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A quasiclassical trajectory study of the $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$ reaction dynamics at 1.4 eV collision energy on a new ab initio potential energy surface

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Abstract

A quasi-classical trajectory (QCT) study of the $\text{H} + \text{H}_2\text{O}$ reaction is reported on the new fully ab initio YZCL2 potential energy surface calculated by Collins and co-workers. OH and H_2 rotational distributions, H_2 co-product internal energy release distributions and state-resolved differential cross sections have been calculated at a collision energy of 1.4 eV. The theoretical results are compared with recent experimental determinations showing a good general agreement. The present QCT calculations support the accuracy of the YZCL2 PES in predicting the dynamics of the title reaction. © 2002 Elsevier Science B.V. All rights reserved.

1. Introduction

The gas-phase $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$ reaction is considered a benchmark for the development of ab initio potential energy surfaces (PESs) and reactive scattering methodologies applied to four-atom reactions [1–6]. Along the years, several versions of the PES for the electronic ground state of the H_3O system have been released, but only the most recent ones have yielded dynamical results in quantitative agreement with the available experimental data. Among these PESs, the Ochoa and Clary (OC) PES [7] has been widely used both in quasi-classical trajectory (QCT) and quantum

mechanical (QM) scattering calculations for the $\text{H} + \text{H}_2\text{O}$ and $\text{OH} + \text{H}_2$ reactions and their isotopic variants. QM calculations using the rotating bond approximation [8] on this PES have proved to be quite successful in reproducing the HOD product vibrational populations of the $\text{OH} + \text{D}_2$ reaction observed in the recent cross molecular beam experiments by Davis and co-workers [9] using the Rydberg D-atom ‘tagging’ technique. More recently, QCT studies on the OC PES by Lakin et al. [10] and Rodríguez et al. [11] have reproduced very well the experimental HOD vibrational distribution.

For the $\text{H} + \text{H}_2\text{O}$ and $\text{H} + \text{D}_2\text{O}$ reactions, experimental rotational populations of the OH and OD products in the collision energy range 1–2.5 eV have been reported [12–19]. QCT calculations by Castillo and Santamaría [20] on the OC PES at a

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collision energy of 2.20 eV yielded OH and OD rotational distributions somewhat hotter than the experimental determinations by Wolfrum and co-workers [16]. Similarly, very recent experiments performed by Brouard and co-workers [19] at 1.43 ± 0.1 eV collision energy provided OH and OD rotational populations which were colder than the QCT predictions on the OC PES [21]. Recently, Wu et al. [22] have reported a new PES, hereafter WSLFH, based on a more extensive set of multireference configuration interaction (MRCI) ab initio points in the transition state region than the OC PES. Comprehensive QCT and variational transition state (VTST) calculations for the OH + H₂ and H + H₂O reactions and their isotopic variants have been performed on that PES [10,23–26]. From the comparison between theory and the available experimental data, it can be concluded that the WSLFH PES is of high accuracy. However, this PES is not fully ab initio since it considers semi-empirical functions for some of the ‘spectator’ degrees of freedom (OH stretch, H₂O bend and the torsion mode) and is not completely symmetric with respect to the exchange of the three H-atoms and, thus, it cannot be used to study the H' + H₂O → H'OH + H exchange reaction [22]. Very recently, a substantial progress have been made in the construction of a global ab initio PES for the H₃O system by Collins et al. [27–29]. These authors have constructed two PESs, namely YZCL1 and YZCL2, as an interpolation of quantum chemistry data evaluated over a large range of molecular geometries. In particular, the YZCL2 PES was constructed by using the UCCSD(T)/aug-cc-pvQZ level of theory [29]. The functional form of the corresponding global PES is given by interpolation of second order Taylor expansions centered at the calculated ab initio data points [29]. Full dimensional time-dependent wave packet calculations were performed on the YZCL1 PES and a good agreement was obtained between theory and experiment on thermal rate constants and the effect of reagent vibrational excitation on reactivity [27]. However, the calculations yielded integral cross sections for the H + H₂O(000) reaction smaller by a factor of 10 than the available experimental data [27]. The calculated integral cross sections for the exchange

reaction H + D₂O → HOD + D were in excellent agreement with experiment. For the reverse OH + H₂ and OH + HD reactions, the QM rate constants calculated on the YZCL2 PES were very close to the experimental values [28,30].

