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

SUPPLEMENTARY MATERIALS

I. The optimized structures of neutral and anionic 5′-dCMPH moieties at the (a) HF, and (b) MP2 methods with 6-31+G(d) basis set.

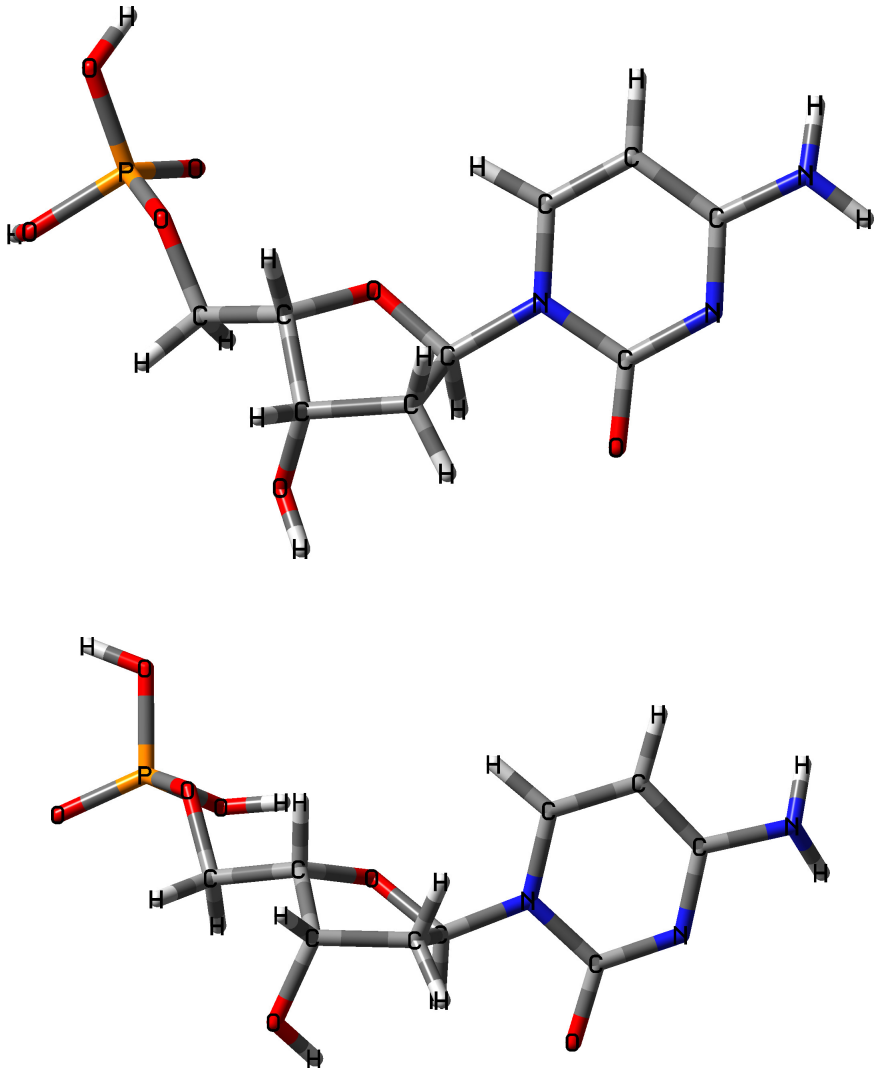

FIG. S1(A). The optimized structures of (i) neutral [above] and (ii) anionic [below] 5′-dCMPH moieties at the HF/6-31+G(d) accuracy level.

