Theoretical investigation of the electronic structure and photophysical properties of a series of mixed-carbene cyclometalated iridium(III) complexes with different ancillary ligands applied in phosphorescent organic light-emitting diodes

Tong Chen1 · Deming Han2,3 · Lihui Zhao2 · Bao Wang1 · Xiaohong Shang1

Received: 14 August 2020 / Accepted: 31 May 2021 / Published online: 13 July 2021 © The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2021

Abstract
By using density functional theory and time-dependent density functional theory, the geometrical structure, electronic structure and photophysical properties of a series of mixed-carbene cyclometalated iridium(III) complexes with different ancillary ligands have been explored. The frontier molecular orbital components and energy levels for all studied complexes have been investigated. The lowest-lying absorptions were calculated as 327, 322, 333, 332 and 332 nm for these complexes, which have a HOMO → LUMO transition configuration. The lowest energy emissions for these complexes are localized at 413, 399, 498, 418 and 415 nm, respectively, simulated in a CH2Cl2 medium at the M062X level. One designed complex possessed the largest radiative decay rate (kr) value and could be a candidate for blue emitters in organic light-emitting diodes. This theoretical study can provide useful guidance for the design and synthesis of new iridium(III) complexes in phosphorescent materials.

Keywords DFT · TDDFT · OLEDs · Iridium · Phosphorescence

1 Introduction
In the past two decades, organic light-emitting diodes (OLEDs) have been widely studied due to their applications in flat display and light sources [1–5]. Phosphorescent OLEDs can capture singlet excitons and triplet excitons at the same time due to the heavy atom effect, so theoretically 100% internal quantum yield can be achieved. Among these OLEDs, phosphorescent iridium complexes have received the most attention [6–10]. Recently, the phosphorescent color and quantum efficiency have been widely investigated by theoretical and experimental researchers. Many green- and red-emitting OLED devices with excellent performance have been reported. However, in the development of blue-emitting phosphors, achieving high efficiency and stability for blue phosphorescence remains a challenging task [11–13]. In order to obtain full-color display, it is necessary to obtain commercially available red, green, and blue light materials. Among these, the blue emitters require a wide energy gap between the excited triplet state and the ground state. The approaches to obtain efficient blue phosphorescence-emitting materials are to either seek ligands with high triplet energy or use electron-withdrawing ancillary ligands to increase the emission energy by stabilizing/destabilizing the highest occupied/lowest unoccupied molecular orbitals (HOMO/LUMO).

N-heterocyclic carbenes (NHCs) are typical carbene ligands incorporated into blue-emitting iridium complexes [14–16]. The acyclic diaminocarbenes (ADCs) can be even stronger σ-donors than NHCs on account...
of the greater 2p character in their σ orbital [17, 18], which could potentially destabilize the metal-centered triplet excited state (3MC) to an even greater extent than is possible with NHCs and improve the photostability of blue phosphorescent complexes. Recently, Na et al. investigated a class of cyclometalated iridium complexes with the general structure Ir(C^C: NHC)_2(C^C: ADC), where C^C: NHC is an N-heterocyclic carbene (NHC)-derived cyclometalating ligand and C^C: ADC is a different type of cyclometalating ligand featuring an acyclic diamino-carbene (ADC) [19]. In this study, on the basis of complex 3b [19], that is, complex 1 in Fig. 1, four complexes [2, 3, 4 and 5 in Fig. 1a] have been designed. The electronic structures and photophysical properties of these complexes have been theoretically studied using density functional theory (DFT) and time-dependent density functional theory (TDDFT). The ancillary ligand with different substituent groups will have an effect on the electronic structure and photophysical properties of all the studied complexes.

