

Supporting Information: Quantum and Quasi-classical Dynamics of the $\text{C}(^3\text{P}) + \text{O}_2(^3\Sigma_g^-)$ $\rightarrow \text{CO}(^1\Sigma^+) + \text{O}(^1\text{D})$ Reaction on Its Electronic Ground State

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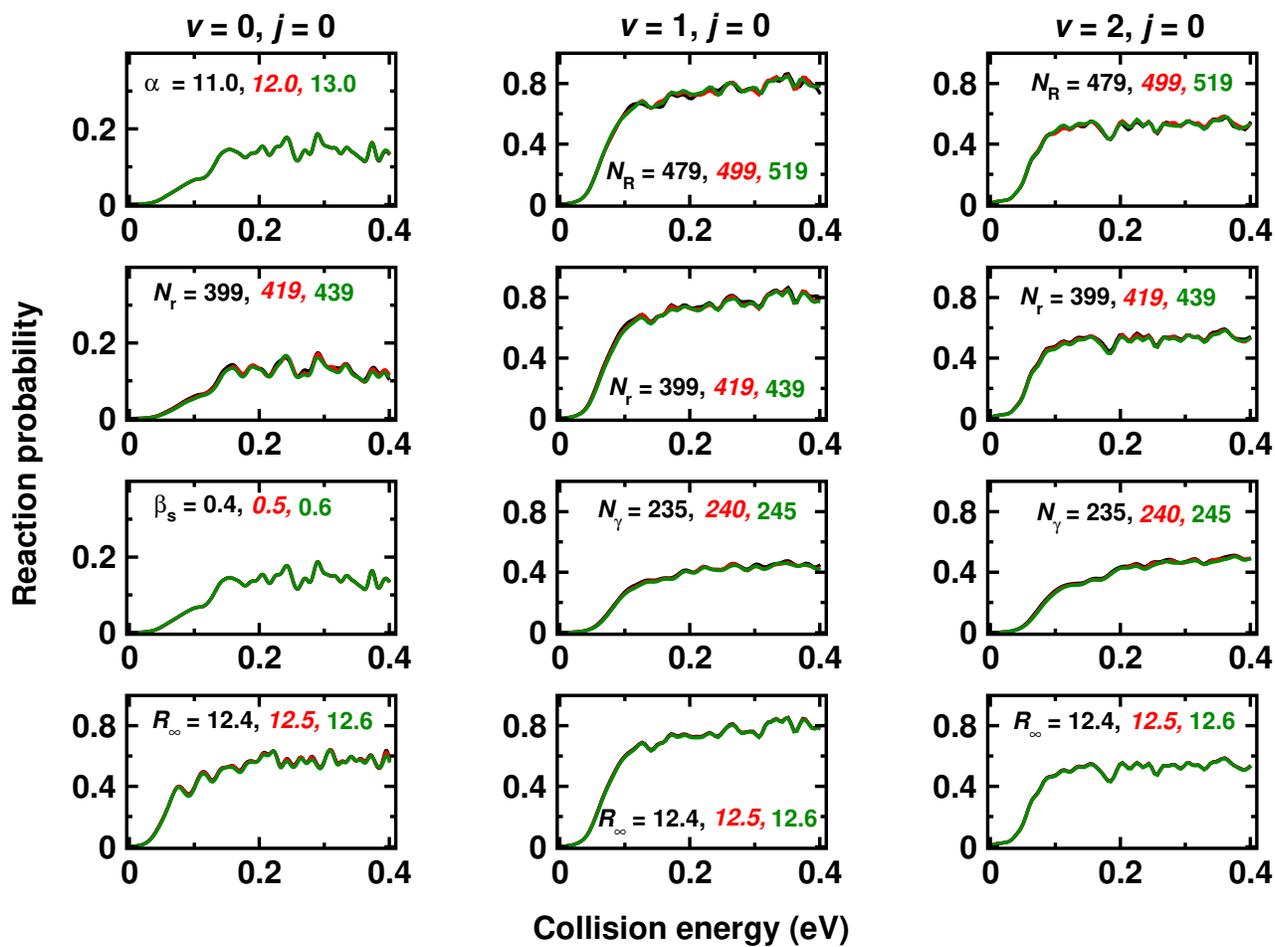


Figure S1: Convergence tests for the TDWP simulations for selected parameters. Line colors correspond to colors of the numerals. The values used in the production simulations are in italics, see Table 1. The converged parameters for $O_2(v = 0, 1, 2)$ are identical.

