Scientific paper

Synthesis and Characterization of High-Efficiency Red Phosphorescent Iridium(III) Complexes with 1-(4-(Trifluoromethyl)phenyl)isoquinoline Ligand

Zheng Zhao,1 Xiao-Han Yang,1 Zi-Wen Tao,1 Han-Ru Xu,1 Kai Liu,1 Guang-Ying Chen,2 Zheng-Rong Mo,2 Shui-Xing Wu,1 Zhi-Gang Niu,1,2 and Gao-Nan Li1,*

1 Key Laboratory of Electrochemical Energy Storage and Energy Conversion of Hainan Province, College of Chemistry and Chemical Engineering, Hainan Normal University, Haikou 571158, China
2 Key Laboratory of Tropical Medicinal Plant Chemistry of Ministry of Education, Hainan Normal University, Haikou 571158, China
* Corresponding author: E-mail: ligaonan2008@163.com (G.-N. Li)
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Abstract
Two new tfmpiq-based bis-cyclometalated iridium(III) complexes, [(tfmpiq)2Ir(idzppo)] (2a) and [(tfmpiq)2Ir(idzppo)] (2b) (where tfmpiq = 1-(4-(trifluoromethyl)phenyl)isoquinoline, imdzppo = 2-(imidazo[1,2-a]pyridin-2-yl)phenol, idzpo = 2-(2H-indazol-2-yl)phenol), have been synthesized and fully characterized. The single crystal structure of 2b has been determined. The relationship between the structures and photophysical properties of both complexes are considered, and the DFT calculations have been used to further support the deduction. These Ir(III) complexes emit red light with quantum yields of 39.9–51.9% in degassed CH2Cl2 solution at room temperature. Also, their emission originates from a hybrid 3MLCT/3LLCT/3LC excited state. All these results show that iridium(III) complexes 2a-2b are suitable for red-phosphorescent materials in OLEDs.

Keywords: Iridium(III) complex; 1-(4-(Trifluoromethyl)phenyl)isoquinoline; Red phosphorescence; DFT calculation

1. Introduction

Organic light-emitting diodes (OLEDs) have attracted great attention on the development of modern optoelectronic technologies such as full-color displays and solid-state lighting sources.1-3 Particularly, cyclometalated iridium(III) complexes ([Ir(C^N)3] or [(C^N)2Ir(LX)]) are the most valuable emitting materials in the fabrication of OLEDs, owing to their relatively short excited-state lifetime, high phosphorescence efficiency and excellent color-tuning capability.4,5 As compared to other colors, red electrophosphorescent emitting phosphors are difficult to maintain high device efficiency, since their quantum efficiencies tend to decrease as the emission wavelength increases in accordance with the energy gap law.6-8 Thus, the design and syntheses of highly efficient red-emitting iridium complexes remain a challenge.

1-Phenylisoquinoline (piq) is one typical ligand framework to construct red iridium complexes. A large number of piq-based Ir(III) complexes have been reported during the past decade.9-13 Among these examples, iridium complexes of fluorinated phenylisoquinoline show strong electroluminescence brightness and efficiency. This is because the fluorine groups could not only modify the electronic properties but also decrease the rate of nonradiative deactivation and improve phosphorescence quantum yields.14 Therefore, in 2006, K.-H. Fang and co-workers first reported Ir(tfmpiq)2acac (acac = acetylacetonate) complex, which emitted red phosphorescence with a wavelength maximum at 631 nm, and the quantum yield was up to 31%.15 Subsequently, in 2014, S. Zhang et al. developed red Ir(tfmpiq)2tpip complex (tpip = tetraphenylimidodiphosphinate), which achieved emission at 622 nm with quantum efficiency of 15%.16 In the same
year, we employed 2,2-bipyridine as the ancillary ligand to synthesize Ir(tfmpiq)_2bipy complex, which exhibited a maximum emission peak at 594 nm with quantum yield of 14%. Recently, in 2016, S. Aoki group reported tris-cyclometalated iridium complex, Ir(tfpiq)_3, which displayed red phosphorescence at 600 nm with quantum yield of 25%.