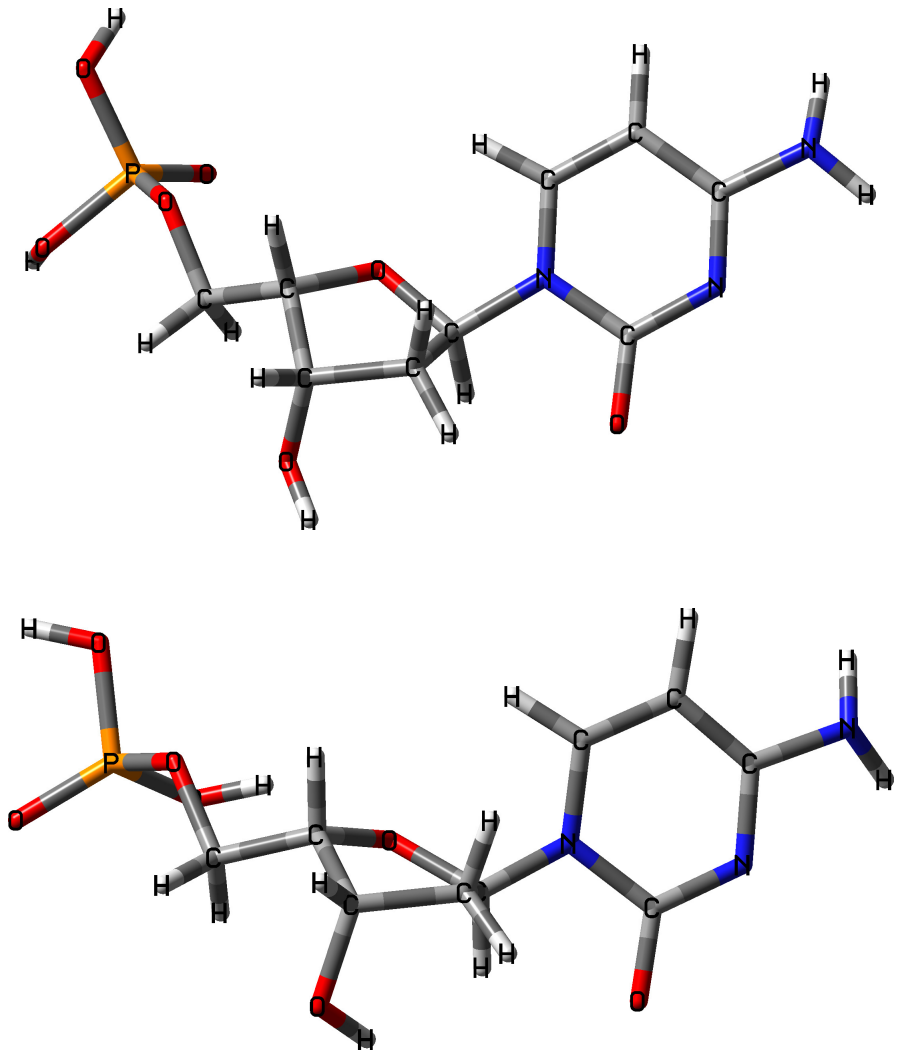

FIG. S1(B). The optimized structures of (i) neutral [above] and (ii) anionic [below] 5′-dCMPH moieties at the MP2/6-31+G(d) accuracy level.

II. Wave packet propagation for the ground state wave function $\phi_0(\mathrm{R})$ of HF potential for target 5′-dCMPH molecule.

