Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Exploration of photophysics of 2,2′-pyridil at room temperature and 77 K: A combined spectroscopic and quantum chemical approach

Pronab Kundu, Saptarshi Ghosh and Nitin Chattopadhyay*

Department of Chemistry, Jadavpur University, Kolkata - 700 032, India

*Corresponding author: Fax: 91-33-2414-6584

E-mail: nitin.chattopadhyay@yahoo.com

Electronic supplementary information

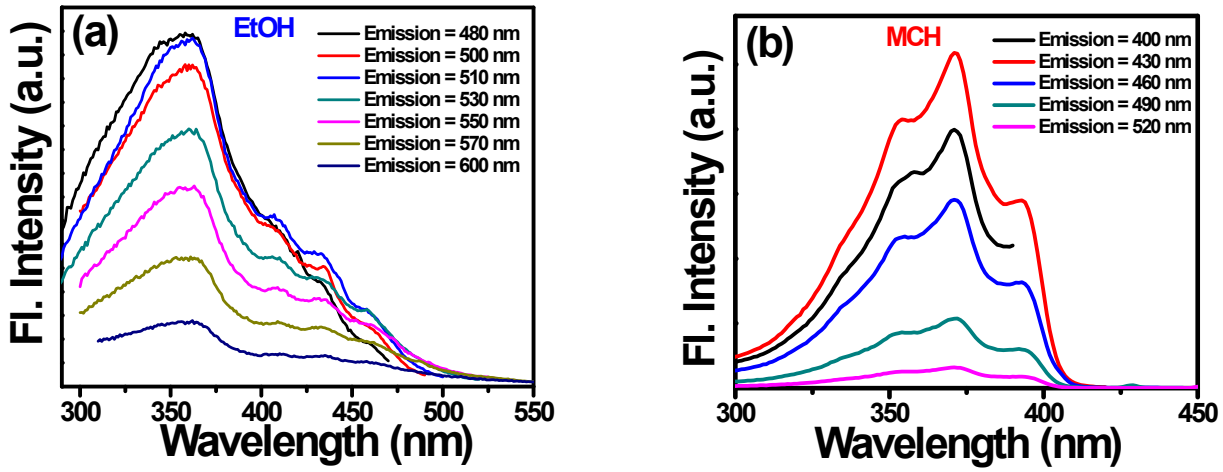

Fig. S1 Room Temperature excitation spectra of 2,2′-pyridil monitoring at different wavelengths under the entire emission band in both (a) EtOH and (b) MCH solvents upon photoexcitation at the nπ* absorption band. Monitoring emission wavelengths are shown in the legends.

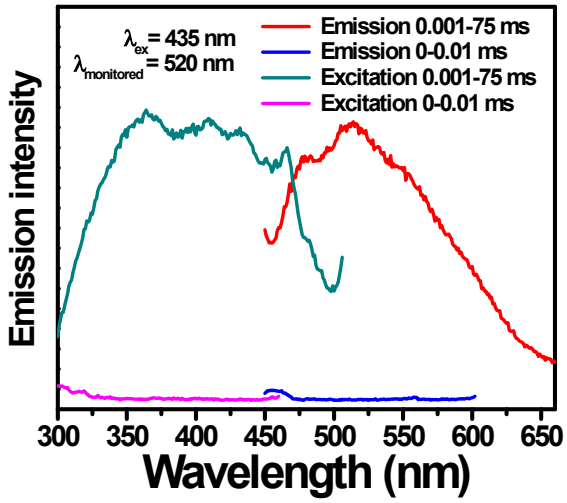

Fig. S2 Room temperature emission and excitation spectra of 2,2´-pyridil in ethanol at different time windows as labeled in the legends.

