(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
9 September 2011 (09.09.2011)

PCT

(10) International Publication Number
WO 2011/109042 A1

(51) International Patent Classification:
C09K 11/06 (2006.01) *H05B 33/14* (2006.01)

(21) International Application Number:
PCT/US2010/051076

(22) International Filing Date:
1 October 2010 (01.10.2010)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
61/339,337 3 March 2010 (03.03.2010) US
12/868,350 25 August 2010 (25.08.2010) US

(71) Applicant *(for all designated States except US)*: **UNIVERSAL DISPLAY CORPORATION** [US/US]; 375 Phillips Boulevard, Ewing, New Jersey 08618 (US).

(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: **XIA, Chuanjun** [CN/US]; 16 Cliveden Court, Lawrenceville, New Jersey 08648 (US). **ALLEYNE, Bert** [TT/US]; 543 Masterson Court, Ewing, New Jersey 08618 (US). **ANSARI, Nasrin** [US/US]; 24 Jamie Court, Monmouth, New Jersey 08852 (US).

(74) Agents: **MCGROARTY, John P.** et al.; Townsend and Townsend and Crew LLP, Two Embarcadero Center, 8th Floor, San Francisco, CA 94111 (US).

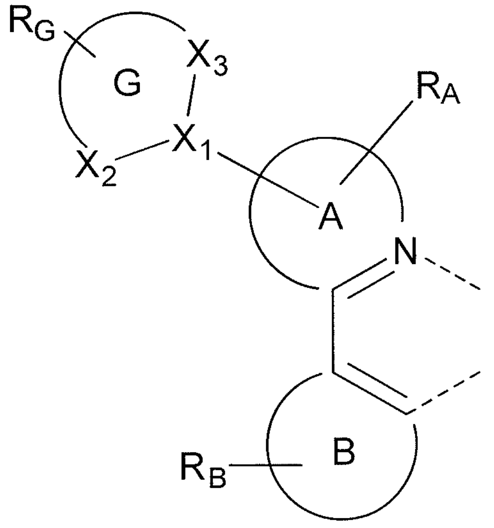
(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report (Art. 21(3))*

(54) Title: PHOSPHORESCENT MATERIALS

FIGURE 3



(I)

(57) Abstract: Compounds comprising a 2-phenylpyridine ligand further substituted with a heterocyclic group are provided. In particular, the compound comprises a 2-phenylpyridine ligand further substituted with a nitrogen-containing heterocycle. The compounds may be used in organic light emitting devices to provide devices having improved efficiency and lifetime.

WO 2011/109042 A1

PHOSPHORESCENT MATERIALS

[0001] This application claims priority to U.S. Provisional Application Serial No. 61/339,337, filed on March 3, 2010, the disclosure of which is herein expressly incorporated by reference in its entirety. The disclosure of WO2010/028151 is also herein expressly incorporated by reference in its entirety.

[0002] The claimed invention was made by, on behalf of, and/or in connection with one or more of the following parties to a joint university corporation research agreement: Regents of the University of Michigan, Princeton University, The University of Southern California, and the Universal Display Corporation. The agreement was in effect on and before the date the claimed invention was made, and the claimed invention was made as a result of activities undertaken within the scope of the agreement.

FIELD OF THE INVENTION

[0003] The present invention relates to organic light emitting devices (OLEDs). More specifically, the present invention relates to phosphorescent materials comprising a 2-phenylpyridine ligand further substituted with a heterocyclic group. These materials may provide devices having improved efficiency and lifetime.

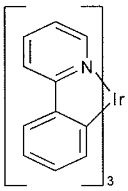
BACKGROUND

[0004] Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer emits light may generally be readily tuned with appropriate dopants.

[0005] OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.

[0006] One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Color may be measured using CIE coordinates, which are well known to the art.

[0007] One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)$_3$, which has the structure:



[0008] In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

[0009] As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core moiety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule," and it is believed that all dendrimers currently used in the field of OLEDs are small molecules.

[0010] As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

[0011] As used herein, "solution processible" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

[0012] A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

[0013] As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level of the same material. A "higher" HOMO or LUMO energy level appears closer to the top of such a diagram than a "lower" HOMO or LUMO energy level.

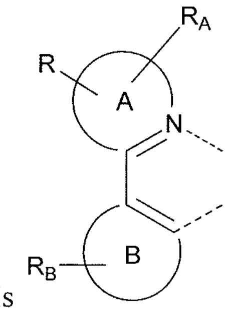
[0014] As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a "higher" work function is more negative. On a conventional energy level diagram, with the vacuum level at the top, a "higher" work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

[0015] More details on OLEDs, and the definitions described above, can be found in US Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

SUMMARY OF THE INVENTION

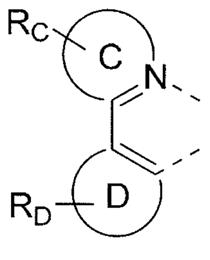
[0016] Compounds having the formula $M(L)_x(L_1)_y(L_2)_z$ are provided.

[0017] L is



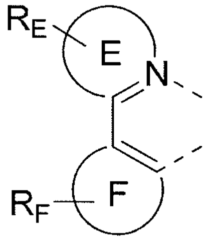
Formula I.

[0018] L_1 is



Formula II.

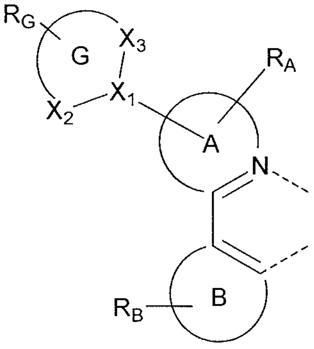
[0019] L_2 is



Formula III.

[0020] L_1 and L_2 can be the same or different. M is a metal having an atomic number greater than 40. Preferably, the metal M is Ir. x is 1, 2 or 3. y is 0, 1 or 2. z is 0, 1 or 2. x+y+z is the oxidation state of the metal M. A is a 6-membered heterocyclic ring. B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. Preferably, B is phenyl. R is a 5 or 6-membered heterocyclic ring. R is attached to A at a position para to the metal M. R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions. Each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated bidentately to the metal M. R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom.

[0021] In one aspect, the ligand L has the formula:



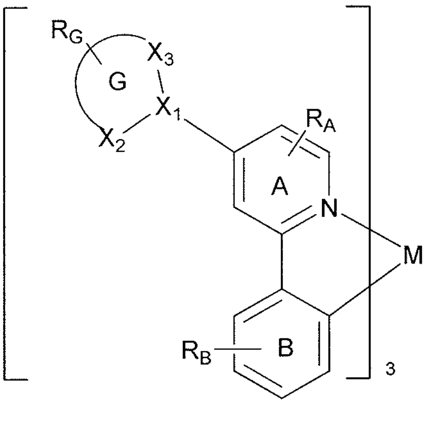
Formula IV.

[0022] G is a 5 or 6-membered heterocyclic ring. Preferably, G is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. X_1, X_2, and X_3 are independently selected from carbon, oxygen, sulfur and nitrogen. Preferably, X_1, X_2, and X_3 are independently carbon or nitrogen. R_G may represent mono, di, tri, tetra, or penta substitutions. R_G is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

[0023] In one aspect, at least one of X_1, X_2, and X_3 is nitrogen. In another aspect, each of X_1, X_2, and X_3 is carbon.

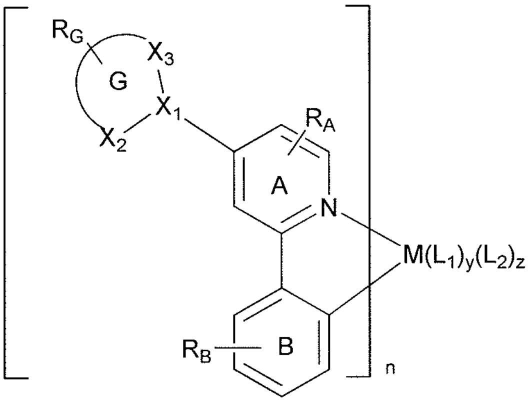
[0024] In another aspect, L, L_1 and L_2 are connected to form a tetradentate ligand and a bidentate ligand or a hexadentate ligand. For example, L and L_1 may be connected to form a tetradentate ligand and L_2 is a bidentate ligand. Similarly, L and L_2 or L_1 and L_2 may be connected to form a tetradentate ligand while L_1 or L is a bidentate ligand. Additionally, L, L_1 and L_2 may all be connected to form a hexadentate ligand.

[0025] In one aspect, the compound is homoleptic. In another aspect, the compound has the formula:



Formula V.

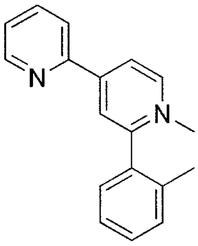
[0026] In one aspect, the compound is heteroleptic. In another aspect, the compound has the formula:

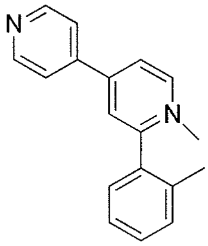


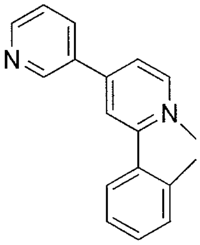
Formula VI.

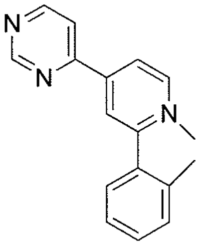
[0027] $n+y+z$ is the oxidation state of the metal M. n is at least 1. y is 0, 1 or 2. x is 0, 1, or 2.

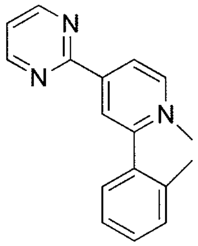
[0028] In one aspect, the ligand L is selected from the group consisting of:

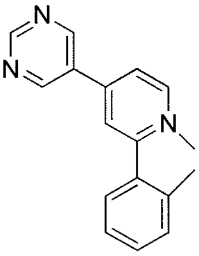


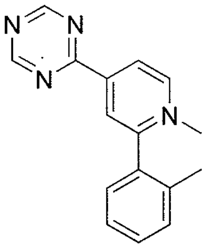


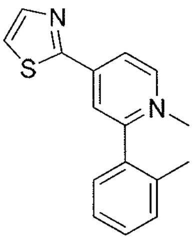


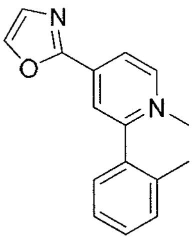


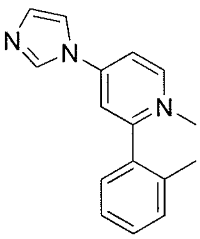




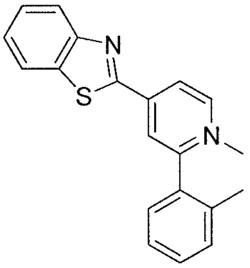


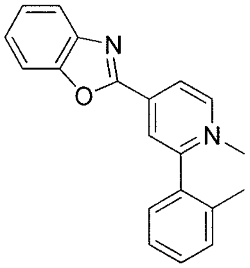






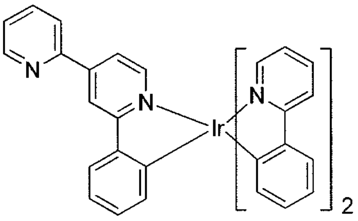
.



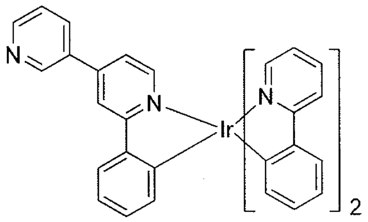


.

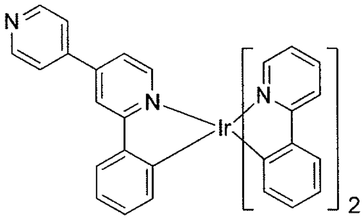
[0029] Specific examples of compounds comprising a phenyl pyridine ligand further substituted with a heterocyclic ring are also provided. In particular, the compound is selected from the group consisting of:



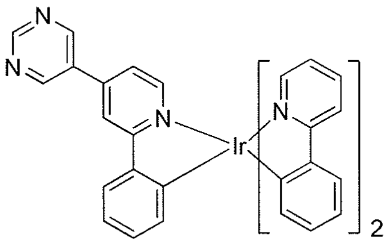
Compound 1



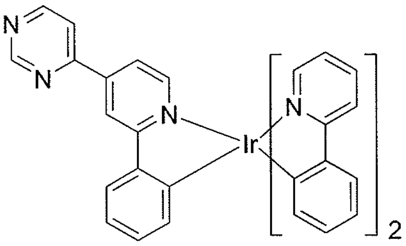
Compound 2



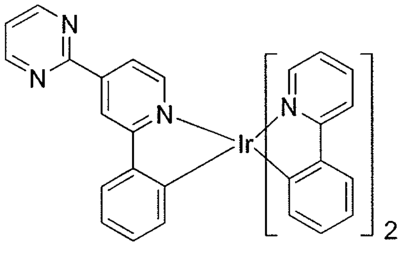
Compound 3



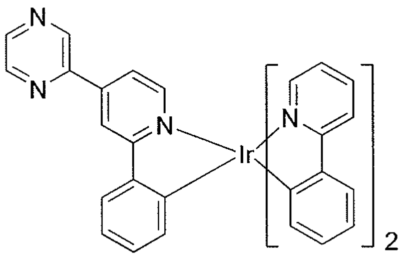
Compound 4



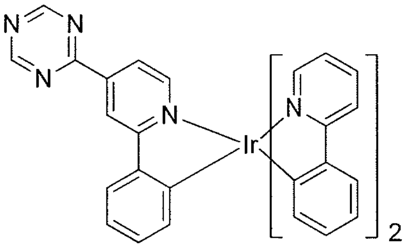
Compound 5



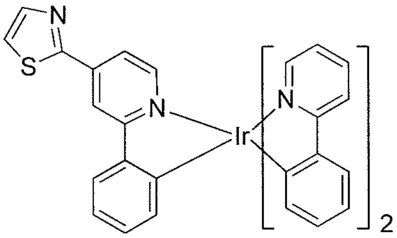
Compound 6



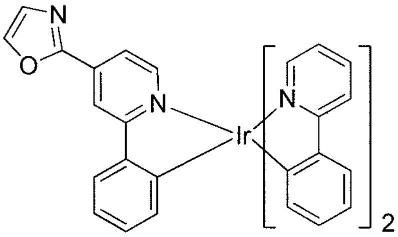
Compound 7



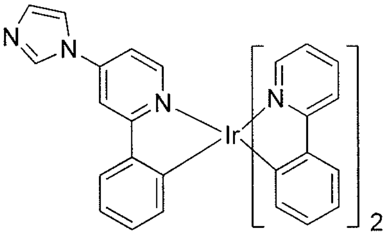
Compound 8



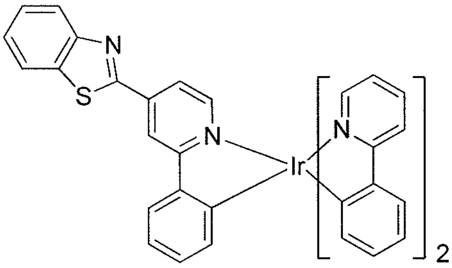
Compound 9



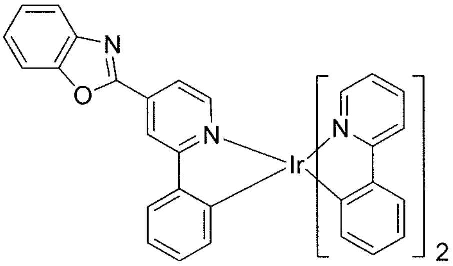
Compound 10



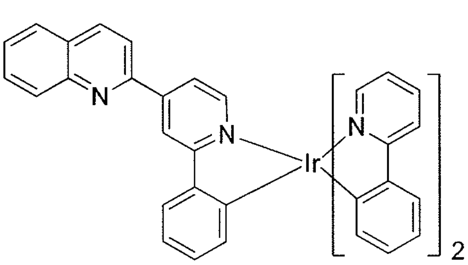
Compound 11



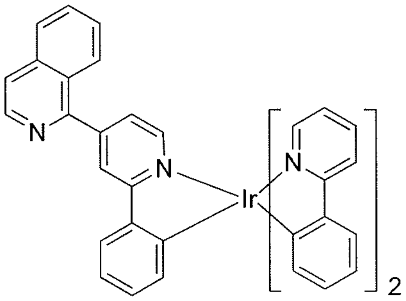
Compound 12



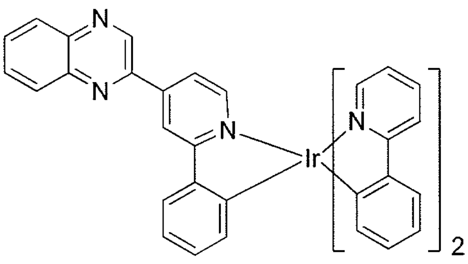
Compound 13



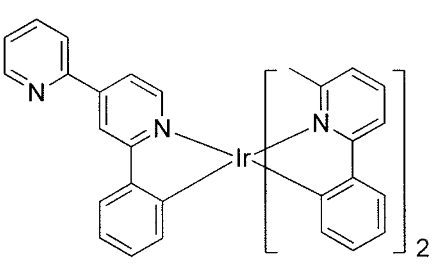
Compound 14



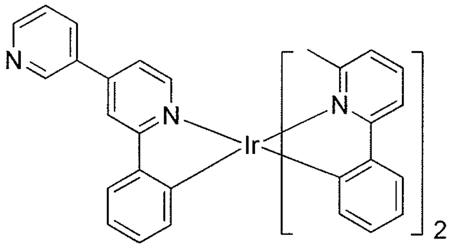
Compound 15



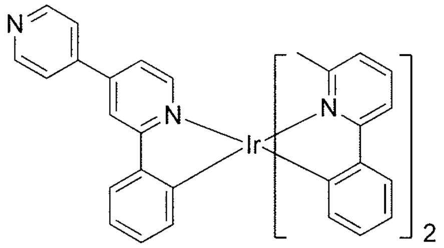
Compound 16



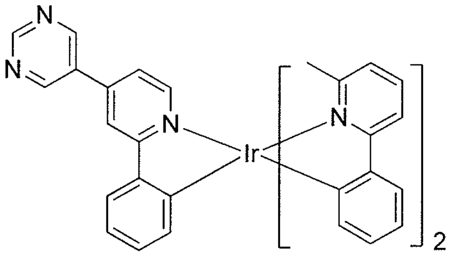
Compound 17



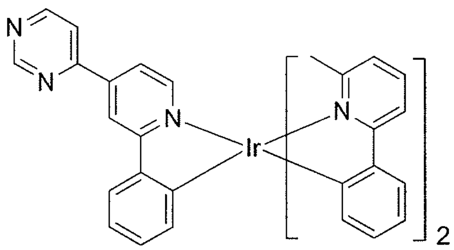
Compound 18



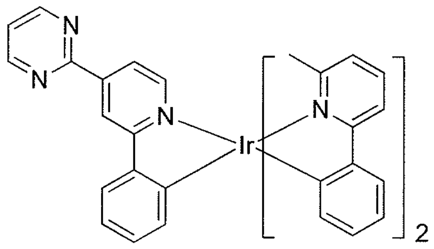
Compound 19



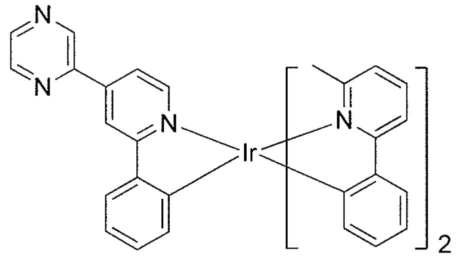
Compound 20



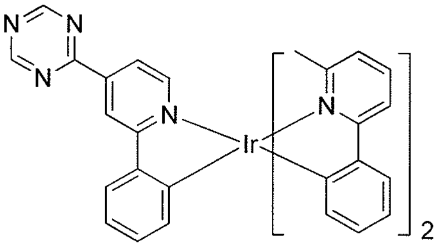
Compound 21



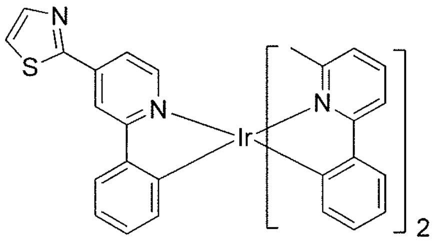
Compound 22



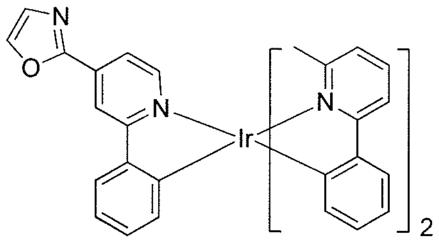
Compound 23



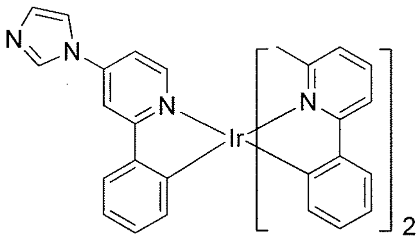
Compound 24



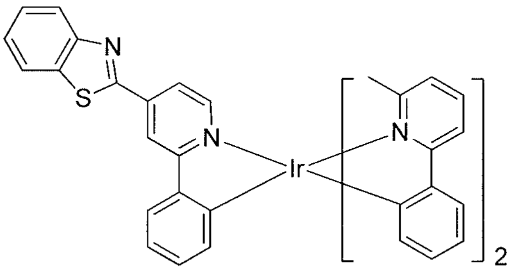
Compound 25



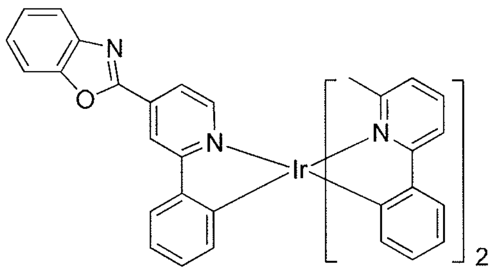
Compound 26



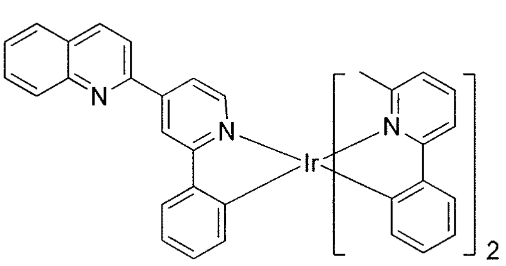
Compound 27



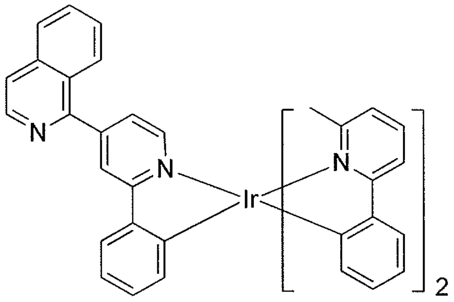
Compound 28



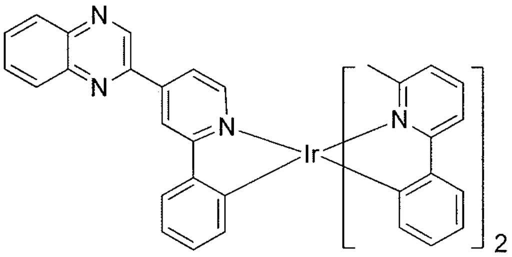
Compound 29



Compound 30



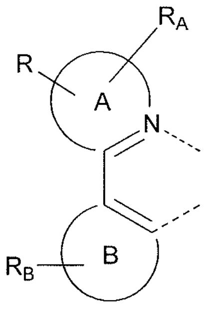
Compound 31



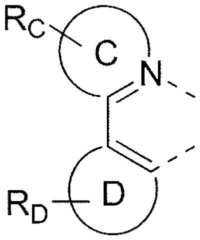
Compound 32

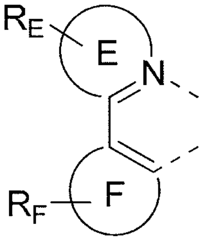
[0030] A first device is also provided. The first device comprises an organic light emitting device, further comprising an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprising a first compound having the formula $M(L)_x(L_1)_y(L_2)_z$.

[0031] L is



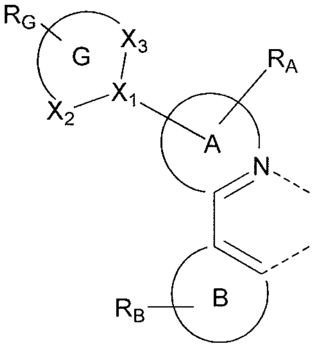
Formula I.

[0032] L_1 is  Formula II.

[0033] L_2 is  Formula III.

[0034] L_1 and L_2 can be the same or different. M is a metal having an atomic number greater than 40. Preferably, the metal M is Ir. x is 1, 2 or 3. y is 0, 1 or 2. z is 0, 1 or 2. x+y+z is the oxidation state of the metal M. A is a 6-membered heterocyclic ring. B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. Preferably, B is phenyl. R is a 5 or 6-membered heterocyclic ring. Preferably, R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. R is attached to A at a position para to the metal M. R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions. Each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated bidentately to the metal M.

[0035] In one aspect, the ligand L has the formula:



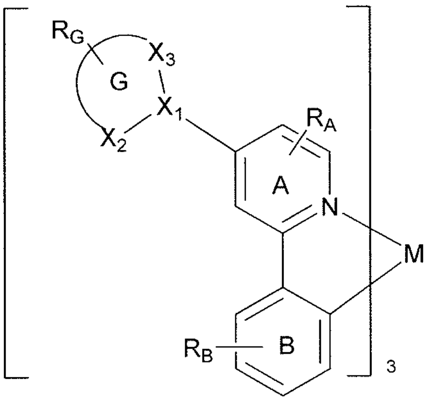
Formula IV.

[0036] G is a 5 or 6-membered heterocyclic ring. Preferably, G is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. X_1, X_2, and X_3 are independently selected from carbon, oxygen, sulfur and nitrogen. Preferably, X_1, X_2, and X_3 are independently carbon or nitrogen. R_G may represent mono, di, tri, tetra, or penta substitutions. R_G is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

[0037] In one aspect, at least one of X_1, X_2, and X_3 is nitrogen. In another aspect, each of X_1, X_2, and X_3 is carbon.

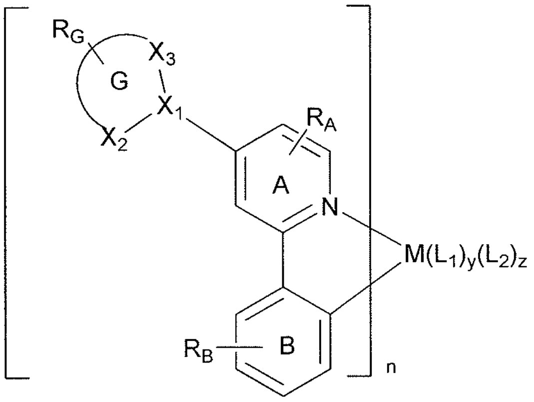
[0038] In another aspect, L, L_1 and L_2 are connected to form a tetradentate ligand and a bidentate ligand or a hexadentate ligand.

[0039] In one aspect, the compound is homoleptic. In another aspect, the compound has the formula:



Formula V.

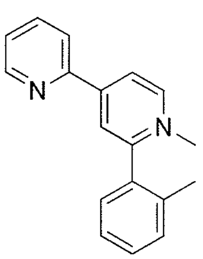
[0040] In one aspect, the compound is heteroleptic. In another aspect, the compound has the formula:

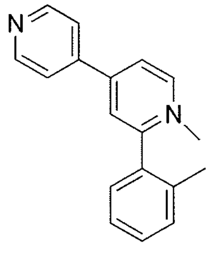


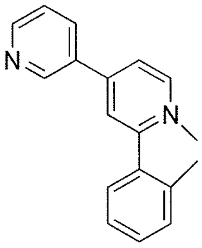
Formula VI.

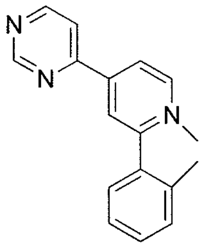
[0041] n+y+z is the oxidation state of the metal M. n is at least 1. y is 0, 1 or 2. x is 0, 1, or 2.

