Electronic Supplementary Material (ESI) for Dalton Transactions.

Room Temperature Phosphorescent Triarylborane Functionalized Iridium Complexes

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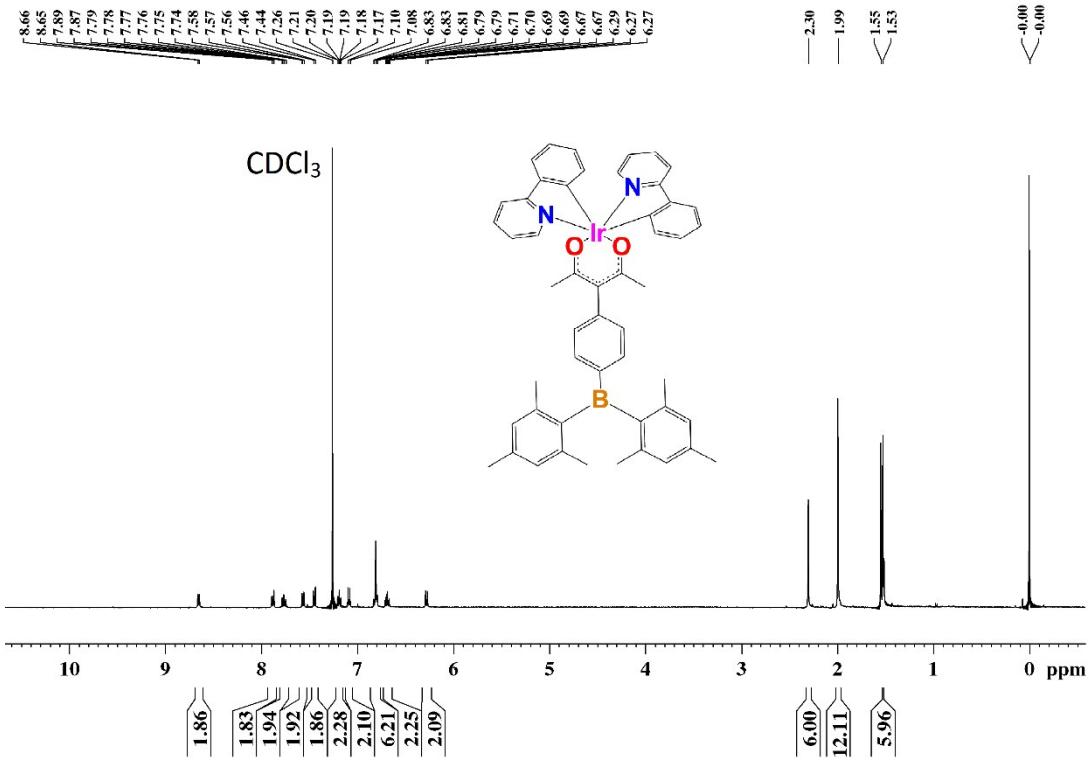


