

SUPPORTING INFORMATION

Dynamics of the Excited State of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ with triple Phosphorescence

Shih-Hsiang Wu, Jung-Wei Ling, Szu-Hsueh Lai, Min-Jie Huang, Chien Hong Cheng, and I-Chia Chen*

Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 30013,

Republic of China

SUPPORTING INFORMATION: the optimized geometry of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$, emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm in various solvents and the best-fitted exponential curves and picosecond measurements on decay curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ in toluene/ CHCl_3 volume ratio 1:1 and CHCl_3 .

Captions of figures

- Figure S1.** Optimized geometry of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ calculated at level B3LYP/6-31G* restricted to symmetry C_2 . The bond distance of Ir-C and Ir-N is 2.028 Å and 2.085 Å, respectively to ppy. The bond distances of C-C in ppy are ~ 1.460 Å and the dihedral angle C-C-C-N is 1.3° . The bond distance of Ir-N is 2.211 Å to bpy. The bond distances of C-C in bpy are ~ 1.483 Å and the dihedral angle N-C-C-N is 4° .
- Figure S2.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in toluene and the best-fitted exponential curves.
- Figure S3.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in toluene/ CHCl_3 at volume ratio 1:1 and the best-fitted exponential curves.
- Figure S4.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in CHCl_3 and the best-fitted exponential curves.
- Figure S5.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in THF and the best-fitted exponential curves.
- Figure S6.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in CH_2Cl_2 and the best-fitted exponential curves.

- Figure S7.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in acetone and the best-fitted exponential curves.
- Figure S8.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in acetonitrile and the best-fitted exponential curves.
- Figure S9.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in DMF and the best-fitted exponential curves.
- Figure S10.** Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in DMSO and the best-fitted exponential curves.
- Figure S11.** Emission decay curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ in toluene/ CHCl_3 volume ratio 1:1 excited at wavelength 355 nm.
- Figure S12.** Emission decay curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ in CHCl_3 excited at wavelength 355 nm.

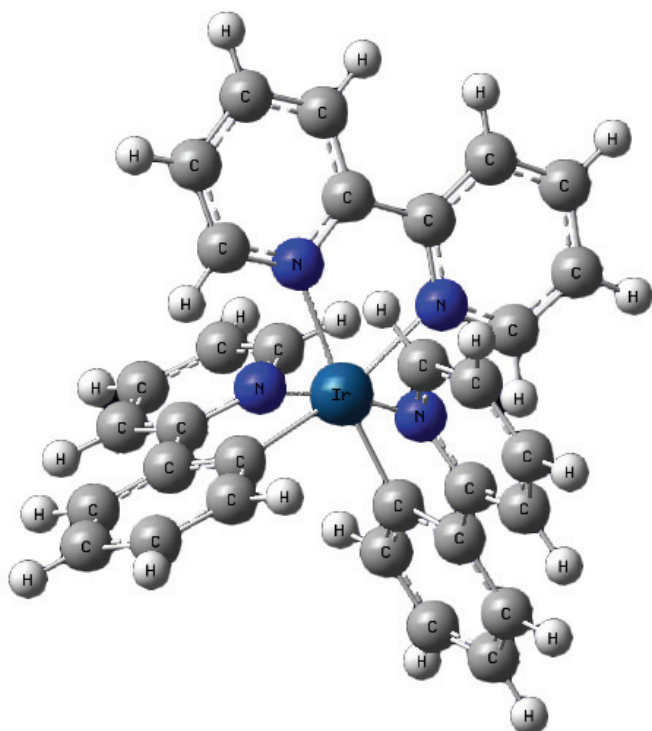


Figure S1. Optimized geometry of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ calculated at level B3LYP/6-31G* restricted to symmetry C_2 . The bond distance of Ir-C and Ir-N is 2.028 Å and 2.085 Å, respectively to ppy. The bond distances of C-C in ppy are ~ 1.460 Å and the dihedral angle C-C-C-N is 1.3° . The bond distance of Ir-N is 2.211 Å to bpy. The bond distances of C-C in bpy are ~ 1.483 Å and the dihedral angle N-C-C-N is 4° .