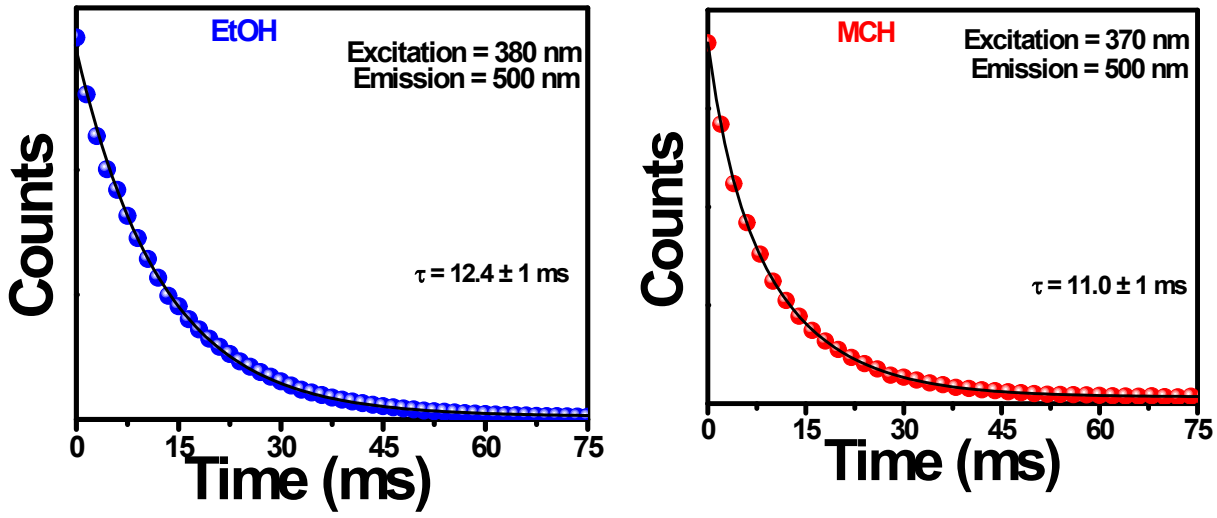

Fig. S3 Phosphorescence decays of 2,2´-pyridil in EtOH and MCH matrices at 77 K. Excitation and monitoring wavelengths are given in the legends.

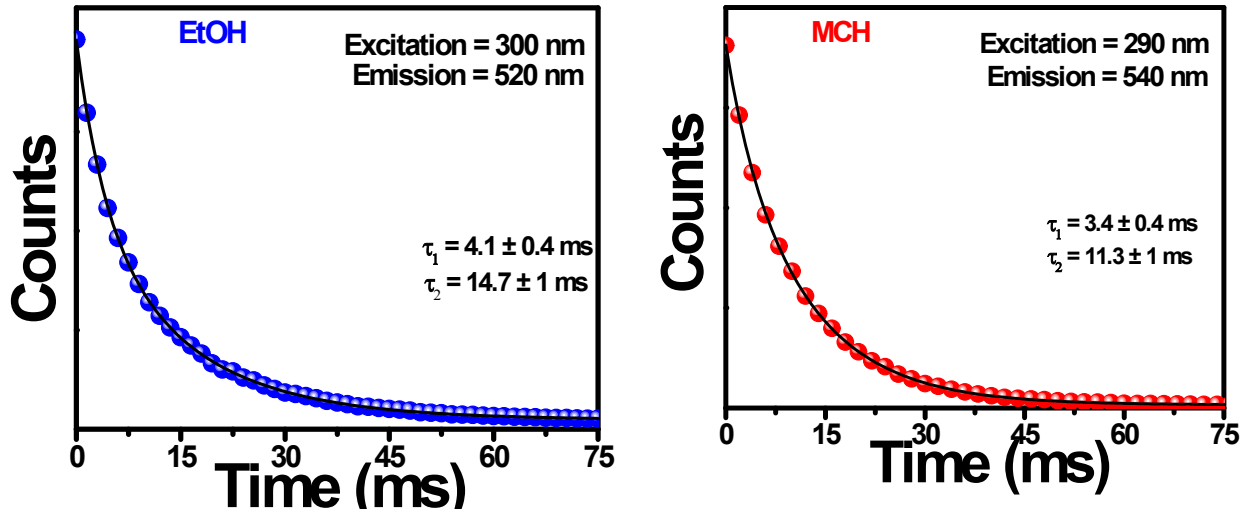

Fig. S4 Lower energy phosphorescence decays of 2,2´-pyridil in EtOH and MCH matrices at 77 K. Excitation and monitoring wavelengths are given in the legends.

