Dynamics of Ultrafast Twisting of the Nitro Group in 1-(p-Nitrophenyl)-2-hydroxymethylpyrrolidine

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Supporting information:

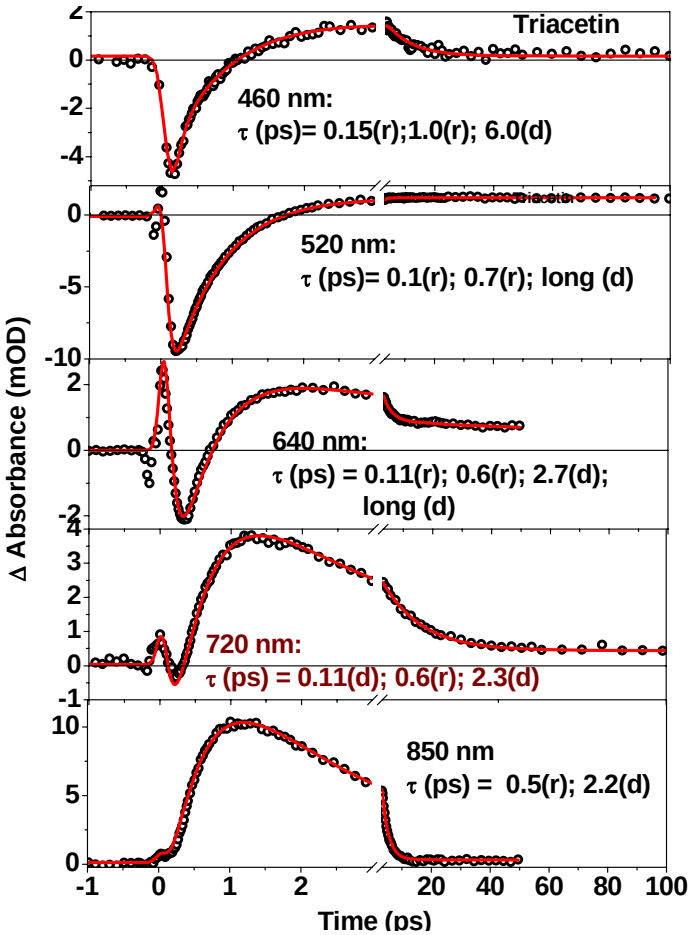


Figure S1: Temporal profiles recorded at few selective wavelengths following photoexcitation of *p*-NPP in triacetin using 400 nm laser pulses, along with best fit multiexponential fit functions and the associated lifetimes.

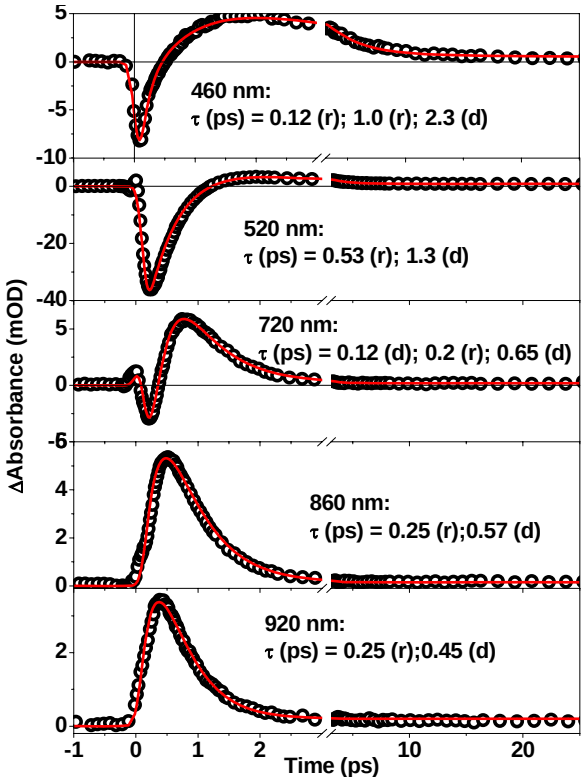


Figure S2: Temporal profiles recorded at few selective wavelengths following photoexcitation of *p*-NPP in acetonitrile using 400 nm laser pulses, along with best fit multiexponential fit functions and the associated lifetimes.

