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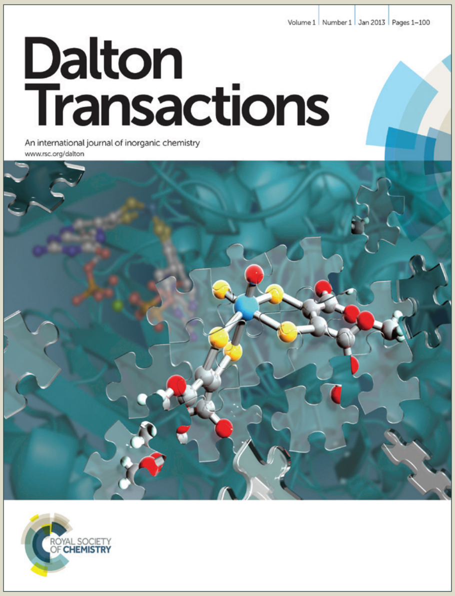

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Tetraphenylborate *versus* tetraimidazolylborate as counterions for cationic iridium(III) complexes: enhanced electrochemical stabilities and electroluminescence

Dongxin Ma, Lian Duan* and Yong Qiu

Tetraimidazolylborate is first used as the counterion of two novel ionic iridium complexes, instead of tetraphenylborate. Both the electrochemical stabilities and electroluminescence are sharply improved. Organic light-emitting diodes have been successfully fabricated with a high current efficiency of 9.48 cd A^{-1} and a maximum brightness of 5163 cd m^{-2}.

Introduction

Organic light-emitting diodes (OLEDs) are regarded as promising candidates in flat panel display and solid state lighting, since C. W. Tang's ground-breaking work in 1987.[1] In OLEDs, singlet and triplet excitons are generated with a ratio of 1:3 through recombination of holes and electrons. For OLEDs doped with fluorescent emitters, only singlet excitons can generate photons, so the maximum efficiency in theory is 25 %.[2] However, for OLEDs based on phosphorescent emitters, both singlet and triplet excitons can generate photons, so the maximum efficiency in theory is 100 %.[3] Consequently, phosphorescent emitters are more favourable choices for OLEDs.

Common phosphorescent emitters always contain transition metals,[4] which can be categorized into ionic transition metal complexes (iTMCs) and neutral ones. As is well-known, neutral transition metal complexes such as iridium(III),[5,6] platinum(II),[7,8] and osmium(II)[9,10] complexes are widely used as phosphorescent emitters in OLEDs. By contrast, iTMCs have many advantages such as good solubilities, abundant photophysical properties and high electrochemical stabilities. However, in the past, iTMCs were only used in another kind of devices called light-emitting electrochemical cells (LECs).[11] In 2002, Carlson *et al.* first reported red-emitting OLEDs based on ionic osmium complexes.[12] Zhang *et al.* then fabricated green-emitting devices based on ionic copper complexes.[13] In 2005, Plummer *et al.* reported devices with ionic iridium complexes as yellow phosphorescent emitters.[14] Our group also reported blue devices doped with ionic iridium complexes.[15] However, application of iTMCs in OLEDs is still scarce. Many key problems remain to be solved, such as charge transport abilities of iTMCs and effect of the counterions on device performance.

In our previous work, ionic iridium(III) complexes with tetraphenylborate as the counterion were reported with high photoluminescent yields, suggesting a series of promising emitters.[16] However, OLEDs based on ionic iridium complexes with tetraphenylborate as counterions gave no luminance, suffering from poor electrochemical stabilities. In tetraphenylborate, the centre boron is surrounded by four phenyl groups with high electron density, easily to be oxidized. As imidazolyl groups are electron-withdrawing, we introduce tetraimidazolylborate as counterions into ionic iridium complexes instead of tetraphenylborate to improve the electrochemical stabilities.

In this communication, two novel ionic iridium complexes with tetraimidazolylborate as the counterion have been synthesized. Their photophysical and electrochemical properties were investigated and compared with the corresponding complexes with tetraphenylborate as the counterion. OLEDs were successfully fabricated, with a high efficiency of 9.48 cd A^{-1} and a maximum brightness of 5163 cd m^{-2}.