However, these conventional ancillary ligands used in tfmpiq-based iridium (III) complexes didn’t show significantly red-shift with high quantum efficiencies. Thus, we wanted to attempt other types of ancillary ligands for Ir(tfmpiq)_2(LX) complexes, aiming to increase quantum efficiencies and further reduce the energy gap to reach to longer wavelength region. Our group previously reported four btp-based deep-red phosphorescent iridium(III) complexes with different ancillary ligands. Among them, the Ir(III) complex with the picolinic acid as ancillary ligand could achieve a more red-shift relative to ones with N^N ancillary ligands. The N^O-type ancillary ligand containing –OH group could dramatically raise the highest occupied molecular orbital (HOMO) level and lead to a narrow HOMO-LUMO energy gap. Unfortunately, the quantum yield is very low (12%), as results of the fluorine-free main ligands in [Ir(btq)_2pic] complex.

Herein, we chose fluorinated 1-phenylisoquinoline (tfmpiq) as the cyclometalated ligand and N^O-type ligand (imidzppo/idzpo) as the ancillary ligand to synthesize two iridium(III) complexes (Scheme 1). Their photophysical and electrochemical properties are investigated, and the lowest-lying triplet excited state are calculated with density functional theory (DFT) and time-dependent DFT (TD-DFT).

2. Experimental

2.1. Materials and Instrumentations

IrCl_3 · 3H_2O was purchased from Energy Chemical and all reagents were used without further purification unless otherwise stated. All solvents were dried using standard procedures. Solvents used for electrochemistry and spectroscopy were spectroscopic grade. The target ligands, 1-(4-(trifluoromethyl)phenyl)isoquinoline (1), 2-(imidazo[1,2-a]pyridin-2-yl)phenol (a) and 2-(2H-indazol-2-yl)phenol (b) were prepared according to the literature procedures.

^1H NMR spectra were recorded on a Bruker AM 400 MHz instrument. Chemical shifts were reported in ppm relative to Me_4Si as internal standard. MALDI-TOF-MS spectra were recorded on a Bruker Autoflex II™ TOF/TOF instrument. Elemental analyses were performed on a Vario EL Cube Analyzer system. UV–vis spectra were recorded on a Hitachi U3900/3900H spectrophotometer. Fluorescence spectra were carried out on a Hitachi F-7000 spectrophotometer in deaerated CH_2Cl_2 solutions at 298 K and 77 K.

Cyclic voltammetry (CV) was performed on a CHI 1210B electrochemical workstation, with a glassy carbon electrode as the working electrode, a platinum wire as the counter electrode, an Ag/Ag^+ electrode as the reference electrode, and 0.1 M n-Bu_4NClO_4 as the supporting electrolyte.

2.2. Synthesis of (tfmpiq)_2Ir(imdzppo) (2a)

A mixture of IrCl_3·3H_2O (295 mg, 0.84 mmol) and the 1-(4-(trifluoromethyl)phenyl)isoquinoline (500 mg,
1.82 mmol) in 15 mL of 2-ethoxyethanol and H2O (v:v = 2:1) was heated at 120 °C under nitrogen for 12 hours. Upon cooling to room temperature, the orange-red precipitate was collected by filtration and washed with cooled ether and MeOH. After drying, the crude product of chloro-bridged dimer complex [(tfmpiq)2Ir(μ-Cl)]2 was used directly in next step without further purification. Then a slurry of the crude chloro-bridged dimer (100 mg, 0.065 mmol), 2-(imidazo[1,2-a]pyridin-2-yl)phenol (35 mg, 0.16 mmol) and Na2CO3 (55 mg, 0.52 mmol) in 2-ethoxyethanol (10 mL) was heated at 120 °C under nitrogen for 10 hours. After the solvent was removed, the mixture was poured into water and extracted with CH2Cl2, three times, and then evaporated. The residue was purified by flash column chromatography (petroleum ether : dichloromethane = 5:1~1:1) to afford the iridium complex 2a as a red solid (55 mg, yield: 45%). 1H NMR (400 MHz, CDCl3) δ (ppm) 8.95 (d, J = 8.0 Hz, 1H), 8.92 (d, J = 6.4 Hz, 1H), 8.78 (d, J = 4.8 Hz, 2H), 8.29 (s, 1H), 8.24 (d, J = 8.0 Hz, 1H), 7.81–7.92 (m, 10H), 7.71–7.75 (m, 3H), 7.38–7.40 (m, 2H), 7.18 (d, J = 4.8 Hz, 2H), 7.08–7.10 (m, 2H), 6.61 (d, J = 6.4 Hz, 1H), 6.21 (s, 1H). MALDI-TOF calcd for C45H27F6IrN4O: 946.172 ([M+H]+). Found: 946.386. Anal. Calcd. for C45H27F6IrN4O: C 57.14, H 2.88, N 5.92.