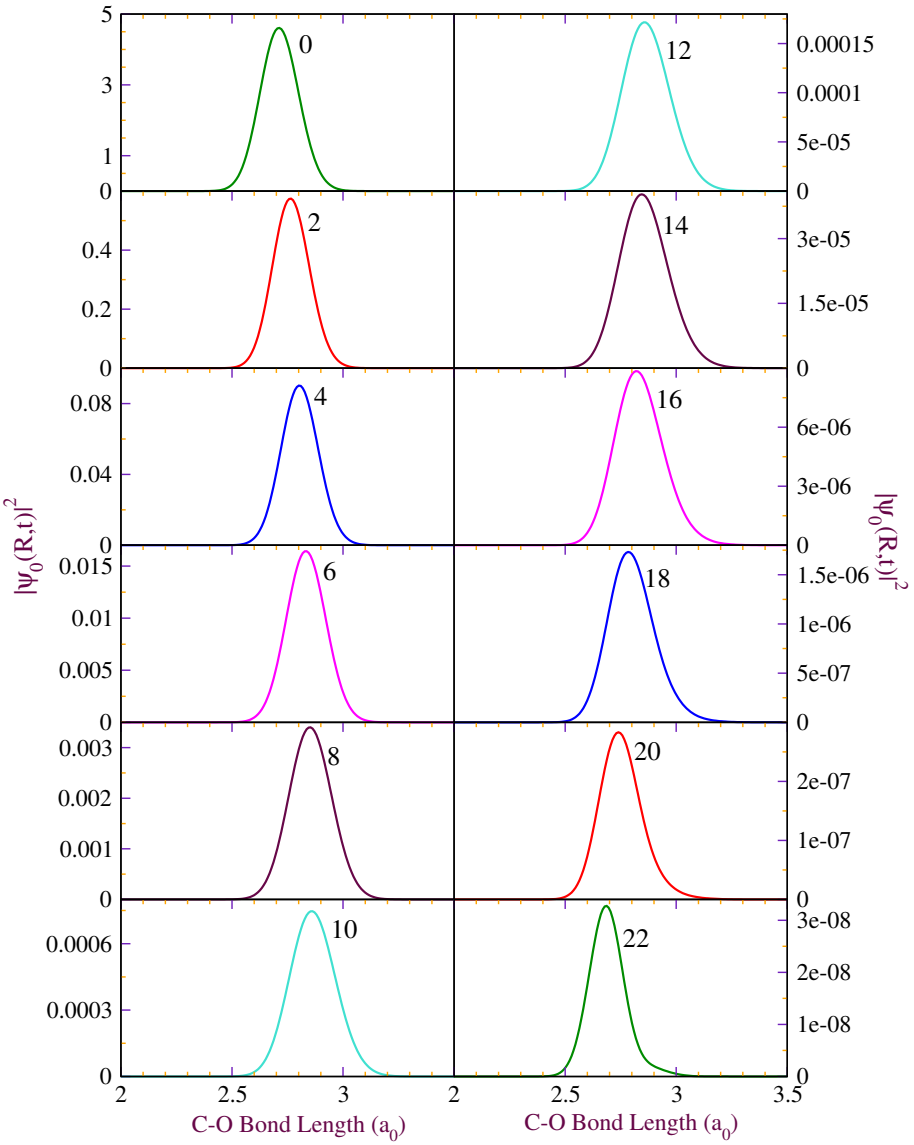

FIG. S2 Plots of wave packet propagation from time t = 0–22 fs for the ground state wave function $\phi_0(\mathrm{R})$ of the target 5′-dCMPH molecule under the effect of anionic Hamiltonian.

III. Plot of transmission coefficient (T) of the 5′ C–O bond from the anionic vibrational states of HF and MP2 potentials.

