Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

Fermi Resonance Controlled Product Branching in the H+HOD reaction

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Results presented here are obtained by a reactant-coordinate based (RCB) method for state-to-state calculation[1] on the neural network fitted potential energy surface (PES) of the H_3O system.[2] Parameters of the calculation are listed in Table S-I.

Table S-I. Parameters used in the calculations for the HD + OH and H_2 + OH abstraction channels (Atomic units are used if not otherwise stated)

Initial wave packet				
R_0	10.0			
δ	0.3			
k_0	$k_0 = \sqrt{2E_0\mu}$ with $E_0 = \begin{cases} 1.35\ \text{e}V\ for\ (000) \\ 0.90\ eV\ for\ (010), (100)\ (020)\ and\ (001) \end{cases}$			
Grid range and size for the reactant coordinates				
	HD + OH channel		**H_2 + OD channel**	
R	$R \in (0.4,16.0),\ N_R^1=96,\ N_R^2=120$		$R \in (0.4,16.0),\ N_R^1=96,\ N_R^2=120$	
r_1	$r_1 \in (0.7,12.0),\ \upsilon_{int}^1=96,\ \upsilon_{asy}^1=8$		$r_1 \in (0.7,12.0),\ \upsilon_{int}^1=80,\ \upsilon_{asy}^1=8$	
r_2	$r_2 \in (0.7,5.0),\ \upsilon_{int}^2=\upsilon_{\text{asy}}^2=4$		$r_2 \in (0.7,5.0),\ \upsilon_{int}^2=\upsilon_{\text{asy}}^2=4$	
j_1	$j_1 \in (0,100)$		$j_1 \in (0,100)$	
j_2	$j_2 \in (0,20)$		$j_2 \in (0,20)$	
Grid range and size for the product coordinates				
r_1'	$r_1' \in (0.7,5.0),\ \upsilon_1'=4$		$r_1' \in (0.7,5.0),\ \upsilon_1'=4$	
r_2'	$r_2' \in (0.7,5.0),\ \upsilon_2'=4$		$r_2' \in (0.7,5.0),\ \upsilon_2'=4$	
j_1'	$j_1' \in (0,28)$		$j_1' \in (0,28)$	
j_2'	$j_2' \in (0,20)$		$j_2' \in (0,20)$	
Product projection planes: $R_p^{\infty}=8.0$				
Absorbing Potential				
	C	x_s	x_e	n
R	0.1	12.2	16.0	1.5
r_1	0.045	10.0	12.0	1.5
Total time/time step: 8000/10				
Flux plane: $r_1^{flux}=7.0$				
Partial waves: J_{tot} = 0-50				
Reactant helicity quantum number: (0-6)				
Product helicity quantum number: (0-13)				

The initial wave packet is constructed as the direct product of an HOD eigenstate and a Gaussian wave packet in the translational coordinate *R* located in the reactant asymptote. The Gaussian wave packet is expressed in the following form,

$$G(R) = \left(\frac{1}{\pi\delta^2}\right)^{1/4} \exp\left[-\frac{(R-R_0)^2}{2\delta^2} - ik_0 R\right], \tag{S1}$$

where R_0, δ, and k_0 are the central position, width, and momentum, respectively.

Absorbing potentials are used to prevent wave function reaching the boundary of grids and following form for $x = R, r_1$ is used:

$$V_{abs}(x) = -iC\left(\frac{x - x_s}{x_e - x_s}\right)^n, \qquad x_s \le x \le x_e, \tag{S2}$$

where x_s and x_e denote the starting and ending positions of the absorbing potential, respectively, *C* is the strength parameter and *n* is the order of absorbing potential.

References:

1. B. Zhao, Z. Sun and H. Guo, J. Chem. Phys. **145** (18), 184106 (2016).
2. J. Chen, X. Xu, X. Xu and D. H. Zhang, J. Chem. Phys **138** (15), 154301 (2013).