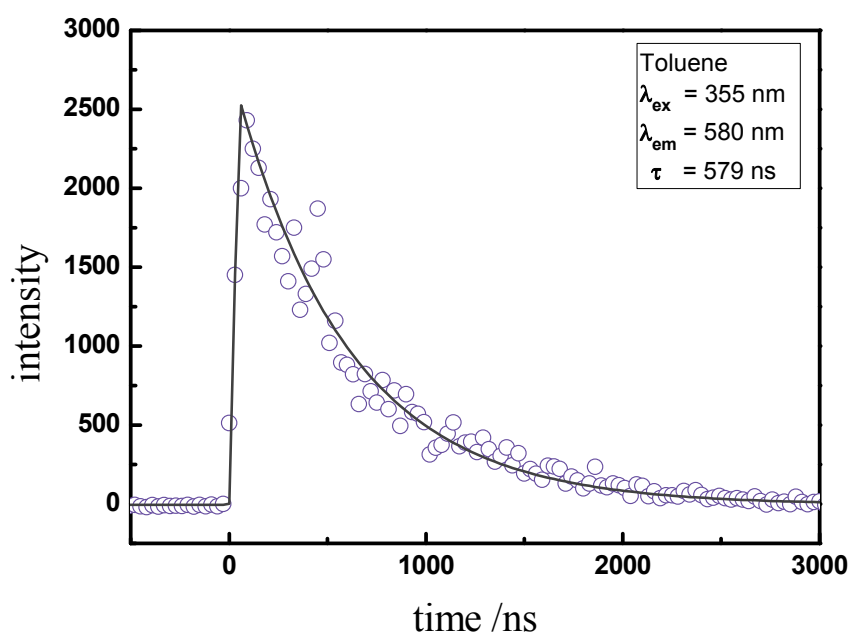
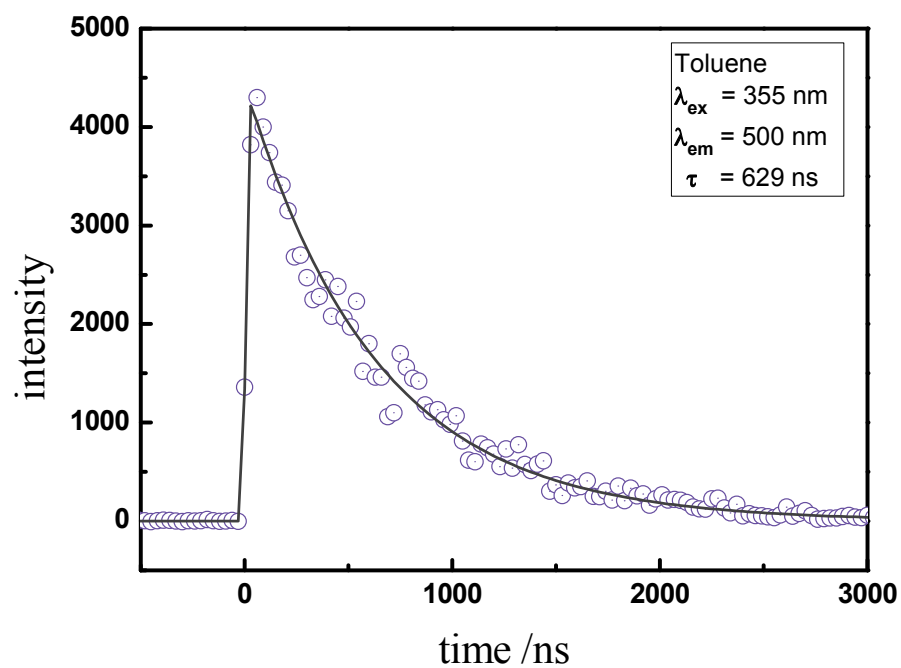


Figure S2. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in toluene and the best-fitted exponential decay curves.

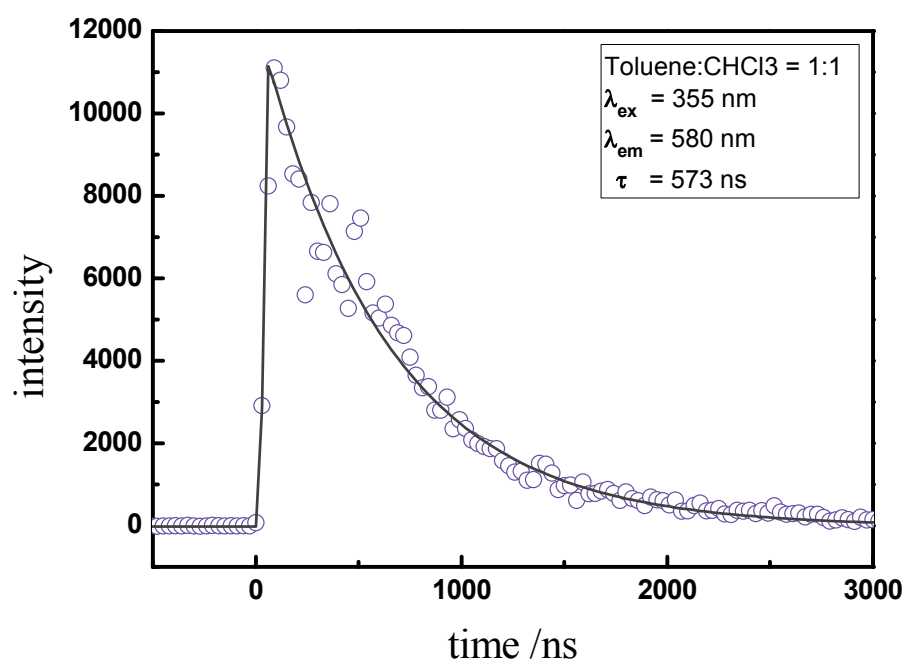
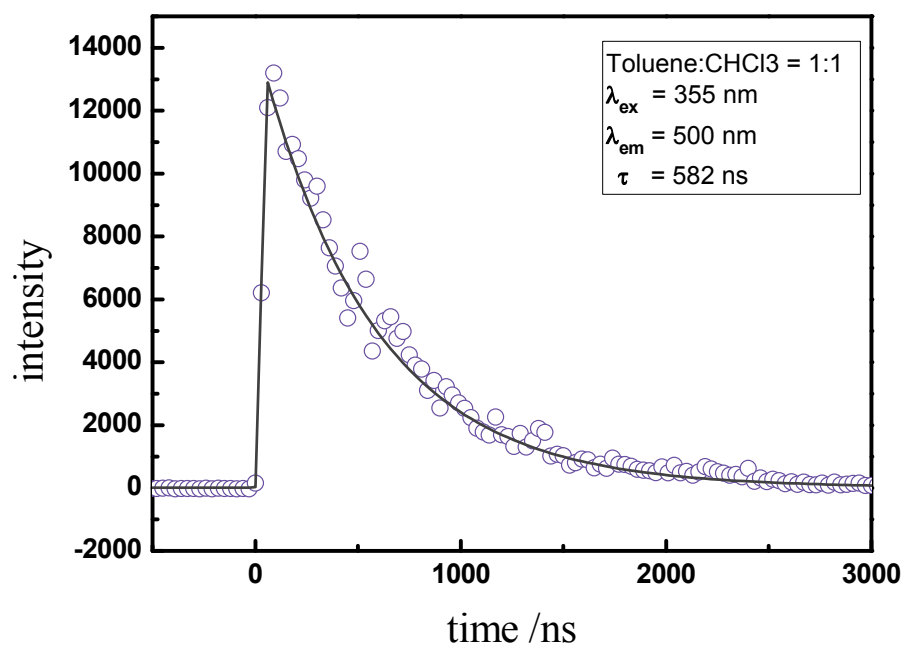


