

Ultrafast Excited-state Dynamics of 4-Hydroxychalcone: Role of Intramolecular Charge Transfer and Photoacidity

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Supporting Information

4-HC in MeOH

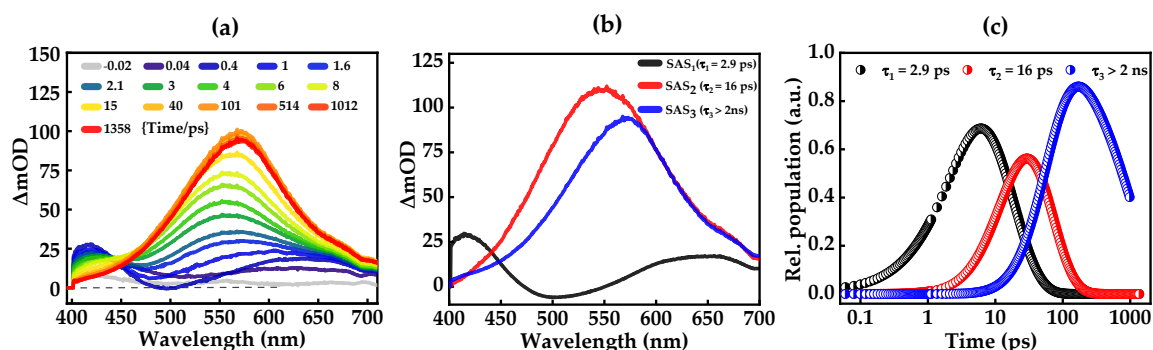
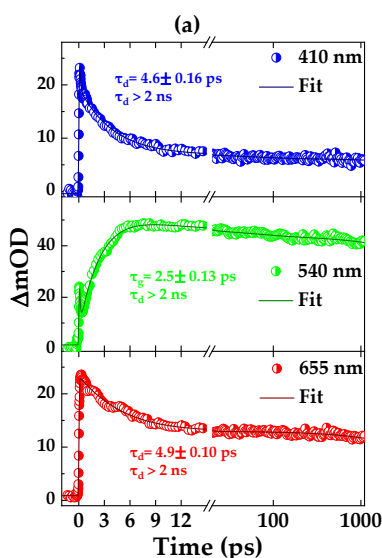
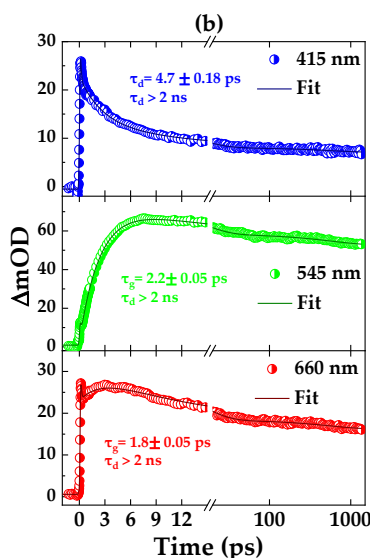


Figure S1: fs-TA of 4-HC in MeOH, (b) species-associated spectra, and (c) kinetic decay profiles. The concentration of 4-HC is 0.5 mM.

4-HC in TOL



4-HC in MeCN



4-HC in MeOH

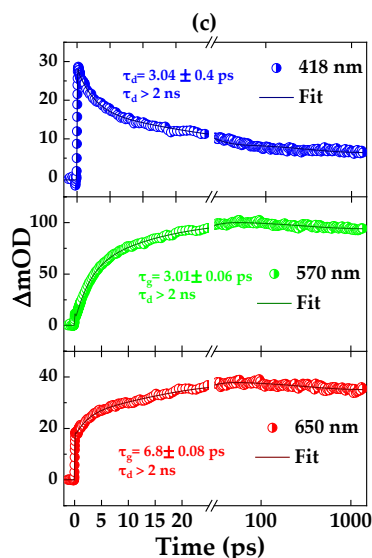


Figure S2: Single wavelength kinetics with best fitted decay profiles of fs-TA data in (a) TOL at 410 nm (blue trace), 540 nm (green trace), 655 nm (red trace), (b) MeCN at 415 nm (blue trace), 545 nm (green trace), 660 nm (red trace), and (c) MeOH at 418 nm (blue trace), 570 nm (green trace), 650 nm (red trace). The amplitude kinetics are best fitted with exponential-growth and exponential-decay functions that are identified as τ_g and τ_d parameters.

