

## Supplementary Materials

### Unusual differential cross sections for the $\text{H} + \text{D}_2\text{O} \rightarrow \text{D} + \text{HOD}$ exchange reaction induced by the $\text{C}_{3v}$ transition state and quantum interference

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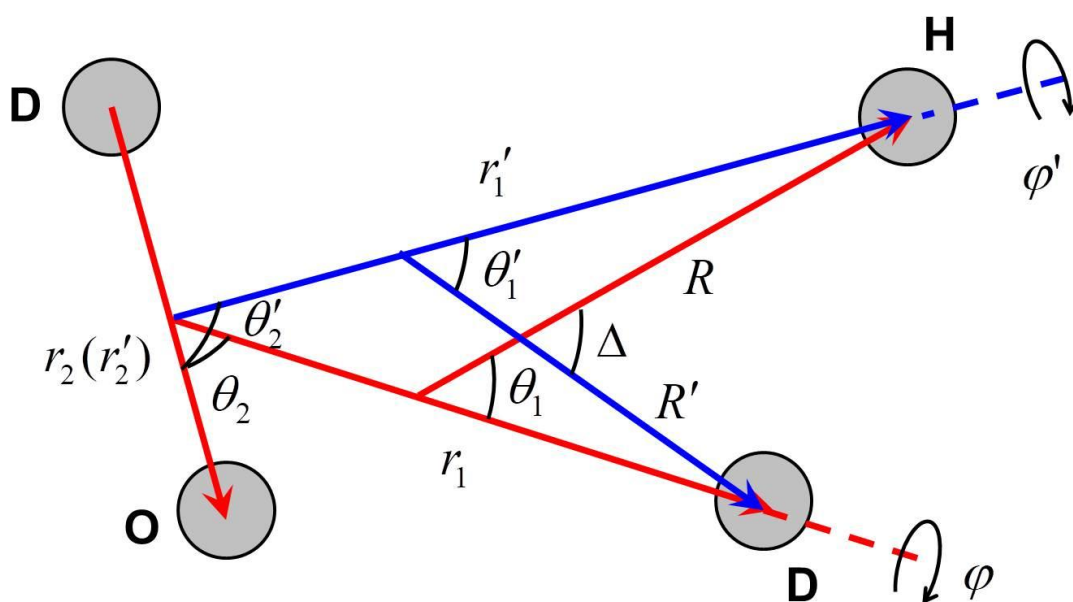


Fig. S1 Reagent Jacobi coordinates ( $R, r_1, r_2, \theta_1, \theta_2, \varphi$ ) for the  $\text{H} + \text{D}_2\text{O}$  atom–triatom arrangement and product Jacobi coordinates ( $R', r_1', r_2', \theta_1', \theta_2', \varphi'$ ) for the  $\text{D} + \text{HOD}$  atom–triatom arrangement.

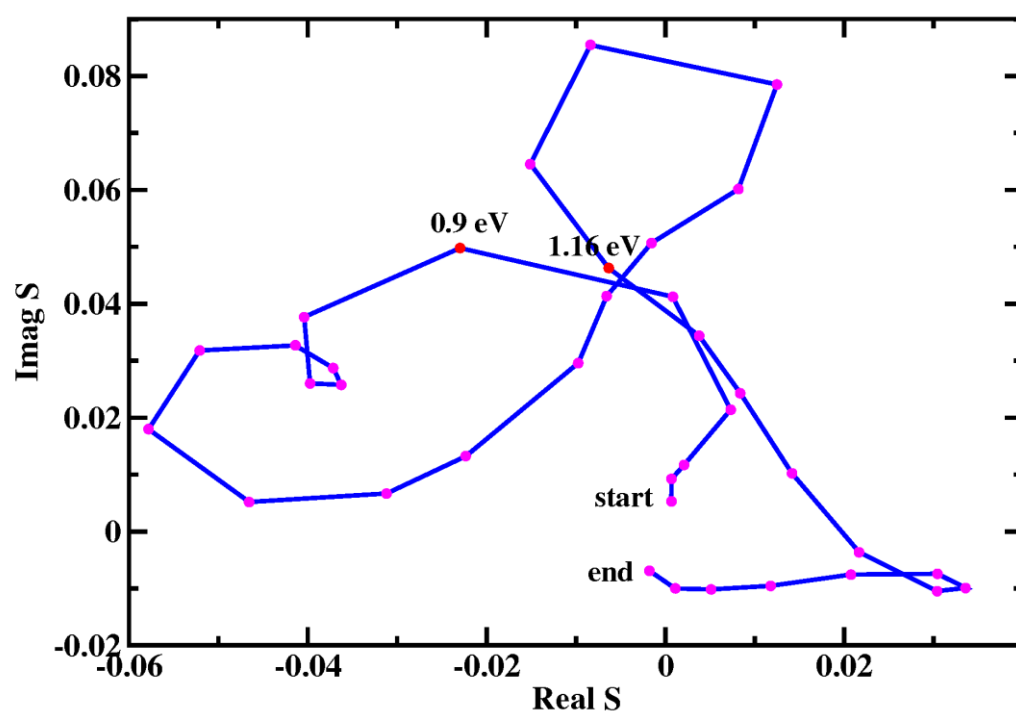


Fig S2 Argand diagram for the ground state product with total angular momentum  $J=0$ , over the collision energy range from 0.85 to 1.4 eV.