Figure S3. Emission curves of [Ir(ppy)₂bpy]⁺ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in toluene/CHCl₃ at volume ratio 1:1 and the best-fitted exponential curves.

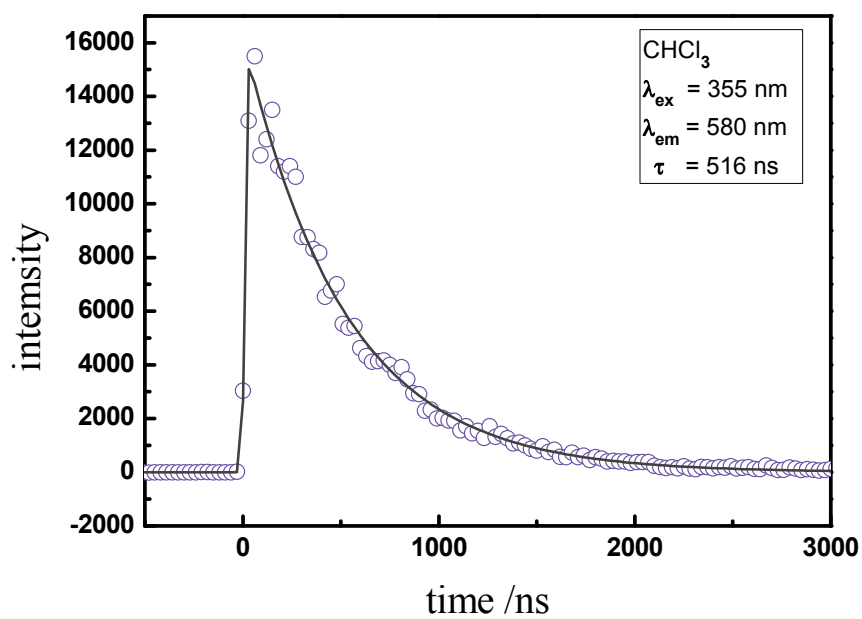
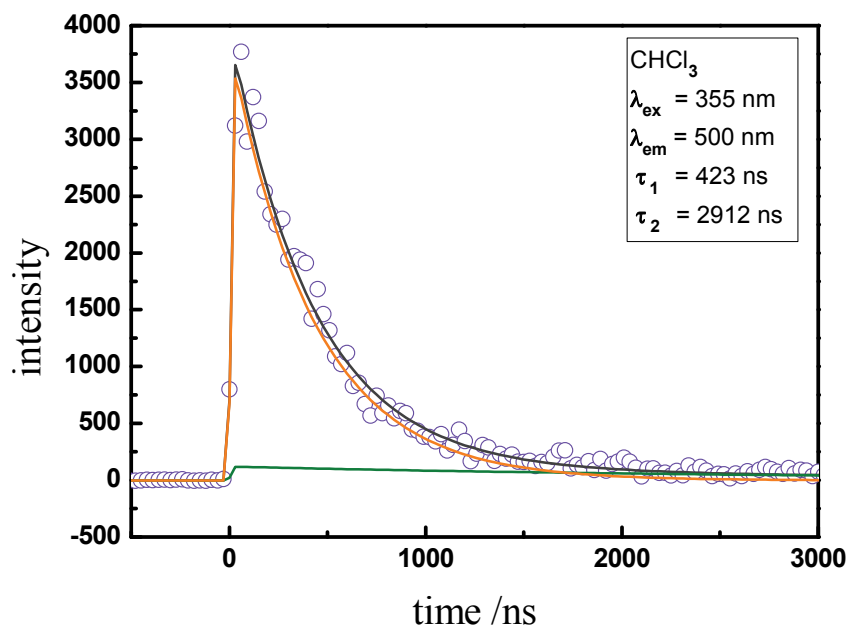


Figure S4. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in CHCl_3 and the best-fitted exponential curves.