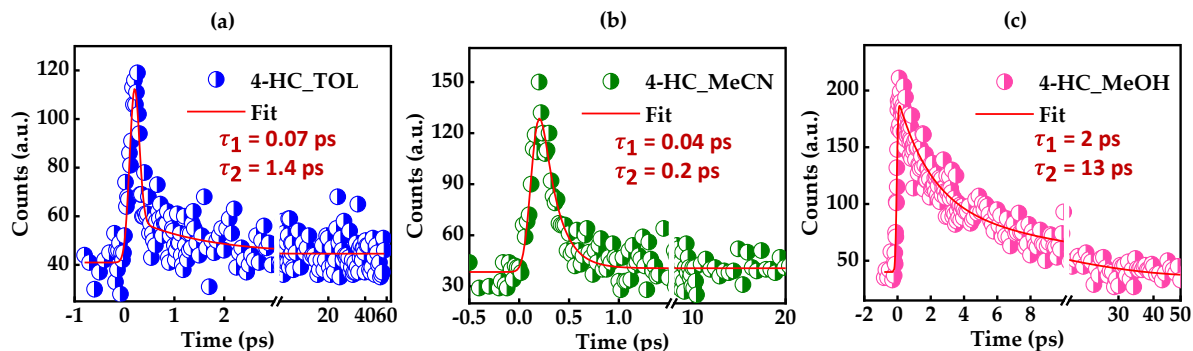


Figure S3: Fluorescence upconversion decay profiles at 440 nm with fitted curves for 4-HC in (a) TOL, (b) MeCN, and (c) MeOH, while exciting at 387 nm.

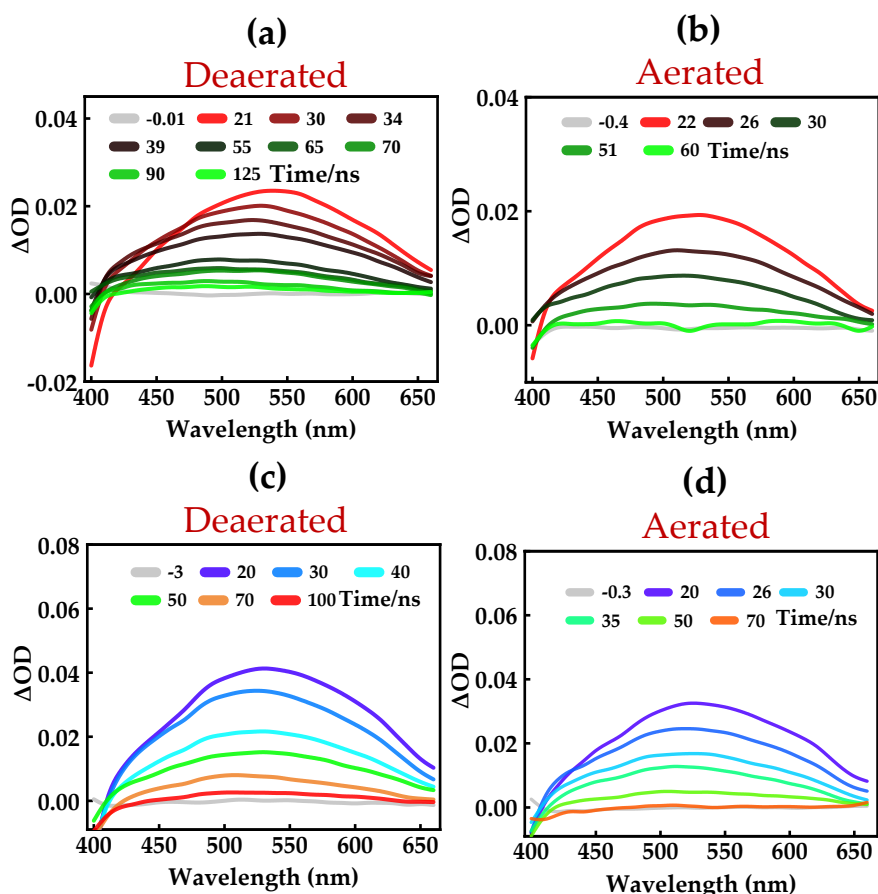


Figure S4: ns-Transient absorption spectra of 4-HC in (a) TOL, Deaerated, (b) TOL, Aerated conditions, (c) MeCN, Deaerated, and (d) MeCN, Aerated conditions while exciting at 355 nm.

