

Accepted Manuscript

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PII: S0277-5387(17)30796-9
DOI: <https://doi.org/10.1016/j.poly.2017.12.014>
Reference: POLY 12970

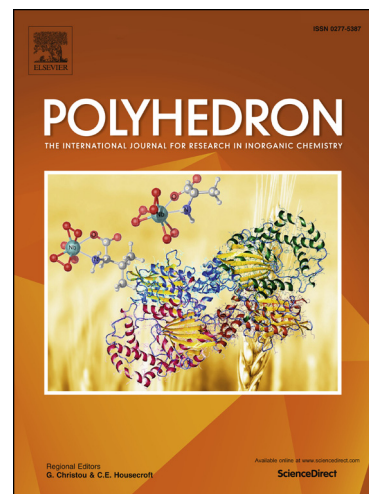
To appear in: *Polyhedron*

Received Date: 16 November 2017

Accepted Date: 12 December 2017

Please cite this article as: W. Wei, S.A.M. Lima, P.I. Djurovich, A. Bossi, M.T. Whited, M.E. Thompson, Synthesis and Characterization of Phosphorescent Isomeric Iridium Complexes with a Rigid Cyclometalating Ligand, *Polyhedron* (2017), doi: <https://doi.org/10.1016/j.poly.2017.12.014>

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Synthesis and Characterization of Phosphorescent Isomeric Iridium Complexes with a Rigid Cyclometalating Ligand

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Abstract

The synthesis, structures and photophysical properties of three phosphorescent isomeric heteroleptic iridium complexes are reported. The complexes are bis-cyclometalated with a rigid 9-*tert*-butyl-pyrazolo[1,5-*f*]phenanthridine (tpzp) ligand. The isomers (**I1**, **I2** and **I3**) of the heteroleptic complex Ir(tpzp)₂pic (pic = picolate) were isolated from reactions and characterized by 2D NMR experiments and X-ray crystallography. The tpszp ligands in isomer **I1** have a trans-N,N configuration, whereas the tpszp ligands in isomers **I2** and **I3** both have a cis-N,N configuration, with the three coordinated nitrogens being facial in **I2** and meridional in **I3**. The **I1** complex was found to isomerize during the sublimation under high vacuum (0.5×10^{-6} torr) at 300 °C, giving a ratio of **I1**:**I2**:**I3** = 3:1:6. Reduction potentials and DFT calculations of the Ir(tpzp)₂pic isomers indicate that the LUMO for these heteroleptic complexes is localized on the picolate moiety. The Ir(tpzp)₂pic isomers all display broad, featureless emission at room temperature ($\lambda_{em} \sim 530$ nm) consistent with emission from a triplet metal-ligand to ligand (Ir-tpzp to picinate) charge transfer (³MLLCT) state. Broad ³MLLCT emission ($\lambda_{em} \sim 520$ nm) is still observed from isomers **I2** and **I3** in rigid media at 77K. However, under the same conditions structured blue phosphorescence ($\lambda_{em} = 452$ nm) is observed from isomer **I1**, consistent with emission from a metal perturbed ³LC state on the tpszp ligand.

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