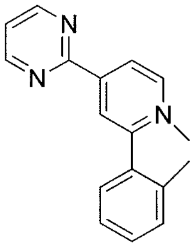
[0042] In one aspect, the ligand L is selected from the group consisting of:

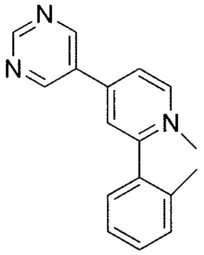


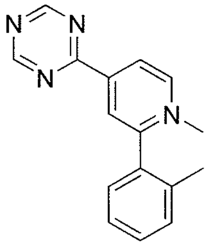


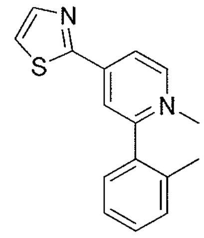


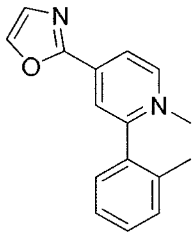


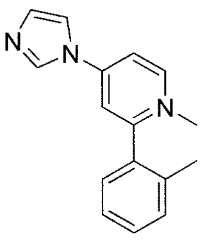


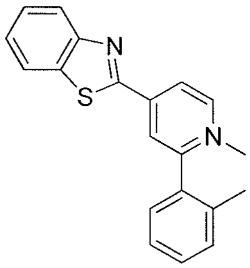


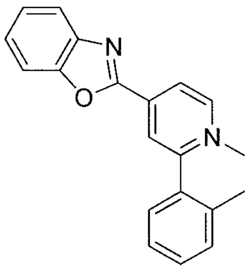










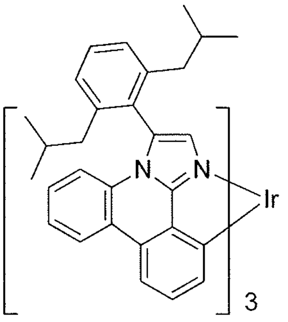


.

[0043] Specific examples of devices containing compounds comprising a phenyl pyridine ligand further substituted with a heterocyclic ring. In particular, the compound is selected from the group consisting of Compound 1 – Compound 32.

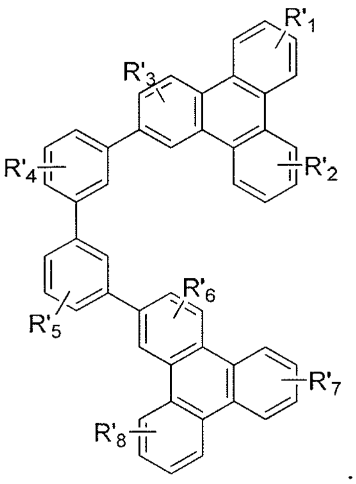
[0044] In one aspect, the organic layer is an emissive layer and the first compound is an emissive compound.

[0045] In another aspect, the organic layer further comprises a second emissive compound. Preferably, the second emissive compound is

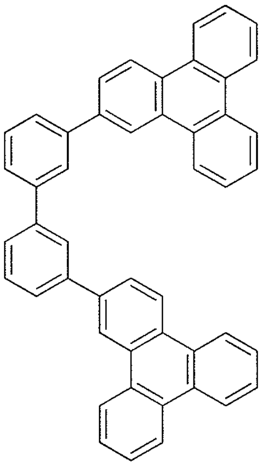


Compound H .

[0046] In another aspect, the organic layer further comprises a host having the formula:



[0047] R'$_1$, R'$_2$, R'$_3$, R'$_4$, R'$_5$, R'$_6$, R'$_7$, and R'$_8$ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Preferably, the host is:



Compound F .

[0048] In one aspect, the first device is a consumer product. In another aspect, the first device is an organic light emitting device.

BRIEF DESCRIPTION OF THE DRAWINGS

[0049] FIG. 1 shows an organic light emitting device.

[0050] FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

[0051] FIG. 3 shows a compound comprising a 2-phenylpyridine ligand further substituted with a heterocyclic group.

DETAILED DESCRIPTION

[0052] Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, an "exciton," which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

[0053] The initial OLEDs used emissive molecules that emitted light from their singlet states ("fluorescence") as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

[0054] More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in US Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

[0055] FIG. 1 shows an organic light emitting device 100. The figures are not necessarily drawn to scale. Device 100 may include a substrate 110, an anode 115, a hole injection layer 120, a hole transport layer 125, an electron blocking layer 130, an emissive layer 135, a hole blocking layer 140, an electron transport layer 145, an electron injection layer 150, a protective layer 155, and a cathode 160. Cathode 160 is a compound cathode having a first conductive layer 162 and a second conductive layer 164. Device 100 may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in US 7,279,704 at cols. 6-10, which are incorporated by reference.

[0056] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F.sub.4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

[0057] FIG. 2 shows an inverted OLED 200. The device includes a substrate 210, a cathode 215, an emissive layer 220, a hole transport layer 225, and an anode 230. Device 200 may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device 200 has cathode 215 disposed under anode 230, device 200 may be referred to as an "inverted" OLED. Materials similar to those described with respect to device 100 may be used in the corresponding layers of device 200. FIG. 2 provides one example of how some layers may be omitted from the structure of device 100.

[0058] The simple layered structure illustrated in FIGS. 1 and 2 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. For example, in device 200, hole transport layer 225 transports holes and injects holes into emissive layer 220, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.

[0059] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

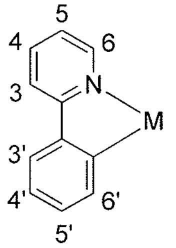
[0060] Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. patent application Ser. No. 10/233,470, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and organic vapor jet deposition (OVJD). Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processibility than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

[0061] Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.).

[0062] The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

[0063] The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, arylkyl, heterocyclic group, aryl, aromatic group, and heteroaryl are known to the art, and are defined in US 7,279,704 at cols. 31-32, which are incorporated herein by reference.

[0064] Novel compounds containing a phenylpyridine ligand further substituted with a heterocyclic ring are provided. In particular, the heterocyclic ring is attached to the pyridine ring of the 2-phenylpyridine ligand at the position para to the metal, i.e., the 4 position, to which the ligand is coordinated (illustrated in FIG. 3). The compounds may be used as emissive materials for phosphorescent OLEDs. All ligands in the compound are phenylpyridine-based, because these ligands may have higher stability. For example, a compound with all phenylpyridine-based ligands may have higher stability than a compound comprising an acetylacetone, i.e., acac, ligand.



[0065] Phenylpyridine and alkyl substituted 2-phenylpyridine ligands have been reported in the literature. In particular, these ligands can bind strongly with iridium(III) to provide good chemical stability. Additionally, the tris complexes of iridium and 2-phenylpyridine ligands may evaporate under high vacuum at low temperatures (i.e., <250 °C). However, the use of these compounds in phosphorescent OLEDs is limited. The operational stability of OLEDs comprising these complexes as the emissive material is poor. Aryl and heterocyclic substitution on 2-phenylpyridine can improve device stability. As reported herein, homoleptic and heteroleptic compounds comprising of at least one ligand with a heterocyclic substituent provide improved devices. In particular, the compounds provided herein may provide high efficiency, high luminous efficiency : quantum efficiency ratio (LE:EQE) and high stability.

[0066] Phenyl groups substituted on the pyridine ring of the 2-phenylpyridine ligand may increase the conjugation of the ligand and, in some cases, result in a red shifted emission. This red-shifting effect may be desirable for emission with longer wavelengths (between 540 nm and 560 nm) in the yellow part of the spectrum. Heterocyclic groups substituted on the pyridine ring of the 2-phenylpyridine ligand may also increase the conjugation of the ligand resulting in even further red shifted emission of up to 590 nm. Without being bound by theory, it is believed that the heterocyclic group located at the 4 position of the pyridine ring of the 2-phenylpyridine ligand provides significant red shifting impact and broadens the emission spectra. That is, heterocyclic rings at the 4 position of the 2-phenylpyridine ligand may provide a broad organce spectrum, which may be especially desirable for white devices. In particular, a nitrogen containing heterocycle may be particularly beneficial for color tuning.

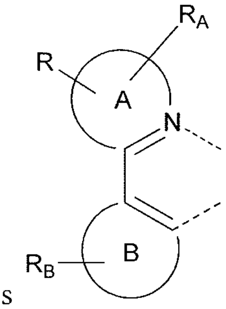
[0067] These materials can be very useful in certain applications, for example, the development of white OLEDs. Typical white OLEDs can be prepared by using a combination of emissive components with different wavelengths, which when optimized can produce white light. White OLEDs can typically be prepared by using a combination of 3 emissive components. In particular, a combination of blue, green and red emissive components can be used to generate white light. For manufacturing purposes, it is most desirable to incorporate a minimum number of materials into a device. Therefore, white OLEDs containing only two emissive components are highly desirable.

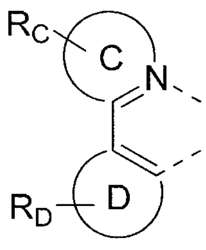
[0068] Generating a commercial device using two emissive components to generate white light is far more challenging than generating a commercial device using three components. Emitters with more specific colors are required. Without being bound by theory, it is believed that the compounds provided herein emit in an energy range suitable for use in two emitting component white devices. In addition, these compounds can also be used in a three emitting component white device.

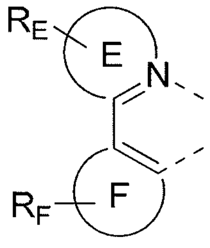
[0069] Heterocyclic groups substituted at the 4 position on the pyridine ring of the 2-phenylpyridine not only provides the optimum desired color but in addition the ligand may also lower and stabilize the LUMO of the metal complex, thereby providing further device operational stability. The homoleptic and heteroleptic compounds provided herein comprise at least one 2-phenylpyridine ligand with a heterocyclic substituent attached to the pyridine para to the metal, i.e., the 4 position. These ligands result in a stabilized LUMO and red shifted emission of the metal complex. Therefore, the compounds provided herein may have emission energies red shifted from the target range of phenyl substituted or unsubstituted counterparts, i.e., 550 nm and 600 nm.

[0070] The compounds provided herein may provide devices having high efficiency, high stability and improved processiblity. These compounds are suitable for both monochrome displays and white devices for displays, medical backlight and lighting.

[0071] Compounds having the formula $M(L)_x(L_1)_y(L_2)_z$ are provided.

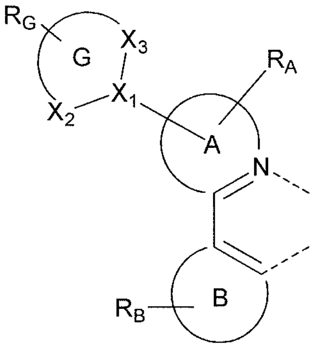
[0072] L is  Formula I.

[0073] L_1 is  Formula II.

[0074] L_2 is  Formula III.

[0075] L_1 and L_2 can be the same or different. M is a metal having an atomic number greater than 40. Preferably, the metal M is Ir. x is 1, 2 or 3. y is 0, 1 or 2. z is 0, 1 or 2. x+y+z is the oxidation state of the metal M. A is a 6-membered heterocyclic ring. B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. Preferably, B is phenyl. R is a 5 or 6-membered heterocyclic ring. R is attached to A at a position para to the metal M. R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions. Each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated bidentately to the metal M. R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom.

[0076] In one aspect, the ligand L has the formula:



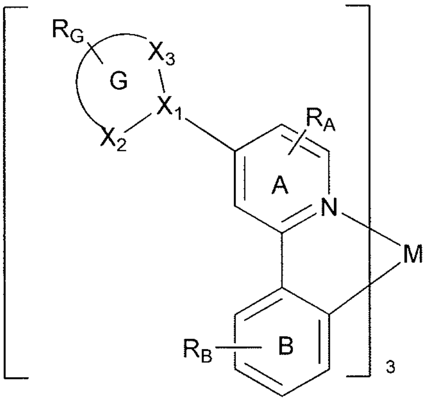
Formula IV.

[0077] G is a 5 or 6-membered heterocyclic ring. Preferably, G is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. X_1, X_2, and X_3 are independently selected from carbon, oxygen, sulfur and nitrogen. Preferably, X_1, X_2, and X_3 are independently carbon or nitrogen. R_G may represent mono, di, tri, tetra, or penta substitutions. R_G is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

[0078] In one aspect, at least one of X_1, X_2, and X_3 is nitrogen. In another aspect, each of X_1, X_2, and X_3 is carbon.

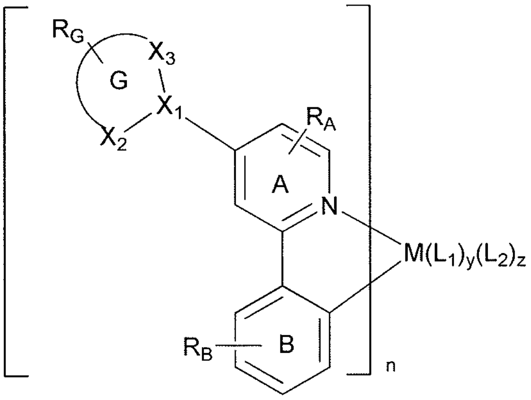
[0079] In another aspect, L, L_1 and L_2 are connected to form a tetradentate ligand and a bidentate ligand or a hexadentate ligand. For example, L and L_1 may be connected to form a tetradentate ligand and L_2 is a bidentate ligand. Similarly, L and L_2 or L_1 and L_2 may be connected to form a tetradentate ligand while L_1 or L is a bidentate ligand. Additionally, L, L_1 and L_2 may all be connected to form a hexadentate ligand.

[0080] In one aspect, the compound is homoleptic. In another aspect, the compound has the formula:



Formula V.

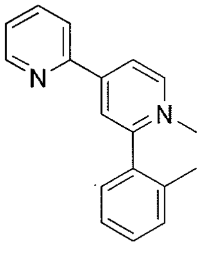
[0081] In one aspect, the compound is heteroleptic. In another aspect, the compound has the formula:

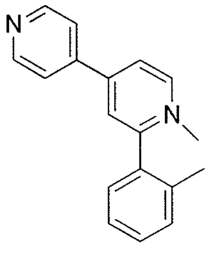


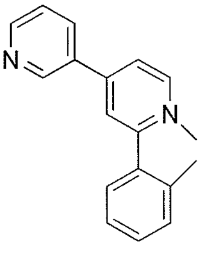
Formula VI.

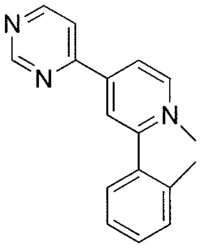
[0082] n+y+z is the oxidation state of the metal M. n is at least 1. y is 0, 1 or 2. x is 0, 1, or 2.

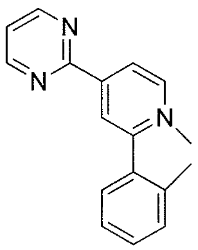
[0083] In one aspect, the ligand L is selected from the group consisting of:

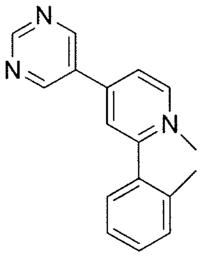


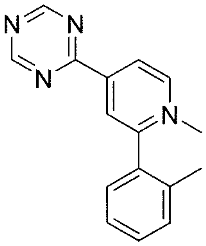


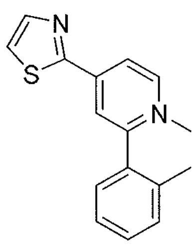


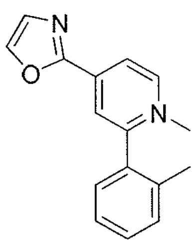


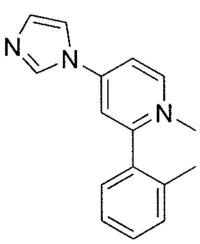


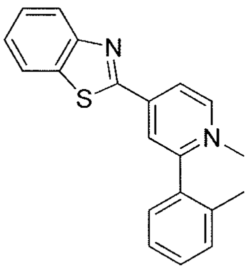


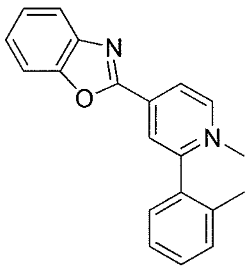






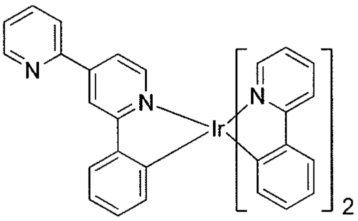




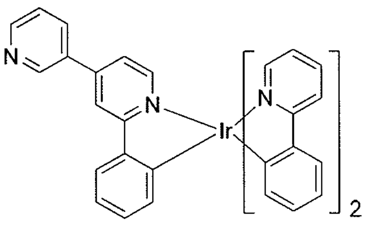


.

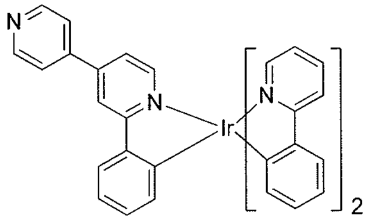
[0084] Specific examples of compounds comprising a phenyl pyridine ligand further substituted with a heterocyclic ring are also provided. In particular, the compound is selected from the group consisting of:



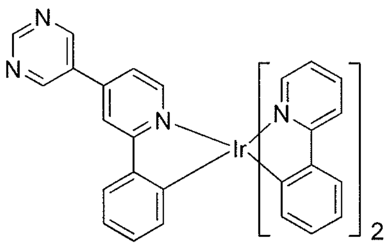
Compound 1



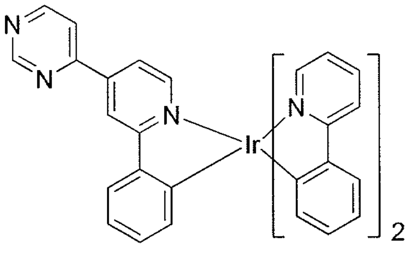
Compound 2



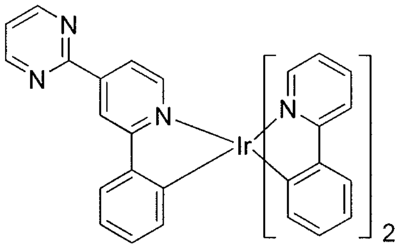
Compound 3



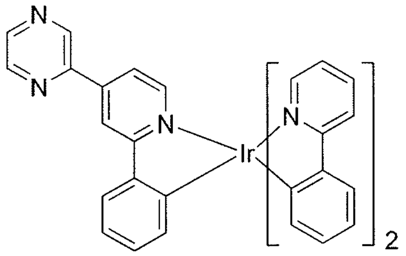
Compound 4



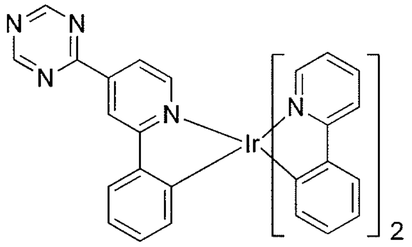
Compound 5



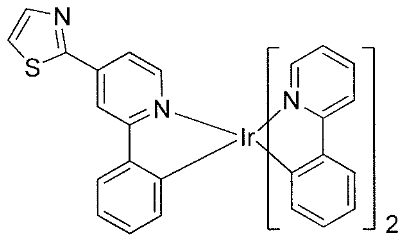
Compound 6



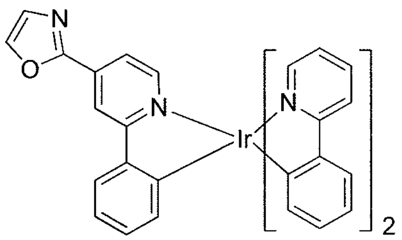
Compound 7



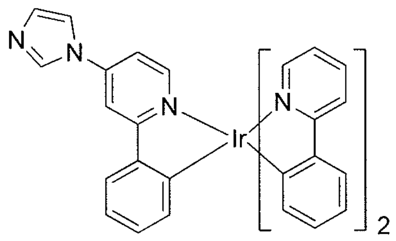
Compound 8



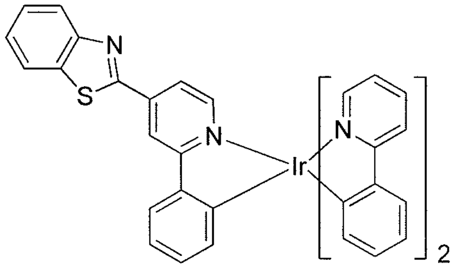
Compound 9



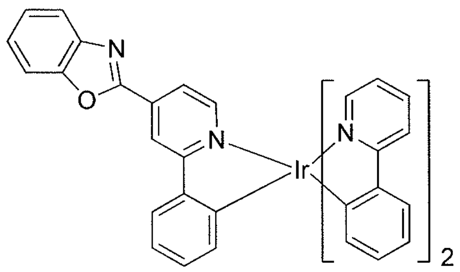
Compound 10



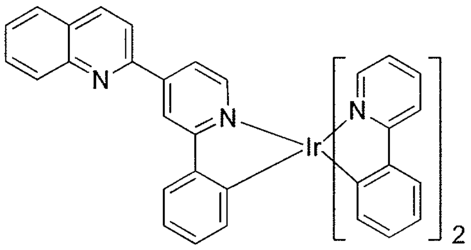
Compound 11



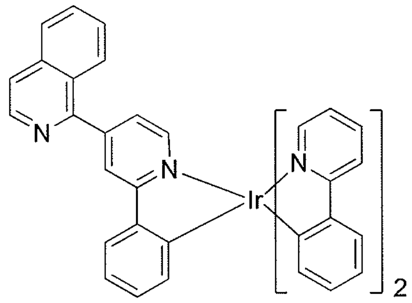
Compound 12



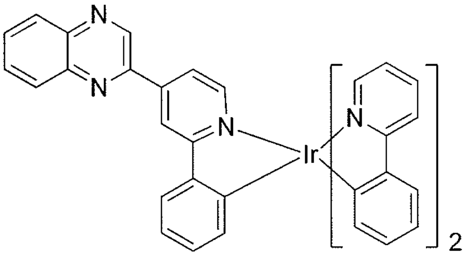
Compound 13

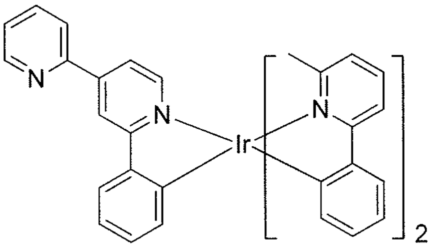


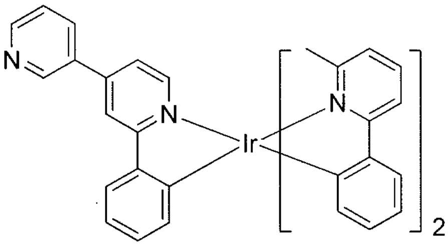
Compound 14

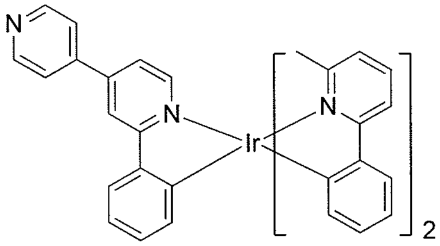


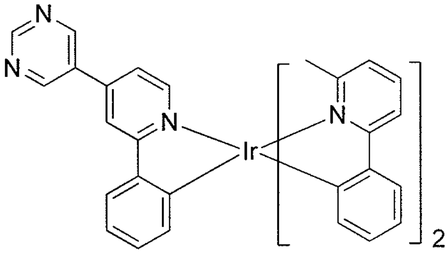
Compound 15

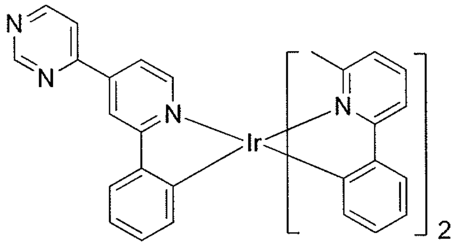

Compound 16

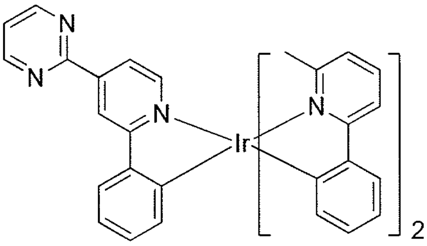

Compound 17

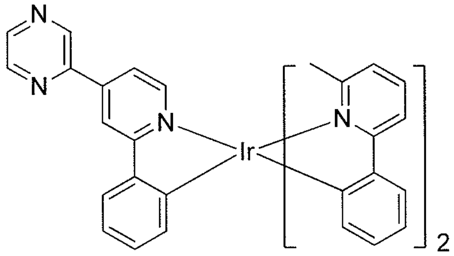

Compound 18

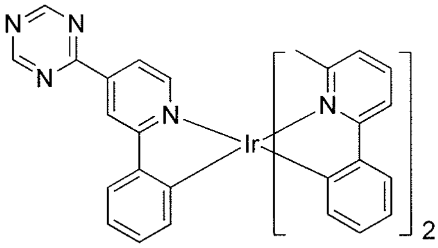

Compound 19

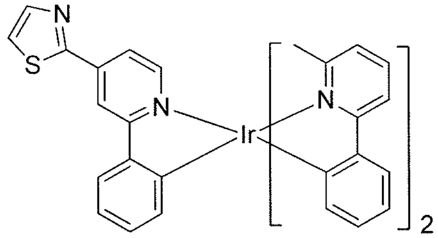

Compound 20

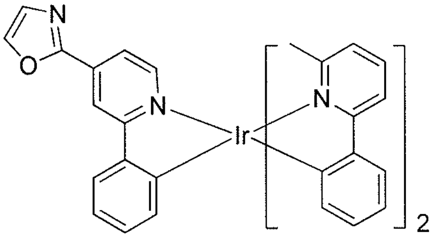

Compound 21


Compound 22

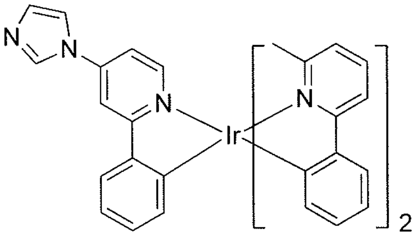

Compound 23


Compound 24

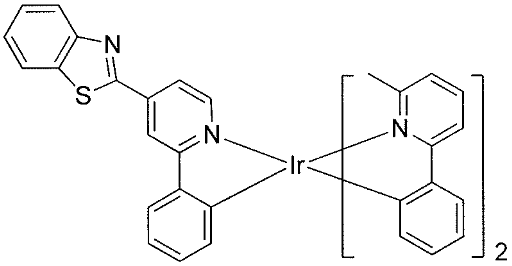

Compound 25



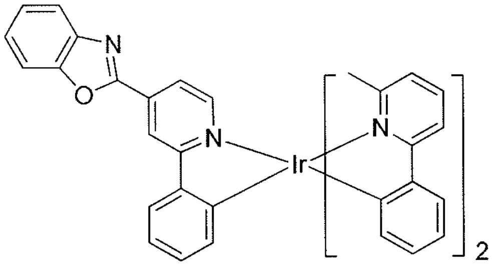
Compound 26



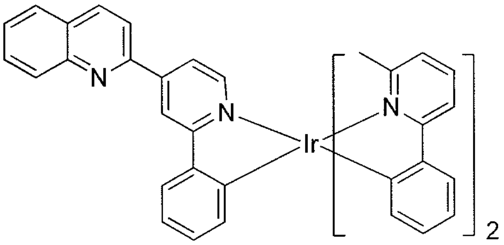
Compound 27



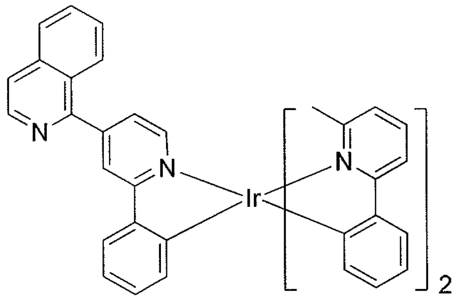
Compound 28



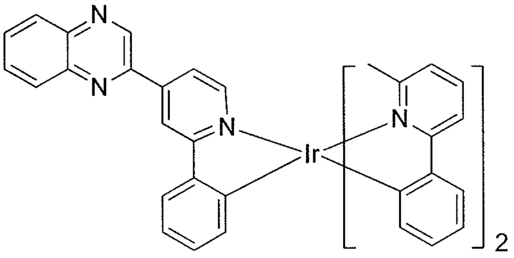
Compound 29



Compound 30

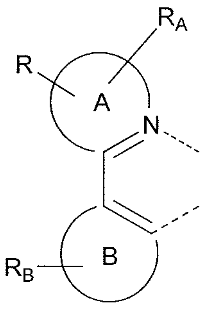


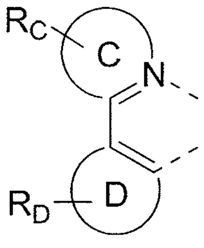
Compound 31

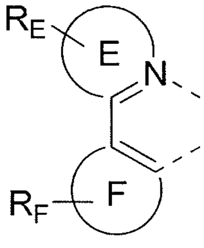


Compound 32

[0085] A first device is also provided. The first device comprises an organic light emitting device, further comprising an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprising a first compound having the formula $M(L)_x(L_1)_y(L_2)_z$.

