## Electronic Supplementary Information

# Franck–Condon simulations of transition state spectra for the OH + $H_2O$ and OD + $D_2O$ reactions

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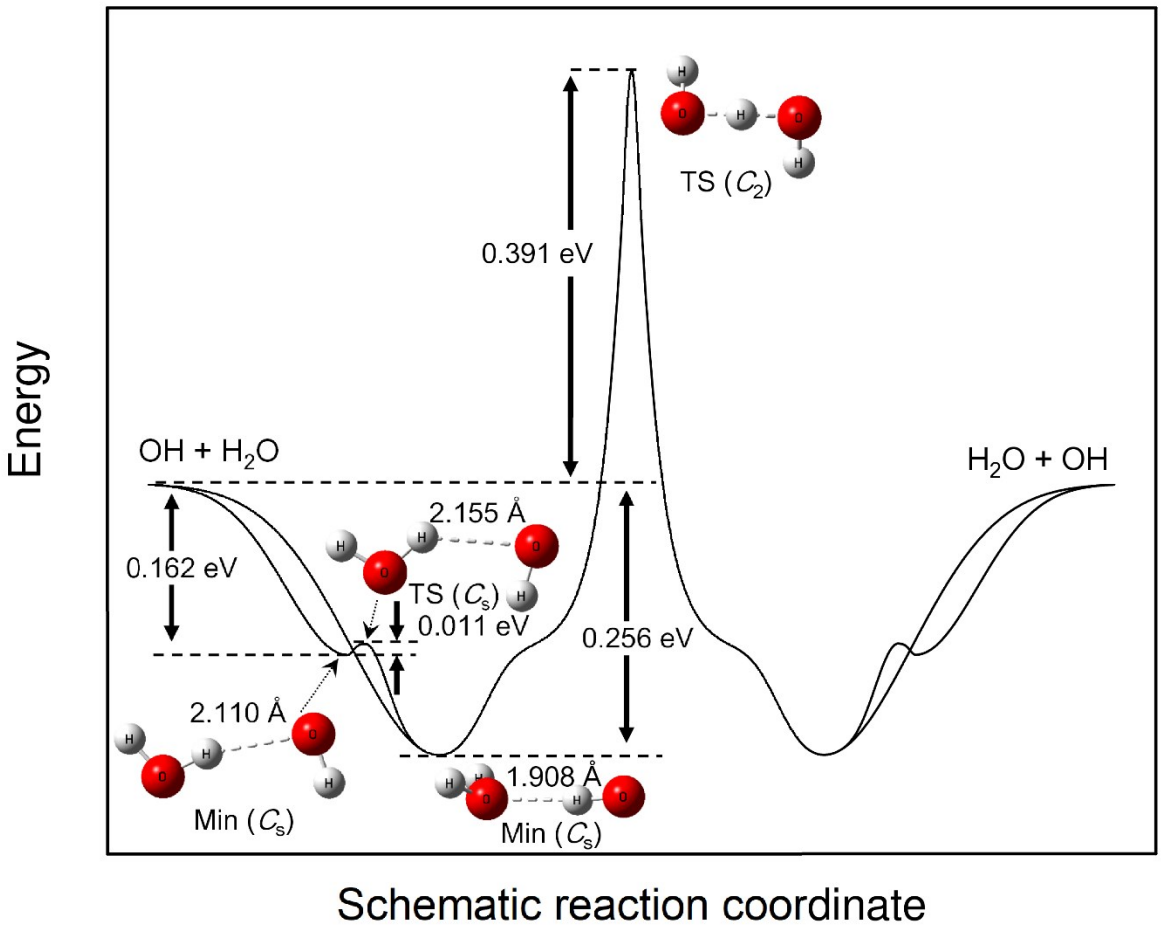


**Figure S1**

Schematic energy diagram of the neutral $H_3O_2$ rection system. Energies at stationary points are obtained from the *ab initio*-level PIP-NN potential energy surface employed in the present study.

