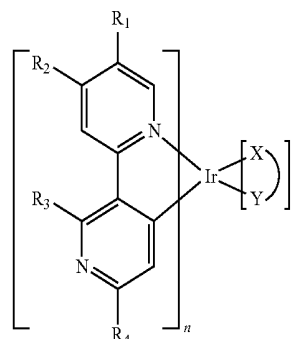


(19) **United States**(12) **Patent Application Publication**
LIN et al.(10) **Pub. No.: US 2017/0162804 A1**(43) **Pub. Date: Jun. 8, 2017**(54) **ORGANOMETALLIC COMPOUND AND ORGANIC LIGHT-EMITTING DEVICE EMPLOYING THE SAME**(71) Applicant: **INDUSTRIAL TECHNOLOGY RESEARCH INSTITUTE**, Hsinchu (TW)(72) Inventors: **Jin-Sheng LIN**, Taipei City (TW); **Jia-Lun LIOU**, Hengshan Township (TW); **Meng-Hao CHANG**, New Taipei City (TW); **Han-Cheng YEH**, Taipei City (TW)(73) Assignee: **INDUSTRIAL TECHNOLOGY RESEARCH INSTITUTE**, Hsinchu (TW)(21) Appl. No.: **15/178,761**(22) Filed: **Jun. 10, 2016**(30) **Foreign Application Priority Data**

Dec. 4, 2015 (TW) 104140698

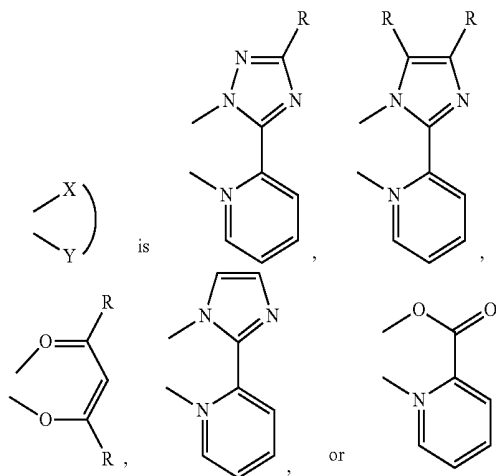
Publication Classification(51) **Int. Cl.****H01L 51/00** (2006.01)**C09K 11/06** (2006.01)**C07F 15/00** (2006.01)(52) **U.S. Cl.**CPC **H01L 51/0094** (2013.01); **C07F 15/0033** (2013.01); **C09K 11/06** (2013.01); **H01L 51/5016** (2013.01)(57) **ABSTRACT**

Organometallic compounds and organic electroluminescence devices employing the same are provided. The organometallic compound has a chemical structure represented below:

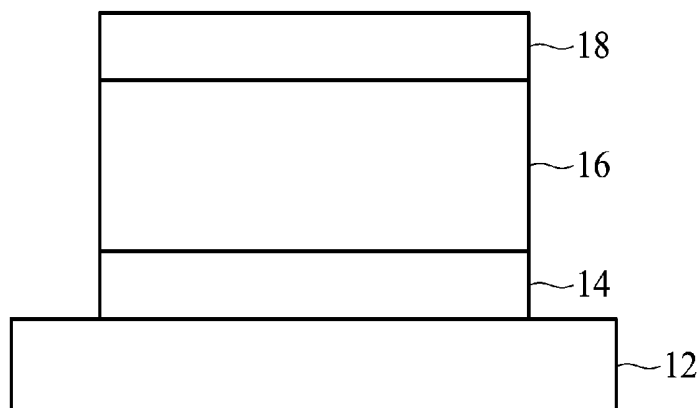


Formula (I)

In Formula (I), one of R1 and R2 is trimethylsilyl (TMS) and the other is hydrogen, at least one of R3 and R4 is fluorine or C1-6 alkyl, or one of R3 and R4 is fluorine and the other is C1-6 alkyl,



n is 2 or 3, and m is 0 or 1, wherein n+m=3.

10

10

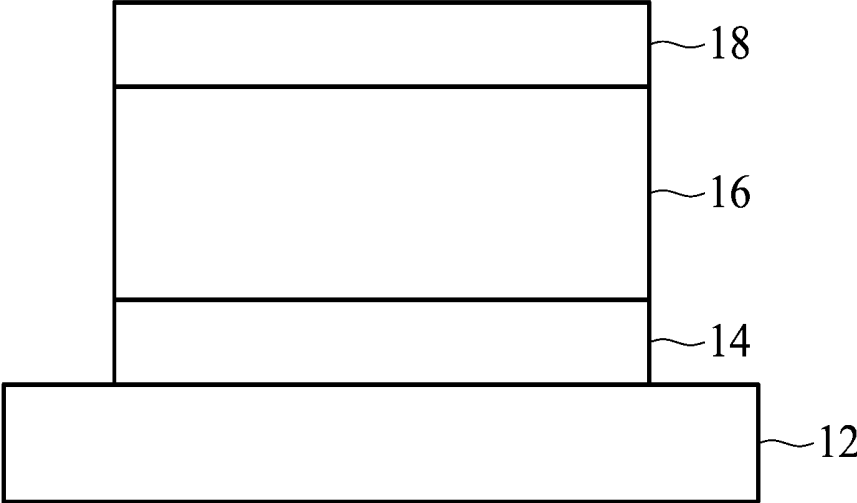


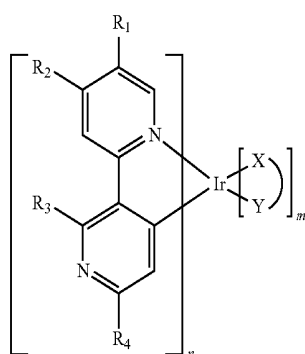
FIG. 1

[0014] FIG. 1 shows a cross section of an organic light-emitting device disclosed by an embodiment of the disclosure.

DETAILED DESCRIPTION

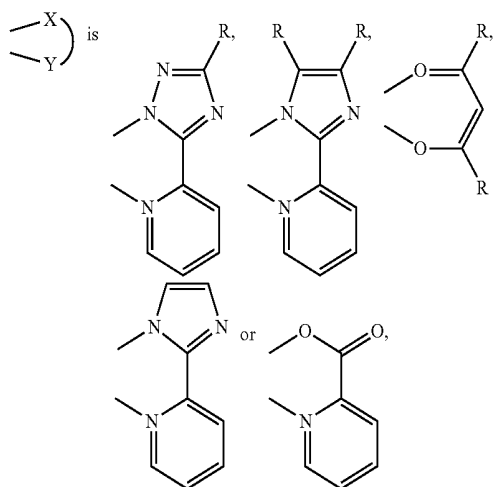
[0015] The following description is of the best-contemplated mode of carrying out the disclosure. This description is made for the purpose of illustrating the general principles of the disclosure and should not be taken in a limiting sense. The scope of the disclosure is best determined by reference to the appended claims.

[0016] According to an embodiment of the disclosure, the disclosure provides an organometallic compound having a structure represented by the following Formula (I):



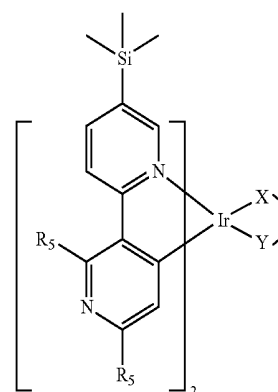
Formula (I)

[0017] In Formula (I), one of R_1 and R_2 may be trimethylsilyl (TMS) and the other is hydrogen, at least one of R_3 and R_4 is fluorine or C_{1-6} alkyl, or one of R_3 and R_4 may be fluorine and the other may be C_{1-6} alkyl,



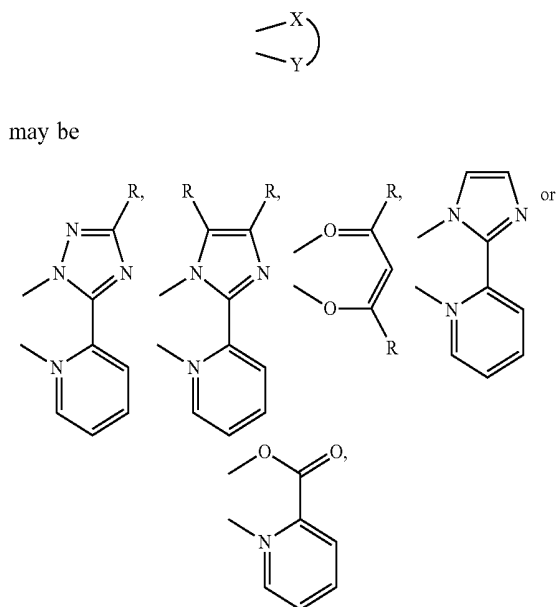
R may be CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl, n may be 2 or 3, and m may be 0 or 1, wherein $n+m=3$.

[0018] According to an embodiment of the disclosure, the organometallic compound may have a structure represented by Formula (II):



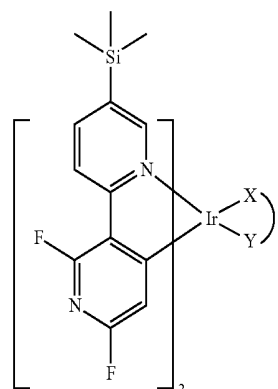
Formula (II)

[0019] In Formula (II), R_5 may be fluorine or C_{1-6} alkyl,



R may be CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl.

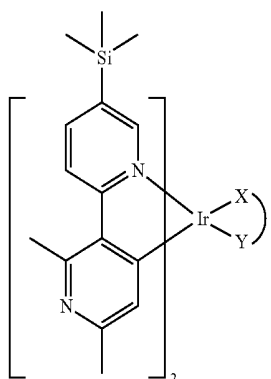
[0020] According to an embodiment of the disclosure, the organometallic compound may have a structure represented by Formula (III) or Formula (IV):



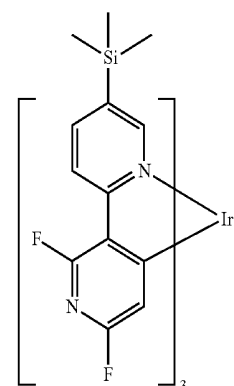
Formula (III)

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Formula (IV)



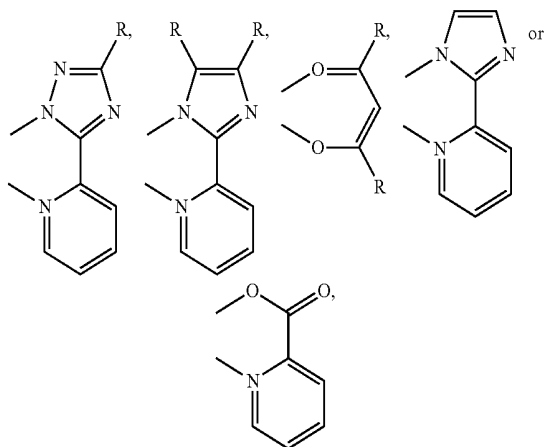
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[0021] In Formula (III) or Formula (IV)

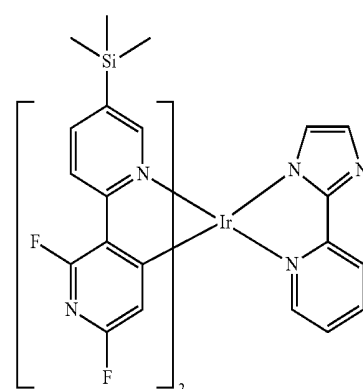
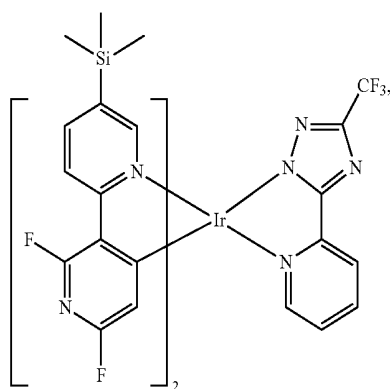
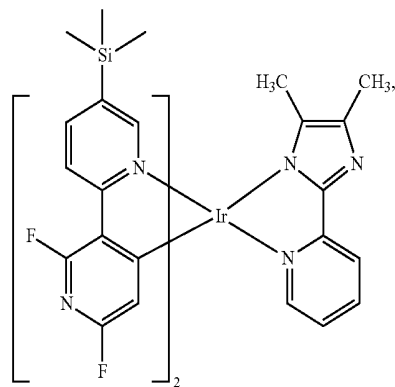
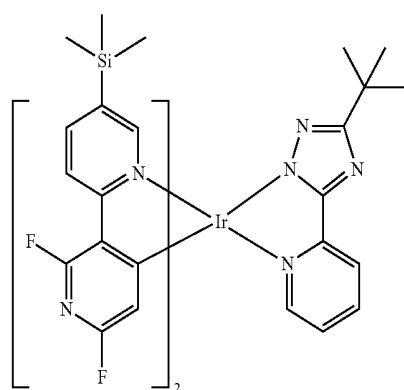


may be

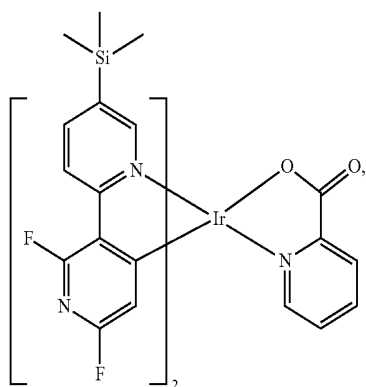


R may be CH₃, CH₂CH₃, CH(CH₃)₂, C(CH₃)₃, CF₃, CHF₂, C₃F₈ or phenyl.

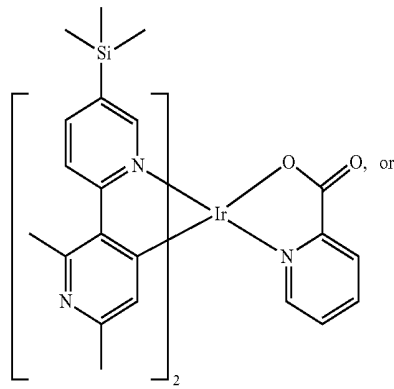
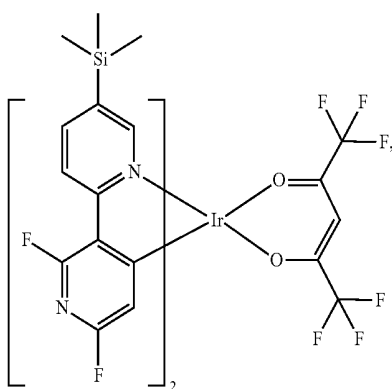
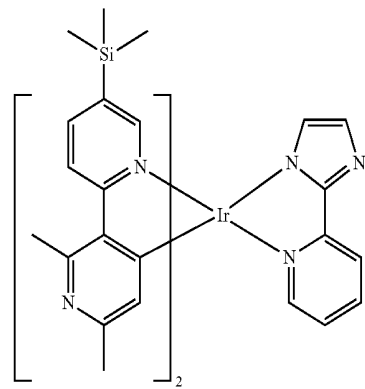
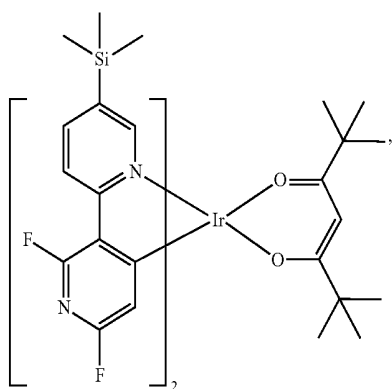
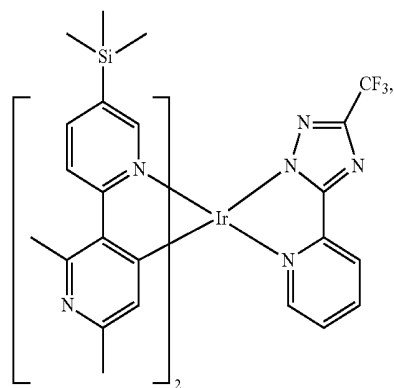
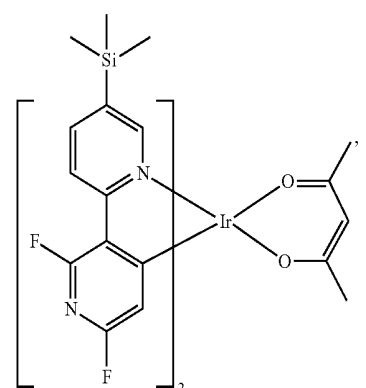
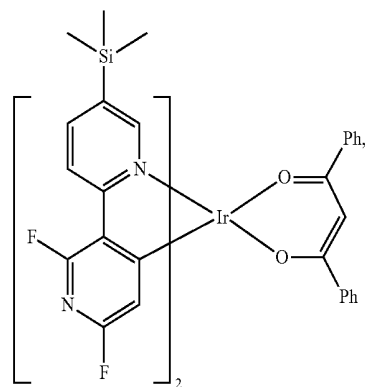
[0022] According to an embodiment of the disclosure, the organometallic compound may be



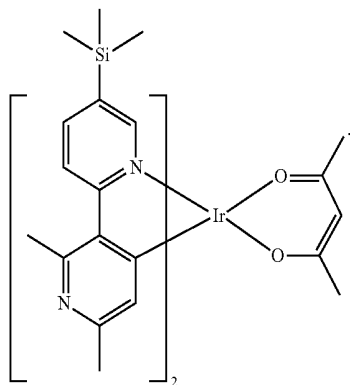
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-continued



[0023] According to another embodiment of the disclosure, the disclosure provides an organic light-emitting device. The device includes an anode, a cathode and an

organic light-emitting element disposed between the anode and the cathode. The organic light-emitting element includes the aforementioned organometallic compound.