2. 3. Synthesis of (tfmpiq)2Ir(idzpo) (2b)

Complex 2b (52 mg, yield: 46%) was obtained by the method similar to the preparation of 2a using 2-(2H-indazol-2-yl)phenol instead of 2-(imidazo[1,2-a]pyridin-2-yl)phenol. 1H NMR (400 MHz, CDCl3) δ (ppm) 9.01 (d, J = 8.4 Hz, 1H), 8.87 (d, J = 6.4 Hz, 1H), 8.84 (d, J = 8.4 Hz, 1H), 8.49–8.51 (m, 2H), 8.25 (d, J = 6.4 Hz, 1H), 8.18 (d, J = 8.4 Hz, 1H), 7.87–8.89 (m, 1H), 7.67–7.83 (m, 5H), 7.61 (d, J = 8.4 Hz, 1H), 7.35 (d, J = 6.4 Hz, 1H), 7.30 (dd, J = 1.6 Hz, 8.4 Hz, 1H), 7.13–7.15 (m, 2H), 7.04–7.09 (m, 2H), 6.85–6.88 (m, 1H), 6.69–6.73 (m, 1H), 6.44–6.48 (m, 1H), 6.32–6.36 (m, 1H), 6.16–6.21 (m, 2H). MALDI-TOF calcd for C45H27F6IrN4O: 946.172 ([M+H]+). Found: 946.386. Anal. Calcd. for C45H27F6IrN4O: C 57.14, H 2.88, N 5.92. Found: C 55.70, H 2.97, N 5.89.

2. 4. Crystallographic Studies

X-ray diffraction data were collected with an Agilent Technologies Gemini A Ultra diffractometer equipped with graphite-monochromated Mo-Kα radiation (λ = 0.7107 Å) at room temperature. Data collection and reduction were processed with CrysalisPro software. The structure was solved and refined using full-matrix least-squares based on F2 with program SHELXS-97 and SHELXL-97 within Olex2. Crystallographic data (excluding structure factors) for the structural analysis have been deposited with the Cambridge Crystallographic Data Center as supplementary publication No. CCDC 1836887 (2b). Copies of the data can be obtained free of charge via www.ccdc.ac.uk/conts/retrieving.html (or from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, Fax: +44-1223-336-033. E-mail: deposit@ccdc.cam.ac.uk).

2. 5. Computational Method

All calculations were carried out with Gaussian 09 software package. The density functional theory (DFT) and time-dependent DFT (TD-DFT) were employed with no symmetry constraints to investigate the optimized geometries and electron configurations with the Becke three-parameter Lee-Yang-Parr (B3LYP) hybrid density functional theory. The LANL2DZ basis set was used for the iridium(III), whereas the 6-31G* basis set was adopted for the ligands. Solvent effects were considered within the SCRF (self-consistent reaction field) theory using the polarized continuum model (PCM) approach to model the interaction with the solvent.

3. Results and Discussion

3. 1. Synthesis and Characterization

Scheme 1 outlines the synthetic routes for iridium complexes 2a–2b investigated in this work. The main ligand, 1-(4-(trifluoromethyl)phenyl)isoquinoline (tfmpiq), was prepared from the synthesis of 1-chloroisooquinoline and 4-(trifluoromethyl)phenylboronic acid according to the literature procedure. The two constitutional isomer ligands, 2-(imidazo[1,2-a]pyridin-2-yl)phenol (imidzppo) and 2-(2H-indazol-2-yl)phenol (idzpo), were formed by an Ortoleva–King reaction and a PIII/PV = O redox cycling reaction, respectively. Complexes 2a–2b were obtained in moderate yields from the above ligands by a conventional two-step reaction. In the first step, a chloro-bridged dimer was formed by the reaction of iridium trichloride hydrate with an excess of main ligand. Then this dimer was cleaved via treatment with ancillary ligand in the presence of Na2CO3 to produce the heteroleptic iridium complex. The two complexes were structurally characterized by 1H NMR spectroscopy, mass spectrometry and elemental analysis.

3. 2. Structural Description

The crystal of 2b was obtained by slow evaporation of CH2Cl2/MeOH solution and the structure was determined through X-ray diffraction analysis (Fig. 1a). The crystallographic data and structure refinement details are listed in Table 1; selected bond lengths and bond angles are collected in Table 2.