Figure S1: ^{1}H NMR spectrum of complex **1**

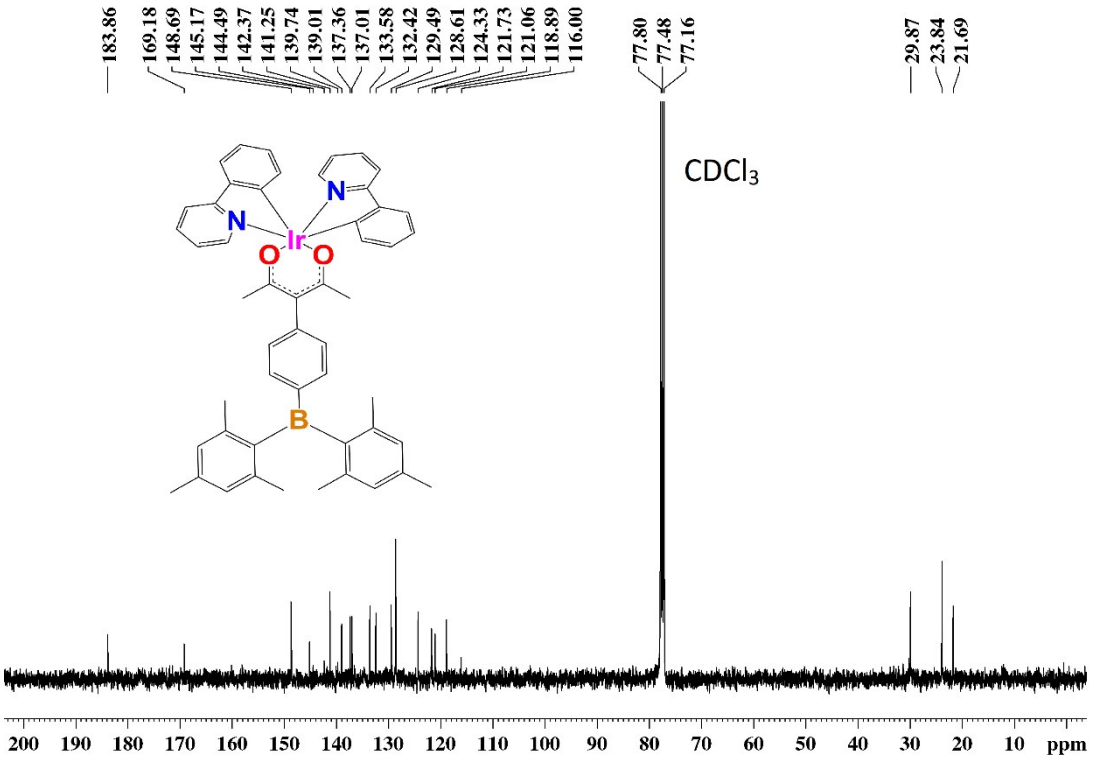


Figure S2: ^{13}C NMR spectrum of complex **1**

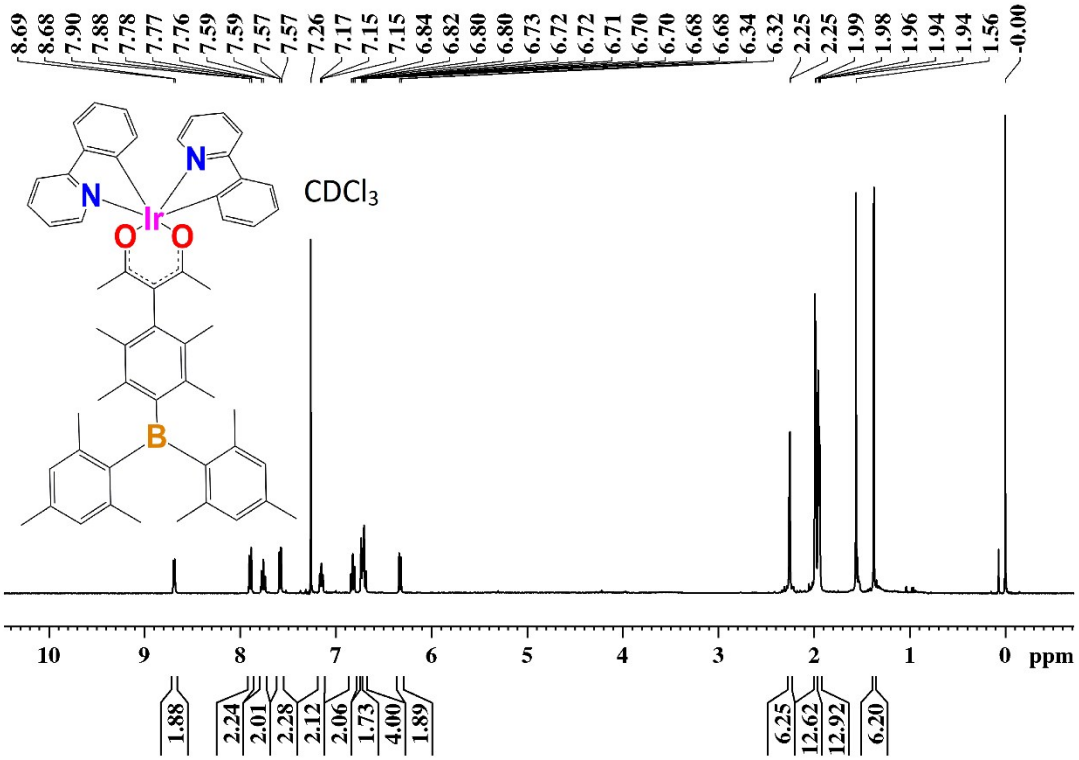


Figure S3: [1]H NMR spectrum of complex **2**

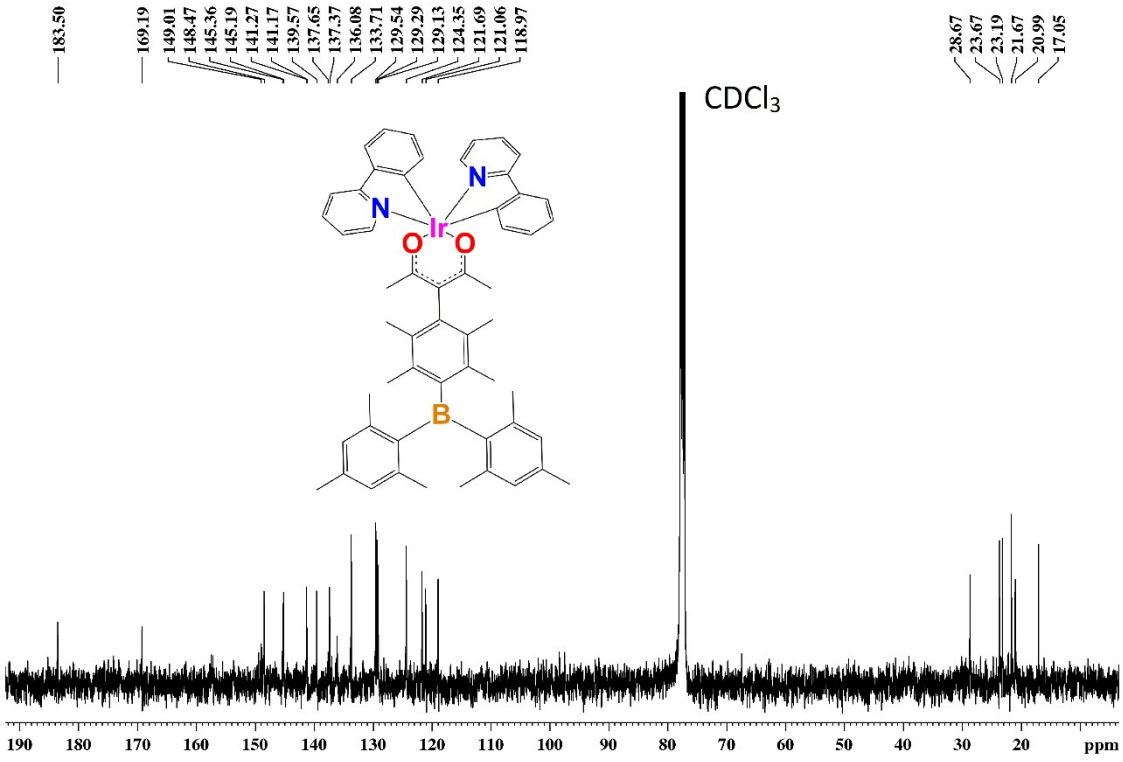


Figure S4: [13]C NMR spectrum of complex **2**

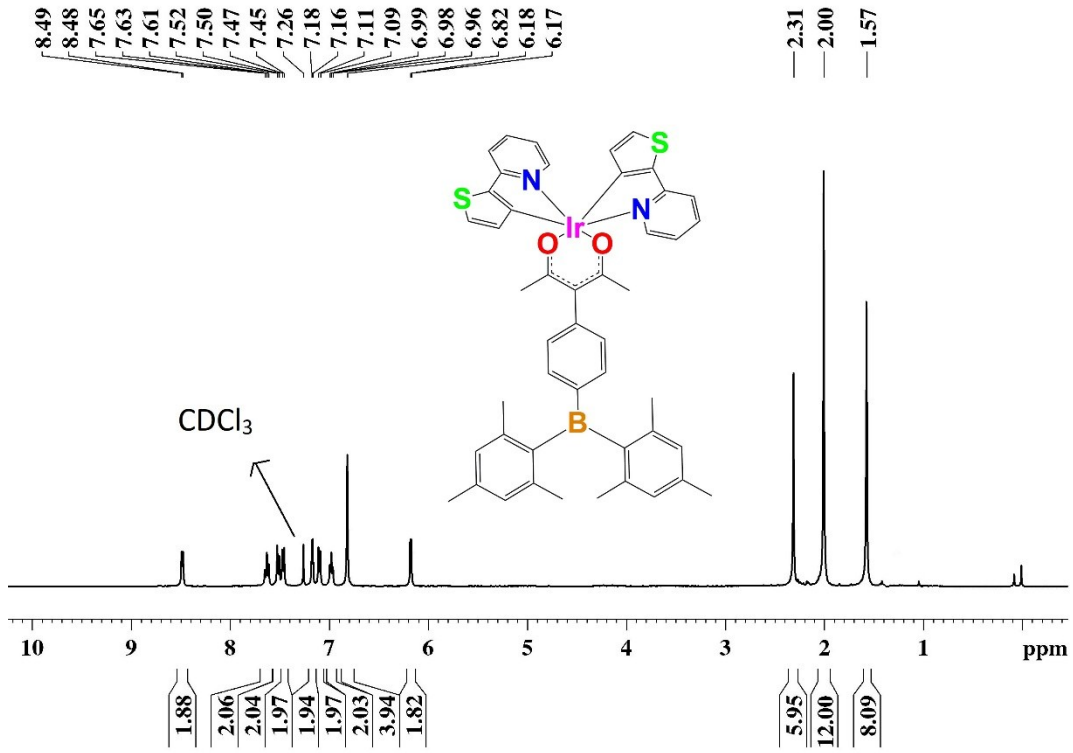


Figure S5: ^{1}H NMR spectrum of complex **3**

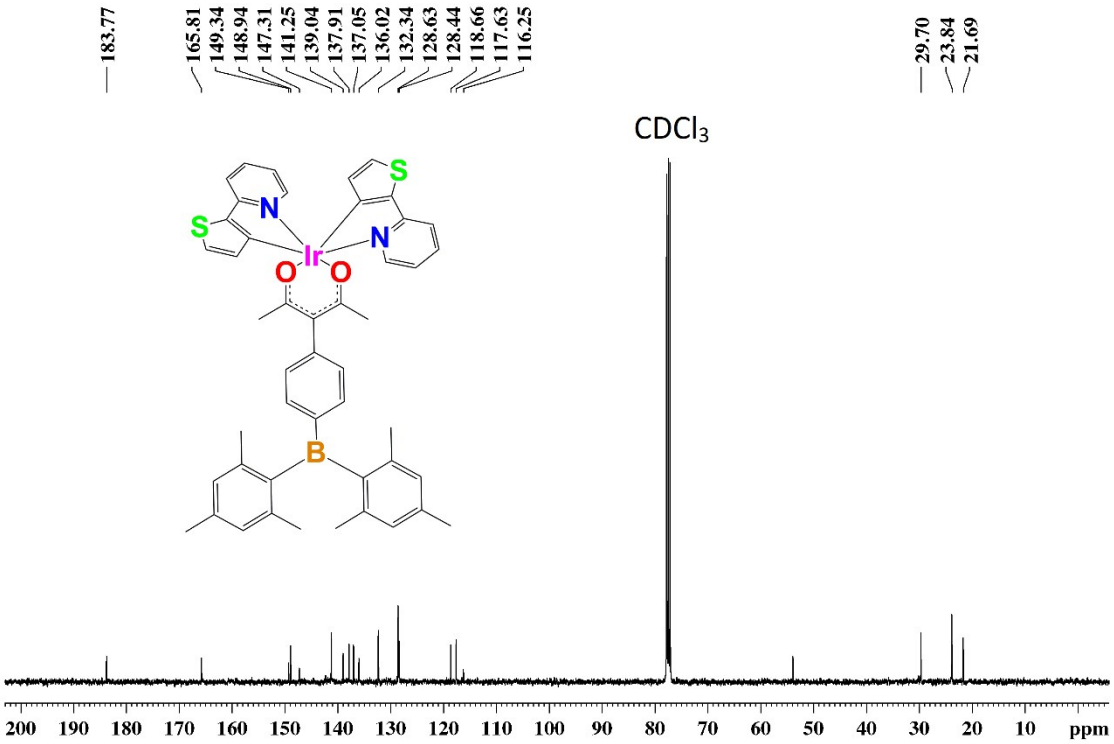


Figure S6: ^{13}C NMR spectrum of complex **3**

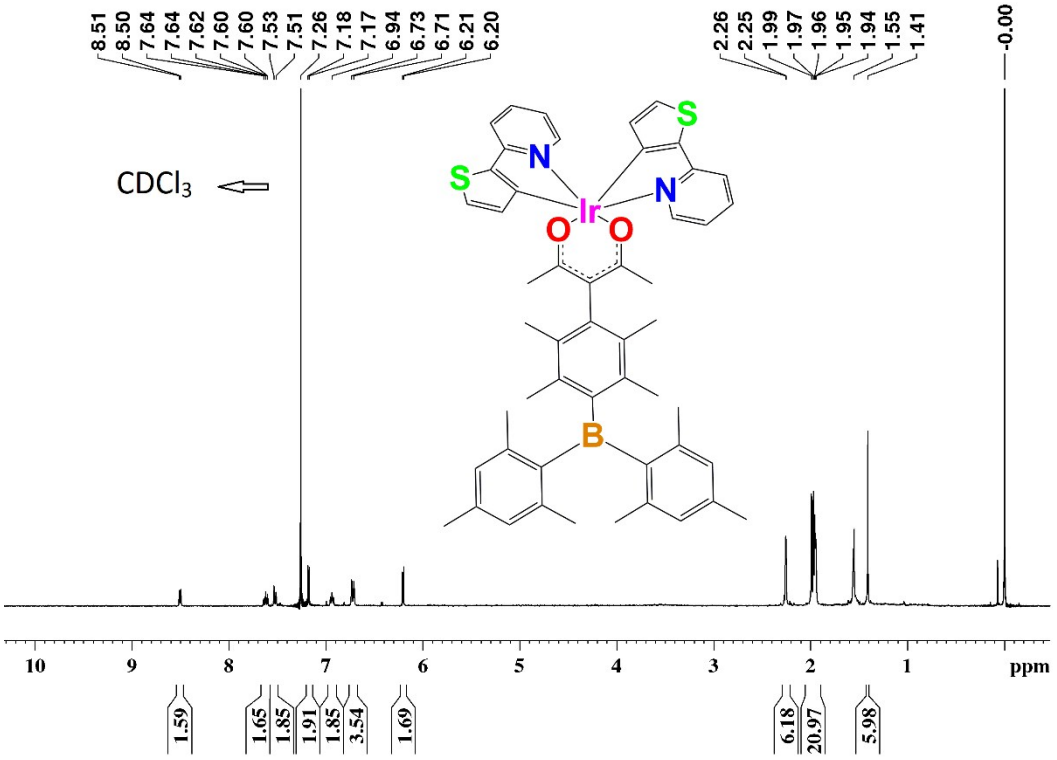


Figure S7: ^{1}H NMR spectrum of complex **4**

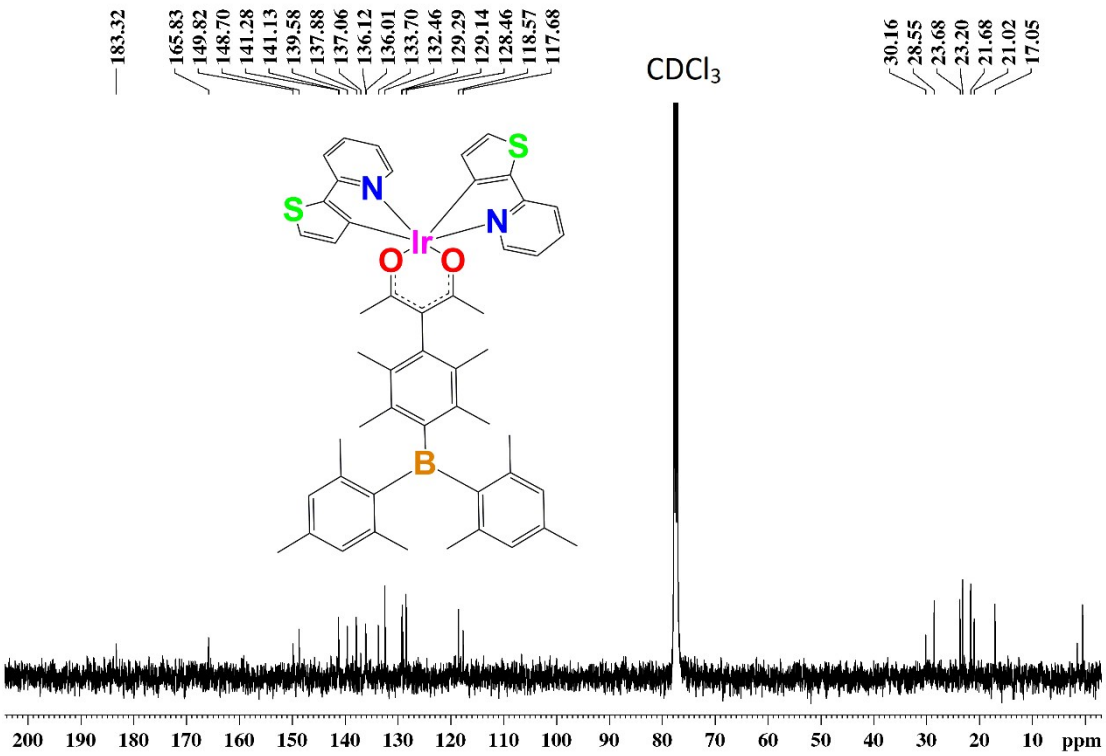


Figure S8: ^{13}C NMR spectrum of complex **4**

