

Supporting Information

Excited-State Dynamics of 3-Hydroxyflavone Anion in Alcohols

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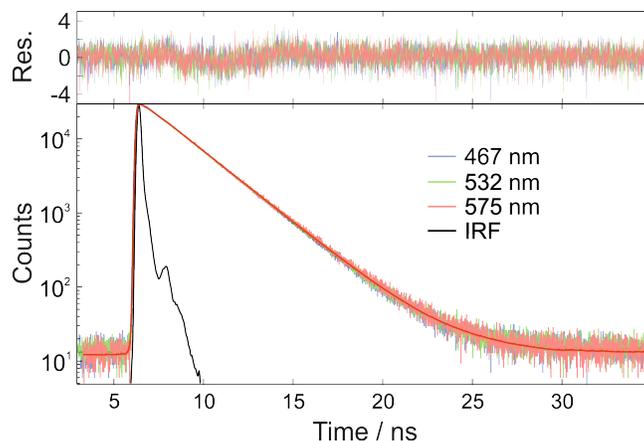


Figure S1: Intensity-normalized fluorescence decay profiles recorded at various wavelengths with a neutral methanol solution of 3HF, instrument response function (IRF), best fits (solid lines) and weighted residuals distribution (top).

Table S1: Time constants and relative amplitudes (in brackets) obtained from a multiexponential analysis of the fluorescence time profiles recorded by TCSPC at various wavelengths with solutions of 3HF at different base concentrations, c .

$c(\text{CH}_3\text{ONa})$	τ_1 / ns	τ_2 / ns	τ_3 / ns
$\lambda_{\text{fl}} = 467 \text{ nm}$			
0 M	0.02 (0.63)	2.2 (0.37)	
10^{-4} M	0.02 (0.96)	0.53 (0.03)	1.7 (0.01)
10^{-3} M	0.03 (0.87)	0.87 (0.08)	1.6 (0.05)
$\lambda_{\text{fl}} = 532 \text{ nm}$			
0 M	0.02 (0.65)	2.2 (0.35)	
10^{-4} M	0.01 (0.96)	0.53 (0.03)	1.7 (0.01)
10^{-3} M	0.02 (0.93)	0.82 (0.04)	1.6 (0.03)
$\lambda_{\text{fl}} = 575 \text{ nm}$			
0 M	0.02 (0.65)	2.2 (0.35)	
10^{-4} M	0.01 (0.97)	0.55 (0.03)	1.8 (<0.01)
10^{-3} M	0.02 (0.96)	0.81 (0.03)	1.6 (0.01)

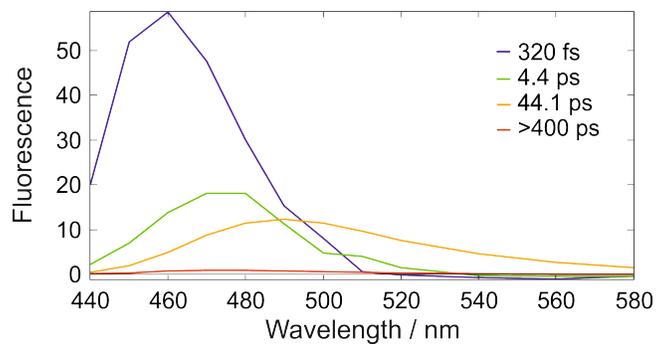


Figure S2: Decay-associated spectra obtained from a global analysis of the fluorescence time profiles in basic (10^{-3} M CH_3ONa) methanol solution of 3HF.