[0024] According to another embodiment of the disclosure, the disclosure provides an organic light-emitting device. The device includes an anode, a cathode and an organic light-emitting element disposed between the anode and the cathode. The organic light-emitting element includes a first light-emitting layer. The first light-emitting layer includes the aforementioned organometallic compound.

[0025] According to another embodiment of the disclosure, the organic light-emitting element further includes a second light-emitting layer disposed between the anode and the first light-emitting layer or between the first light-emitting layer and the cathode. The second organic light-emitting layer includes the aforementioned organometallic compound.

[0026] According to another embodiment of the disclosure, the organic light-emitting device may emit blue light.

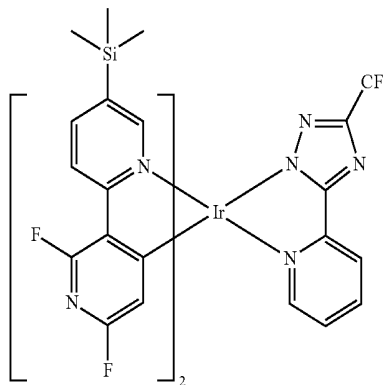
[0027] The organometallic compounds according to Formula (I)-(IV) of the disclosure include the compounds shown in Table 1.

TABLE 1

Example	Structure	abbreviation
1		DFTIr(taz)

1

DFTIr(taz)



2

DFTIr(iaz)

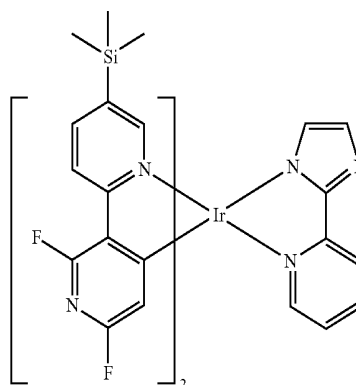


TABLE 1-continued

Example	Structure	abbreviation
3	<p>The structure shows an iridium (Ir) center coordinated to two bidentate ligands. One ligand is a 2,6-difluoropyridine-3,5-dicarboxylate derivative, where the 2 and 6 positions are fluorinated and the 3 and 5 positions are coordinated to the Ir. The other ligand is a picolinic acid derivative (pic), which is a 2-pyridinecarboxylic acid. A tert-butylsilyl group (SiMe₃) is attached to the 4-position of the pyridine ring of the first ligand. The entire complex is shown within brackets with a subscript 2, indicating a dimeric species.</p>	DFTIr(pic)
4	<p>The structure shows an iridium (Ir) center coordinated to two bidentate ligands. One ligand is a 2,6-difluoropyridine-3,5-dicarboxylate derivative, where the 2 and 6 positions are fluorinated and the 3 and 5 positions are coordinated to the Ir. The other ligand is a 2-tert-butyl-1H-tetrazol-5-ylpyridine derivative (taz2), where the 2-position of the pyridine ring is substituted with a tert-butyl group and the 5-position is coordinated to the Ir. A tert-butylsilyl group (SiMe₃) is attached to the 4-position of the pyridine ring of the first ligand. The entire complex is shown within brackets with a subscript 2, indicating a dimeric species.</p>	DFTIr(taz2)
5	<p>The structure shows an iridium (Ir) center coordinated to two bidentate ligands. One ligand is a 2,6-difluoropyridine-3,5-dicarboxylate derivative, where the 2 and 6 positions are fluorinated and the 3 and 5 positions are coordinated to the Ir. The other ligand is a 2,4-dimethyl-1H-imidazole-5-ylpyridine derivative (Miaz), where the 2 and 4 positions of the imidazole ring are substituted with methyl groups and the 5-position is coordinated to the Ir. A tert-butylsilyl group (SiMe₃) is attached to the 4-position of the pyridine ring of the first ligand. The entire complex is shown within brackets with a subscript 2, indicating a dimeric species.</p>	DFTIr(Miaz)
6	<p>The structure shows an iridium (Ir) center coordinated to two bidentate ligands. One ligand is a 2,6-difluoropyridine-3,5-dicarboxylate derivative, where the 2 and 6 positions are fluorinated and the 3 and 5 positions are coordinated to the Ir. The other ligand is an acetylacetonate (acac) derivative, which is a 1,5-diketone. A tert-butylsilyl group (SiMe₃) is attached to the 4-position of the pyridine ring of the first ligand. The entire complex is shown within brackets with a subscript 2, indicating a dimeric species.</p>	DFTIr(acac)

TABLE 1-continued

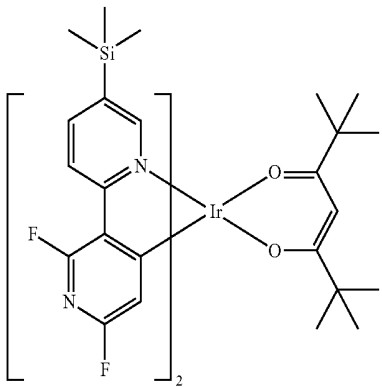
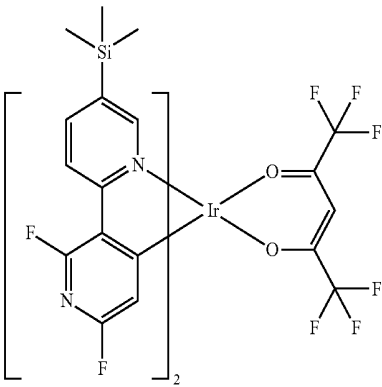
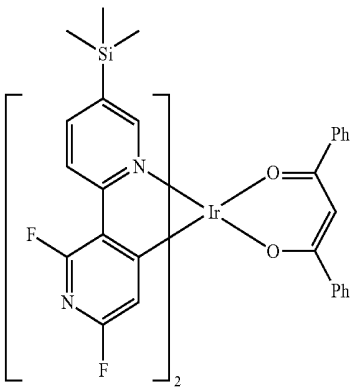
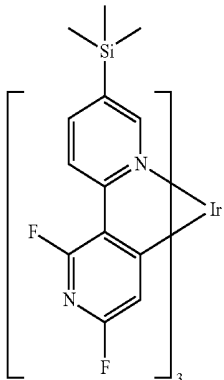
Example	Structure	abbreviation
7		DFTIr(tmd)
8		DFTIr(hf)
9		DFTIr(dbm)
10		DFTIr

TABLE 1-continued

Example	Structure	abbreviation
11		DMTIr(taz)
12		DMTIr(iaz)
13		DMTIr(pic)
14		DMTIr(acac)

[0028] FIG. 1 shows an embodiment of an organic light-emitting device 10. The organic light-emitting device 10

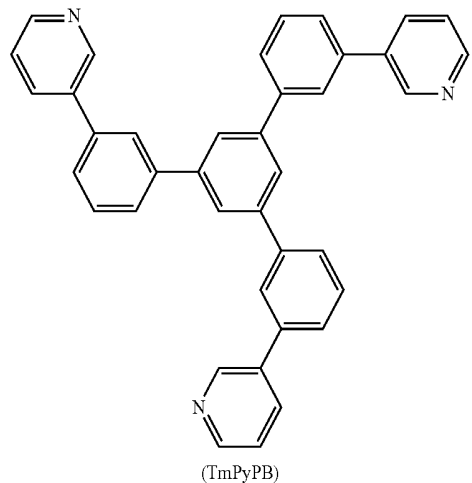
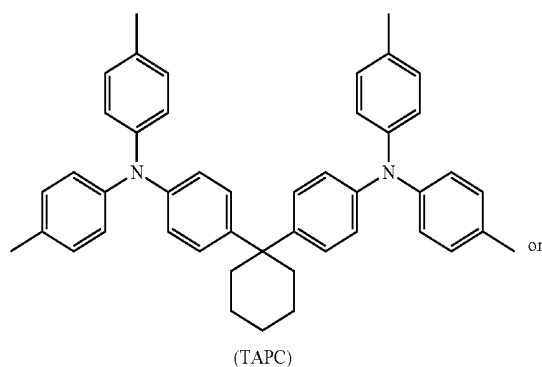
includes a substrate 12, an anode 14, an organic light-emitting element 16, and a cathode 18, as shown in FIG. 1.

The anode **14** is disposed on the substrate **12**, the organic light-emitting element **16** is disposed on the anode **14**, and the cathode **18** is disposed on the organic light-emitting element **16**.

[0029] The organic light-emitting element **16** at least includes a first organic light-emitting layer, and can further include a hole injection layer, a hole transport layer, an electron transport layer, and an electron injection layer. In an embodiment of the disclosure, at least one layer of the organic light-emitting element **16** includes the aforementioned organometallic compounds.

[0030] The organic light-emitting device can be a top-emission, bottom-emission, or dual-emission device. The substrate **12** can be a glass, plastic, or semiconductor substrate. Suitable materials for the anode **14** can be indium tin oxide (ITO), indium zinc oxide (IZO), aluminum zinc oxide (AZO), or zinc oxide (ZnO). Suitable materials for the cathode **18** can be Ca, Ag, Mg, Al, Li, In, Au, Ni, W, Pt, or Cu. The organic light-emitting layer can be formed by sputtering, electron beam evaporation, thermal evaporation, or chemical vapor deposition. Furthermore, at least one of the anode **14** and cathode **18** is transparent.

[0031] According to embodiments of the disclosure, Suitable materials for the hole transport layer and the electron transport layer can be



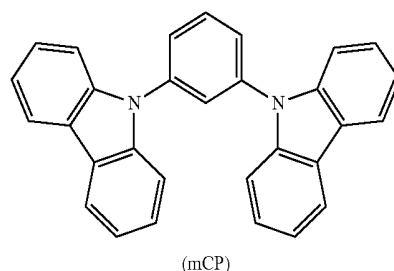
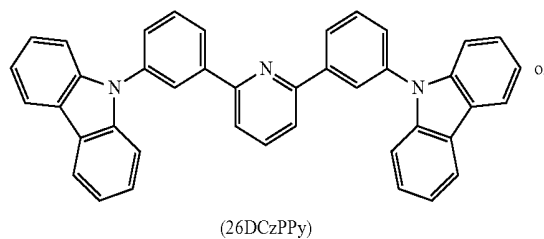
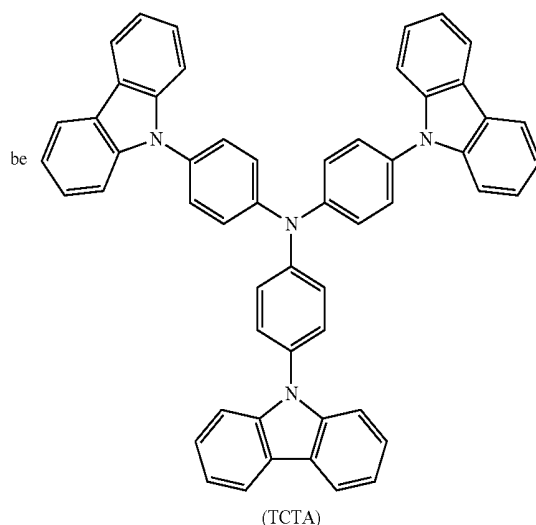
[0032] According to embodiments of the disclosure, the organic light-emitting element **16** can emit blue or green light under a bias voltage.

[0033] According to embodiments of the disclosure, the organic light-emitting element **16** can further include a second organic light-emitting layer disposed between the

anode **14** and the first light-emitting layer or between the first light-emitting layer and the cathode **18**. The second organic light-emitting layer includes the aforementioned organometallic compound.

[0034] According to embodiments of the disclosure, the first and second organic light-emitting layers at least include a host and a dopant.

[0035] According to embodiments of the disclosure, Suitable materials for the host can



[0036] According to embodiments of the disclosure, Suitable materials for the dopant can include the aforementioned organometallic compounds.

[0037] The simple layered structure illustrated in FIG. 1 is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost

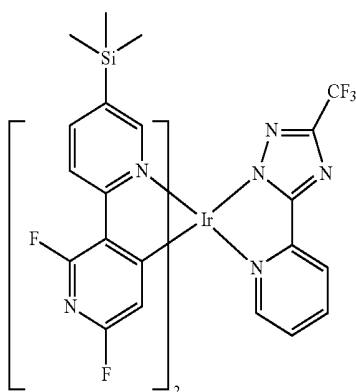
factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting.

[0038] In order to clearly disclose the organic light-emitting devices of the disclosure, the following examples (employing the organometallic compounds of the disclosure) are intended to illustrate the disclosure more fully without limiting their scope, since numerous modifications and variations will be apparent to those skilled in this art. For example, when the organometallic compounds of the disclosure serves as a dopant material, the organometallic compounds of the disclosure can have a weight percentage from 0.1 wt % to 15 wt %, based on the weight of the host material.

EXAMPLE 1

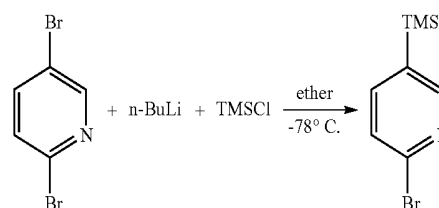
Preparation of Organometallic Compound DFTIr(taz)

[0039]

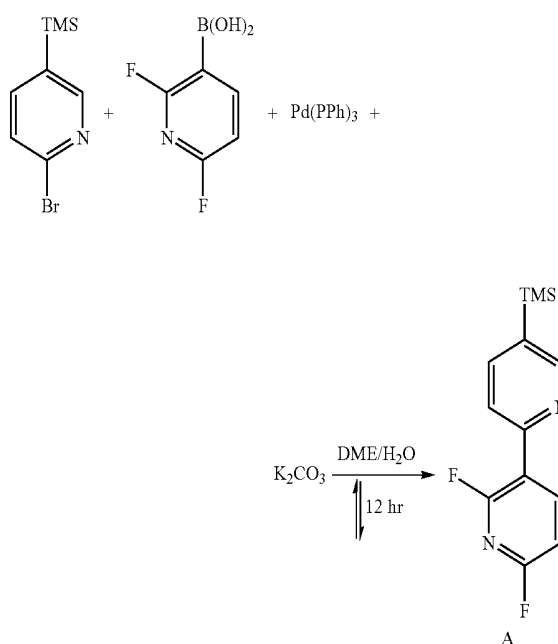


Organometallic compound DFTIr(taz)

[0040] Firstly, after a 100 mL double-neck bottle was dried to remove the moisture and the air several times, 2,5-dibromopyridine (1 g, 4.22 mmol) and dehydrated ether (40 mL) were dropwise added into the bottle under nitrogen atmosphere. Next, after cooling to -78°C . and temperature equilibrating, *n*-BuLi (3 mL, 4.64 mmol) was dropwise added into the reaction bottle and subjected to reaction at -78°C . for 1 hours, and then TMSCl (0.65 mL, 5 mmol) was added thereto. The reaction was then warmed to room temperature and the reaction mixture was extracted three times using ethyl acetate (EA) and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), 2-bromo-5-trimethylsilylpyridine was obtained. The synthesis pathway of the above reaction was as follows:

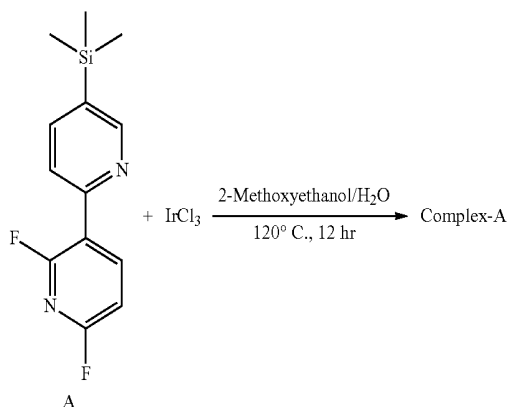


[0041] Next, 2-Bromo-5-trimethylsilylpyridine (0.7 g, 3 mmol), 2,4-difluoropyridine boric acid (0.52 g, 3.3 mmol), K_2CO_3 (0.4 g, 1 mmol), dimethoxyethane (20 mL), water (10 mL) and tetrakis(triphenylphosphine)palladium $\text{Pd}(\text{PPh}_3)_4$ (0.17 g, 0.15 mmol) were added into a 100 mL double-neck bottle. After the reaction bottle was dried to remove the moisture and the air therein, the reaction bottle was heated to reflux under nitrogen atmosphere and keep refluxing overnight. After cooling to room temperature, the reaction mixture was neutralized to weak alkalinity (pH 8 to 10) with saturated sodium hydrogen carbonate (NaHCO_3) aqueous solution, and then the mixture was extracted with ethyl acetate (EA) and water. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), a compound (A) was obtained. The synthesis pathway of the above reaction was as follows:

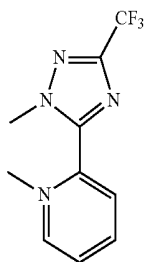


[0042] The compound A (1.7 g, 6.6 mmol), IrCl_3 (0.89 g, 3 mmol), 2-methoxyethanol (24 mL) and water (8 mL) were added into a 100 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120°C . under nitrogen atmosphere and keep reacting overnight.

