5]$, $N_{\text{int}} = 36$, $N_{\text{asy}} = 36$
r_1	$[2.0, 7.0]$, $v_{\text{int}}^1 = 100$, $v_{\text{asy}}^1 = 10$
r_2	$[1.9, 3.0]$, $v_{\text{int}}^2 = v_{\text{asy}}^2 = 8$
j	(0, 95)
l	(0, 110)
Time increment: 10	
Dividing surface: $r_1^{\text{flux}} = 5.5$	
Initial Gaussian wave packet	
R_0	10
σ_0	0.3
E_{k0}	1.7 eV

tion, which is a very large value to ensure that almost no trajectory trapped in the complex well. In fact, at the collision energy of 1.6 eV, more than 95% trajectories finish within 2 ps in the current calculation. The maximal impact parameter (b_{max}) was set to 2.0 Å. The scattering parameters (vibrational phases, and spatial orientation of the initial reactants) were selected with a Monte Carlo approach. The gradient of the PES was obtained numerically by the central-difference algorithm.

The total ICSs were computed according to the following formula:

$$\sigma_r = \pi b_{\text{max}}^2 \frac{N_{\text{reac}}}{N_{\text{tot}}}, \quad (9)$$

where N_{reac} and N_{tot} are the number of reactive trajectories and total number of trajectories, respectively. The standard error is given by

$$\Delta = \sqrt{(N_{\text{tot}} - N_{\text{reac}})/N_{\text{tot}}N_{\text{reac}}}. \quad (10)$$

3. Results and discussion

Fig. 2 shows the $J = 30$ total reaction probabilities for the ground initial state calculated with different number of K -blocks. Apparently, the CS approximation does not work well for the title reaction as the $J = 30$ CS probability is considerably smaller than the 2K probability. The threshold energy difference between CS and 2K probabilities reaches 0.6 eV. As mentioned in Ref. [39], the cis-HOCO TS2 transition state is the major bottleneck in the

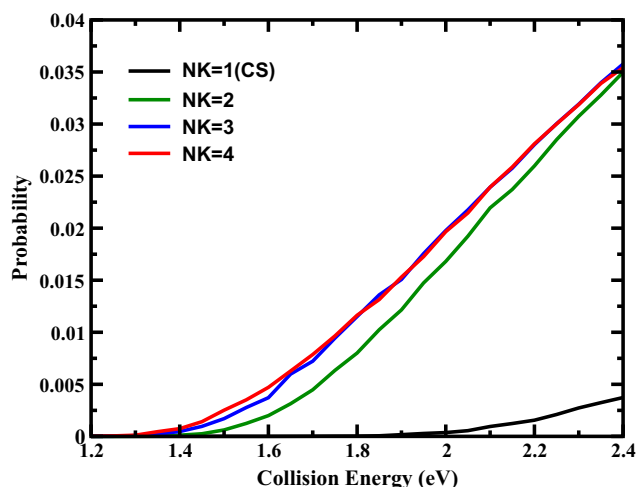


Fig. 2. The total reaction probabilities for the ground initial state for $J = 30$ calculated using different number of K -blocks.

title reaction, with the H-OCO bending angle being 115.1° , away from the collinear geometry. Because CO_2 is a linear molecule, $K = 0$ means the collinear approach of reactants, making the TS2 geometry less accessible, and leading to tiny reactivity. In contrast, $K > 0$ excitation can help the molecule get to the TS2 transition state, consequently dramatically enhance the reactivity. That's why the CS approximation, which limits K to zero, is inadequate. As can be seen, the $NK = 3$ reaction probabilities agree with the $NK = 4$ results quite well, in particular above $E_c = 2$ eV. Therefore, 3 K -blocks are sufficient to yield a well converged total reaction probability for $J = 30$ (also for $J = 60$ after calculation), and even the $NK = 2$ probability is rather close to the CC result in high energy region.

To obtain the converged CC ICSs for collision energy up to 2.4 eV of the title reaction, we calculated the reaction probabilities for total angular momentum J from 0 to 60 with a step size of 10, and with 3 K -blocks included. The energy dependence of the total reaction probabilities for different J are presented in Fig. 3. The overall behavior of $J > 0$ reaction probabilities resembles that of $J = 0$ probability, which increase monotonically with the collision energy. With the increase of J , the probabilities shift toward the lower energy first, and then shift to higher energy because of the increasingly higher centrifugal barrier. With the increase of total angular momentum, the coupling between different K -blocks becomes stronger, resulting in larger distributions on $K > 0$. Because $K > 0$ is substantially more effective on promoting the reaction than $K = 0$, $J = 30$ has lower threshold energy and larger probabilities in the collision energy region considered here than $J = 0$.

Fig. 4 shows the changing of CC reaction probabilities with partial waves at the collision energy of 2.0 eV. For this collision energy, partial wave of $J = 30$ have the biggest contribution. The probabilities first rise and then fall down as J increases, and become negligible when $J = 60$. The QCT partial wave contributions on the same PES are represented by black dots, which show almost identical trend as the QM curve.