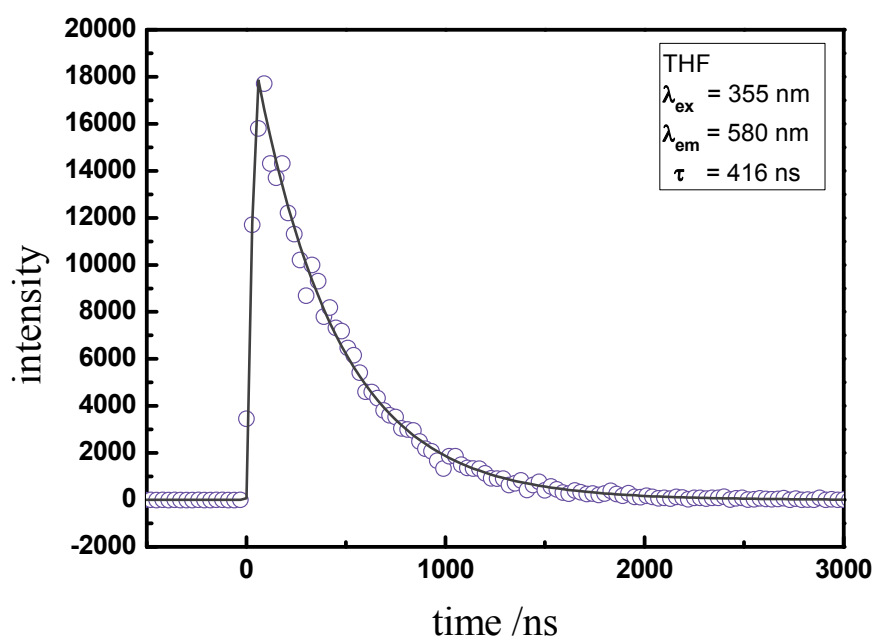
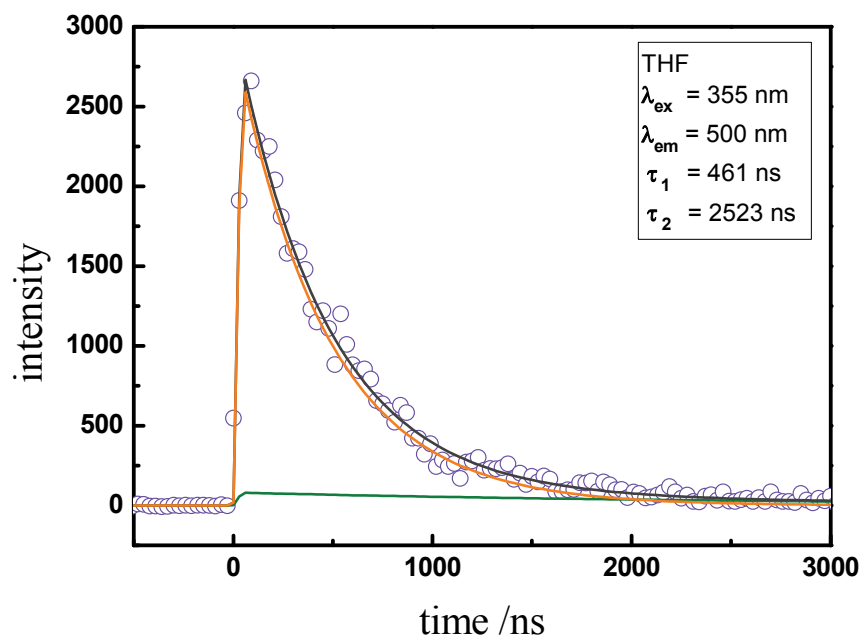


Figure S5. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in THF and the best-fitted exponential curves.

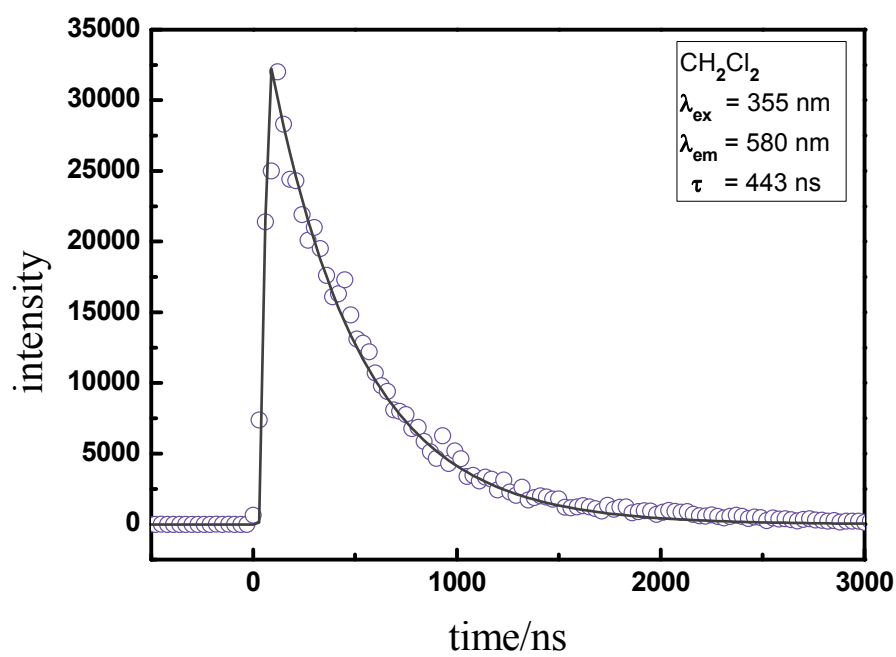
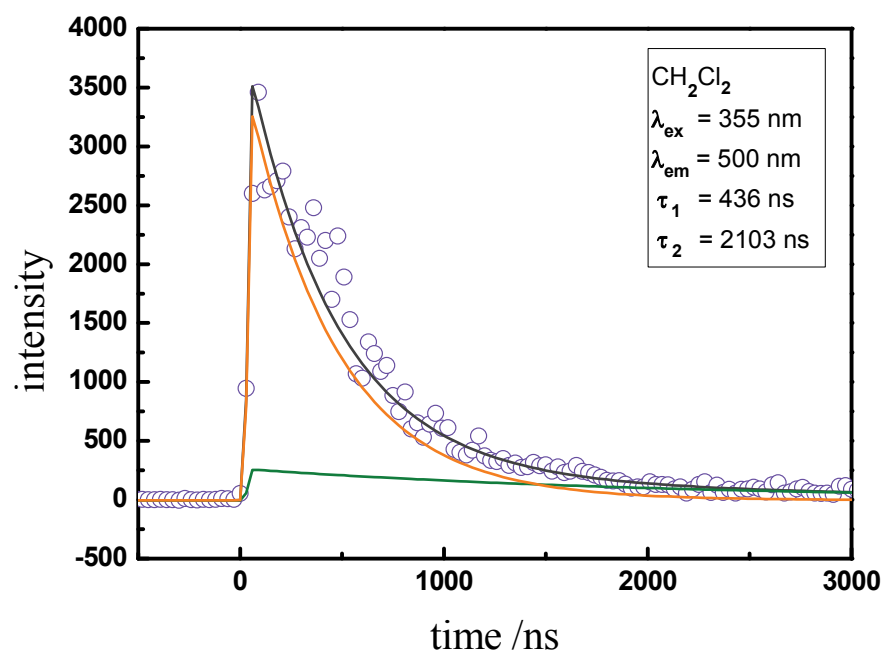