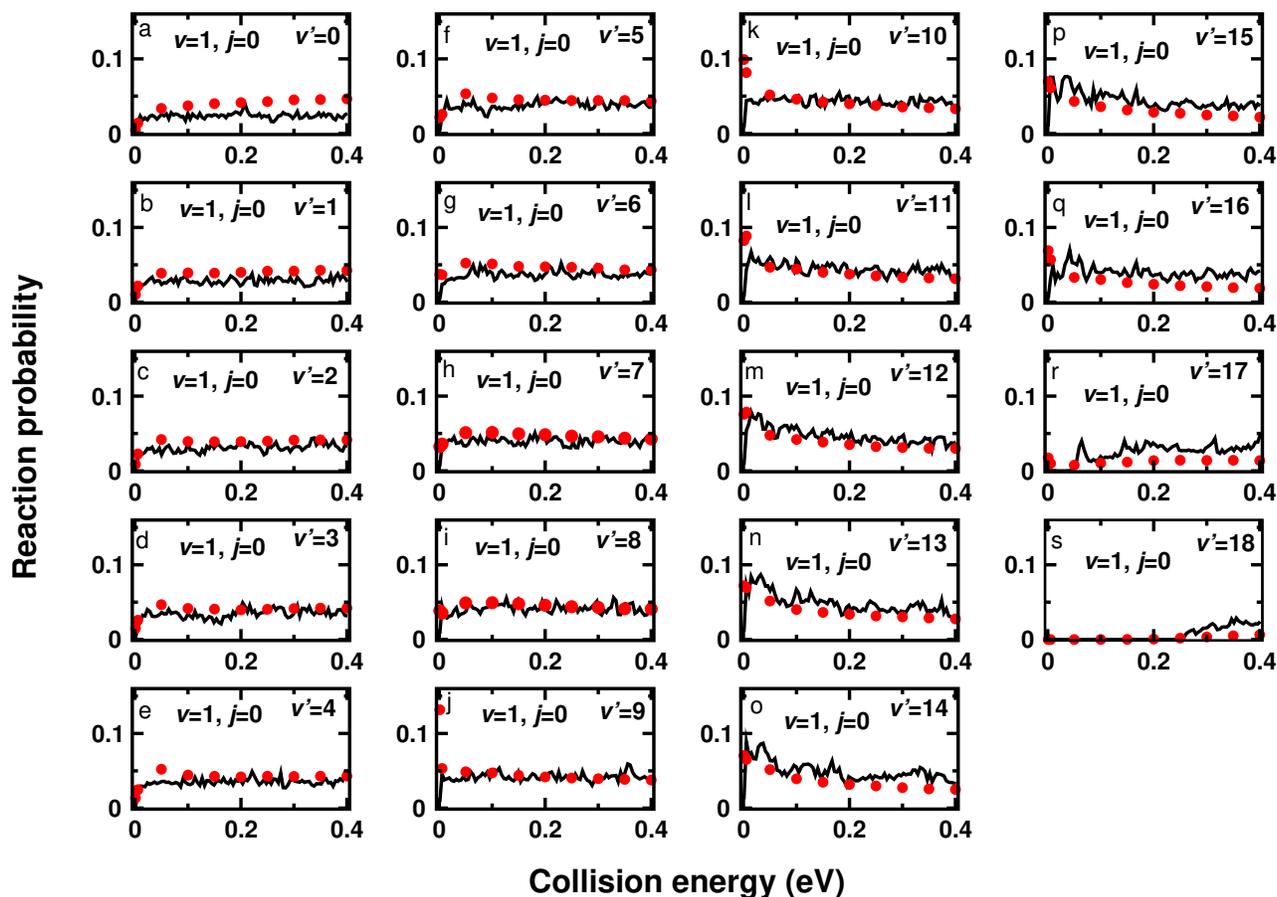


Figure S2: Product diatom vibrational level resolved state-to-state reaction probabilities for the $C(^3P) + O_2(^3\Sigma_g^-, v=1, j=0) \rightarrow CO(^1\Sigma^+, v', \sum j') + O(^1D)$ reaction on its electronic ground state and for $J=0$ as function of collision energy. The probabilities calculated from the TDWP approach and QCT(HB) method are shown by solid (black) lines and solid (red) dots, respectively.