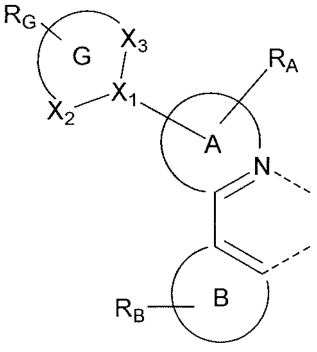
[0086] L is  Formula I.

[0087] L_1 is  Formula II.

[0088] L_2 is  Formula III.

[0089] L_1 and L_2 can be the same or different. M is a metal having an atomic number greater than 40. Preferably, the metal M is Ir. x is 1, 2 or 3. y is 0, 1 or 2. z is 0, 1 or 2. x+y+z is the oxidation state of the metal M. A is a 6-membered heterocyclic ring. B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. Preferably, B is phenyl. R is a 5 or 6-membered heterocyclic ring. Preferably, R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. R is attached to A at a position para to the metal M. R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions. Each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated bidentately to the metal M.

[0090] In one aspect, the ligand L has the formula:



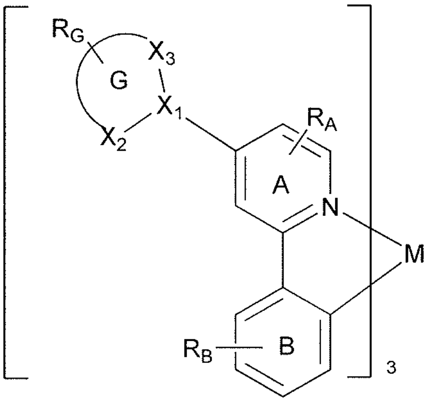
Formula IV.

[0091] G is a 5 or 6-membered heterocyclic ring. Preferably, G is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. X_1, X_2, and X_3 are independently selected from carbon, oxygen, sulfur and nitrogen. Preferably, X_1, X_2, and X_3 are independently carbon or nitrogen. R_G may represent mono, di, tri, tetra, or penta substitutions. R_G is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

[0092] In one aspect, at least one of X_1, X_2, and X_3 is nitrogen. In another aspect, each of X_1, X_2, and X_3 is carbon.

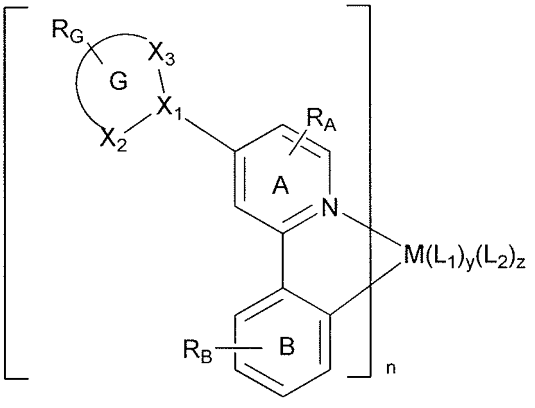
[0093] In another aspect, L, L_1 and L_2 are connected to form a tetradentate ligand and a bidentate ligand or a hexadentate ligand.

[0094] In one aspect, the compound is homoleptic. In another aspect, the compound has the formula:



Formula V.

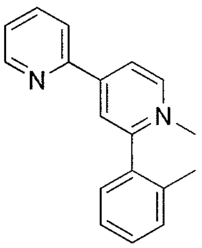
[0095] In one aspect, the compound is heteroleptic. In another aspect, the compound has the formula:

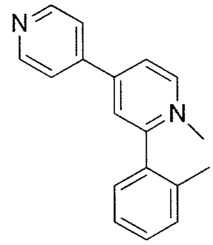


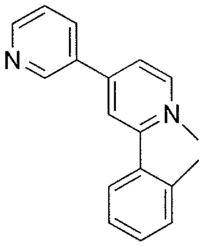
Formula VI.

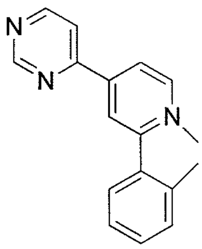
[0096] n+y+z is the oxidation state of the metal M. n is at least 1. y is 0, 1 or 2. x is 0, 1, or 2.

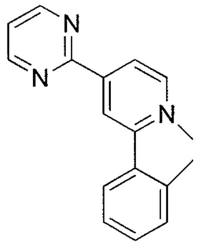
[0097] In one aspect, the ligand L is selected from the group consisting of:

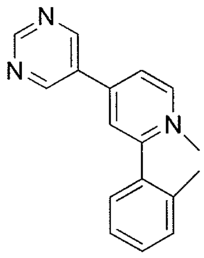


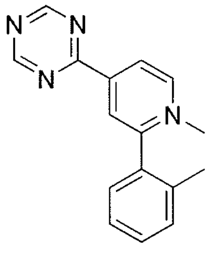


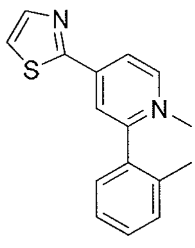


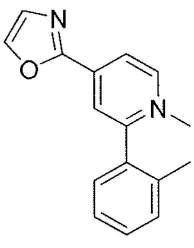


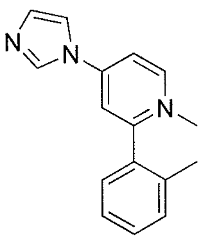


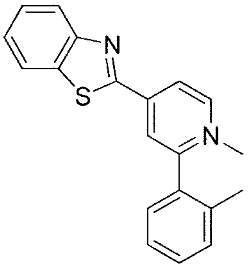


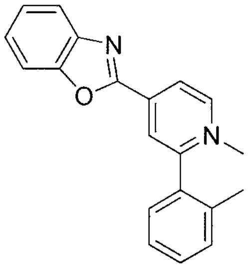






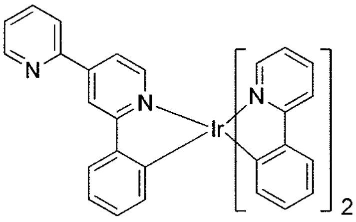




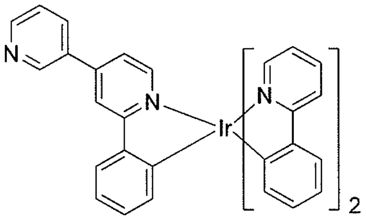


.

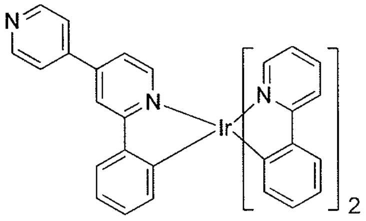
[0098] Specific examples of devices containing compounds comprising a phenyl pyridine ligand further substituted with a heterocyclic ring. In particular, the compound is selected from the group consisting of:



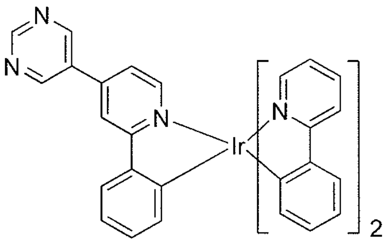
Compound 1



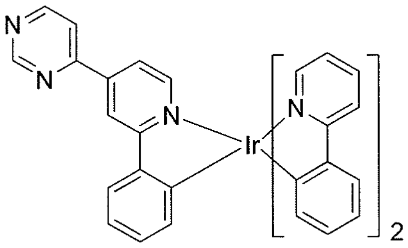
Compound 2



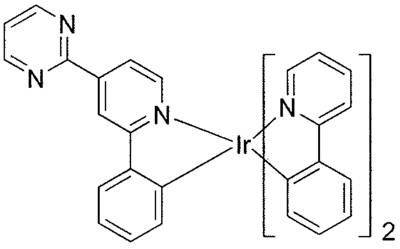
Compound 3



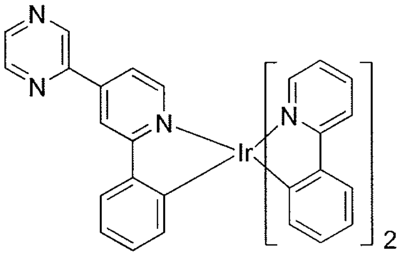
Compound 4



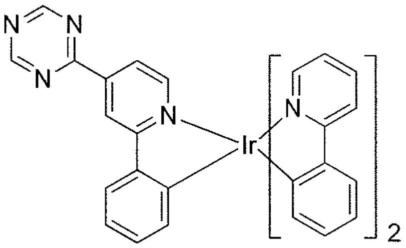
Compound 5



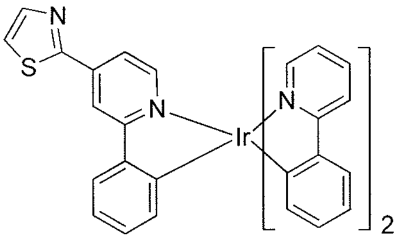
Compound 6



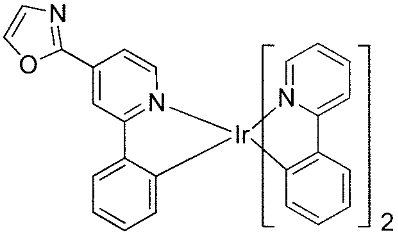
Compound 7



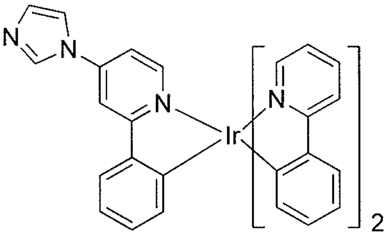
Compound 8



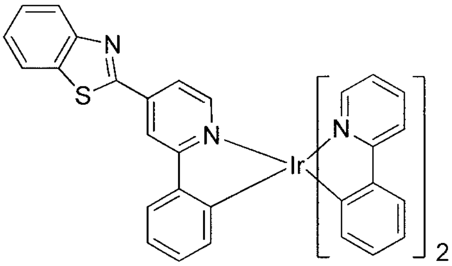
Compound 9



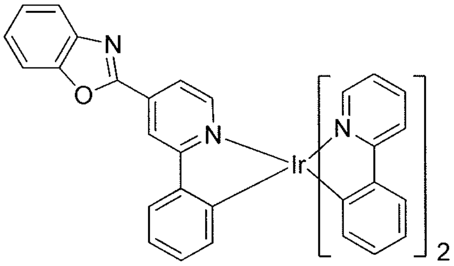
Compound 10



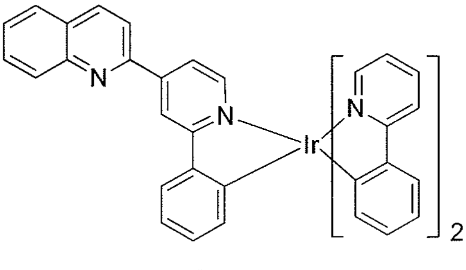
Compound 11



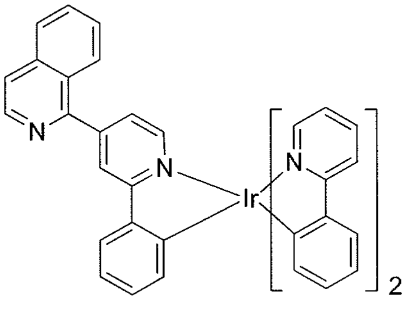
Compound 12



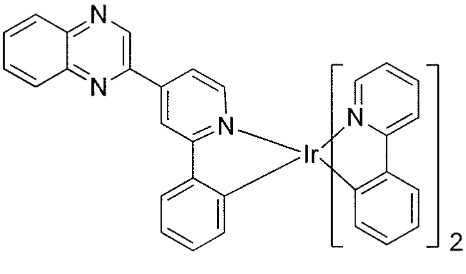
Compound 13



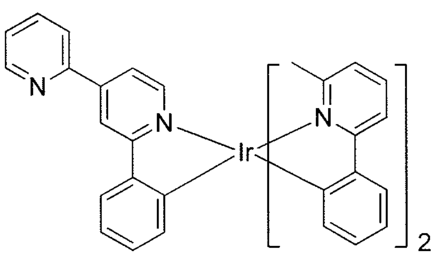
Compound 14



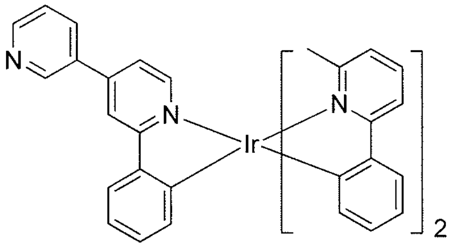
Compound 15



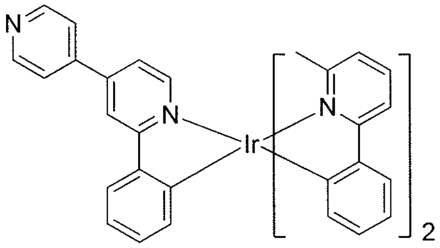
Compound 16



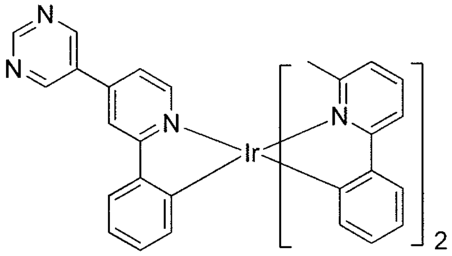
Compound 17



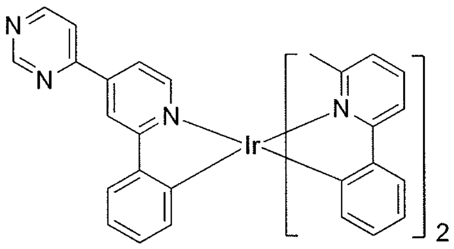
Compound 18



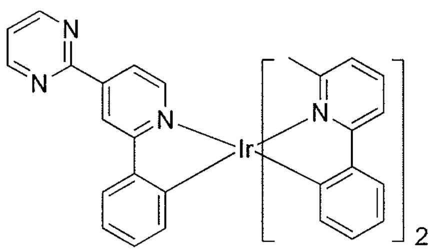
Compound 19



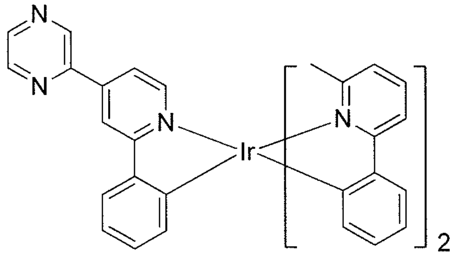
Compound 20



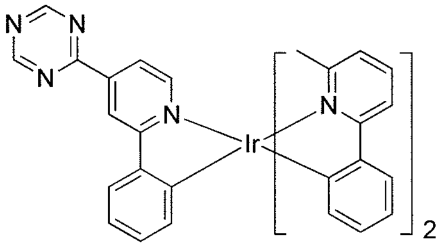
Compound 21



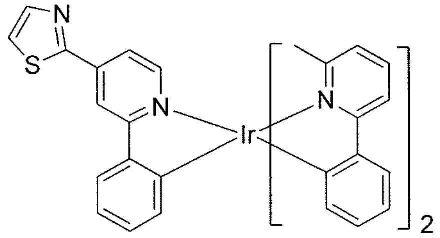
Compound 22



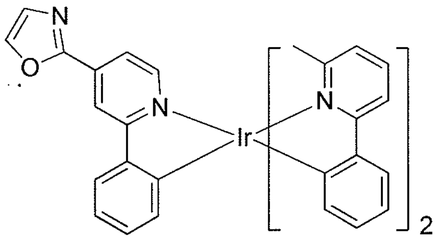
Compound 23



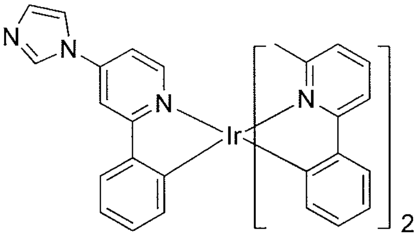
Compound 24



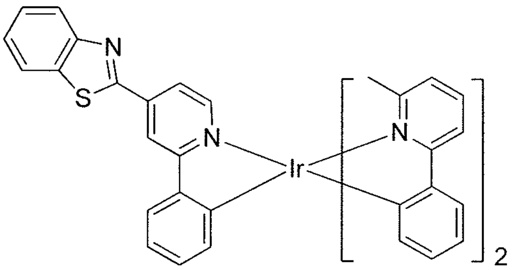
Compound 25



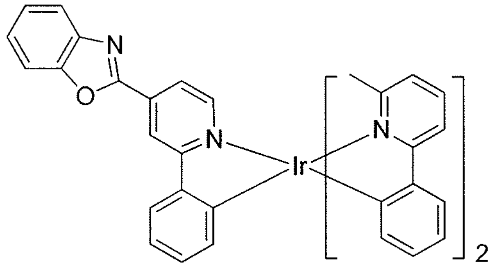
Compound 26



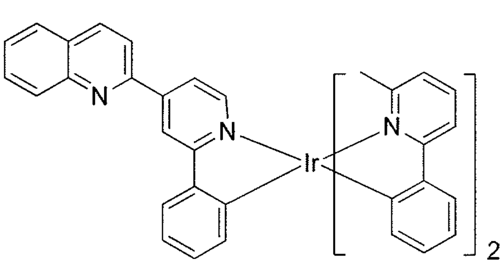
Compound 27



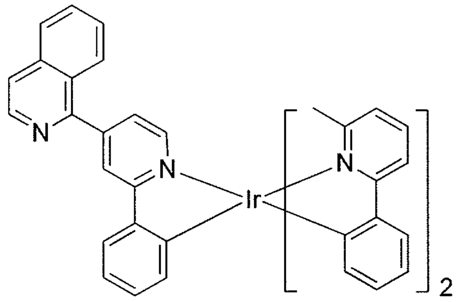
Compound 28



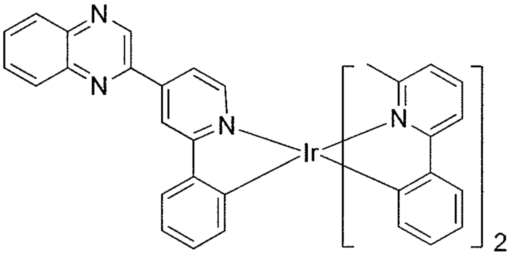
Compound 29



Compound 30



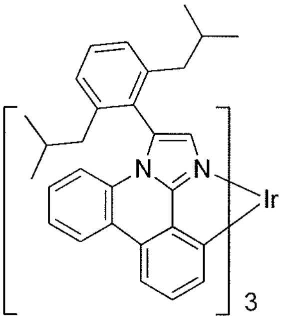
Compound 31



Compound 32

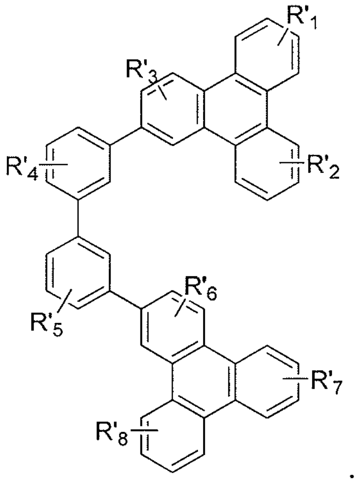
[0099] In one aspect, the organic layer is an emissive layer and the first compound is an emissive compound.

[0100] In another aspect, the organic layer further comprises a second emissive compound. Preferably, the second emissive compound is

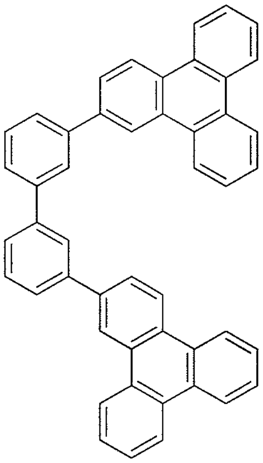


Compound H

[0101] In another aspect, the organic layer further comprises a host having the formula:



[0102] R'$_1$, R'$_2$, R'$_3$, R'$_4$, R'$_5$, R'$_6$, R'$_7$, and R'$_8$ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. Preferably, the host is:

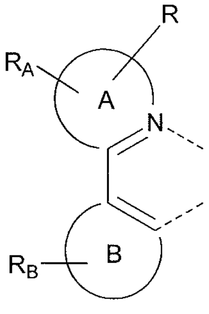


Compound F .

[0103] In one aspect, the first device is a consumer product. In another aspect, the first device is an organic light emitting device.

[0104] In addition, there are several other embodiments. However, these additional embodiments are less preferred.

[0105] Compounds comprising a 2-phenylpyridine ligand further substituted with a heterocyclic ring are provided. The compounds comprise a ligand L having the formula:

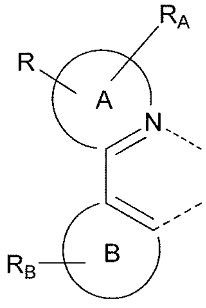


Formula VII.

[0106] A and B are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. Preferably, B is phenyl. R is a 5 or 6-membered heterocyclic ring. Preferably, R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. R_A and R_B may represent mono, di, tri, tetra, or penta substitutions. R_A and R_B is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated to a metal M having an atomic number greater than 40. Preferably, the metal M is Ir.

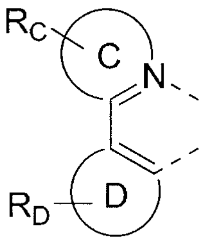
[0107] In one aspect, the compounds have the formula $M(L)_x(L_1)_y(L_2)_z$.

[0108] L is



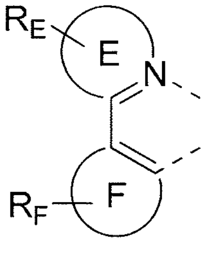
Formula VIII.

[0109] L_1 is



Formula IX.

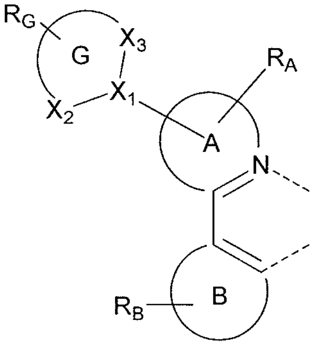
[0110] L_2 is



Formula X.

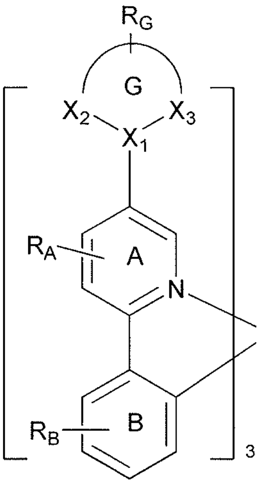
[0111] L_1 and L_2 can be the same or different. x is 1, 2 or 3, y is 0, 1 or 2, z is 0, 1 or 2. x+y+z is the oxidation state of the metal M. A, B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. R is a 5 or 6-membered heterocyclic ring. R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions. Each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated bidentately to a metal M having an atomic number greater than 40.

[0112] In one aspect, the compound is homoleptic. In a particular aspect, the compound has the formula:

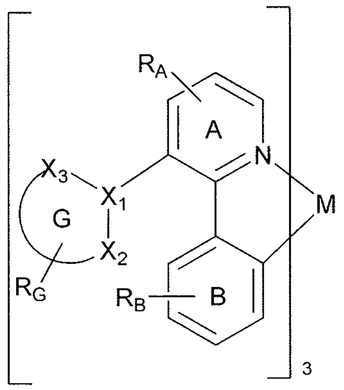


Formula XI.

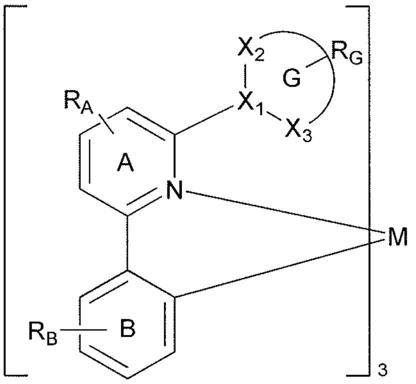
[0113] In another aspect, the compound has a formula selected from the group consisting of:



Formula XII

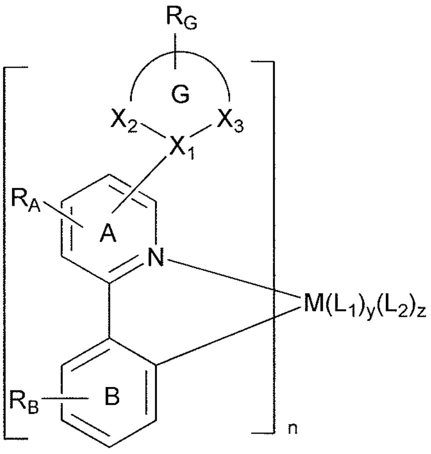


Formula XIII



Formula XIV

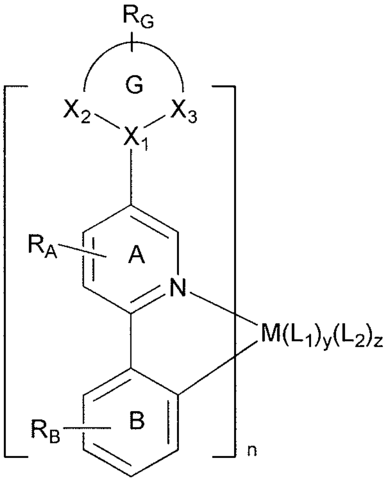
[0114] In one aspect, the compound is heteroleptic. In a particular aspect, the compound has the formula:



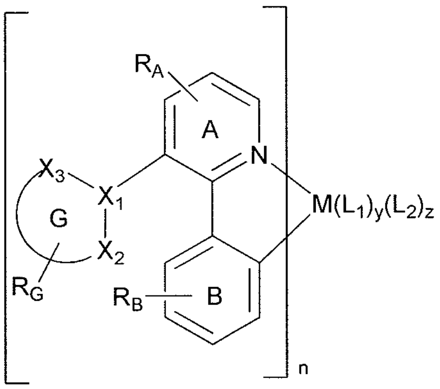
Formula XV.

[0115] $n+y+z$ is the oxidation state of the metal M. n is at least 1. y is 0, 1 or 2. x is 0, 1, or 2.

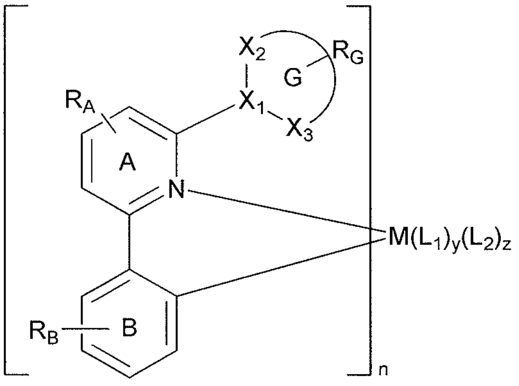
[0116] In another aspect, the compound has a formula selected from the group consisting of:



Formula XVI



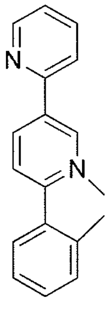
Formula XVII

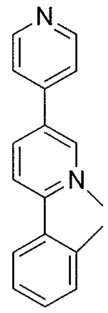


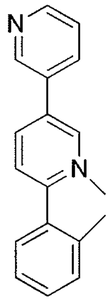
Formula XVIII

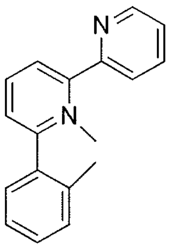
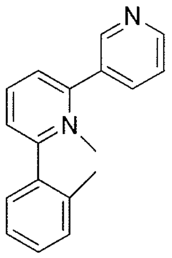
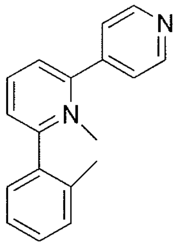
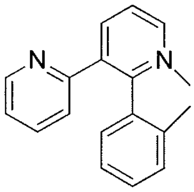
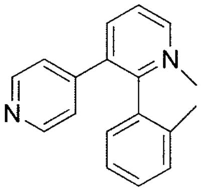
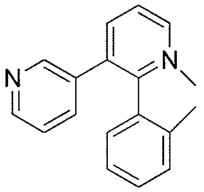
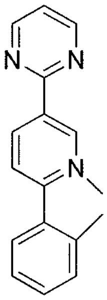
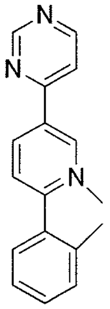
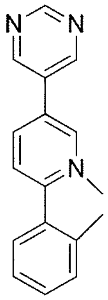
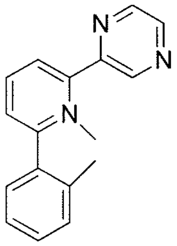
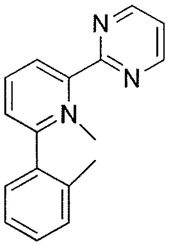
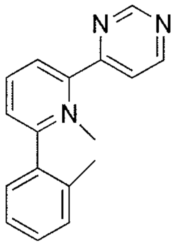
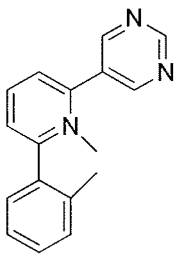
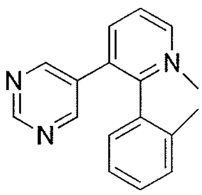
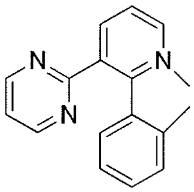
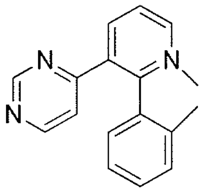
.