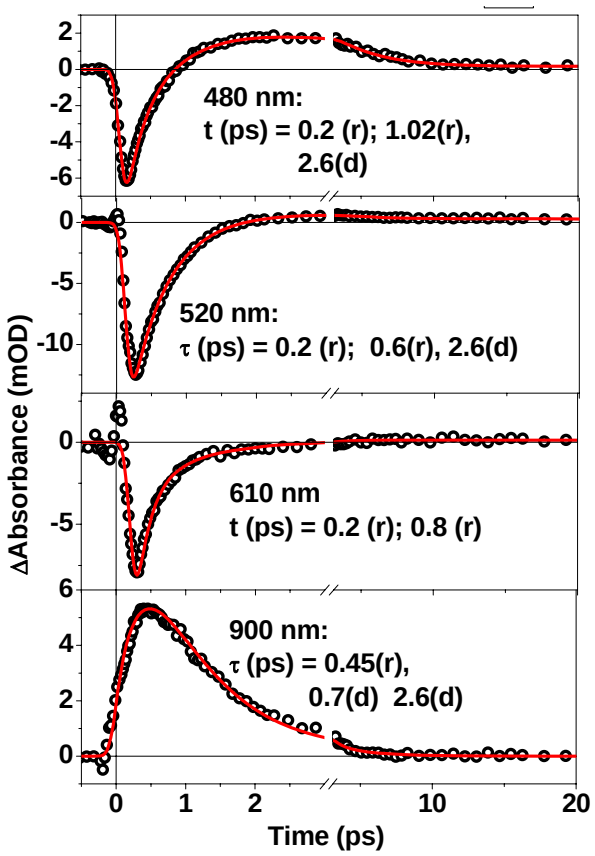


Figure S3: Temporal profiles recorded at few selective wavelengths following photoexcitation of *p*-NPP in EG using 400 nm laser pulses, along with the best multiexponential fit functions and the associated lifetimes.

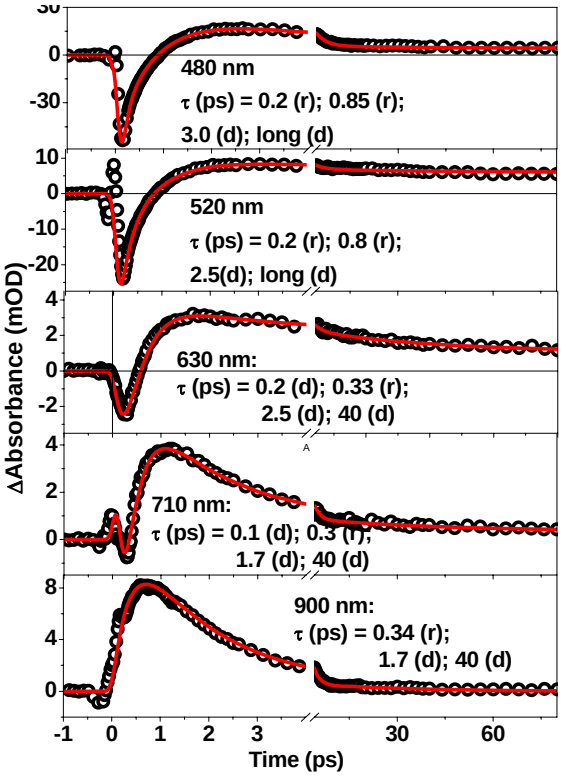


Figure S4: Temporal profiles recorded at few selective wavelengths following photoexcitation of *p*-NPP in 1-propanol using 400 nm laser pulses, along with best fit multiexponential fit functions and the associated lifetimes.

