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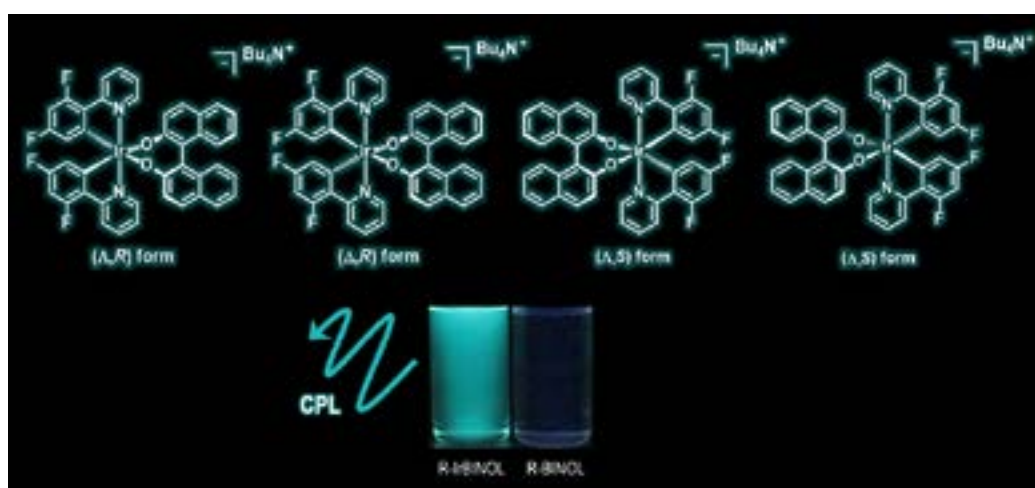
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Circularly polarized phosphorescence from cyclometalated Ir(III) complexes having axially chiral ligands

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Circularly polarized luminescence (CPL) refers to the differential emission of right- and left-handed circularly polarized light. CPL finds various photonic utility, including 3D electroluminescence displays, optical storage, spintronics, enantioselective biological probes, security tags, lasers, and asymmetric photosynthesis. In particular, organic light-emitting devices based on CPL emitters are considered as promising alternatives to the existing 3D displays, because they can significantly improve brightness. CPL is typically observed in luminescence systems having molecular and environmental chiral components. The most representative molecular class showing CPL are lanthanides having chiral ligands. Strong CPL properties are also found in nematic liquid crystals doped with achiral fluorophore. However, despite the significant effort, many of molecular CPL materials suffer from small $|g_{\text{PL}}|$ values ($<10^{-2}$) and low photoluminescence quantum yields. As our initial step toward developing CPL molecules, we designed and synthesized bis-cyclometalated iridium (III) complexes having dual chiral components. The complexes possessed a N, N trans disposition between two C, N² cyclometalating ligands (dfppy) which generated Ir-centered Δ and Λ helicity. The octahedral geometry of the complexes was completed by coordination of a di-anionic form of either (*R*)-BINOL or (*S*)-BINOL (BINOL=1,1'-bi(2-naphthol)) having axial chirality. Therefore, formally four isomers could be created: (Δ ,*R*), (Λ ,*R*), (Δ ,*S*), and (Λ ,*S*). Quantum chemical calculations based on time-dependent density functional theory at the level of CAM-B3LYP predicted chiroptical properties. The negatively charged complexes were easily prepared through base-mediated substitution of chloride in a μ -chloride Ir(III) dimer precursor, followed by cation metathesis with NH_4PF_6 . Structural characterization with employing ^1H NMR spectroscopy revealed the presence of one set of peaks, which indicated selective formation of either a Δ form or a Λ form. Electronic circular dichroism spectra of the complexes contained a cotton effect in the metal-to-ligand charge-transfer (MLCT) transition regions. Photophysical properties, including photoluminescence quantum yields, were determined, which promises potential applications into 3D OLEDs showing CPL.



Biography

Gyurim Park is pursuing her Graduation at Ewha Womans University, Korea. Her recent research interests include "Sensors for bio-imaging, photo-redox catalysis, and circularly polarized luminescence". She has strong knowledge in research fields, including molecular photo-physics, organic chemistry, and coordination chemistry. She is experienced with a wide range of research methods, such as organic and organometallic synthesis, spectroscopic techniques, and electrochemistry.

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