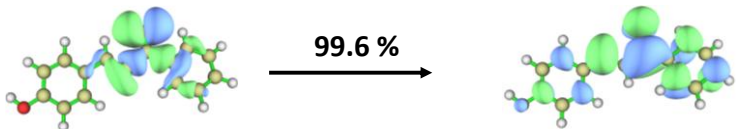
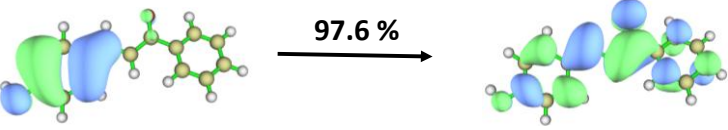
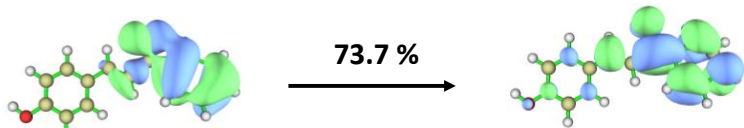
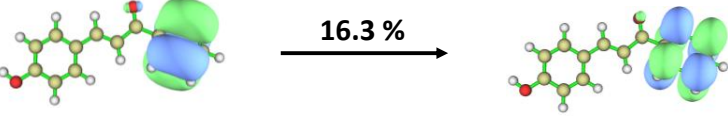
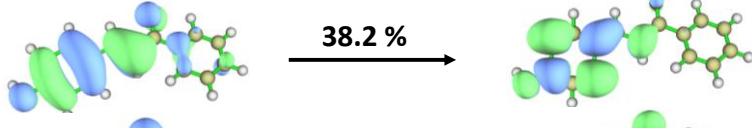
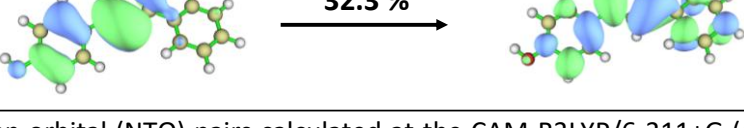
$S_1(n\pi^*)$	
$S_2(\pi\pi^*)$	
$T_3(n\pi^*)$	
	
$T_4(\pi\pi^*)$	
	

Figure S5: Natural transition orbital (NTO) pairs calculated at the CAM-B3LYP/6-311+G (d,p) level of theory in TOL.

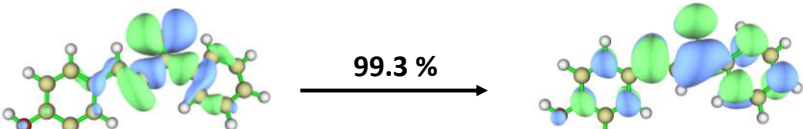
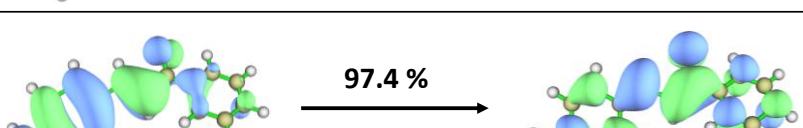
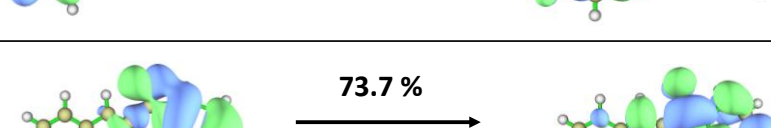
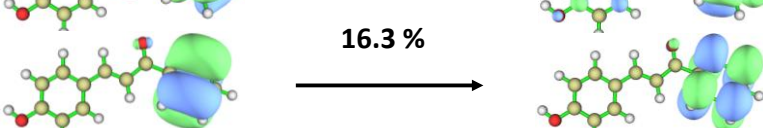
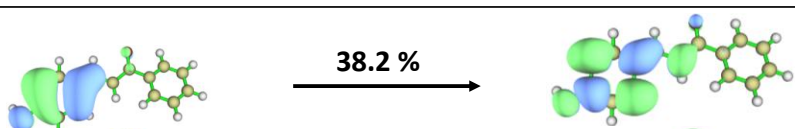
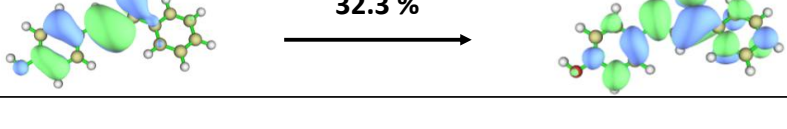
$S_1(n\pi^*)$	
$S_2(\pi\pi^*)$	
$T_3(n\pi^*)$	
	
$T_4(\pi\pi^*)$	
	

Figure S6: Natural transition orbital (NTO) pairs calculated at the CAM-B3LYP/6-311+G (d,p) level of theory in MeCN.