As shown in Fig. 1a, the Ir(III) adopts a distorted octahedral geometry with the C=N ligands in cis-C,C’ and trans-N,N’ configurations. The average distance of Ir–C

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bonds (Ir–Cav = 1.989 Å) is shorter than that of the Ir–N bonds (Ir–Nav = 2.082 Å), as reported in other iridium(III) complexes.32,33 Notably, bonds between iridium and the N^O ligand (Ir–N3 = 2.156 Å, Ir–O1 = 2.153 Å) are longer than those between iridium and the C^N ligands (Ir–C15 = 1.985 Å, Ir–C31 = 1.993 Å, Ir–N1 = 2.040 Å, Ir–N2 = 2.051 Å), resulting from strong trans influence of the carbon donors.34 The angles of atoms on the para positions of the octahedron range from 171.61(18)° to 172.59(17)°, which are close to straight lines. For comparison, the two C–Ir–N bite angles of the C^N ligand are 79.23° and 79.47°, while the N–Ir–O bite angle of the ancillary ligand is 82.78°. This may be due to the rigid effect of the five-membered ring at the metal center.35 In addition, the hydrogen-bonding interactions in the crystal structure are presented in Fig. 1b and the details are summarized in Table 3. From Fig. 1b, the three selected non-covalent contacts of the C–H···O, C–H···F and C–H···N types are attributed to intramolecular hydrogen bonds, making three five-membered rings, respectively.

### Table 2. Selected bond distances (Å) and angles (°) for complex 2b·H2O.

<table>
<thead>
<tr>
<th>Bond/Angle</th>
<th>Value (Å/°)</th>
</tr>
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<tbody>
<tr>
<td>Ir1–N1</td>
<td>2.040(4)</td>
</tr>
<tr>
<td>Ir1–O1</td>
<td>2.153(4)</td>
</tr>
<tr>
<td>Ir1–N3</td>
<td>2.156(4)</td>
</tr>
<tr>
<td>N1–Ir1–O1</td>
<td>93.51(15)</td>
</tr>
<tr>
<td>N1–Ir1–N3</td>
<td>97.49(19)</td>
</tr>
<tr>
<td>C15–Ir1–N1</td>
<td>98.77(19)</td>
</tr>
<tr>
<td>C15–Ir1–N3</td>
<td>171.61(18)</td>
</tr>
</tbody>
</table>

### Table 3. Hydrogen bonding arrangements for complex 2b·H2O (Å, °).

<table>
<thead>
<tr>
<th>D–H···A</th>
<th>D–H</th>
<th>H···A</th>
<th>D···A</th>
<th>D–H···A</th>
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</thead>
<tbody>
<tr>
<td>C1–H1···O1</td>
<td>0.93</td>
<td>2.52</td>
<td>3.075(6)</td>
<td>118</td>
</tr>
<tr>
<td>C12–H12···F2</td>
<td>0.93</td>
<td>2.42</td>
<td>2.732(1)</td>
<td>100</td>
</tr>
<tr>
<td>C30–H30···N1</td>
<td>0.93</td>
<td>2.58</td>
<td>3.091(6)</td>
<td>115</td>
</tr>
</tbody>
</table>

### 3.3. Electronic Absorption Spectra

The UV-vis absorption spectra of complexes 2a–2b measured in CH2Cl2 solution at room temperature are depicted in Fig. 2, and the data are provided in Table 4. The absorption spectra reveal strong absorption bands below 400 nm, which are assigned to intraligand π–π* transitions centered on the C^N main ligand and the N^O ancillary ligand. The weak absorption bands extending from 400 nm to 550 nm are attributed to the metal to ligand 1MLCT/3MLCT transitions.36–38 In comparison...
with 2a, the lowest lying absorption band for complex 2b is slightly red-shifted, presumably depending on the different N-heterocycle ancillary ligands. This assumption will be proved by electrochemistry analyses and DFT calculations.

### 3.4. Emission Properties

Photoluminescence (PL) emission spectra of complexes 2a–2b in degassed CH$_2$Cl$_2$ solution at 298 K and 77 K are displayed in Fig. 3 and the corresponding data are also summarized in Table 4. In both cases, the emission spectra show the broad emission maxima at 618–628 nm together with a shoulder peak at 662–670 nm, which makes them red emitters. For their emission, the excited states are attributed to a mixing of 3MLCT and 3LC state.\(^{39,40}\) As seen, the emission band of 2b is also red-shifted relative to 2a, in good agreement with absorption analyses. When the temperature is decreased to 77 K, the emission maxima of 2a–2b are a slightly bathochromic shift compared to the 298 K spectra, as reported in our earlier literature.\(^{13}\) Clearly, these complexes exhibit vibronic bands at 77 K, which again demonstrate that their emission states are hybrid states with 3MLCT and 3LC characters.