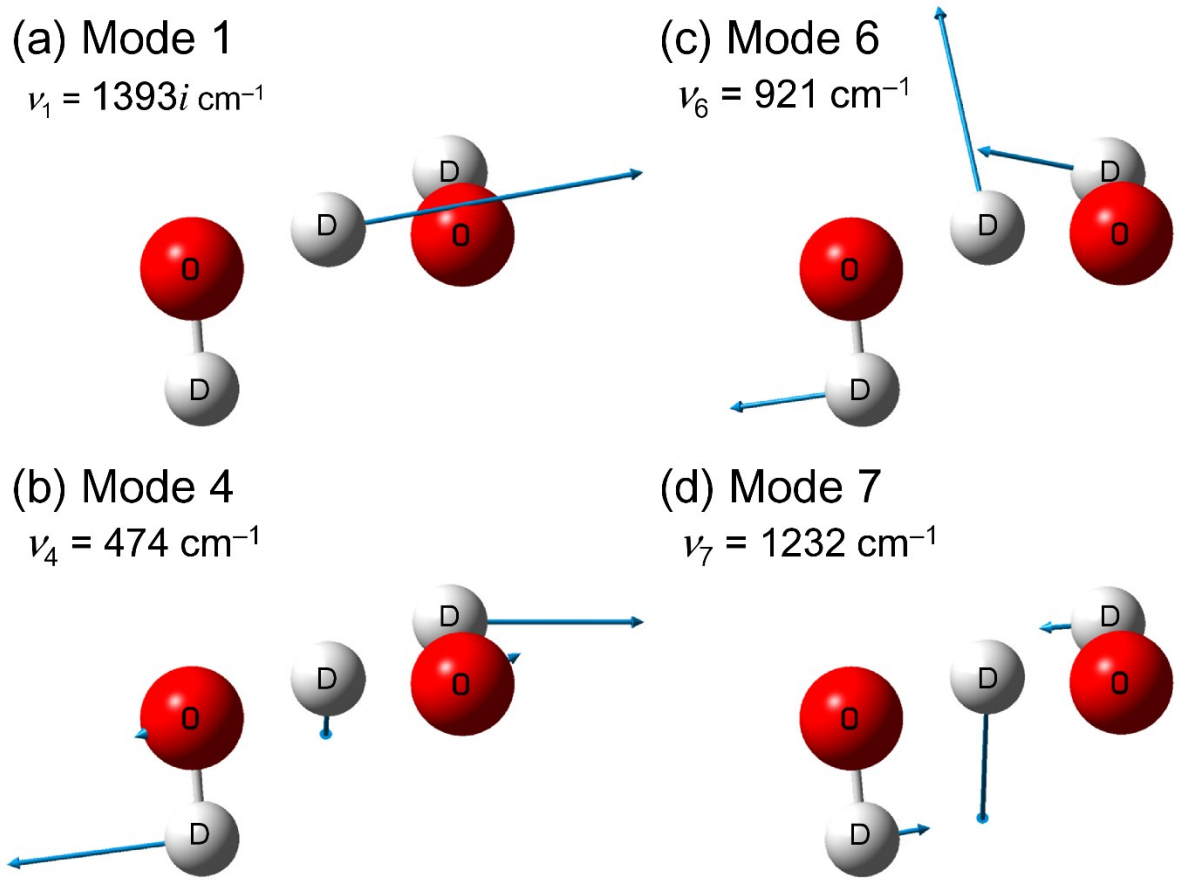


**Figure S2**

Normal-mode coordinates used in the quantum dynamics calculations as active nuclear degrees of freedom, obtained from vibrational frequency analysis of the $C_2$ transition-state structure for the OD + $D_2O$ → $D_2O$ + OD reaction. Mode 1 corresponds to the vibrational mode with an imaginary frequency.

