

# **A Family of Ir(III) Complexes with High Nonlinear Optical Response and Their Potential Use in Light-Emitting Devices**

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## **Abstract**

We synthesized a new family of Ir III complexes  $[\text{Ir}(\text{R}_1\text{-ppy})_2(\text{R}_2\text{-ppl})](\text{PF}_6)$ , where  $\text{R}_1\text{-ppy}$  = 2-phenylpyridine (ppy) or 2,4-difluorophenylpyridine (F2-ppy) and  $\text{R}_2\text{-ppl}$  = pyrazino[2,3-f][1,10]phenanthroline (ppl) or 2,3-diethoxycarbonylpyrazino [2,3-f][1,10]phenanthroline (deeppl). The complexes were experimentally and theoretically characterized, noting the importance of the  $\text{R}_1$  substituent on the modulation of HOMO level and its impact on the electronic properties. These compounds exhibit high second-order nonlinear optics (NLO) activity, especially, those with F2-ppy ligands; this substituent modulates the charge transfer, optimizing the NLO response. The compounds also show blueshifted emissions, both in solution and as a solid film, which is desirable for use in light-emitting devices. This is the first use of the synthesized complexes for application in the two tasks.