Fig. 5 shows the CC ICSs for the ground initial state as a function of the collision energy, in comparison with the CS ones, the QCT results on the same PES at $E_c = 1.6, 2.0$, and 2.4 eV and on the CCSD-3/d PES [30], and experimental data of Hoffmann et al. [8]. To obtain the QCT ICSs, 2,400,000 trajectories were run for the collision energy of 1.6 eV, and 600,000 trajectories for 2.0 and 2.4 eV, with standard errors less than 1% in this energy range. As reported in our previous investigations of the reverse $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$

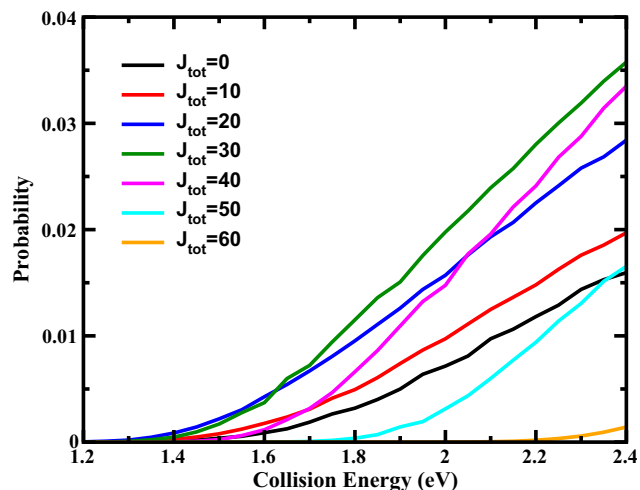


Fig. 3. The converged CC reaction probabilities of the title reaction for the ground initial state for J up to 60.

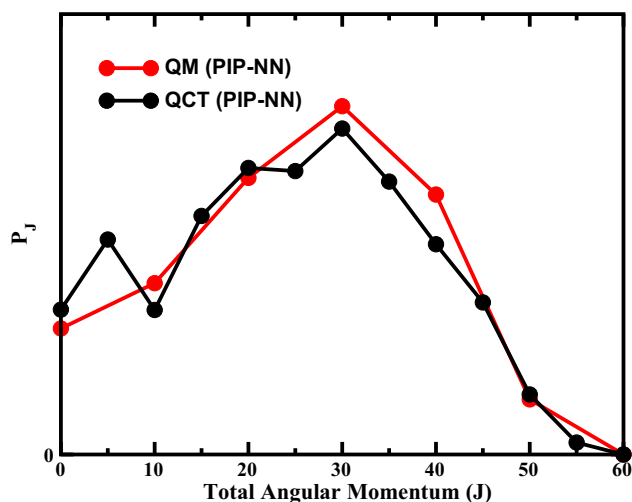


Fig. 4. The changing of QM and QCT reaction probabilities with partial waves at the collision energy of 2.0 eV.

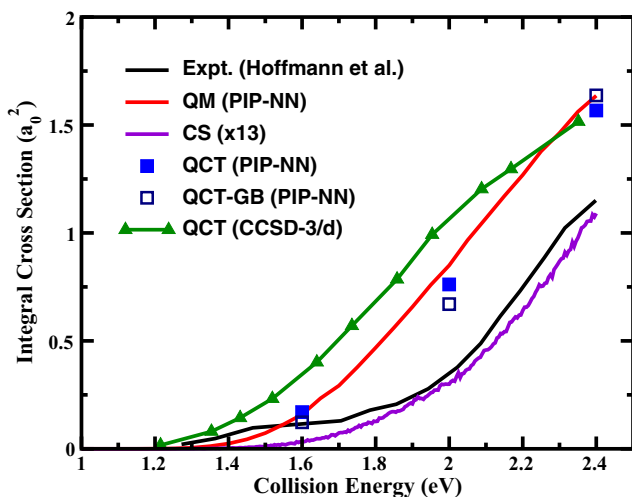


Fig. 5. CC ICSs for the ground initial state as a function of the collision energy, compared with the CS ones, the QCT results on the same PES and on the CCSD-3/d PES, and experimental data of Hoffmann et al.

reaction [38], the zero point energy (ZPE) problem is an important issue in QCT calculations. As for this reaction, some OH or CO products can have vibrational energies below their ZPE level. Hence, we also calculated the QCT results with ZPE constraint by using the Gaussian binning (GB) approach. As can be seen, the CS approximation substantially underestimated ICSs for the title reaction, which is consistent with the conclusion obtained from $J = 30$ reaction probabilities. The agreement between the QM and QCT ICSs are quite satisfactory, indicating that the QCT method is rather accurate on describing dynamics of this complex-forming reaction on the PIP-NN PES. The ZPE constraint QCT ICSs are similar to the original QCT ones, except a slightly higher reaction threshold, indicating a trivial tunneling effect of this heavy atom migration reaction. In addition, when compared with the previous QCT results on the CCSD-3/d PES, our QCT ICSs are smaller at $E_c = 1.6$ and 2.0 eV and have a larger threshold energy, because of a narrower reaction path and tighter TS2 of the PIP-NN PES. The QM ICSs were close to experimental data below 1.6 eV, but larger than them at higher collision energy region.

4. Conclusions

To investigate the accuracy of the CS approximation for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ reaction, we perform a further quantum dynamics calculation with more than one K -block. The $J = 30$ reaction probabilities show that the CS approximation is inadequate for the title reaction, because of the bending geometry of the cis-TS2 transition state. It was found that 3 K -blocks are sufficient to yield converged CC reaction probabilities for total angular momentum J up to 60. With the increase of J , the CC probabilities as a function of collision energy shift toward the lower energy first, and then shift to higher energy. Well converge ICSs for the ground initial state with collision energy up to 2.4 eV were obtained from the CC probabilities. The CC ICSs are found to be substantially larger than the corresponding CS ones. The QCT ICSs were also calculated for some collision energies on the same PES, which are in very good agreement with QM results, indicating that the QCT method is rather accurate on describing dynamics of the title reaction on the PIP-NN PES.

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