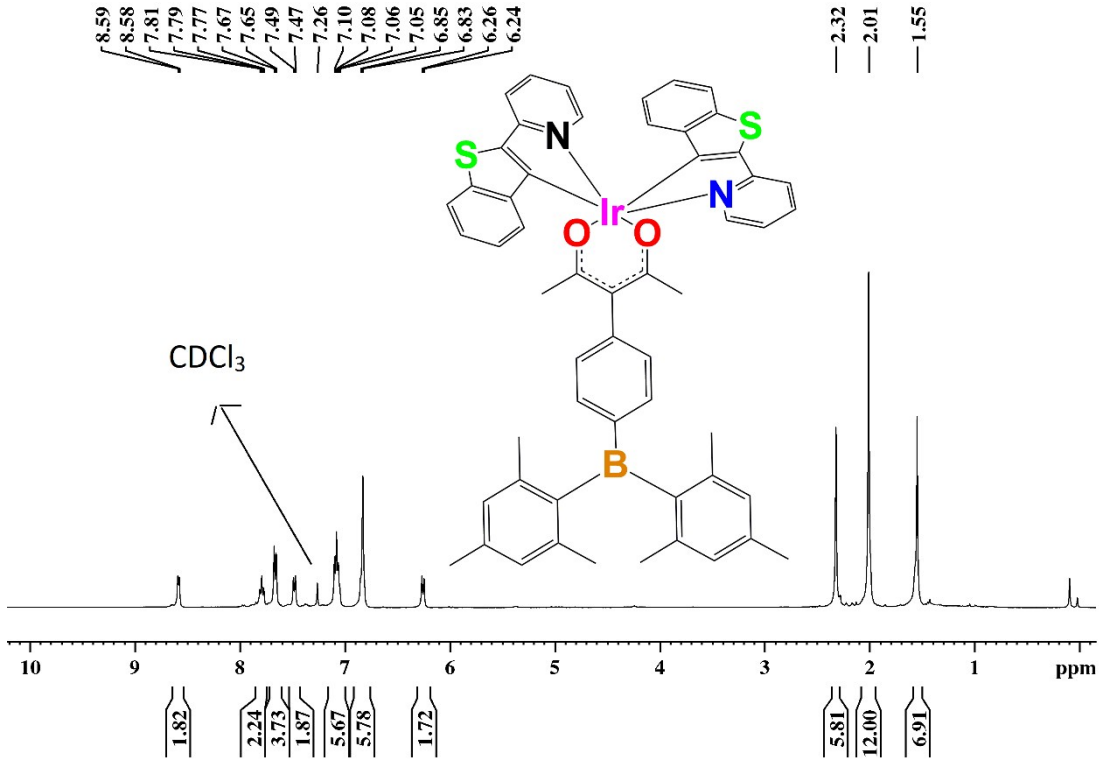


Figure S9: [1]H NMR spectrum of complex **5**

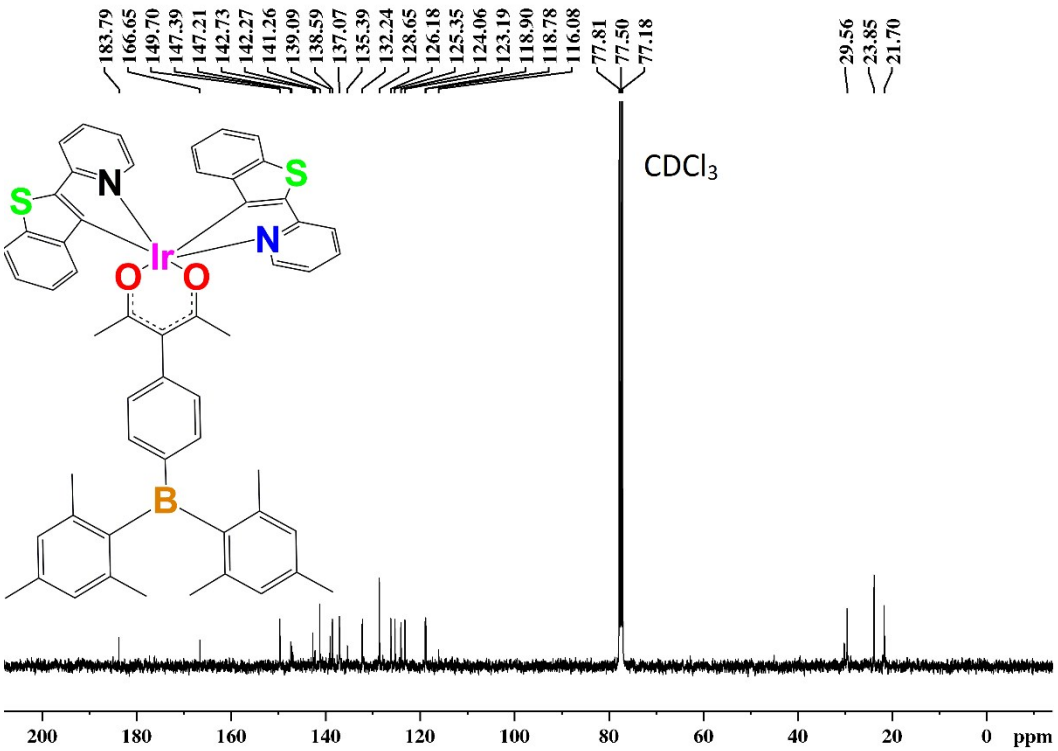


Figure S10: [13]C NMR spectrum of complex **5**

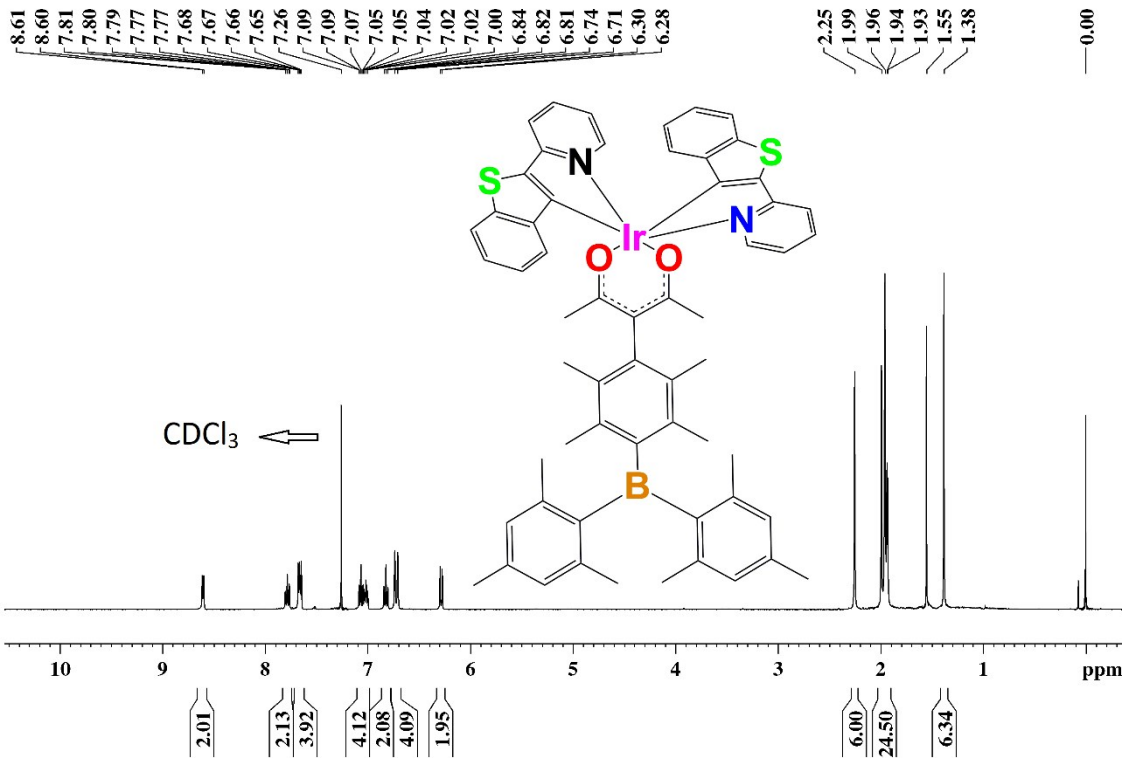


Figure S11: [1]H NMR spectrum of complex **6**

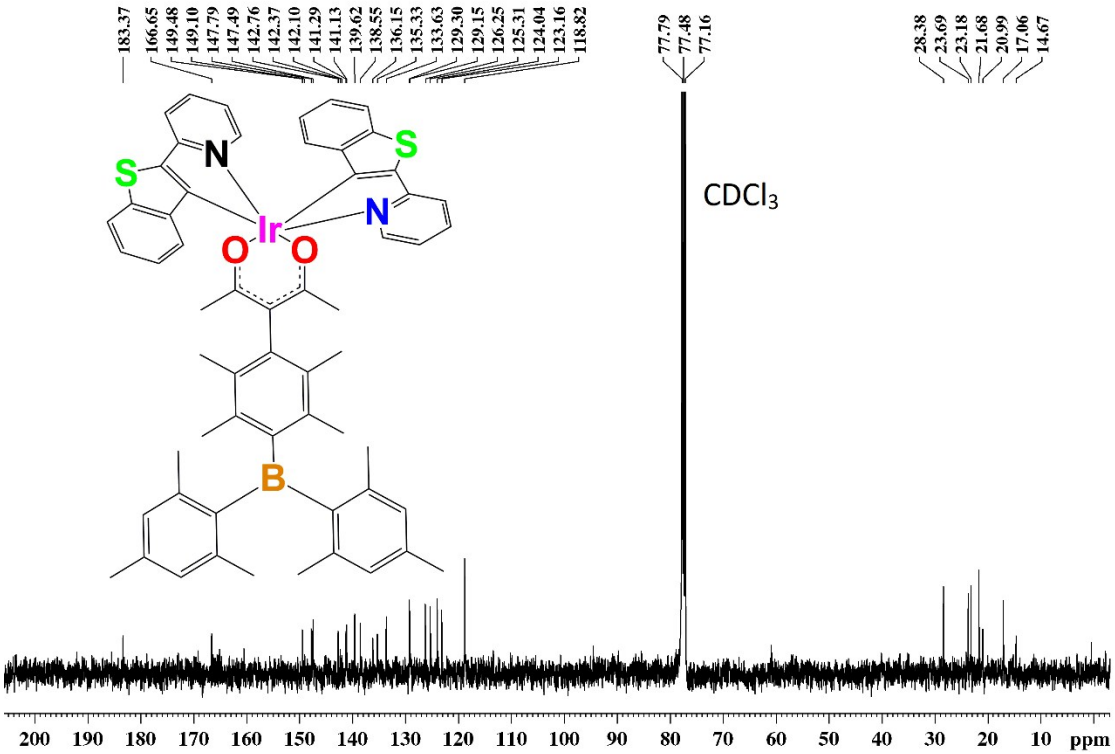


Figure S12: [13]C NMR spectrum of complex **6**

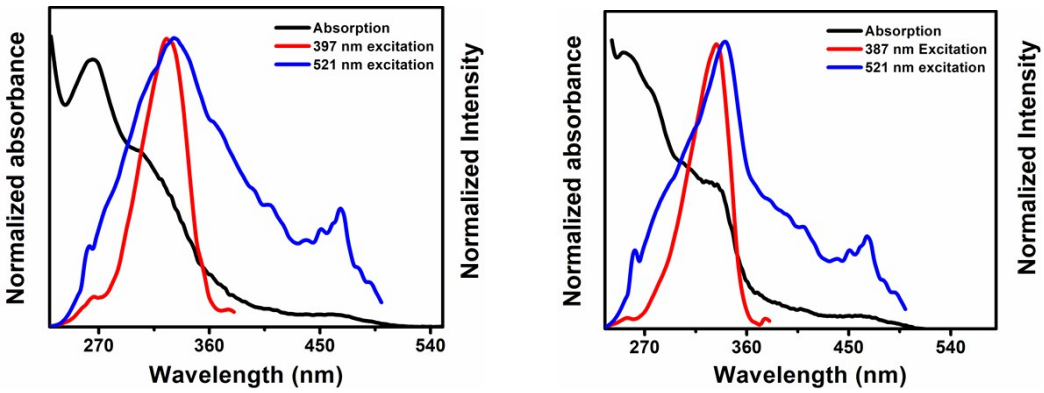


Figure S13: Combined absorption and excitation spectra of **1** (left) and **2** (right) in CH_2Cl_2.

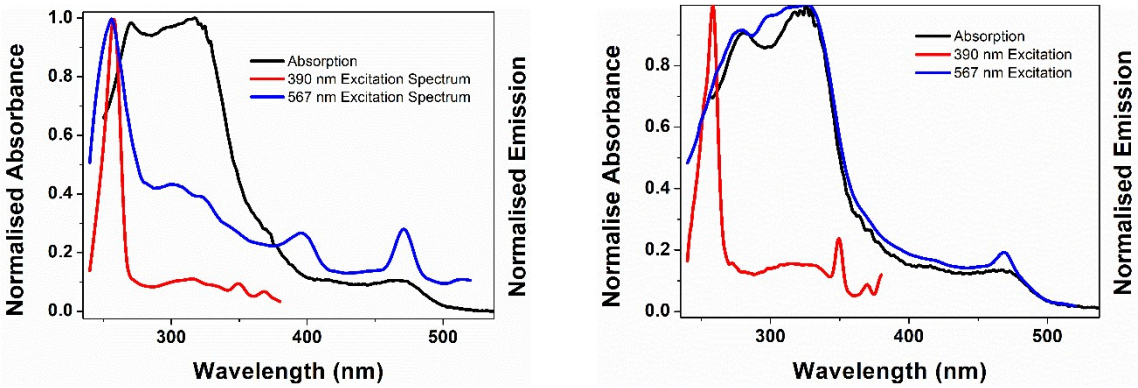


Figure S14: Combined absorption and excitation spectra of **3** (left) and **4** (right) in CH_2Cl_2.