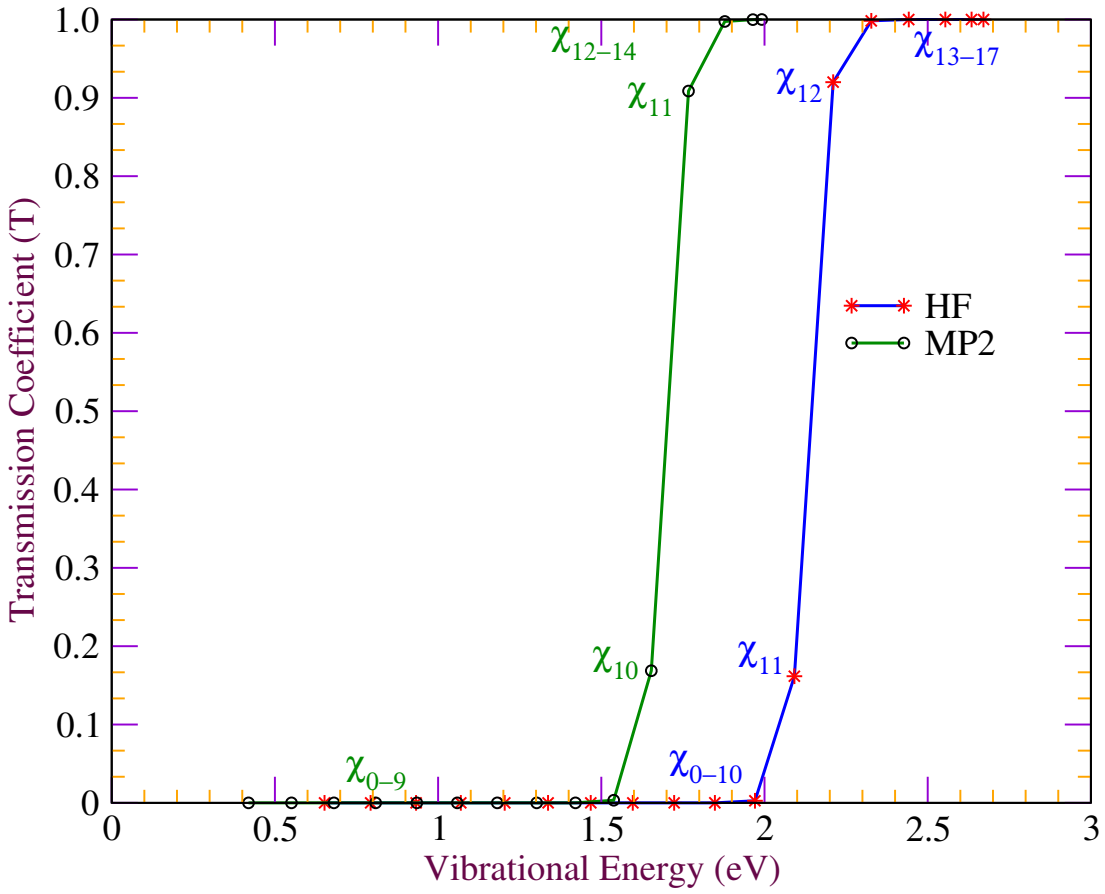

FIG. S3. "S-shaped" Transmission coefficient (T) curve of the 5′ C–O bond from (a) HF anionic vibrational states $\chi_{i=0-17}$ [blue line], and (b) MP2 anionic vibrational states $\chi_{i=0-14}$ [green line] .

IV. Plots of wave packet propagation from time t = 0–55 fs for the ϕ_{12}(R) excited vibrational state function of the 5′-dCMPH molecule.