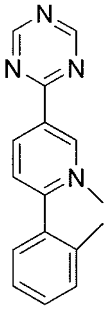
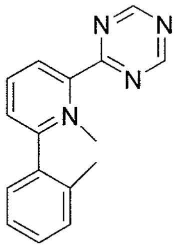
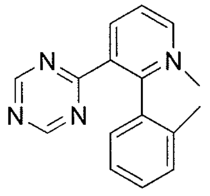
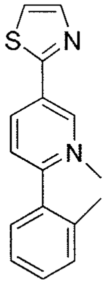
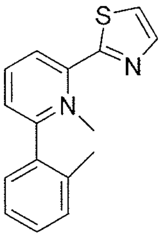
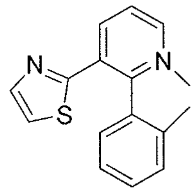
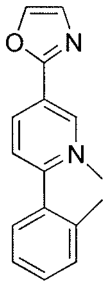
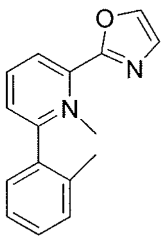
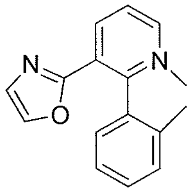
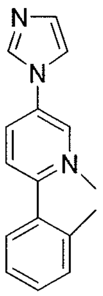
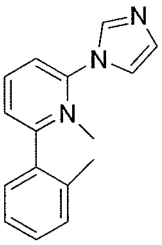
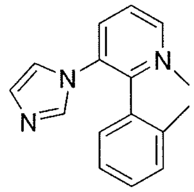
[0117] In one aspect, the ligand L is selected from the group consisting of:



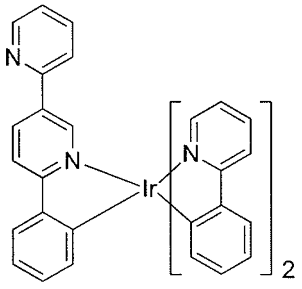




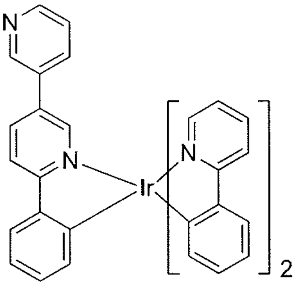

















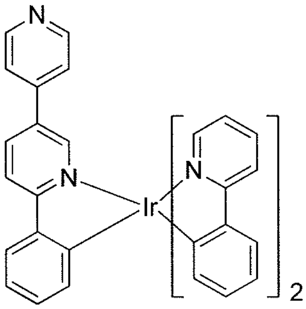
[0118] Specific examples of compounds comprising a phenyl pyridine ligand further substituted with a heterocyclic ring are also provided. In particular, the compound is selected from the group consisting of:



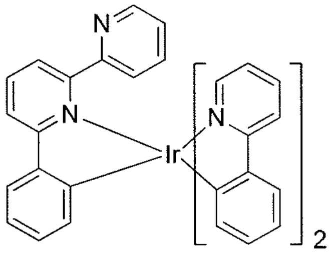
Compound 33



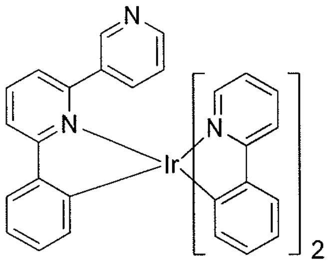
Compound 34



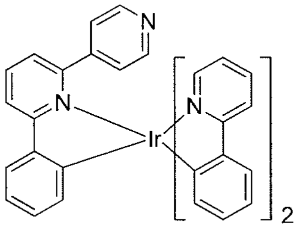
Compound 35



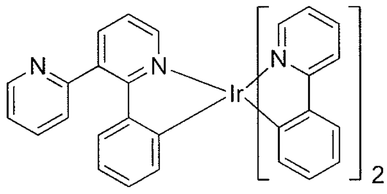
Compound 36



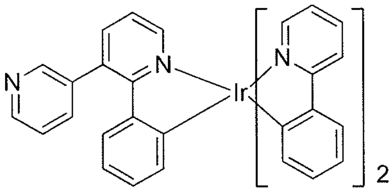
Compound 37



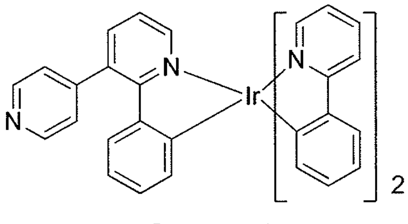
Compound 38



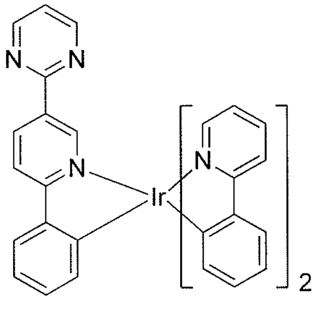
Compound 39



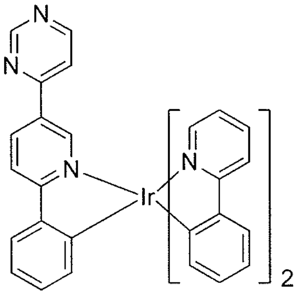
Compound 40



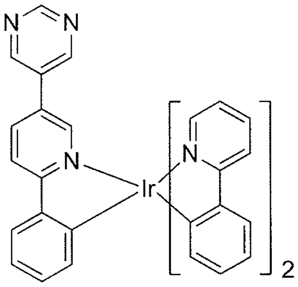
Compound 41



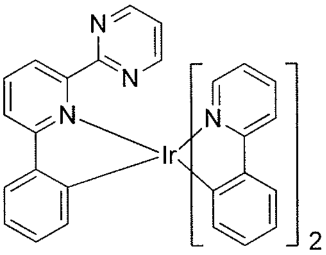
Compound 42



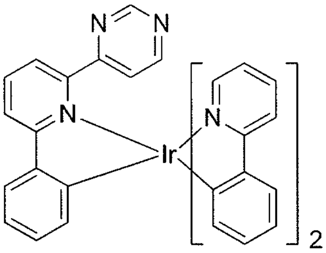
Compound 43



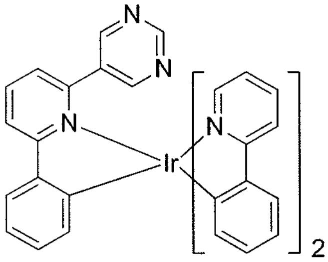
Compound 44



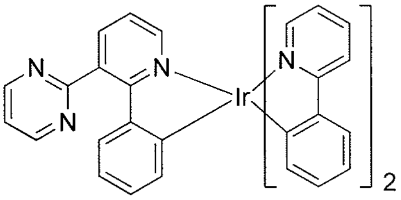
Compound 45



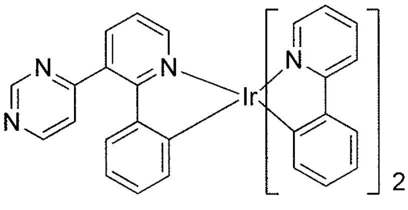
Compound 46



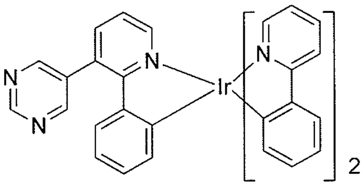
Compound 47



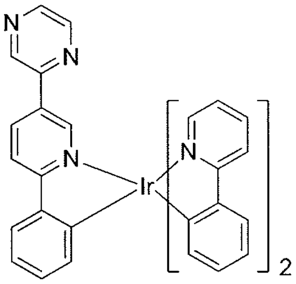
Compound 48



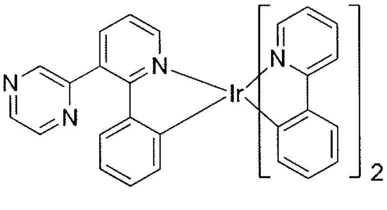
Compound 49



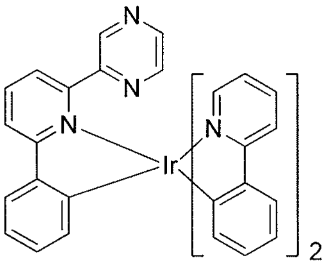
Compound 50



Compound 51

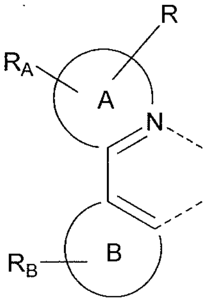


Compound 52



Compound 53 .

[0119] A first device comprising an organic light emitting device is also provided. The device further comprises an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprises a first compound having the formula:

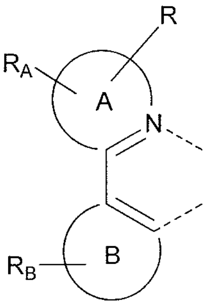


Formula VII.

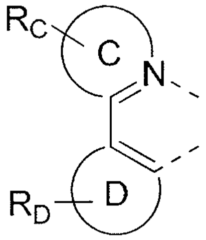
[0120] A and B are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. Preferably, B is phenyl. R is a 5 or 6-membered heterocyclic ring. Preferably, R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom. R_A and R_B may represent mono, di, tri, tetra, or penta substitutions. R_A and R_B is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated to a metal M having an atomic number greater than 40. Preferably, the metal M is Ir.

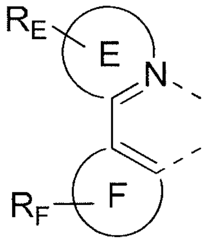
[0121] In one aspect, the device comprises a compound having the formula $M(L)_x(L_1)_y(L_2)_z$.

[0122] L is



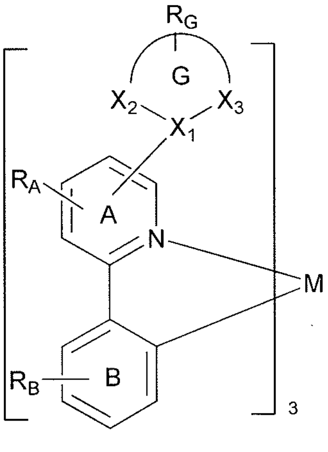
Formula VIII.

[0123] L_1 is  Formula IX.

[0124] L_2 is  Formula X.

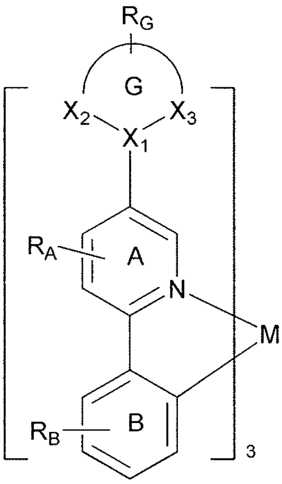
[0125] L_1 and L_2 can be the same or different. x is 1, 2 or 3, y is 0, 1 or 2, z is 0, 1 or 2. x+y+z is the oxidation state of the metal M. A, B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring. R is a 5 or 6-membered heterocyclic ring. R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions. Each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl. The ligand L is coordinated bidentately to a metal M having an atomic number greater than 40.

[0126] In one aspect, the compound is homoleptic. In a particular aspect, the compound has the formula:

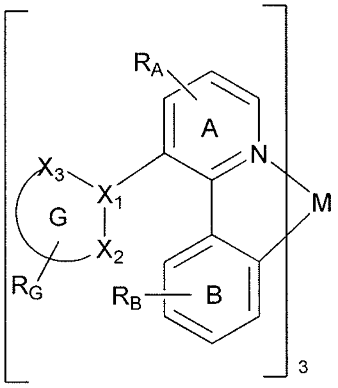


Formula XI.

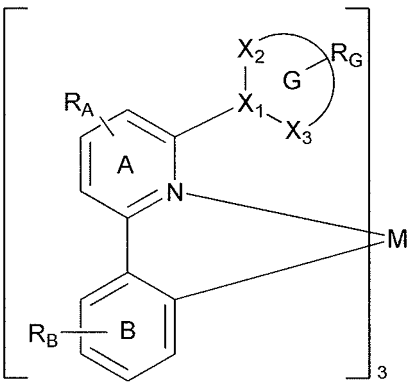
[0127] In another aspect, the compound has a formula selected from the group consisting of:



Formula XII

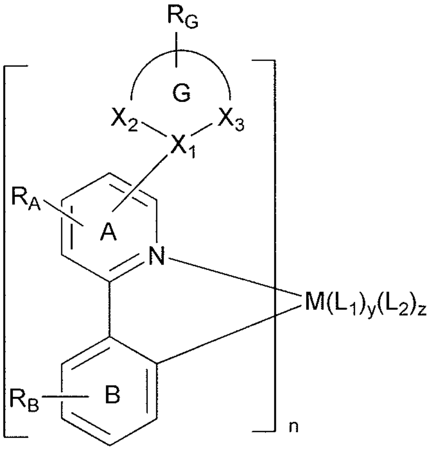


Formula XIII



Formula XIV.

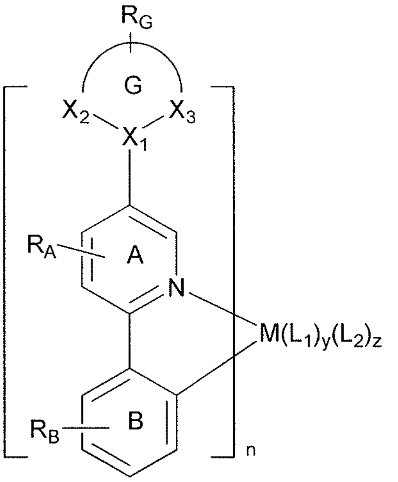
[0128] In another aspect, the compound is heteroleptic. In a particular aspect, the compound has the formula:



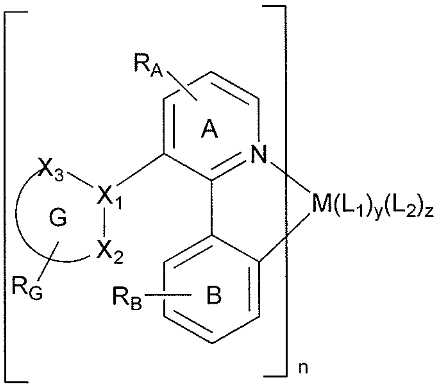
Formula XV.

[0129] n+y+z is the oxidation state of the metal M. n is at least 1. y is 0, 1 or 2. x is 0, 1, or 2.

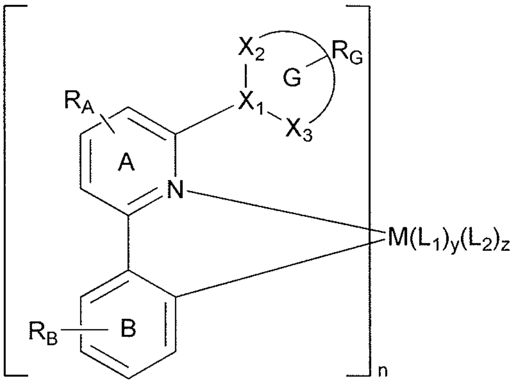
[0130] In yet another aspect, the compound has a formula selected from the group consisting of:



Formula XVI

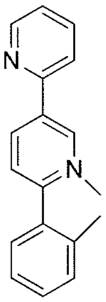


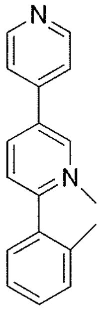
Formula XVII

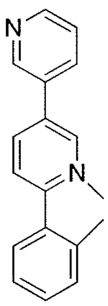


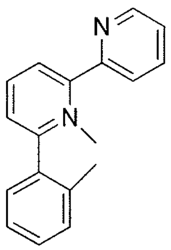
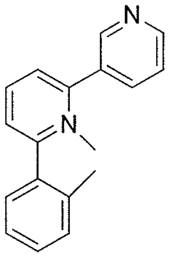
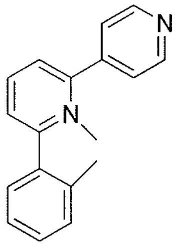
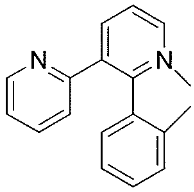
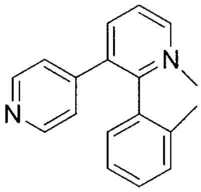
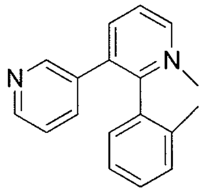
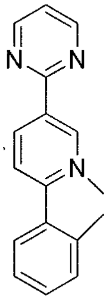
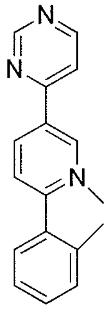
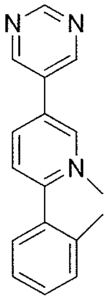
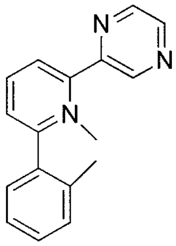
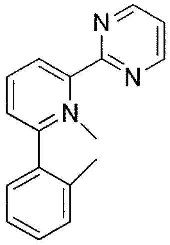
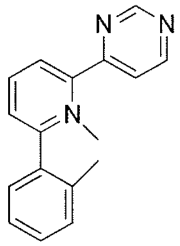
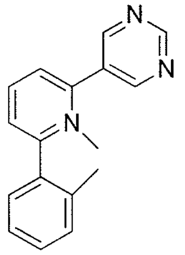
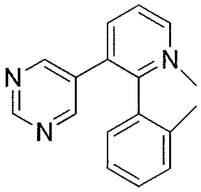
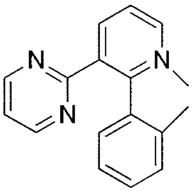
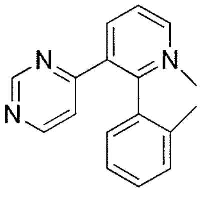
Formula XVIII

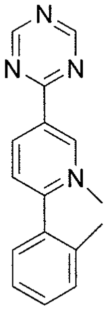
[0131] In one aspect, the ligand L is selected from the group consisting of:

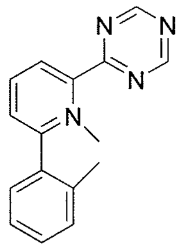


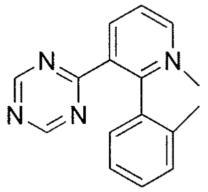


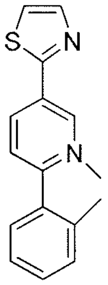


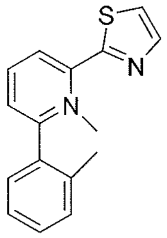

















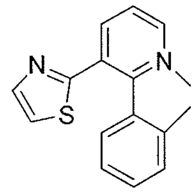


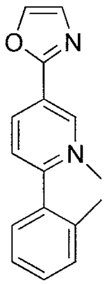


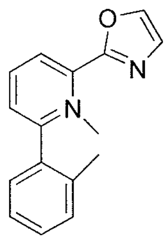


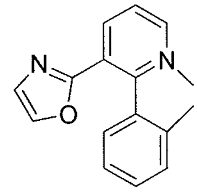


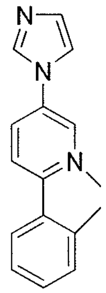


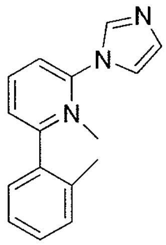


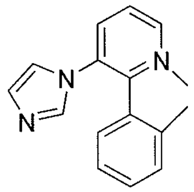






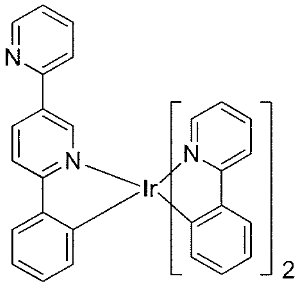


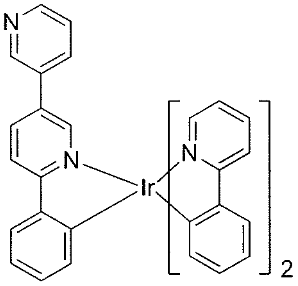


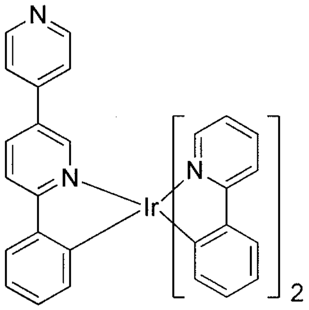


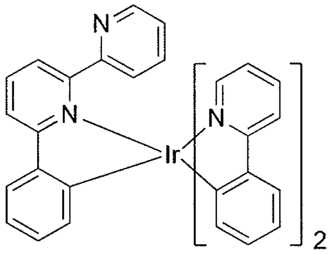
.

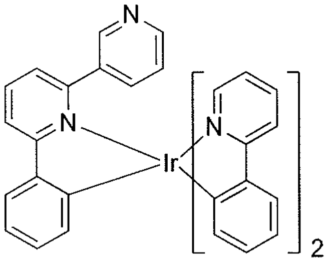
[0132] Specific examples of devices containing compounds comprising a phenyl pyridine ligand further substituted with a heterocyclic ring. In particular, the compound is selected from the group consisting of:

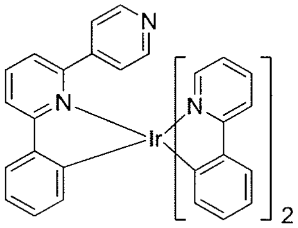

Compound 33

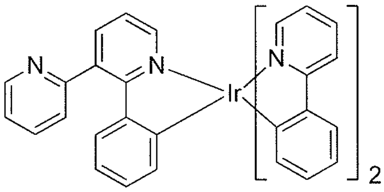

Compound 34

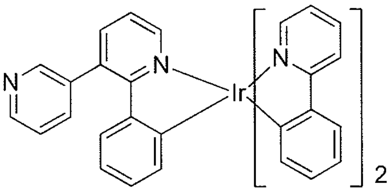

Compound 35

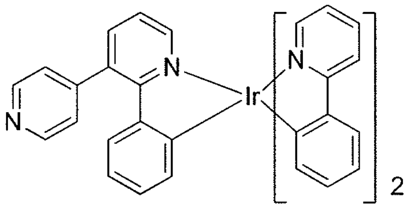

Compound 36

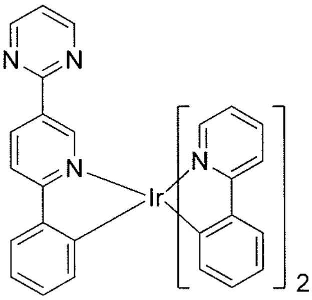

Compound 37

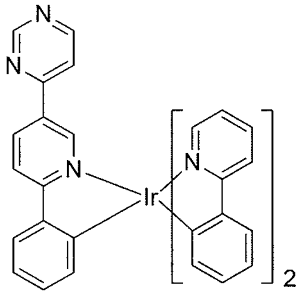

Compound 38


Compound 39

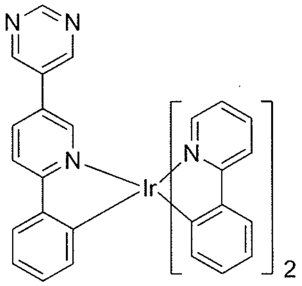

Compound 40


Compound 41

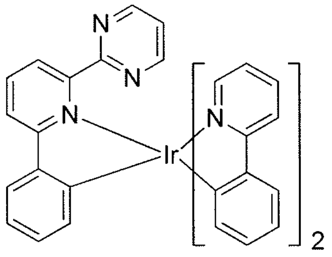

Compound 42



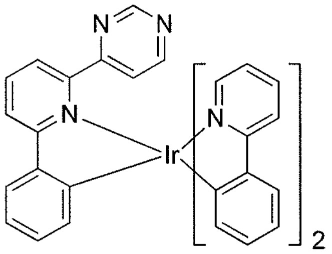
Compound 43



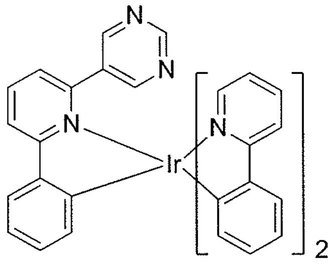
Compound 44



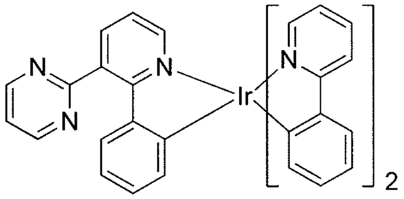
Compound 45



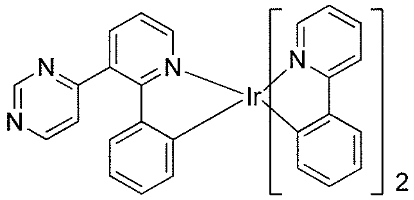
Compound 46



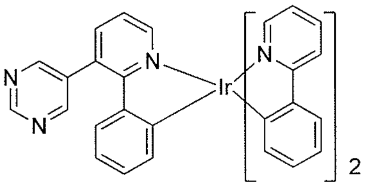
Compound 47



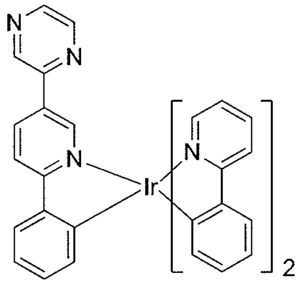
Compound 48



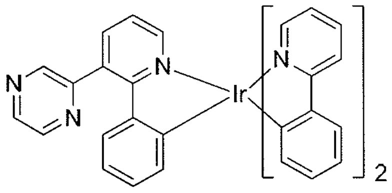
Compound 49



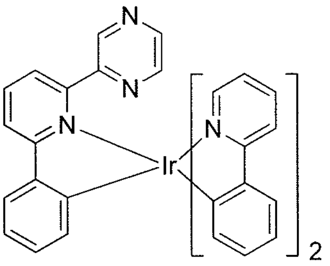
Compound 50



Compound 51



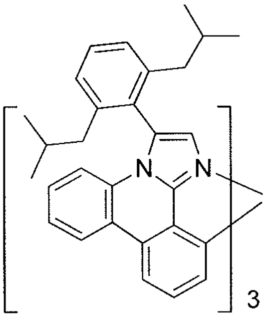
Compound 52



Compound 53 .

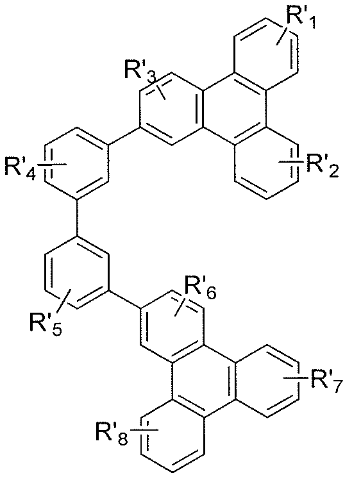
[0133] In one aspect, the organic layer is an emissive layer and the first compound having Formula I is an emissive compound.

[0134] In another aspect, the organic layer further comprises a second emissive compound. Preferably, the second emissive compound is



Compound H .