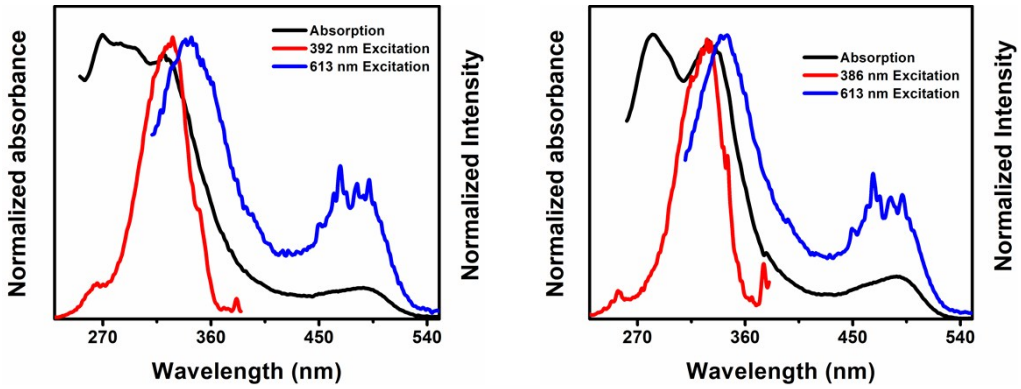


Figure S15: Combined absorption and excitation spectra of **5** (left) and **6** (right) in CH_2Cl_2.

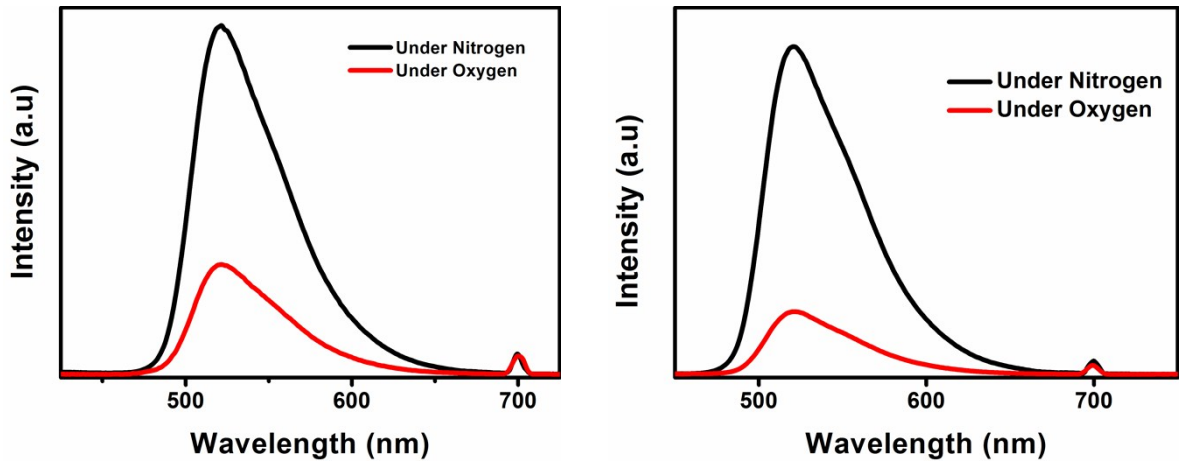


Figure S16: Photoluminescence spectra (λ_{ex} = 350 nm) of complexes **1** (left) and **2** (right).

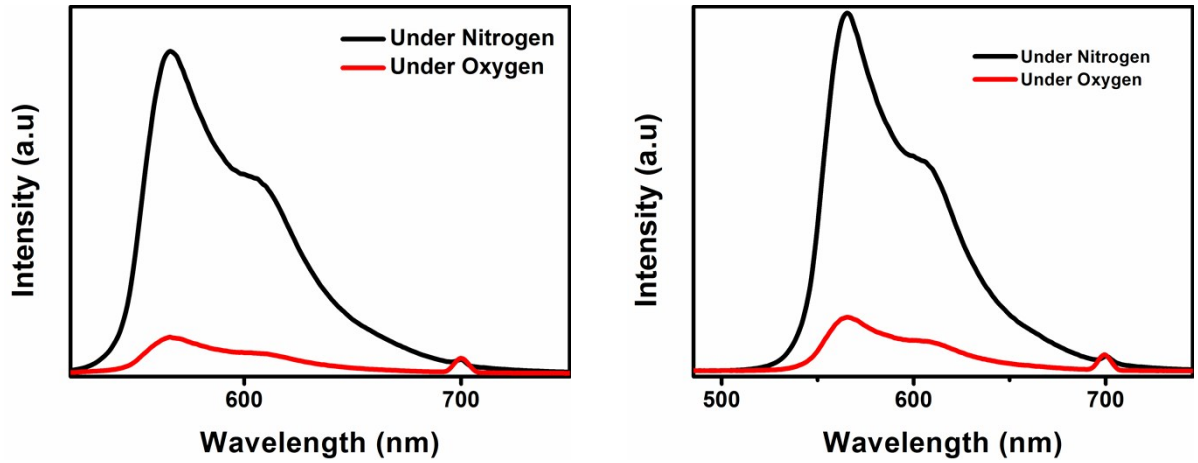


Figure S17: Photoluminescence spectra (λ_{ex} = 350 nm) of complexes **3** (left) and **4** (right).

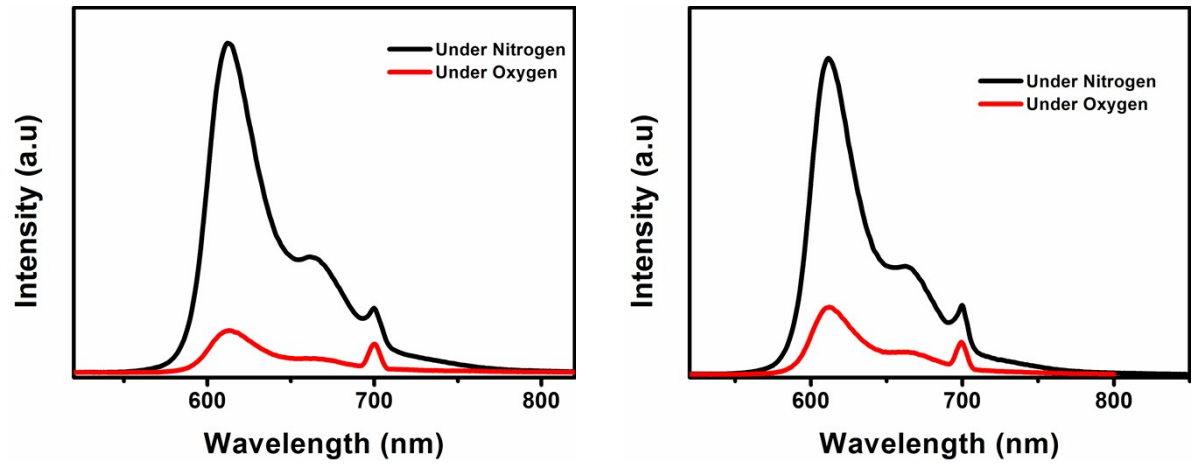


Figure S18: Photoluminescence spectra (λ_{ex} = 350 nm) of complexes **5** (left) and **6** (right).

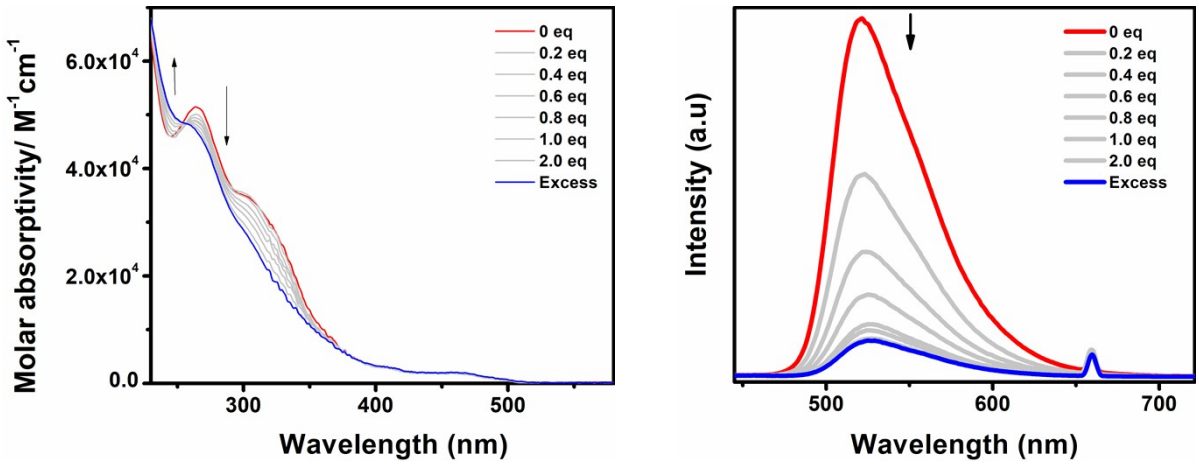


Figure S19: UV-Vis absorption (left) and photoluminescence spectra (right, λ_{ex} = 330 nm) of **1** in presence of TBAF.

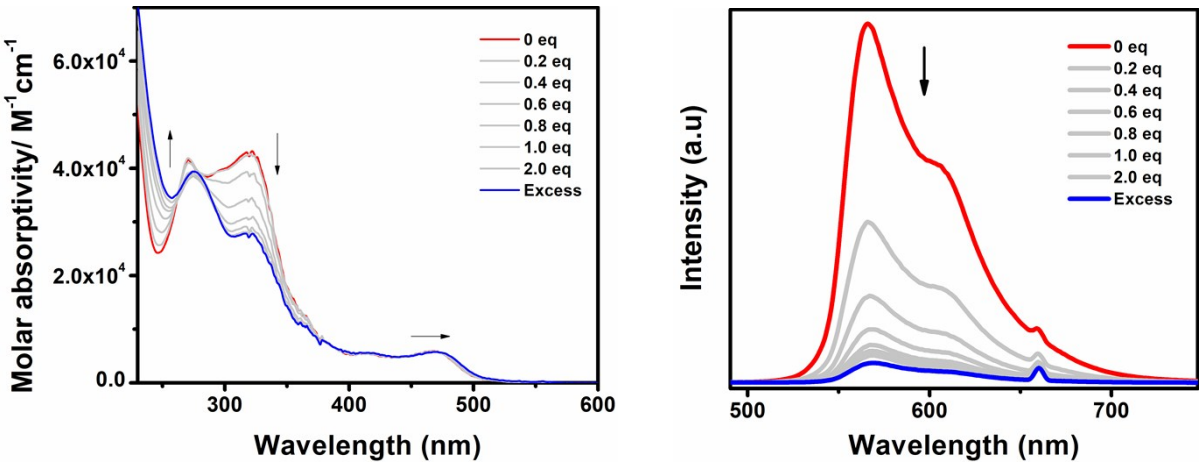


Figure S20: UV-Vis absorption (left) and photoluminescence spectra (right, λ_{ex} = 330 nm) of **3** in presence of TBAF.

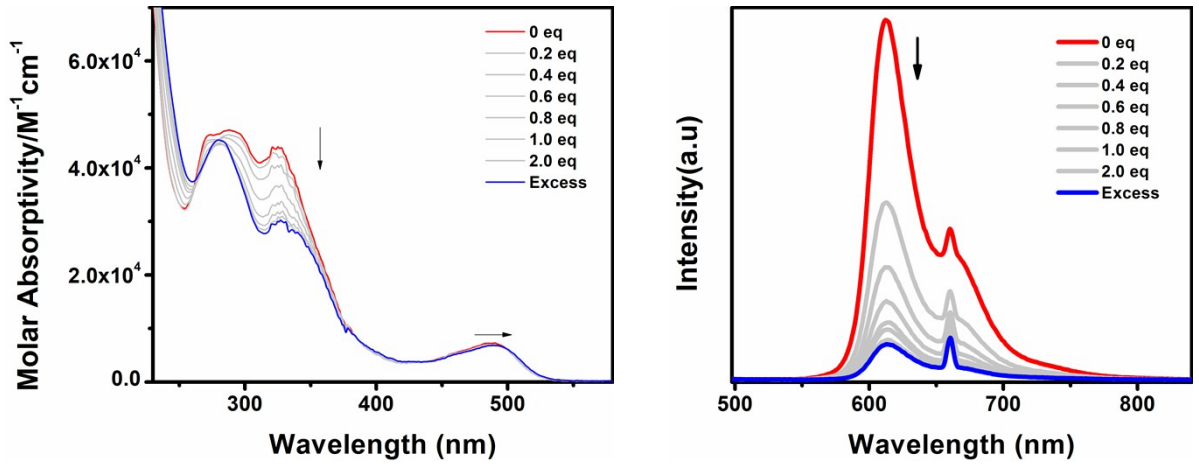


Figure S21: UV-Vis absorption (left) and photoluminescence spectra (right, λ_{ex} = 330 nm) of **5** in presence of TBAF.