Phosphorescence relative quantum yields (Φ$_{em}$) of 2a and 2b in dichloromethane solution at room temperature were measured to be 39.9 and 51.9% (Table 4) respectively, using typical phosphorescent fac-Ir(ppy)$_3$ as a standard (Φ$_{em}$ = 0.40).\(^{41}\) As expected, complexes 2a–2b have relatively high quantum yields, due to the effect of fluorinated backbones.\(^{42,43}\) Specially, the quantum efficiency of 2b is larger than that of 2a. The results manifest nitrogen atoms at 1,2-positions are more effective than 2,8-positions.

### 3.5. Theoretical Calculations

Density functional theory (DFT) and time-dependent DFT (TDDFT) calculations have been performed for complexes 2a–2b to gain insights into the lowest-energy
electronic transitions. The most representative molecular frontier orbital diagrams for these complexes are presented in Fig. 4. The calculated spin-allowed electronic transitions are provided in Table 5, as well as compared with the experimental absorption spectra data. The electron density distributions are summarized in Table S1.

As shown in Fig. 4, the HOMOs of these complexes are mainly localized on the metal center and the phenyl ring of ancillary ligands, whereas the LUMOs are primarily dominated on the whole C=N ligands. Besides, the HOMO-1 of complex 2a is located on iridium ion, the cyclometalated ligands and a little part of the ancillary ligands. The theory calculations of DFT reveal that the lowest-energy spin-allowed transitions of 2a–2b are derived from HOMO/HOMO-1→LUMO and HOMO→LUMO transitions (Table 5), consequently assigned to metal-to-ligand charge transfer transitions and ligand-to-ligand π–π* transitions. These calculations support the photophysical properties discussed above.

To gain the origins of emission for complexes 2a–2b, we also employed the DFT calculations to investigate the triplet excited-state characters. The results of the TD-DFT calculations for the triplet states are listed in Table 6. For both the studied complexes, the two lowest lying triplet states (T1 and T2) are predominantly from HOMO→LUMO, HOMO-1→LUMO, HOMO→LUMO+1, HOMO→LUMO+1, HOMO-2→LUMO and HOMO-3→LUMO transitions. According to electron density distributions in Table S1, the HOMOs are mainly localized at the ancillary ligands, while LUMOs/LUMO+1s at the C=N ligands. The HOMO-1s/HOMO-2s/HOMO-3s are composed of Ir d-orbital, C=N ligands and ancillary ligands. Thereby, both of the two lowest-lying triplet states (T1 and T2) have a mixed 3MLCT/3LLCT/3LC character for the two complexes, except T2 of 2a with limited 3MLCT contribution. The lowest-lying triplet states of 2a have similar transition paths with those of 2b, indicating that the different positions of N atoms on ancillary ligands have no obvious effect on emissive behavior.

### 3. 6. Electrochemical Properties

The electrochemical behaviors of both iridium complexes were investigated by cyclic voltammetry and the electrochemical waves are shown in Fig. 5. The respective electrochemical data and estimated HOMO energy levels are also reported in Table 4. Complexes 2a–2b exhibit a

<table>
<thead>
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<th>Complex</th>
<th>HOMO Configuration</th>
<th>Transition</th>
<th>Character</th>
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<tr>
<td>2a</td>
<td>S1 HOMO→LUMO (93%)</td>
<td>LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
</tr>
<tr>
<td></td>
<td>S2 HOMO-1→LUMO (94%)</td>
<td>MLCT/LC</td>
<td>dπ_{Ir}/π_{tffmpiq}→π^{*}_{tffmpiq}</td>
</tr>
<tr>
<td>2b</td>
<td>S1 HOMO→LUMO (91%)</td>
<td>MLCT/LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
</tr>
</tbody>
</table>