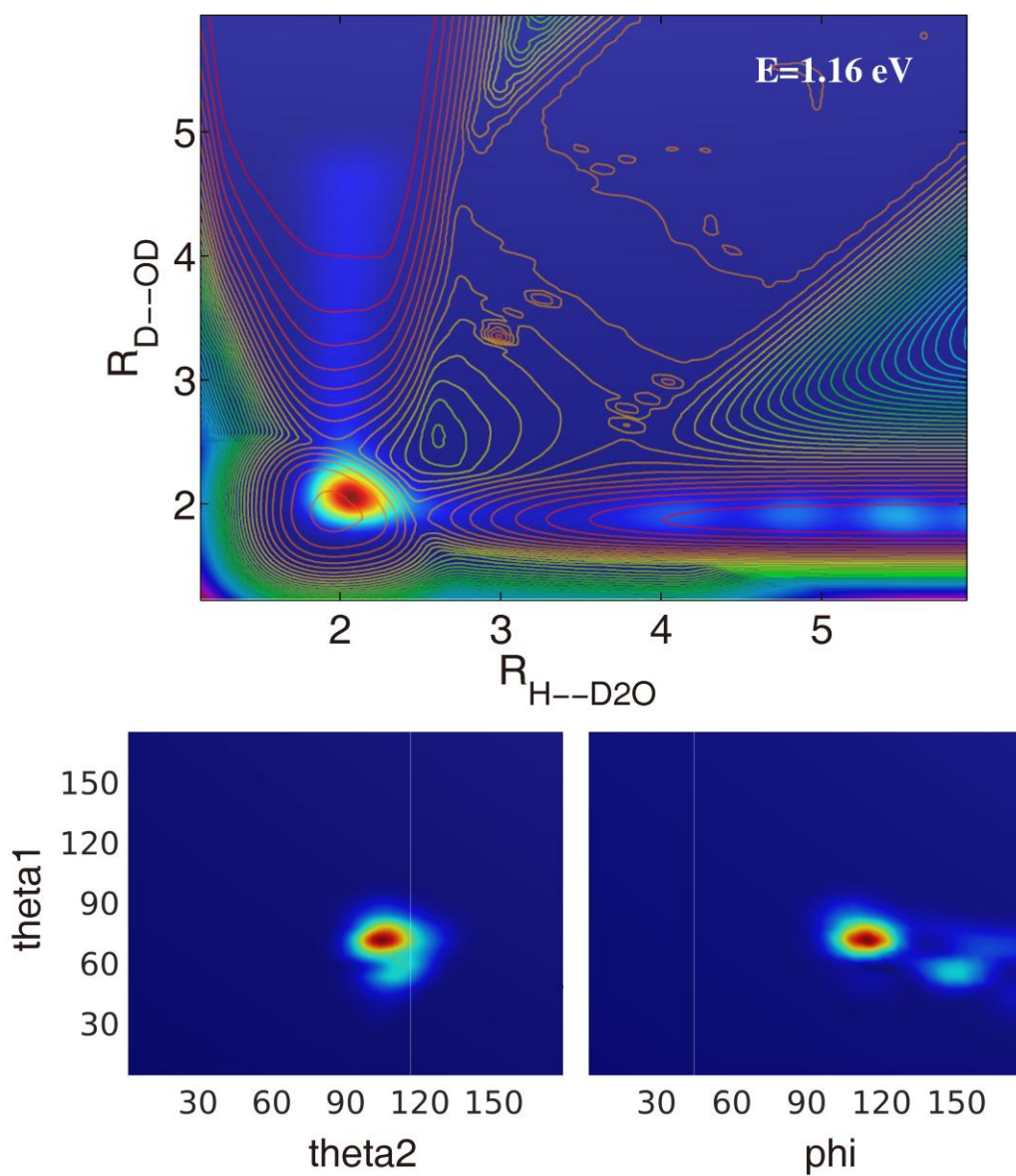


Fig S3 Reactive scattering wave functions at the collision energy of 1.16 eV in the two Jacobi coordinates  $R_{\text{H-D2O}}$  and  $r_{\text{D-OD}}$  with other coordinates integrated, and in the angle coordinates with  $R$ ,  $r_1$ , and  $r_2$  fixed at the peak position.