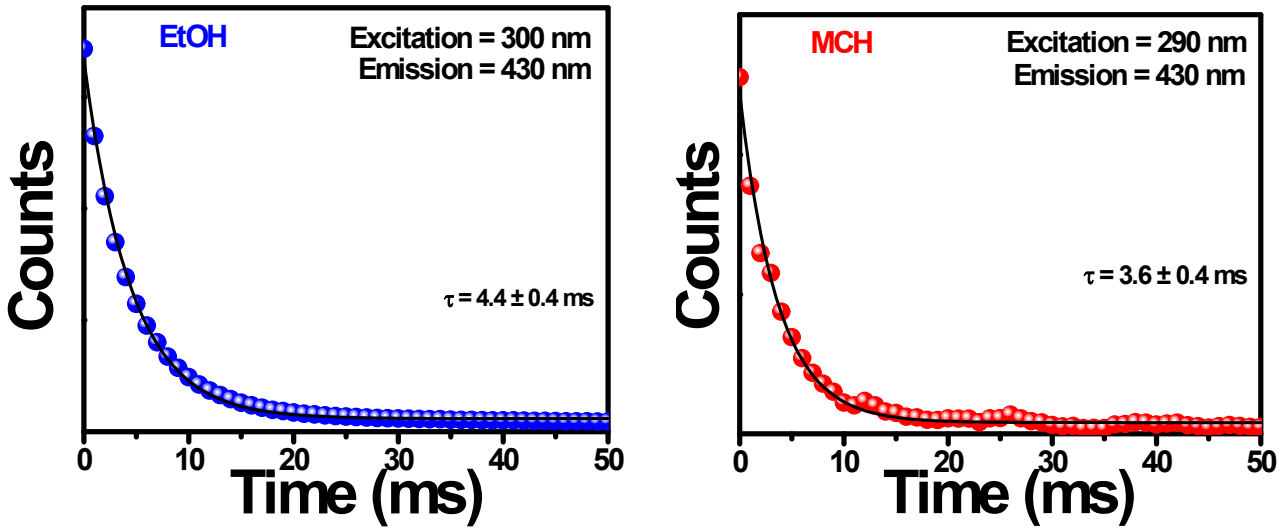

Fig. S5 Higher energy phosphorescence decays of 2,2´-pyridil in EtOH and MCH matrices at 77 K upon excitation at the ππ* band. Excitation and monitoring wavelengths are given in the legends.

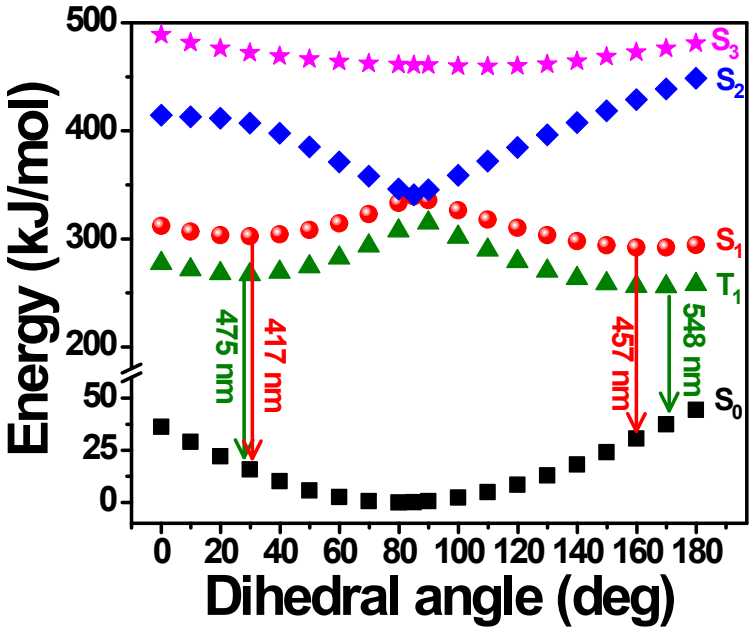

Fig. S6 Potential energy curves (PECs) of 2,2´-pyridil in S_0, S_1, S_2, S_3 and T_1 electronic states as a function of intercarbonyl dihedral angle (Φ) in vacuum.

Table S1 Phosphorescence decay parameters of 2,2´-pyridil in EtOH and in MCH matrices at 77 K.

Solvent	λ_{ex} (nm)	λ_{em} (nm)	τ_1 (ms)	τ_2 (ms)	a_1	a_2	R^2
EtOH	300	430	4.4 ± 0.4	14.7 ± 1	0.43	0.57	0.9983
	300	520	4.1 ± 0.4				0.9999
	380	500	12.4 ± 1				0.9991
MCH	290	430	3.6 ± 0.4	11.3 ± 1	0.13	0.87	0.9930
	290	540	3.4 ± 0.4				0.9999
	370	500	11.0 ± 1				0.9999

Table S2 Experimental and theoretical absorption wavelengths of 2,2´-pyridil in EtOH and MCH.

Solvent	Absorption positions	
	Experimental	Calculated
EtOH	~ 360 nm and ~ 340 nm ($n\pi^*$); 270 nm ($\pi\pi^*$)	~ 348 nm and ~ 336 nm; 284 nm
MCH	~ 370 nm and ~ 350 nm ($n\pi^*$); 268 nm ($\pi\pi^*$)	~ 354 nm and ~ 341 nm; 282 nm