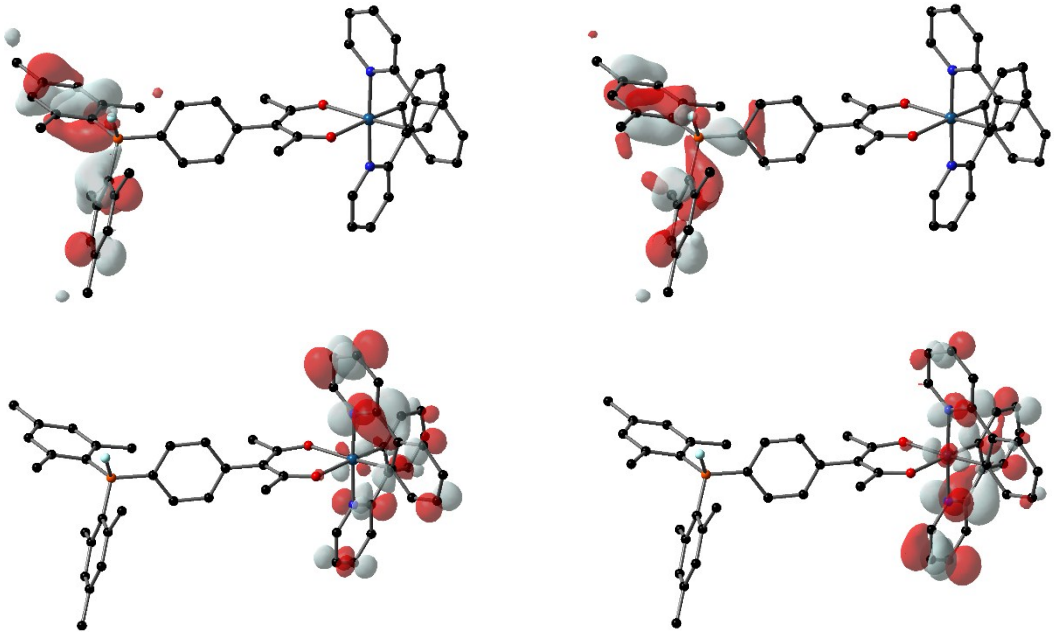
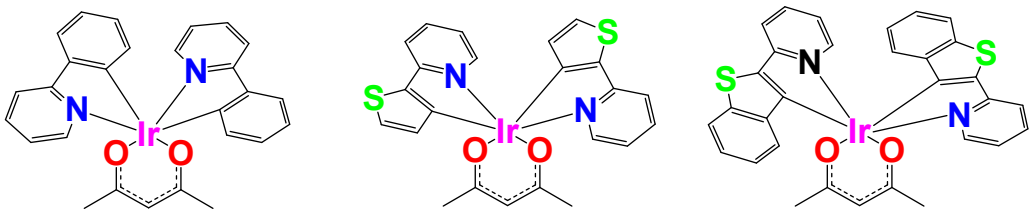


Figure S22: Frontier molecular orbitals of **1**•F^- [HOMO-1 (top left), HOMO (top right), LUMO (bottom left) and LUMO+1 (bottom right)].



7 **8** **9**

Figure S23: Complexes without TAB moiety.[1]

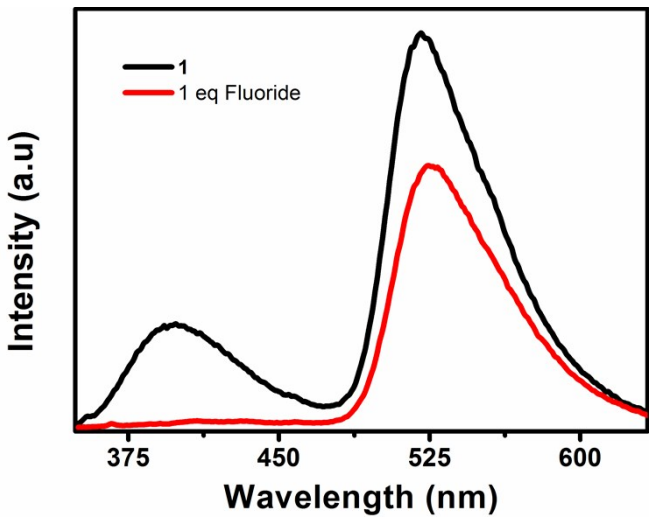


Figure S24: Photoluminescence spectra of 1 in presence of fluoride ions under open atmospheric conditions.

Table S1: Photoluminescence lifetime (τ) of lower energy band under open atm and N_2 condition, radiative rate (k_r, s^{-1}) and non-radiative rate (k_{nr}, s^{-1}) of complexes **1**–**6**.

	τ (μs) (λ_{max} at lower energy band) Under open atm Condition	k_r ($10^6 s^{-1}$)	k_{nr} (10^6 s^{-1})	τ (μs) (λ_{max} at lower energy band) Under N_2 atm	k_r (10^6 s^{-1})	k_{nr} (10^6 s^{-1})
1	0.08	2.1	10.37	0.10	5.4	4.61
2	0.09	2.0	9.11	0.10	9.5	0.53
3	0.002	27.0	472.50	0.12	4.0	4.34
4	0.10	0.75	9.25	0.13	3.8	3.91
5	0.11	0.12	8.97	0.23	0.38	3.97
6	0.005	4.20	195.8	0.22	0.42	4.12

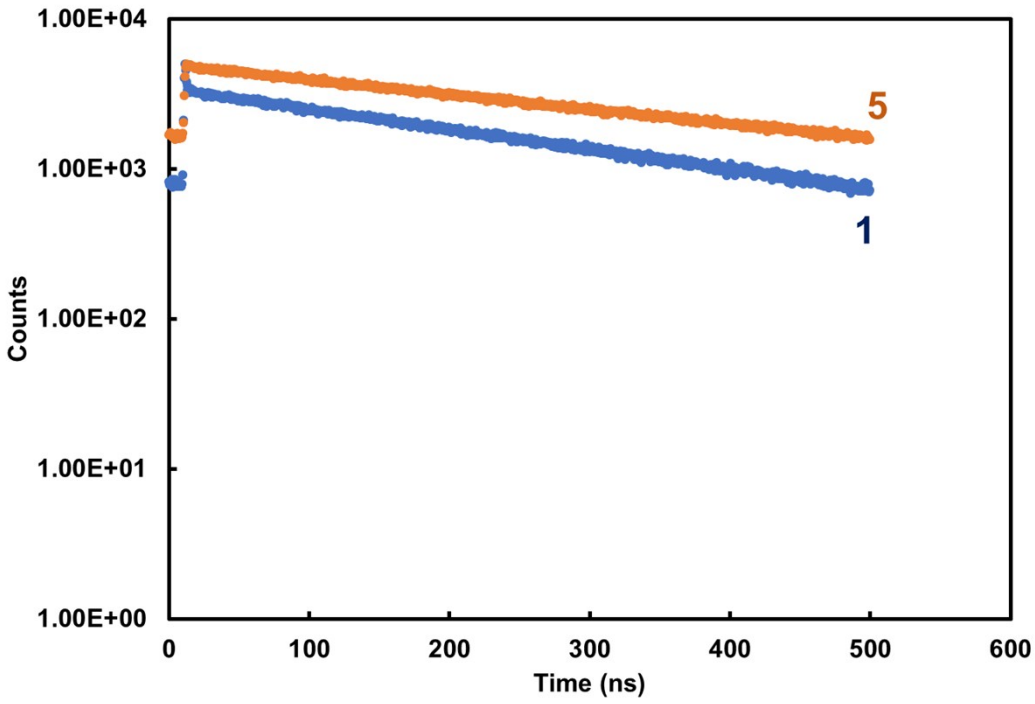


Figure S25: Luminescence decay profile of complex **1 and 5** with 375 excitation.

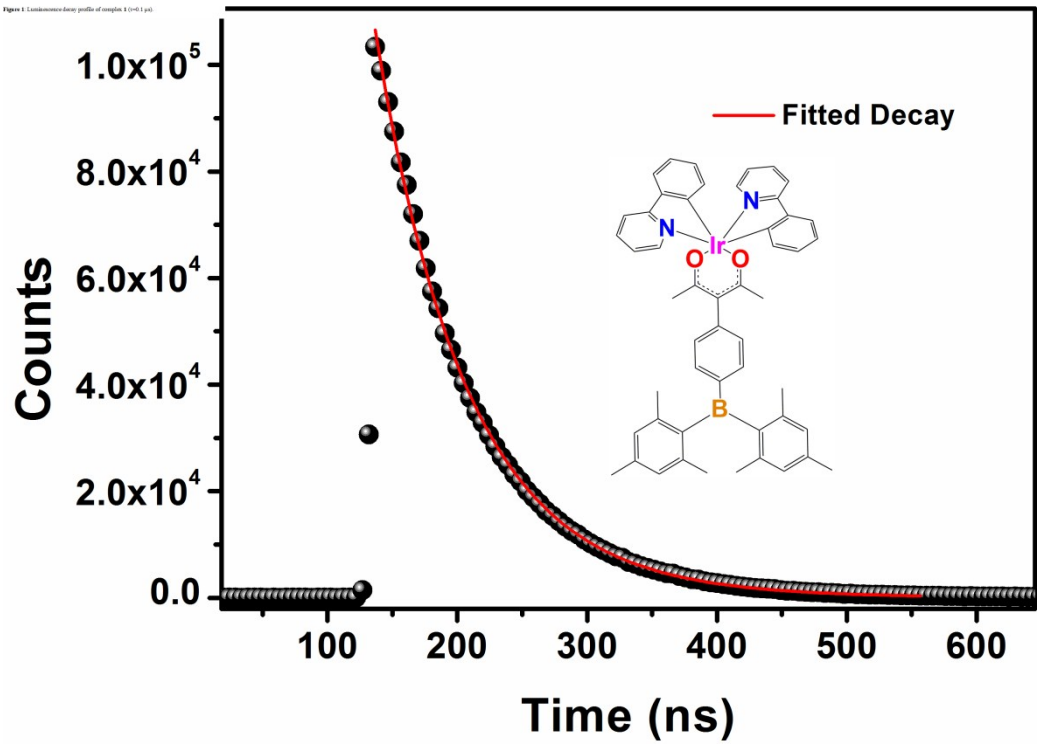


Figure S26: Luminescence decay profile of complex **1** (λ_{max}= 521 nm).