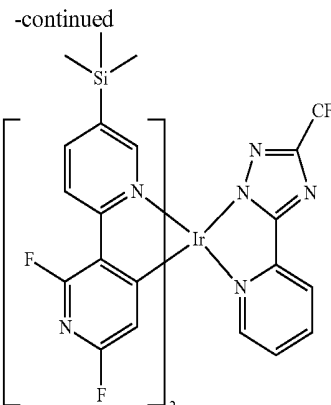
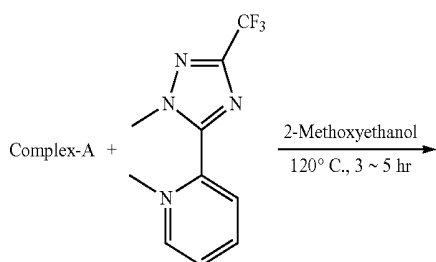
After cooling to room temperature, water was added into the reaction mixture to produce precipitate. Then, the precipitate purified and dried under vacuum, and, obtaining a complex A. The synthesis pathway of the above reaction was as follows:



[0043] The complex A (0.5 g, 0.33 mmol), ligand



(285 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to produce precipitate. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DFTIr(taz) was obtained. The synthesis pathway of the above reaction was as follows:

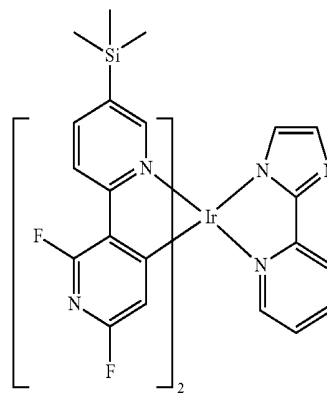


[0044] The physical measurement of the compound DFTIr(taz) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.37 (d, 1H), 8.25 (d, 1H), 8.21 (d, 1H), 8.02 (t, 1H), 7.90 (d, 2H), 7.83 (d, 1H), 7.58 (s, 1H), 7.38~7.32 (m, 2H), 5.74 (t, 1H), 5.64 (t, 1H), 0.15 (s, 9H), 0.06 (s, 9H).

EXAMPLE 2

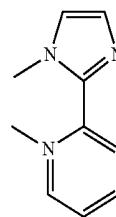
Preparation of Organometallic Compound DFTIr(iaz)

[0045]



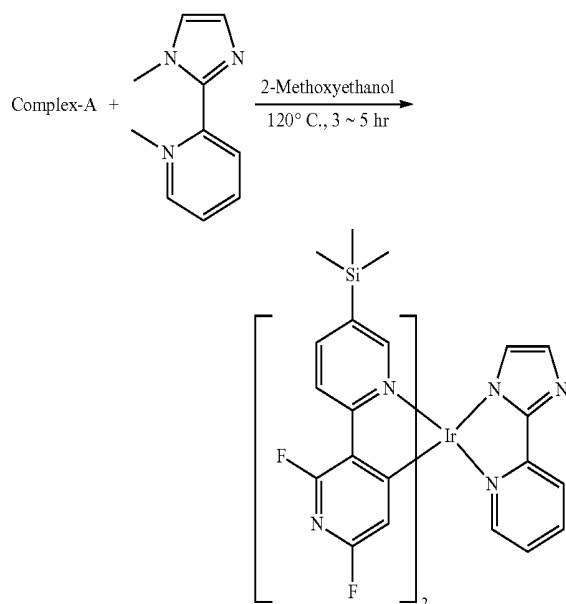
Organometallic compound DFTIr(iaz)

[0046] The complex A (0.5 g, 0.33 mmol), ligand (



) (193 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce

precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH_2Cl_2 . The result was extracted three times with CH_2Cl_2 and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), Compound DFTIr(iaz) was obtained. The synthesis pathway of the above reaction was as follows:

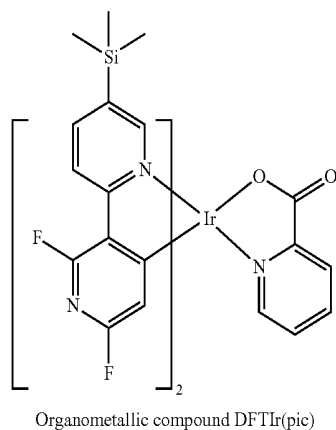


[0047] The physical measurement of the compound DFTIr(iaz) is listed below: $^1\text{H NMR}$ (200 MHz, CDCl_3 , 294 K): δ 8.29~8.17 (m, 3H), 7.88~7.77 (m, 3H), 7.67 (d, 1H), 7.62 (s, 1H), 7.52 (s, 1H), 7.32 (s, 1H), 7.06 (t, 1H), 6.61 (s, 1H), 5.80 (t, 1H), 5.68 (t, 1H), 0.13 (s, 9H), 0.09 (s, 9H).

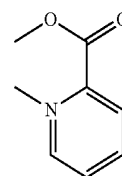
EXAMPLE 3

Preparation of Organometallic Compound DFTIr(pic)

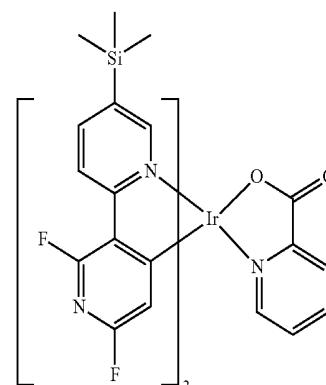
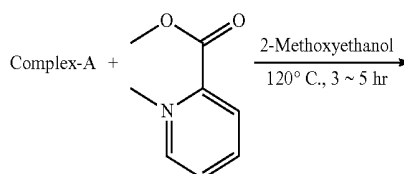
[0048]



[0049] The complex A (0.5 g, 0.33 mmol), ligand (



) (193 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH_2Cl_2 . The result was extracted three times with CH_2Cl_2 and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), Compound DFTIr(pic) was obtained. The synthesis pathway of the above reaction was as follows:

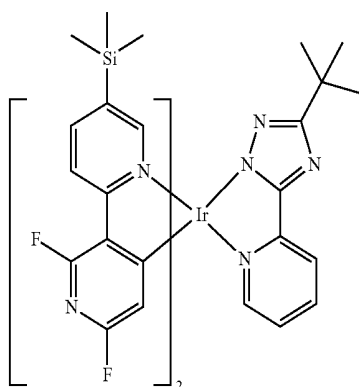


[0050] The physical measurement of the compound DFTIr(pic) is listed below: $^1\text{H NMR}$ (200 MHz, CDCl_3 , 294 K): δ 8.78 (s, 1H), 8.38 (d, 1H), 8.27~8.20 (m, 2H), 8.05 (dt, 1H), 7.80~7.91 (m, 2H), 7.83 (d, 1H), 7.53 (t, 1H), 7.31 (s, 1H), 5.80 (s, 1H), 5.57 (s, 1H), 0.31 (s, 9H), 0.08 (s, 9H).

EXAMPLE 4

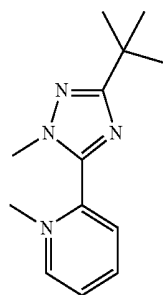
Preparation of Organometallic Compound
DFTIr(taz2)

[0051]

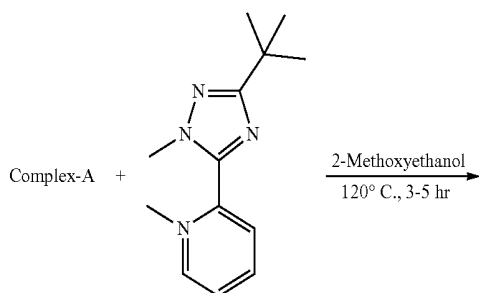


Organometallic compound DFTIr(taz2)

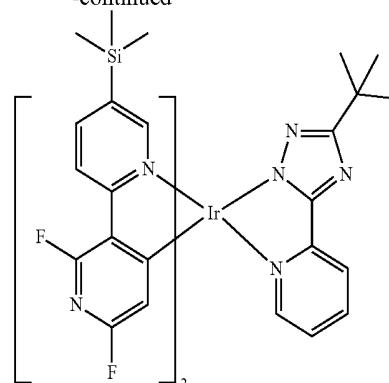
[0052] The complex A (0.5 g, 0.33 mmol), ligand (



) (269 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DFTIr(taz2) was obtained. The synthesis pathway of the above reaction was as follows:



-continued

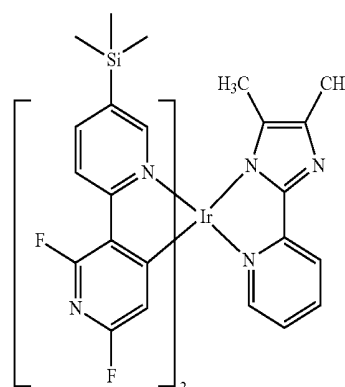


[0053] The physical measurement of the compound DFTIr(taz2) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.28~8.16 (m, 3H), 7.91~7.83 (m, 3H), 7.72 (s, 1H), 7.70 (d, 1H), 7.45 (s, 1H), 7.15 (t, 1H), 5.69~5.66 (m, 2H), 1.37 (s, 9H), 0.17 (s, 9H), 0.08 (s, 9H).

EXAMPLE 5

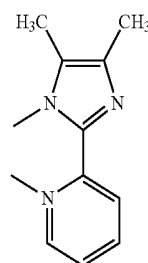
Preparation of Organometallic Compound
DFTIr(Miaz)

[0054]



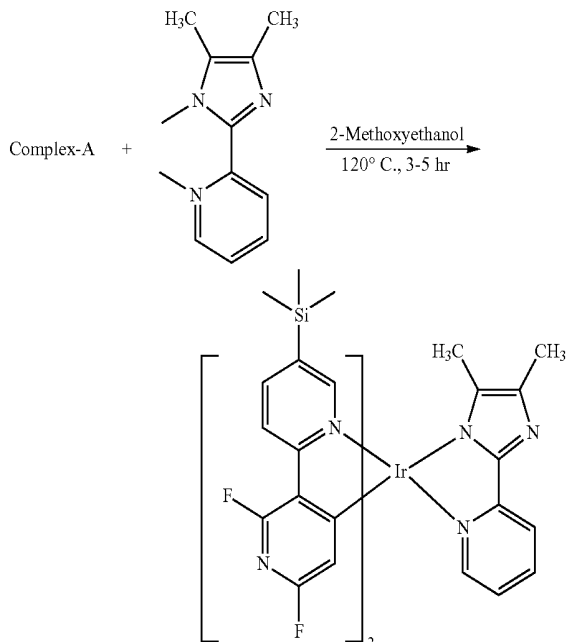
Organometallic compound DFTIr(Miaz)

[0055] The complex A (0.5 g, 0.33 mmol), ligand (



) (299 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatog-

raphy (SiO_2 , EA/Hexane=1/40), Compound DFTIr(Miaz) was obtained. The synthesis pathway of the above reaction was as follows:

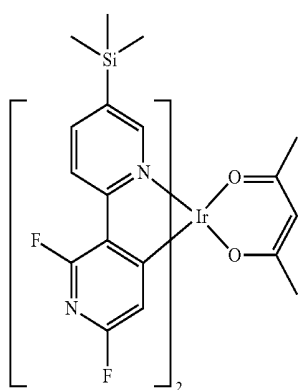


[0056] The physical measurement of the compound DFTIr(Miaz) is listed below: $^1\text{H NMR}$ (200 MHz, CDCl_3 , 294 K): δ 8.35~8.22 (m, 3H), 7.95~7.80 (m, 3H), 7.70 (d, 1H), 7.65 (s, 1H), 7.50 (s, 1H), 7.35 (s, 1H), 7.10 (t, 1H), 6.61 (s, 1H), 3.51 (s, 3H), 3.12 (s, 3H), 0.15 (s, 9H), 0.08 (s, 9H).

EXAMPLE 6

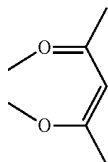
Preparation of Organometallic Compound DFTIr(acac)

[0057]

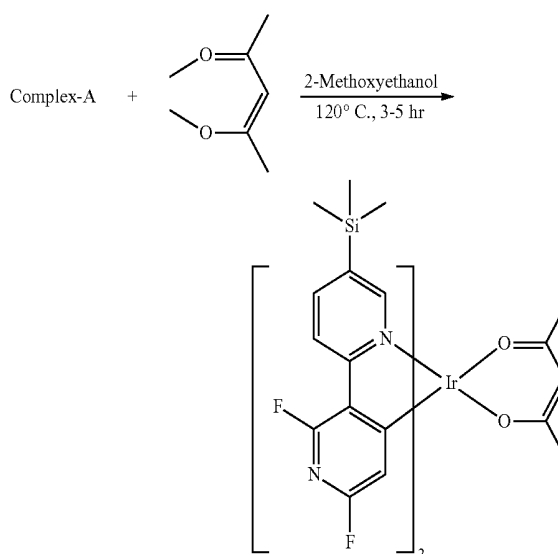


Organometallic compound DFTIr(acac)

[0058] The complex A (0.5 g, 0.33 mmol), ligand (



) (133 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH_2Cl_2 . The result was extracted three times with CH_2Cl_2 and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), Compound DFTIr(acac) was obtained. The synthesis pathway of the above reaction was as follows:

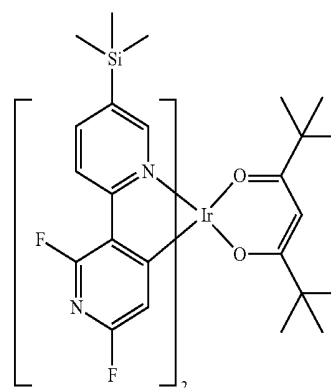


[0059] The physical measurement of the compound DFTIr(acac) is listed below: $^1\text{H NMR}$ (200 MHz, CDCl_3 , 294 K): δ 8.45 (s, 2H), 8.22 (d, 2H), 7.97 (d, 2H), 5.65 (t, 2H), 5.33 (s, 1H), 1.85 (s, 6H), 0.35 (s, 18H).

