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# **ACCEPTED MANUSCRIPT**

#### Redox cycling of iridium(III) complexes gives versatile materials for

#### photonics applications

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#### Abstract

The cyclometallated iridium(III)  $[Me_4N][Ir(ppy)_2(cat)]$ complex (Hppy = 2-phenylpyridine;  $H_2$ cat = benzene-1,2-diol) has been prepared under inert atmosphere and structurally characterized by single crystal X-ray diffraction. Under ambient conditions, the fully reduced complex (as formulated) undergoes rapid one-electron oxidation both in solution and in the solid state to a species containing a semiquinone ligand. The resultant neutral complex  $[Ir(ppy)_2(sq)]$  (sq = *o*-semiquinone) was also prepared by exposing the reaction mixture to  $O_2$  during the course of the reaction. Electron paramagnetic resonance (EPR) spectroscopy confirms the diamagnetic nature of the complex  $[Me_4N][Ir(ppy)_2(cat)]$  and indicates that the unpaired electron in  $[Ir(ppy)_2(sq)]$  resides primarily on the sq ligand. The photophysical, electrochemical, and spectroelectrochemical properties of  $[Ir(ppy)_2(sq)]$  were investigated and reveal the changes in absorption as the complex is converted into the catecholate and quinone forms.

Keywords: iridium; semiquinone; spectroelectrochemistry; X-ray structure

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