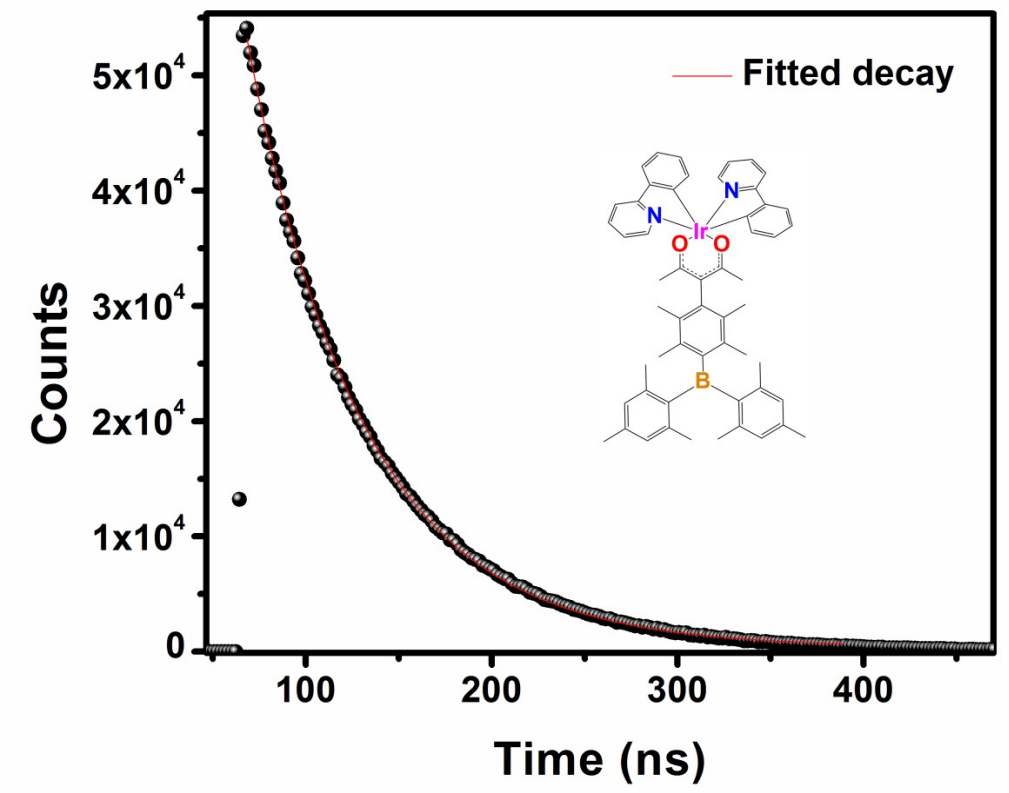


Figure S27: Luminescence decay profile of complex **2** (λ_{max}= 521 nm).

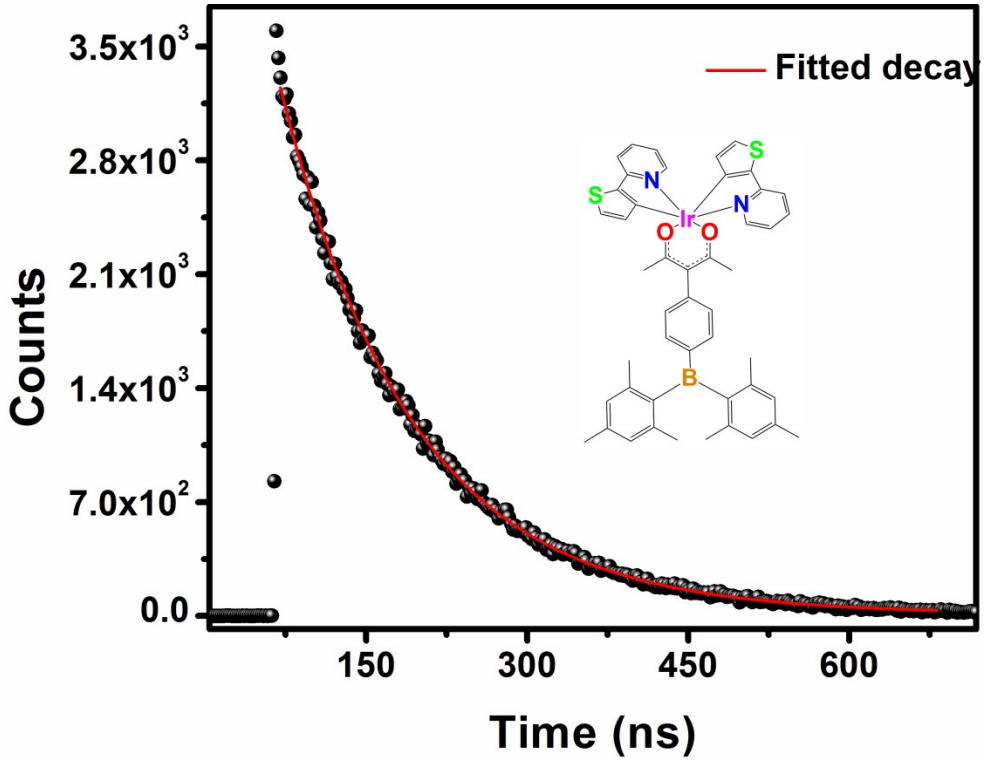


Figure S28: Luminescence decay profile of complex **3** (λ_{max}= 566 nm).

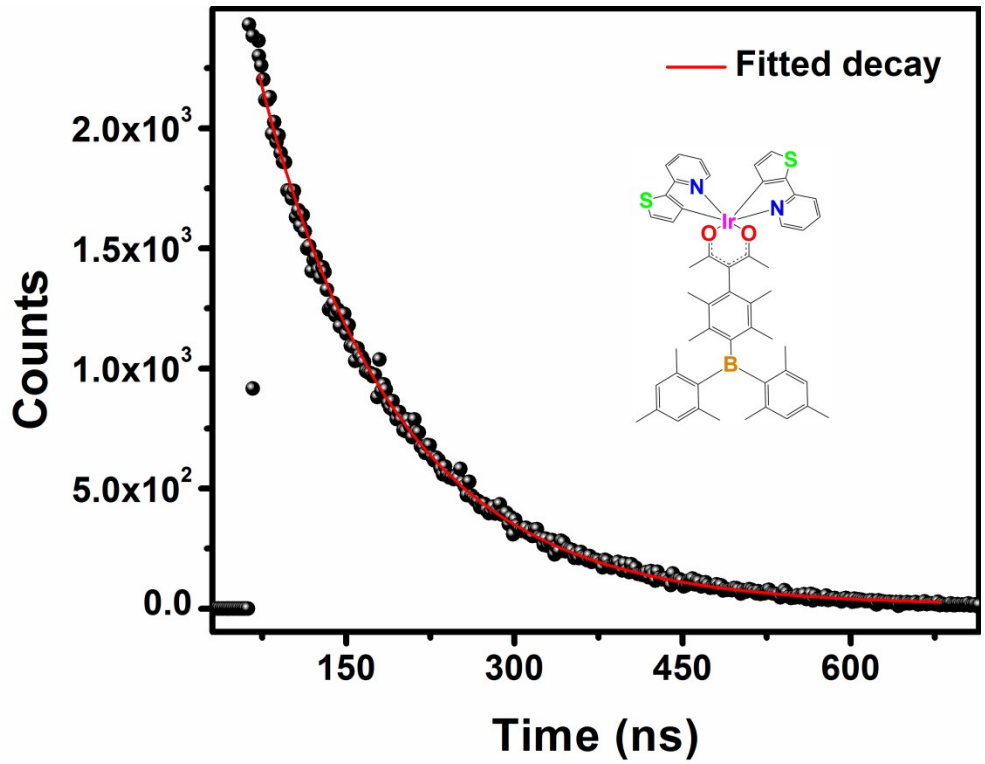


Figure S29: Luminescence decay profile of complex **4** (λ_{max}= 566 nm).

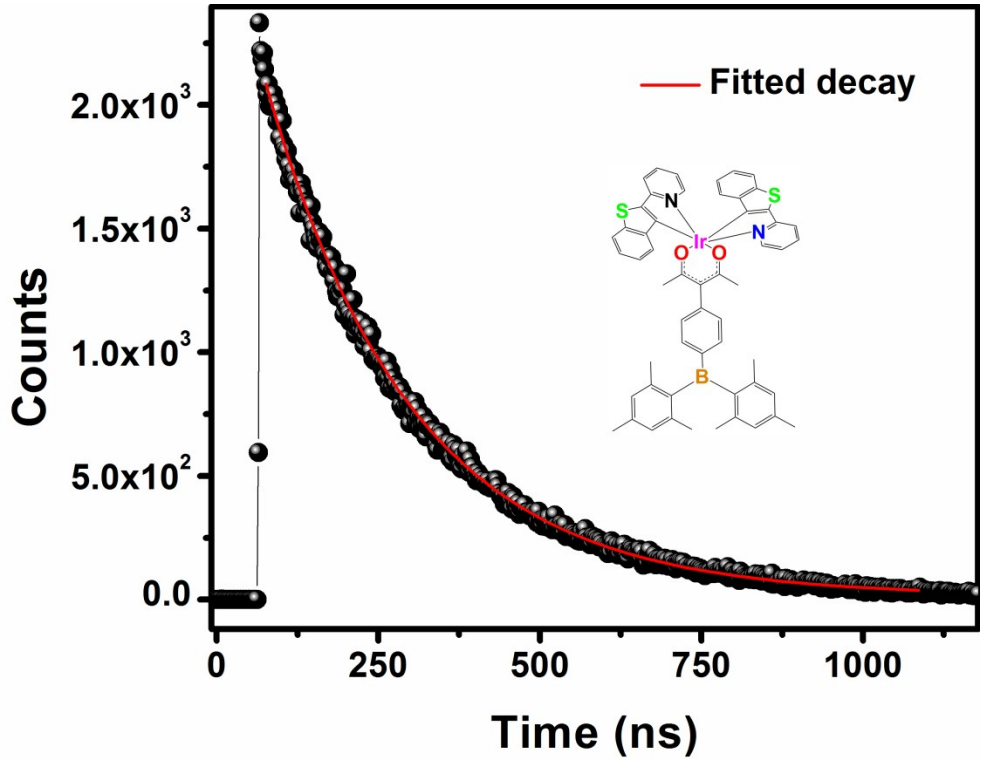


Figure S30: Luminescence decay profile of complex **5** (λ_{max}= 612 nm).

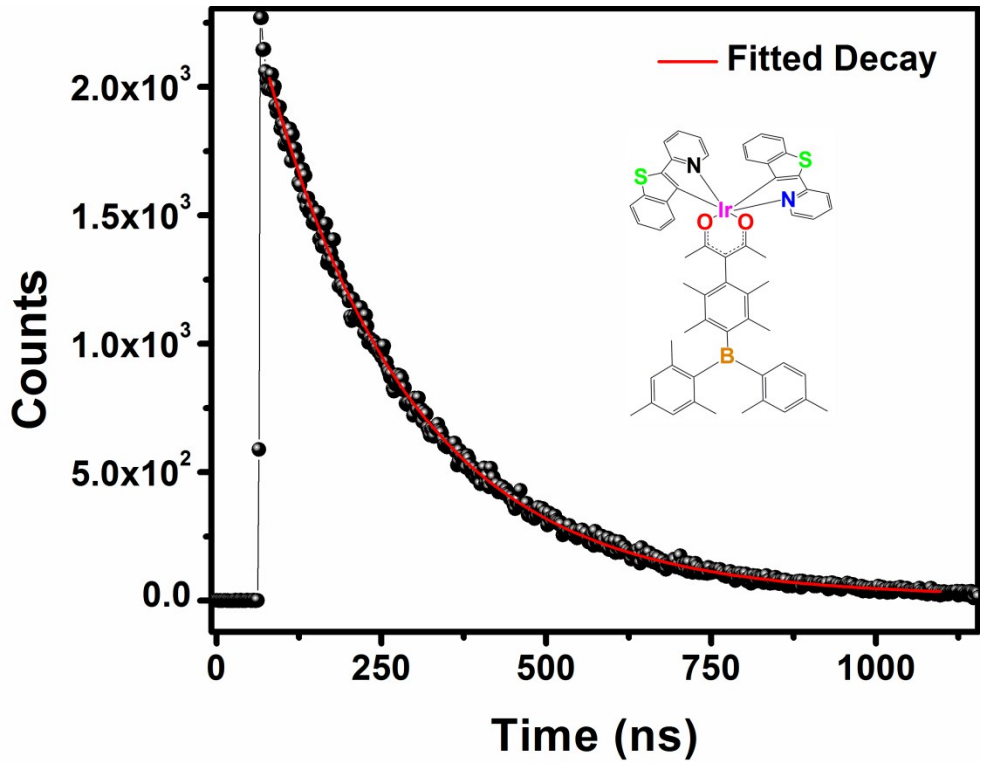


Figure S31: Luminescence decay profile of complex **6** (λ_{max}= 612 nm).