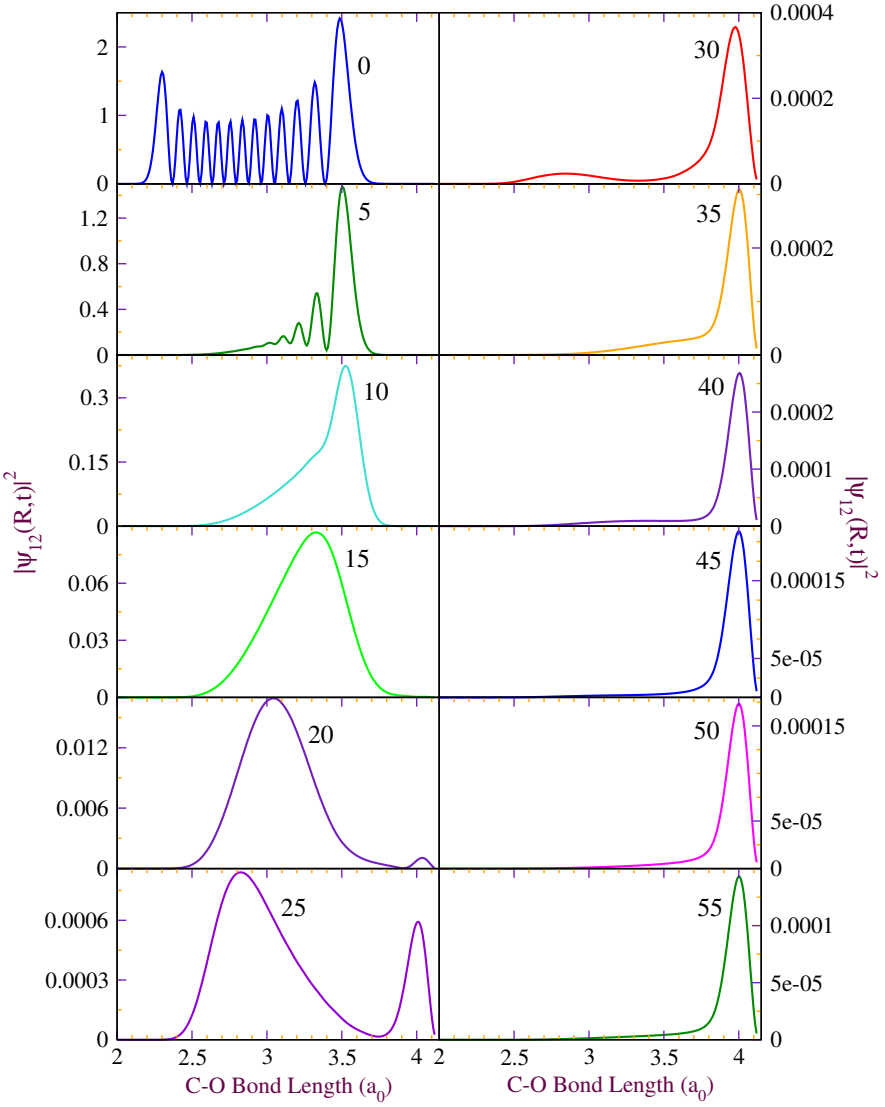

FIG. S4. Plots of wave packet propagation from time t = 0–55 fs for the excited state wave function ϕ_{12}(R) of the target 5′-dCMPH molecule under the effect of anionic Hamiltonian.

V. Singly occupied molecular orbital (SOMO)s generated at the HF/6-31+G(d) accuracy level at various instances of 5′ C–O bond breaking event.

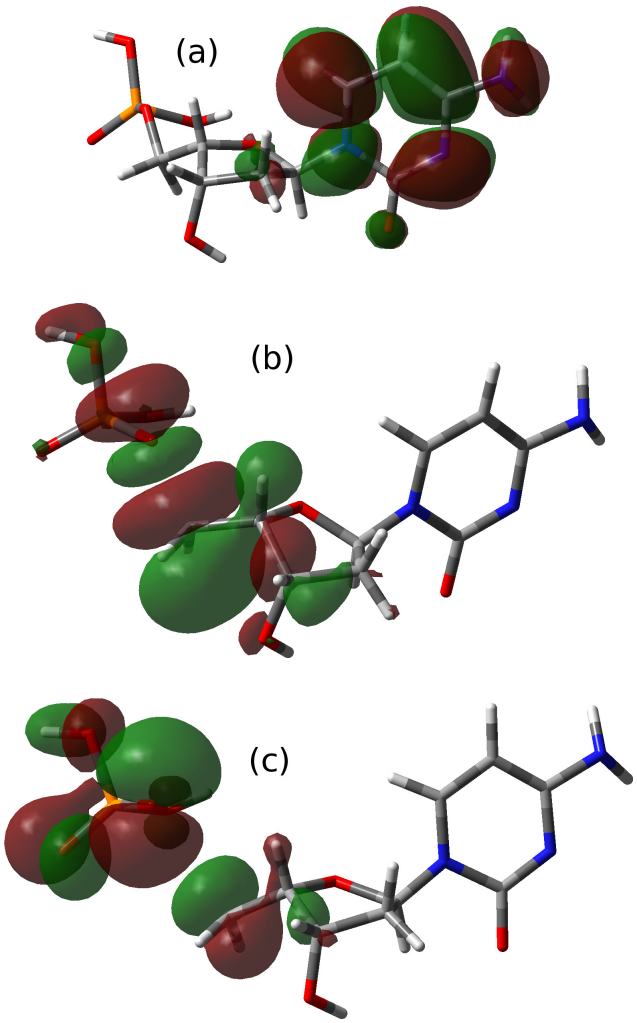

FIG. S5. Singly occupied molecular orbital (SOMO)s generated at the HF/6-31+G(d) accuracy level for anionic 5′-dCMPH moiety for the 5′ C–O bond lengths of (a) 2.75 a_0 (1.45 Å), (b) 3.69 a_0 (1.95 Å), and (c) 5.67 a_0 (3.00 Å).