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Photophysical, electrochemical properties and DFT calculations of highly phosphorescent homoleptic cyclometalated iridium (III) complexes based on 4-fluorophenylvinyl- and 4-methoxy phenylvinyl-quinoline derivatives

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This study reports the synthesis and comparative investigation of the substituent effects of new series of highly luminescent homoleptic tris-cyclometalated iridium (III) complexes of the type [Ir(N^C)$_3$]. These are based on two ligand type derivatives comprising of 4-fluorophenylvinylquinolines and 4-methoxy phenylvinylquinolines with electron-donating and/or electron-withdrawing groups as aryl-substituents at 2-position. The ligands and complexes were structurally characterized by FT-IR, UV-Vis, NMR, photoluminescence and cyclic voltammetry. In addition, 2-aryl-4-(4-fluorophenylvinyl) quinoline and its corresponding complex were also studied using density functional theory method. The photoluminescent properties of the ligands and complexes showed high fluorescent intensities and quantum yields in solvents of different polarities. The photoluminescence spectra of the complexes in solid film showed very high emission intensity analogous to individual ligands and complexes when in solutions at common wavelength maximum (λ_{em}=698 nm). The reported Ir (III) complexes may find use as potential emissive dopants, fluorescent marker, sensors, electronics, electron transport materials for OLEDs application and drug discovery.

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