In this Letter, we report a QCT study of the title reaction using the YZCL2 PES with the aim of calculating OH and H₂ rotational populations, the distribution $P(f_i)$ of the fraction of the available energy released as translational energy, f_i , and differential cross sections (DCS) determined for specific final quantum states of the OH product. The calculations have been performed at 1.43 eV collision energy and the results compared with the newest available experimental data by Brouard and co-workers [19].

2. Quasi-classical trajectory method

The QCT methodology employed in this work has been described in detail in [20,21,31]. A batch of 200 000 trajectories was run using a maximum impact parameter of 1.5 Å and the initial distance from the H–H₂O molecule was set to 8 Å. The reagent rotationless H₂O ground vibrational state was determined by means of a quasi-periodic trajectory calculation where actions were converged to $0.05\hbar$. Another batch of 200,000 trajectories was calculated with the same initial conditions and adding a rotational energy about each axis of the H₂O molecule of $E_{\text{rot}} = RT/2 = 0.9 \text{ kcal mol}^{-1}$, with $T = 300 \text{ K}$. An accurate calculation would have required to perform several batches of trajectories with a semiclassical quantization of rotational levels of water and should include rotational states up to $j = 10$. Integration of the equations of motion have been carried out using a slightly modified version of the VENUS 96 program [32]. A time step of 0.025 fs was employed, which gave a conservation of energy better than 1 in 10^5 . The pseudo-quantization of the final diatomic products has been performed by equating the modulus of the classical rotational quantum number to $\sqrt{j'(j' + 1)}\hbar$. The vibrational quantum number v' is found by equating the internal energy of the molecule to a rovibrational Dunham expansion in $(v' + 1/2)$ and $j'(j' + 1)$, whose coeffi-

cients are calculated by fitting the semiclassical or quantum rovibrational energies given by the asymptotic diatomic potentials of the PES. The results presented in this work do not consider energy constraints imposed either on the OH or the H₂ diatoms [23]; that is, trajectories yielding a diatom with an internal energy smaller than zero point vibrational energy have not been discarded. We have checked that the present results are not affected noticeably by imposing such energy constraint on the H₂ product molecule. As in previous works [21], the scattering angle is defined for the title reaction as that formed between the incoming H₂O and the outgoing OH molecule. The DCSs were calculated by the method of moments expansion in Legendre polynomials [31] using the Smirnov–Kolmogorov statistical test to decide when to truncate the series. Significance levels higher than 90% are achieved using 3–4 moments, ensuring good convergence, such that the inclusion of more terms did not produce significant change. Note that the experimental DCS were obtained by fitting the composite Doppler profiles with three basis functions, each of them corresponding to a Legendre moment of the distribution [19]. The $P(f_i)$ distributions have been calculated as in [21].

3. Results and discussion

3.1. Product rotational distributions and energy disposal

Before discussing the product rotational distributions and the results of the energy disposal, it is worthwhile to compare the total integral cross section (ICS) calculated for the title reaction using the YZCL2 PES with those obtained on other PESs. The present QCT calculations yield an ICS of $0.024 \pm 0.001 \text{ \AA}^2$ for $\text{H} + \text{H}_2\text{O}(000)$ and $0.027 \pm 0.001 \text{ \AA}^2$ for $\text{H} + \text{H}_2\text{O}(000, E_{\text{rot}} = 0.9 \text{ kcal/mol})$. Notice the small effect of the rotational excitation of water on the total ICS. If we apply an energy constraint on the newly formed H₂ molecule [23] (see above), the ICSs reduce to 0.017 and 0.019 \AA^2 , respectively. The present QCT ICSs calculated with the zero point energy constraint are about two times larger than the corresponding

QM ICSs obtained on the YZCL1 PES [27]. Troya et al. [23] obtained a QCT ICS of 0.015 ± 0.003 on the WSLFH PES at $E_{\text{col}} = 1.5 \text{ eV}$, which is in reasonable agreement with the present results. However, all the calculated ICSs are lower by almost an order of magnitude than the existing experimental data [13,16]. This fact suggests that new experiments would be needed to confirm the disagreement between theory and experiment.