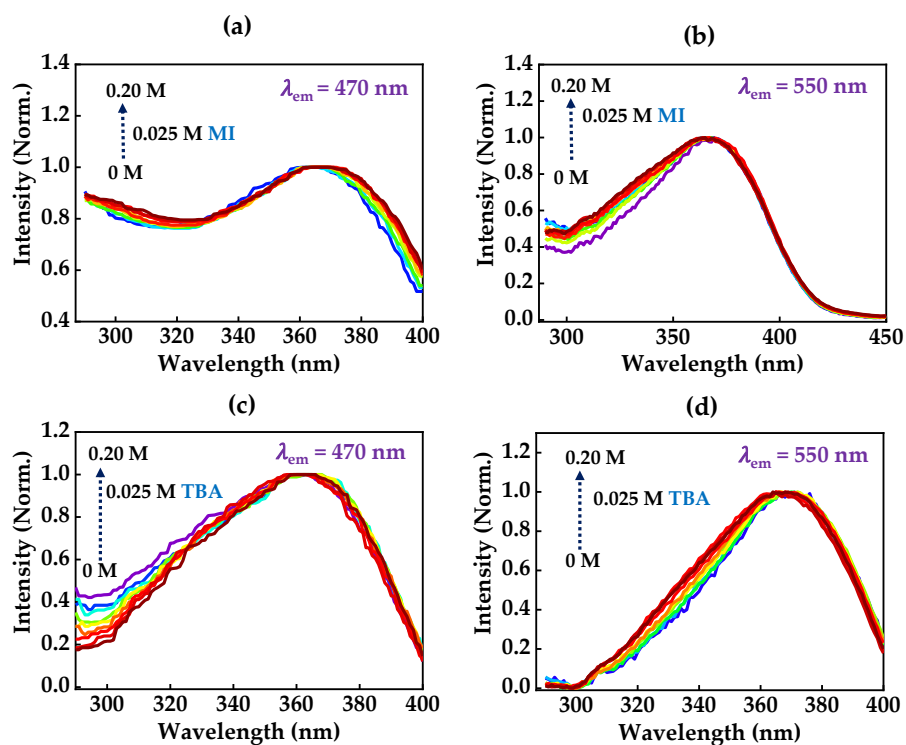


Figure S7: Excitation spectra of 4-HC in MeCN with addition of MI for emission at **(a)** 470 nm, and **(b)** 550 nm; with addition of TBA for emission at **(c)** 470 nm, and **(d)** 550 nm.