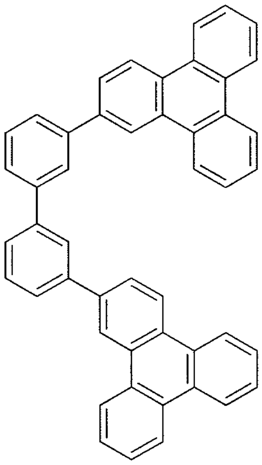
[0135] In yet another aspect, the organic layer further comprises a host having the formula:



.

[0136] R'$_1$, R'$_2$, R'$_3$, R'$_4$, R'$_5$, R'$_6$, R'$_7$, and R'$_8$ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

[0137] Preferably, the host is:



Compound F .

[0138] In one aspect, the first device is a consumer product. In another aspect, the first device is an organic light emitting device.

COMBINATION WITH OTHER MATERIALS

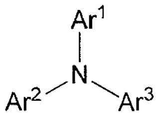
[0139] The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

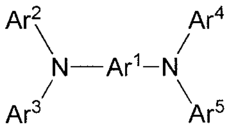
[0140] In addition to and / or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed below. The list includes non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

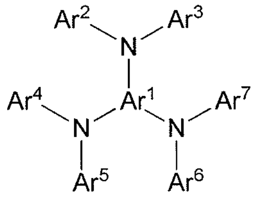
HIL/HTL:

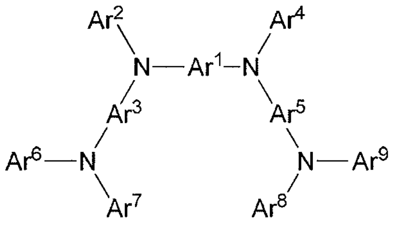
[0141] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphryin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and sliane derivatives; a metal oxide derivative, such as MoO_x; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

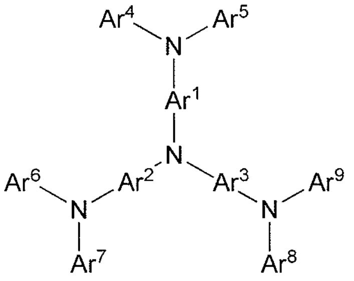
[0142] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:





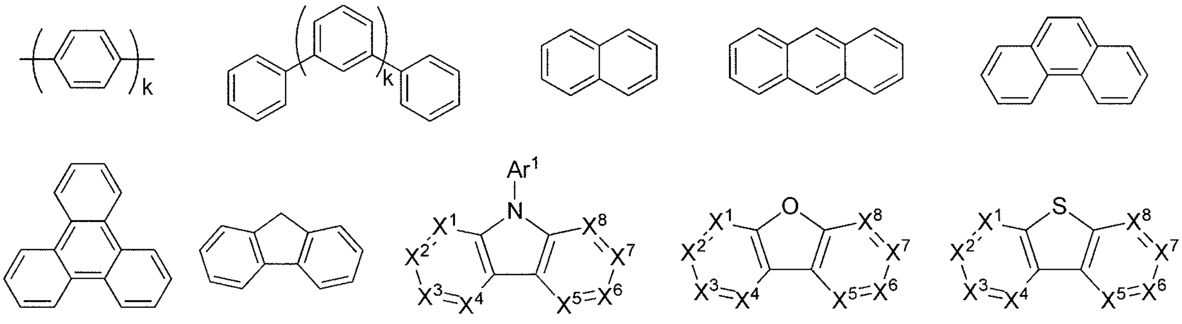






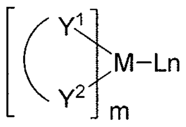
[0143] Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

[0144] In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:



[0145] k is an integer from 1 to 20; X^1 to X^8 is CH or N; Ar^1 has the same group defined above.

[0146] Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:



[0147] M is a metal, having an atomic weight greater than 40; (Y^1-Y^2) is a bidentate ligand, Y^1 and Y^2 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

[0148] In one aspect, (Y^1-Y^2) is a 2-phenylpyridine derivative.

[0149] In another aspect, (Y^1-Y^2) is a carbene ligand.

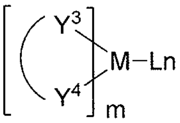
[0150] In another aspect, M is selected from Ir, Pt, Os, and Zn.

[0151] In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

Host:

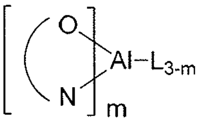
[0152] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant.

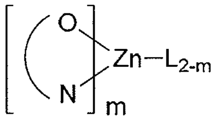
[0153] Examples of metal complexes used as host are preferred to have the following general formula:



[0154] M is a metal; (Y^3-Y^4) is a bidentate ligand, Y^3 and Y^4 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

[0155] In one aspect, the metal complexes are:





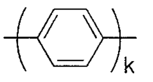
[0156] (O-N) is a bidentate ligand, having metal coordinated to atoms O and N.

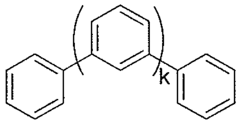
[0157] In another aspect, M is selected from Ir and Pt.

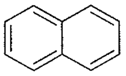
[0158] In a further aspect, (Y^3-Y^4) is a carbene ligand.

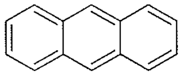
[0159] Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

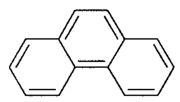
[0160] In one aspect, host compound contains at least one of the following groups in the molecule:

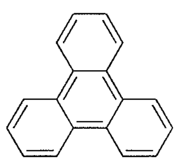


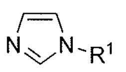


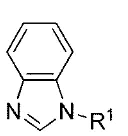


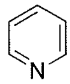


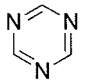


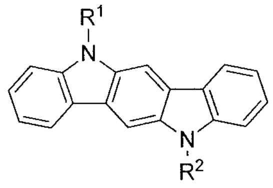


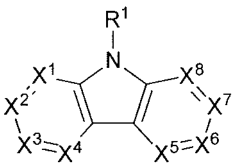


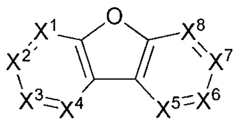


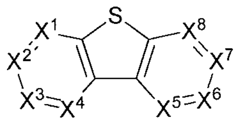


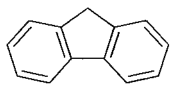


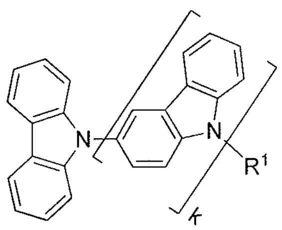


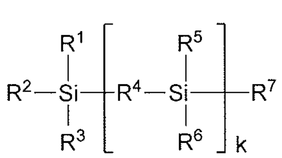


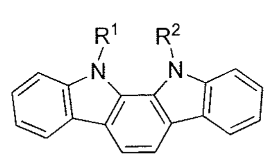












[0161] R^1 to R^7 is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

[0162] k is an integer from 0 to 20.

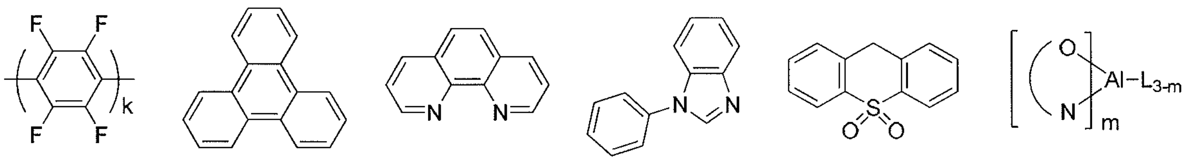
[0163] X^1 to X^8 is selected from CH or N.

HBL:

[0164] A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED.

[0165] In one aspect, compound used in HBL contains the same molecule used as host described above.

[0166] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

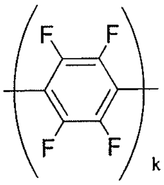
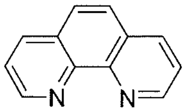
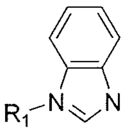
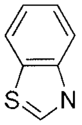
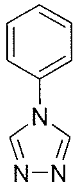
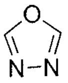
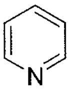
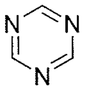


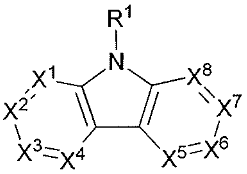
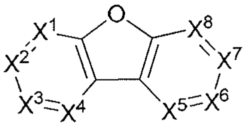
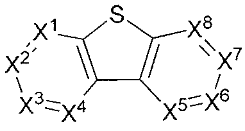
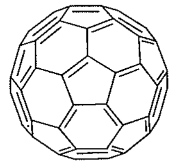
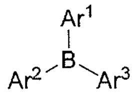
[0167] k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

ETL:

[0168] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

[0169] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

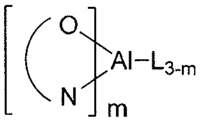
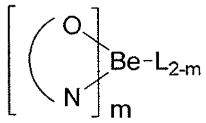
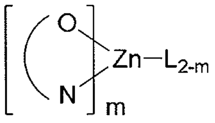
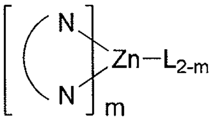
[0170] R^1 is selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

[0171] Ar^1 to Ar^3 has the similar definition as Ar's mentioned above.

[0172] k is an integer from 0 to 20.

[0173] X^1 to X^8 is selected from CH or N.

[0174] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

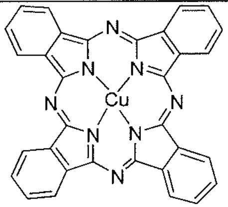
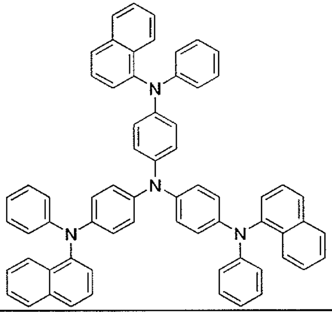
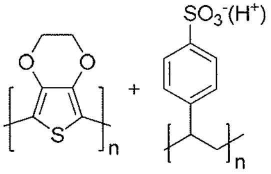
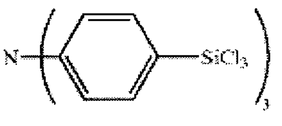
[0175] (O-N) or (N-N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

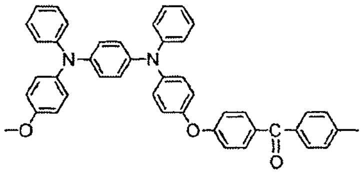
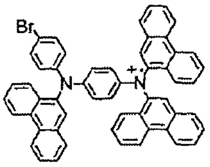
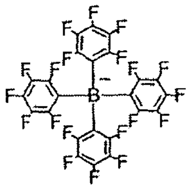
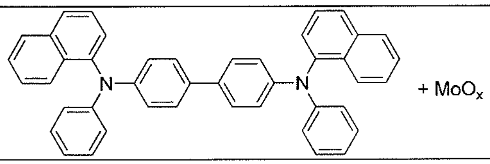
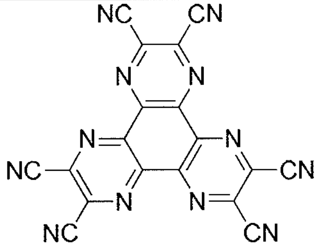
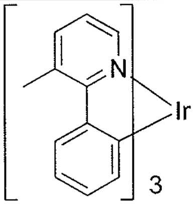
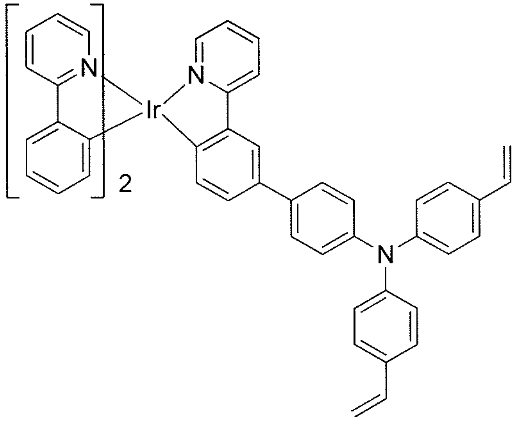
[0176] In any above-mentioned compounds used in each layer of OLED device, the hydrogen atoms attached to conjugated rings can be partially or fully deuterated.

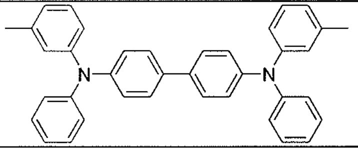
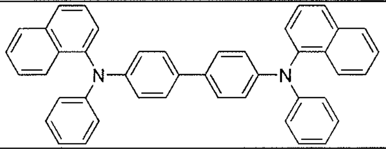
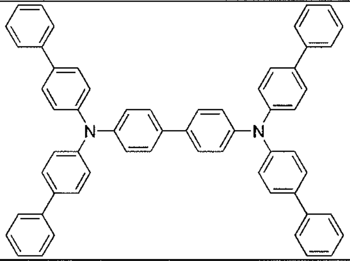
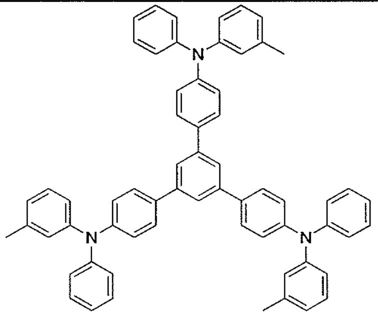
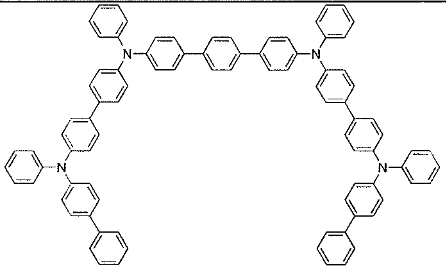
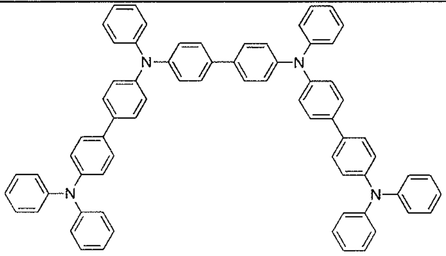
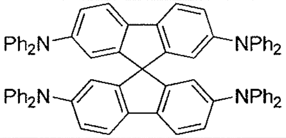
[0177] The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be use din conjunction with a wide variety pf hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

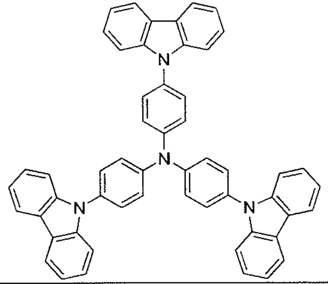
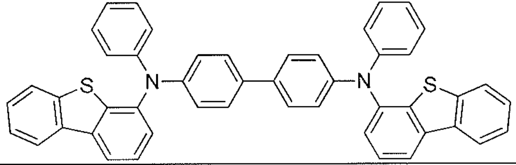
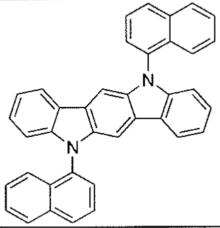
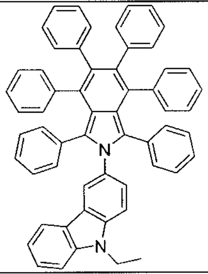
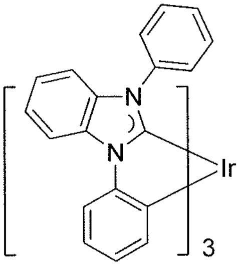
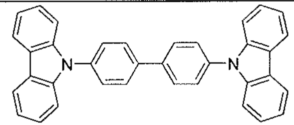
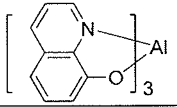
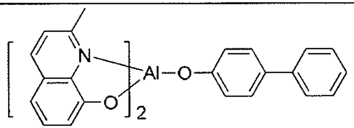
[0178] In addition to and / or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 1 below. Table 1 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

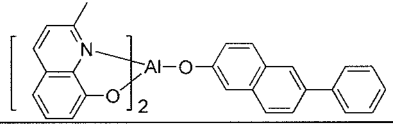
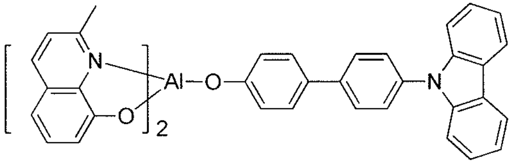
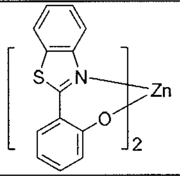
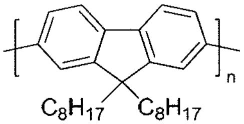
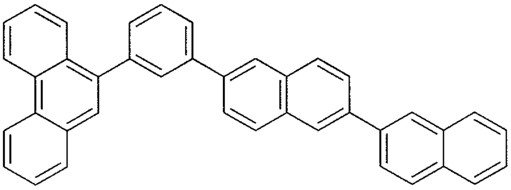
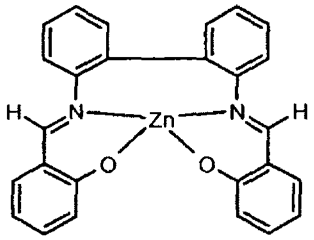
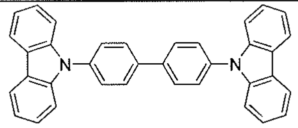
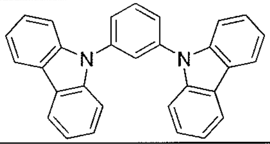
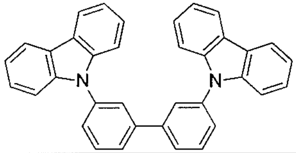
TABLE 1

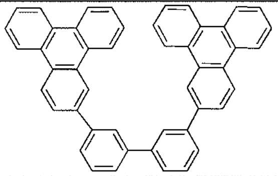
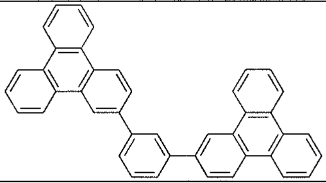
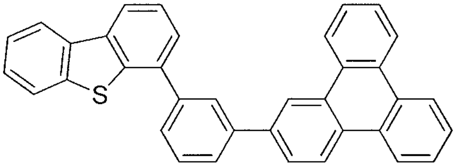
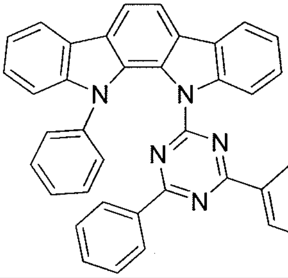
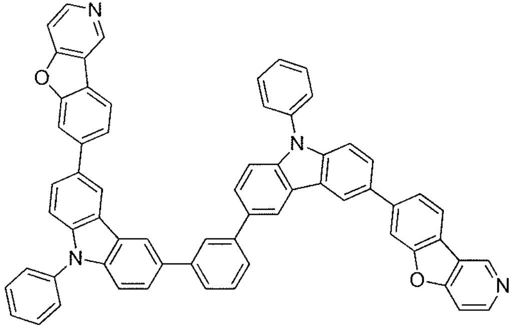
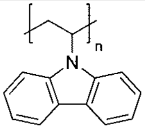
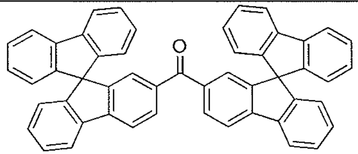
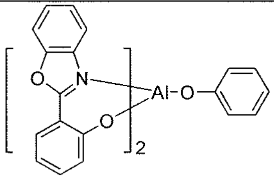
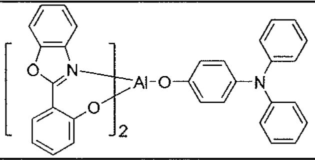
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_X Fluorohydrocarbon polymer	$\left[CH_xF_y \right]_n$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and sliane SAMs		US20030162053

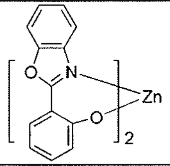
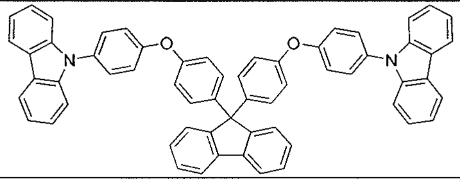
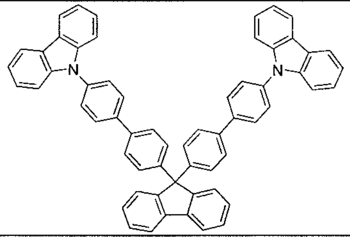
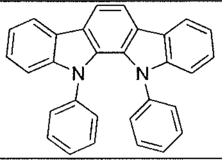
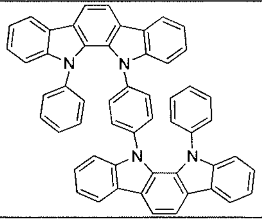
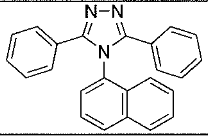
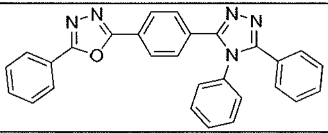
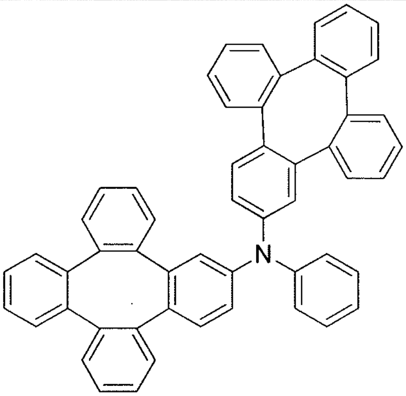
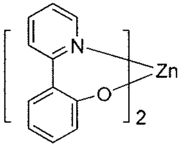
Triarylamine or polythiophene polymers with conductivity dopants	 and  	EA01725079A1
Arylamines complexed with metal oxides such as molybdenum and tungsten oxides		SID Symposium Digest, 37, 923 (2006) WO2009018009
p-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Hole transporting materials		

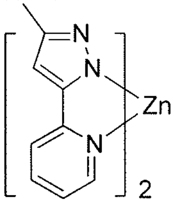
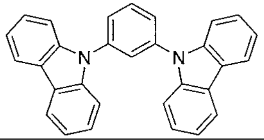
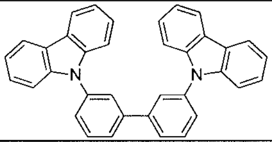
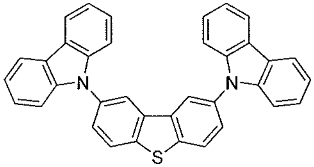
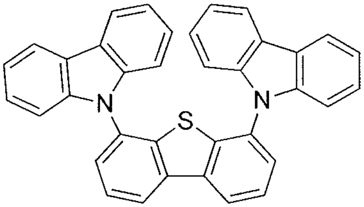
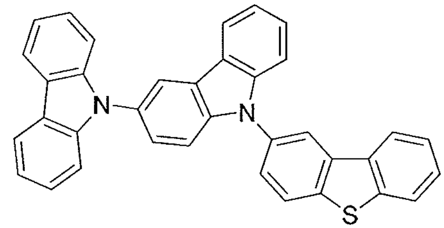
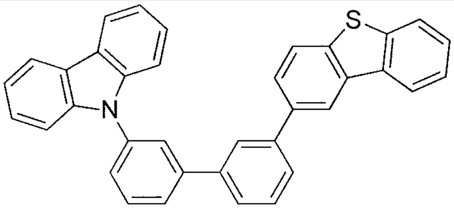
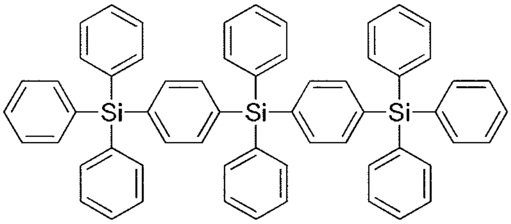
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		US5061569
		EP650955
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)

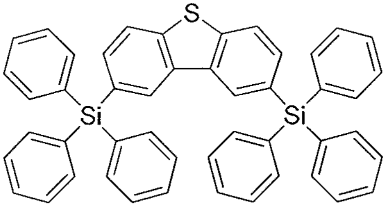
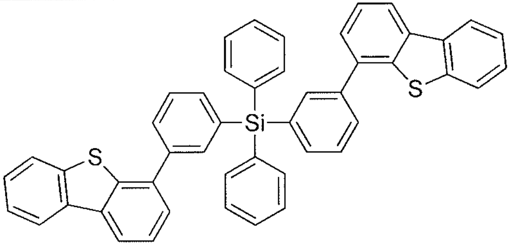
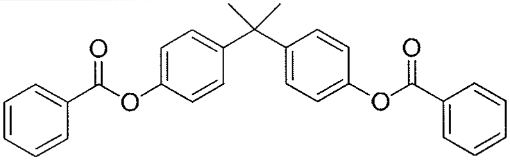
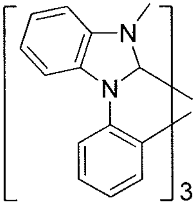
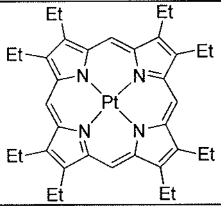
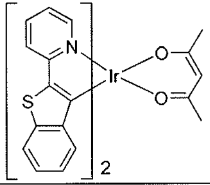
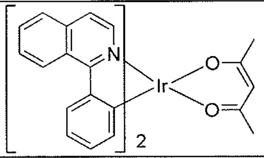
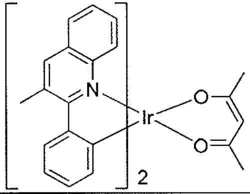
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/(di)benzofuran		US20070278938, US20080106190
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials		
Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq$_3$, BAlq)		Nature 395, 151 (1998)
		US20060202194

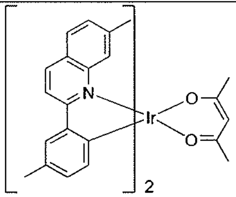
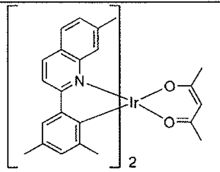
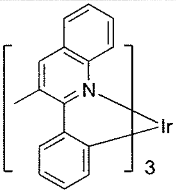
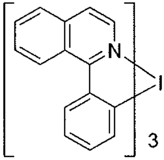
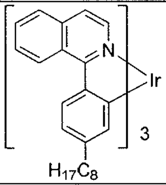
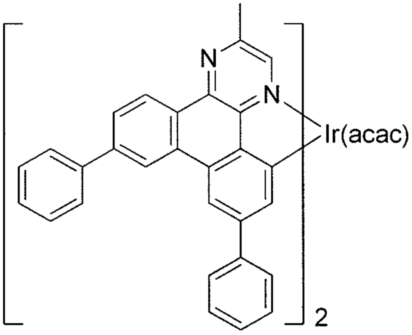
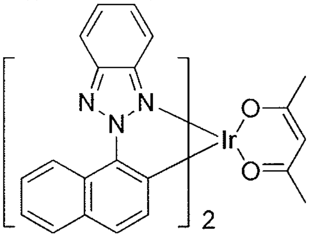
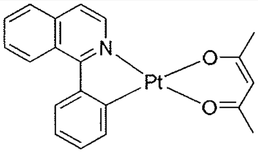
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2009062578
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234

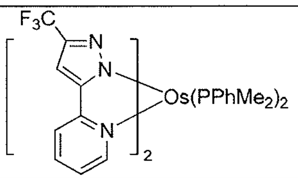
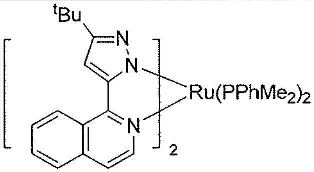
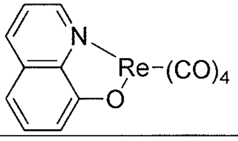
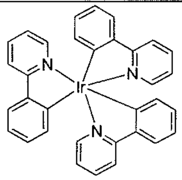
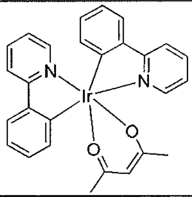
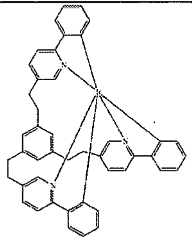
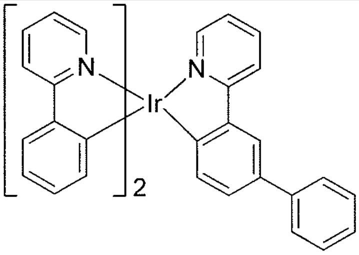
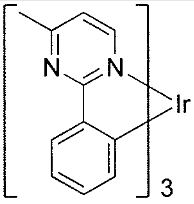
Aryltriphenylene compounds		US20060280965
		US20060280965
		WO2009021126
Donor acceptor type molecules		WO2008056746
Aza-carbazole/DBT/DBF		JP2008074939
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207
Metal phenoxybenzooxazole compounds		WO2005089025
		WO2006132173