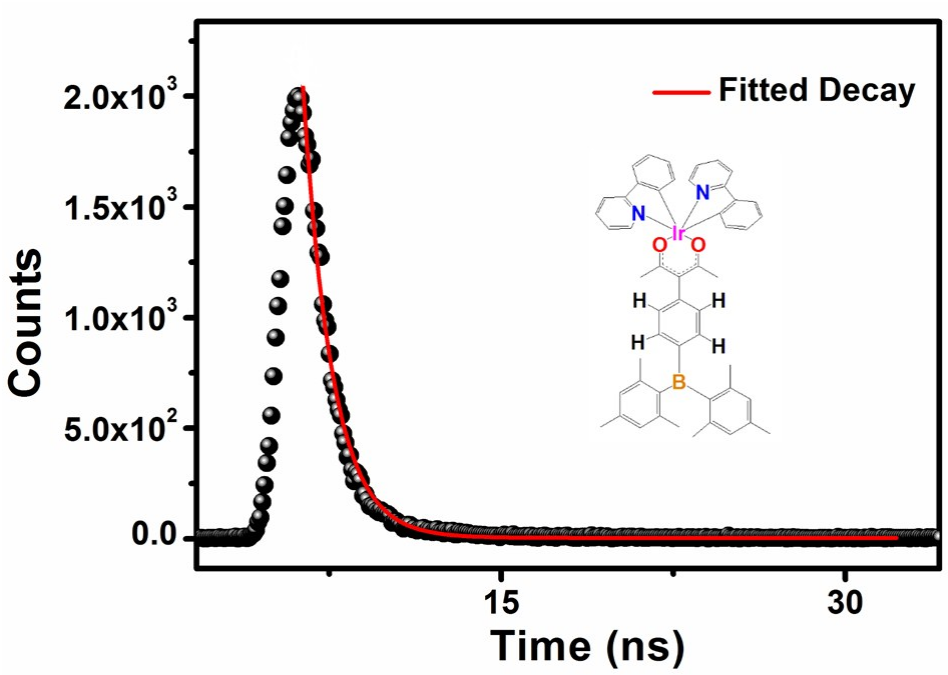


Figure S32: Luminescence decay profile of complex **1** (λ_{max}= 395 nm).

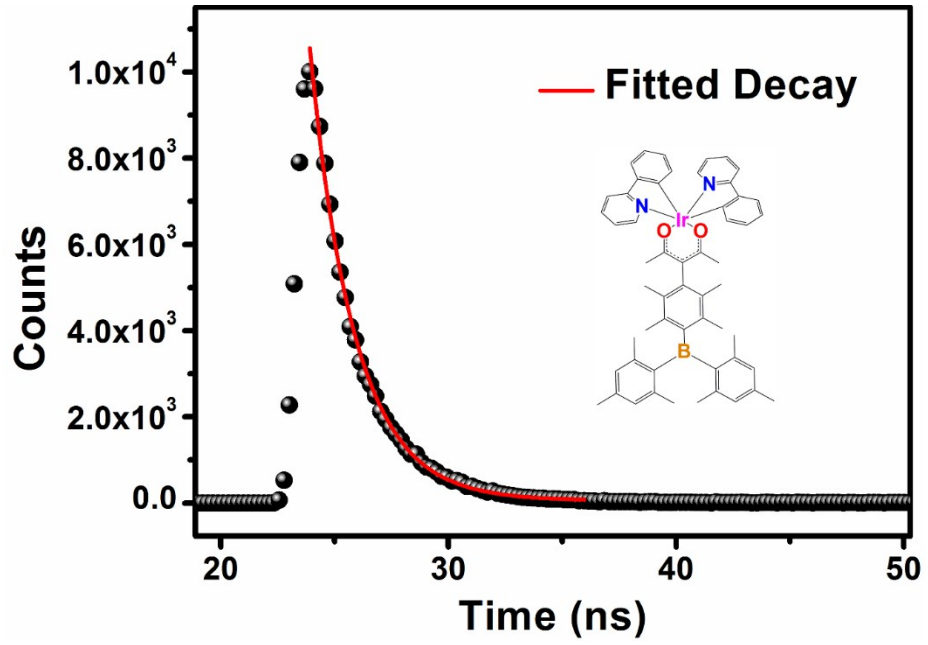


Figure S33: Luminescence decay profile of complex **2** (λ_{max}= 385 nm).

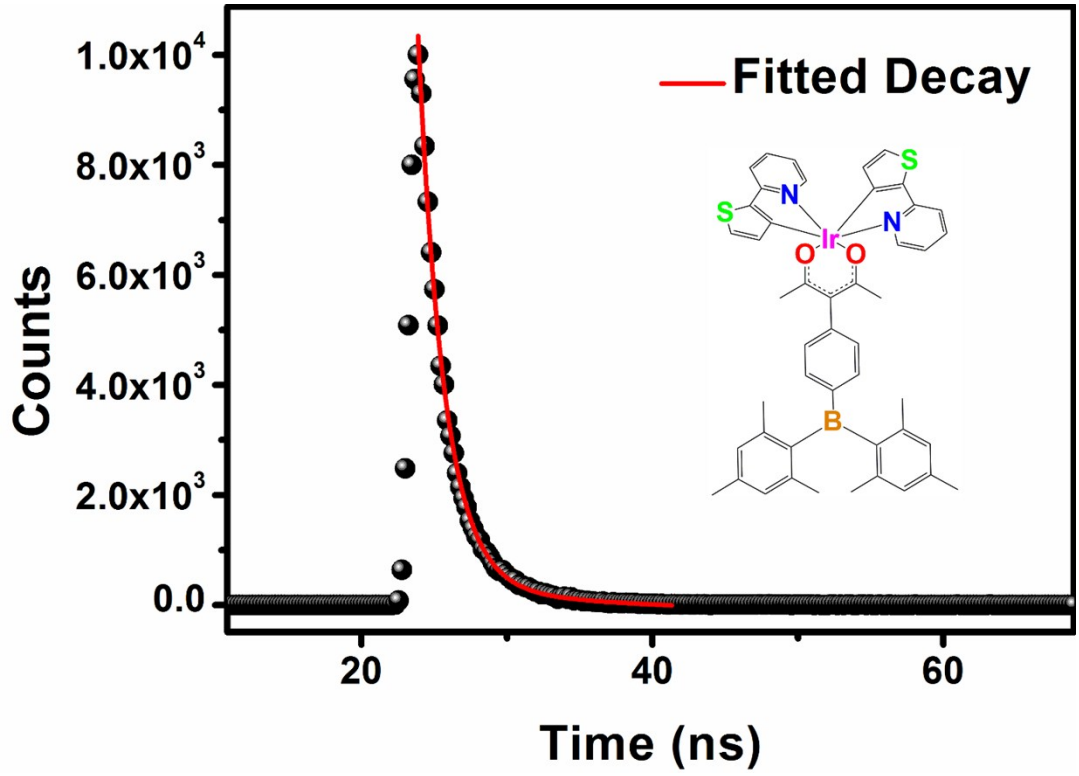


Figure S34: Luminescence decay profile of complex **3** (λ_{max}= 395 nm).

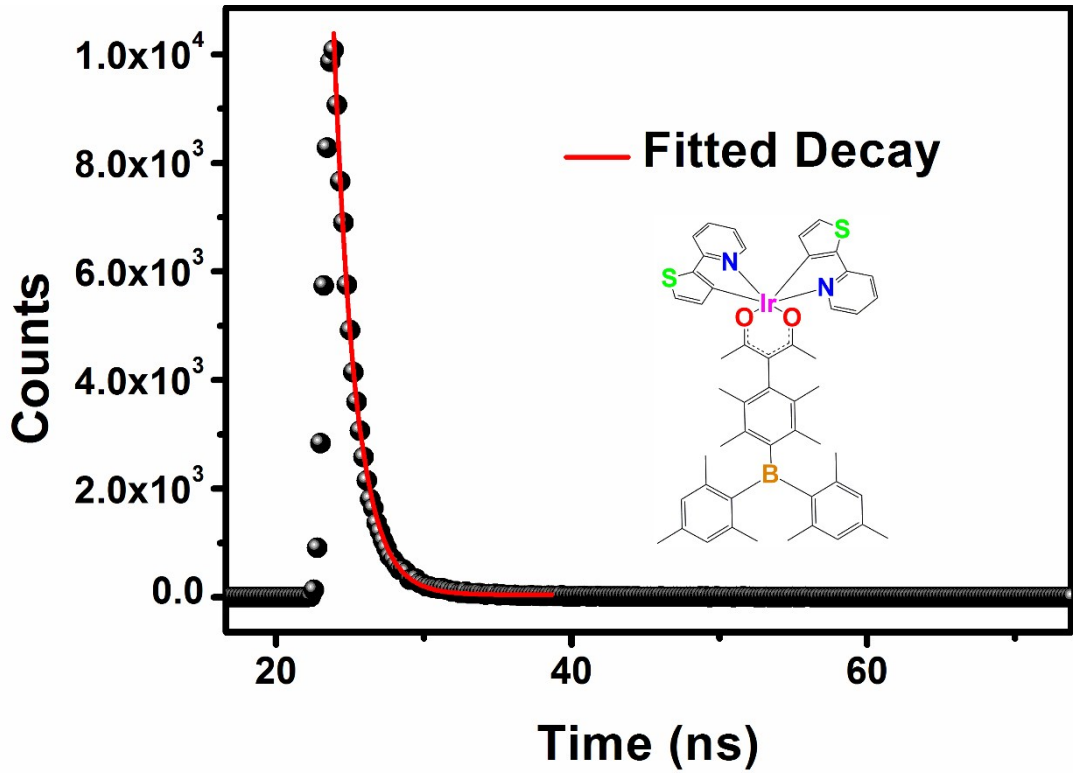


Figure S35: Luminescence decay profile of complex **4** (λ_{max}= 385 nm).

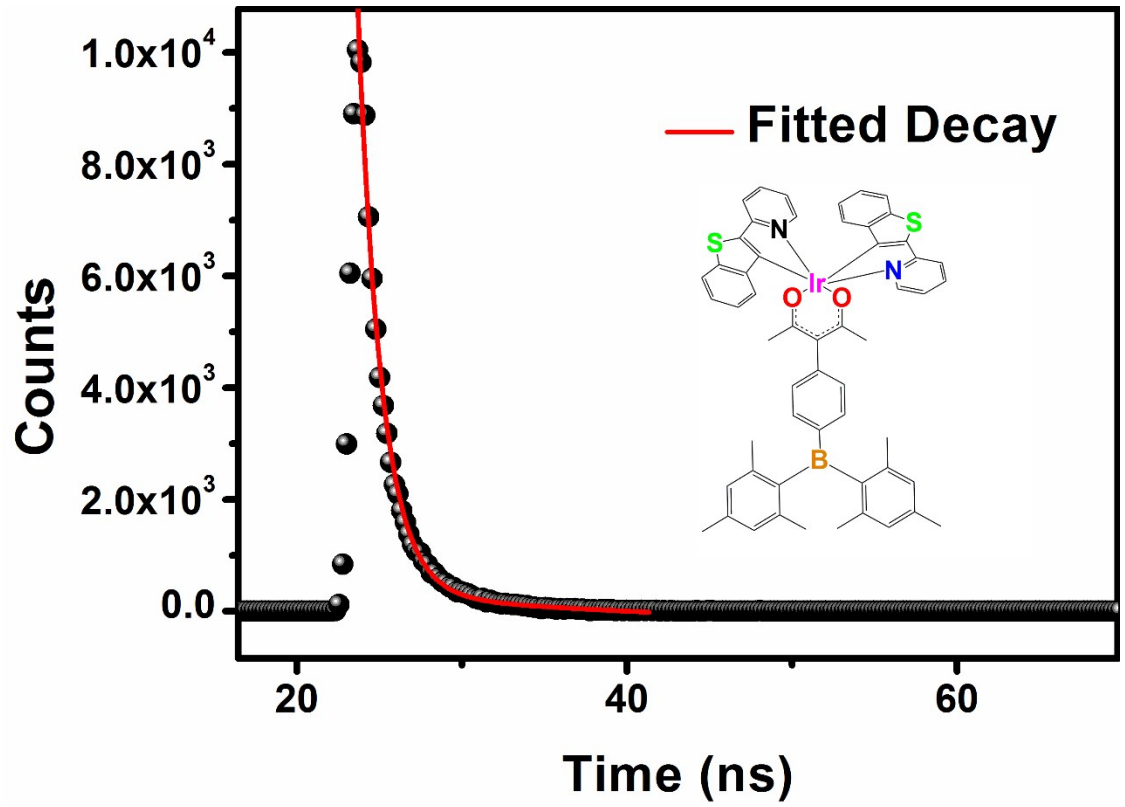


Figure S36: Luminescence decay profile of complex **5** (λ_{max}= 395 nm).

