

Theoretical study on photophysical properties of cyclometalated cationic iridium(III) complexes containing dipyrido[3,2-*f*:2',3'-*h*]quinoxaline ligand

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ABSTRACT

We report a theoretical analysis of a family of cyclometalated cationic iridium(III) complexes: $[\text{Ir}(\text{C}\hat{\text{N}})_2(\text{N}\hat{\text{N}})]^+$ [$\text{N}\hat{\text{N}}$ = dipyrido[3,2-*f*:2',3'-*h*]quinoxaline(dpq), $\text{HC}\hat{\text{N}}$ = 1-phenylpyrazole(Hppz) (**1**); $\text{HC}\hat{\text{N}}$ = 7,8-benzoquinoline(Hbzq) (**2**); $\text{HC}\hat{\text{N}}$ = 2-phenylquinoline(Hpq) (**3**); $\text{HC}\hat{\text{N}}$ = 1-(2,4-difluorophenyl)pyrazole(Hdfppz) (**4**), $\text{HC}\hat{\text{N}}$ = 1-(2,4-dimethylphenyl)pyrazole(Hdmppz) (**5**), $\text{HC}\hat{\text{N}}$ = 1-(2,4-difluorophenyl)-1,2,4-triazole(Hdfptz) (**6**)] by using density functional theory (DFT) method to investigate their optoelectronic properties and understand the phosphorescent efficiency mechanism. Complexes **1–3** exhibit green to yellow luminescence. The different quantum efficiencies of **1–3** in methanol (MeOH), acetonitrile (CH_3CN), and dichloromethane (CH_2Cl_2) solvents have been explained by calculated results. Complexes **4** and **5** show different trend in the absorption and emission spectra comparing with **1** due to the added different substituent on the phenyl of ppzH. The emission wavelength of the assumed complex **6** bearing the triazole in $\text{C}\hat{\text{N}}$ ligand is blue-shifted to the blue region. We suggest complex **6** might be a potential candidate as blue-emitting material.

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1. Introduction

Phosphorescent iridium(III) complexes have been received considerable attention over the past decades [1,2]. These iridium(III) complexes are promising triplet dopant emitters in organic light-emitting diodes (OLED) [3–5] because of their high thermal stability, short lifetime in the excited states, and high quantum efficiency. The high quantum efficiency can be attributed to the strong spin–orbit coupling (SOC) induced by iridium(III), which makes singlet–triplet excited states sufficiently mixed to create the possibility of full utilization of both the singlet and triplet excitons, and facilitates intersystem crossing (ISC). Thus, many efforts have been devoted toward the design and synthesis of new phosphorescent iridium(III) complexes [6–9].

Among phosphorescent iridium(III) complexes, cyclometalated iridium(III) complexes are the most successful phosphorescent emitters due to a number of important features, including solution processability, fairly good stability, good color tunability of emission energy (spanning the visible spectra) [2,10], and high external quantum efficiency. These cyclometalated iridium(III) complexes can be divided into two groups: neutral and ionic iridium(III) complexes. Nowadays, numerous studies revealed that neutral

iridium(III) complexes have remarkable potentials as triplet emitters for OLED. In addition, many researchers have directed their attention to cationic iridium(III) complexes because of their rich photophysical properties, ionic character, and good solubility in polar solvents [11–13]. Cationic cyclometalated iridium(III) complexes are also good candidates as the light-emitting layer for light-emitting electrochemical cells because of high ligand-field splitting energy of the trivalent iridium ion [14].

In comparison with the experimental study on cationic iridium(III) complexes, theoretical study is still limited, especially on deep understanding of phosphorescent emission. Recently, Lam et al. [15] have reported a series of luminescent cyclometalated iridium(III) complexes $[\text{Ir}(\text{C}\hat{\text{N}})_2(\text{N}\hat{\text{N}})]^+$ ($\text{N}\hat{\text{N}}$ = dipyrido[3,2-*f*:2',3'-*h*]quinoxaline(dpq), $\text{HC}\hat{\text{N}}$ = 1-phenylpyrazole(Hppz) (**1**); $\text{HC}\hat{\text{N}}$ = 7,8-benzoquinoline(Hbzq) (**2**); $\text{HC}\hat{\text{N}}$ = 2-phenylquinoline(Hpq) (**3**), Fig. 1a). They explored the photophysical and electrochemical properties of these complexes in different organic solvents. The results showed that complexes with dpq ligand are the first examples of luminescent iridium(III) polypyridines that have nuclear uptake and nuclear staining in live cells. The three complexes displayed intense and long-lived green to orange triplet metal-to-ligand charge-transfer ($^3\text{MLCT}$) [$d\pi(\text{Ir}) \rightarrow \pi^*(\text{dpq})$] emission in aprotic organic solvents at room temperature and in low temperature glass. Interestingly, complexes **1–3** exhibited different emissions and quantum efficiencies in different solvents. In order to shed light on the mechanism of different emissions and quantum