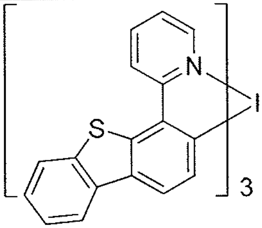
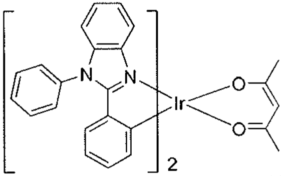
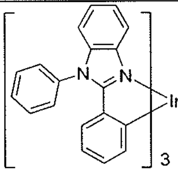
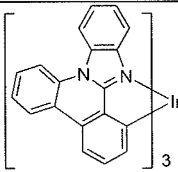
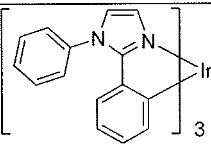
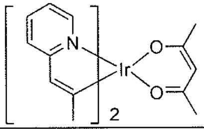
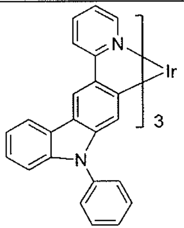
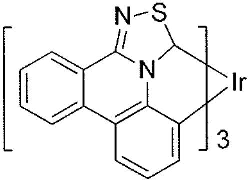
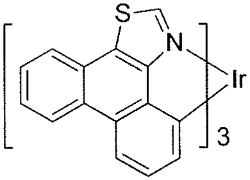
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297
Indolocabazoles		WO2007063796
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900

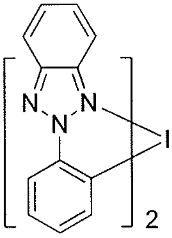
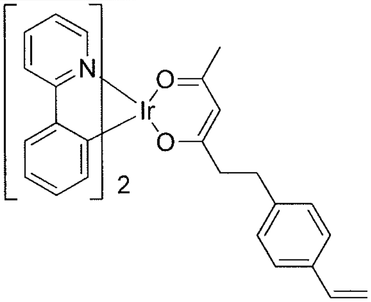
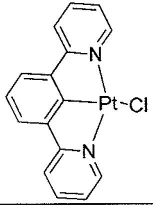
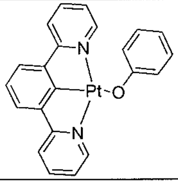
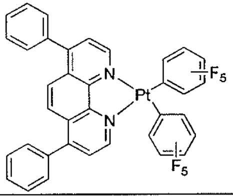
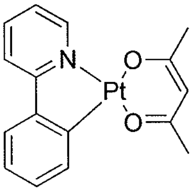
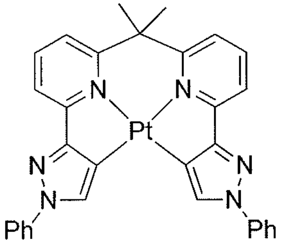
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
Blue hosts		
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162
		WO2009086028
		US20090030202, US20090017330
Silicon aryl compounds		US20050238919

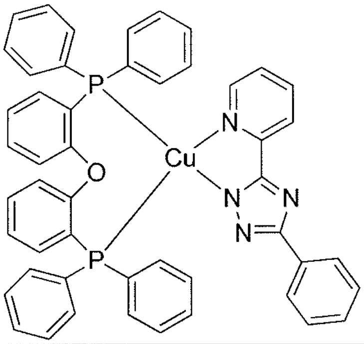
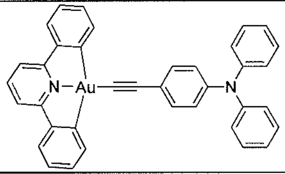
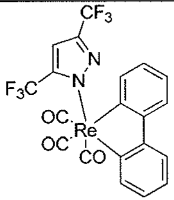
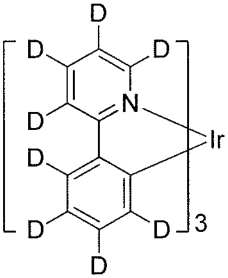
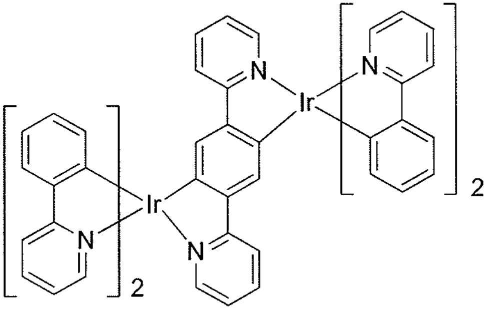
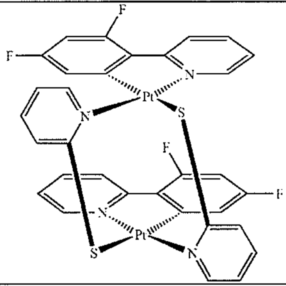
		WO2009003898
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex		US7154114
Phosphorescent dopants		
Red dopants		
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US2006835469
		US2006835469

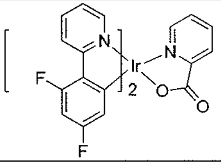
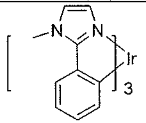
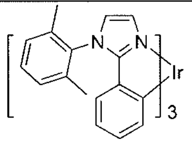
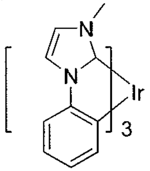
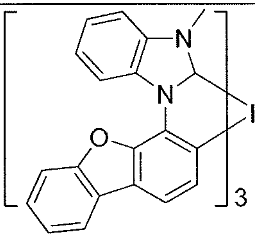
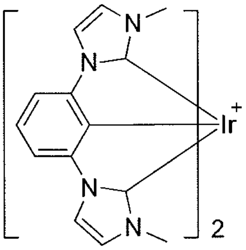
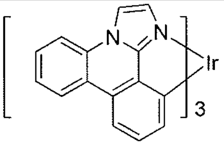
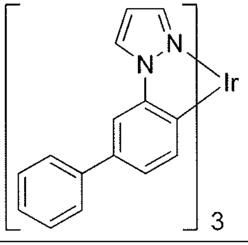
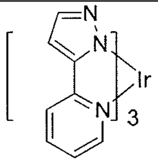
		US20060202194
		US20060202194
		US20070087321
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
Platinum(II) organometallic complexes		WO2003040257

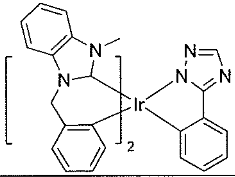
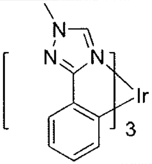
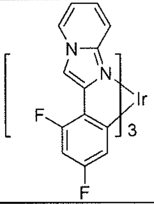
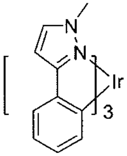
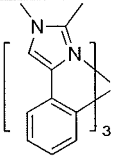
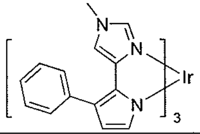
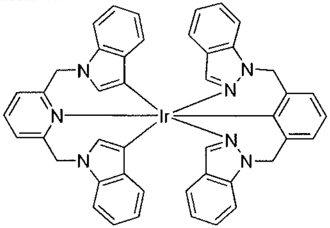
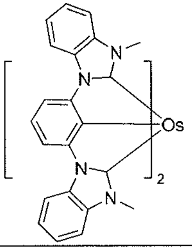
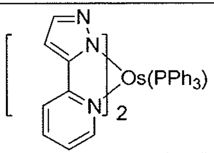
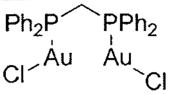
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
Green dopants		
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656
		US7332232
		US20090108737
		US20090039776

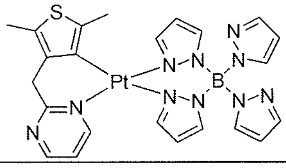
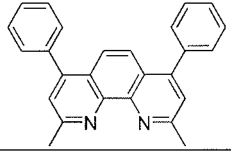
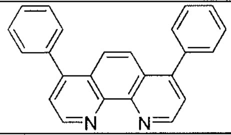
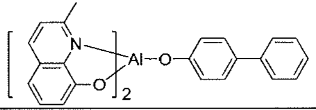
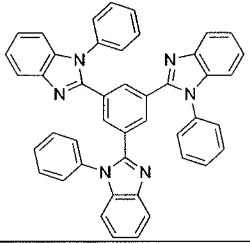
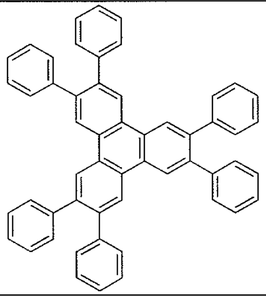
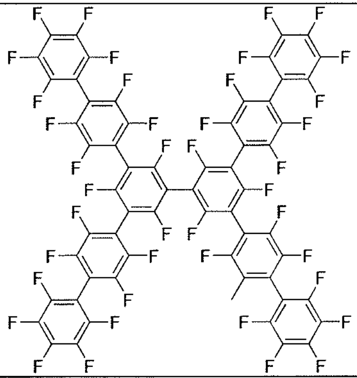
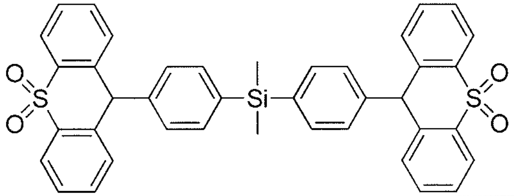
		US6921915
		US6687266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US 20060008670 JP2007123392
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846

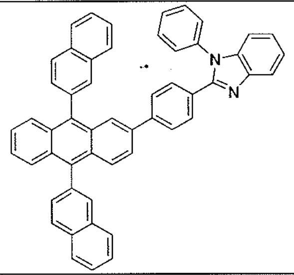
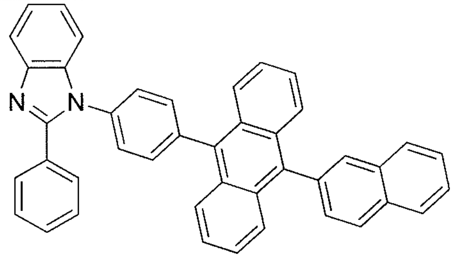
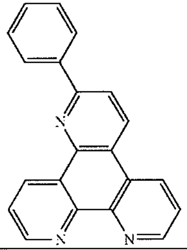
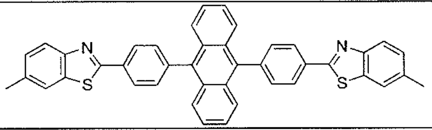
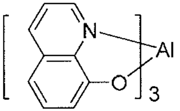
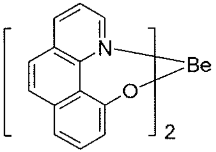
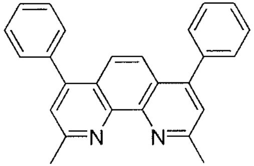
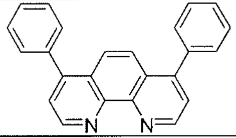
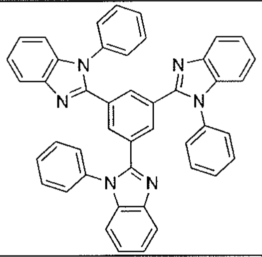
		US20080015355
Monomer for polymeric metal organometallic compounds		US7250226, US7396598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635

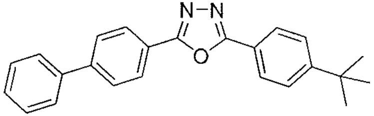
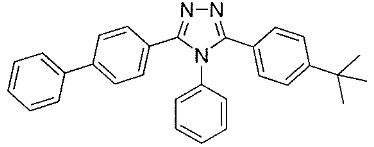
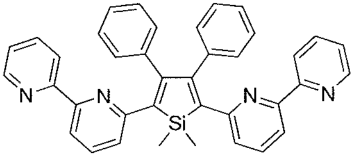
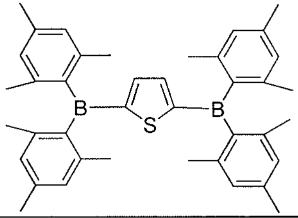
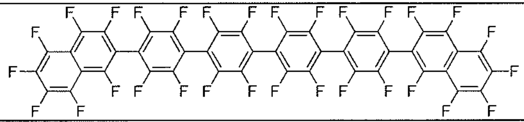
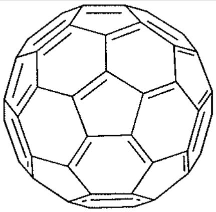
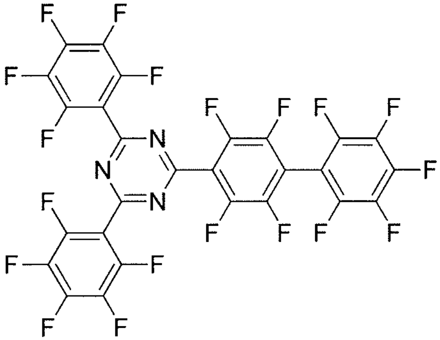
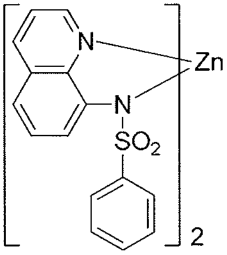
Cu complexes		WO2009000673
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		US7090928
Blue dopants		

Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923
		US7393599, WO2006056418, US20050260441, WO2005019373
		US7534505
		US7445855
		US20070190359, US20080297033
		US7338722
		US20020134984

		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380
		WO2006082742
Osmium(II) complexes		US7279704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett.74,1361 (1999)

Platinum(II) complexes		WO2006098120, WO2006103874
Exciton/hole blocking layer materials		
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085
Electron transporting materials		

Anthracene-benzoimidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) US7230107
Metal hydroxybenoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
		Appl. Phys. Lett. 79, 449 (2001)
5-member ring electron deficient heterocycles (e.g.,triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)

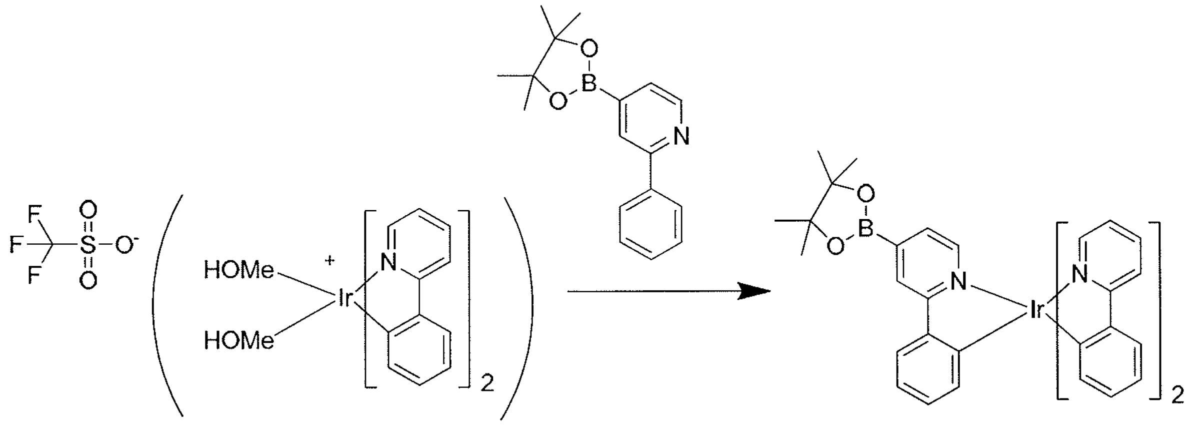
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870
Triazine complexes		US20040036077
Zn (N^N) complexes		US6528187

EXPERIMENTAL

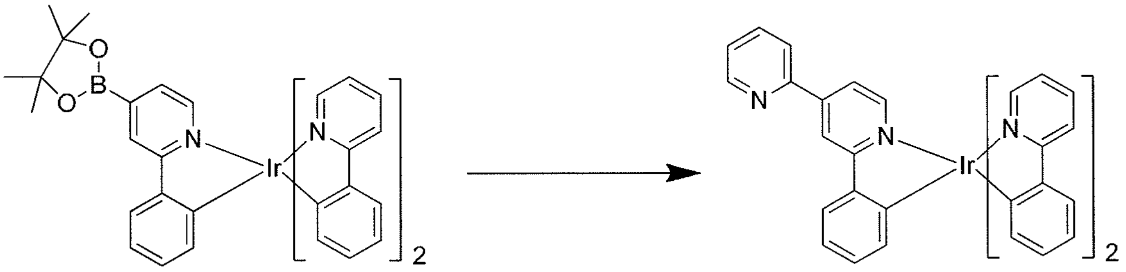
Compound Examples

[0179] Several of the compounds were synthesized as follows:

Example 1. Synthesis of Compound 1

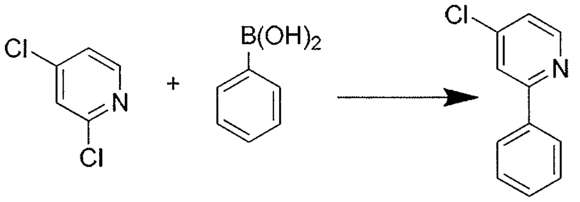


[0180] The iridium phenylpyridine triflate salt was refluxed in ethanol with 2-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (4 g, 14.23 mmol) under nitrogen for 24 h. After cooling to room temperature, the mixture was filtered through a Celite pad and washed with ethanol and hexanes to give 60% yield of the desired product. The product was used for the next step without further purification.

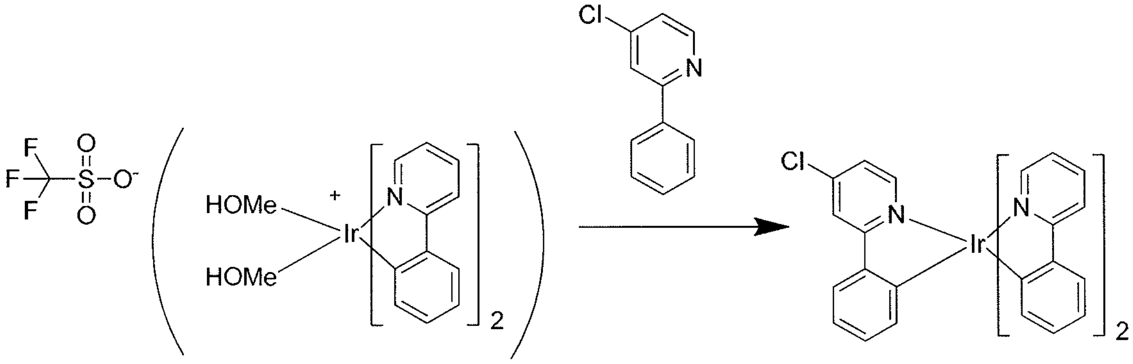


[0181] A mixture of Iridium phenylpyridine boronic ester complex (2.5 g, 3.20 mmol), 2-chloropyridine (0.545 g, 4.80 mmol), and Potassium phosphate (1.699 g, 8.01 mmol) in 100 mL of toluene and 10 mL of H_2O was bubbled with N_2 for 20 minutes. $Pd_2(dba)_3$ (0.029 g, 0.032 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.053 g, 0.128 mmol) were then added, and the mixture was heated to reflux under N_2 for 14 h. The mixture was cooled and extracted with dichloromethane. The organic extracts were dried over $MgSO_4$, filtered and evaporated to a residue. The residue was coated on Celite and purified by column using dichloromethane as solvent. 0.8 g product was obtained.

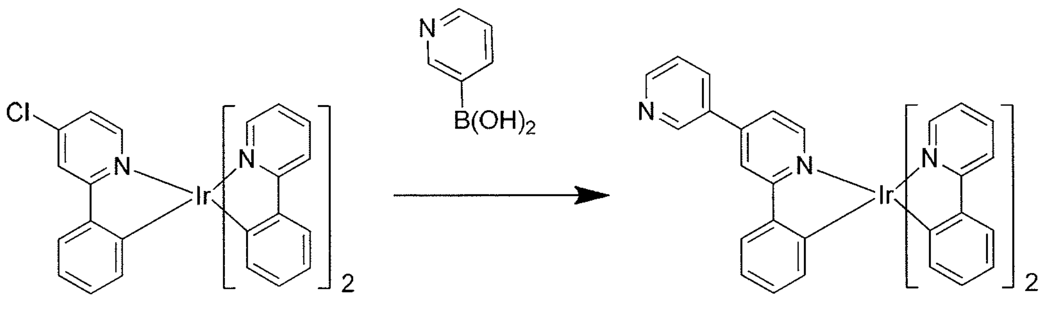
Example 2. Synthesis of Compound 2



[0182] 2,4-dichloropyridine (21.90 mL, 203 mmol), phenylboronic acid (24.72 g, 203 mmol) and Potassium carbonate (84.0 g, 608 mmol), dimethoxy ethane (500 mL) and water (150 mL) were placed in a 3-neck round bottom flask. Nitrogen gas was bubbled through the reaction mixture for 30 minutes. Tetrakis triphenylphosphine Pd(0) (2.343 g, 2.027 mmol)) was then added and the reaction mixture was refluxed for 18 h. The aqueous layer was removed and organic layer was concentrated to dryness. The crude product was purified using silica gel chromatography.

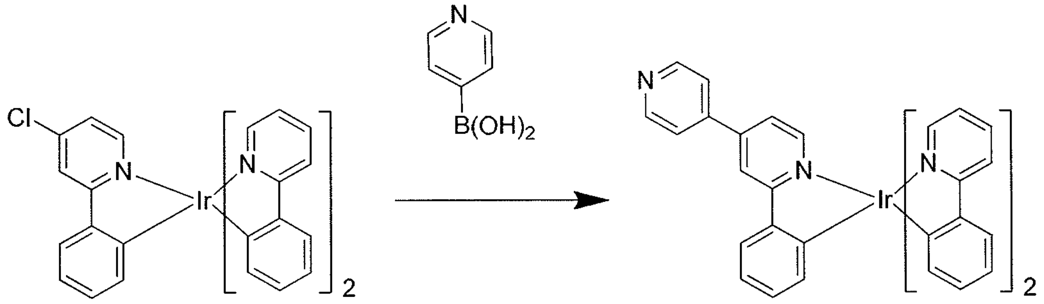


[0183] 4-chloro-2-phenylpyridine (14.0 g, 73.8 mmol) and the Iridium phenylpyridine triflate (14.0 g, 19.61 mmol) was placed in a 500mL round bottom flask. A 50:50 mixture of ethanol and methanol (100mL) was then added. The reaction mixture was refluxed for 18h. The reaction mixture was cooled to room temperature, diluted with ethanol and filtered through a plug of silica gel. The product was washed with ethanol and hexanes and then eluted with dichloromethane. Solvent was concentrated and residue was obtained as solid yield (11.0 g, 81%).



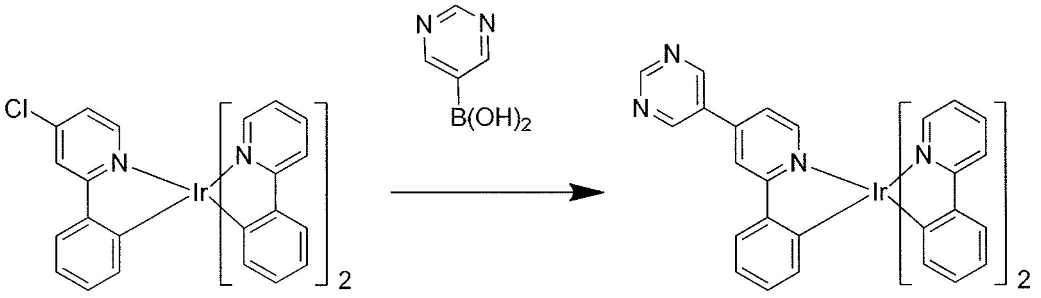
[0184] The heteroleptic Iridium pre cursor (4.0 g, 5.80 mmol), pyridin-3-ylboronic acid (3.57 g, 29.0 mmol), Potassium phosphate tribasic monohydrate (4.01 g, 17.41 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.095 g, 0.232 mmol), toluene (250 mL) and Water (25 mL) were all placed in a 500mL 3-neck round bottom flask. Nitrogen gas was bubbled through the reaction mixture 30 minutes. $Pd_2(dba)_3$ (0.053 g, 0.058 mmol) was then added and the reaction mixture was refluxed for 18h. They reaction was cooled to room temperature and the aqueous layer was removed. The organic fraction was concentrated and the crude product was obtained. The crude was further purified using deactivated neutral alumina to give 1.2 g of product (Yield = 28.2%).

Example 3. Synthesis of Compound 3



[0185] The heteroleptic Iridium pre cursor (4.0 g, 5.80 mmol), pyridin-4-ylboronic acid (1.0 g, 9 mmol), Potassium phosphate tribasic monohydrate (4.01 g, 17.41 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.095 g, 0.232 mmol), toluene (250 mL) and Water (25 mL) were all placed in a 500 mL 3-neck round bottom flask. Nitrogen gas was bubbled through the reaction mixture 30 minutes. $Pd_2(dba)_3$ (0.106 g, 0.116 mmol) was then added and the reaction mixture was refluxed for 18h. The reaction was cooled to room temperature and the aqueous layer was removed. The organic fraction was concentrated and the crude product was obtained. The crude was further purified using deactivated neutral alumina to give 2.9g of product (68.2% yield).

Example 4. Synthesis of Compound 4



[0186] The heteroleptic Iridium pre cursor (5.56g, 8.09 mmol), pyrimidin-5-ylboronic acid (5.01g, 40.5mmol), Potassium phosphate tribasic monohydrate (5.59g, 24.27 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.133g, 0.324 mmol), toluene (250 mL) and water (25 mL) were all placed in a 500 mL 3-neck round bottom flask. Nitrogen gas was bubbled through the reaction mixture 30 minutes. $Pd_2(dba)_3$ (0.222g, 0.243 mmol) was then added and the reaction mixture was refluxed for 18h. The reaction was cooled to room temperature and the aqueous layer was removed. The organic fraction was concentrated and the crude product was obtained. The crude was further purified using deactivated neutral alumina to give 3.9g of product (66.4% yield).

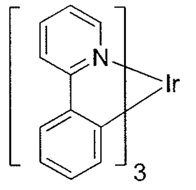
Device Examples

[0187] All device examples were fabricated by high vacuum ($<10^{-7}$ Torr) thermal evaporation. The anode electrode is 1200Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1000 Å of Al. All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H_2O and O_2) immediately after fabrication, and a moisture getter was incorporated inside the package.

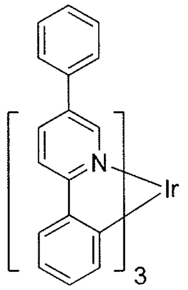
[0188] The organic stack of the Device Example consisted of sequentially, from the ITO surface, 100 Å of hole injection layer (HIL), 300 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (α-NPD) as the hole transporting later (HTL), 300 Å of host doped with 7-10% of Compound 1-4 as the emissive layer (EML), 100 Å of blocking layer (BL) and 400 Å of Alq_3 (tris-8-hydroxyquinoline aluminum) as the ETL1. For devices in which LG101 was used as the HIL, LG101 was purchased from LG Chem and used as received.

[0189] Examples 6 and 7 were fabricated similarly to other device examples except there were two emissive compounds in the EML.