Results and discussion

As shown in **Scheme 1**, ionic iridium complexes with different counterions are $[Ir(ppy)_2(pzpy)][Bph_4]$ (complex 1), $[Ir(ppy)_2(pzpy)][BIm_4]$ (complex 2), $[Ir(dfppy)_2(pzpy)][Bph_4]$ (complex 3) and $[Ir(dfppy)_2(pzpy)][BIm_4]$ (complex 4), respectively. Ppy is 2-phenylpyridine, pzpy is 2-(1*H*-pyrazol-1-yl) pyridine, $[Bph_4]^-$ is tetraphenylborate, and $[BIm_4]^-$ is tetrakis(1-imidazolyl)borate (tetraimidazolylborate for short), respectively. The synthetic routes are shown in **Scheme 2**.

Photophysical properties of complexes 1-4 in degassed CH_3CN solutions and neat films are shown in **Figure 1**. Details are summarized in **Table 1**. As we can see, the absorption and emission spectra of complexes 1 and 2, 3 and 4 in solutions are quite similar, respectively. The intense absorption bands in the ultra-violet region ranging from 230 nm to 350 nm are ascribed to spin-allowed $^1\pi$-π^* transitions from the ligands, while the weaker absorption bands from

350 nm extending to the visible region are ascribed to ^{1}MLCT (metal-to-ligand charge-transfer), ^{1}LLCT (ligand-to-ligand charge-transfer), ^{3}MLCT, ^{3}LLCT, and ligand-centred (LC) $^3\pi$-π^* transitions. For complexes 1-4 at room temperature, the vibronically structured emission spectra indicate that the emissive excited states have predominantly ^{3}LC π-π^* characters other than ^{3}MMCT or ^{3}LLCT characters. However, the emission peak and shoulder peak of complex 4 in neat films and solutions are exchanged, due to the different vibronic structures in different conditions, as a similar phenomenon described in our previous work.[16] Photoluminescent quantum yields (PLQYs) of complexes 1 and 2 are similar in both solutions and neat films. However, PLQY of complex 4 is quite lower than that of complex 3 in solution, while completely opposite in neat films.

Cyclic voltammetry was then used to measure electrochemical properties of complexes 1-4 in degassed solutions. As depicted in **Figure 2**, the reduction potentials of complexes 1-4 are similar, while the oxidation potentials are quite different. For complexes 1 and 3, an anodic peak is observed at 0.42 V, which is ascribed to the same counterion, $[Bph_4]^-$. For complexes 2 and 4, the anodic peak is different, which is ascribed to the different cation, $[Ir(ppy)_2(pzpy)]^+$ or $[Ir(dfppy)_2(pzpy)]^+$, respectively, rather than $[BIm_4]^-$. As a result, from tetraphenylborate to tetraimidazolylborate as the counterion of ionic iridium complexes, the electrochemical stabilities are sharply improved.

Furthermore, quantum chemical calculations were performed to gain insight into the electrochemical behaviors of different counterions. The highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) of $[Bph_4]^-$ and $[BIm_4]^-$ are shown in **Figure 3**. The highest occupied molecular orbital (HOHO) energy of $[Bph_4]^-$ is -2.44 eV, while HOMO energy of $[BIm_4]^-$ is -2.81 eV, much stabilized. Similarly, the lowest unoccupied molecular orbital (LUMO) energy of $[Bph_4]^-$ is 3.31 eV, while LUMO energy of $[BIm_4]^-$ is 3.79 eV. Mulliken charges of all the atoms in the counterions were also calculated and summarized in **Table 2** and **Scheme 3**. Mulliken charge of the boron in $[Bph_4]^-$ is 0.16, lower than that of the boron in $[BIm_4]^-$ (0.82). It shows that from tetraphenylborate to tetraimidazolylborate, electron densities of the boron are decreased significantly, and electrochemical stabilities are sharply improved.

To investigate the electroluminescent (EL) properties of complexes 1-4, OLEDs were fabricated with the structure of ITO/ PEDOT: PSS (60 nm)/ PVK: OXD-7: 10 wt. % Ir-complex (85 nm)/ TPBi (30 nm)/ Mg: Ag (150 nm)/ Ag (50 nm) (as shown in **Schemes 4-5**). Devices were grown on a 100 nm-indium-tinoxide (ITO) by sputter etching, and then passivated with a 60 nm layer of PEDOT: PSS by spin-coating in the atmosphere. PVK: OXD-7 served as the host, doped with complexes 1-4, respectively. The light-emitting layer was spin-coated in the glove box filled with nitrogen. The devices were transferred into the vacuum chamber afterwards and TPBi was evaporated as a hole blocking layer. Finally, magnesium was doped in the silver cathode to help electron injection.