Figure S6. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in CH_2Cl_2 and the best-fitted exponential curves.

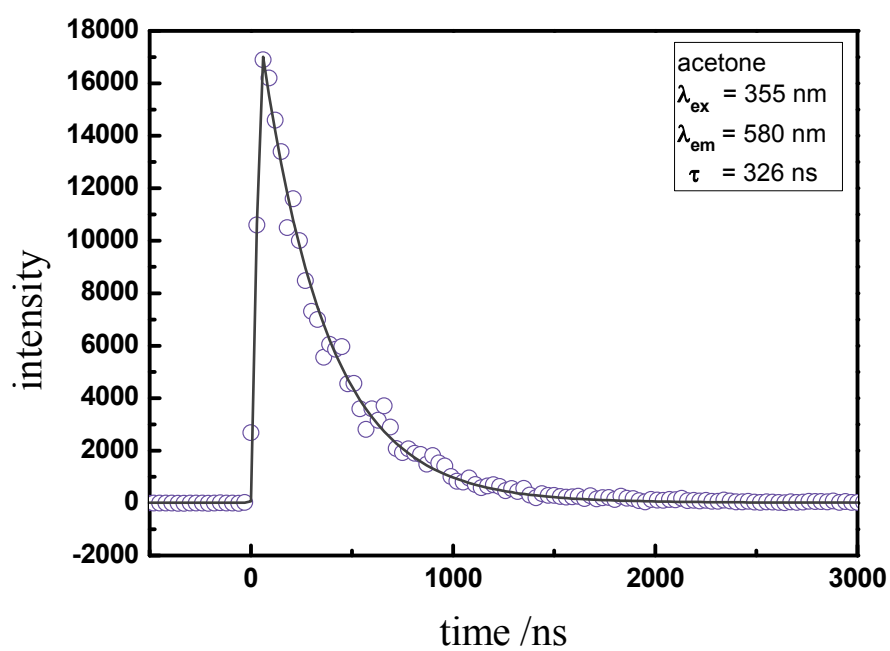
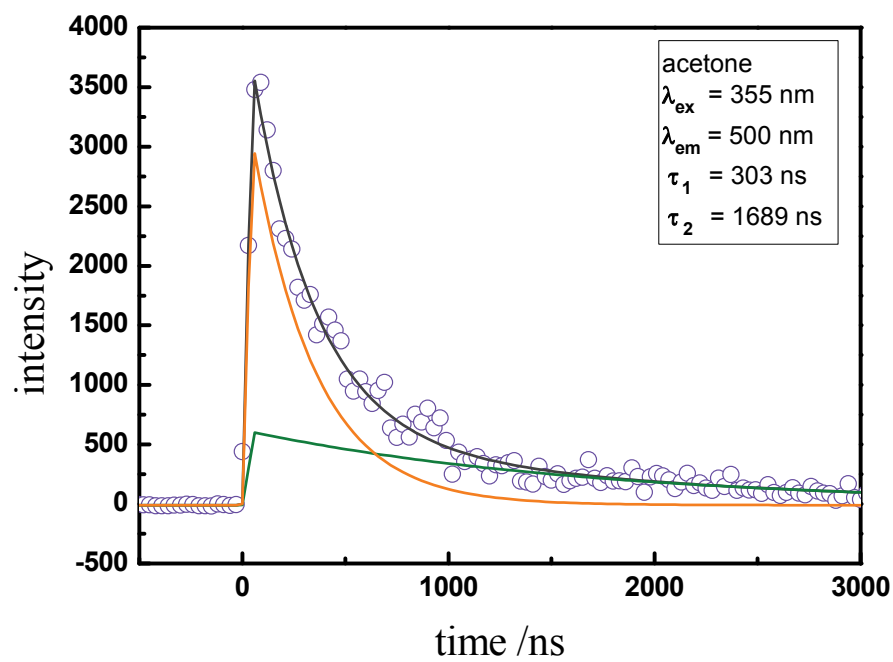


Figure S7. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in acetone and the best-fitted exponential curves.