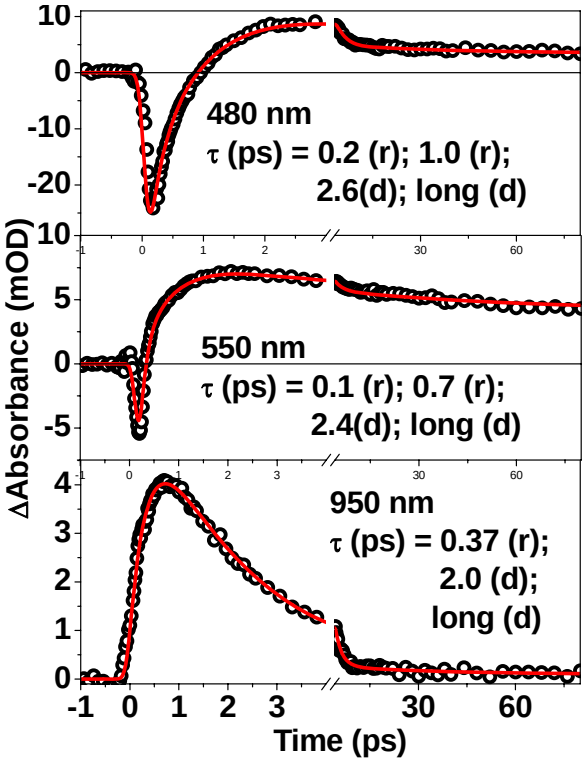
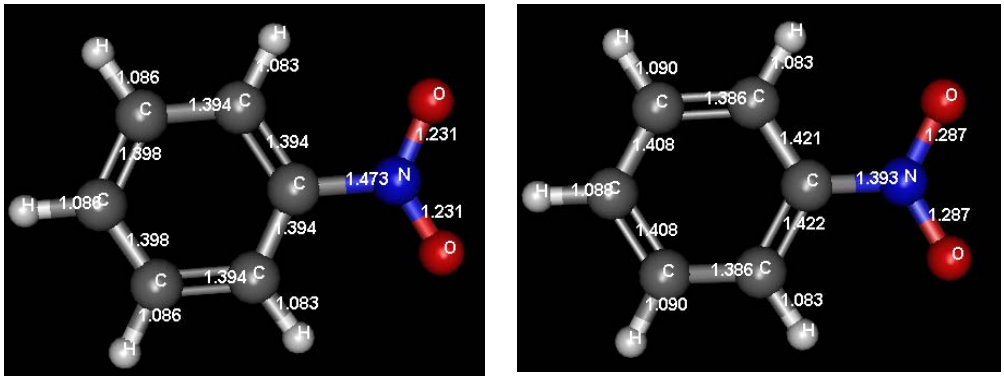


Figure S5: Temporal profiles recorded at few selective wavelengths following photoexcitation of *p*-NPP in 1-butanol using 400 nm laser pulses, along with best fit multiexponential fit functions and the associated lifetimes.



Nitrobenzene

Nitrobenzene anion

Figure S6: optimized ground state geometry of nitrobenzene and nitrobenzene anion.

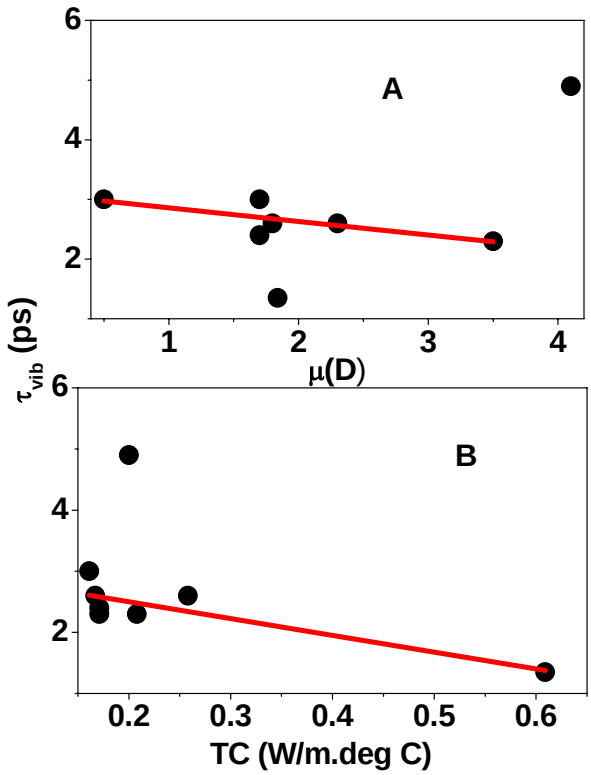


Figure S7: Correlation between τ_{vib} with μ(D) and Thermal conductivity of the solvents.

Table S1: Excitation energies, oscillator strengths and dipole moments (μ) in the S_0 and S_1 states of the *p*-NPP molecule in the gas phase at different dihedral angles between the nitro group and the 2-hydroxymethyl-pyrolidinophenyl group calculated by DFT and TDDFT methods using B3LYP/6-31G(d,p.) basis set.

Twisting angle	Excitation energy (eV)	Oscillator Strength	$\mu(S_0)$ (D)	$\mu(S_1)$ (D)
0	3.734	0.443	8.27	14.03
10	3.68	0.311	8.22	11.68
20	3.60	0.272	8.12	11.60
30	3.53	0.236	8.02	11.55
40	3.43	0.199	7.84	12.25
50	3.31	0.151	7.62	13.28
60	3.16	0.097	7.37	14.56
70	3.00	0.047	7.13	15.94
80	2.87	0.012	6.95	17.10
90	2.82	0.00	6.88	17.57