The current-voltage-brightness characteristics of devices were measured and shown in **Figure 4**. Devices based on complexes 1 and 3 show no luminescence, while devices based on complexes 2 and 4 are green-blue emitting. We obtained devices based on complex 4 with a current efficiency of 0.27 cd A^{-1}. While OLED based on complex 2 shows a quite better performance with a high current efficiency of 9.48 cd A^{-1} and a maximum brightness of 5163 cd m^{-2}. The current density of the device based on complex 2 is 1111 A m^{-2} at 15 V, while that of the device based on complex 4 is only 0.62 A m^{-2} at 15 V. It indicates that charge-transport ability of complex 2 is much better than that of complex 4. However, the emission wavelength is 514 nm, with CIE (Commission Internarionale de I'Eclairage) coorinates of (0.31, 0.54), quite red-shifted compared with the PL emission of complex 2 in neat films and solutions. We speculate that the EL spectra shift is ascribed to the polarization effect of molecular orbitals under electric field in the device.[17]

Experimental

In this paper, all the reactants and solvents mentioned were purchased from commercial sources and used as received unless otherwise stated. Mass spectrometry was performed with a Theromo Electron Corporation Finnigan LTQ. ^{1}H NMR spectra were recorded on JOEL JNM-ECA600 NMR spectrometer with tetramethylsilane as the internal standard. Elemental analysis was determined on an Elementar Vario EL CHN elemental analyser. Absorption spectra were performed with a UV-vis spectrophotometer (Agilent 8453) and PL spectra were recorded with a fluorospectrophotometer (Jobin Yvon, FluoroMax-3). The excited state lifetimes were perfomed with a transient spectrofluorimeter (Edinburgh Instruments, FLSP920) with time-correlated single-photon counting technique at the peak PL wavelength. PLQYs of complexes 1-4 in neat films were measured with Quantaurus-QY (C11347-11). Cyclic voltammetry was performed on a Princeton Applied Research potentiostat/galvanostat model 283 voltammetrice analyser in CH_3CN solutions (1×10^{-3} mol L^{-1}) at a scan rate of 100 mV s-1 with a platinum plate as the working electrode, a silver wire as the pseudo-reference electrode and a platinum wire as the couner electrode. Tetrabutylammonium tetrafluoroborate (0.1 mol L^{-1}) was used as supporting electrolyte, and ferrocene was selected as the internal standard. The solution was bubbled with nitrogen for 10 min before measurements.

Synthesis and characterization of complex 1. The ancillary ligand 2-(1*H*-pyrazol-1-yl)pyridine (pzpy) was conveniently synthesized from 2-bromopyridine and pyrazole. As reported,[18] the dichloro-bridged diiridium complex $[Ir(ppy)_2Cl]_2$ (0.4378 g, 0.408 mmol) and the ancillary ligand pzpy (0.1337 g, 0.921 mmol) were dissolved in 20 mL 1,2-ethanediol, refluxed at 150 ºC for 12 h under an argon atmosphere to form a clear bright yellow solution. After cooling to room temperature, the reaction mixture was added with an aqueous solution of $Na[Bph_4]$ (1.3688 g, 4.000 mmol in 100 mL water) under stirring, and then filtrated. The resulting precipitate was washed with deionized water and dried under vacuum at 70 ºC overnight. The crude product was purified by column chromatography on silica gel (200-300 mesh) with CH_2Cl_2 as the eluent, yielding a bright light-yellow powder