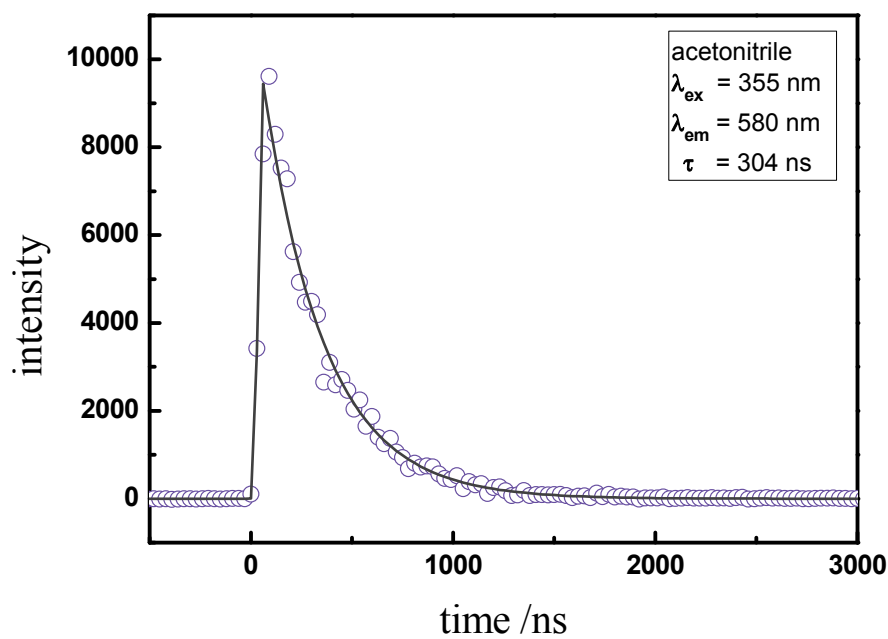
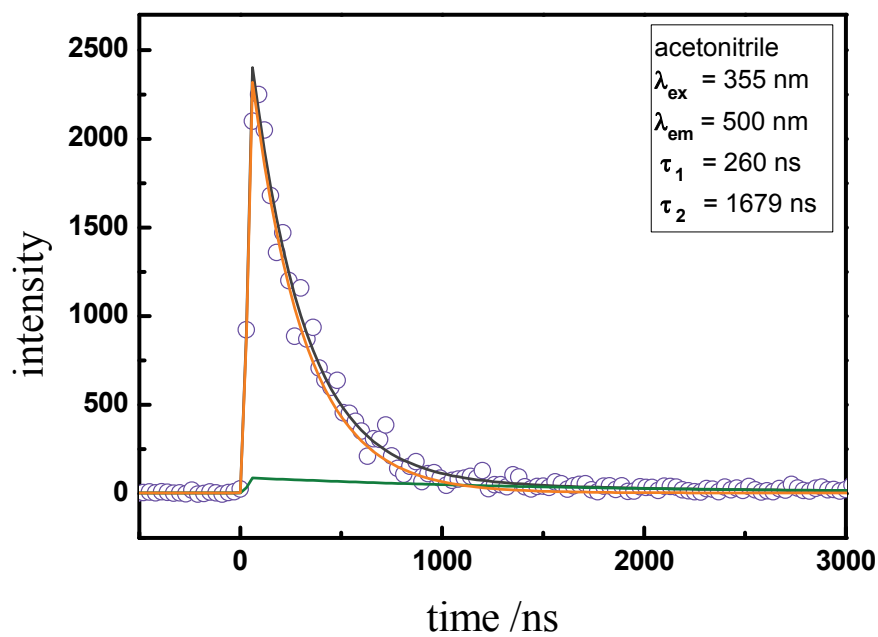


Figure S8. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in acetonitrile and the best-fitted exponential curves.