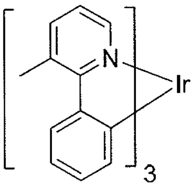
[0190] As used herein, the following compounds have the following structures:



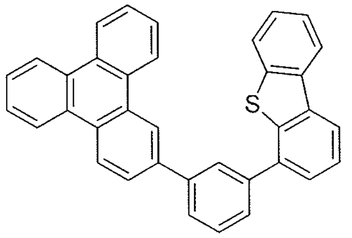
Compound A



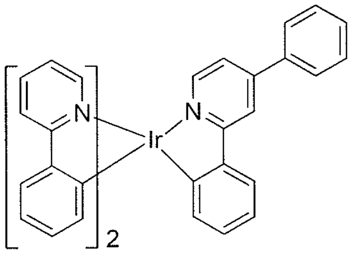
Compound B



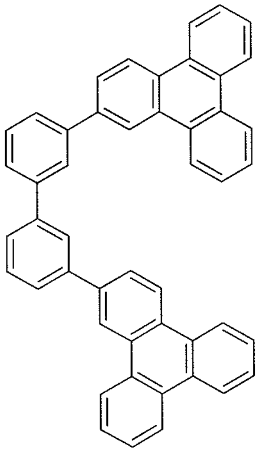
Compound C



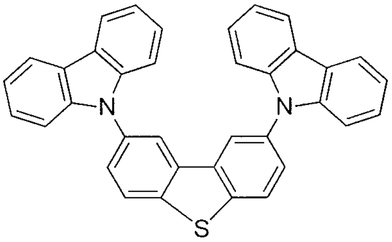
Compound D



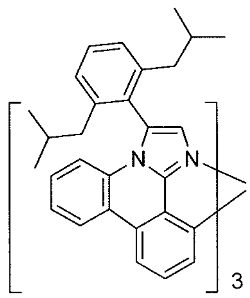
Compound E



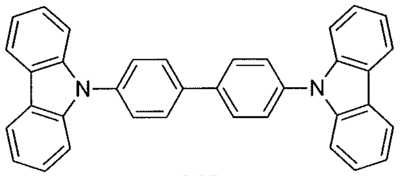
Compound F



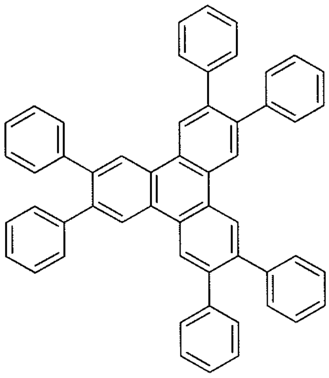
Compound G



Compound H



CBP



HPT

[0191] Particular emissive dopants for the emissive layer of an OLED are provided. These compounds may lead to devices having particularly good properties. The device structures are provided in Table 2, and the corresponding device data is provided in Table 3.

Table 2. VTE PHOLEDs

Device Example	HIL	HTL	EML(doping%)		BL	ETL
Example 1	Compound C	NPD	Compound D	Compound 1 (7%)	Compound D	Alq3
Example 2	LG101	NPD	Compound F	Compound 1 (10%)	Compound F	Alq3
Example 3	LG101	NPD	Compound F	Compound 2 (10%)	Compound F	Alq3
Example 4	LG101	NPD	Compound F	Compound 3 (10%)	Compound F	Alq3
Example 5	LG101	NPD	Compound F	Compound 4 (10%)	Compound F	Alq3
Example 6	LG101	NPD	Compound G	Compound 1 (10%)	Compound G	Alq3
			Compound G	Compound H (20%)		
Example 7	LG101	NPD	Compound G	Compound 3 (10%)	Compound G	Alq3
			Compound G	Compound H (20%)		
Comparative Example 1	Compound C	NPD	CBP	Compound A (7%)	HPT	Alq3
Comparative Example 2	Compound C	NPD	Compound F	Compound B (9%)	HPT	Alq3
Comparative Example 3	LG101	NPD	Compound F	Compound E (10%)	Compound F	Alq3

Table 3. VTE Device data

	CIE				At 1000 cd/m2					at J = 40mA/cm2	
Device Example	**Imax**	**FWHM/ nm**	**CIE (x)**	**CIE (y)**	**V [V]**	**cd/A**	**EQE %**	**lm/W**	**cd/A/ EQE**	**Lo, nits**	**RT$_{80\%}$ (h)**
Example 1	578	84	0.51	0.48	6.3	41.4	15.1	20.7	2.7	14,019	700
Example 2	574	88	0.51	0.48	6.1	41.8	15.3	21.7	2.7	12,550	1150
Example 3	572	86	0.49	0.51	6.1	43.5	14.6	22.3	3	13,567	216
Example 4	588	90	0.54	0.45	6.8	29.7	12.7	13.8	2.3	9,696	1800
Example 5	588	88	0.54	0.46	6.9	30.4	12.6	13.8	2.4	9,753	547
Example 6	574	176	0.4	0.41	5.7	30	12.1	16.6	2.5	9,994	38
Example 7	462	178	0.37	0.36	5.9	24.7	11.8	13.2	2.1	8,525	25
Comparative example 1	519	74	0.32	0.62	6	45.1	12.6	23.6	3.6	13,835	196
Comparative example 2	548	70	0.44	0.55	5.5	56.0	16.0	32	3.5	15,970	348
Comparative example 3	560	84	0.44	0.54	5.6	53.5	16	30.3	3.3	16,415	252

[0192] In particular Device Examples 1-5 are significantly red shifted from Comparative Device Examples 1-3. This supports that the LUMO of the complex has been lowered, reducing the HOMO-LUMO gap and the triplet energy. The external quantum efficiencies of Devices 1-5 are comparable to comparative examples 1-3. In particular the device lifetimes of devices 1,2,4 and 5 are significantly better than comparative examples 1-3 which shows that complexes with heterocyclic groups substituted at the 4 position on the pyridine ring of the 2-phenylpyridine may also lower and stabilize the LUMO of the metal complex, thereby providing further device operational stability.

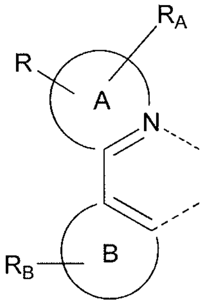
[0193] Device Example 6 shows a warm white with CIE (x=0.4. y=0.4) and Device Example 7 shows a cooler white with CIE (x=0.37. y=0.36). This supports that the compounds herein can be used to make white OLEDs with two component emitters.

[0194] It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore includes variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

CLAIMS:

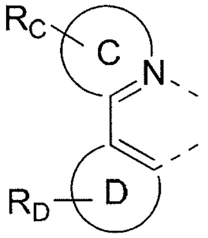
1. A compound having the formula $M(L)_x(L_1)_y(L_2)_z$:

wherein L is



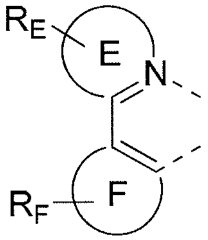
Formula I;

wherein L_1 is



Formula II;

wherein L_2 is



Formula III;

wherein L_1 and L_2 can be the same or different;

wherein M is a metal having an atomic number greater than 40;

wherein x is 1, 2 or 3, y is 0, 1 or 2, z is 0, 1 or 2;

wherein x+y+z is the oxidation state of the metal M;

wherein A is a 6-membered heterocyclic ring;

B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring;

wherein R is a 5 or 6-membered heterocyclic ring;

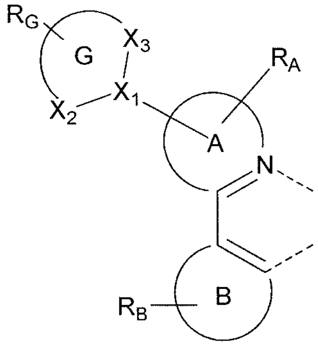
wherein R is attached to A at a position para to the metal M;

wherein R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions;

wherein each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl; and wherein the ligand L is coordinated bidentately to the metal M.

2. The compound of claim 1, wherein R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom.

3. The compound of claim 1, wherein the ligand L has the formula:



Formula IV,

wherein G is a 5 or 6-membered heterocyclic ring;

wherein X_1, X_2, and X_3 are independently selected from carbon, oxygen, sulfur and nitrogen;

wherein R_G may represent mono, di, tri, tetra, or penta substitutions;

wherein R_G is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

4. The compound of claim 3, wherein X_1, X_2, and X_3 are independently carbon or nitrogen.

5. The compound of claim 3, wherein G is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom.

6. The compound of claim 3, wherein at least one of X_1, X_2, and X_3 is nitrogen.

7. The compound of claim 3, wherein each of X_1, X_2, and X_3 is carbon.

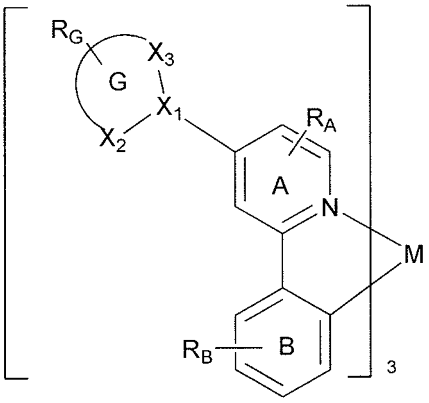
8. The compound of claim 1, wherein the metal M is Ir.

9. The compound of claim 1, wherein B is phenyl.

10. The compound of claim 1, wherein L, L_1 and L_2 are connected to form a tetradentate ligand and a bidentate ligand or a hexadentate ligand.

11. The compound of claim 1, wherein the compound is homoleptic.

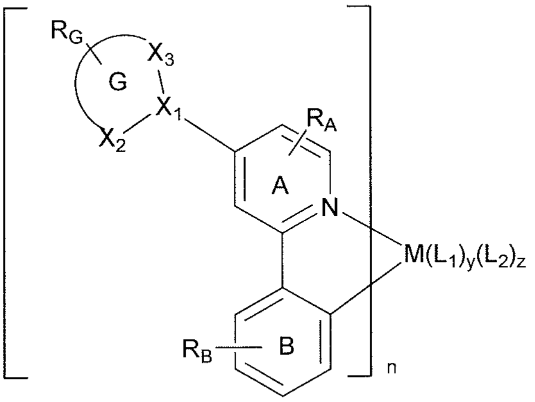
12. The compound of claim 11, wherein the compound has the formula:



Formula V.

13. The compound of claim 1, wherein the compound is heteroleptic.

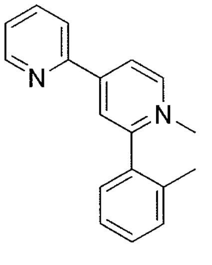
14. The compound of claim 13, wherein the compound has the formula:

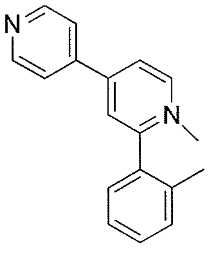


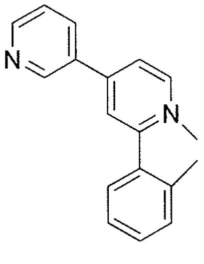
Formula VI,

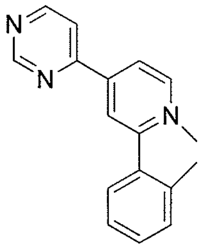
wherein $n+y+z$ is the oxidation state of the metal M;
wherein n is at least 1; and
wherein y is 0, 1 or 2 and x is 0, 1, or 2.

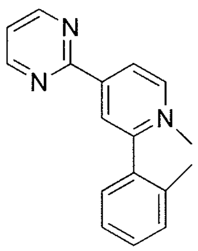
15. The compound of claim 1, wherein the ligand L is selected from the group consisting of:

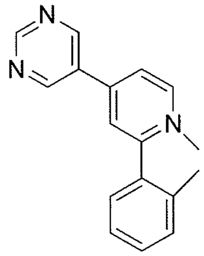


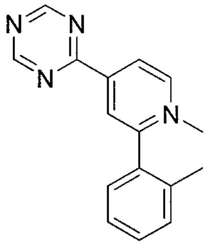


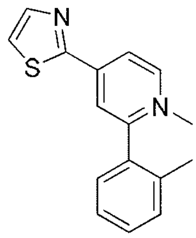


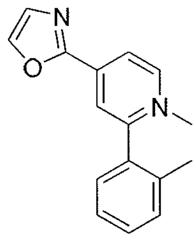


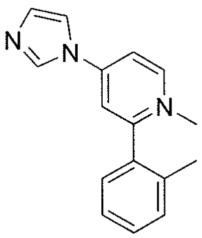


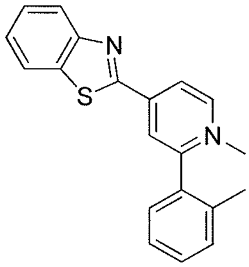


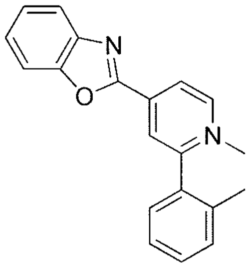






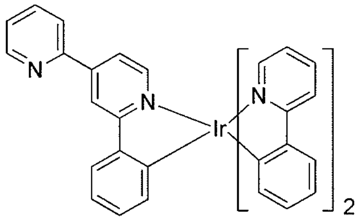




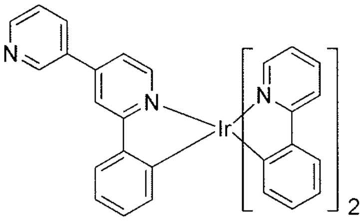


.

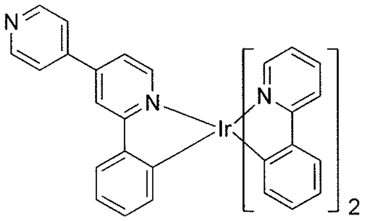
16. The compound of claim 1, wherein the compound is selected from the group consisting of:



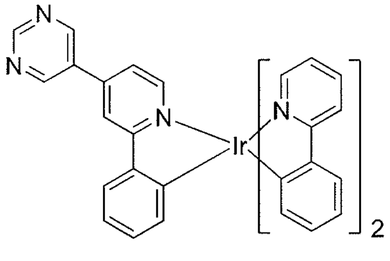
Compound 1



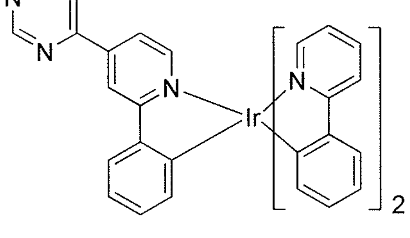
Compound 2



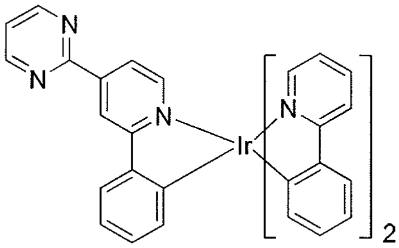
Compound 3



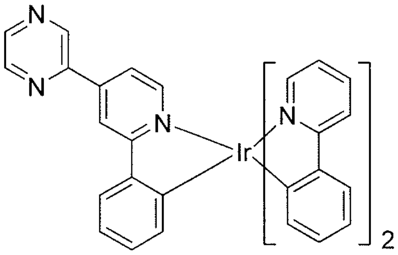
Compound 4



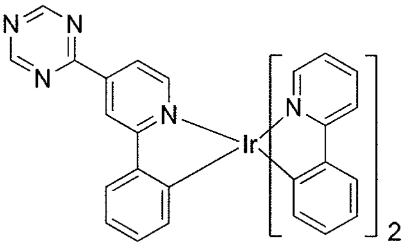
Compound 5



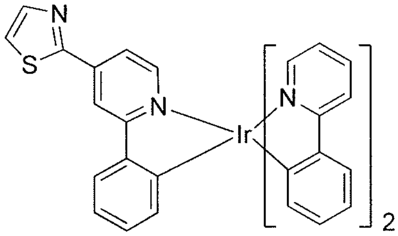
Compound 6



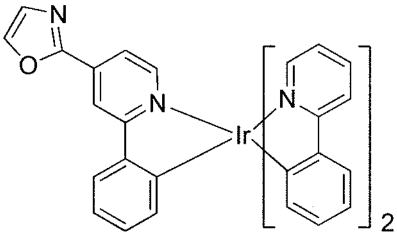
Compound 7



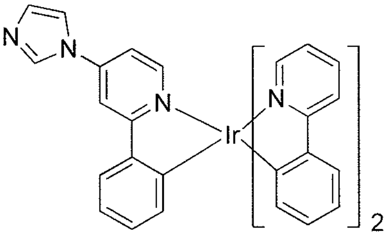
Compound 8



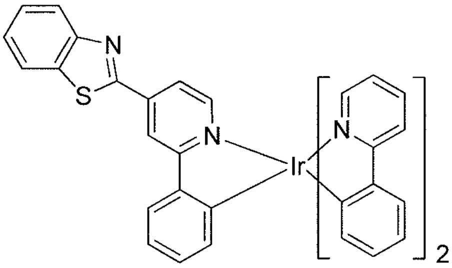
Compound 9



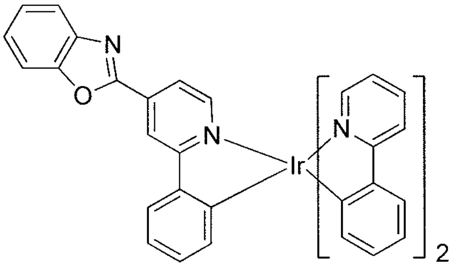
Compound 10



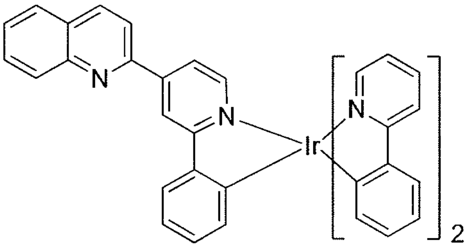
Compound 11



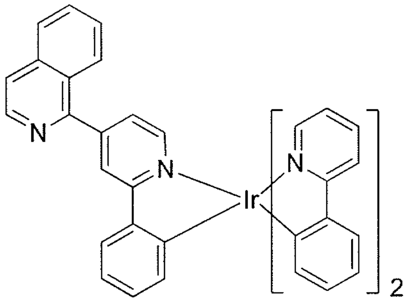
Compound 12



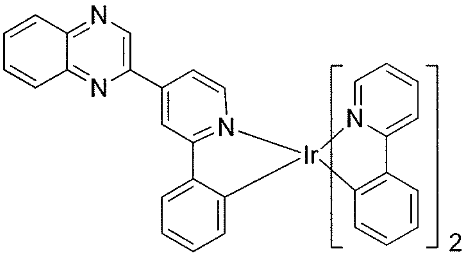
Compound 13



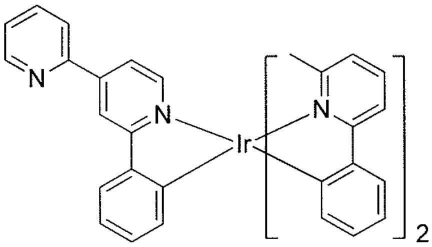
Compound 14



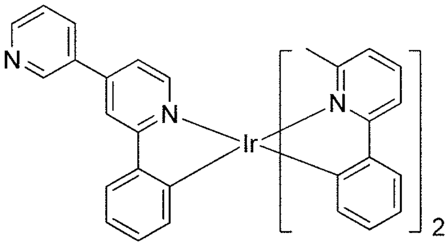
Compound 15



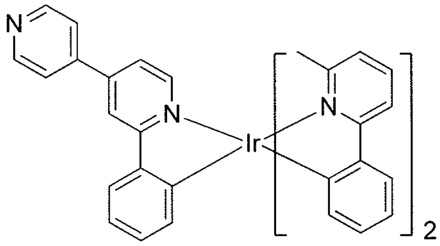
Compound 16



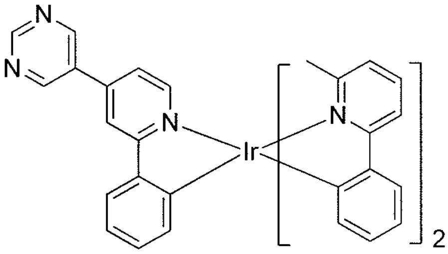
Compound 17



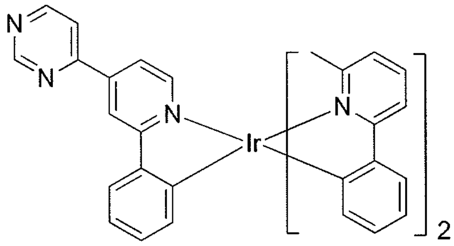
Compound 18



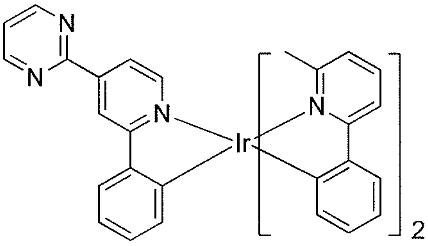
Compound 19



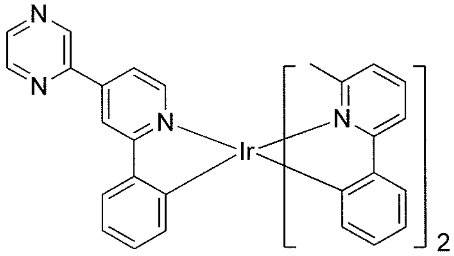
Compound 20



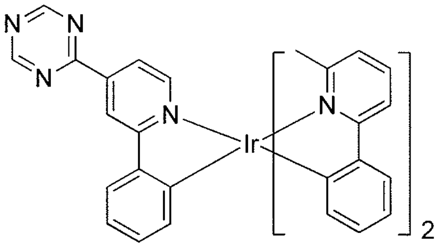
Compound 21



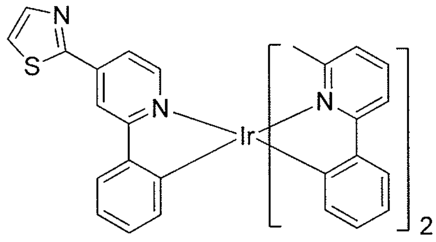
Compound 22



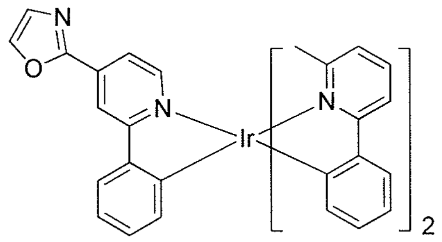
Compound 23



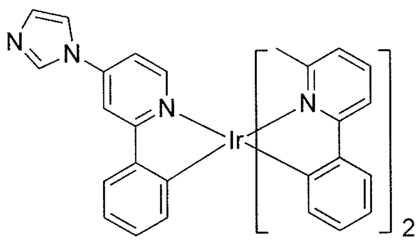
Compound 24



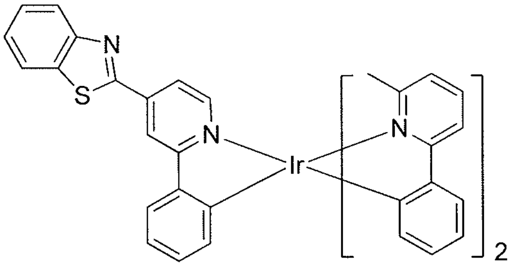
Compound 25



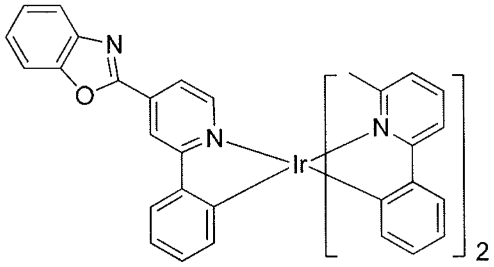
Compound 26



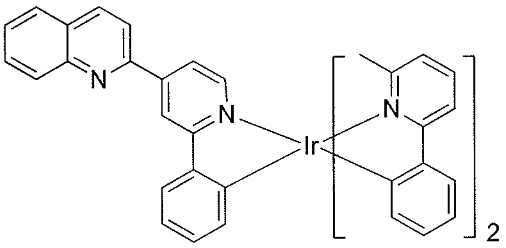
Compound 27



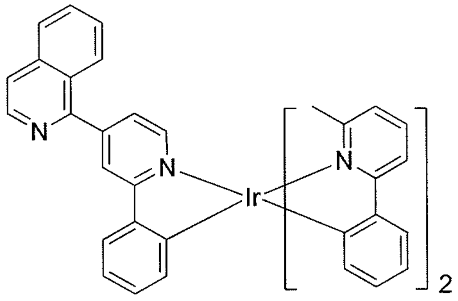
Compound 28



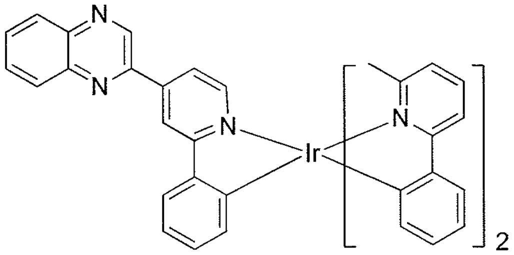
Compound 29



Compound 30



Compound 31



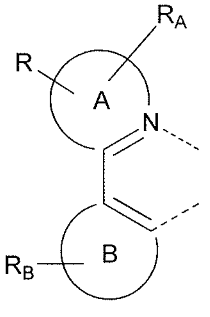
Compound 32

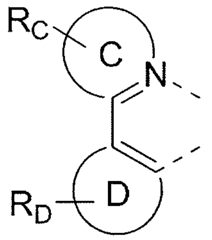
17. A first device comprising an organic light emitting device, further comprising:

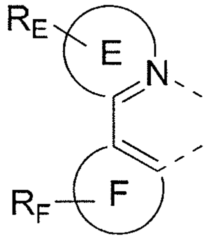
an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, the organic layer comprising a first compound having the formula $M(L)_x(L_1)_y(L_2)_z$:

wherein L is  Formula I;

wherein L_1 is  Formula II;

wherein L_2 is  Formula III;

wherein L_1 and L_2 can be the same or different;

wherein M is a metal having an atomic number greater than 40;

wherein x is 1, 2 or 3, y is 0, 1 or 2, z is 0, 1 or 2;

wherein x+y+z is the oxidation state of the metal M;

wherein A is a 6-membered heterocyclic ring;

B, C, D, E and F are each independently a 5 or 6-membered carbocyclic or heterocyclic ring;

wherein R is a 5 or 6-membered heterocyclic ring;

wherein R is attached to A at a position para to the metal M;

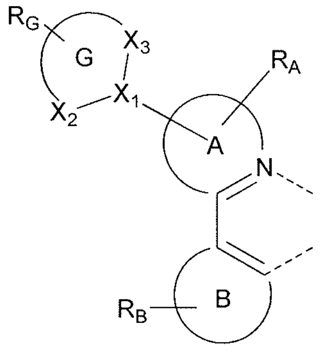
wherein R_A, R_B, R_C, R_D, R_E and R_F may represent mono, di, tri, tetra, or penta substitutions;

wherein each of R_A, R_B, R_C, R_D, R_E and R_F is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl; and

wherein the ligand L is coordinated bidentately to the metal M.

18. The device of claim 17, wherein R is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom.

19. The device of claim 17, wherein the ligand L has the formula:



Formula IV,

wherein G is a 5 or 6-membered heterocyclic ring;

wherein X_1, X_2, and X_3 are independently selected from carbon, oxygen, sulfur and nitrogen;

wherein R_G may represent mono, di, tri, tetra, or penta substitutions;

wherein R_G is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

20. The device of claim 19, wherein X_1, X_2, and X_3 are independently carbon or nitrogen.

21. The device of claim 19, wherein G is a 5 or 6-membered heterocyclic ring that contains at least one nitrogen atom.

22. The compound of claim 19, wherein at least one of X_1, X_2, and X_3 is nitrogen.

23. The device of claim 19, wherein each of X_1, X_2, and X_3 is carbon.

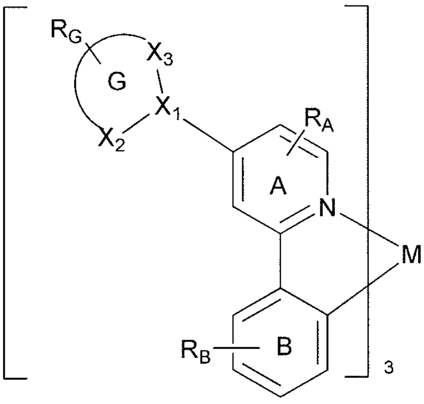
24. The device of claim 17, wherein the metal M is Ir.

25. The device of claim 17, wherein B is phenyl.

26. The device of claim 17, wherein L, L_1 and L_2 are connected to form a tetradentate ligand and a bidentate ligand or a hexadentate ligand.

27. The device of claim 17, wherein the compound is homoleptic.

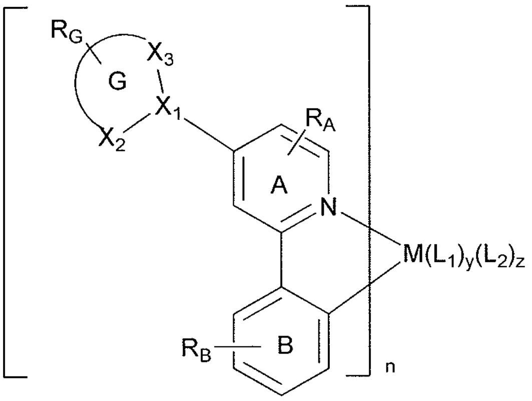
28. The device of claim 27, wherein the compound has the formula:



Formula V.