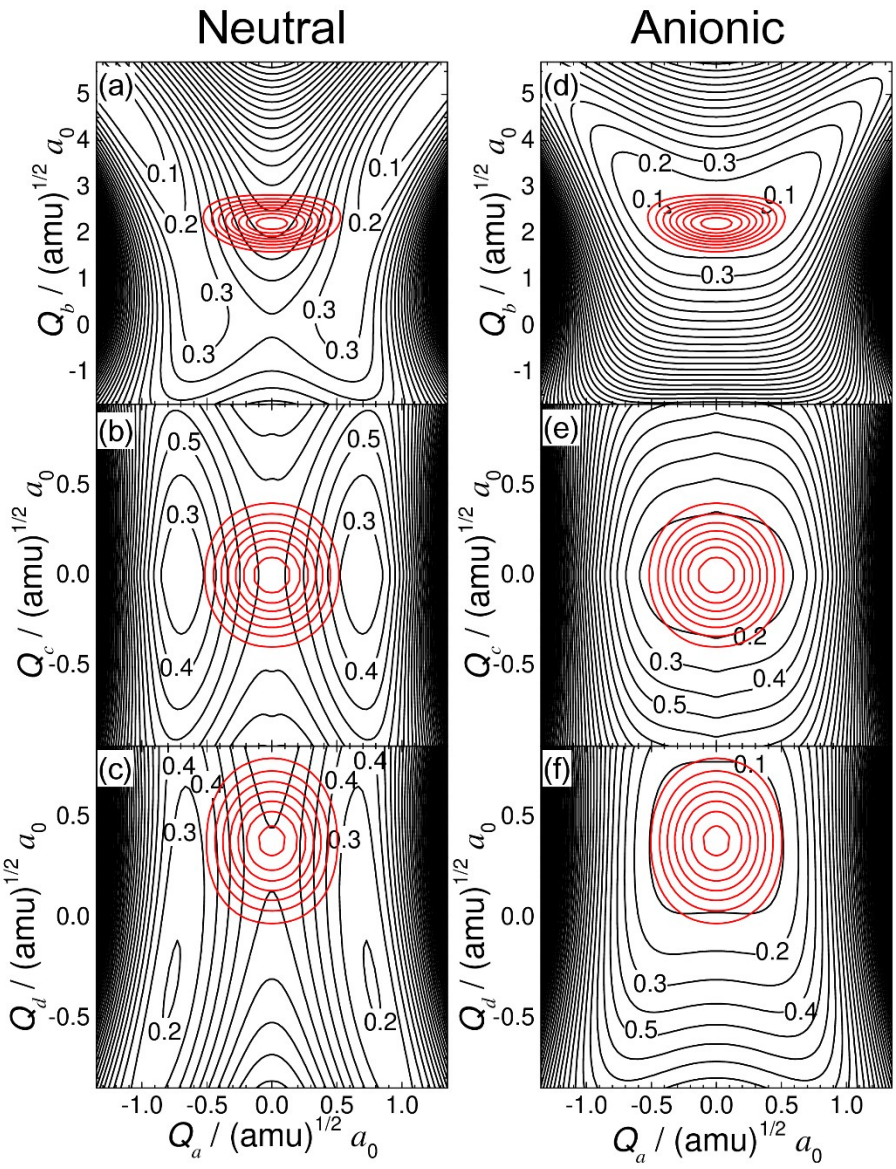


**Figure S3**

Two-dimensional contour plots of the potential energy surfaces of $D_3O_2$ and $D_3O_2^-$. The contour increment was set to 0.1 eV. Left and right panels show the neutral and anionic potential energy surfaces, respectively. Panels (a) and (d) depict the surfaces plotted as a function of $Q_a$ and $Q_b$. Panels (b) and (e) depict the surfaces plotted as a function of $Q_a$ and $Q_c$. Panels (c) and (f) depict the surfaces plotted as a function of $Q_a$ and $Q_d$. The superimposed red contour lines indicate the projection of the initial anion wavefunction density in the ground vibrational state.