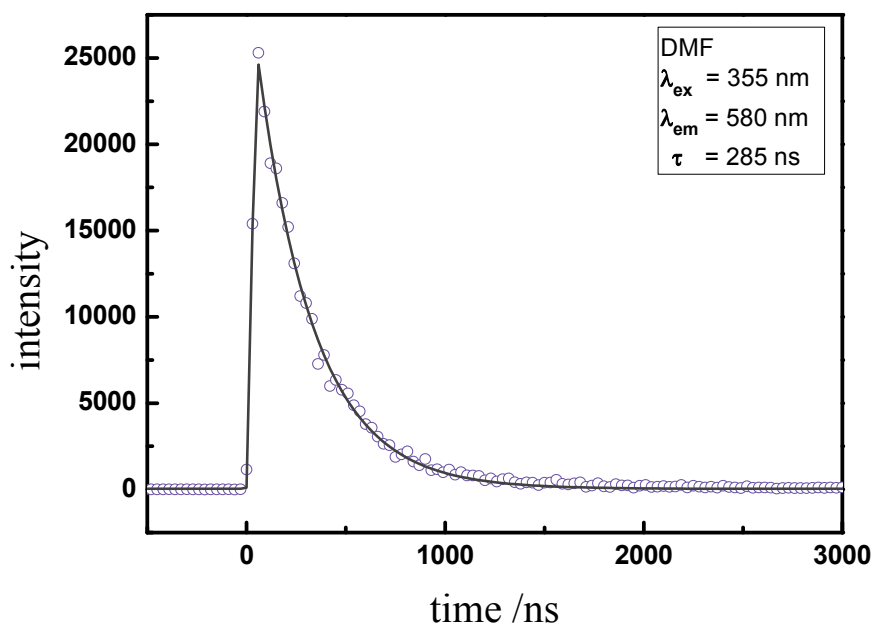
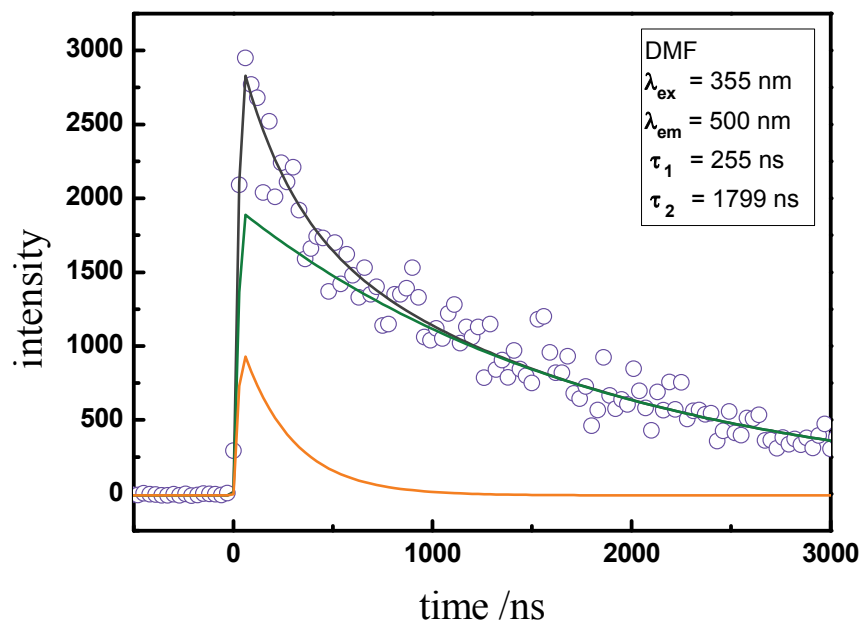


Figure S9. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in DMF and the best-fitted exponential curves.

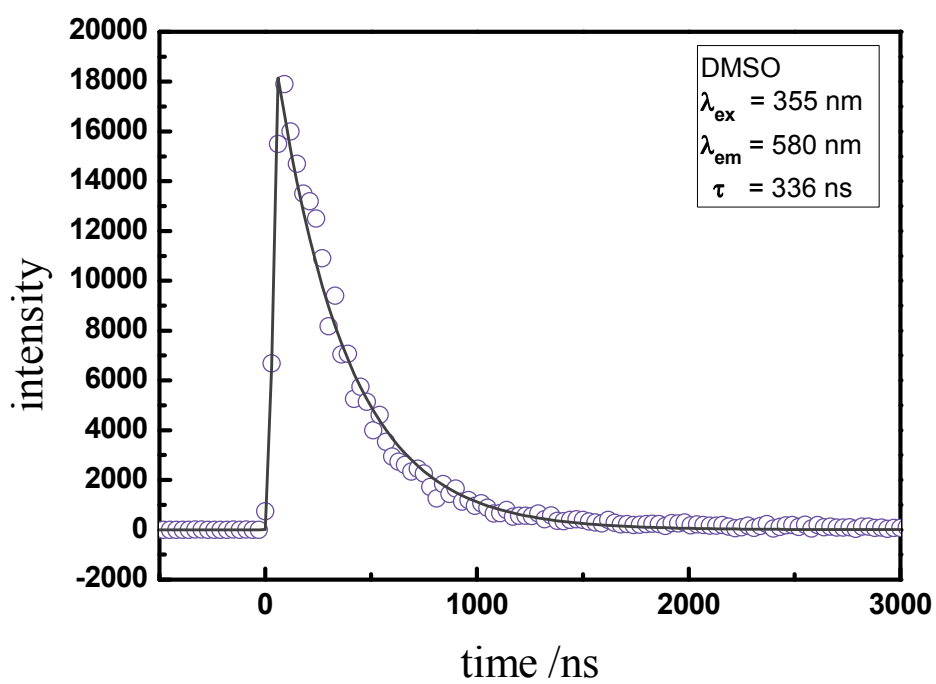
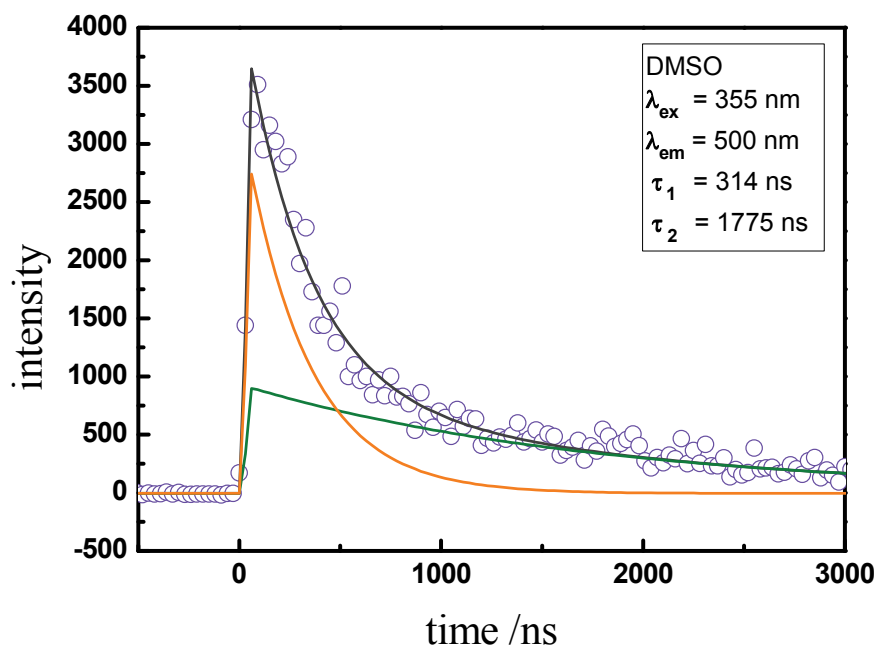


Figure S10. Emission curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ at excitation wavelength 355 nm and detected at wavelength 500 and 580 nm in DMSO and the best-fitted exponential curves.