Table S1. The energy levels of the HOD vibrational states (with respect to the ground rovibrational state of HOD) and the collision energies at which they become populated.

| HOD vibrational state | $E_v$ (eV) | $E_c$ (eV) |
|-----------------------|------------|------------|
| (000)                 | 0          | 0.88       |
| (010)                 | 0.174      | 0.96       |
| (001)                 | 0.338      | 1.14       |
| (020)                 | 0.345      | 1.14       |
| (100)                 | 0.46       | 1.26       |
| (011)                 | 0.509      | 1.34       |
| (030)                 | 0.514      | 1.34       |

### Animation From QCT Calculations

To illustrate the reaction mechanism, three animations of typical H + D<sub>2</sub>O direct exchange trajectories at  $E_c=1.2$  eV from quasiclassical trajectory (QCT) calculations are presented.

Animation S1: A direct exchange trajectory with small initial impact parameter leading to sideward scattering.

Animation S2: A direct exchange trajectory with large impact parameter leading to late-sideward scattering.

Animation S3: A direct exchange trajectory with large impact parameter leading to backward scattering.

### Numerical parameters of quantum wave packet calculations

Figure S1 illustrates the reagent Jacobi coordinates ( $R, r_1, r_2, \theta_1, \theta_2, \varphi$ ) for the H + D<sub>2</sub>O arrangement, as well as the product Jacobi coordinates ( $R', r_1', r_2', \theta_1', \theta_2', \varphi'$ ) for the D + HOD arrangements. The numerical parameters used in the wave packet

propagation in reactant atom-triatom coordinates are as follows, with both OD bonds in the D<sub>2</sub>O reactant treated as reactive bonds. The interaction region was defined by a rectangular box of [1.0,6.0] $a_0$  in the  $r_1$  coordinate, [1.0,5.0] $a_0$  in the  $r_2$  coordinate, and [1.0,6.0] $a_0$  for the  $R$  coordinate. The number of vibrational basis functions used was 65 for  $r_1$  and 32 for  $r_2$  coordinates. For the  $R$  coordinate, we used 40 sine discrete variable representation (DVR) points. The asymptotic region was defined from 6.0 to 12.0  $a_0$  with 42 sine DVR points for the  $R$  coordinate, and 8 vibrational basis functions for both the  $r_1$  and  $r_2$  coordinates. For the rotational motion, we used  $j_{1\max}=28$  and  $j_{2\max}=50$ , which results in 18125 rotational basis functions for  $K=0$  and even parity. The number of  $K$  blocks used in the calculation increases with the total angular momentum, from 1 for  $J=0$ , up to 8 for  $J=20$ . Thus, the maximum number of the rotational basis functions reaches 257714 in the 8  $K$ -block case. The initial wave packet located at  $R_0=10 a_0$ . For lower  $J$ , we propagate the wave packets for 10000 a.u. of time with a time step of 10 to converge the reaction probability in the low energy region, especially near the resonance peak.

In product atom-triatom coordinates, we used a total number of 100 sine functions for the translational coordinate  $R'$  in a range of [3.0,15.0] $a_0$ , 5 vibrational basis functions for  $r_1'$ , and 3 vibrational basis functions for  $r_2'$ . We used  $j_{1\max}'=28$  and  $j_{2\max}'=30$ , resulting in a total of 9425 rotational basis functions for  $K'=0$  with even parity. The number of  $K$  blocks used for product propagation must be full ( $J+1$ ) to get the accurate state-to-state probabilities. A dividing surface is placed at  $R'=10 a_0$  to extract  $S$  matrix elements. To minimize the computational cost, the coordinate transformation, which transfers the absorbed wave packet in the reactant coordinates to the product coordinates, is carried out at every 8 propagation time steps.

## The quasi-classical trajectory study

The quasi-classical trajectories (QCT) simulations were performed at collision energies ranging from 0.80 to 1.5 eV, with the D<sub>2</sub>O reactant prepared in its ground rovibrational state. For each collision energy, the maximum impact parameter was

determined using 50,000 test trajectories. The initial H and D<sub>2</sub>O were separated by 8.0 Å and the trajectories were terminated when products (or reactants for non-reactive trajectories) reached a separation of 8.0 Å. The propagation time step was 2 a.u., and the scattering parameters (vibrational phases and spatial orientation of initial reactants) were selected with a Monte Carlo approach. The gradient of the PES was obtained numerically by the central-difference algorithm. A total of 10,000,000 trajectories were simulated at each collision energy.