2 Computational methods

To calculate the electronic singlet and triplet states of all the studied complexes, we use density functional theory (DFT) with a hybrid-type Perdew–Burke–Ernzerhof exchange correlation functional (PBE0) and unrestricted PBE0 (UPBE0), respectively [20–22]. The value of the lowest-lying emission wavelength of complex 1 is calculated by the M062X functional, which is in good agreement with the experimental wavelength value [19]. The quasi-relativistic pseudo-potentials of the Ir atom proposed by Hay and Wadt with 17 valence electrons were employed, and a “double-ξ” quality basis set LANL2DZ was adopted as the basis set [23]. The 6–31G(d) basis set was applied to other atoms. Based on the optimized structures of the ground and excited states, the time-dependent DFT (TDDFT) approach associated with the self-consistent reaction field (SCRF) theory using the integral equation formalism polarized continuum model (IEFPCM) [24–26] in dichloromethane (CH_2Cl_2) media was applied to simulate the absorption and emission
spectral properties from the experimental results by Na et al. [19]. All calculations were performed using the Gaussian 09 software package [27]. GaussSum 2.5 was used for UV/Vis absorption spectra analysis with a full width at half maximum (FWHM) of 3000 cm\(^{-1}\) based on the present TDDFT computational results [28].

3 Results and discussion

3.1 Geometries in the ground state \(S_0\) and triplet excited state \(T_1\)

The sketch map of Ir(III) complexes 1–5 is shown in Fig. 1a, and the partial atomic number of complex 1 as a representative is shown in Fig. 1b. In order to describe these complexes, the main ligand and ancillary ligand have been respectively labeled as NHC and ADC moieties. The main optimized geometrical parameters of the ground state \(S_0\) and triplet excited state \(T_1\) are presented in Table 1.

The optimized bond distances of complex 1 are in quite good agreement with available experimental data [19], and the deviation is within 1.8%. The bond angles C1–Ir–C2, C3–Ir–C6 and C4–Ir–C5 are larger than 77°. The bond angles C1–Ir–C6, C2–Ir–C5 and C3–Ir–C4 are larger than 166°. This indicates that all studied Ir(III) complexes with a \(d^6\) configuration adopt a pseudo-octahedral coordination geometry. The dihedral angles C1–C3–C6–C4 in complexes 1–5 are less than 2°, which shows a nearly planar structure around the central Ir atom. In particular, the dihedral angle C1–C2–C6–C5 in complex 2 is less than those of other four complexes, which is probably due to the introduction of the strong electron-donating group \(-\text{N(CH}_3)_2\). From the \(S_0\) to \(T_1\) states, the bond lengths Ir–C4 and Ir–C5 in complexes 1–5 decrease and increase slightly, respectively. The bond angles C3–Ir–C6 and C4–Ir–C5 in complexes 1–5 also slightly decrease and increase, respectively.

3.2 Frontier molecular orbital properties

The frontier molecular orbital (FMO) properties are bound to the photophysical properties of these Ir(III) complexes. The energy levels and distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of all studied Ir(III) complexes have been investigated by DFT/PBE0. The contour plots of HOMO and LUMO are shown in Fig. 2. The detailed descriptions of the molecular orbitals, in terms of energies, composition and the assignment of different fragments are shown in Tables S1–S5 (Supplementary Information). From Fig. 2 and Tables S1–S5, it can be seen that the HOMO of complexes 1–4 resides mainly on the Ir atom and NHC ligand.

