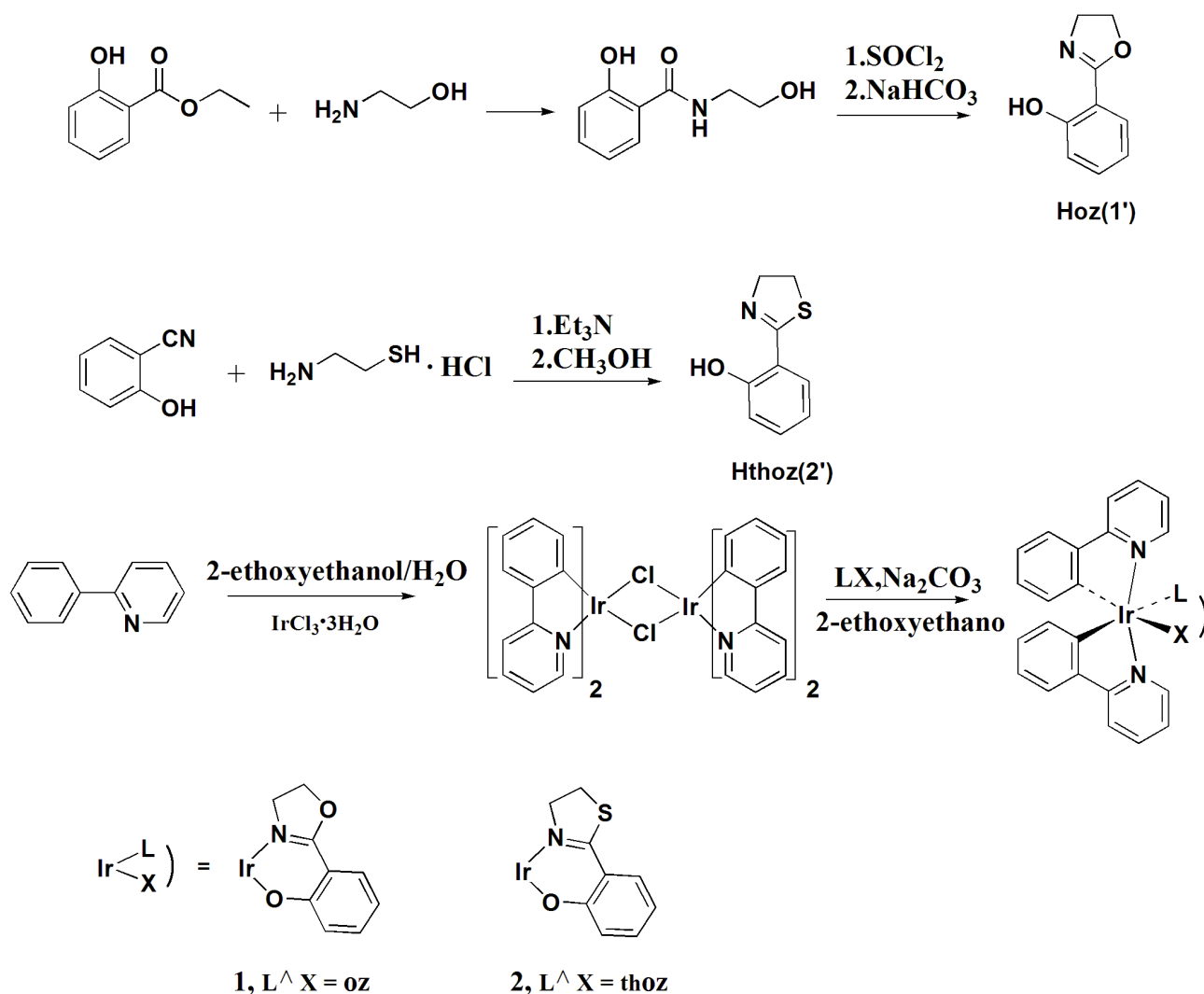


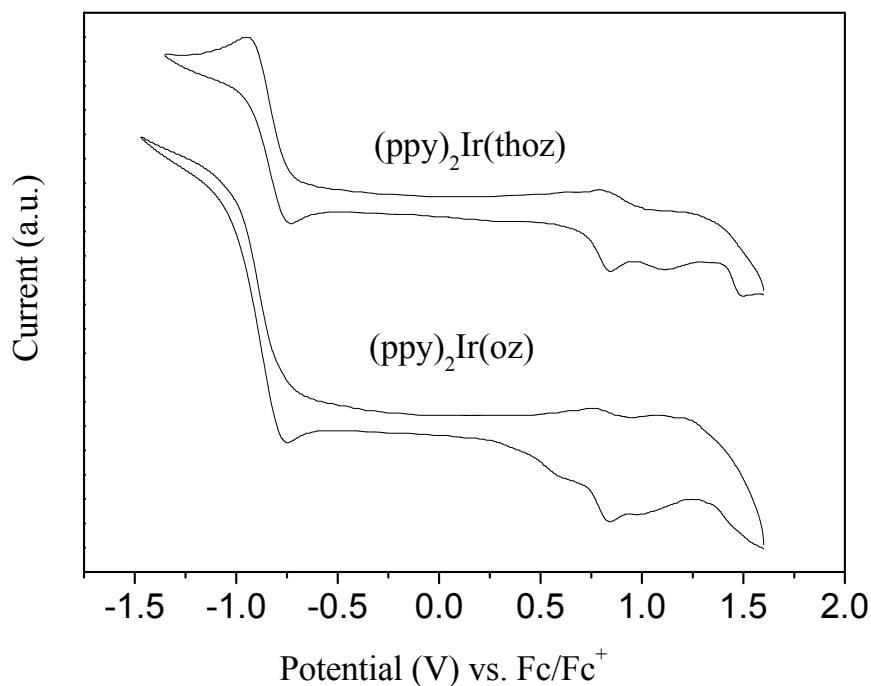
## Supporting Information

### New oxazoline- and thiazoline-containing heteroleptic iridium(III) complexes for highly-efficient phosphorescent organic light-emitting devices (PhOLEDs): colour tuning by varying the electroluminescence bandwidth

Kai Chao, Kuizhan Shao, Tai Peng, Dongxia Zhu\*, Yue Wang, Yu Liu\*, Zhongmin Su, Martin R. Bryce\*

Scheme 1. Synthesis of the Ir complexes (ppy)<sub>2</sub>Ir(oz) (1) and (ppy)<sub>2</sub>Ir(thoz) (2) used in this study.





**Figure S1.** Cyclic voltammograms of complexes  $(ppy)_2Ir(oz)$  (**1**) and  $(ppy)_2Ir(thoz)$  (**2**) in  $CH_3CN$  solutions ( $10^{-3}$  M). Potentials were recorded versus  $Fc/Fc^+$ .

