Theoretical Exploration on Phosphorescent Pt(II) Complexes with 2,2'-bipyridine Ligand: Influence of Isotope Effect and Ligand Modification on OLED Quantum Yield

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Abstract

In order to explore the influence of isotope effect and ligand modification on the quantum yield of OLED, three classes Pt(II) complexes with 2,2'-bipyridine ligand have been investigated by using density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The explored Pt(II) complexes, class 1 included Pt(RC[?]CBpyC[?]CR)(C[?]CBpy)2, (R = trimethylsilyl,1a or H, 1b, C[?]CBpyC[?]C = 5,5-bis(ethynyl)-2,2-bipyridine, C[?]CBpy corresponds to bipyridineacetylene) and Pt(Bpy)(C[?]CBpy)2 (Bpy = bipyridine, 1c); class 2, Pt(Bpy)(C[?]CPy)2 (C[?]CPy = pyridineacetylene, 2a) , Pt(Bpy)(C[?]CPh)2 (C[?]CPh =phenylethynyl, 2b), Pt(dbBpy)(C[?]CPh)2(dbBpy = 4,4'-di-tert-butyl-2,2'-bipyridine, 2c); and class 3, Pt(Bpy)(Tda) (Tda = tolan-2,2'-diacetylide, 3a), Pt(dbBpy)(Tda) (3b), Pt(3,3',4,4'-OH-Bpy)(Tda) (3c). The calculation results reveal that the heavy isotope effect effectively reduces the overall vibration frequency of these complexes, and in turn decreases the non-radiative decay rate ϰnr, which lead to the promotion of phosphorescent quantum yield em. Theoretical studies also reveal the influence of ligand modification on the phosphorescence quantum yields of OLED, and a new Pt(II) complex 3c was designed based on the theoretical study.

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