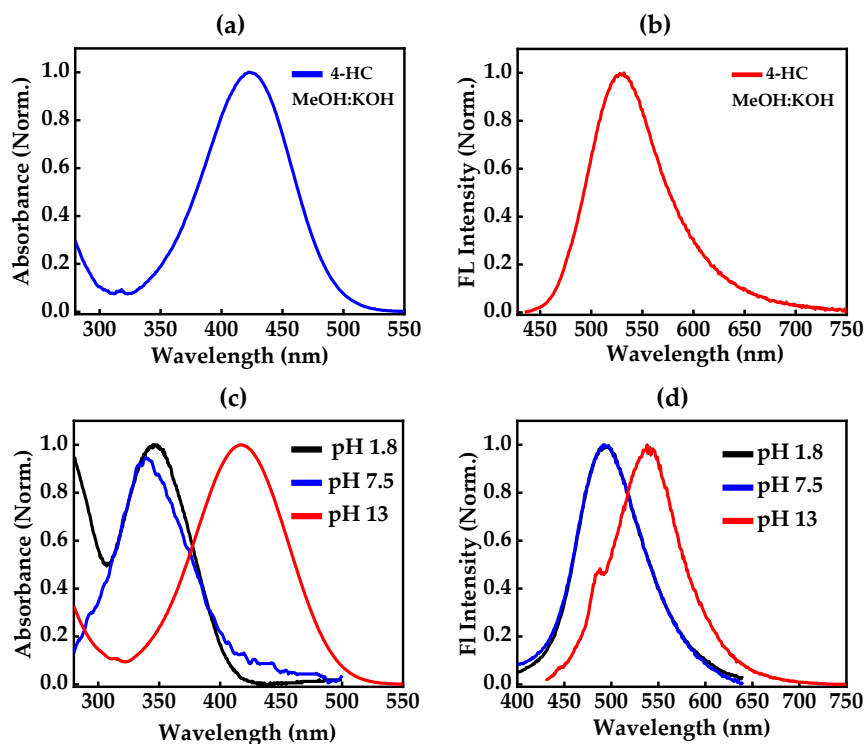


Figure S8: (a) Steady-state absorption, and (b) fluorescence spectra of 4-HC in MeOH:KOH. (c) steady-state absorption, and (d) emission spectrum of 4-HC in pH 1.8, pH 7.5, and pH 13, which were prepared using phosphate buffer in water.

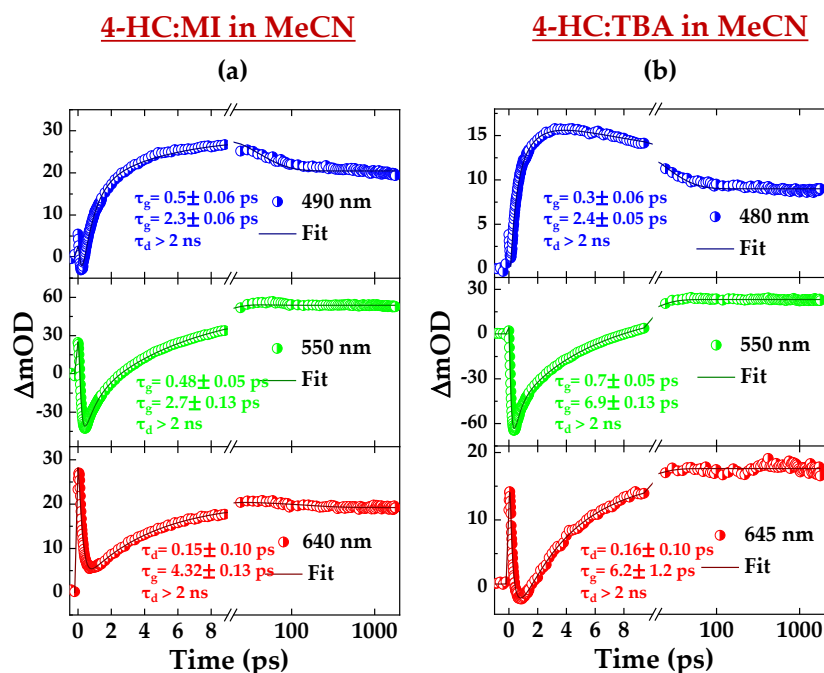


Figure S9: Single wavelength kinetics with best fitted decay profiles of fs-TA data in MeCN with addition of (a) MI at 490 nm (blue trace), 550 nm (green trace), 640 nm (red trace), and (b) TBA at 480 nm (blue trace), 550 nm (green trace), 645 nm (red trace). The amplitude kinetics are best fitted with exponential-growth and exponential-decay functions that are identified as τ_g and τ_d parameters.

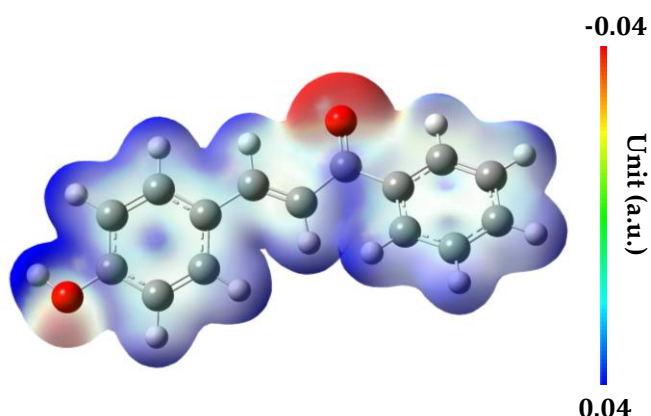


Figure S10: Molecular electrostatic potential surface of 4-HC in MeCN as solvent obtained through the CAM-B3LYP/6-311+G (d,p) level of theory.