EXAMPLE 7

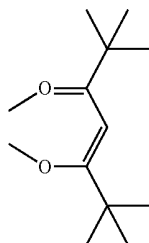
Preparation of Organometallic Compound DFTIr(tmd)

[0060]

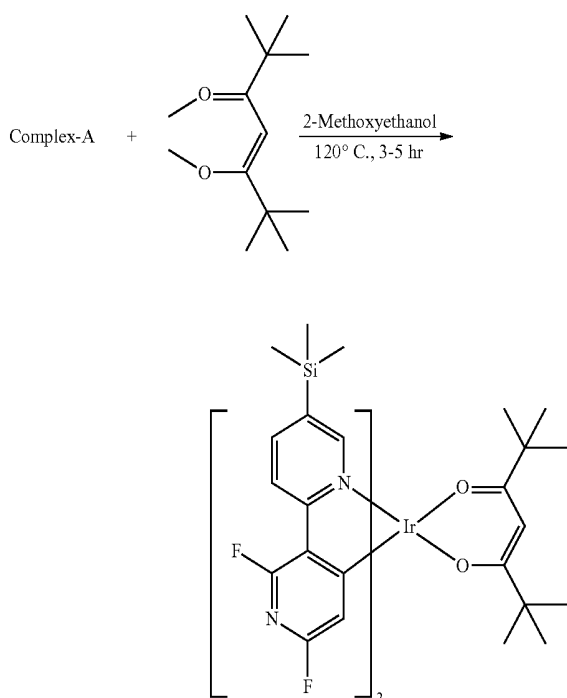


Organometallic compound DFTIr(tmd)

[0061] The complex A (0.5 g, 0.33 mmol), ligand (



) (245 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DFTIr(tmd) was obtained. The synthesis pathway of the above reaction was as follows:

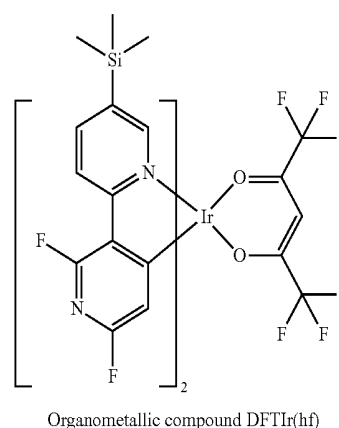


[0062] The physical measurement of the compound DFTIr(tmd) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.31 (s, 2H), 8.17 (d, 2H), 7.90 (d, 2H), 5.81 (t, 2H), 5.613 (s, 1H), 0.84 (s, 18H), 0.29 (s, 18H).

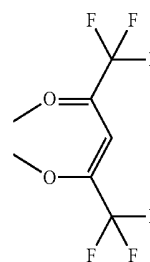
EXAMPLE 8

Preparation of Organometallic Compound DFTIr(hf)

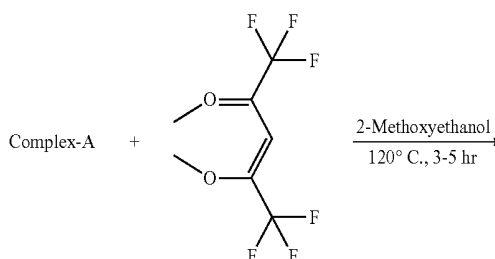
[0063]

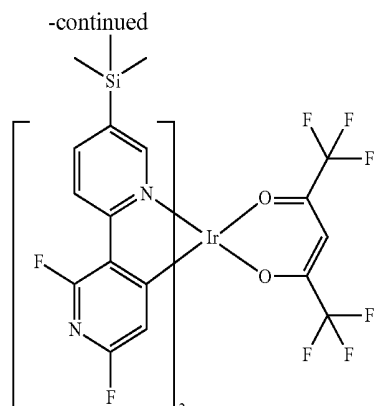


[0064] The complex A (0.5 g, 0.33 mmol), ligand (



) (277 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DFTIr(hf) was obtained. The synthesis pathway of the above reaction was as follows:



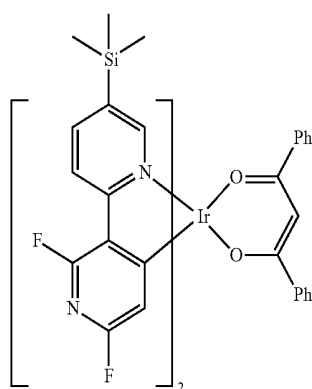


[0065] The physical measurement of the compound DFTIr (hf) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.27 (d, 2H), 8.25 (s, 2H), 8.06 (d, 2H), 6.09 (s, 1H), 5.60 (t, 2H), 0.34 (s, 18H).

EXAMPLE 9

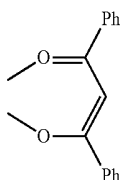
Preparation of Organometallic Compound DFTIr(dbm)

[0066]



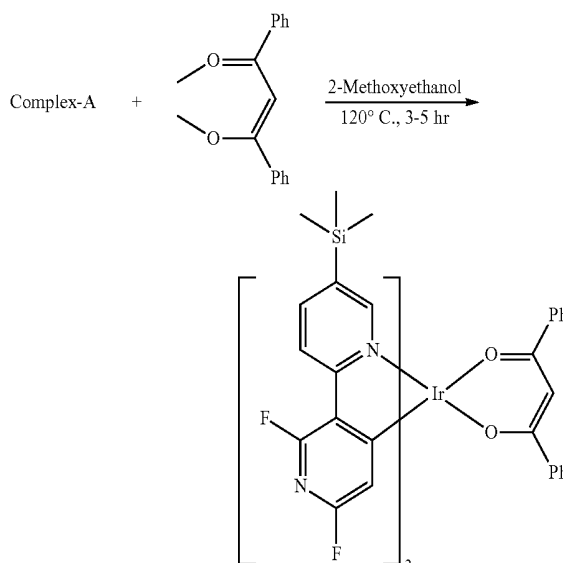
Organometallic compound DFTIr(dbm)

[0067] The complex A (0.5 g, 0.33 mmol), ligand (



) (311 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DFTIr(dbm)

was obtained. The synthesis pathway of the above reaction was as follows:



[0068] The physical measurement of the compound DFTIr (dbm) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.56 (s, 2H), 8.22 (d, 2H), 7.92 (d, 2H), 7.80 (d, 4H), 7.47~7.31 (m, 6H), 6.67 (s, 1H), 5.76 (t, 2H), 0.15 (s, 18H).

[0069] The photoluminescence (PL) emission spectra of the organometallic compounds (a series of DFTIr) of the disclosure

[0070] As shown in Table 2, the organometallic compounds of the disclosure having a stronger electron-withdrawing ligand (such as: pic, taz or taz2) can exhibit a blue-shifted emission and serve as blue phosphorescent material. For example, the PL spectra (452 nm) of the organometallic compound DFTIr(pic) can have a 23 nm blue-shift in comparison with the PL spectra (475 nm) of the conventional phosphorescent material Ir(pic).

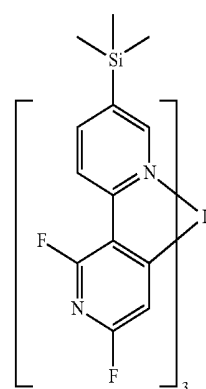
TABLE 2

DFTIr (aac)	DFTIr (pic)	DFTIr (taz)	DFTIr (taz2)
465 nm	452 nm	447 nm	452 nm

EXAMPLE 10

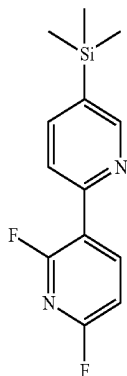
Preparation of Organometallic Compound DFTIr

[0071]

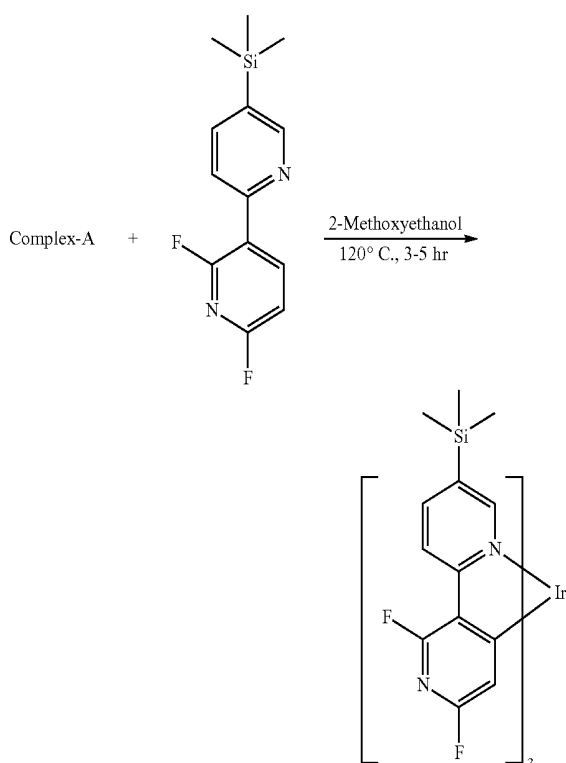


Organometallic compound DFTIr

[0072] The complex A (0.37 g, 0.25 mmol), ligand (



) (200 mg, 0.25 mmol), AgOCOCF_3 (160 mg, 0.75 mmol) and diphenyl ether (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 165°C . under nitrogen atmosphere and keep reacting for two hours. After cooling down to room temperature, purified by column chromatography (SiO_2 , EA/Hexane=1/8), Compound DFTIr was obtained. The synthesis pathway of the above reaction was as follows:



[0073] The physical measurement of the compound DFTIr is listed below: $^1\text{H NMR}$ (200 MHz, CDCl_3 , 294 K): δ 8.33 (d, 1H), 8.21 (t, 2H), 8.05~7.77 (m, 5H), 7.31 (s, 1H), 6.43 (t, 1H), 5.92 (t, 1H), 5.70 (s, 1H), 0.14 (s, 9H), 0.12 (s, 9H), 0.05 (s, 9H).

[0074] The photoluminescence (PL) emission spectra of the organometallic compounds (a series of DFTIr) of the disclosure

[0075] The organometallic compound DFTIr have a property of the PL spectra (448 nm) and the half maximum wavelength (57 nm), that is, it is a high colorimetric purity and serves as blue phosphorescent material. Thus, it can be used for lighting application of color temperature adjusting and display application of pure blue light emission.

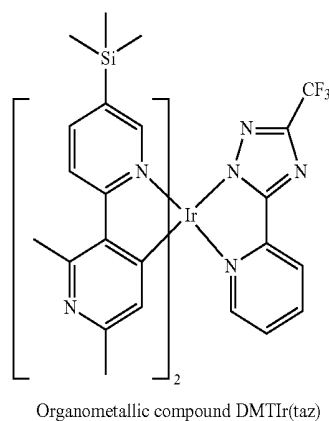
[0076] The sublimation purification of the organometallic compounds (a series of DFTIr) of the disclosure

[0077] The organometallic compounds (a series of DFTIr) of the disclosure have a sublimation yield that is close to 100% due to their good thermal stability. The devices in Examples of the disclosure show high yield as compared with the conventional phosphorescent material Ir(pic) (its yield is about 50%). For example, after the compound DFTIr(acac) was purified by a sublimation process, there's almost nothing in the tube after sublimation and almost all the compound DFTIr(acac) was sublimated into the collection tube.

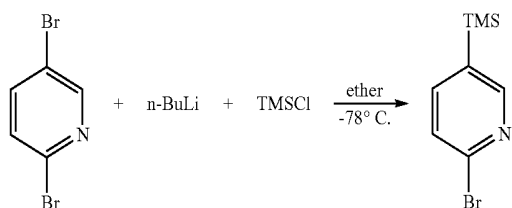
EXAMPLE 11

Preparation of Organometallic Compound DMTIr(taz)

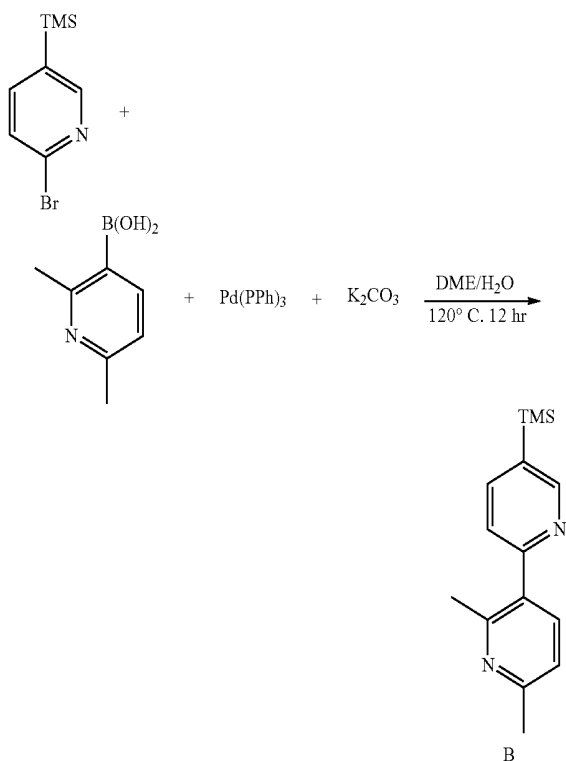
[0078]



[0079] Firstly, after a 100 mL double-neck bottle was dried to remove the moisture and the air several times, 2,5-dibromopyridine (1 g, 4.22 mmol) and dehydrated ether (40 mL) were dropwise added into the bottle under nitrogen atmosphere. Next, after cooling to -78°C . and temperature equilibrating, n-BuLi (3 mL, 4.64 mmol) was dropwise added into the reaction bottle and subjected to reaction at -78°C . for 1 hours, and then TMSCl (0.65 mL, 5 mmol) was added thereto. The reaction was then warmed to room temperature and the reaction mixture was extracted three times using ethyl acetate (EA) and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), 2-bromo-5-trimethylsilylpyridine was obtained. The synthesis pathway of the above reaction was as follows:

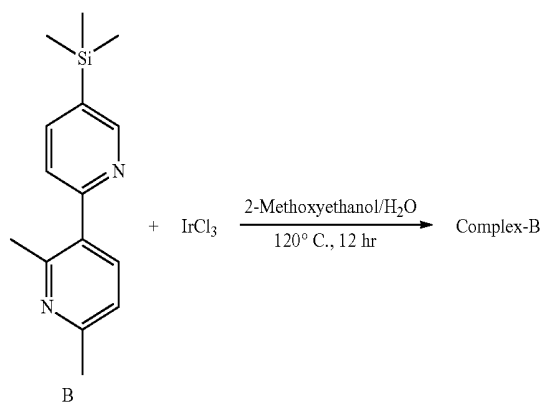


[0080] Next, 2-Bromo-5-trimethylsilylpyridine (0.7 g, 3 mmol), 2,4-dimethylpyridine bromic acid (0.52 g, 3.3 mmol), K_2CO_3 (0.4 g, 1 mmol), dimethoxyethane (20 mL), water (10 mL) and tetrakis(triphenylphosphine)palladium $Pd(PPh_3)_4$ (0.17 g, 0.15 mmol) were added into a 100 mL double-neck bottle. After the reaction bottle was dried to remove the moisture and the air therein, the reaction bottle was heated to reflux under nitrogen atmosphere and keep refluxing overnight. After cooling to room temperature, the reaction mixture was neutralized to weak alkalinity (pH 8 to 10) with saturated sodium hydrogen carbonate ($NaHCO_3$) aqueous solution, and then the mixture was extracted with ethyl acetate (EA) and water. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), and compound (B) was obtained. The synthesis pathway of the above reaction was as follows:

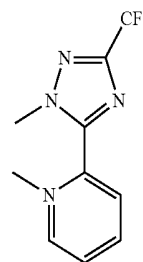


[0081] The compound B (1.7 g, 6.6 mmol), $IrCl_3$ (0.89 g, 3 mmol), 2-methoxyethanol (24 mL) and water (8 mL) were added into a 100 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting overnight. After cooling to room temperature, water was added into the reaction mixture to induce precipitation. Then, the precipi-

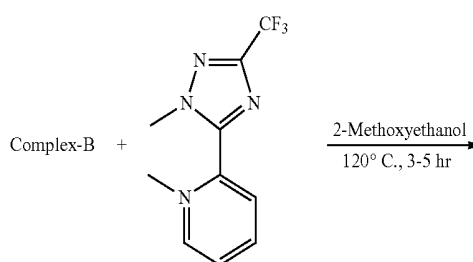
tate was purified and dried under vacuum, and a complex B was obtained. The synthesis pathway of the above reaction was as follows:

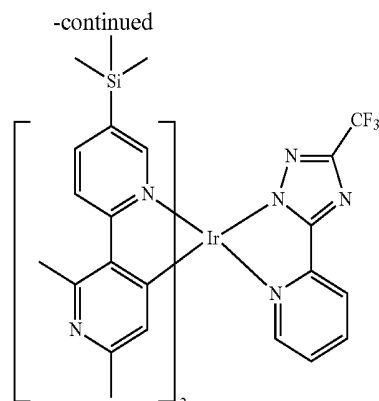


[0082] The complex B (0.5 g, 0.33 mmol), ligand (



) (285 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH_2Cl_2 . The result was extracted three times with CH_2Cl_2 and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), Compound DMTIr(taz) was obtained. The synthesis pathway of the above reaction was as follows:



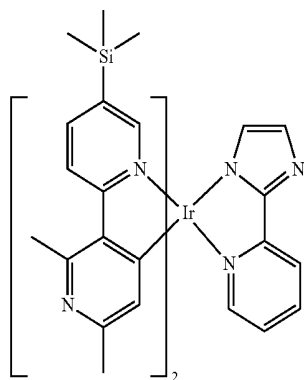


[0083] The physical measurement of the compound DMTIr(taz) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.31 (d, 1H), 8.11 (d, 1H), 8.04 (d, 1H), 7.91 (t, 1H), 7.84~7.78 (m, 3H), 7.69 (d, 1H), 7.50 (s, 1H), 7.22 (t, 1H), 5.92 (s, 1H), 5.83 (s, 1H), 2.86 (s, 6H), 2.29 (s, 3H), 2.23 (s, 3H), 0.15 (s, 9H), 0.04 (s, 9H).