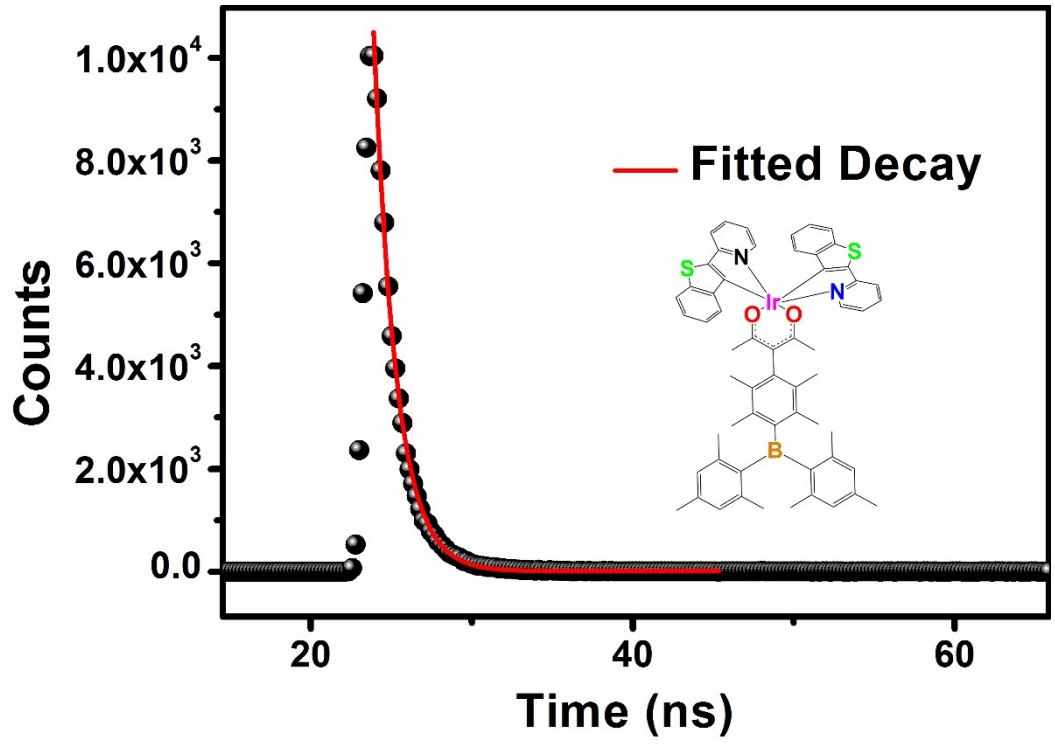


Figure S37: Luminescence decay profile of complex **6** (λ_{max}= 385 nm).

Table S2: Electronic transitions, calculated energies and oscillator strengths obtained form TDDFT calculations

Complexes	Singlet Transition		Calculated energy/eV	*f*	Triplet Transition		Calculated energy/eV	*f*
1	S_1	HOMO to LUMO+1 96.23%	2.62	0.0306	T_1	HOMO-3 to LUMO+2 6.38 % HOMO to LUMO+1 87.1 %	2.4014	0.0000
	S_2	HOMO to LUMO+2 96.93 %	2.65	0.0001	T_2	HOMO-3 to LUMO+1 7.23 % HOMO to LUMO+2 87.0 %	2.4099	0.0000
	S_3	HOMO to LUMO 99.30 %	2.83	0.0001	T_3	HOMO to LUMO 98.6 %	2.6729	0.0000
2	S_1	HOMO to LUMO+1 96.80 %	2.61	0.0294	T_1	HOMO-3 to LUMO+2 5.64 % HOMO to LUMO+1 87.6 %	2.3938	0.0000
	S_2	HOMO to LUMO+2 96.83 %	2.64	0.0001	T_2	HOMO-3 to LUMO+1 6.25 % HOMO to LUMO+2 87.7 %	2.3962	0.0000
	S_3	HOMO to LUMO 99.43 %	2.89	0.0001	T_3	HOMO-12 to LUMO+5 2.26 % HOMO-7 to LUMO+5 5.39 % HOMO-1 to LUMO+2 7.79 % HOMO-1 to LUMO+5 80.7 %	2.6168	0.0000
	S_4	HOMO-1 to LUMO+2 93.8 % HOMO to LUMO+3 2.09 %	3.03	0.0279	T_4	HOMO-12 to LUMO+3 2.20 % HOMO-8 to LUMO+4 3.08 % HOMO-7 to LUMO+1 6.64 % HOMO-3 to LUMO+1 7.81 % HOMO-2 to LUMO+2 11.0 % HOMO-1 to LUMO+1 46.8 % HOMO to LUMO+2 4.89 % HOMO to LUMO+4 3.18 %	2.7350	0.0000
	S_5	HOMO-1 to LUMO 2.56 % HOMO-1 to LUMO+1 90.6 %	3.07	0.0060	T_5	HOMO-8 to LUMO+1 2.55 % HOMO-8 to LUMO+3 3.14 % HOMO-7 to LUMO+2 6.29 % HOMO-3 to LUMO+2 2.85 %	2.7571	0.0000

		HOMO to LUMO+4 2.23 %				HOMO-3 to LUMO+4 2.11 % HOMO-2 to LUMO+1 10.8 % HOMO-1 to LUMO+2 40.8 % HOMO-1 to LUMO+5 7.44 % HOMO to LUMO+1 4.65 % HOMO to LUMO+3 5.36 %		
	S_6	HOMO-1 to LUMO 95.5 % HOMO-1 to LUMO+1 2.45 %	3.08	0.0024	T_6	HOMO-10 to LUMO+6 2.19 % HOMO-6 to LUMO 23.8 % HOMO to LUMO 67.7 %	2.9451	0.0000
3	S_1	HOMO to LUMO+1 94.2 %	2.63	0.0648	T_1	HOMO-3 to LUMO+1 2.14 % HOMO-2 to LUMO+2 13.7 % HOMO-2 to LUMO+4 2.18 % HOMO-1 to LUMO+2 2.30 % HOMO to LUMO+1 75.0 %	2.1346	0.0000
	S_2	HOMO to LUMO+2 95.4 %	2.72	0.0003	T_2	HOMO-2 to LUMO+1 18.6 % HOMO-1 to LUMO+1 3.07 % HOMO to LUMO+2 68.8 % HOMO to LUMO+4 3.39 %	2.1705	0.0000
	S_3	HOMO to LUMO 98.4 %	2.86	0.0002	T_3	HOMO-3 to LUMO+2 8.30 % HOMO-2 to LUMO+1 11.3 % HOMO-2 to LUMO+3 8.88 % HOMO-1 to LUMO+1 19.5 % HOMO to LUMO+2 24.1 % HOMO to LUMO+4 11.2 %	2.6794	0.0000
	S_4	HOMO-2 to LUMO 3.44 % HOMO-1 to LUMO 93.1 %	3.03	0.0031	T_4	HOMO to LUMO 97.8 %	2.7142	0.0000
4	S_1	HOMO to LUMO+1 94.8 %	2.62	0.0631	T_1	HOMO-4 to LUMO+1 2.06 % HOMO-2 to LUMO+2 14.1 % HOMO-2 to LUMO+4 2.25 %	2.1310	0.0000

						HOMO to LUMO+1 75.3 %		
	S_2	HOMO to LUMO+2 95.2 %	2.70	0.0006	T_2	HOMO-2 to LUMO+1 19.3 % HOMO-1 to LUMO+1 2.32 % HOMO to LUMO+2 69.1 % HOMO to LUMO+4 3.48 %	2.1668	0.0000
	S_3	HOMO to LUMO 99.2 %	3.05	0.0001	T_3	HOMO-4 to LUMO+2 7.61 % HOMO-2 to LUMO+1 12.7 % HOMO-2 to LUMO+3 8.69 % HOMO-1 to LUMO+1 20.2 % HOMO to LUMO+2 23.4 % HOMO to LUMO+4 16.3 %	2.6244	0.0000
	S_4	HOMO-1 to LUMO+1 90.7 % HOMO to LUMO+4 3.83 %	3.06	0.0045	T_4	HOMO-12 to LUMO+5 2.36 % HOMO-9 to LUMO+5 19.6 % HOMO-2 to LUMO+5 3.80 % HOMO-1 to LUMO+2 5.76 % HOMO-1 to LUMO+4 2.08 % HOMO to LUMO+5 76.5 %	2.6937	0.0000
	S_5	HOMO-1 to LUMO+2 93.1 % HOMO to LUMO+3 2.90 %	3.07	0.0079	T_5	HOMO-4 to LUMO+1 7.87 % HOMO-2 to LUMO+2 6.20 % HOMO-2 to LUMO+4 9.07 % HOMO-1 to LUMO+2 12.2 % HOMO-1 to LUMO+5 6.86 % HOMO to LUMO+1 13.8 % HOMO to LUMO+3 30.9 %	2.7461	0.0000
	S_6	HOMO-1 to LUMO 96.0 %	3.08	0.0249	T_6	HOMO-6 to LUMO 3.50 % HOMO to LUMO 94.27 %	2.9227	0.0000
5	S_1	HOMO to LUMO+2 94.3 %	2.50	0.0608	T_1	HOMO-1 to LUMO+2 15.6 % HOMO to LUMO+1 77.6 %	2.0033	0.0000
	S_2	HOMO to LUMO+1 96.5 %	2.52	0.0039	T_2	HOMO-1 to LUMO+1 15.7 % HOMO to LUMO+1 77.1 %	2.0085	0.0000
	S_3	HOMO to LUMO 98.5 %	2.76	0.0002	T_3	HOMO to LUMO 98.5 %	2.6891	0.0000

6	S_1	HOMO to LUMO+2 95.5 %	2.50	0.0591	T_1	HOMO-1 to LUMO+2 15.1 % HOMO to LUMO+1 77.6 %	2.0012	0.0000
	S_2	HOMO to LUMO+1 96.4 %	2.52	0.0045	T_2	HOMO-1 to LUMO+1 15.1 % HOMO to LUMO+2 77.6 %	2.0067	0.0000
	S_3	HOMO to LUMO 99.8 %	2.92	0.0039	T_3	HOMO-12 to LUMO+1 2.52 % HOMO-2 to LUMO+2 5.5 % HOMO-1 to LUMO+2 18.1 % HOMO-1 to LUMO+4 8.28 % HOMO to LUMO+1 15.1 % HOMO to LUMO+3 39.4 %	2.6524	0.0000
	S_4	HOMO-2 to LUMO+2 9.57 % HOMO-1 to LUMO+2 11.5 % HOMO to LUMO+3 76.5 %	2.94	0.0001	T_4	HOMO-12 to LUMO+2 2.47 % HOMO-2 to LUMO+1 6.30 % HOMO-1 to LUMO+1 17.4 % HOMO-1 to LUMO+3 9.30 % HOMO to LUMO+2 14.5 % HOMO to LUMO+4 38.6 %	2.6779	0.0000
	S_5	HOMO-2 to LUMO+1 39.1 % HOMO-1 to LUMO+1 14.9 % HOMO to LUMO+4 43.4 %	3.07	0.0003	T_5	HOMO-12 to LUMO+5 5.39 % HOMO-4 to LUMO+5 3.52 % HOMO-2 to LUMO+5 85.8 % HOMO-1 to LUMO+5 3.45 %	2.7103	0.0000
	S_6	HOMO-2 to LUMO+1 55.6 % HOMO-1 to LUMO+1 3.37 % HOMO to LUMO+4 37.7 %	3.08	0.0052	T_6	HOMO to LUMO 99.0 %	2.8795	0.0000

References:

1. Lamansky, S.; Djurovich, P.; Murphy, D.; Razzaq, F. A.; Lee, H. E. Adachi, C.; Burrows, P. E.; Forrest, S. R.; Thompson, M. E. *J. Am. Chem. Soc*. **2001**, *123*, 4304-4312.