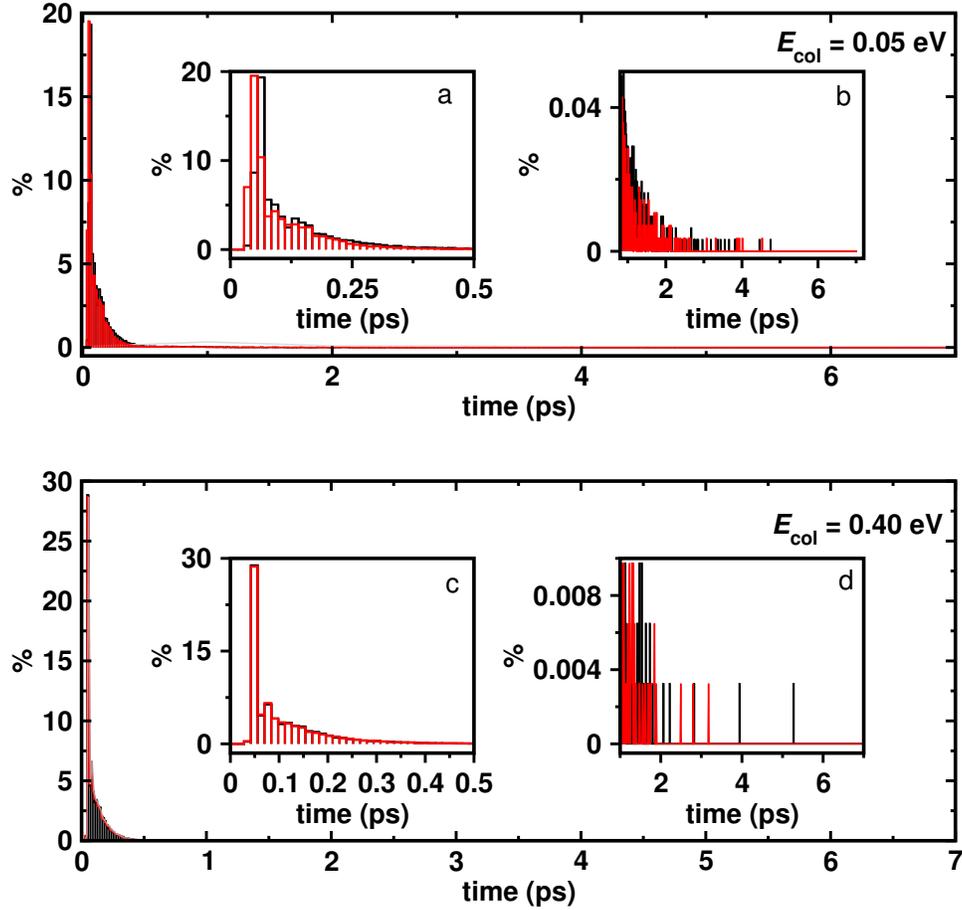


Figure S3: Distribution of collision times (or lifetime) of the intermediate collision complex as a function of time analyzed with a cutoff of $14 a_0$ (black) and $12 a_0$ (red) for the sum of distances as the criterion for formation of the complex. The distributions at 0.05 eV and 0.40 eV collision energies are shown in the top and bottom panels, respectively, together with detailed views for short and long collision times in the insets. The maxima for the two distributions with a distance cutoff at $14 a_0$ are at ~ 0.07 ps and ~ 0.056 ps and the longest collision times encountered are ~ 4.8 ps and ~ 5.3 ps for the two cases considered, respectively. These values change to ~ 0.056 ps and ~ 0.056 ps and ~ 4.5 ps and ~ 3.2 ps for the maxima and longest collision time, respectively, if a cutoff of $12 a_0$ is used.

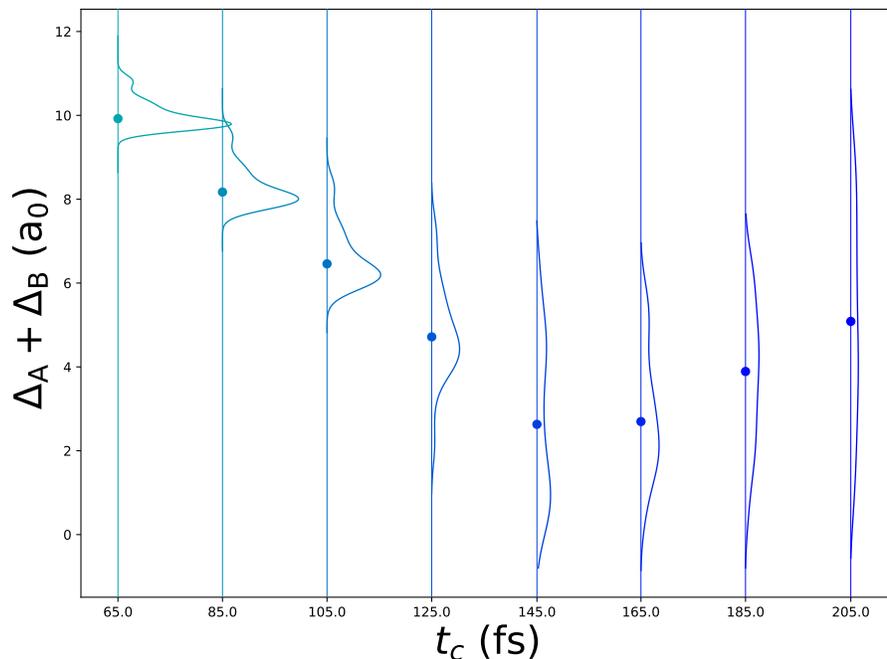


Figure S4: Distributions $P(\Delta_A + \Delta_B)$ for the deviation of each instantaneous CO-separation (CO_A and CO_B) from the equilibrium distance $r_{\text{eq}} = 2.1504 a_0$ for the minimum energy structure of CO_2 as a function of time t after synchronization. For each trajectory a time t_s is determined when the trajectory reaches $\Delta_A + \Delta_B = 15.0 a_0$ to synchronize all trajectories in time. After synchronization the distributions $P(\Delta_A + \Delta_B)$ are determined at intervals $\Delta t = 0.05$ fs from a total of 100 reactive trajectories (50 leading to $\text{CO}_A + \text{O}_B$ and 50 leading to $\text{CO}_B + \text{O}_A$). Selective distributions are plotted for $t_s = 65 - 205$ fs. The solid lines represent the 5-95th percentile, and the black circles are the median of each distribution.