EXAMPLE 12

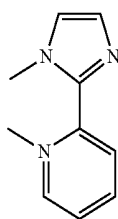
Preparation of Organometallic Compound DMTIr(iaz)

[0084]



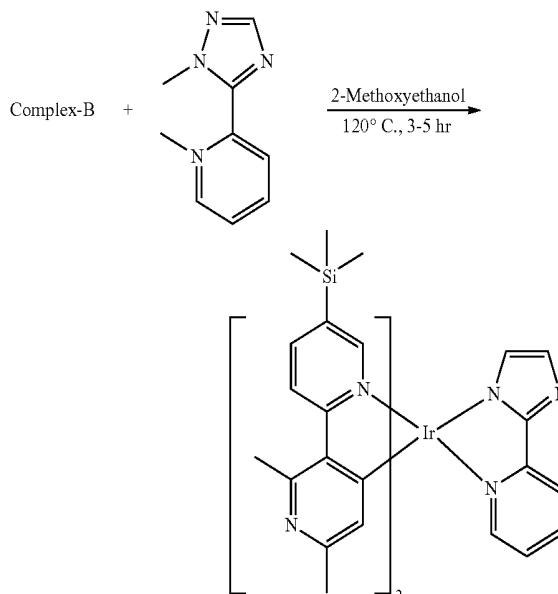
Organometallic compound DMTIr(iaz)

[0085] The complex B (0.5 g, 0.33 mmol), ligand (



) (193 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce

precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DMTIr(iaz) was obtained. The synthesis pathway of the above reaction was as follows:

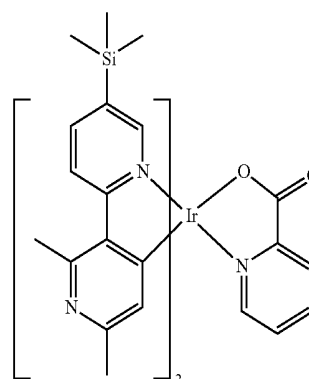


[0086] The physical measurement of the compound DFMIr(iaz) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.29~8.17 (m, 3H), 7.88~7.77 (m, 3H), 7.67 (d, 1H), 7.62 (s, 1H), 7.52 (s, 1H), 7.32 (s, 1H), 7.06 (t, 1H), 6.61 (s, 1H), 5.80 (t, 1H), 5.68 (t, 1H), 0.13 (s, 9H), 0.09 (s, 9H).

EXAMPLE 13

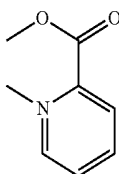
Preparation of Organometallic Compound DMTIr(pic)

[0087]

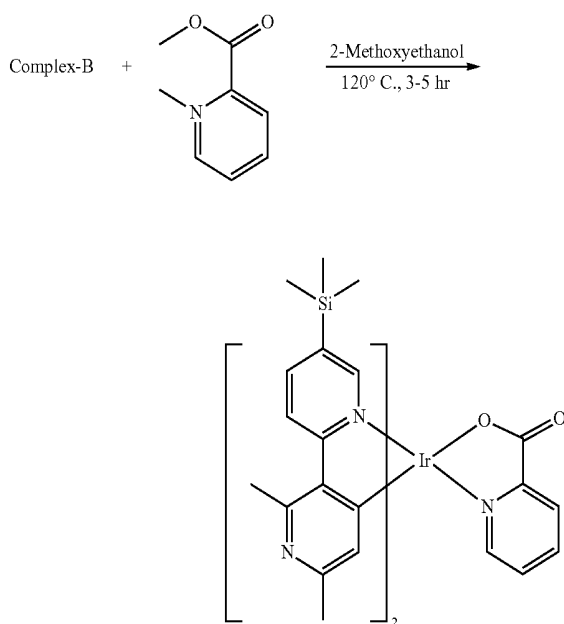


Organometallic compound DMTIr(pic)

[0088] The complex B (0.5 g, 0.33 mmol), ligand (



) (193 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DMTIr(pic) was obtained. The synthesis pathway of the above reaction was as follows:

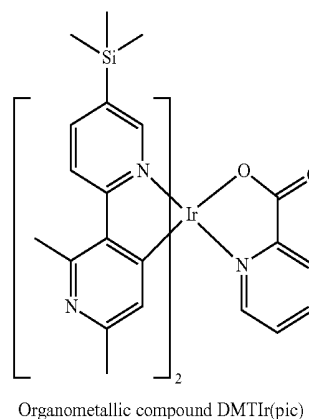


[0089] The physical measurement of the compound DMTIr(pic) is listed below: ¹H NMR (200 MHz, CDCl₃, 294 K): δ 8.87 (s, 1H), 8.33 (d, 1H), 8.10 (dd, 2H), 7.99~7.85 (m, 3H), 7.71 (d, 1H), 7.45~7.39 (m, 2H), 6.02 (s, 1H), 5.78 (s, 1H), 2.92 (s, 3H), 2.86 (s, 3H), 2.26 (s, 3H), 2.23 (s, 3H), 0.31 (s, 9H), 0.07 (s, 9H).

EXAMPLE 13

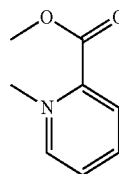
Preparation of Organometallic Compound DMTIr(pic)

[0090]

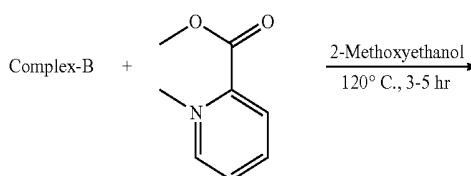


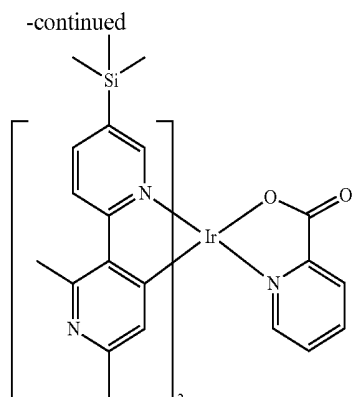
Organometallic compound DMTIr(pic)

[0091] The compound complex B (0.5 g, 0.33 mmol), ligand (



) (193 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH₂Cl₂. The result was extracted three times with CH₂Cl₂ and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO₂, EA/Hexane=1/40), Compound DMTIr(pic) was obtained. The synthesis pathway of the above reaction was as follows:



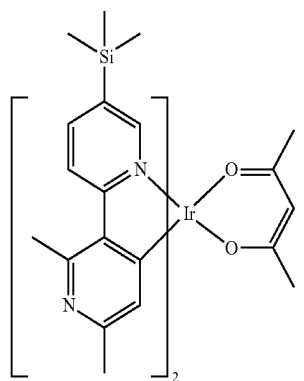


[0092] The physical measurement of the compound DMTIr(pic) is listed below: ^1H NMR (200 MHz, CDCl_3 , 294 K): δ 8.87 (s, 1H), 8.33 (d, 1H), 8.10 (dd, 2H), 7.99~7.85 (m, 3H), 7.71 (d, 1H), 7.45~7.39 (m, 2H), 6.02 (s, 1H), 5.78 (s, 1H), 2.92 (s, 3H), 2.86 (s, 3H), 2.26 (s, 3H), 2.23 (s, 3H), 0.31 (s, 9H), 0.07 (s, 9H).

EXAMPLE 14

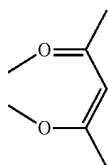
Preparation of Organometallic Compound DMTIr(acac)

[0093]



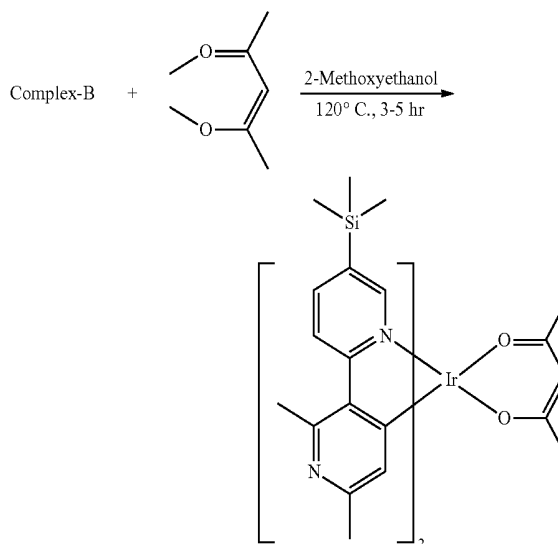
Organometallic compound DMTIr(acac)

[0094] The complex B (0.5 g, 0.33 mmol), ligand (



) (133 mg, 1.33 mmol), trimethylamine (0.1 mL, 1.33 mmol) and 2-methoxyethanol (5 mL) were added into a 10 mL flask. After removing the moisture and the air therein, the reaction bottle was heated to 120° C. under nitrogen atmosphere and keep reacting for three hours. After cooling to room temperature, water was added into the result to induce precipitation. The precipitate was collected and washed with water and hexane, and then dissolved into CH_2Cl_2 . The

result was extracted three times with CH_2Cl_2 and water as the extraction solvent. Next, an organic phase was separated and concentrated, and then purified by column chromatography (SiO_2 , EA/Hexane=1/40), Compound DMTIr(pic) was obtained. The synthesis pathway of the above reaction was as follows:



[0095] The physical measurement of the compound DMTIr(pic) is listed below: ^1H NMR (200 MHz, CDCl_3 , 294 K): δ 8.57 (s, 2H), 8.07 (d, 2H), 7.89 (d, 2H), 5.90 (s, 2H), 5.24 (s, 1H), 2.84 (s, 6H), 2.19 (s, 6H), 1.79 (s, 6H), 0.33 (s, 18H).

EXAMPLE 15

Fabrication of the Organic Light-Emitting Device (1) (Dry Process)

[0096] A glass substrate with an indium tin oxide (ITO) film with a thickness of 110 nm was provided and then washed with a cleaning agent, acetone, and isopropanol with ultrasonic agitation. After drying with nitrogen flow, the ITO film was subjected to a UV/ozone treatment for 30 min. Next, TAPC(1,1-bis[4-[N,N'-di (p-tolyl)amino]phenyl]cyclohexane, with a thickness of 40 nm), 26DCzPPY doped with the organometallic compound DFTIr(acac) of Example 6 (the ratio between 26DCzPPY and the organometallic compound DFTIr(acac) was 10:1, with a thickness of 10 nm), TmPyPB (1,3,5-tri(p-pyrid-3-yl-phenyl)benzene, with a thickness of 50 nm), LiF (with a thickness of 0.8 nm), and Al (with a thickness of 120 nm) were subsequently deposited on the ITO film at 10^{-6} torr, obtaining the organic light-emitting device (1). The materials and layers formed therefrom are described in the following: ITO (150 nm)/TAPC (40 nm)/26DCzPPY:organometallic DFTIr(acac)(10%)(10 nm)/TmPyPB (50 nm)/LiF (0.8 nm)/Al (120 nm)

[0097] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y) of the light-emitting device (1), as described in Example 15, were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 3

EXAMPLE 16

Fabrication of the Organic Light-Emitting Device
(2) (Dry Process)

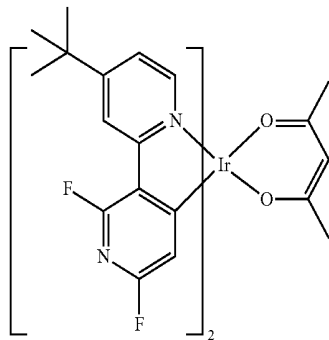
[0098] Example 16 was performed in the same manner as in Example 15 except that TATC was substituted for 26DCzPPy (TCTA doped with the organometallic compound DFTIr(acac) of Example 6), obtaining the organic light-emitting device (2). The materials and layers formed therefrom are described in the following: ITO (150 nm)/TAPC (40 nm)/TCTA:organometallic DFTIr(acac)(10%)(10 nm)/TmPyPB (50 nm)/LiF (0.8 nm)/Al (120 nm)

[0099] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (1), as described in Example 15, were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 3

COMPARATIVE EXAMPLE 1

Fabrication of a Traditional Organic Light-Emitting Device (Dry Process)

[0100] Comparative Example 1 was performed in the same manner as in Example 15 except that mCP doped with FK306 (



) was substituted for 26DCzPPy doped with the organometallic compound DFTIr(acac), obtaining the traditional organic light-emitting device.

[0101] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (1), as described in Example 15, were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 3

TABLE 3

Light-emitting layer	current efficiency (cd/A)	power efficiency (lm/W)	λ_{\max} (nm)	C.I.E coordinate (x, y)
Comparative Example 1 mCP:FK306	21.5	16.1	454	(0.16, 0.25)

TABLE 3-continued

Light-emitting layer	current efficiency (cd/A)	power efficiency (lm/W)	λ_{\max} (nm)	C.I.E coordinate (x, y)
Example 15 26DCzPPy:DFTIr(acac)	25.2	18.7	464	(0.15, 0.25)
Example 16 TCTA:DFTIr(acac)	22.0	17.2	464	(0.15, 0.25)

[0102] In accordance with Table 3, in the examples, the optical properties of the organic light emitting diodes fabricated with host material 26DCzPPy or TCTA combined with the dopant DFTIr(acac) are shown in Table 3. Particularly, the current efficiency of the organic light emitting diode (1) fabricated with host material 26DCzPPy combined with the dopant DFTIr(acac) (25.2 cd/A) was about 16% times higher than that of the organic light-emitting diode (2) fabricated with host material TCTA combined with the dopant DFTIr(acac) (22.0 cd/A) (measured at a brightness of 1000 Cd/m²).

EXAMPLE 17

[0103] The optical properties of the organometallic compounds of the disclosure

[0104] As shown in Table 4, in the example, the optical properties of organic light emitting diodes fabricated by host material 26DCzPPy combined with various dopants was measured, because the organic light emitting diode (1) fabricated with host material 26DCzPPy exhibited higher optical properties than the organic light emitting diode (2). Due to the organometallic compound DFTIr(tmd) showing great steric hindrance, the optical properties and light of the organic light emitting diode with it was similar to that of the organic light emitting diode with DFTIr(acac). The organometallic compounds having a stronger electron-withdrawing ligand (such as: pic, taz or taz2) had a 12-16 nm blue-shift, but the luminescence efficiencies of the organic light emitting diodes with these dopants were over 10 lm/W. The organometallic compound DMTIr(acac) emitted bluish green light, but the luminescence efficiency of the organic light emitting diode with that achieved 57.2 lm/W.