**Table S2.** Calculated energy levels of selected molecular orbitals and the corresponding orbital compositions of complex **1**.

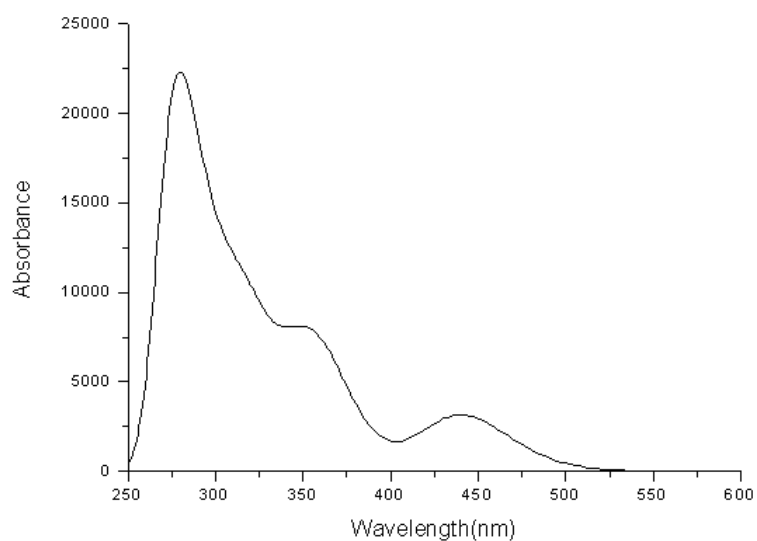
Complex 1	Energies (eV)	Composition
HOMO-5	-6.00	$d(Ir) + \pi(ppy)_{ab}$
HOMO-4	-5.75	$d(Ir) + \pi(ppy)_{ab}$
HOMO-3	-5.68	$d(Ir) + \pi(ppy)_{ab}$
HOMO-2	-5.50	$d(Ir) + \pi(c)$
HOMO-1	-4.77	$d(Ir) + \pi(ppy)_b$
HOMO	-4.53	$d(Ir) + \pi(c)$
Energy gap	3.22	
LUMO	-1.31	$\pi^*(ppy)_a$
LUMO+1	-1.05	$\pi^*(ppy)_b$
LUMO+2	-0.77	$\pi^*(ppy)_{ab}$
LUMO+3	-0.66	$\pi^*(ppy)_{ab}$
LUMO+4	-0.40	$\pi^*(c)$
LUMO+5	0.68	$\pi^*(ppy)_a$

