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Phosphorescent Iridium(III) Cyclometalates Supported by 2,2',4,4'-Biphenyl-1,1'-diylpyridine Ligand

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Abstract

Novel Ir(III) cyclometalates, $(\text{dnpy})_2\text{Ir}(\text{acac})$ (**2**) and $\text{fac-}(\text{dnpy})_3\text{Ir}$ (**3**), supported by 2,2'-bis(4-pyridyl)dihydronaphthalene (**1**) were synthesized and characterized. X-ray diffraction study on **3** revealed facial arrangement of three dnpy ligands around the Ir center. Photoluminescence (PL) spectra of **2** exhibited orange emission centered at 590 nm, which is almost similar to that

observed for 2-*thiophen-2-yl*-1-*naphthyl*pyridine complex, (napy)₂Ir(acac) (**III**). In contrast, compound **3** displayed blue-shifted, yellow emission at 550 nm. Tris-*thiophen-2-yl*-1-*naphthyl*pyridine complex **3** showed higher quantum efficiencies than **2** in both the solution and film states. Cyclic voltammetry measurements indicated that replacing naphthyl with 1,2-dihydronaphthyl ring raises both the metal-centered HOMO level and ligand-centered LUMO level in **2** and **3**. It was suggested that 1,2-dihydronaphthyl ring has a stronger electron-donating effect than naphthyl ring, while the π^* orbital of dnpy ligand is less stabilized due to partial conjugation of the dihydronaphthyl ring.

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```