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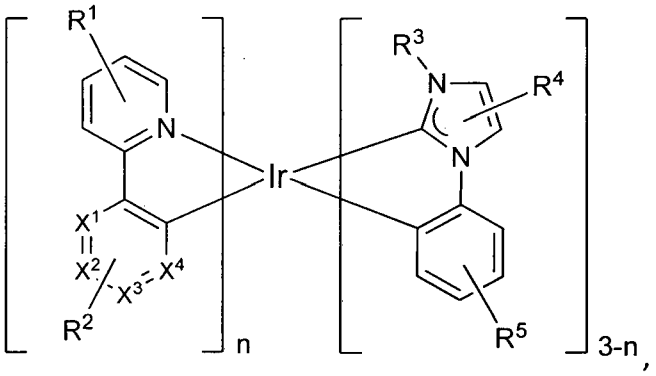
(54) **Organic eletroluminescent materials and devices**

(57) A compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



Formula I, is described. In formula $Ir(L_A)_n(L_B)_{3-n}$, n is either 1 or 2; R^1, R^2, R^4, and R^5 each independently represent up to the maximum number of substitutions or no substitutions; X^1, X^2, X^3, and X^4 are each independently C or N; and at least one of X^1, X^2, X^3, and X^4 is N. In addition, any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring, and each R^1, R^2, R^3, R^4, and R^5 is independently selected from hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof. Formulations and devices, such as an OLEDs, that include the compound of formula $Ir(L_A)_n(L_B)_{3-n}$ are also described.

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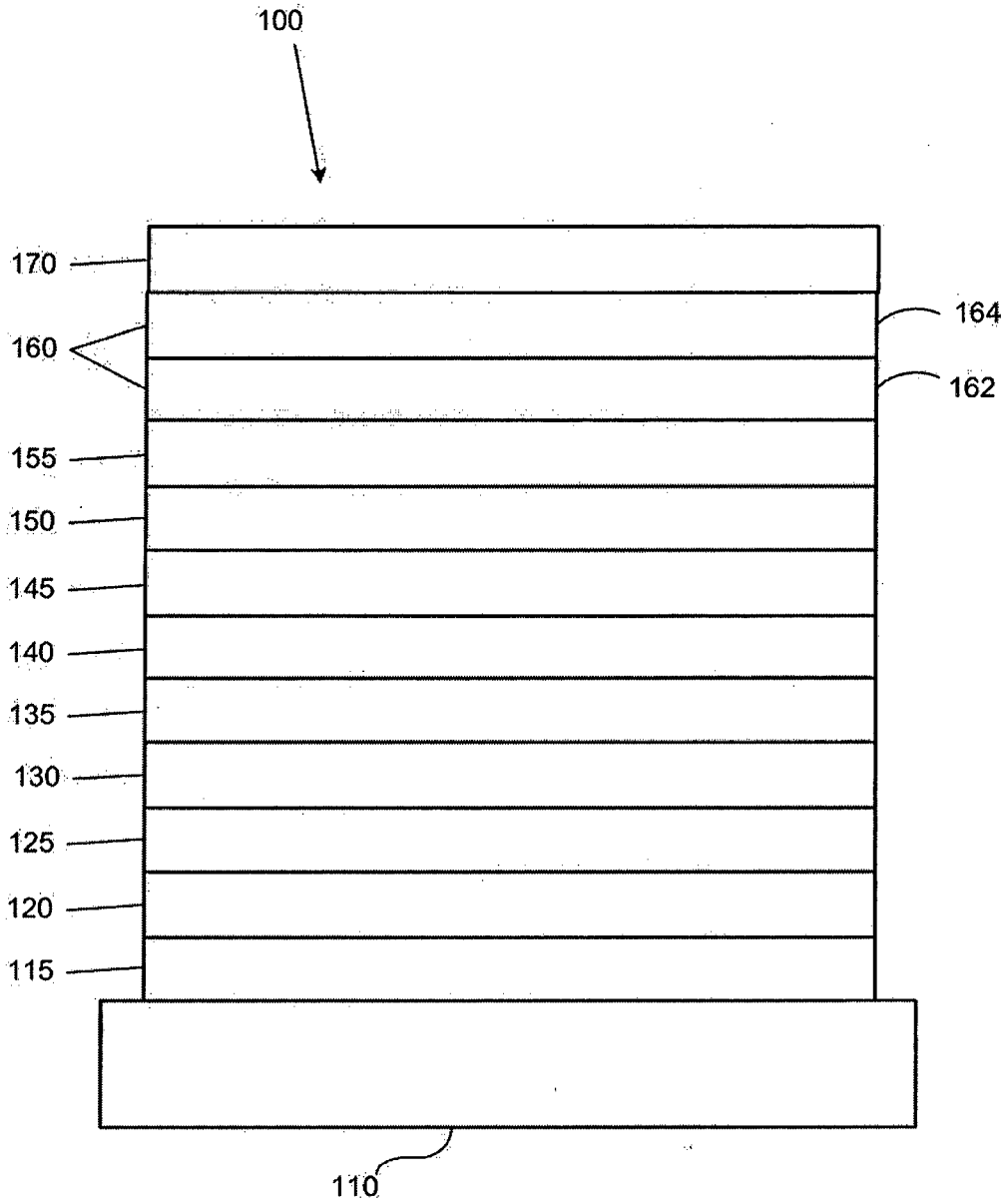


FIGURE 1

Description

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application claims priority to U.S. Provisional Patent Application Serial No. 61/904,530, filed November 15, 2013, and U.S. Provisional Patent Application Serial No. 61/907,450, filed November 22, 2013, the entire contents of which are incorporated herein by reference.