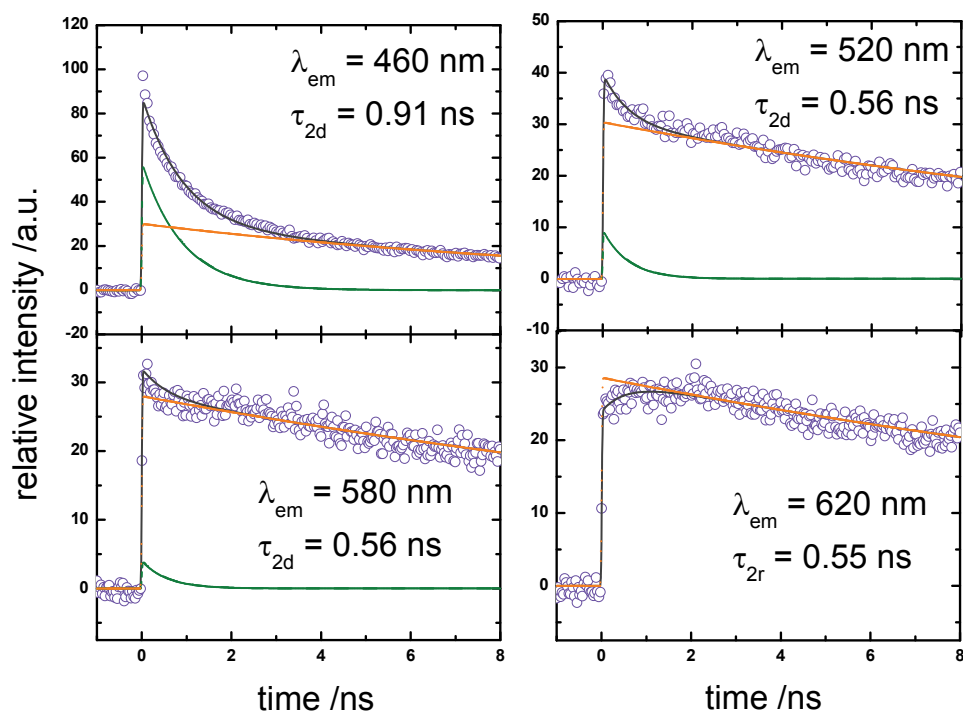


Figure S11. Emission decay curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ in toluene/ CHCl_3 volume ratio 1:1 excited at wavelength 355 nm.

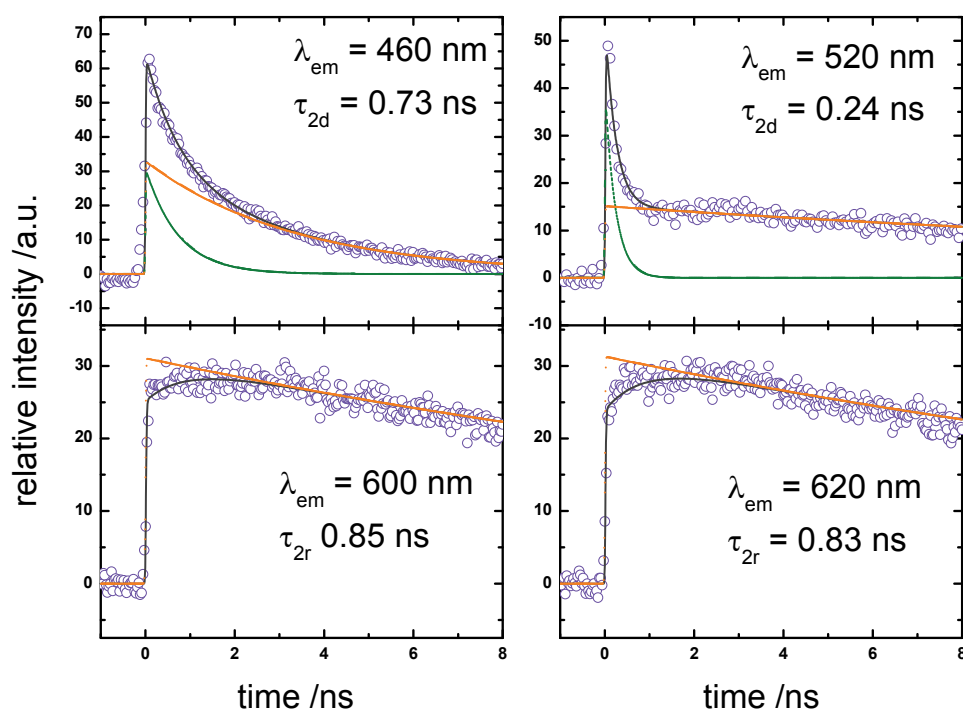


Figure S12. Emission decay curves of $[\text{Ir}(\text{ppy})_2\text{bpy}]^+$ in CHCl_3 excited at wavelength 355 nm.