TABLE 4

	current efficiency (cd/A)	power efficiency (lm/W)	λ_{\max} (nm)	C.I.E coordinate (x, y)
DFTIr (acac)	25.2	18.7	464	(0.15, 0.25)
DFTIr (tmd)	24.9	17.4	464	(0.15, 0.25)
DFTIr (pic)	18.2	12.0	452	(0.15, 0.23)
DFTIr (taz)	20.2	14.5	448	(0.15, 0.22)
DFTIr (taz2)	19.7	14.1	452	(0.15, 0.23)
DMTIr (acac)	65.3	57.2	492	(0.19, 0.52)
DMTIr (pic)	30.2	22.4	476	(0.18, 0.37)

EXAMPLE 18

Fabrication of the Organic Light-Emitting Device
(3) (Wet Process)

[0105] A glass substrate with an indium tin oxide (ITO) film with a thickness of 150 nm was provided and then washed with a cleaning agent, acetone, and isopropanol with

ultrasonic agitation. After drying with nitrogen flow, the ITO film was subjected to a UV/ozone treatment for 30 min.

[0106] Next, PEDOT(poly(3,4)-ethylenedioxythiophen):PSS (e-polystyrenesulfonate) was coated on the ITO film by a blade and spin coating process (with a rotation rate of 2000 rpm) and baked at 130° C. for 10 min to form a PEDOT:PSS film serving as a hole injection layer (with a thickness of 40 nm). Next, a composition was used for forming a light-emitting layer coated on the PEDOT:PSS film by a blade coating process and baked at 100° C. for 40 min to form the light-emitting layer (with a thickness of 30 nm). The composition used for forming a light-emitting layer includes mCP and the organometallic compound DFTIr(acac), wherein the weight ratio of mCP to the organometallic compound DFTIr(acac) was 4:1, dissolved in chlorobenzene. Next, TmPyPB (1,3,5-tri(p-pyrid-3-yl-phenyl)benzene) was coated on the light-emitting layer by a spin coating process to form a TmPyPB film (with a thickness of 45 nm). Next, LiF (with a thickness of 1 nm), and Al (with a thickness of 100 nm) were subsequently formed on the TmPyPB film at 1×10^{-6} Pa, obtaining the organic light-emitting device (3) after encapsulation. The materials and layers formed therefrom are described in the following:

[0107] ITO(150 nm)/PEDOT:PSS(40 nm)/mCP:organometallic compound DFTIr(acac) (30 nm)/TmPyPB(45 nm)/LiF(1 nm)/Al (100 nm)

[0108] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the organic light-emitting device (3) were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 5.

EXAMPLE 19

Fabrication of the Organic Light-Emitting Device (4) (Wet Process)

[0109] Example 19 was fabricated in the same manner as in Example 18 except that TATC was substituted for mCP (TCTA doped with the organometallic compound DFTIr(acac) of Example 6), obtaining the organic light-emitting device (4). The materials and layers formed therefrom are described in the following:

[0110] ITO(150 nm)/PEDOT:PSS(40 nm)/TCTA:organometallic compound DFTIr(acac) (30 nm)/TmPyPB(45 nm)/LiF(1 nm)/Al (100 nm)

[0111] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (4) were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 5

EXAMPLE 20

Fabrication of the Organic Light-Emitting Device (5) (Wet Process)

[0112] Example 20 was fabricated in the same manner as in Example 19 except that the organometallic compound DFTIr(tmd) was substituted for the organometallic compound DFTIr(acac) (TCTA doped with the organometallic compound DFTIr(tmd) of Example 7), obtaining the organic

light-emitting device (5). The materials and layers formed therefrom are described in the following:

[0113] ITO(150 nm)/PEDOT:PSS(40 nm)/TCTA:organometallic compound DFTIr(tmd) (30 nm)/TmPyPB(45 nm)/LiF(1 nm)/Al (100 nm)

[0114] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (5) were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 5

EXAMPLE 21

Fabrication of the Organic Light-Emitting Device (6) (Wet Process)

[0115] Example 21 was fabricated in the same manner as in Example 19 except that the organometallic compound DMTIr(acac) was substituted for the organometallic compound DFTIr(acac) (TCTA doped with the organometallic compound DMTIr(acac) of Example 14), obtaining the organic light-emitting device (6). The materials and layers formed therefrom are described in the following:

[0116] ITO(150 nm)/PEDOT:PSS(40 nm)/TCTA:organometallic compound DMTIr(acac) (30 nm)/TmPyPB(45 nm)/LiF(1 nm)/Al (100 nm)

[0117] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (6) were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 5

EXAMPLE 22

Fabrication of the Organic Light-Emitting Device (7) (Wet Process)

[0118] Example 22 was fabricated in the same manner as in Example 19 except that the organometallic compound DMTIr(pic) was substituted for the organometallic compound DFTIr(acac) (TCTA doped with the organometallic compound DMTIr(pic) of Example 13), obtaining the organic light-emitting device (7). The materials and layers formed therefrom are described in the following:

[0119] ITO(150 nm)/PEDOT:PSS(40 nm)/TCTA:organometallic compound DMTIr(pic) (30 nm)/TmPyPB(45 nm)/LiF(1 nm)/Al (100 nm)

[0120] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (6) were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 5

COMPARATIVE EXAMPLE 2

Fabrication of a Traditional Organic Light-Emitting Device (Wet Process)

[0121] Comparative Example 2 was fabricated in the same manner as in Example 19 except that TCAC doped with the

organometallic compound FTIr(pic) was substituted for TCAC doped with the organometallic compound DFTIr(acac), obtaining the traditional organic light-emitting device.

[0122] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the traditional light-emitting device were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 5

TABLE 5

	OLED device	current efficiency (cd/A)	power efficiency (lm/W)	λ_{\max} (nm)	C.I.E coordinate (x, y)
Example 18	device (3)	14.3	9.8	464	(0.16, 0.28)
Example 19	device (4)	14.2	10.7	464	(0.16, 0.29)
Example 20	device (5)	13.3	10.9	464	(0.16, 0.29)
Example 21	device (6)	34.1	30.5	492	(0.20, 0.56)
Example 22	device (7)	21.2	17.1	476	(0.18, 0.37)
Comparative Example 2	—	—	15.0	475	(0.18, 0.39)

[0123] During the formation of the light-emitting device via a wet process, it showed that the organometallic compounds (a series of DFTIr) of the disclosure exhibited high solubility (the solution has a solid content that is more than 4 wt %), the organometallic compounds of the disclosure can be uniformly mixed with the TCTA or mCP. The luminescence efficiency of the organic light emitting diode (4) with the dopant DFTIr(acac) achieved 10.7 lm/W, and the luminescence efficiency of the organic light emitting diode (5) with the dopant DFTIr(tmd) achieved 10.9 lm/W (measured at a brightness of 1000 Cd/m²), that is, the devices in Examples of the disclosure showed high driving durability. Moreover, the luminescence efficiency of the organic-light emitting diode (7) with the dopant DFTIr(pic) of the disclosure fabricated via the wet process is 17.1 lm/W (measured at a brightness of 1000 Cd/m²), that is, it was about 1.14 times higher than that of the organic light-emitting diode with the dopant FTIr(pic).

EXAMPLE 23

Fabrication of the organic light-emitting device (8) (dry process)

[0124] A glass substrate with an indium tin oxide (ITO) film with a thickness of 110 nm was provided and then washed with a cleaning agent, acetone, and isopropanol with ultrasonic agitation. After drying with nitrogen flow, the ITO film was subjected to a UV/ozone treatment for 30 min. Next, TAPC(1,1-bis[4-[N,N'-di (p-tolyl)amino]phenyl]cyclohexane, with a thickness of 35 nm), TCTA doped with the organometallic compound DFTIr(tmd) (the ratio between TATC and the organometallic compound DFTIr(tmd) was 1:0.05, with a thickness of 6 nm), 26DCzPPY doped with the organometallic compound DFTIr(tmd) (the ratio between 26DCzPPY and the organometallic compound DFTIr(tmd) was 1:0.06, with a thickness of 6 nm), TmPyPB (1,3,5-tri (p-pyrid-3-yl-phenyl)benzene, with a thickness of 110 nm), LiF (with a thickness of 1 nm), and Al (with a thickness of 100 nm) were subsequently formed on the ITO film at 10⁻⁶

torr, obtaining the organic light-emitting device (8). The materials and layers formed therefrom are described in the following:

[0125] ITO (150 nm)/TAPC (35 nm)/TATC:organometallic DFTIr(tmd)(5%)(6 nm)/26DCzPPY:organometallic DFTIr(tmd)(6%)(6 nm)/TmPyPB(110 nm)/LiF(1 nm)/Al (100 nm)

[0126] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (8), as described in Example 15, were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 3

EXAMPLE 24

Fabrication of the Organic Light-Emitting Device (9) (Dry Process)

[0127] Example 24 was fabricated in the same manner as in Example 23 except that the organometallic compound DFTIr(acac) was substituted for the organometallic compound DFTIr(tmd), obtaining the organic light-emitting device (9). The materials and layers formed therefrom are described in the following:

[0128] ITO (150 nm)/TAPC (35 nm)/TATC:organometallic DFTIr(acac)(6%)(6 nm)/26DCzPPY:organometallic DFTIr(acac)(8%)(6 nm)/TmPyPB(110 nm)/LiF(1 nm)/Al (100 nm)

[0129] Next, the optical properties (such as current efficiency (cd/A), power efficiency (lm/W), emission wavelength (nm), and C.I.E coordinates (x, y)) of the light-emitting device (9) were measured by a spectra colorimeter PR650 (purchased from Photo Research Inc.) and a luminance meter LS110 (purchased from Konica Minolta). The results are shown in Table 6

TABLE 6

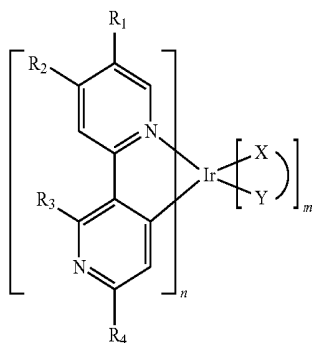
	OLED device	current efficiency (cd/A)	power efficiency (lm/W)	λ_{\max} (nm)	C.I.E coordinate (x, y)
Comparative Example 1	—	21.5	16.1	454	(0.16, 0.25)
Example 23	device (8)	32.4	30.2	464	(0.15, 0.25)
Example 24	device (9)	29.5	27.2	464	(0.15, 0.25)
Comparative Example 2	—	—	15.0	475	(0.18, 0.39)

[0130] As can be apparently seen from the above results, with dual light emitting layers, the luminescence efficiency of the organic light emitting diode (9) with the dopant DFTIr(acac) achieved 27.2 lm/W. The luminescence efficiency of the organic light emitting diode (8) with the dopant DFTIr(tmd) achieved 30.2 lm/W, that is, it was about 1.88 times higher than that of the organic light-emitting diode with the dopant FK306 in Comparative Example 1. In addition, the luminescence efficiency of the organic light emitting diode with dual light emitting layers of the disclosure is better than that of organic light emitting diode with single light emitting layer in Comparative Example 2.

[0131] While the disclosure has been described by way of example and in terms of the preferred embodiments, it should be understood that the disclosure is not limited to the disclosed embodiments. On the contrary, it is intended to cover various modifications and similar arrangements (as would be apparent to those skilled in the art). Therefore, the scope of the appended claims should be accorded the broadest interpretation so as to encompass all such modifications and similar arrangements.

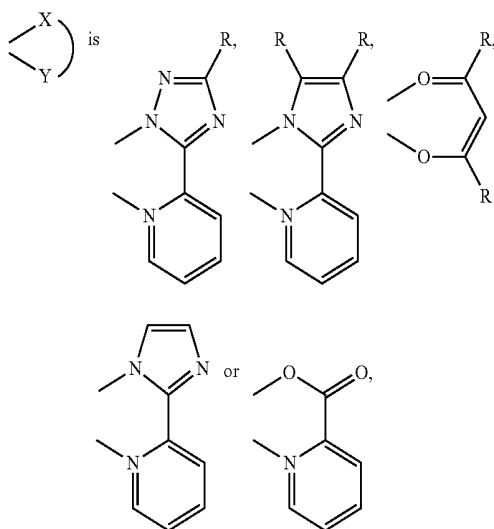
What is claimed is:

1. An organometallic compound having a structure represented by Formula (I):



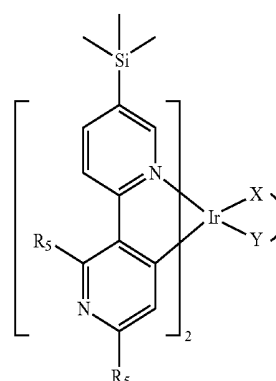
Formula (I)

wherein, one of R₁ and R₂ is trimethylsilyl (TMS) and the other is hydrogen, at least one of R₃ and R₄ is fluorine or C₁₋₆ alkyl, or one of R₃ and R₄ is fluorine and the other is C₁₋₆ alkyl,



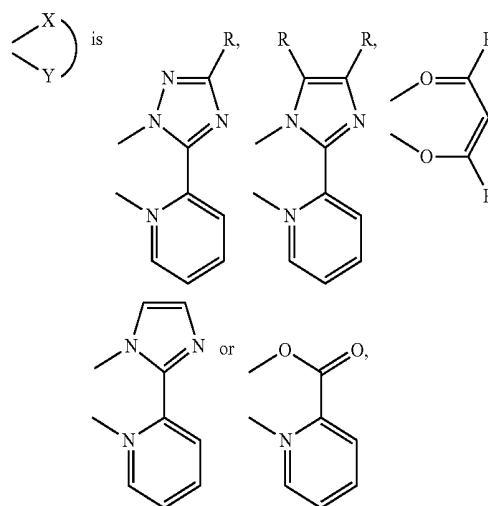
R is CH₃, CH₂CH₃, CH(CH₃)₂, C(CH₃)₃, CF₃, CHF₂, C₃F₈ or phenyl, and n is 2 or 3, and m is 0 or 1, wherein n+m=3.

2. The organometallic compound as claimed in claim 1, wherein the organometallic compound has a structure represented by Formula (II):



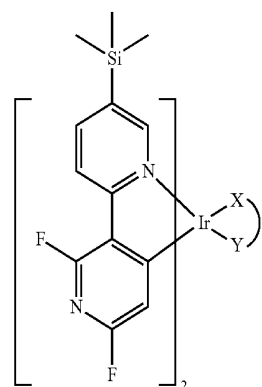
Formula (II)

wherein R₅ is fluorine or C₁₋₆ alkyl,



R is CH₃, CH₂CH₃, CH(CH₃)₂, C(CH₃)₃, CF₃, CHF₂, C₃F₈ or phenyl.