PARTIES TO A JOINT RESEARCH AGREEMENT

[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, 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 compounds for use as emitters and devices, such as organic light emitting diodes, including the same.

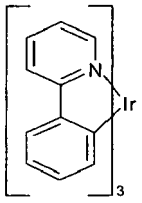
BACKGROUND

[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 following 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.

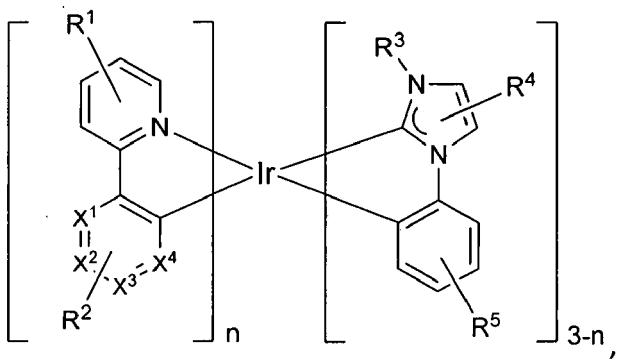
[0013] As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer 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] According to one embodiment, a compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



Formula I, is provided. In the structure of Formula I:

R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;

R^2 represents up to tri-substitution, or no substitution;

R^4 represents mono, or di-substitution, or no substitution;

X^1, X^2, X^3, and X^4 are each independently C or N;

at least one of X^1, X^2, X^3, and X^4 is N;

any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;

each of R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

n is either 1 or 2.

[0017] According to another embodiment, a first device comprising a first organic light emitting device is also provided. The first organic light emitting device can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer can include a compound of the formula $Ir(L_A)_n(L_B)_{3-n}$. The first device can be one or more of a consumer product, an electronic component module, an organic light-emitting device, and a lighting panel.

[0018] Formulations containing a compound of the formula $Ir(L_A)_n(L_B)_{3-n}$ are also provided.

BRIEF DESCRIPTION OF THE DRAWINGS

[0019]

FIG. 1 shows an organic light emitting device.

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

FIG. 3 shows Formula I as disclosed herein.

FIG. 4 shows Formula II as disclosed herein.

DETAILED DESCRIPTION

[0020] 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.

[0021] 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.

[0022] 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.

[0023] 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, a cathode 160, and a barrier layer 170. 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.

[0024] 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_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.

[0025] 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.

[0026] 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.

[0027] 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.

[0028] 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. Pat. No. 7,431,968, 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 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.

[0029] Devices fabricated in accordance with embodiments of the present invention may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer

may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a mixture of a polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a "mixture", the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a non-polymeric material consists essentially of polymeric silicon and inorganic silicon.

[0030] Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of electronic component modules (or units) that can be incorporated into a variety of electronic products or intermediate components. Examples of such electronic products or intermediate components include display screens, lighting devices such as discrete light source devices or lighting panels, etc. that can be utilized by the end-user product manufacturers. Such electronic component modules can optionally include the driving electronics and/or power source(s). Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of consumer products that have one or more of the electronic component modules (or units) incorporated therein. Such consumer products would include any kind of products that include one or more light source(s) and/or one or more of some type of visual displays. Some examples of such consumer products include flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads-up displays, fully or partially transparent displays, flexible displays, laser printers, telephones, cell phones, tablets, phablets, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, 3-D 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), but could be used outside this temperature range, for example, from -40 degree C to + 80 degree C.

[0031] 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.

[0032] The term "halo," "halogen," or "halide" as used herein includes fluorine, chlorine, bromine, and iodine.

[0033] The term "alkyl" as used herein contemplates both straight and branched chain alkyl radicals. Preferred alkyl groups are those containing from one to fifteen carbon atoms and includes methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tert-butyl, and the like. Additionally, the alkyl group may be optionally substituted.

[0034] The term "cycloalkyl" as used herein contemplates cyclic alkyl radicals. Preferred cycloalkyl groups are those containing 3 to 7 carbon atoms and includes cyclopropyl, cyclopentyl, cyclohexyl, and the like. Additionally, the cycloalkyl group may be optionally substituted.

[0035] The term "alkenyl" as used herein contemplates both straight and branched chain alkene radicals. Preferred alkenyl groups are those containing two to fifteen carbon atoms. Additionally, the alkenyl group may be optionally substituted.

[0036] The term "alkynyl" as used herein contemplates both straight and branched chain alkyne radicals. Preferred alkynyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group may be optionally substituted.

[0037] The terms "aralkyl" or "arylalkyl" as used herein are used interchangeably and contemplate an alkyl group that has as a substituent an aromatic group. Additionally, the aralkyl group may be optionally substituted.

[0038] The term "heterocyclic group" as used herein contemplates aromatic and non-aromatic cyclic radicals. Hetero-aromatic cyclic radicals also means heteroaryl. Preferred hetero-non-aromatic cyclic groups are those containing 3 or 7 ring atoms which includes at least one hetero atom, and includes cyclic amines such as morpholino, piperdino, pyrrolidino, and the like, and cyclic ethers, such as tetrahydrofuran, tetrahydropyran, and the like. Additionally, the heterocyclic group may be optionally substituted.