(0.4433 g, 0.459 mmol). Yields: 57 %. ^{1}H NMR (600 MHz, DMSO-d_6, δ) 9.30 (d, J = 2.8 Hz, 1H), 8.52 (d, J = 8.5 Hz, 1H), 8.35-8.30 (m, 1H), 8.26 (dd, J = 8.2, 4.1 Hz, 2H), 7.99-7.93 (m, 2H), 7.91 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 7.8 Hz, 1H), 7.76 (d, J = 5.8 Hz, 1H), 7.71 (d, J = 5.8 Hz, 1H), 7.65 (d, J = 5.5 Hz, 1H), 7.55-7.51 (m, 1H), 7.28 (s, 1H), 7.19-7.15 (m, 9H), 7.02 (t, J = 7.6 Hz, 1H), 6.99 (t, J = 7.5 Hz, 1H), 6.92 (t, J = 7.3 Hz, 9H), 6.89 (d, J = 7.4 Hz, 1H), 6.85 (t, J = 7.4 Hz, 1H), 6.78 (t, J = 7.1 Hz, 4H), 6.20 (d, J = 8.9 Hz, 1H), 6.21-6.17 (m, 2H). MS (ESI) [m/z]: 646.25 (M-Bph$_4$)$^+$, 319.39 (M-[Ir(ppy)$_2$(pzpy)])$^-$. Anal. calcd. for $C_{54}H_{43}N_5BIrH_2O$: C, 65.58; H, 4.61; N, 7.12. Found: C, 66.24; H, 4.62; N, 7.31. Space group of $P2_1/n$ with a = 9.5427(19), b = 13.247(3), c = 35.237(7) Å; α = 90.00, β = 93.01(3), γ = 90.00 º; V = 4448.2(15) Å^3; Z = 4, d_{calcd} = 1.472 g cm^{-3}; R_1 = 0.0321; ωR_2 = 0.0621 for 7674 observed reflections [$I \geq 2\sigma(I)$].

Synthesis and characterization of complex 2. The synthesis of complex 2 was similar to that of complex 1 except that Na[Bph$_4$] was replaced with Na[BIm$_4$]. Yields: 70 %. ^{1}H NMR (600 MHz, DMSO-d_6, δ) 9.26 (d, J = 2.8 Hz, 1H), 8.52 (d, J = 6.5 Hz, 1H), 8.48 (d, J = 8.3 Hz, 1H), 8.29 (t, J = 8.0 Hz, 1H), 8.22 (dd, J = 7.8 Hz, 4.0 Hz, 2H), 8.05 (d, J = 8.3 Hz, 1H), 7.92 (t, J = 7.1 Hz, 2H), 7.85 (dd, J = 12.5 Hz, 7.8 Hz, 2H), 7.73 (d, J = 5.7 Hz, 1H), 7.67 (d, J = 5.8 Hz, 1H), 7.61 (d, J = 5.0 Hz, 2H), 7.51-7.48 (m, 1H), 7.25 (s, 1H), 7.15 (d, J = 11.3 Hz, 3H), 7.00-6.96 (m, 4H), 6.95-6.83 (m, 4H), 6.84-6.77 (m, 4H), 6.47 (s, 1H), 6.18-6.13 (m, 2H). MS (ESI) [m/z]: 646.16 (M-[BIm$_4$])$^+$, 279.13 (M-[Ir(ppy)$_2$(pzpy)])$^-$. Anal. calcd. for $C_{42}H_{35}BIrN_{13}$: C, 54.54; H, 3.81; N, 19.69. Found: C, 54.84; H, 4.05; N, 18.21.

Synthesis and characterization of complex 3. The synthesis of complex 3 was similar to that of complex 1 except that the dichloro-bridged diiridium complex [Ir(ppy)$_2$Cl]$_2$ was replaced with [Ir(dfppy)$_2$Cl]$_2$. Yields: 75 %. ^{1}H NMR (600 MHz, DMSO-d_6, δ) 9.29 (d, J = 3.0 Hz, 1 H), 8.50 (d, J = 8.5 Hz, 1H), 8.30 (dt, J = 15.6, 4.3 Hz, 1 H), 8.26 (d, J = 6.2 Hz, 2H), 8.01 (ddd, J = 5.6, 5.2, 2.6 Hz, 2 H), 7.80 (d, J = 5.3 Hz, 1H), 7.74 (d, J = 5.2 Hz, 1H), 7.71 (d, J = 4.8 Hz, 1 H), 7.16 (d, J = 1.3 Hz, 10 H), 6.97-6.86 (m, 10H), 6.76 (t, J = 7.2 Hz, 5 H), 5.63 (d, J = 2.3 Hz, 1 H), 5.62 (d, J = 2.3 Hz, 1 H), 5.60 (d, J = 2.3 Hz, 1H), 5.58 (d, J = 2.3 Hz, 1H). MS (ESI) [m/z]: 718.37 (M-Bph$_4$)$^+$, 319.39 (M-[Ir(dfppy)$_2$(pzpy)])$^-$. Anal. calcd. for $C_{54}H_{39}BF_4IrN_5$: C, 62.55; H, 3.79; N, 6.75. Found: C, 63.13; H, 3.64; N, 6.89. Space group of P_{-1} with a = 12.694(3), b = 15.159(3), c = 17.350(4) Å; α = 79.17(3), β = 69.47(3), γ = 72.48(3) º; V = 2968.8(10) Å^3; Z = 2, d_{calcd} = 1.420 g cm^{-3}; R_1 = 0.0843; ωR_2 = 0.1965 for 10956 observed reflections [$I \geq 2\sigma(I)$].

