Electronic Supplementary Information

A Novel Route Towards Water-Soluble Luminescent Iridium(III) Complexes via a Hydroxy-bridged Dinuclear Precursor

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PHOTOPHYSICAL STUDIES: Materials and methods

Spectrofluorimetric grade water was used for the photophysical investigations in solution without further purification. A Perkin Elmer Lambda 900 spectrophotometer was employed to obtain the UV/Vis absorption spectra. Steady-state emission spectra were recorded on a Horiba Jobin Yvon Fluorolog 3 spectrofluorimeter, equipped with a Hamamatsu R-928 photomultiplier tube. The luminescence quantum yields were determined using the optical dilution method[1] using $Ru(bpy)_3Cl_2$ in air-equilibrated water solution as a reference standard ($\Phi = 0.028$).[2] Solutions were degassed by bubbling argon into quartz cells prior to measurements. Time-resolved measurements were performed using the time-correlated single-photon counting (TCSPC) on the Fluorolog-3 apparatus. A NanoLED pulses centered at 379 nm (FWHM 750 ps with 1 MHZ repetition rate) was used as excitation source and fixed directly on the sample chamber at 90° to a single-grating emission monochromator (2.1 nm/mm dispersion; 1200 grooves/mm). Data analysis was performed using the commercially available DAS6 software (HORIBA Jobin Yvon IBH). The quality of the fit was assessed by minimizing the reduced χ^2 function. The experimental uncertainties were 1 nm on the band maximum for the absorption and luminescence spectra, 10% on the molar extinction coefficient, 20% on the emission quantum yields and 5% on the lifetime values.

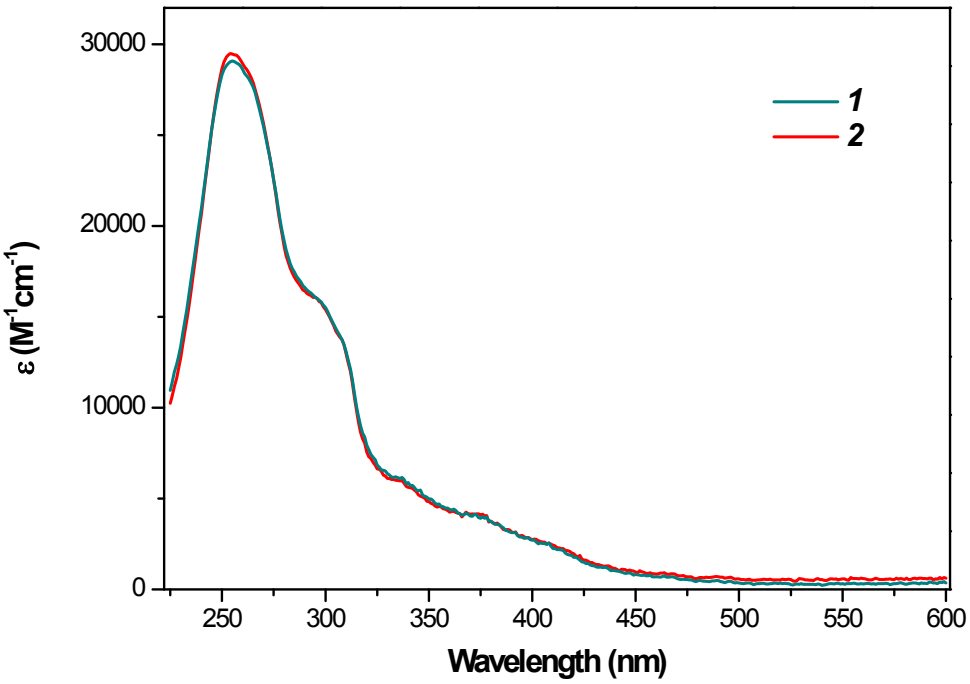

Figure S1. Absorption spectra of complexes **[(*ppy*)$_2$Ir(*bpy*)](EtO)** (**1**) and **[(*ppy*)$_2$Ir(*bpy*)](OH)** (**2**) in deaerated water solution.

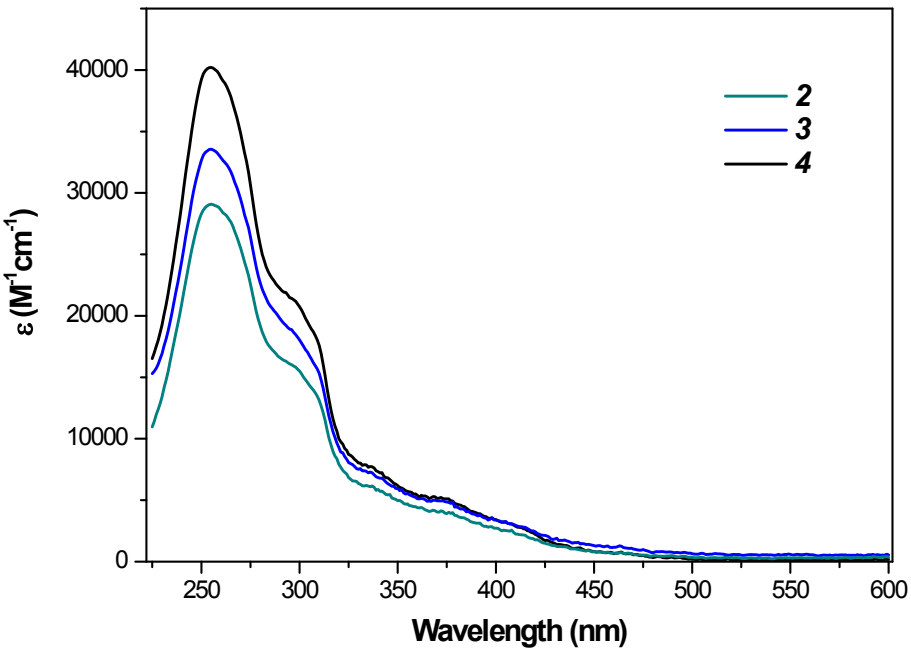

Figure S2. Absorption spectra of complexes **[(*ppy*)$_2$Ir(*bpy*)](OH) (2)**, **[(*ppy*)$_2$Ir(*bpy*)](CH$_3$CH$_2$OCH$_2$CO$_2$) (3)**, **[(*ppy*)$_2$Ir(*bpy*)](CH$_3$OCH$_2$CO$_2$) (4)** in deaerated water solution (C = 5.0 x 10^{-6}M).