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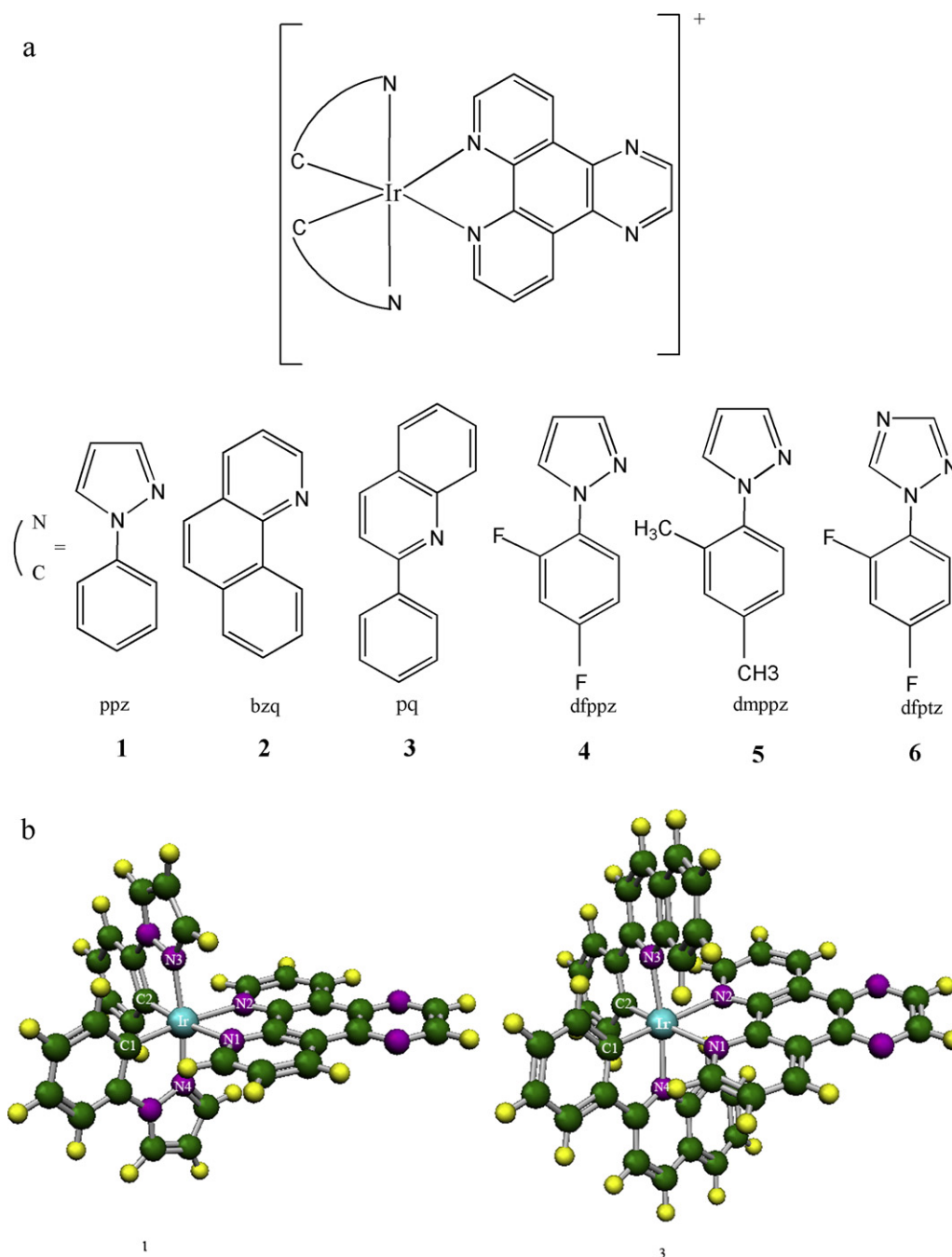


Fig. 1. (a) The schematic structures of complexes 1–6. (b) The optimized geometrical structure of complexes 1 and 3.

efficiencies in different organic solvents, we performed quantum chemistry calculations on the three complexes **1**, **2**, and **3**.

To the best of our knowledge, obtaining highly efficient blue phosphorescence materials at room temperature remains a challenge. From the experimental study, we noted that complex **1** exhibits strong phosphorescence and shortest emission wavelength. Based on the structure of complex **1**, we designed another three complexes, i.e., $\text{N}\hat{\text{N}}$ = dipyrdo[3,2-*f*:2',3'-*h*] quinoxaline(dpq), $\text{HC}\hat{\text{N}}$ = 1-(2,4-difluorophenyl) pyrazole(Hdfppz) (**4**), $\text{HC}\hat{\text{N}}$ = 1-(2,4-dimethylphenyl) pyrazole(Hdmppz) (**5**), $\text{HC}\hat{\text{N}}$ = 1-(2,4-difluorophenyl)-1,2,4-triazole(Hdfptz) (**6**) (Fig. 1a), aiming to give theoretical suggestions for designing new highly efficient materials. With an attempt to investigate the influence of the substituent effect on properties, the electron-withdrawing groups –F

and electron-donating groups – CH_3 were added on phenyl of $\text{C}\hat{\text{N}}$ ligands of **1** to give **4** and **5**, respectively. We expect that complex **6**, bearing the triazole derivative ligands ($\text{C}\hat{\text{N}}$), could exhibit blue-shifted emission wavelength and to be a blue emitter.

2. Computational methods

The calculations were performed with Gaussian 03 software package [16]. The ground state for each molecule was optimized by the DFT method [17] with the hybrid-type Perdew–Burke–Ernzerhof exchange correlation functional (PBE0) [18–20]. This approach has been shown to be particularly efficient and accurate for the calculation of transition metal complexes and

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