Fig. 1 compares the QCT OH($v' = 0$) relative rotational populations with the experimental measurements by Brouard and co-workers [19]. It

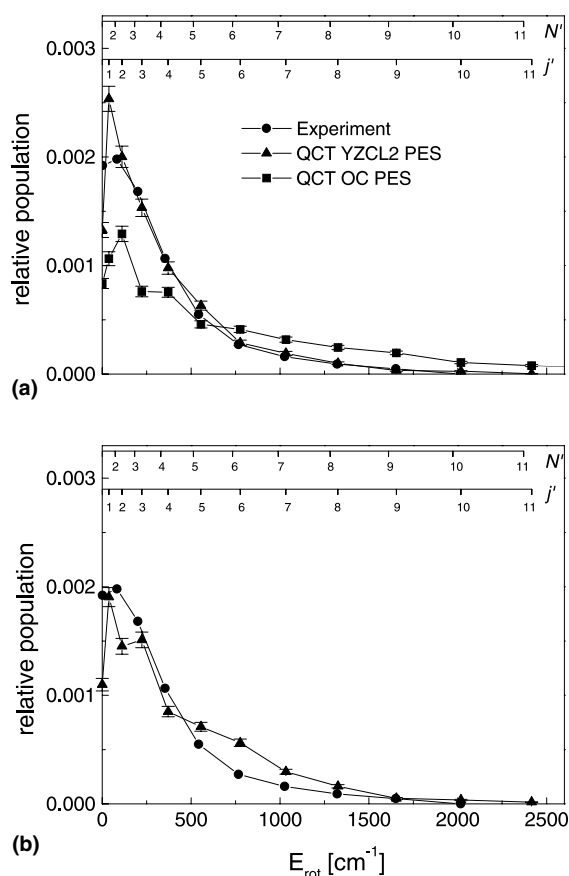


Fig. 1. Comparison between experimental and QCT OH($v' = 0, N'$) relative rotational populations as a function of OH rotational energy for the $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$ reaction at 1.4 eV collision energy. Filled circles: experimental results from [19]. (a) Filled triangles: present QCT results for $\text{H}_2\text{O}(000)$ on the YZCL2 PES. Filled squares: QCT results for $\text{H}_2\text{O}(000)$ on the OC PES [21]. (b) Filled triangles: present QCT results for $\text{H}_2\text{O}(000, E_{\text{rot}} = 0.9 \text{ kcal mol}^{-1})$ on the YZCL2 PES.

must be noted that the reported experimental OH populations are the average over all OH spin–orbit and *A*-doublet levels. To make a proper comparison between the QCT and experimental distributions we have adopted the method suggested by Clary et al. [33] in which the distributions are represented as a function of rotational energy. The procedure employed in this work is as follows: (a) the QCT OH(*v*' = 0) rotational distribution $P(j')$, normalized to unity, is calculated considering the OH as a closed shell molecule, (b) the $P(j')$ distribution is transformed to a distribution $P(E_{\text{rot}})$ that depends on the OH rotational energy E_{rot} using

$$P(E_{\text{rot}}) = P(j') \left(\frac{dj'}{dE_{\text{rot}}} \right), \quad (1)$$

where dj'/dE_{rot} is the Jacobian of the transformation. This Jacobian is calculated by differentiation of the Dunham expansion in $(v' + 1/2)$ and $j'(j' + 1)$. The above transformation ensures that the normalization is preserved. A similar procedure is employed to transform the experimental rotational distribution $P(N')$ to $P(E_{\text{rot}})$. In this case, each rotational level, N' , is considered to have a rotational energy which is the one corresponding to the $^2\Pi_{3/2}$ spin–orbit state with the lowest *A*-doublet sublevel [34]. The energy levels are fitted to a Dunham expansion and the expansion differentiated in order to obtain the Jacobian dN'/dE_{rot} . This procedure is more flexible than the usual correspondence rule $N' = j' + 1$ employed to assign the OH N' quantum number to the j' rotational quantum number obtained when this radical is considered as a closed shell molecule. Actually, on the basis of comparison of rotational energies, the $N' = j' + 1$ rule is only valid for the first levels and rapidly deviates to the $N' = j'$ rule as N' increases. We stress that what is actually calculated in the QCT method is the rotational angular momentum of the product diatom and from that the rotational energy is determined. Therefore, it must be emphasized that there is no a general and unambiguous procedure to make the correspondence between j' and N' .

As can be seen in Fig. 1a, the agreement between theory and experiment is quite good. For comparison purposes, we have included the rotational distribution calculated on the OC PES [21].