[0039] The term "aryl" or "aromatic group" as used herein contemplates single-ring groups and polycyclic ring systems. The polycyclic rings may have two or more rings in which two carbons are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is aromatic, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Additionally, the aryl group may be optionally substituted.

[0040] The term "heteroaryl" as used herein contemplates single-ring hetero-aromatic groups that may include from one to three heteroatoms, for example, pyrrole, furan, thiophene, imidazole, oxazole, thiazole, triazole, pyrazole, pyridine, pyrazine and pyrimidine, and the like. The term heteroaryl also includes polycyclic hetero-aromatic systems having two

or more rings in which two atoms are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Additionally, the heteroaryl group may be optionally substituted.

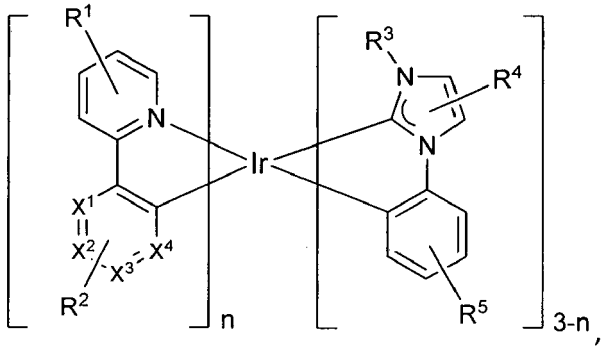
[0041] The alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, heterocyclic group, aryl, and heteroaryl may be optionally substituted with one or more substituents selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, cyclic amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0042] As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant position, such as carbon. Thus, for example, where R^1 is mono-substituted, then one R^1 must be other than H. Similarly, where R^1 is di-substituted, then two of R^1 must be other than H. Similarly, where R^1 is unsubstituted, R^1 is hydrogen for all available positions.

[0043] The "aza" designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzothiophene, etc. means that one or more of the C-H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[*f*,*h*]quinoxaline and dibenzo[*f*,*h*]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein.

[0044] It is to be understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it were a fragment (e.g. phenyl, phenylene, naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. benzene, naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[0045] According to one embodiment, a compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



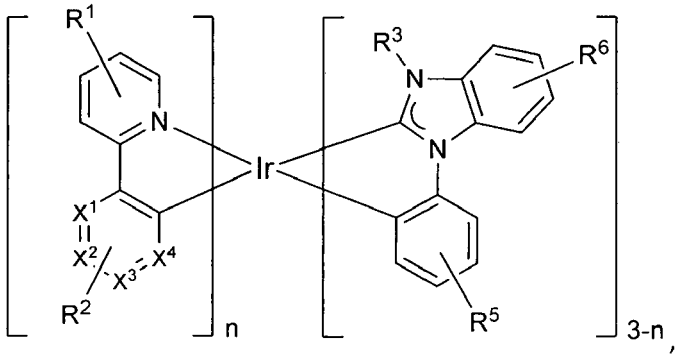
[0046] Formula I, is disclosed. In the structure of Formula I:

R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;
R^2 represents up to tri-substitution, or no substitution;
R^4 represents mono, or di-substitution, or no substitution;
X^1, X^2, X^3, and X^4 are each independently C or N;
at least one of X^1, X^2, X^3, and X^4 is N;
any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;
each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and
n is either 1 or 2.

[0047] In some embodiments, two adjacent substituents of R^4 can form a fused ring. In some embodiments, the fused ring can be aryl or heteroaryl. In some embodiments, the fused ring can be phenyl or pyridyl.

[0048] In some embodiments, n is 1. In some embodiments, n is 2.

[0049] In some embodiments, the compound has the structure of Formula II:



In the structure of Formula II:

R^6 represents mono, di, tri, or tetra-substitution, or no substitution;

any adjacent substitutions of R^6 are optionally linked together to form a ring; and

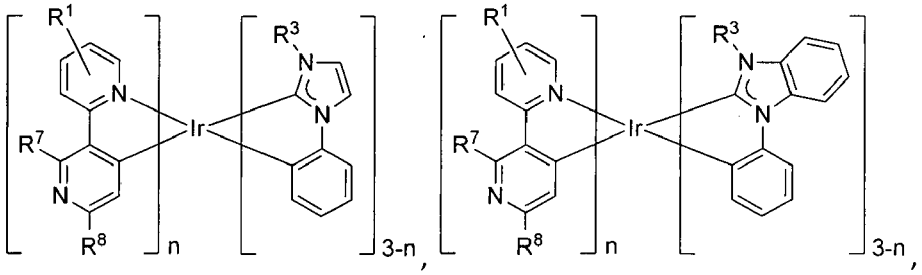
each R^6 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

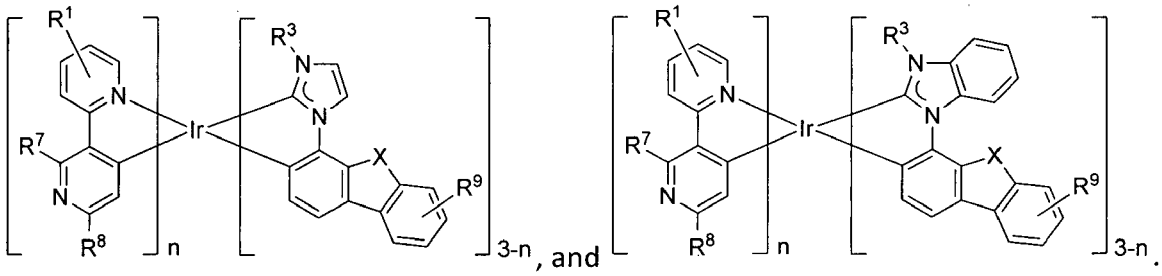
[0050] In some embodiments, only one of X^1, X^2, X^3, and X^4 is N. In some embodiments, only two of X^1, X^2, X^3, and X^4 are N. In some embodiments, exactly three of X^1, X^2, X^3, and X^4 are N, while in some embodiments all four of X^1, X^2, X^3, and X^4 are N. In some embodiments, X^2 is N.