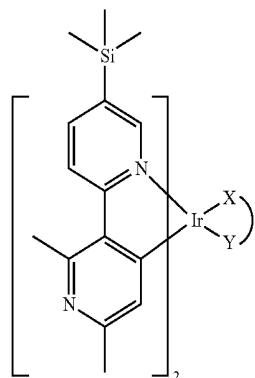
3. The organometallic compound as claimed in claim 1, wherein the organometallic compound has a structure represented by Formula (III) or Formula (IV):



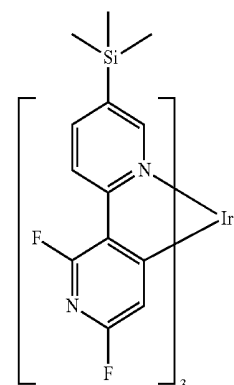
Formula (III)

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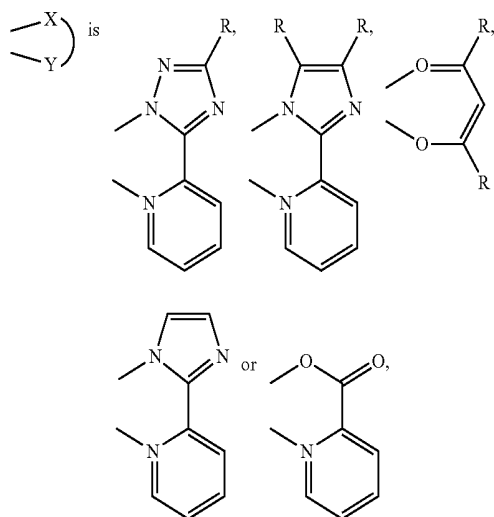
Formula (IV)



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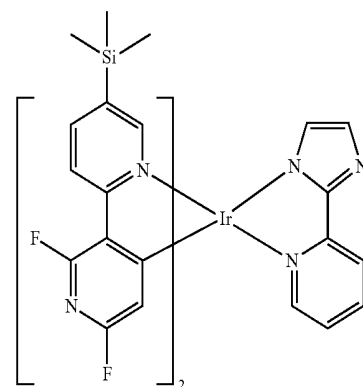
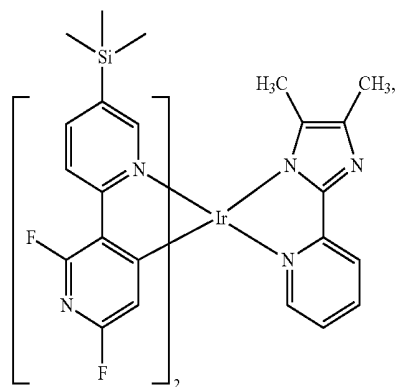
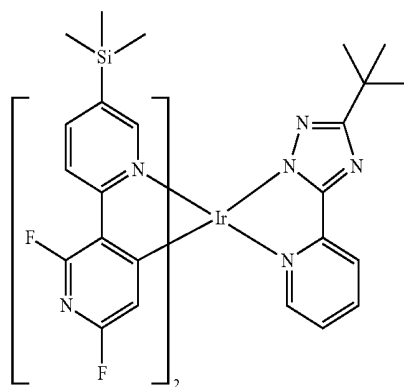
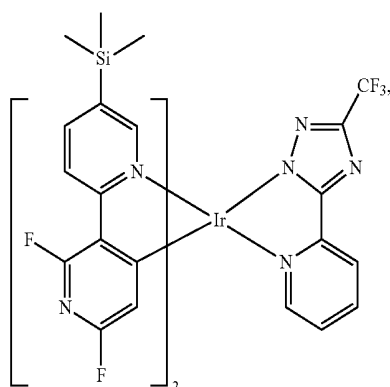


wherein

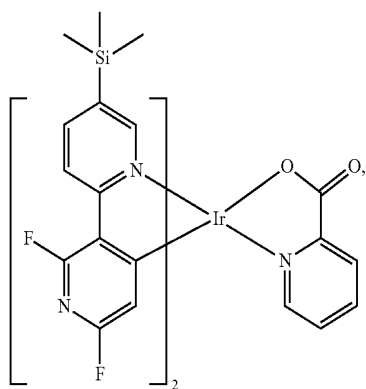


R is CH_3 , CH_2CH_3 , $\text{CH}(\text{CH}_3)_2$, $\text{C}(\text{CH}_3)_3$, CF_3 , CHF_2 , C_3F_8 or ph.

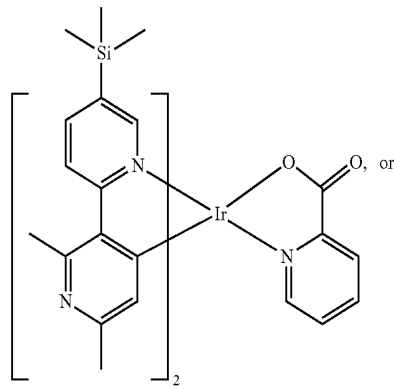
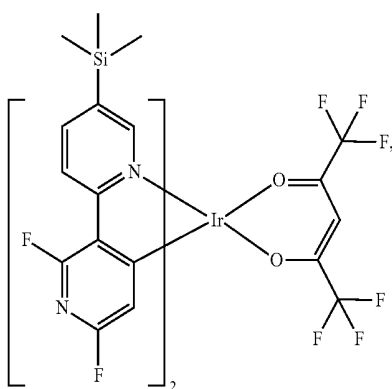
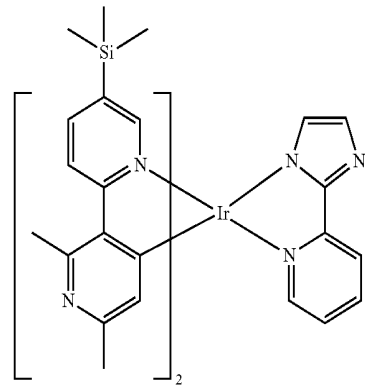
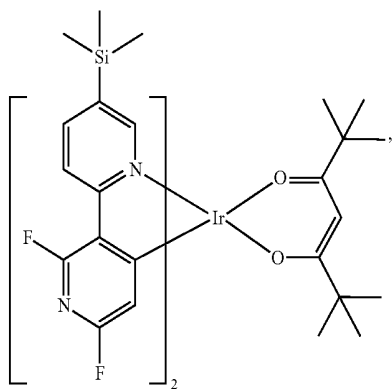
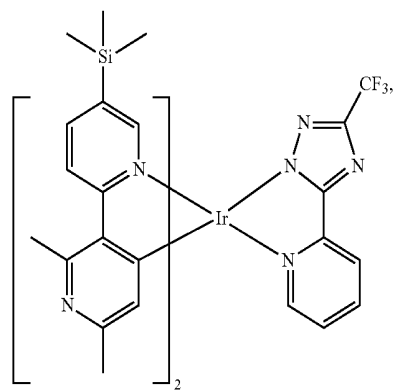
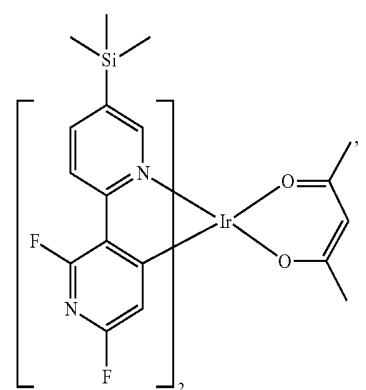
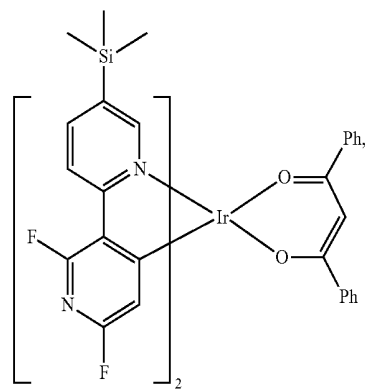
4. The organometallic compound as claimed in claim 1, wherein the organometallic compound is

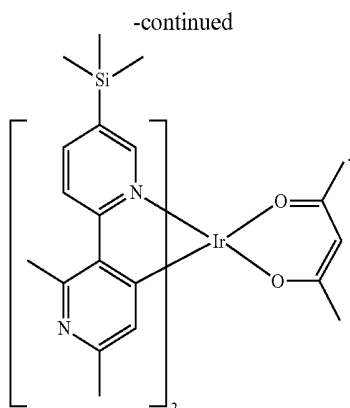


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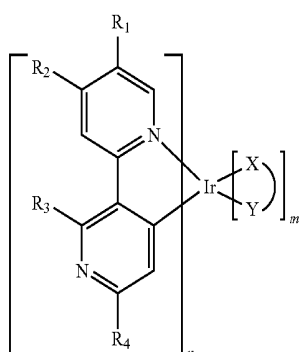


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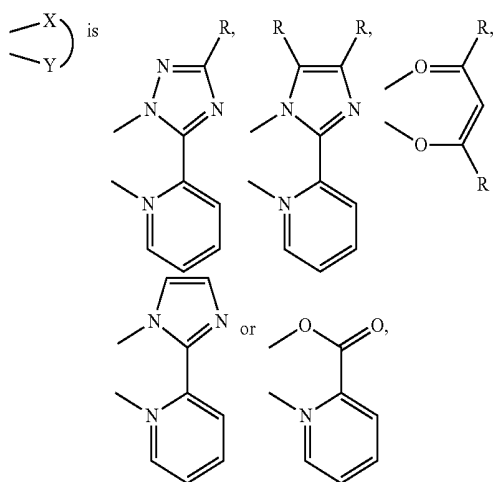




5. An organic light-emitting device, comprising:
 an anode and a cathode; and
 an organic light-emitting element disposed between the anode and the cathode,
 wherein the organic light-emitting element comprises a organometallic compound having a structure represented by the following Formula (I):

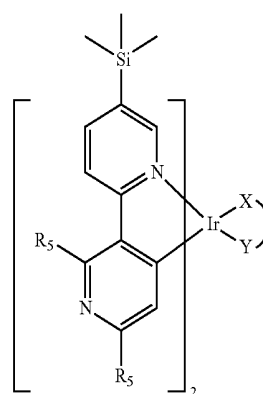


wherein, one of R_1 and R_2 is trimethylsilyl (TMS) and the other is hydrogen, at least one of R_3 and R_4 is fluorine or C_{1-6} alkyl, or one of R_3 and R_4 is fluorine and the other is C_{1-6} alkyl,

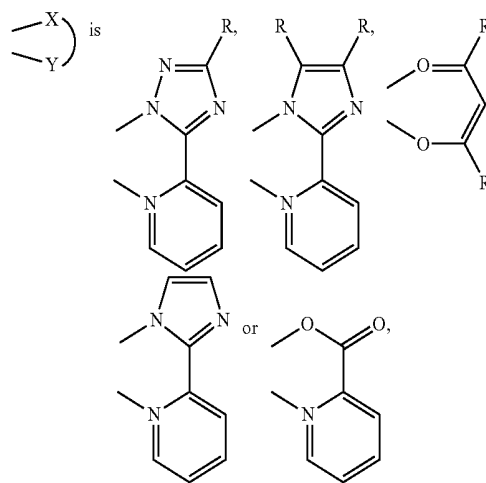


R is CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl, n is 2 or 3, and m is 0 or 1, wherein $n+m=3$.

6. The organic light-emitting device as claimed in claim 5, wherein the organometallic compound has a structure as defined by Formula (II):

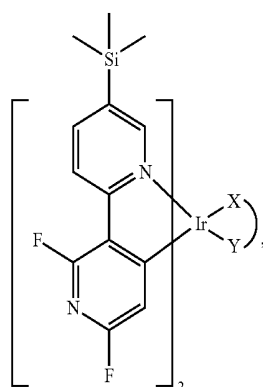


wherein R_5 is fluorine or C_{1-6} alkyl,



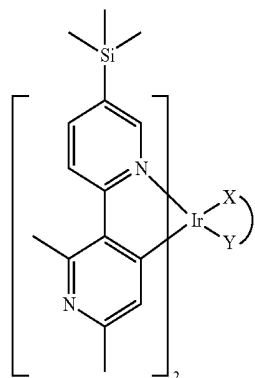
R is CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl.

7. The organic light-emitting device as claimed in claim 5, wherein the organometallic compound has a structure represented by Formula (III) or Formula (IV):

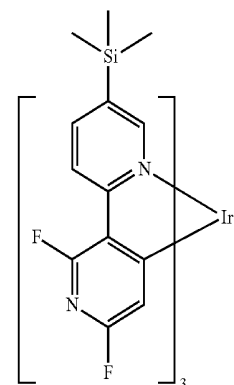


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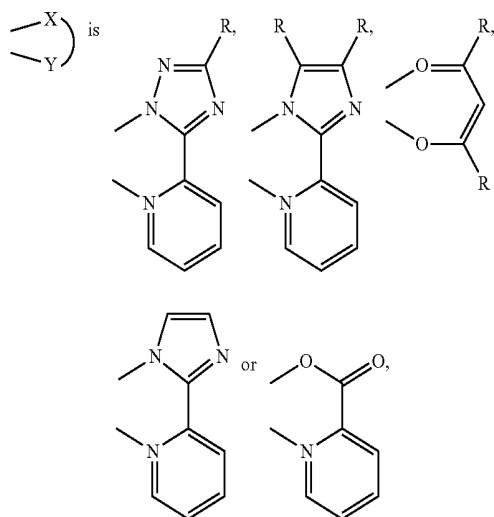
Formula (IV)



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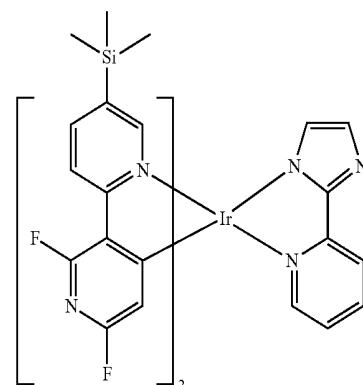
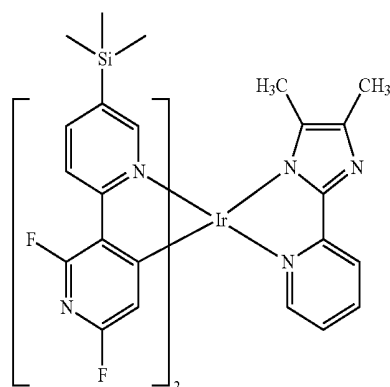
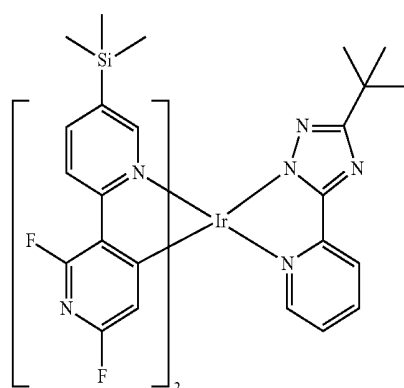
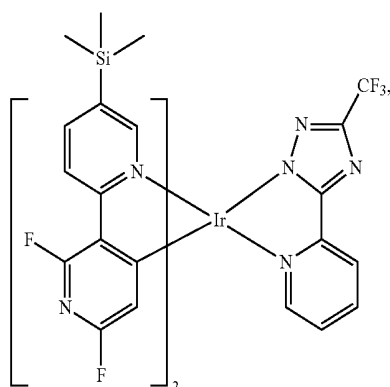


wherein

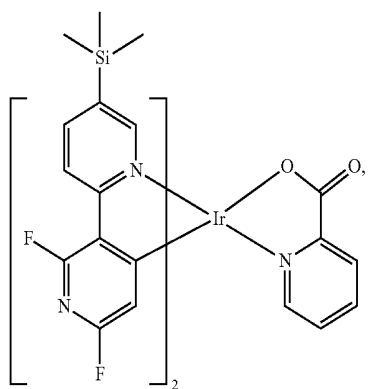


R is CH₃, CH₂CH₃, CH(CH₃)₂, C(CH₃)₃, CF₃, CHF₂, C₃F₈ or phenyl.

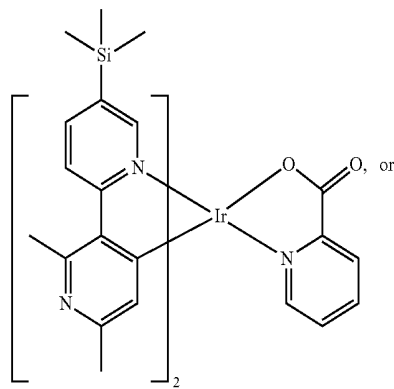
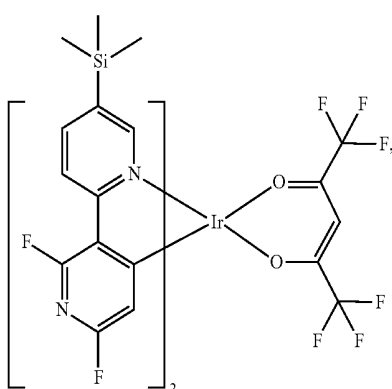
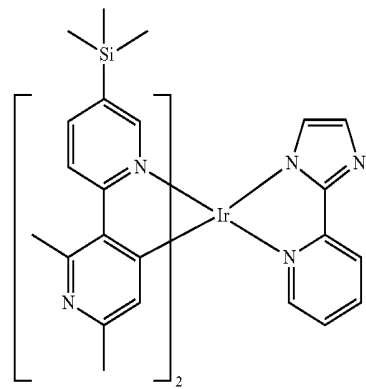
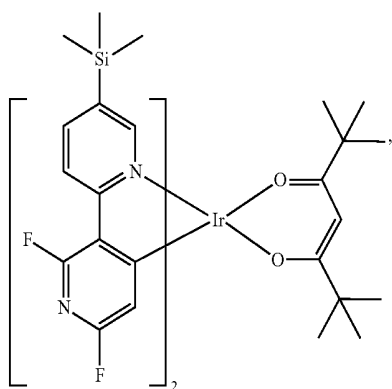
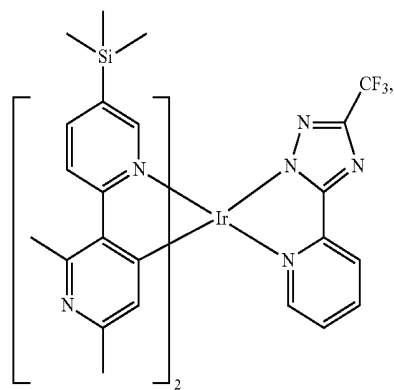
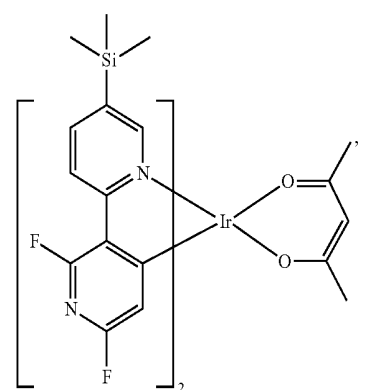
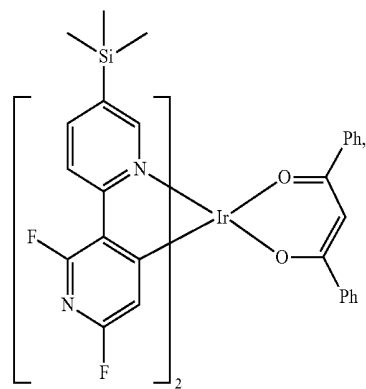
8. The organic light-emitting device as claimed in claim 5, wherein the organometallic compound is