| Table 1 | Main optimized geometrical parameters of complexes 1–5 in the ground and the lowest-lying triplet states, together with the experimental values |
|---------|-------------------------------------------------------------------------------------|
| \(1\)   | \(2\)   | \(3\)   | \(4\)   | \(5\)   |
| \(S_0\) | \(T_1\) | \(S_0\) | \(T_1\) | \(S_0\) | \(T_1\) | \(S_0\) | \(T_1\) |
| PBE0/ExptL \(^a\) |
| Bond length (Å) | 2.085/2.096 | 2.058 | 2.094 | 2.101 | 2.085 | 2.053 | 2.086 | 2.067 | 2.086 | 2.061 |
| Ir–C1 | 2.034/2.026 | 2.105 | 2.032 | 2.030 | 2.034 | 2.037 | 2.032 | 2.098 | 2.099 |
| Ir–C2 | 2.055/2.019 | 2.102 | 2.114 | 2.129 | 2.050 | 2.151 | 2.057 | 2.111 | 2.058 | 2.110 |
| Ir–C3 | 2.074/2.081 | 2.028 | 2.063 | 2.019 | 2.077 | 2.035 | 2.075 | 2.030 | 2.073 | 2.030 |
| Ir–C4 | 2.018/1.997 | 2.028 | 2.021 | 2.034 | 2.021 | 2.028 | 2.018 | 2.026 | 2.018 | 2.029 |
| Ir–C5 | 2.101/2.094 | 2.106 | 2.099 | 2.100 | 2.100 | 2.129 | 2.106 | 2.102 | 2.106 | 2.106 |
| Bond angle (°) | 77.04/77.81 | 79.36 | 77.96 | 77.94 | 77.97 | 79.15 | 78.00 | 79.35 | 78.03 | 79.39 |
| C1–Ir–C2 | 78.61/79.57 | 78.72 | 78.46 | 78.57 | 76.71 | 76.64 | 76.73 | 76.70 |
| C3–Ir–C6 | 78.11/77.70 | 78.76 | 79.62 | 77.95 | 79.04 | 78.05 | 78.58 | 78.04 | 78.67 |
| C1–Ir–C6 | 170.71/168.19 | 162.63 | 177.17 | 177.64 | 171.25 | 160.74 | 170.41 | 161.48 | 170.45 | 161.95 |
| C2–Ir–C5 | 166.82/170.67 | 170.93 | 167.79 | 168.79 | 166.73 | 174.03 | 167.40 | 170.38 | 167.55 | 170.83 |
| C3–Ir–C4 | 172.75/171.99 | 169.43 | 169.72 | 168.58 | 171.98 | 166.21 | 172.43 | 171.05 | 172.47 | 170.51 |
| Dihedral angle (°) | 14.36/12.19 | 17.59 | 3.74 | 3.02 | 13.97 | 16.92 | 14.30 | 18.56 | 14.15 | 18.27 |
| C1–C2–C6–C5 | 10.49/11.18 | 11.88 | 13.09 | 13.85 | 11.28 | 14.05 | 10.50 | 11.03 | 10.43 | 11.02 |
| C1–C3–C6–C4 | 0.77/4.19 | 3.29 | 0.59 | 0.51 | 0.03 | 1.28 | 1.09 | 4.85 | 1.27 | 3.45 |

\(^a\)Ref. [19]
For example, the HOMO of 1 is distributed over the d-orbital of Ir (36%) and the π-orbital of NHC (58%). However, the HOMO of complex 5 is distributed on the Ir atom (31%), NHC (40%) and ADC (29%) ligand. The LUMO of all studied complexes resides mainly on the NHC ligand, except complex 3, which is mainly distributed on the ADC ligand. In addition, the HOMO/LUMO energy levels for complexes 1–5 are not largely different. The largest and smallest energy gaps between LUMO and HOMO ($\Delta E_{L\rightarrow H}$) values are 4.76 and 4.61 eV for complexes 2 and 5, respectively.

### 3.3 Absorption spectra

The vertical electronic excitation energies, oscillator strengths ($f$), dominant orbital excitations and their assignments of the singlet excited state are presented in Table S6 (Supplementary Information). Simulated absorption curves for complexes 1–5 in CH$_2$Cl$_2$ medium are shown in Fig. 3.