[0051] In some embodiments, R^1 is selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, and combinations thereof. In some embodiments, R^2 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, nitrile, and combinations thereof. In some embodiments, each halide is independently selected from the group consisting of fluoride, chloride, dromide, and iodide.

[0052] In some embodiments, R^3 is alkyl or cycloalkyl. In some embodiments, R^3 is aryl or substituted aryl. In some embodiments, R^3 is selected from the group consisting of: ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, cyclopentyl, and cyclohexyl, wherein each group is optionally partially or fully deuterated.

[0053] In some embodiments, the compound is selected from the group consisting of:





In these structures:

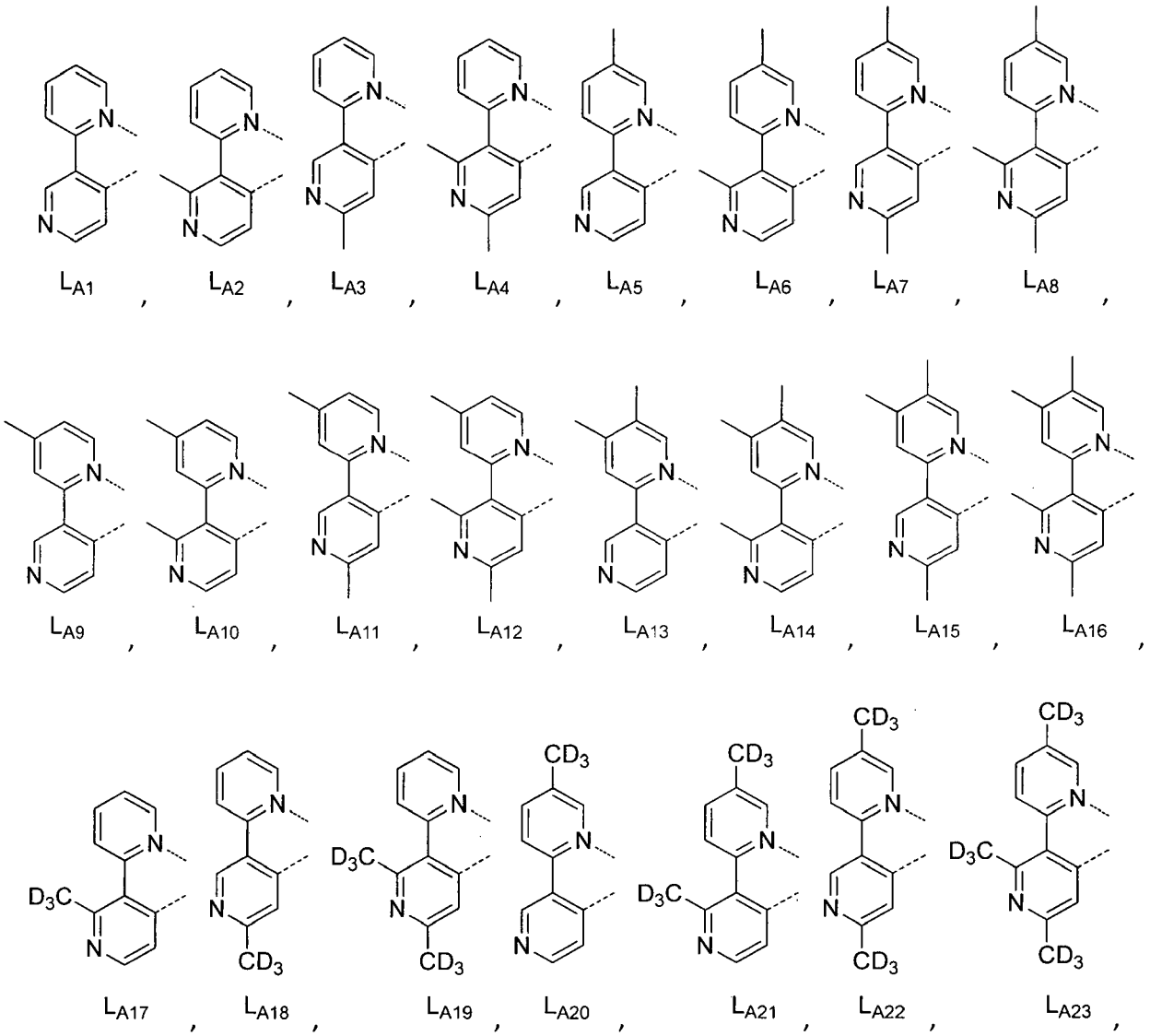
R^9 represents mono, di, tri, or tetra-substitution, or no substitution;

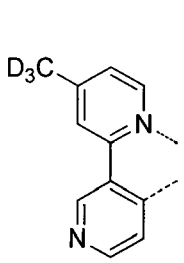
each R^7, R^8, and R^9 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

XisOorS.