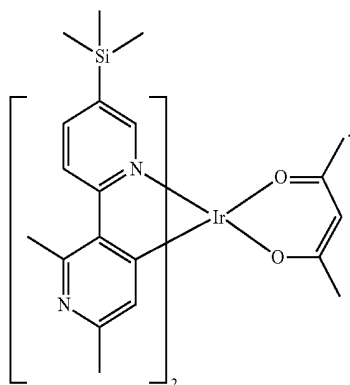
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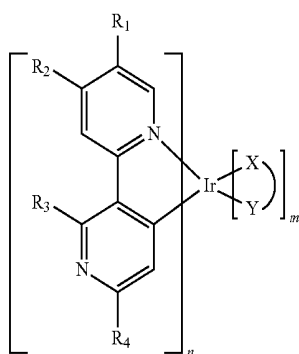


9. An organic light-emitting device, comprising:

an anode and a cathode; and

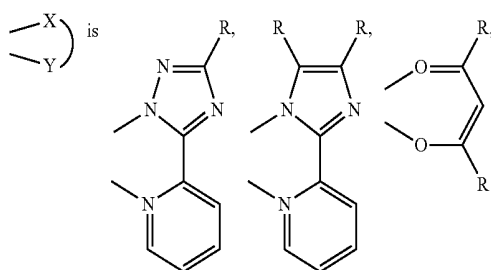
an organic light-emitting element disposed between the anode and the cathode,

wherein the organic light-emitting element comprises a first light-emitting layer, and the first light-emitting layer comprises a organometallic compound having a structure represented by the following Formula (I):

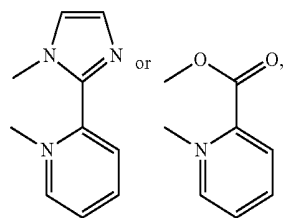


Formula (I)

wherein, one of R_1 and R_2 is trimethylsilyl (TMS) and the other is hydrogen, at least one of R_3 and R_4 is fluorine or C_{1-6} alkyl, or one of R_3 and R_4 is fluorine and the other is C_{1-6} alkyl,

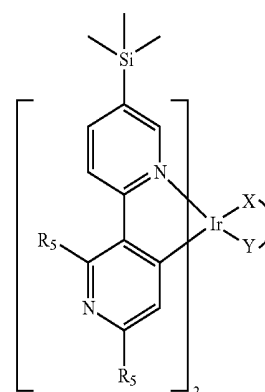


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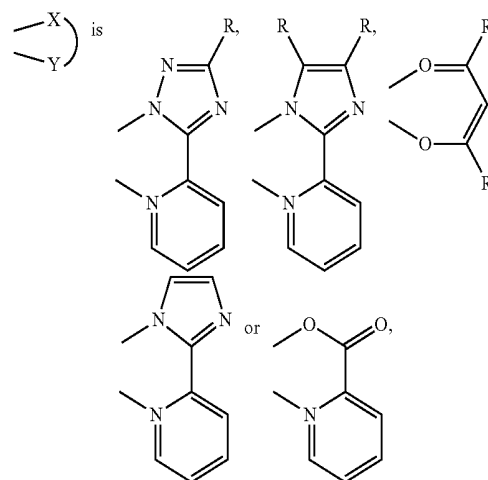
R is CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl, n is 2 or 3, and m is 0 or 1, wherein $n+m=3$.

10. The organic light-emitting device as claimed in claim 9, wherein the first organometallic compound has a structure as defined by Formula (II):



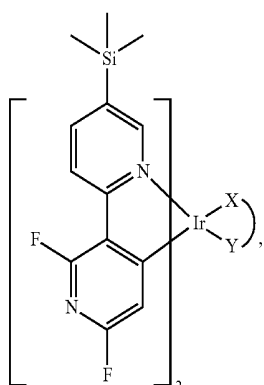
Formula (II)

wherein R_5 is fluorine or C_{1-6} alkyl,

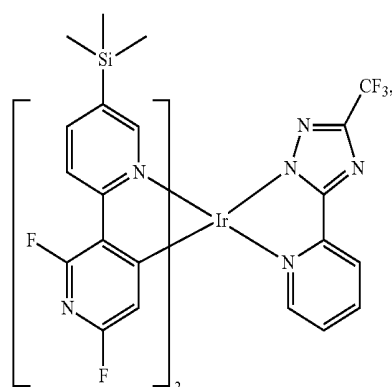


R is CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl.

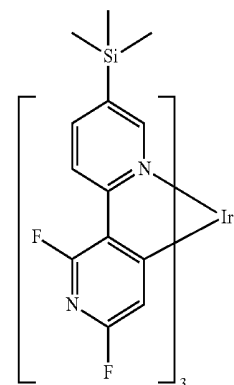
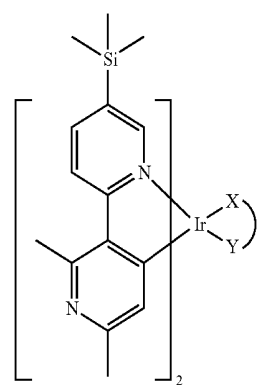
11. The organic light-emitting device as claimed in claim 9, wherein the first organometallic compound has a structure represented by Formula (III) or Formula (IV):



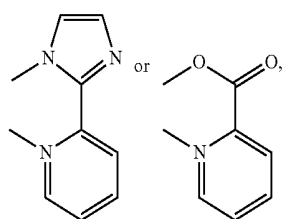
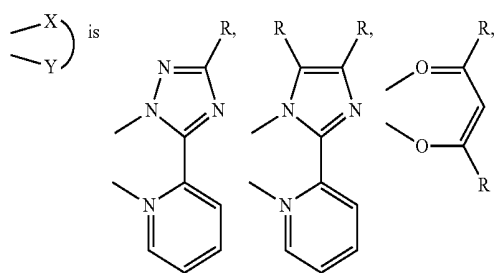
Formula (III)



Formula (IV)

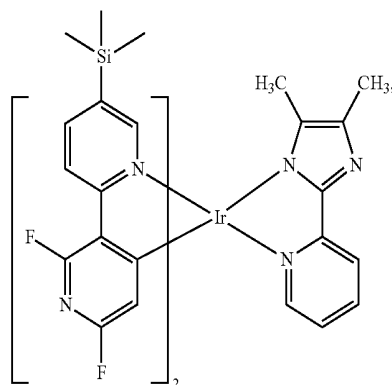
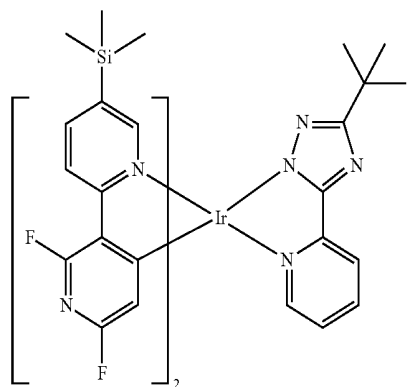


wherein

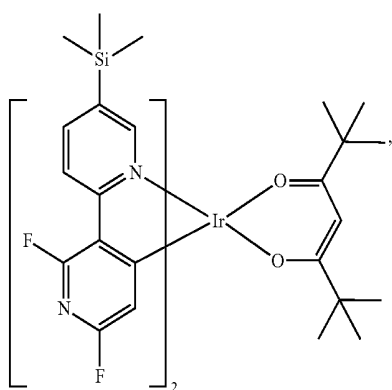
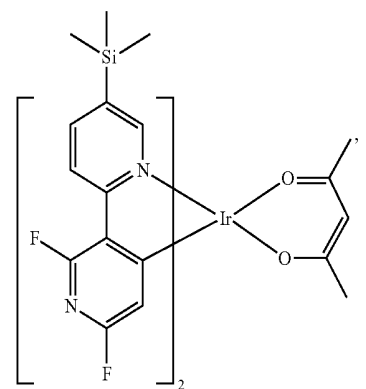
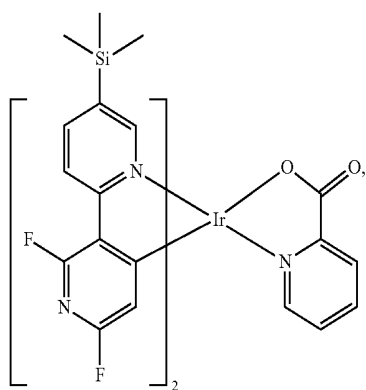
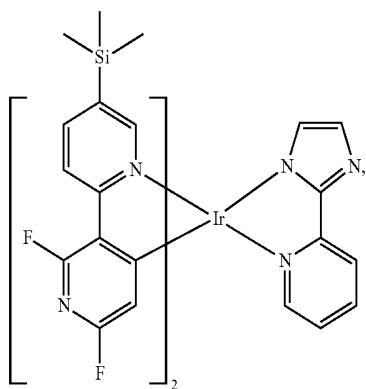


R is CH₃, CH₂CH₃, CH(CH₃)₂, C(CH₃)₃, CF₃, CHF₂, C₃F₈ or phenyl.

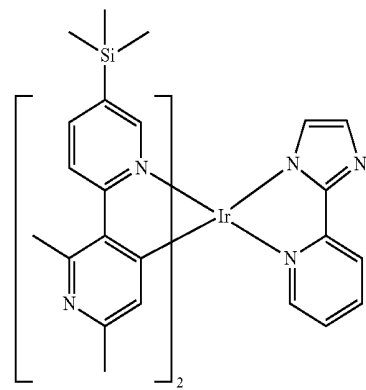
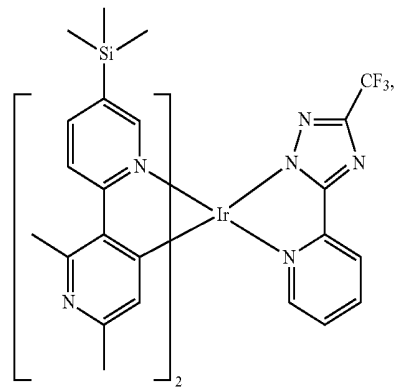
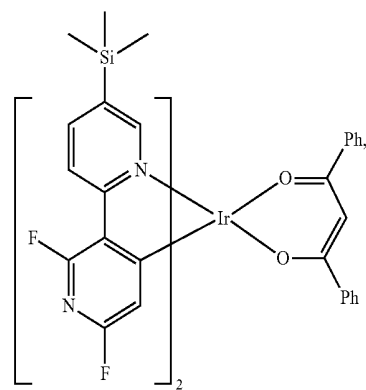
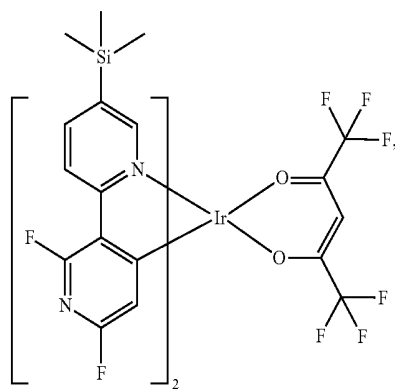
12. The organic light-emitting device as claimed in claim 9, wherein the first organometallic compound is



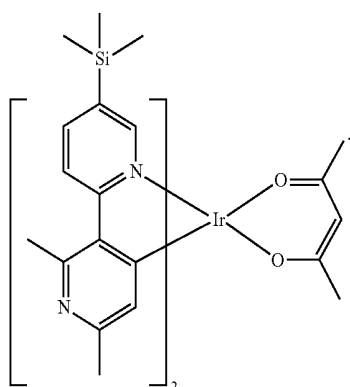
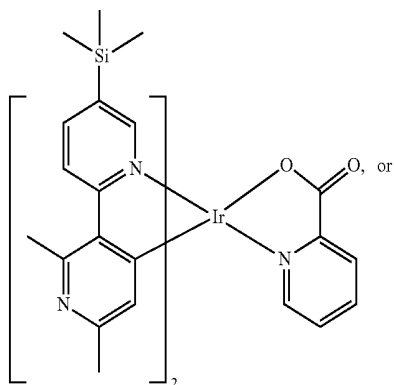
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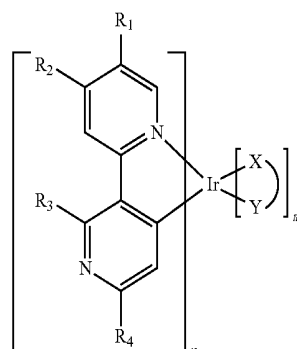
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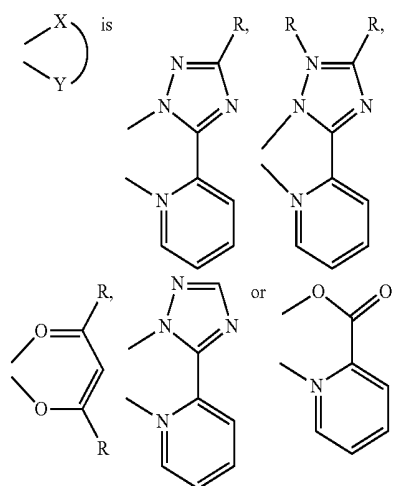
13. The organic light-emitting device as claimed in claim 9, further comprising a second light-emitting layer disposed between the anode and the first light-emitting layer or between the first light-emitting layer and the cathode.

14. The organic light-emitting device as claimed in claim 9, wherein the second light-emitting layer comprises an organometallic compound having a structure represented by the following Formula (I):

Formula (I)



wherein, one of R_1 and R_2 is trimethylsilyl (TMS) and the other is hydrogen, at least one of R_3 and R_4 is fluorine or C_{1-6} alkyl, or one of R_3 and R_4 is fluorine and the other is C_{1-6} alkyl,



R is CH_3 , CH_2CH_3 , $CH(CH_3)_2$, $C(CH_3)_3$, CF_3 , CHF_2 , C_3F_8 or phenyl, n is 2 or 3, and m is 0 or 1, wherein $n+m=3$.

15. The organic light-emitting device as claimed in claim 9, wherein the organic light-emitting element emits blue light.

* * * * *

专利名称(译)	有机金属化合物和使用其的有机发光器件		
公开(公告)号	US20170162804A1	公开(公告)日	2017-06-08
申请号	US15/178761	申请日	2016-06-10
[标]申请(专利权)人(译)	财团法人工业技术研究院		
申请(专利权)人(译)	工业技术研究院		
当前申请(专利权)人(译)	工业技术研究院		
[标]发明人	LIN JIN SHENG LIOU JIA LUN CHANG MENG HAO YE HAN CHENG		
发明人	LIN, JIN-SHENG LIOU, JIA-LUN CHANG, MENG-HAO YE H, HAN-CHENG		
IPC分类号	H01L51/00 C09K11/06 C07F15/00		
CPC分类号	H01L51/0094 C07F15/0033 C09K11/06 H01L51/5016 C09K2211/1044 C09K2211/185 H01L51/0085 H01L51/504 C09K2211/1059 C09K2211/1029		
优先权	104140698 2015-12-04 TW		
外部链接	Espacenet USPTO		

摘要(译)

提供了有机金属化合物和使用其的机电致发光器件。有机金属化合物具有如下化学结构：在式(1)中，R₁和R₂中的一个是三甲基甲硅烷基(TMS)而另一个是氢，R₃和R₄中的至少一个是氟或C₁₋₆烷基，或者R₃和R₄中的一个是氟，另一个是C₁₋₆烷基，n为2或3，m为0或1，其中n + m = 3。

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