The absorption spectra shapes of complexes 1–5 are very similar. In addition, there is a small absorption peak at about 260 nm for complexes 4 and 5. It can be seen from Table S6 that the lowest-lying singlet $\rightarrow$ singlet absorption of 1–5 is located at 327 nm ($f=0.0103$), 322 nm ($f=0.0038$), 333 nm ($f=0.0023$), 332 nm ($f=0.0092$) and 332 nm ($f=0.0077$), respectively. The calculated 327 nm absorption for complex 1 is comparable to the experimental value of 302 nm [19]. The lowest-lying absorptions for complexes 1, 2 and 4 mainly have a HOMO $\rightarrow$ LUMO transition configuration contributing to the $S_0$ $\rightarrow$ $S_1$ state, and they have the same transitions; for example, the lowest energy absorption of 1 is characterized as metal-to-ligand charge transfer (MLCT)/intraligand charge transfer (ILCT) [d(Ir) $+$ $\pi$(NHC) $\rightarrow$ $\pi^*$ (NHC)] character. The lowest-lying absorptions for complex 3 have a HOMO $\rightarrow$ LUMO transition configuration contributing to the $S_0$ $\rightarrow$ $S_1$ state characterized as MLCT/ligand-to-ligand charge transfer (LLCT) d(Ir) $+$ $\pi$(NHC) $\rightarrow$ $\pi^*$ (ADC) character. For complex 5, the lowest energy absorption is characterized as MLCT/LLCT/ILCT [d(Ir) $+$ $\pi$(NHC + ADC) $\rightarrow$ $\pi^*$ (NHC)].

### 3.4 Phosphorescence emission properties

In order to further explore the phosphorescence properties of the complexes, the TDDFT method was used to calculate the emission wavelength and transition properties based on the optimized T$_1$ structure. In order to ensure the accuracy of the data, the density functionals B3LYP [29], PBE0 [21], CAM-B3LYP [30], M052X [31], M062X [32] and BP86 [33] were respectively used to calculate complex 1. The calculated lowest energy emissions at these levels are localized at 2.356, 2.467, 2.808, 3.013, 3.001 and 1.908 eV, deviating from the experimental value 2.952 eV [19] by 0.596, 0.485, 0.144, 0.061, 0.049 and 1.051 eV, respectively. Obviously, good agreement with the measured data was obtained for M062X. Therefore, we have employed the M062X method for emission property calculations of all studied complexes. The calculated emission wavelengths, emission energies and transition nature of complexes 1–5 in CH$_2$Cl$_2$ medium are listed in Table 2. The plots of the molecular orbitals related to emissions of complexes 1–5 are also presented in Table 3. In addition, partial frontier molecular orbital compositions (%) of complexes 1–5 in the triplet excited states are presented in Table S7 (Supplementary Information).

Table 2 shows that the calculated lowest energy emissions of complexes 1–5 are located at 413, 399, 498, 418 and 415 nm, respectively. Complex 3 has the largest emission wavelength of 498 nm among these studied complexes, which shows that the introduction of a phenyl ring to the ancillary ligand has an obvious effect on...
the phosphorescence emission properties. From Table 2 and Table S7, it can be seen that the phosphorescence emission of all studied complexes mainly possesses a LUMO→HOMO transition configuration. For example, complex 1 has the triplet metal-to-ligand charge transfer (3MLCT)/triplet ligand-to-ligand charge transfer (3LLCT)/triplet intraligand charge transfer (3ILCT) [π*(NHC)→d*(Ir) + π*(NHC + ADC)] transition characters. Complex 2 has the smallest emission wavelength, 399 nm, among these studied complexes, which may be due to the introduction of –N(CH3)2 with strong electron-donating ability to the ancillary ligand. For example, the LUMO of complex 1 is distributed on the NHC ligand (91%). From Table 3 and Table S7, it can be seen that the LUMO of all studied complexes are mainly localized on the NHC ligand, except complex 3. The HOMO of all studied complexes are mainly localized on the Ir atom and NHC ligand. For example, the HOMO of complex 1 is distributed on the Ir atom (34%) and NHC ligand (55%).