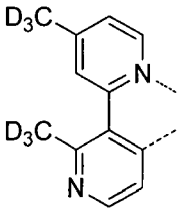
[0054] In some embodiments, R^9 can be selected from the group consisting of ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, wherein each group is optionally partially or fully deuterated.

[0055] In some embodiments, L_A is selected from the group consisting of:

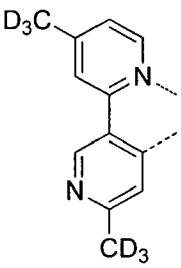




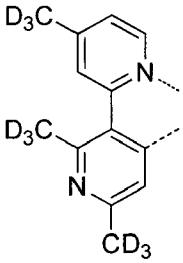
L_{A24} ,



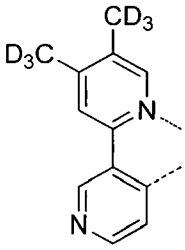
L_{A25} ,



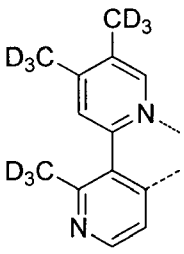
L_{A26} ,



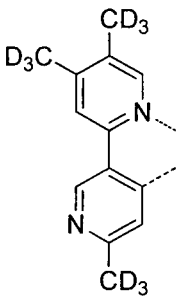
L_{A27} ,



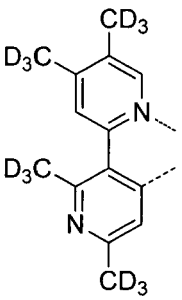
L_{A28} ,



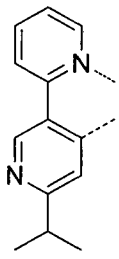
L_{A29} ,



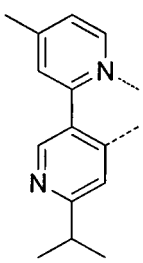
L_{A30} ,



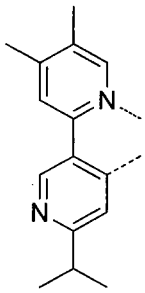
L_{A31} ,



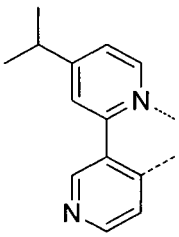
L_{A32} ,



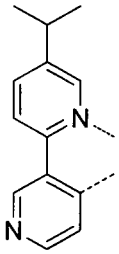
L_{A33} ,



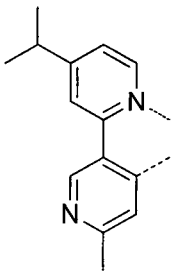
L_{A34} ,



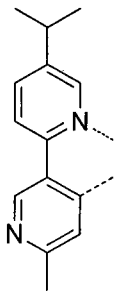
L_{A35} ,