In this case, the QCT distribution shows a long tail at variance with experiment. The OH(*v*' = 0) rotational populations obtained when considering 0.9 kcal mol^{−1} of rotational energy for the H₂O molecule (Fig. 1b) is slightly broader compared to the calculation with rotationless H₂O(000). This result is in agreement with that obtained in a recent QCT calculation on the WSLFH PES [25] in which the rotational state of H₂O(000) was fixed to $j = 2$. The broadening of the OH rotational distribution with the rotational excitation of the H₂O molecule is also consistent with the increase of the average OH rotational energy as j increases found in the QCT study by Troya et al. [23] on the WSLFH PES. The present calculations predict no formation of OH(*v*' = 1) products, in accordance with the experimental findings and the QCT results obtained on the WSLFH PES [25], and in contrast with the QCT calculations on the OC PES [21].

The experiments of Brouard and co-workers [19] provide information about the OH quantum state-resolved kinetic energy release distribution, $P(f_i)$. Due to energy conservation, the $P(f_i)$ reflects the internal energy distribution of the H₂ co-product formed in coincidence with a given quantum state of the OH. Fig. 2 shows the $P(f_i)$ for the OH($^2\Pi_{1/2}(A')$, *v*' = 0, $N' = 1$) product from the H + H₂O reaction at 1.4 eV. The calculation of the $P(f_i)$ has been performed as in a previous work [21] using the QCT state-resolved ICSSs. Briefly, the H₂ rotational state populations in coincidence with the specific OH rotational state are convoluted with a gaussian function of width $\Delta E_t = 0.1$ eV that mimics the experimental resolution. The QCT results shown in Fig. 2 are the average for the OH(*v*' = 0) products born in $j' = 0$ –2. The partial state resolution chosen in the QCT calculations is due to the small number of reactive trajectories in these low j' states, which makes the associated statistics quite poor. In fact, it has been checked that the $P(f_i)$ distribution is quite insensitive with respect to the OH rotational states chosen in the calculation. As can be seen, the theoretical $P(f_i)$ obtained from the QCT calculations with rotationless H₂O or with the 0.9 kcal mol^{−1} rotational excitation are somehow broader than the experimental one. This implies that the experimentally inferred H₂ co-product rotational distribution

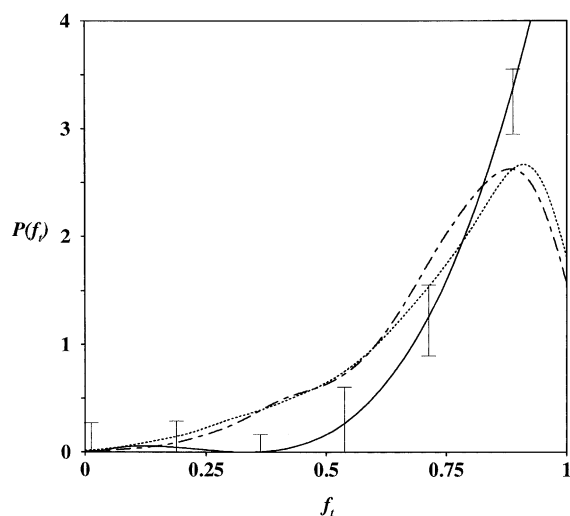


Fig. 2. Comparison between experimental and QCT $\text{OH}(v' = 0, N' = 1)$ kinetic energy release distribution $P(f_i)$ for the $\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$ reaction at 1.4 eV collision energy. Solid line: Experimental results for $\text{OH}(\text{}^2\Pi_{1/2}, v' = 0, N' = 1)$ from [19]. Dot-dashed line: present QCT results for $\text{H}_2\text{O}(000)$ on the YZCL2 PES. Dotted line: present QCT results for $\text{H}_2\text{O}(000, E_{\text{rot}} = 0.9 \text{ kcal mol}^{-1})$ on the YZCL2 PES.

formed in conjunction with $\text{OH}(v' = 0, j' = 0-2)$ molecules must be colder than the QCT ones shown in Fig. 3. In spite of this, the present results are noticeably colder than those obtained on the OC PES [21] (notice that the OC PES predicts the population of H_2 in $v' = 1$ whereas for the YZCL2 PES all the population is in $v' = 0$), and also somewhat colder than that obtained by Troya et al. [25] on the WSLFH PES.