29. The device of claim 17, wherein the compound is heteroleptic.

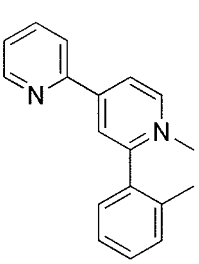
30. The device of claim 29, wherein the compound has the formula:

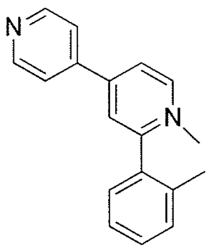


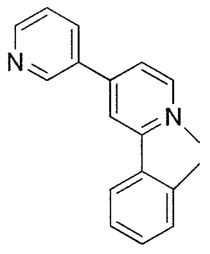
Formula VI,

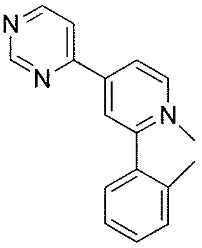
wherein n+y+z is the oxidation state of the metal M;
wherein n is at least 1; and
wherein y is 0, 1 or 2 and x is 0, 1, or 2.

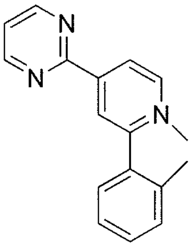
31. The device of claim 17, wherein the ligand L is selected from the group consisting of:

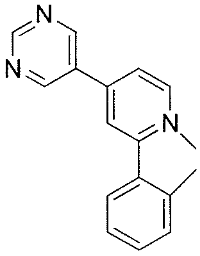


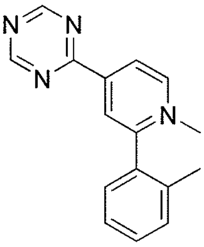


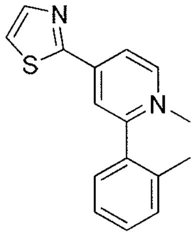


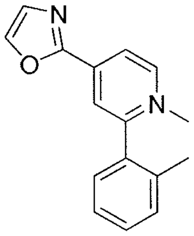


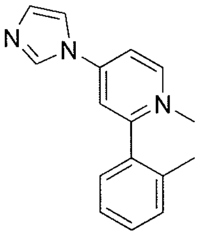


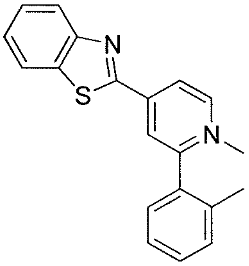


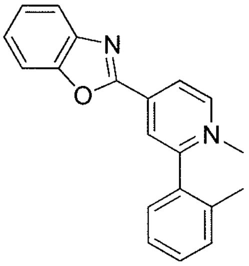






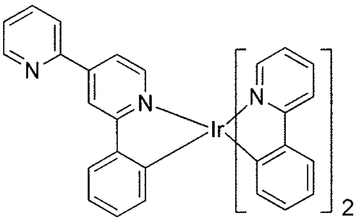




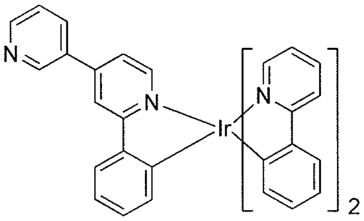


.

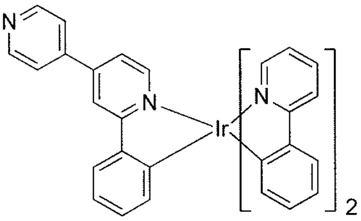
32. The device of claim 17, wherein the compound is selected from the group consisting of:



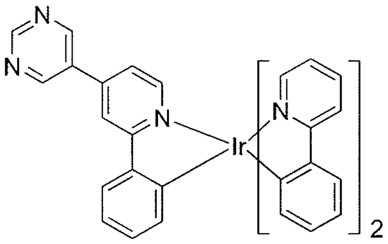
Compound 1



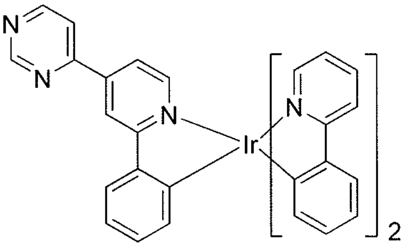
Compound 2



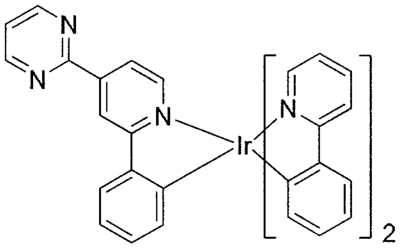
Compound 3



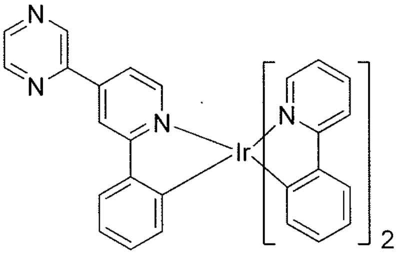
Compound 4



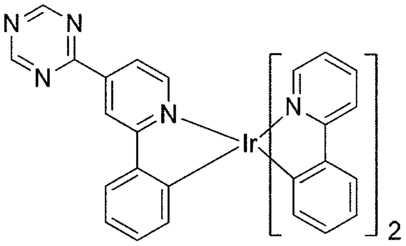
Compound 5



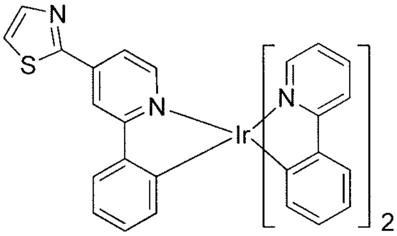
Compound 6



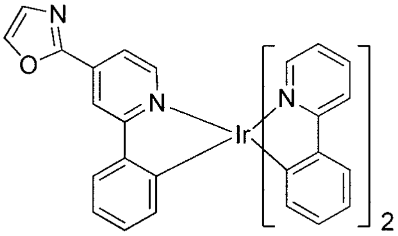
Compound 7



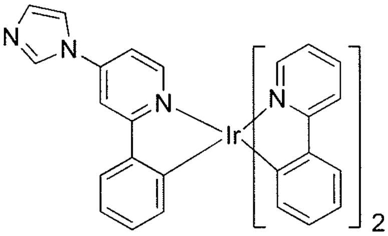
Compound 8



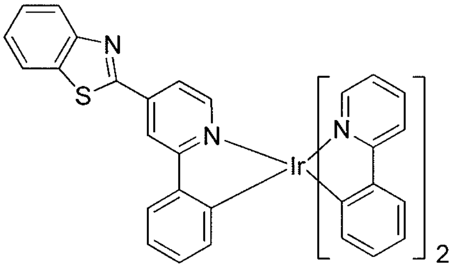
Compound 9



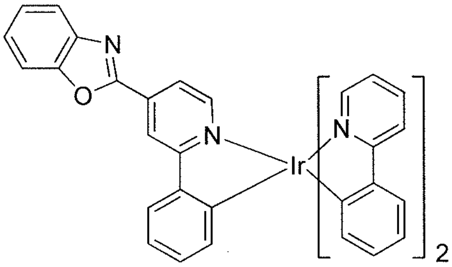
Compound 10



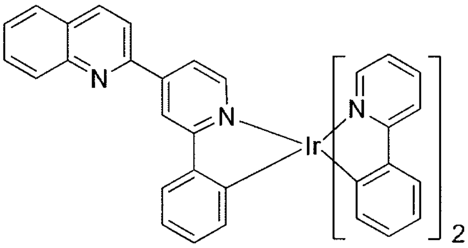
Compound 11



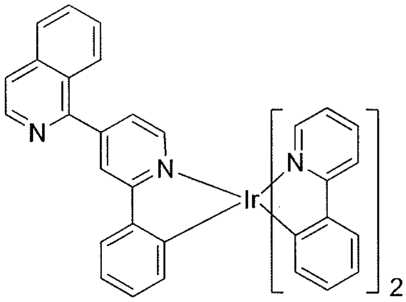
Compound 12



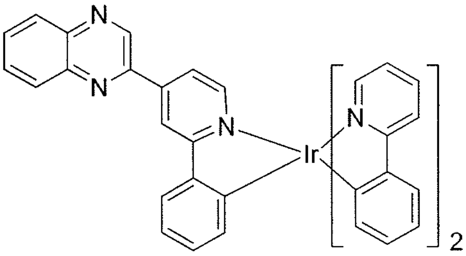
Compound 13



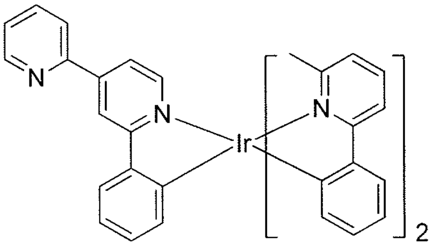
Compound 14



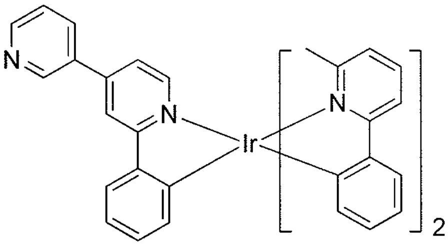
Compound 15



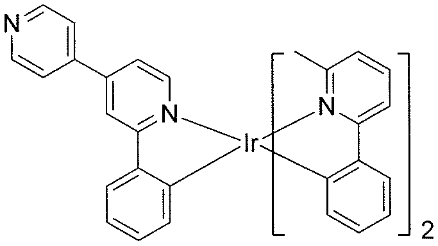
Compound 16



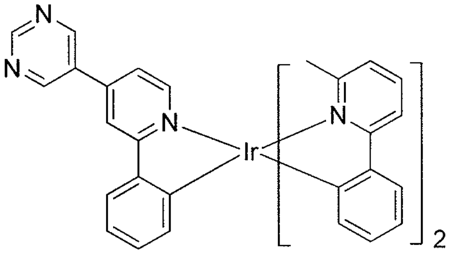
Compound 17



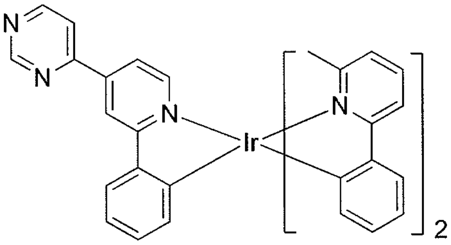
Compound 18



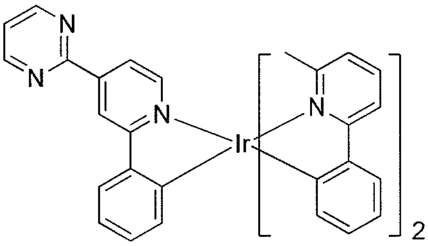
Compound 19



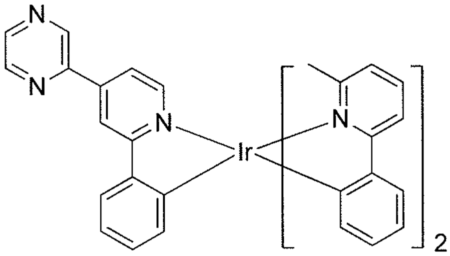
Compound 20



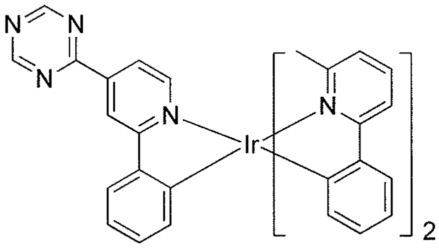
Compound 21



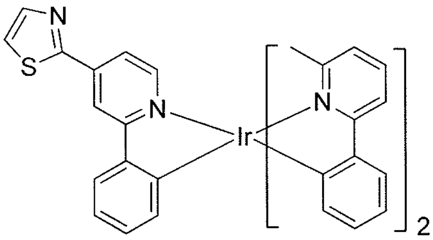
Compound 22



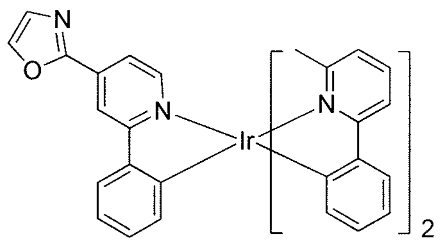
Compound 23



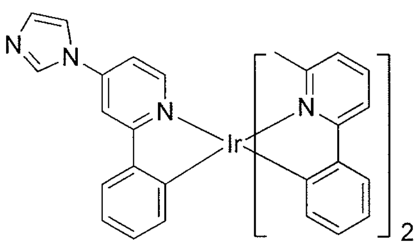
Compound 24



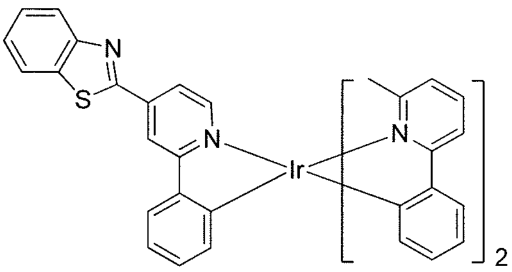
Compound 25



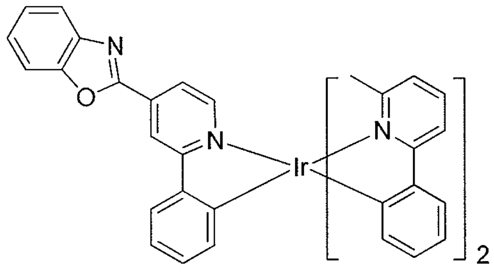
Compound 26



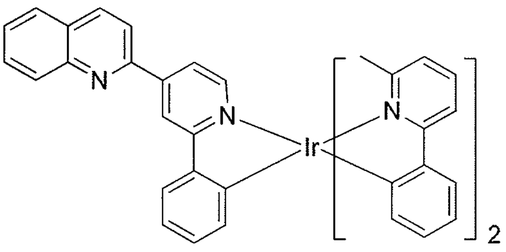
Compound 27



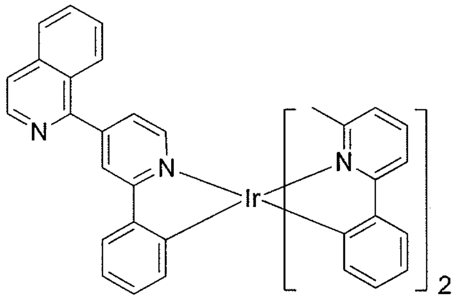
Compound 28



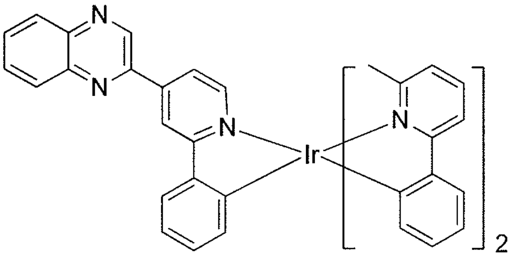
Compound 29



Compound 30



Compound 31

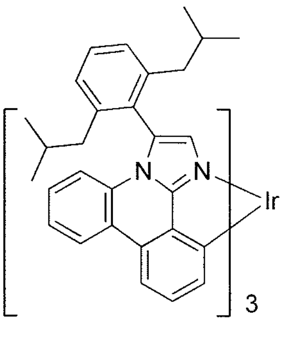


Compound 32

33. The device of claim 17, wherein the organic layer is an emissive layer and the first compound is an emissive compound.

34. The device of claim 17, wherein the organic layer further comprises a second emissive compound.

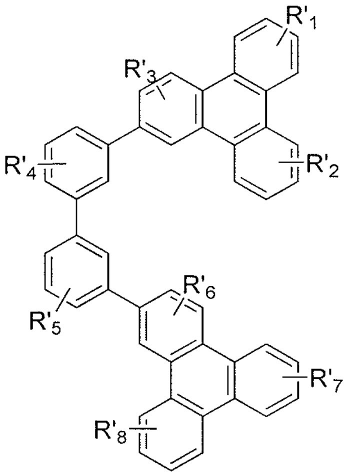
35. The device of claim 34, wherein the second emissive compound is



Compound H

.

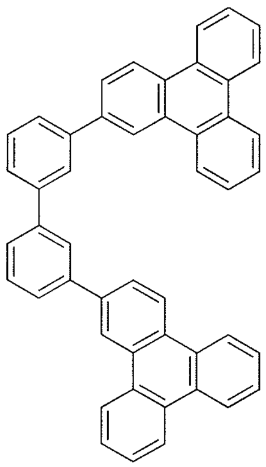
36. The device of claim 17, wherein the organic layer further comprises a host having the formula:



,

wherein R'$_1$, R'$_2$, R'$_3$, R'$_4$, R'$_5$, R'$_6$, R'$_7$, and R'$_8$ are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl, and heteroaryl.

37. The device of claim 36, wherein the host is:



Compound F .

38. The device of claim 17, wherein the first device is a consumer product.

39. The device of claim 17, wherein the first device is an organic light emitting device.

PHOSPHORESCENT MATERIALS
Inventor: Chuanjun XIA, *et al.*
Attorney Docket No.: 027166-005810PC

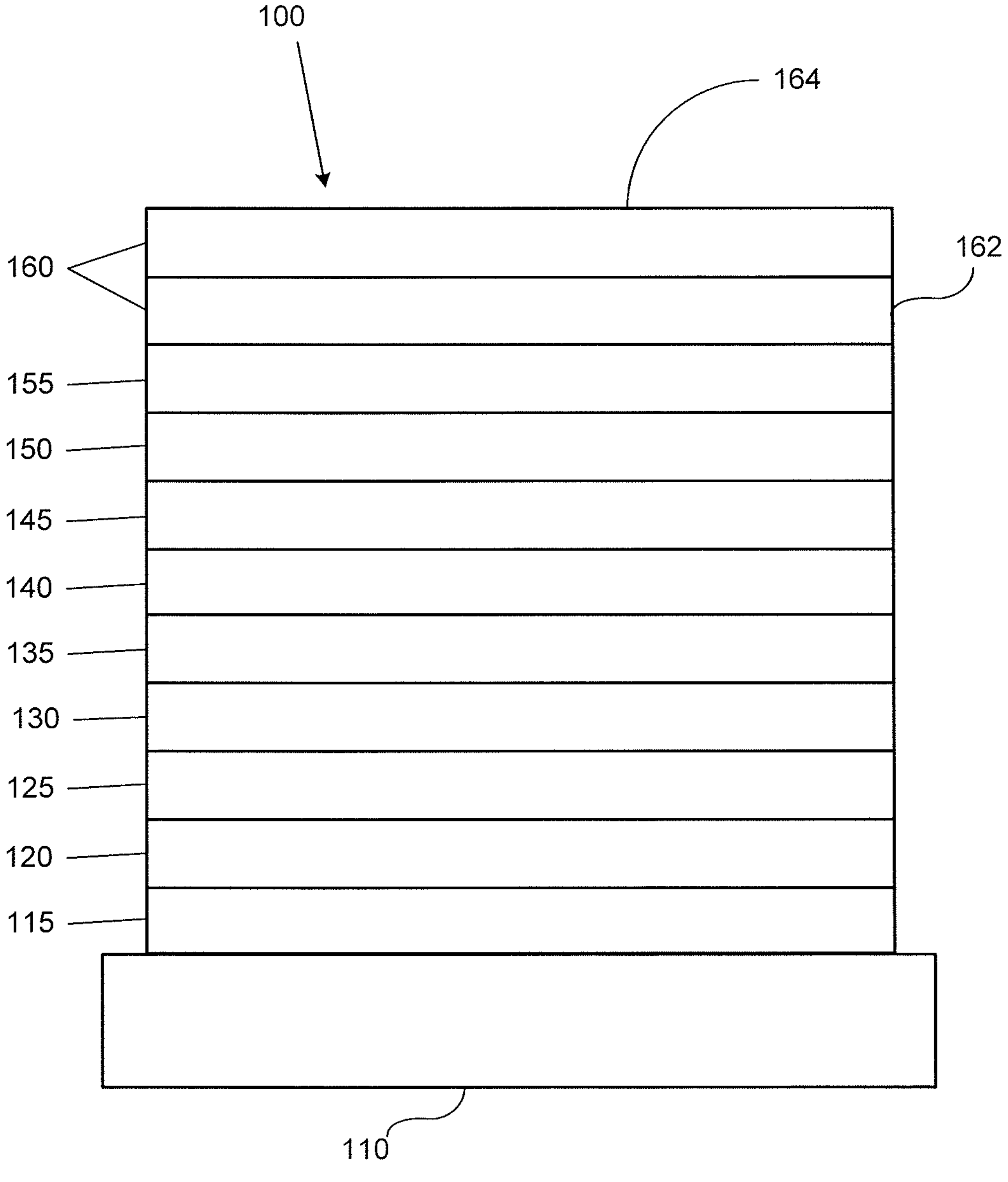


FIGURE 1

PHOSPHORESCENT MATERIALS
Inventor: Chuanjun XIA, *et al.*
Attorney Docket No.: 027166-005810PC

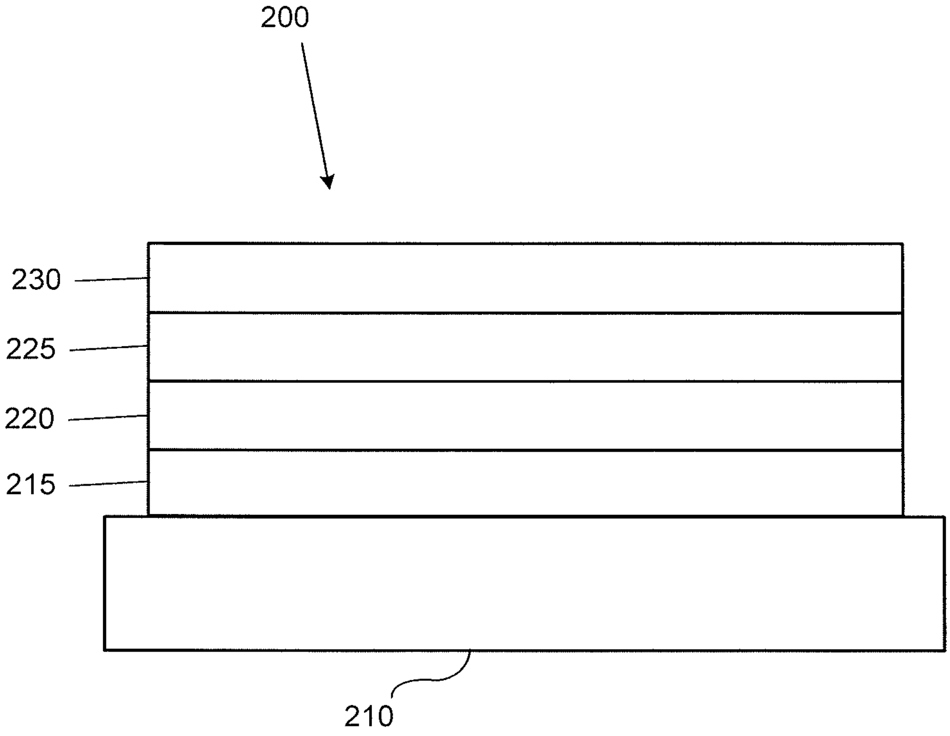


FIGURE 2

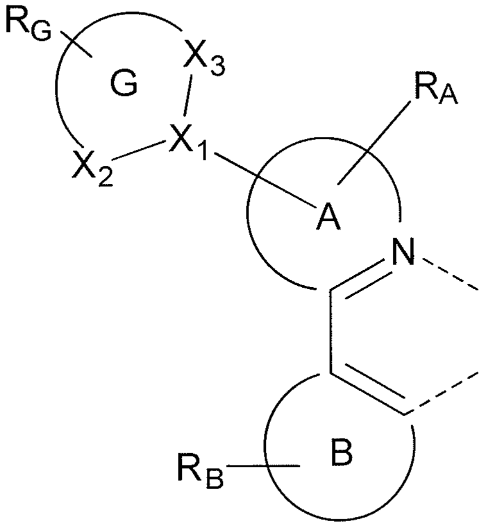


FIGURE 3

INTERNATIONAL SEARCH REPORT

International application No
PCT/US2010/051076

A. CLASSIFICATION OF SUBJECT MATTER
INV. C09K11/06 H05B33/14
ADD.

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
C09K H05B

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, CHEM ABS Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	EP 1 239 526 A2 (CANON KK [JP]) 11 September 2002 (2002-09-11) compounds 43,309-348,522,527 -----	1-39
X	EP 2 062 959 A2 (GRACEL DISPLAY INC [KR]) 27 May 2009 (2009-05-27) claims 2,3 -----	1-39
X	WO 2010/004877 A1 (KONICA MINOLTA HOLDINGS INC [JP]; TAMARU JUNKO [JP]; TAKA HIDEO [JP];) 14 January 2010 (2010-01-14) compounds DD-5,DD-11 -----	1-39
X	JP 2008 101114 A (KONICA MINOLTA HOLDINGS INC) 1 May 2008 (2008-05-01) compounds 16,20,27,39,42,45,67 ----- -/--	1-39

☒ Further documents are listed in the continuation of Box C.

☒ See patent family annex.

* Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance
"E" earlier document but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
"&" document member of the same patent family

Date of the actual completion of the international search 30 December 2010	Date of mailing of the international search report 12/01/2011
Name and mailing address of the ISA/ European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Authorized officer Saldamli, Saltuk

1

INTERNATIONAL SEARCH REPORT

International application No
PCT/US2010/051076

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	JP 2008 210941 A (KONICA MINOLTA HOLDINGS INC) 11 September 2008 (2008-09-11) compounds 2-6,8	1-39
X	JP 2009 267244 A (FUJIFILM CORP) 12 November 2009 (2009-11-12) compounds 4-3	1-39
X	US 2005/027123 A1 (TAKIGUCHI TAKAO [JP] ET AL) 3 February 2005 (2005-02-03) compounds 13,15,24,35,37,41,48,64-65,100,135,137,163-164,167	1-39
X	US 2007/184301 A1 (OSHIYAMA TOMOHIRO [JP] ET AL) 9 August 2007 (2007-08-09) compound 23	1-39

1

Form PCT/ISA/210 (continuation of second sheet) (April 2005)

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/US2010/051076

Patent document cited in search report		Publication date	Patent family member(s)			Publication date
EP 1239526	A2	11-09-2002	JP	4438042	B2	24-03-2010
			JP	2002332292	A	22-11-2002
			US	2003068536	A1	10-04-2003
			US	2006022588	A1	02-02-2006
EP 2062959	A2	27-05-2009	CN	101508673	A	19-08-2009
			JP	2009173630	A	06-08-2009
			KR	20090051856	A	25-05-2009
			US	2009179555	A1	16-07-2009
WO 2010004877	A1	14-01-2010	NONE			
JP 2008101114	A	01-05-2008	NONE			
JP 2008210941	A	11-09-2008	NONE			
JP 2009267244	A	12-11-2009	NONE			
US 2005027123	A1	03-02-2005	NONE			
US 2007184301	A1	09-08-2007	WO	2005083033	A1	09-09-2005

专利名称(译)	磷光材料		
公开(公告)号	EP2542644A1	公开(公告)日	2013-01-09
申请号	EP2010763296	申请日	2010-10-01
[标]申请(专利权)人(译)	环球展览公司		
申请(专利权)人(译)	通用显示器公司		
当前申请(专利权)人(译)	通用显示器公司		
[标]发明人	XIA CHUANJUN ALLEYNE BERT ANSARI NASRIN		
发明人	XIA, CHUANJUN ALLEYNE, BERT ANSARI, NASRIN		
IPC分类号	C09K11/06 H05B33/14		
CPC分类号	C09K11/06 C07F15/0033 C09K2211/1022 C09K2211/1029 C09K2211/1033 C09K2211/1037 C09K2211/1044 C09K2211/1059 C09K2211/185 H01L51/0085 H01L51/5016 H05B33/14		
代理机构(译)	MAIWALD专利ADVOCATE GMBH		
优先权	61/339337 2010-03-03 US 12/868350 2010-08-25 US		
其他公开文献	EP2542644B1		
外部链接	Espacenet		

摘要(译)

提供了包含进一步被杂环基取代的2-苯基吡啶配体的化合物。特别地，该化合物包含进一步被含氮杂环取代的2-苯基吡啶配体。该化合物可用于有机发光器件中，以提供具有改进的效率和寿命的器件。