a, b = 2-phenylpyridine; c = 2-(2'-Hydroxyphenyl)-2-oxazoline

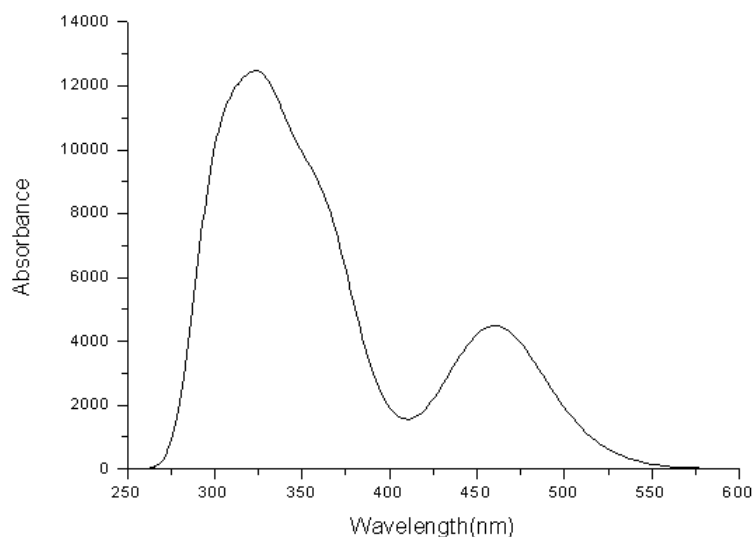
**Table S2.** Calculated energy levels of selected molecular orbitals and the corresponding orbital compositions of complex **2**.

Complex <b>2</b>	Energies (eV)	Composition
HOMO-5	-5.83	$\pi(c)$
HOMO-4	-5.58	$d(\text{Ir}) + \pi(\text{ppy})_b$
HOMO-3	-5.43	$d(\text{Ir}) + \pi(\text{ppy})_{ab}$
HOMO-2	-5.31	$\pi(\text{ppy})_{ab}$
HOMO-1	-5.15	$d(\text{Ir}) + \pi(\text{ppy})_{ab}$
HOMO	-4.41	$\pi(c)$
Energy gap	2.83	
LUMO	-1.58	$\pi^*(\text{ppy})_a$
LUMO+1	-1.37	$\pi^*(\text{ppy})_b$
LUMO+2	-1.32	$\pi^*(c)$
LUMO+3	-0.97	$\pi^*(\text{ppy})_{ab}$
LUMO+4	-0.70	$\pi^*(\text{ppy})_{ab}$
LUMO+5	-0.21	$\pi^*(c)$

a, b = 2-phenylpyridine; c = 2-(2'-Hydroxyphenyl)-2-thiazoline.



**Figure S2.** Simulated absorption spectra of complex **1**.



**Figure S3.** Simulated absorption spectra of complex **2**.

### Theoretical Calculations.

The calculations on the ground and excited electronic states of the iridium complexes **1** and **2** were performed by using density functional theory (DFT) and TDDFT at the B3LYP level.<sup>1</sup> The “Double- $\xi$ ” quality basis sets were employed for C, H, N atoms (6-31G\*) and the Ir atom (LANL2DZ). The effective core potential (ECP) replaces the inner core electrons of iridium leaving the outer core  $(5s)^2(5p)^6$  electrons and the  $(5d)^6$  valence electrons of Ir(III). In addition, the geometries of the singlet ground state ( $S_0$ ) of these complexes were fully optimized with  $C_1$  symmetry constraints. All calculations reported here were carried out with the Gaussian 09 software package using a spin-restricted formalism.<sup>2</sup>

### References for the Supporting Information

- 1 a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648. b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.
- 2 Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.