The results shown in Figs. 2 and 3 indicate that rotational excitation of water has a very small effect on the $P(f_i)$ and H_2 rotational distribution, at least at this collision energy. This is in contrast with the slight increase of OH rotational excitation when a rotating water molecule is considered (see

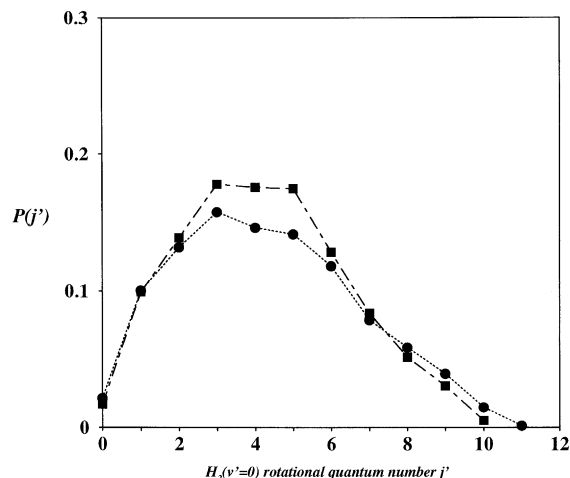


Fig. 3. QCT relative rotational distributions of the $\text{H}_2(v' = 0)$ co-product for $\text{OH}(v' = 0, j' = 0-2)$. Solid squares: present QCT results for rotationless $\text{H}_2\text{O}(000)$ on the YZCL2 PES. Solid circles: present QCT results for $\text{H}_2\text{O}(000, E_{\text{rot}} = 0.9 \text{ kcal mol}^{-1})$ on the YZCL2 PES.

Fig. 1). This finding seems to confirm the idea discussed by Brouard et al. [19] that the non-reactive OH moiety of the reagent H_2O molecule acts as an ‘spectator’ and that the OH product rotational excitation has its origin in the bending and rotational thermal motions of the parent water molecule.

Table 1 summarizes the energy disposal data for the $\text{H} + \text{H}_2\text{O}$ reaction at 1.4 eV collision energy and provides a comparison with the most recent experimental results. Following Schatz and co-workers [22], the fractions for vibration and rotation have been obtained from the rovibrational energies calculated by rounding off the vibrational and rotational actions. This implies to assume that the zero point energies of the H_2 and OH molecules are taken in $v' = 0$ rather than in the minimum of the corresponding diatomic potential. As

Table 1
Energy disposal data for the $\text{H} + \text{H}_2\text{O}$ reaction at 1.4 eV collision energy

$\langle f_i \rangle$	$\langle f_r^{\text{OH}} \rangle$	$\langle f_v^{\text{OH}} \rangle$	$\langle f_{\text{int}}^{\text{H}_2} \rangle$	$\langle f_v^{\text{H}_2} \rangle$	Comments	Ref.
0.80 ± 0.09	0.06 ± 0.01	0.00 ± 0.02	0.14 ± 0.09	$\lesssim 0.05$	Experimental	[19]
0.80	0.05	0.00	0.15	0.01	QCT (YZCL2)	[a]
0.78	0.06	0.00	0.14	0.02	QCT (YZCL2)	[b]

[a] For rotationless $\text{H}_2\text{O}(000)$; [b] for $\text{H}_2\text{O}(000, E_{\text{rot}} = 0.9 \text{ kcal mol}^{-1})$.

can be seen, the present results agree quite well with the experimental data. The comparison with the QCT results using the WSLFH PES [22,25] is good for the OH product but less quantitative for the H₂ product.

