Electronic Supplementary Information for:

Green chemiluminescence from a bis-cyclometalated iridium complex with an ancillary bathophenanthroline disulfonate ligand

Elizabeth M. Zammit, Neil W. Barnett, Luke C. Henderson, Gail A. Dyson, Ming Zhou, Paul S. Francis*

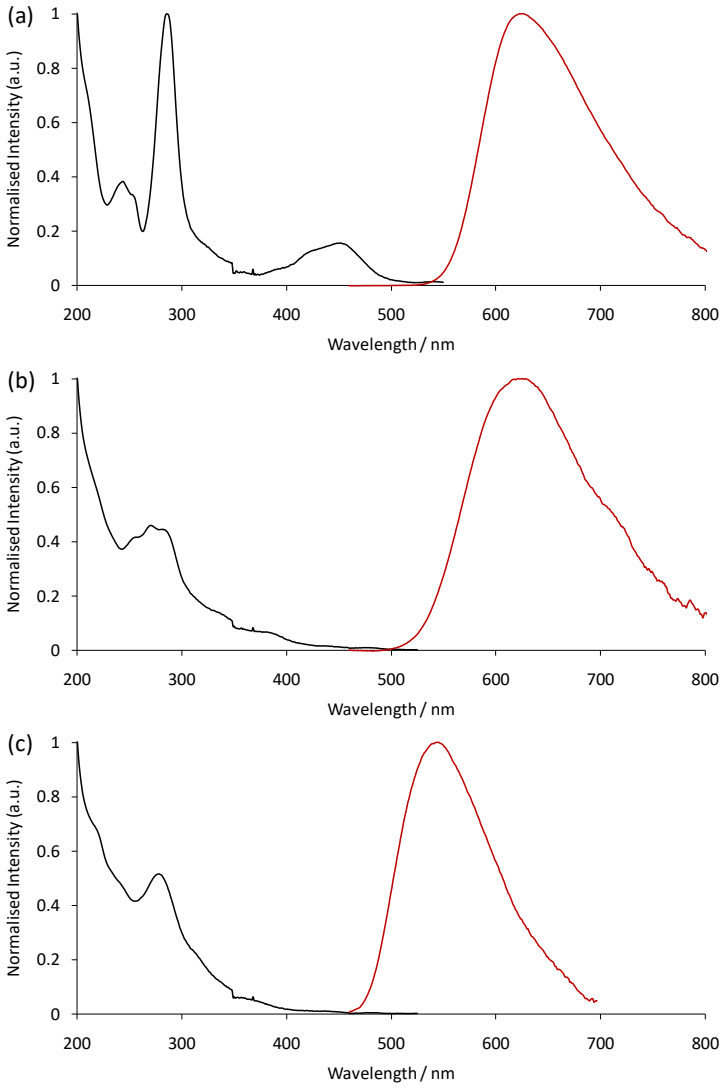


Fig. S1 Absorption spectra (black lines) and photoluminescence emission spectra (red lines) for (a) $[Ru(bipy)_3]^{2+}$, (b) $[(ppy)_2Ir(BPS)]^-$, and (c) $[(df\text{-}ppy)_2Ir(BPS)]^-$. All complexes at a concentration of 1×10^{-5} M in 1:1 acetonitrile:water. Emission spectra were corrected for the wavelength dependence of the detector response and monochromator transmission.