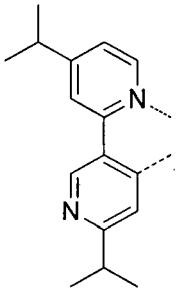
L_{A36} ,



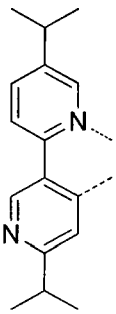
L_{A37} ,



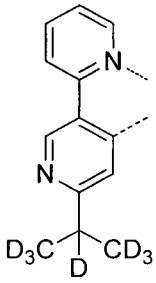
L_{A38} ,



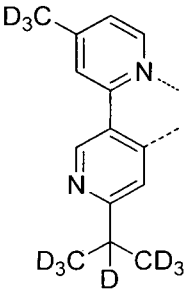
L_{A39} ,



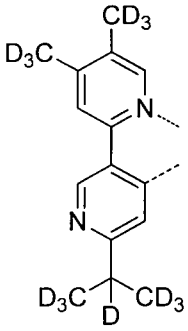
L_{A40} ,



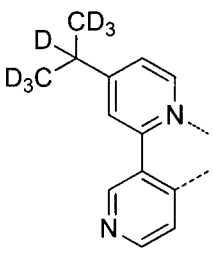
L_{A41} ,



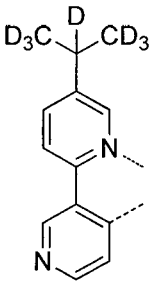
L_{A42} ,



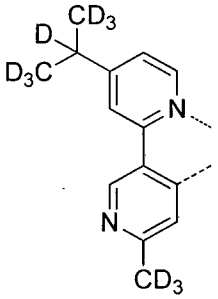
L_{A43} ,



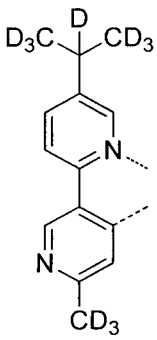
L_{A44} ,



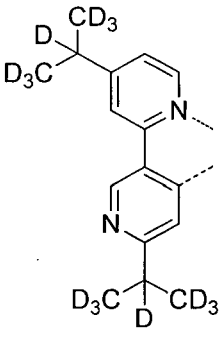
L_{A45} ,



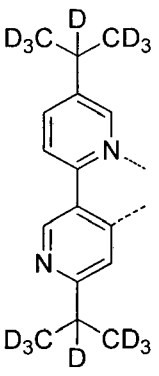
L_{A46} ,



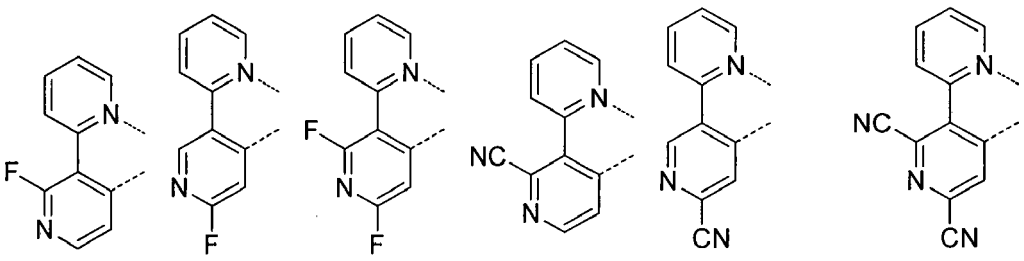
L_{A47} ,



L_{A48} ,

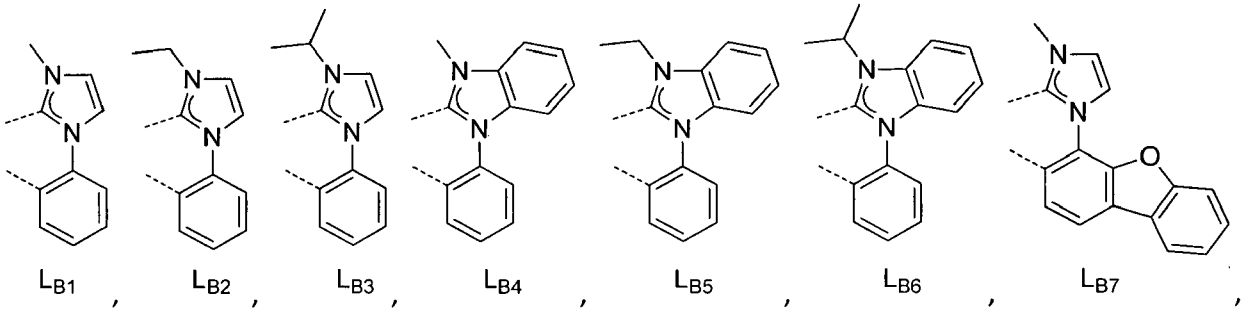


L_{A49} ,

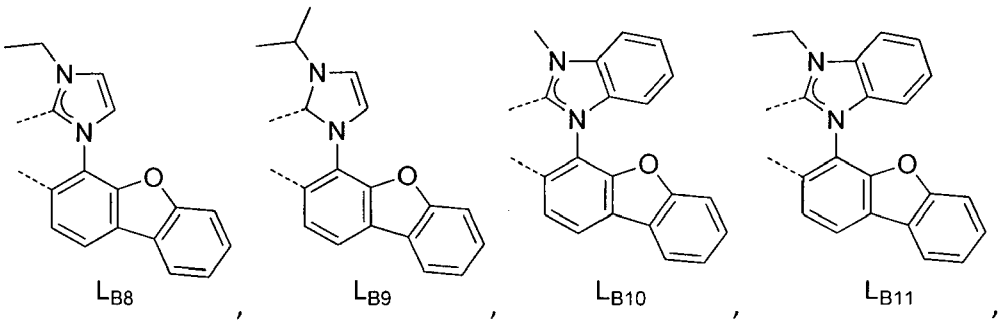


L_{A50}, L_{A51}, L_{A52}, L_{A53}, L_{A54}, and L_{A55}.

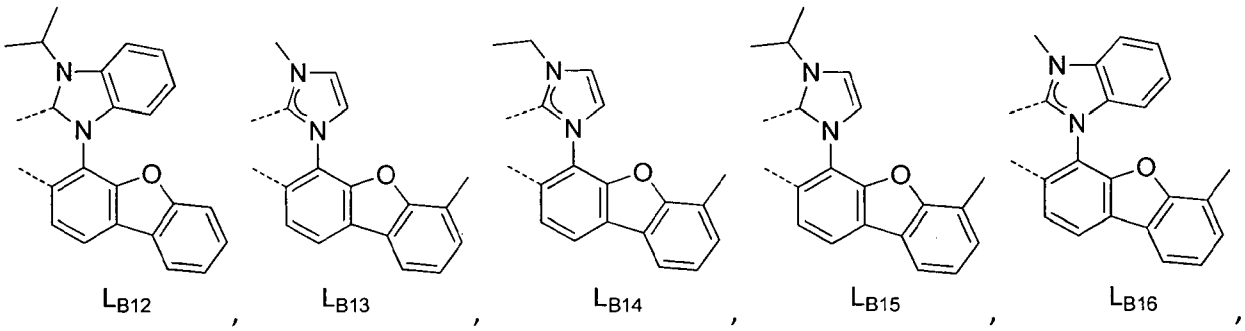
[0056] In some embodiments, L_B is selected from the group consisting of:



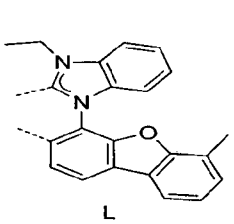
L_{B1}, L_{B2}, L_{B3}, L_{B4}, L_{B5}, L_{B6}, L_{B7},

