Phenanthroline-pyridylidene Ligand Promotes Near Infrared Luminescence up to 840 nm in Ru(II) and Os(II) Complexes

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Abstract

Near-infrared (NIR) luminescence is receiving an increasing deal of attention from various research fields because of its multiple uses such as light communication, night vision, photodynamic therapy and photobiomodulation therapy, just to name a few.[1] Among the most promising materials, transition metal complexes (TMC) possess a great interest because of their thermal and photo-stability, and the facile ligand structure tunability. However, achieving NIR luminescence is extremely challenging since the efficiency of low-energy emissions is inherently very low (energy gap low)[2] and thus, a judicious ligand design plays a crucial role in obtaining such properties. For many TM ions, strong σ-donor units such as N-heterocyclic carbenes (NHC) are typically required to enhance their emission properties upon destabilization of nonradiative metal-centered (MC) states.[3] A poorly investigated class of such NHC ligands are pyridylidenes, which are non-classical NHC carbenes possessing a better σ-donor and π-acceptor character compared to classical imidazolydenes.[4]

In this presentation, I will speak about the design of an unprecedent C^N^N ligand featuring a 2-pyridylidene, which possesses strong σ-donor properties,[4] and 1,10-phenantroline, which is a good π-acceptor and light harvesting moiety,[5] and the corresponding homoleptic ruthenium(II) and osmium(II) complexes. Molecular structures of both complexes have been confirmed by single-crystal X-ray diffraction, and their optical and electrochemical properties investigated. While almost identical panchromatic absorptions are obtained, slightly different NIR emissions are observed, with the Os(II) complex remarkably peaking 840 nm at the crystalline state. Computational data highlighted the important role played by the spin-orbit coupling (SOC) perturbation in modulating the optical properties into the NIR.

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