### 3.5 Phosphorescence quantum yield

The phosphorescence quantum yield (Φ<sub>PL</sub>) is obtained by the following equation [34]:

\[
\Phi_{PL} = \frac{k_r}{k_r + k_{nr}}
\]

in which \(k_r\) is the radiative decay rate and \(k_{nr}\) is the nonradiative decay rate. Therefore, it is necessary to increase \(k_r\) and reduce \(k_{nr}\) to achieve high phosphorescence quantum efficiency. The \(k_{nr}\) from the T<sub>1</sub> to the S<sub>0</sub> states is usually expressed in the form of the energy law, Eq. (2), and \(k_r\) is given by Eq. (3) [35, 36]:

\[
k_r \approx \frac{\mu_{S_i}^2}{(\Delta E_{S_i-T_i})^2}
\]

\[
\gamma = 16\pi^3 10^6 n^3 E_{em}^3 / 3\hbar\epsilon_0
\]

Here \(\alpha\), \(\beta\) and \(\gamma\) are constant, \(\mu_{S_i}\) is the transition electric dipole moment for the S<sub>i</sub>→S<sub>0</sub> transition, \(E_{T_i}\) represents the emission energy in cm<sup>-1</sup>, and \(n\), \(\hbar\), and \(\epsilon_0\) are the refractive index of the medium, Planck’s constant, and the permittivity in vacuo, respectively. \(\langle \Psi_{S_i} | H_{so} | \Psi_{T_i} \rangle\) is the spin–orbit coupling (SOC) matrix element. In addition, the SOC effects can be elucidated by the triplet metal-to-ligand charge transfer (3MLCT) in the T<sub>i</sub> state [37]. It is known that a larger 3MLCT composition and thus intersystem crossing (ISC) can increase the phosphorescence quantum yield. The direct involvement of the d orbital in Ir can increase the first-order SOC in the T<sub>i</sub>→S<sub>0</sub> transition, resulting in a drastic decrease in the radiative lifetime and an increased nonradiative rate constant. The 3MLCT contribution of complex 4 is the largest among these studied complexes. The phosphorescence quantum yield is inversely proportional to the energy gaps between the S<sub>i</sub> and T<sub>i</sub> states (\(\Delta E_{S_i-T_i}\)) [38], in which a minimal \(\Delta E_{S_i-T_i}\) is required for enhancing the intersystem
crossing rate, leading to the increased $k_r$. The $\Delta E_{S_1 \rightarrow T_1}$ and $\mu_{s_1}$ values are presented in Table 4. As mentioned above, according to Eq. (1), a lower $\Delta E_{S_1 \rightarrow T_1}$ and larger 3MLCT contributions and higher $\mu_{s_1}$ values may account for a larger $k_r$. Hence, complex 4 possibly possesses the largest $k_r$ value, and thus represents a potential candidate for blue phosphorescence dopant emitters in OLEDs.

4 Conclusions

In this study the electronic structures and photophysical properties of five iridium(III) complexes with different ancillary ligands have been theoretically investigated. All studied complexes have a distorted octahedral structure around the Ir(III) metal center with d6 configuration. The HOMO/LUMO energy levels for complexes 1–5 in the S0 state are not changed significantly. Complexes 1–5 have similar absorption curves with a large peak. The calculated phosphorescence emission wavelength of complex 1 at TDDFT/M062X level shows very good agreement with the available experimental data. The HOMO of complexes 1–5 in the T1 state are mainly localized on the Ir atom and NHC ligand. Complex 4 has the largest 3MLCT contribution among these studied complexes. It is anticipated that this study will facilitate the further theoretical and experimental design of phosphorescent materials in OLEDs.

Supplementary Information  The online version contains supplementary material available at https://doi.org/10.1007/s10825-021-01738-z.

Acknowledgements  The authors are grateful to the financial aid from the Program of Science and Technology Development Plan of Jilin Province of China (Grant No. 20200201099JC) and Innovation and Entrepreneurship Training Program for College Students in Jilin Province (Grant No. 202010190063). The authors are grateful to Computing Center of Jilin Province of China and Professor Keli Han of Dalian Institute of Chemical Physics, Chinese Academy of Sciences for essential support.

Declarations

Conflict of interest  The authors declare that they have no conflicts of interest.

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