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ACCEPTED MANUSCRIPT

Luminescent Ir(III) complexes bearing benzothiazole or benzoxazole-based

pincer ligand

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ABSTRACT

Ir complexes bearing pincer ligands are expected to be efficient phosphorescent materials. This work

investigated the solid-state structures and photophysical properties of Ir(III) complexes that contain

different **NCN** pincer ligands (NCN 1,3-bis(2-benzothiazolyl)benzene,

1,3-bis(2-benzimidazoyl)benzene 1,3-bis(2-benzoxazoyl)benzene, derivatives), bidentate or

cyclometalating NC ligands (NC = 2-phenylpyridine or 2-phenylbenzothiazole), and anionic

ancillary ligands. The structure of the NCN pincer ligands is a dominant factor for determining the

emission wavelength, rather than the bidentate NC and ancillary ligands. The organic light emitting

diodes (OLEDs) with an Ir(III) complex show electroluminescence with 14% external quantum

efficiency at 1 mAcm⁻². Modification of the device structure improved the efficiency at the high

current density region.

Keywords: Pincer complex; Photoluminescence; Electroluminescence; Ir(III) complex; OLEDs.

1. Introduction

Cyclometalating tridentate ligands (so-called pincer ligands) provide high stability, unique catalytic

activity, and efficient luminescent properties to transition-metal complexes [1–5]. Nitrogen-based

NCN and CNN pincer ligands have been used to develop Pt complexes showing highly efficient

phosphorescence [2,6]. Williams and Haga independently developed Ir complexes bearing NCN

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