<p>| Table 5. Major configuration, transition characters, oscillator strength and calculated/experimental absorption wavelengths for 2a–2b. |
|-----------------|-----------------|-----------------|-----------------|</p>
<table>
<thead>
<tr>
<th>Complex</th>
<th>Major Configuration</th>
<th>Transition</th>
<th>Character</th>
<th>Oscillation Strength</th>
<th>Calcd (nm)</th>
<th>Exptl (nm)</th>
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<tbody>
<tr>
<td>2a</td>
<td>S1 HOMO→LUMO (93%)</td>
<td>LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>S2 HOMO-1→LUMO (94%)</td>
<td>MLCT/LC</td>
<td>dπ_{Ir}/π_{tffmpiq}→π^{*}_{tffmpiq}</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>2b</td>
<td>S1 HOMO→LUMO (91%)</td>
<td>MLCT/LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<p>| Table 6. Contribution of triplet transitions and transition characters for complexes 2a–2b. |
|-----------------|-----------------|-----------------|-----------------|</p>
<table>
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<tr>
<th>Complex</th>
<th>Major Configuration</th>
<th>Transition</th>
<th>Character</th>
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</thead>
<tbody>
<tr>
<td>2a</td>
<td>T1 HOMO→LUMO (57 %)</td>
<td>3LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
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<tr>
<td></td>
<td>T2 HOMO→LUMO+1 (61%)</td>
<td>3LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
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<tr>
<td>2b</td>
<td>T1 HOMO→LUMO (31 %)</td>
<td>3MLCT/3LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
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<td></td>
<td>T2 HOMO→LUMO+1 (25%)</td>
<td>3MLCT/3LLCT</td>
<td>π_{ndzppo}→π^{*}_{tffmpiq}</td>
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Fig. 4. The frontier molecular orbital diagrams of complexes 2a–2b from DFT calculations.
quasi-reversible/irreversible oxidation peak ($E_{on}$) at 0.87 and 1.05 V, respectively. As inferred from DFT calculations (Table S1), the HOMOs are mainly localized on the Ir ion (13.88 % for 2a, 24.74 % for 2b) and ancillary ligands (75.74 % for 2a, 58.06 % for 2b). Therefore, the oxidation is assigned to Ir(III) to Ir(IV) with some contribution from ancillary ligand. On the basis of the potentials of the oxidations (Table S1), the HOMOs are mainly localized on the Ir ion (13.88 % for 2a, 24.74 % for 2b) and ancillary ligands (75.74 % for 2a, 58.06 % for 2b). Therefore, the oxidation is assigned to Ir(III) to Ir(IV) with some contribution from ancillary ligand. On the basis of the potentials of the oxidations, the HOMO energy is deduced by the equation $E_{HOMO} = -(E_{ox} + 4.8 \text{ eV})$, and the trend is quite consistent with theoretical calculation values (Table 4). As it can be seen from these results, through changes of nitrogen atoms from 2,8-positions to 1,2-positions, the HOMO level of 2b is more stable and the oxidation process is more difficult than those of analogue 2a.

4. Conclusions

In conclusion, two red-emitting iridium(III) complexes (2a–2b) equipped with tfmpiq cyclometalated ligand and imdzppo/idzpo ancillary ligand, have been successfully synthesized and characterized. Their photophysical properties, electrochemical behaviors and theoretical calculations have been systematically studied. The calculated absorptions of the two complexes 2a–2b are in full agreement with the experimental data, which indicate that the lowest lying absorptions are assigned to MLCT/LLCT transitions. Both Ir(III) complexes exhibit red phosphorescence in dichloromethane solution at 298 K and at 77 K, and the lowest lying triplet excited states have a mixed $^3\text{MLCT}/^3\text{LLCT}/^3\text{LC}$ character. By changing the positions of N atoms in the ancillary ligand, we have confirmed complex 2b had a further red-shift relative to 2a in the emission spectra. These research results will facilitate the design of new piq-based ligands for red-emitting iridium complexes.

5. Acknowledgments

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References

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Povzetek
Sintetizirali smo dva nova bis-ciklometalirana iridijeva(III) kompleksa s tfmpiq ligandom, \([(\text{tfmpiq})_2\text{Ir(idzppo)}]\) (2a) in \([(\text{tfmpiq})_2\text{Ir(idzppo)}]\) (2b) (tfmpiq = 1-(4-(trifluorometil)fenil)izokinolin, idzppo = 2-(imidazo[1,2-a]piridin-2-il)fenol, idzpo = 2-(2H-indazol-2-il)fenol), in ju okarakterizirali. Določili smo monokristalno strukturo 2b. Določili smo razmerje med strukturo in fotofizikalnimi lastnostmi obeh kompleksov podprto tudi z DFT izračuni. Ir(III) kompleksa emitirata rdečo svetlobo s kvantnim izkoristkom 39.9–51.9 % v degaziranem CH₂Cl₂ pri sobni temperaturi. Emisija izvira iz hibridnega 'MLCT/LLCT/LLC vzbujenega stanja. Vsi ti rezultati kažejo, da sta iridijeva(III) kompleksa 2a-2b primerna kot rdeča fosforescentna materiala v OLED.