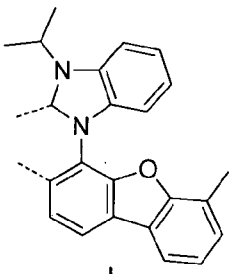


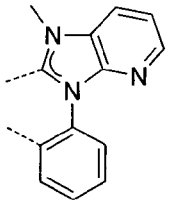
L_{B8}, L_{B9}, L_{B10}, L_{B11},

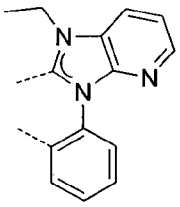


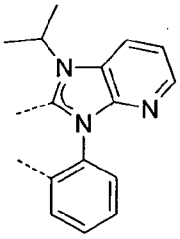
L_{B12}, L_{B13}, L_{B14}, L_{B15}, L_{B16},

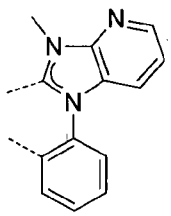

L_{B17},

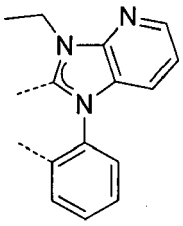

L_{B18},

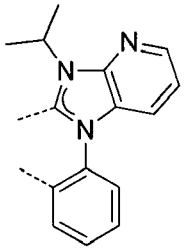

L_{B19},

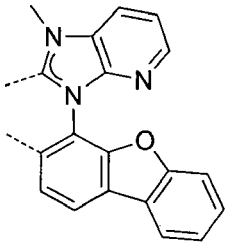

L_{B20},

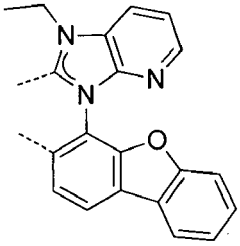

L_{B21},

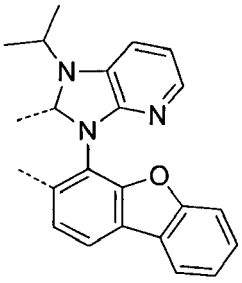

L_{B22},

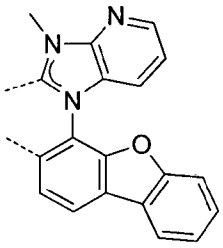

L_{B23},

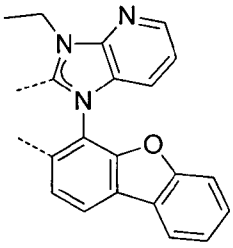

L_{B24},

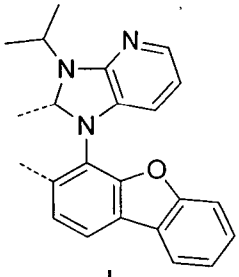

L_{B25},

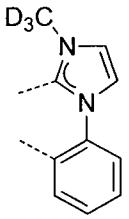

L_{B26},

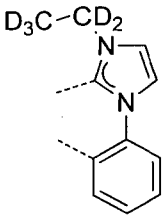

L_{B27},

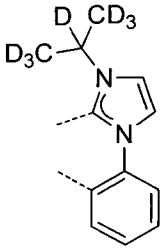

L_{B28},

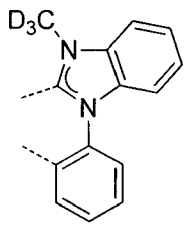

L_{B28},

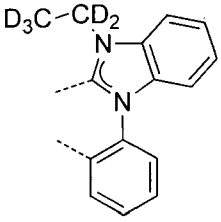

L_{B30},

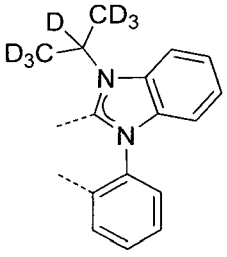

L_{B31},

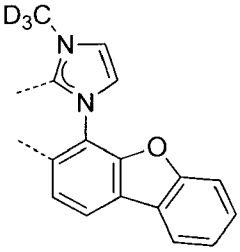

L_{B32},


L_{B33},


L_{B34},


L_{B35},


L_{B36},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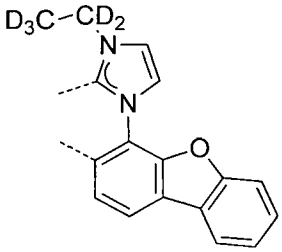
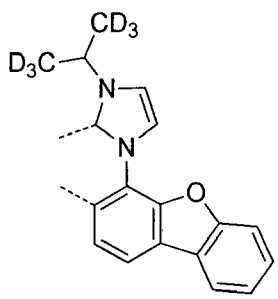
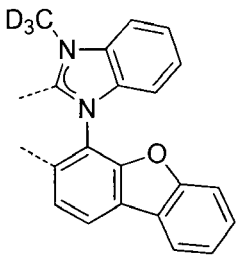
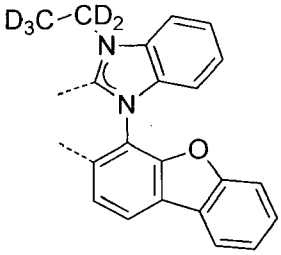