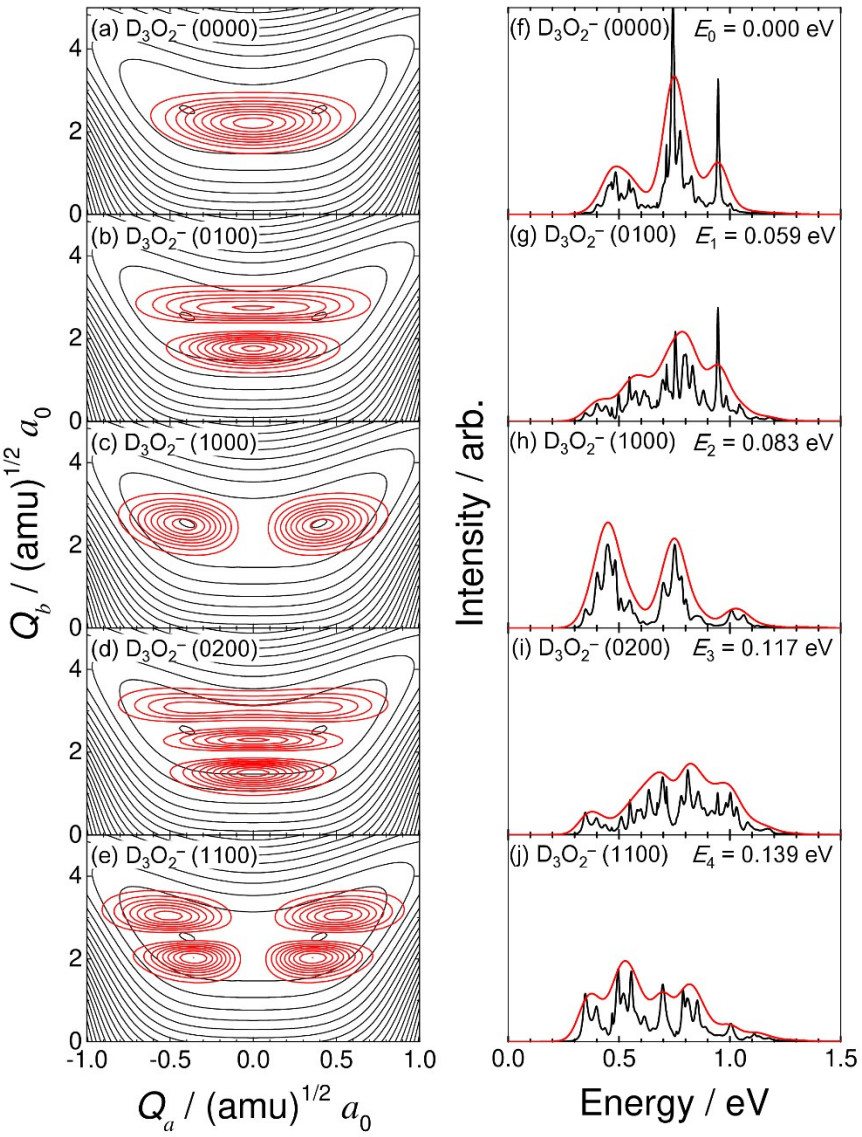


**Figure S4**

Left panels: vibrational wavefunction densities of the $D_3O_2^-$ anion plotted as a function of $Q_a$ and $Q_b$ coordinates. The state can be described by a set of quantum numbers ($v_a$, $v_b$, $v_c$, $v_d$), where $v_a$, $v_b$, $v_c$, and $v_d$ are the vibrational quantum numbers for the $Q_a$, $Q_b$, $Q_c$, and $Q_d$ coordinates, respectively. Right panels: photodetachment spectrum calculated using each vibrational wavefunction as an initial wave packet. The calculated spectra are plotted as a function of the energy defined by the neutral potential energy surface.