3.2. Differential cross sections

Fig. 4 shows the QCT state-resolved DCS for OH($v' = 0, j' = 0-2$) (Fig. 4a) and OH($v' = 0, j' = 4-6$) (Fig. 4b) obtained on the YZCL2 PES with and without rotation of H₂O along with the experimental data of Brouard and co-workers [19]. The QCT OH($v' = 0, j' = 0-2$) DCSs are in very good agreement with the experimental determination for the OH($^2\Pi_{1/2}, v' = 0, N' = 1, A'$) state, showing a forward-backward symmetry. However, the agreement between theoretical and experimental DCSs for the higher OH rotational state is only qualitative. Experiment and theory agree in that the backward scattering is more favored as the rotational quantum state of OH increases. This same behavior has been observed in previous QCT calculations on the OC [21] and WSLFH [25] PESs. Inspection of the reactive trajectories and the corresponding opacity functions indicates that small impact parameters ($b < 0.3$ Å) tend to favor the production of OH in high rotational states ($j' > 4$), whereas high impact parameters ($b > 1.2$ Å) have some propensity to produce OH in low rotational states ($j' < 4$). Since there is a clear correlation between small and large scattering angles and low and high impact parameters, respectively, the OH products in high j' are more backscattered than those produced in low j' . This behavior can be related to the impulsive model for the breakup of the HH–OH collision ‘complex’ suggested by Zare and co-workers [15]. This model has been sustained by QCT calculations on the Walch–Dunning–Schatz–Elgersma (WDSE) PES, the Isaacson 5 (I5) PES [35] and, recently, on the more accurate WLSFH PES [23]. According to the model, the breaking of the H–OH bond will rotationally excite the remaining OH fragment by exerting a force on the O-atom and, hence, a torque on the departing molecule. The formation of the complex is more likely to be by ‘head-on’ collisions; that is, at small

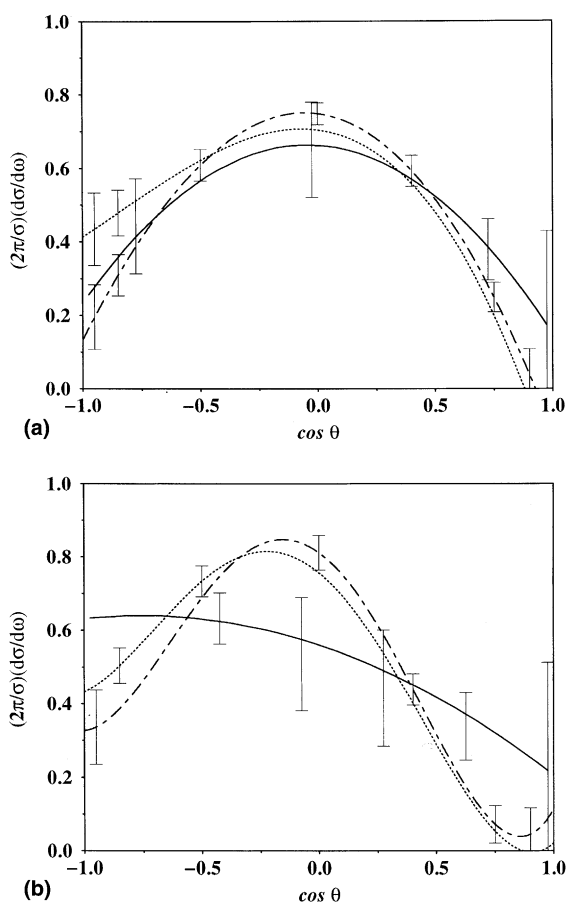


Fig. 4. (a) Comparison between experimental OH($v' = 0, N' = 1$) product and QCT calculated OH($v' = 0, j' = 0-2$) DCSs for the H + H₂O → OH + H₂ reaction at 1.4 eV collision energy. Solid line: experimental results from [19]. Dot-Dashed line: QCT results for H₂O(000) on the YZCL2 PES. Dotted line: QCT results for H₂O(000, $E_{\text{rot}} = 0.9$ kcal mol⁻¹) on the YZCL2 PES. (b) Same as (a) but for the experimental OH($v' = 0, N' = 5$) product and QCT calculated OH($v' = 0, 4 \leq j' \leq 6$) product.

impact parameters. Nevertheless, this mechanism is not truly efficient and the resulting OH rotational distribution is fairly cold.

4. Conclusions

QCT calculations have been performed for the H + H₂O reaction on one of the most recent PESs available for this system, namely the YZCL2 PES by Collins and co-workers [29]. Rotational distri-

butions for the OH and H₂ products as well as kinetic energy release and state-resolved differential cross sections have been calculated and compared with the available experimental data and other theoretical results on different PESs. In most cases, there exists a good agreement between the present calculations and the experimental results, which is better than that obtained when using other PESs available.

It remains to be seen whether the agreement found between theory and experiment extends to the isotopically substituted reactions, H + D₂O and H + HOD, and to other collision energies. Work is in progress in that direction. Besides, accurate full dimensional QM calculations on this PES would be desirable to assess the validity of the QCT method to reproduce the state-to-state dynamics of this prototype reaction.

Acknowledgements

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