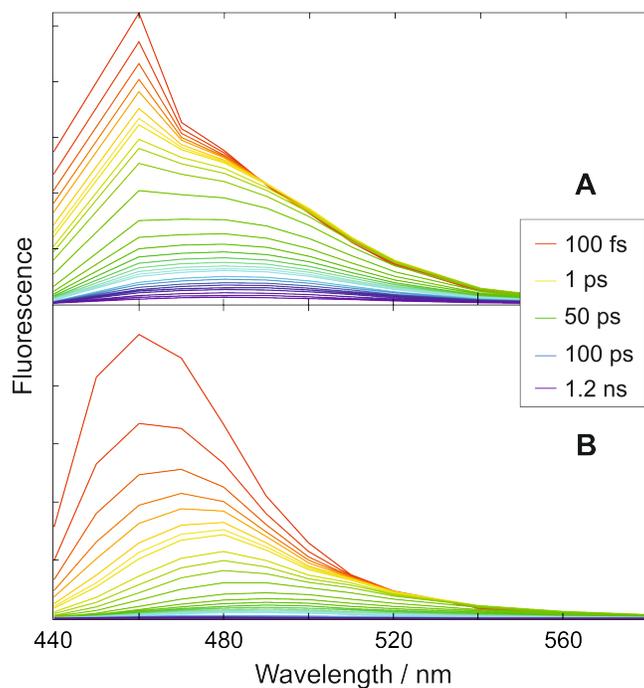


Figure S3: Time-resolved fluorescence spectra of **A)** neutral, and **B)** basic (10^{-4} M CH_3ONa) methanol solutions of 3HF.

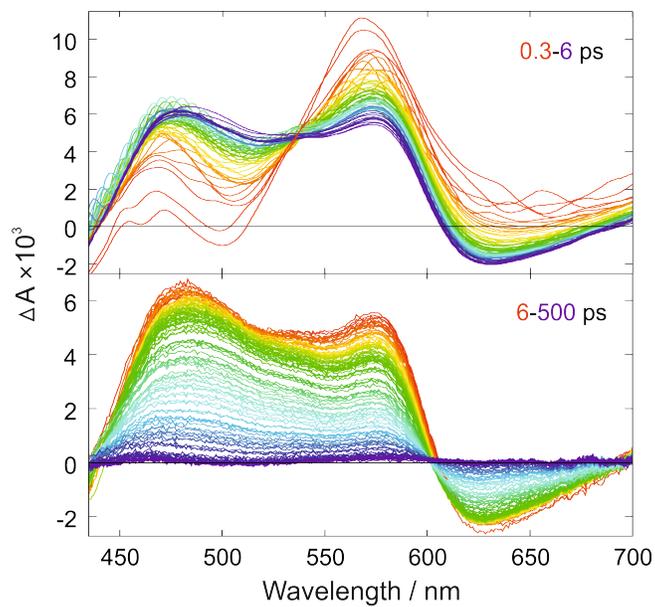


Figure S4: Electronic transient absorption spectra measured at various time delays after 400 nm excitation of a basic (10^{-3} M CH_3ONa) methanol solution of 3HF.

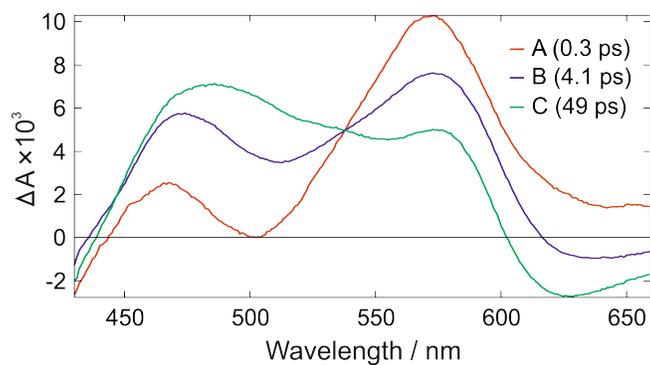


Figure S5: Species-associated difference spectra obtained from a target analysis of electronic transient absorption data measured with 3HF in basic (10^{-3} M CH_3ONa) methanol assuming a $\text{A} \rightarrow \text{B} \rightarrow \text{C} \rightarrow \text{D}$ scheme.

