

Supplementary Information

Spin Mixed Charge Transfer States of Iridium Complex Ir(ppy)₃: Transient Absorption and Time-Resolved Photoluminescence

Mohan Singh Mehata^{†,*}, Yang Yang[†], Zongjing Qu[†], Jun-sheng Chen[†], Feng-jiao Zhao[†] and Ke-Li Han^{†*}

[†]State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics (DICP),
Chinese Academy of Sciences, Dalian 116023, CHINA.

[‡]Laser-Spectroscopy Laboratory, Department of Applied Physics, Delhi Technological University, Bawana
Road, Delhi 110042, INDIA.

*To whom correspondence should be sent: E-mail: (M.S. Mehata) msmehata@gmail.com; (Ke-Li Han)

klhan@dicp.ac.cn.

Table S1: The tri-exponential fitted parameters of transient absorption dynamical curve of Ir (ppy)₃ (pumped wavelength was 355 nm).

Wavelength (nm)	Parameter	Value (τ in μs)	Standard Error
370	y0	0.00122	3.26E-05
	A1	-414.13	659.0228
	t1	1.717414	0.010636
	A2	-407.158	863.7066
	t2	1.705352	0.011175
	A3	821.2928	369.2865
	t3	1.711387	0.012478
410	y0	3.90E-04	3.26E-05
	A1	685.8815	1092.607
	t1	1.717414	0.010636
	A2	682.9857	1444.837
	t2	1.705352	0.011175
	A3	-1368.87	614.8723
	t3	1.711387	0.012478
520	y0	1.44E-04	3.37E-05
	A1	2594.912	4131.83
	t1	1.717414	0.010636
	A2	2583.297	5463.726
	t2	1.705352	0.011175
	A3	-5178.22	2312.803
	t3	1.711387	0.012478
540	y0	-2.99E-04	3.37E-05
	A1	2576.568	4102.788
	t1	1.717414	0.010636
	A2	2565.546	5425.946
	t2	1.705352	0.011175
	A3	-5142.13	2296.994
	t3	1.711387	0.012478

R²=0.96

Table S2: The bi-exponential fitted parameters of transient absorption dynamical curve of Ir (ppy)₃ (pumped wavelength was 355 nm), which does not give reasonable fitting.

Wavelength (nm)	Parameter	Value (τ in μ s)	Standard Error
370	y0	-0.00107	7.21E-05
	A1	-44.9936	1382.973
	t1	3.062248	0.039586
	A2	44.97772	1382.973
	t2	3.061823	0.03958
410	y0	3.11E-04	7.23E-05
	A1	73.9971	2274.979
	t1	3.062248	0.039586
	A2	-74.0056	2274.979
	t2	3.061823	0.03958
520	y0	-1.44E-04	7.79E-05
	A1	273.9078	8421
	t1	3.062248	0.039586
	A2	-273.936	8421
	t2	3.061823	0.03958
540	y0	-5.53E-04	7.73E-05
	A1	259.6686	7983.225
	t1	3.062248	0.039586
	A2	-259.695	7983.225
	t2	3.061823	0.03958

R²=0.89

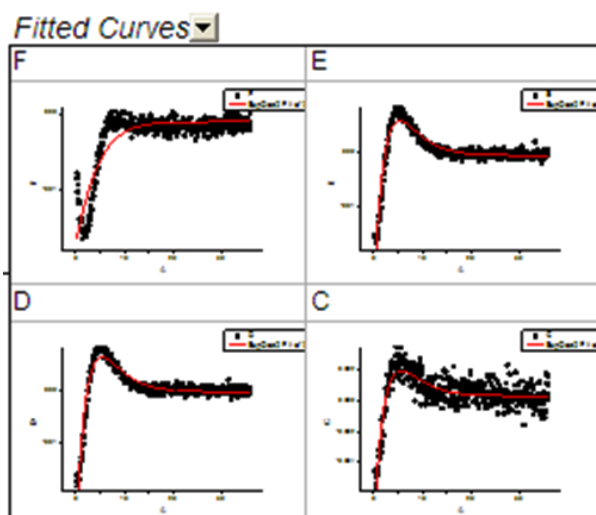


Fig. S1. The bi-exponential fitted parameters of transient absorption dynamical curves C(410), D (520), E (540 nm) and F (370 nm), which does not give reasonable fitting.