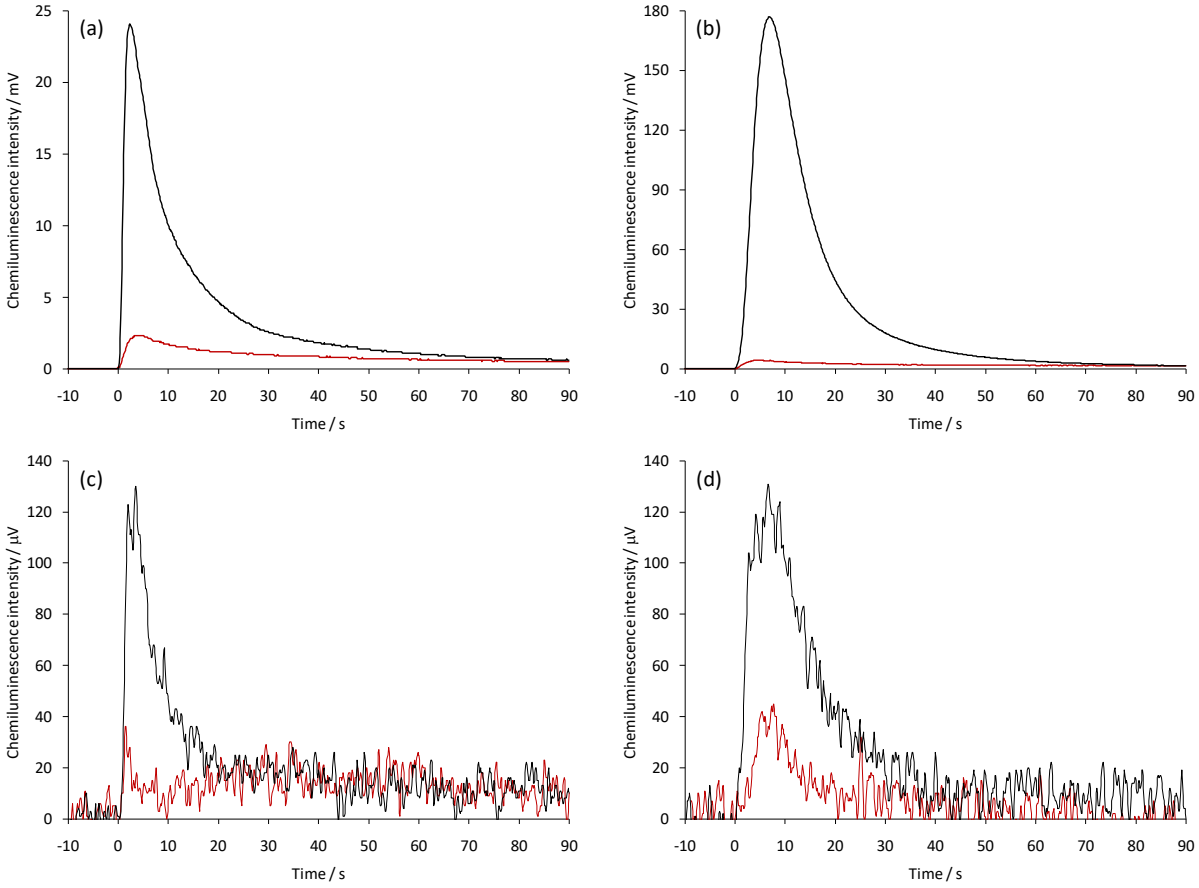
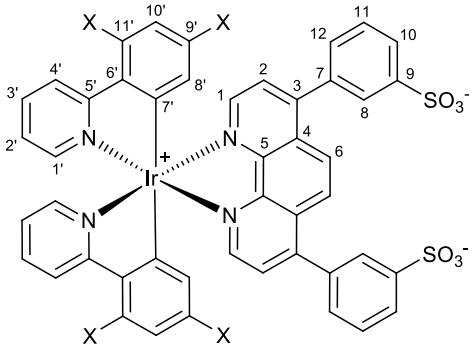


Fig. S2 Intensity versus time profiles for the chemiluminescence reactions of: (a) 1×10^{-3} M $[(df\text{-}ppy)_2Ir(BPS)]^-$ or (b) 1×10^{-3} M $[Ru(bipy)_3]^{2+}$, and 1×10^{-3} M cerium(IV), with (black traces) or without (red traces) 1×10^{-5} M ofloxacin; and (c) 1×10^{-5} M $[(df\text{-}ppy)_2Ir(BPS)]^-$ or (d) 1×10^{-5} M $[Ru(bipy)_3]^{2+}$, and 1×10^{-3} M cerium(IV), with (black traces) or without (red traces) 1×10^{-6} M ofloxacin. The intensity of the red trace in figure S2(b) was multiplied by 5 for comparison purposes. The stopped-flow manifold was constructed as previously described (*Anal. Chem.*, 2010, **82**, 2580-2584). Discrepeancies in the signal/blank ratios obtained in these experiments and the flow-injection analysis procedure described in the paper arise due to differences in the final reactant concentrations, the mode of mixing and the portion of the emission profile measured. Experimental details: the injection loop (70 µL) was filled with reagent and ofloxacin solutions (combined 1:1 (v/v) off-line). The syringe pump was then activated to dispense 120 µL of carrier (1:1 acetonitrile:water) and 120 µL of oxidant (1×10^{-3} M cerium(IV) in 0.05 M H_2SO_4) solutions at a rate of 10 mL min^{-1} per line, which rapidly merged the three reactants in a dual-inlet serpentine flow-cell, where the emission was monitored over time.

Table S1 ^{1}H and ^{13}C NMR chemical shifts (ppm) for $[(ppy)_2Ir(BPS)]^-$ and $[(df\text{-}ppy)_2Ir(BPS)]^-$ in CD_3OD, collected using a Bruker Avance AV400 spectrometer.



	$[(ppy)_2Ir(BPS)]^-$ (X = H)		$[(df\text{-}ppy)_2Ir(BPS)]^-$ (X = F)	
	^{1}H	^{13}C	^{1}H	^{13}C
1′	7.60	150.3	7.69	150.6
2′	6.94	124.6	7.06	125.0
3′	7.82	139.6	7.93	140.8
4′	8.15	121.0	8.39	125.0
5′	-	169.3	-	165.4
6′	-	145.5	-	128.7
7′	-	151.5	-	166.2
8′	6.41	133.0	5.86	115.2
9′	6.89	131.5	-	164.0
10′	7.00	123.9	6.72	101.1
11′	7.84	126.1	-	161.9
1	8.42	152.0	8.47	152.2
2	7.82	128.3	7.95	128.7
3	-	148.7	-	148.4
4	-	130.8	-	130.8
5	-	151.5	-	152.0
6	8.25	127.5	8.25	127.6
7	-	137.2	-	137.0
8	8.06	128.2	8.08	128.3
9	-	147.5	-	147.4
10	8.03	128.3	8.02	128.0
11	7.69	132.7	7.68	130.4
12′	7.66	130.3	7.74	132.7