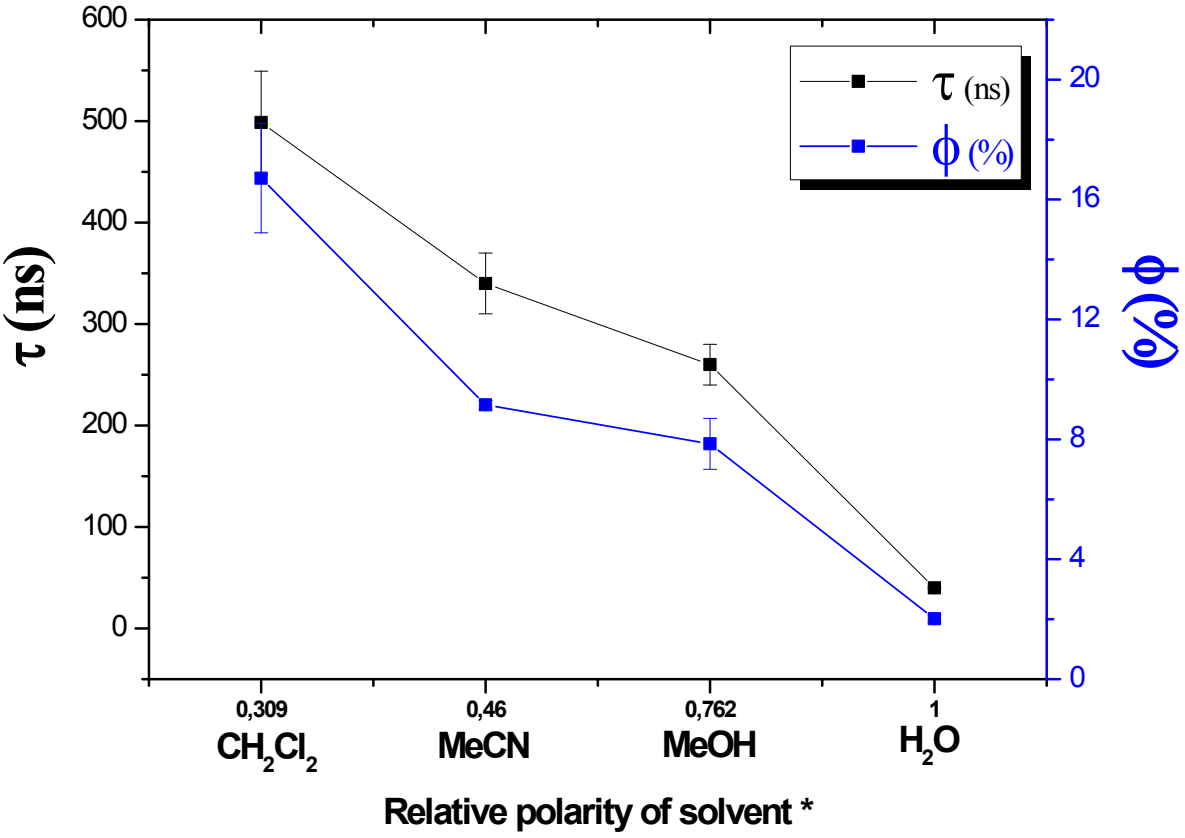

Figure S3. Life time decay (τ, ns) and luminescence quantum yield (ϕ, %) of the exited state of the cation **[(*ppy*)$_2$Ir(*bpy*)]$^+$** with increase of solvent polarity

*Note: Both data from our work and reported literature data[3-5] have been taken into account. The values of relative polarity have been normalised, taken from Christian Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH Publishers, 3rd ed., 2003.

Table S1. Photophysical data of complex **3** in deaerated water solution at various concentrations

	Deaerated water solution		
Complex	Concentration ($mol.L^{-1}$)	Emission, λ_{max}/nm	Lifetime, τ/ns(α/%)
3	**5.0×10^{-6}**	606	40.9 (91.9) 531.0 (8.1)
	1.3×10^{-5}	593	39.4 (81.57), 444.7 (18.43)
	1.3×10^{-4}	592	33.9 (60.72), 77.2 (34.44), 275.0 (4.84)
	1.2×10^{-3}	590	30.2 (47.27), 83.5 (45.85), 277.8 (6.87)
	4×10^{-2} (gel phase)	580	28.5 (17.2), 115.9 (55.0), 336.4 (27.8)

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[2] K. Nakamaru, *Bull. Soc. Chem. Jpn*., 1982, **55**, 2697-2705.

[3] Y. J. Yadav, B. Heinrich, G. De Luca, A. M. Talarico, T. F. Mastropietro, M. Ghedini, B. Donnio and E. I. Szerb, *Adv. Opt. Mater.*, 2013, **1**, 844–854.

[4] K. K.-W. Lo , J. S.-W. Chan , L.-H. Lui , and C.-K. Chung, *Organometallics,* 2004, **23**, 3108-3116

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