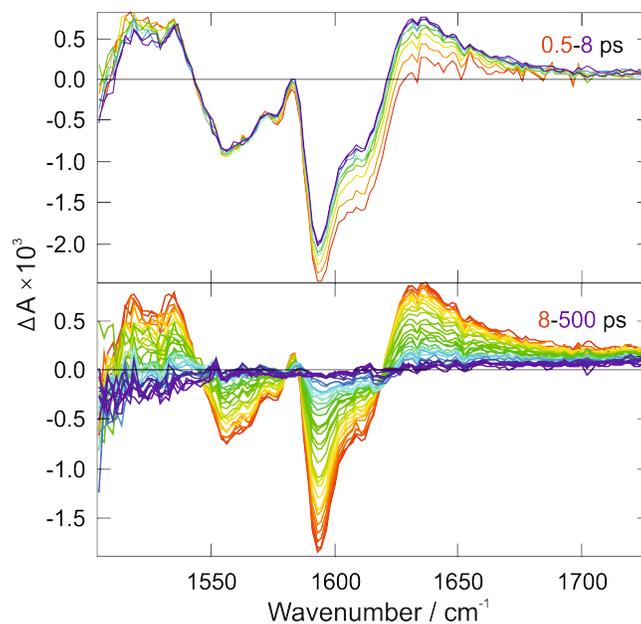


Figure S6: Infrared transient absorption spectra measured at various time delays after 400 nm excitation of basic (10^{-4} M CH_3ONa) methanol solution of 3HF.

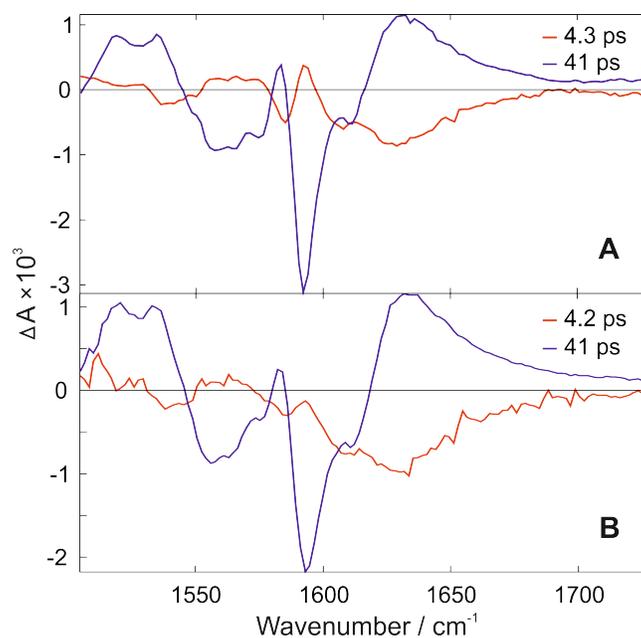


Figure S7: Decay-associated difference spectra obtained from a multiexponential global analysis of infrared transient absorption data measured with 3HF in basic **A)** methanol- d_4 and **B)** methanol solution of 3HF.

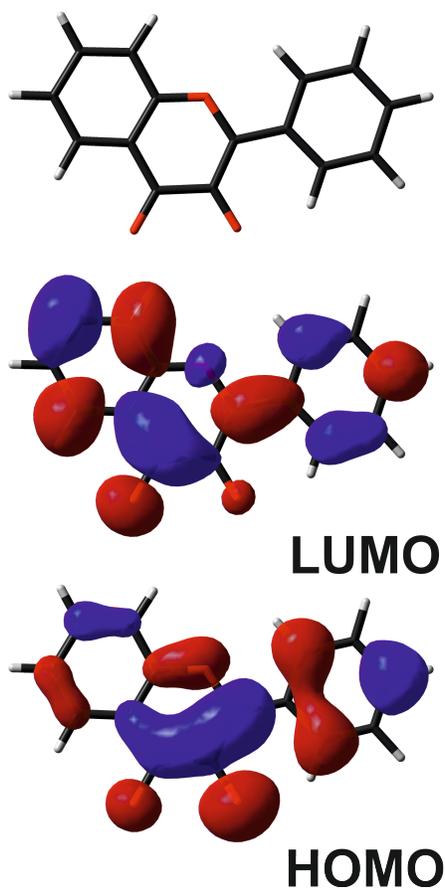


Figure S8: Structure (top) and frontier molecular orbitals of 3HF anion calculated at the B3LYP/aug-N07D level of theory with the PCM model for methanol.