Synthesis and characterization of complex 4. The synthesis of complex 4 was similar to that of complex 1 except that the dichloro-bridged diiridium complex [Ir(ppy)$_2$Cl]$_2$ was replaced with [Ir(dfppy)$_2$Cl]$_2$ and Na[Bph$_4$] was replaced with Na[BIm$_4$]. Yields: 59 %. ^{1}H NMR (600 MHz, DMSO-d_6, δ) 9.28 (d, J = 3.0 Hz, 1H), 8.48 (d, J = 8.5 Hz, 1H), 8.31-8.26 (m, 1H), 8.21 (d, J = 7.5 Hz, 2H), 7.98 (dd, J = 9.9 Hz, 5.6 Hz, 2H), 7.76 (d, J = 5.6 Hz, 1H), 7.69 (d, J = 5.7 Hz, 1H), 7.66 (d, J = 5.4 Hz, 2H), 7.49-7.44 (m, 2H), 7.25-7.18 (m, 2H), 6.97 (s, 4H), 6.91-6.86 (m, 4H), 6.85 (s, 4H), 6.68 (s, 4H). MS (ESI) [m/z]: 718.42 (M-[BIm$_4$])$^+$, 279.28 (M-[Ir(dfppy)$_2$(pzpy)])$^-$. Anal. calcd. for $C_{42}H_{31}BF_4IrN_{13}$: C, 50.61; H, 3.13; N, 18.27. Found: C, 48.76; H, 3.03; N, 16.95.

X-ray crystallography. Single crystals of complexes 1 and 3 were grown from solutions. Acetone was used as good solvent, and ethanol and deionized water was used as poor solvent for complex 1 and 3, respectively. The low-temperature single-crystal X-ray experiments were performed on a Bruker APEX charge-coupled device (CCD) diffractometer equipped with graphite monochromatized $MO_{K\alpha}$ radiation. Crystallographic data of complexes 1 and 3 can be found in CCDC 963326 and 995213, respectively, which can be obtained free of charge from the Cambridge Crystallographic Data Centre from www.ccdc.cam.ac.uk/conts/retrieving.html.

Quantum Chemical Calculations. Calculations on the ground and excited electronic states of the counterions [Bph$_4$]$^-$ and [BIm$_4$]$^-$ were carried out with density functional theory (DFT) according to B3LYP/6-31 G* calculations using Gaussian.[19] The initial ground-state geometry of [Bph$_4$]$^-$ was directly obtained from the X-ray single crystal structure of complex 1,[16] while the initial ground-state geometry of [BIm$_4$]$^-$ was optimized first.

Conclusions

In summary, a series of novel green-blue emitting ionic iridium complexes with tetraphenylborate and tetraimidazolylborate as the counterion, respectively, have been designed and synthesized. Photophysical and electrochemical characteristics were fully investigated with both experimental and theoretical methods. It indicates that from tetraphenylborate to tetraimidazolylborate, electrochemical stabilities are sharply improved. OLEDs based on these compounds were fabricated to study the effect of different counterions on EL properties. Ionic iridium complexes with tetraphenylborate as the counterion gave no luminance in devices, suffering from the strong reducibilities. While OLEDs based on complexes with tetraimidazolylborate as counterions are green-blue emitting, with a high current efficiency of 9.48 cd A^{-1} and a maximum brightness of 5163 cd m^{-2}.

However, the EL spectra of devices are red-shifted compared with PL spectra, which indicates that counterions indeed affect the EL mechanism of devices doped with ionic transition metal complexes. It would be part of our further work.

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[a] Key Lab of Organic Optoelectronics and Molecular Engineering of Ministry of Education, Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China. E-mail: duanl@mail.tsinghua.edu.cn; Fax: +86-10-62795137; Tel: +86-10-62788802.

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Tetraimidazolylborate is first used as the counterion of cationic iridium complexes to improve both electrochemical stabilities and device performance.

Color Graphic