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PHOSPHORESCENT CYCLOMETALATED Ir(III) COMPLEXES WITH ACETYLIDE AND ISOCYANIDE LIGANDS

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Over the last years, numerous studies have been carried out on d^6 phosphors, such as Ru^{II} or Ir^{III} and d^8 Pt^{II} compounds, due to their potential application in different optoelectronic fields. In particular, cyclometalated Ir(III) complexes display very high photophysical performances due their good photostability, high photoluminescent quantum yields (Φ_{PL}), facile color tunability and long-lived triplet excited states. Furthermore, this class of complexes has been applied to a variety of photonic applications including oxygen sensing, biological labeling, photosensitization, and emissive materials in organic light emitting diodes (OLEDs)¹. These complexes usually display mixed metal-to-ligand charge transfer/ $^3MLCT/^3LC$ excited states with some ligand-to-ligand charge transfer (3LLCT) character depending on the auxiliary ligands. Strong field ligand coordination is desirable because it rises the energy of the nonradiative dd metal centered excited states causing enhancement of the quantum yields.

Following the interest of the group in designing photoluminescent cyclometalated systems based on strong field ligands such as CN^- , isocyanide or acetylide,^{2,3} here we present the synthesis and optical properties of a new family of neutral cyclometalated iridium(III) heteroleptic complexes $[Ir(C^*N)_2(CNXyl)(C\equiv CR)]$ (C^*N = difluorophenylpyridinate (dffpy) **1**, 2-phenylbenzothiazolate (pbt) **2**, 2-phenylquinolate (pq) **3**; R = *p*-tolyl **a**, $C_6H_2(OMe)_3$ **b**, pyrene **c**). These complexes are luminescent in different media, originating from $^3MLCT/^3LLCT/^3LC$ states, as supported by TD-DFT studies.

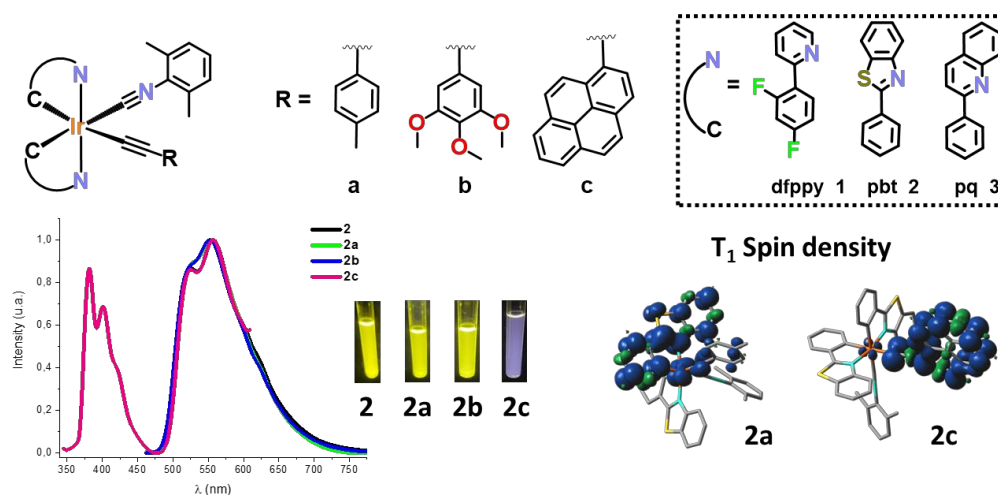


Figure 1: Synthesized cyclometalated Ir(III) complexes with different acetylide ligands.

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