L_{B38},



L_{B39} ,



L_{B40} ,



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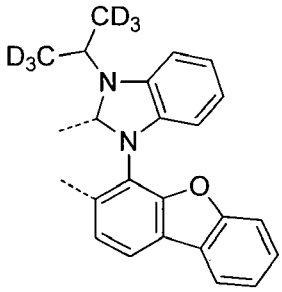
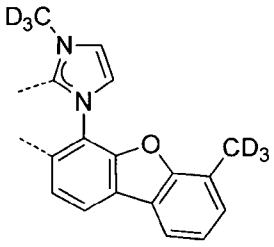
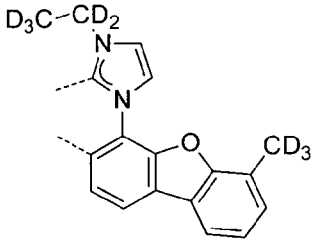


L_{B42} ,



L_{B43} ,



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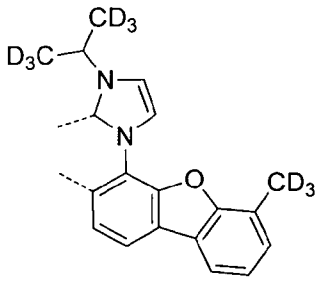
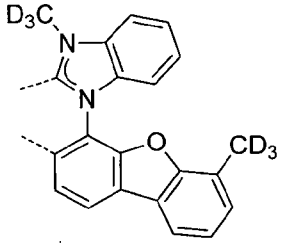


L_{B45} ,



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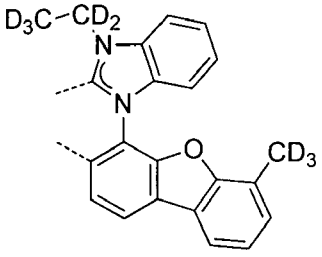
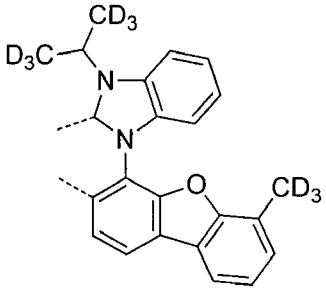
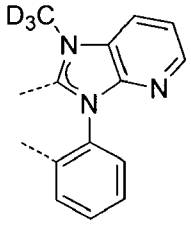


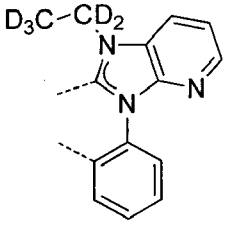
L_{B47} ,



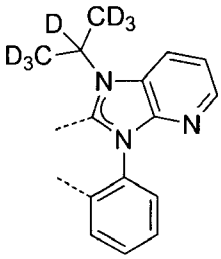
L_{B48} ,



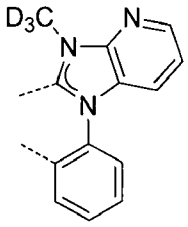
L_{B49} ,



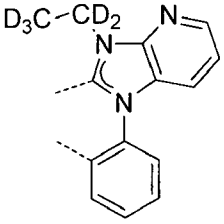
L_{B50} ,



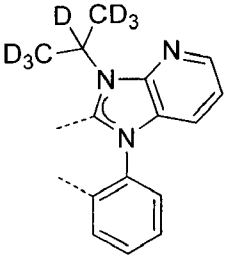
L_{B51} ,



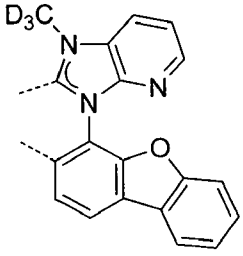
L_{B52} ,



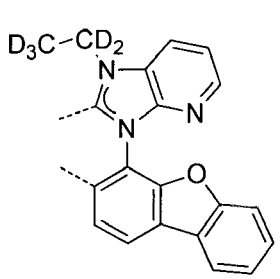
L_{B53} ,



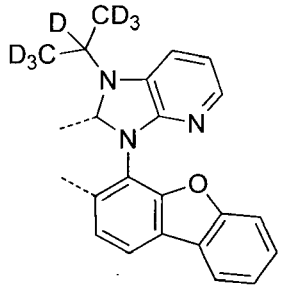
L_{B54} ,



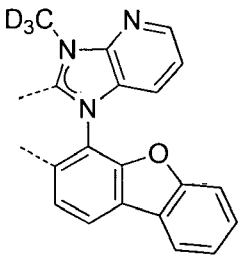
L_{B55} ,



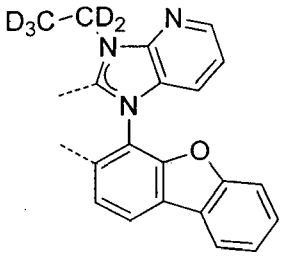
L_{B56} ,



L_{B57} ,

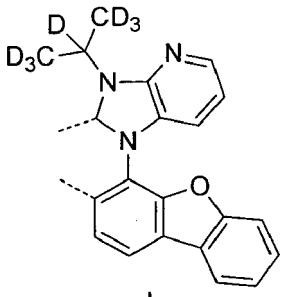


L_{B58} ,



L_{B59} ,

and



L_{B60} .

[0057] In some embodiments, the compound is selected from Compound 1 to 3300, where ligands L_A and L_B are as described herein, n is 2, and where each Compound x has the formula $Ir(L_{Ak})_2(L_{Bj})$, wherein $x = 55j + k - 55$, k is an integer from 1 to 55, and j is an integer from 1 to 60.

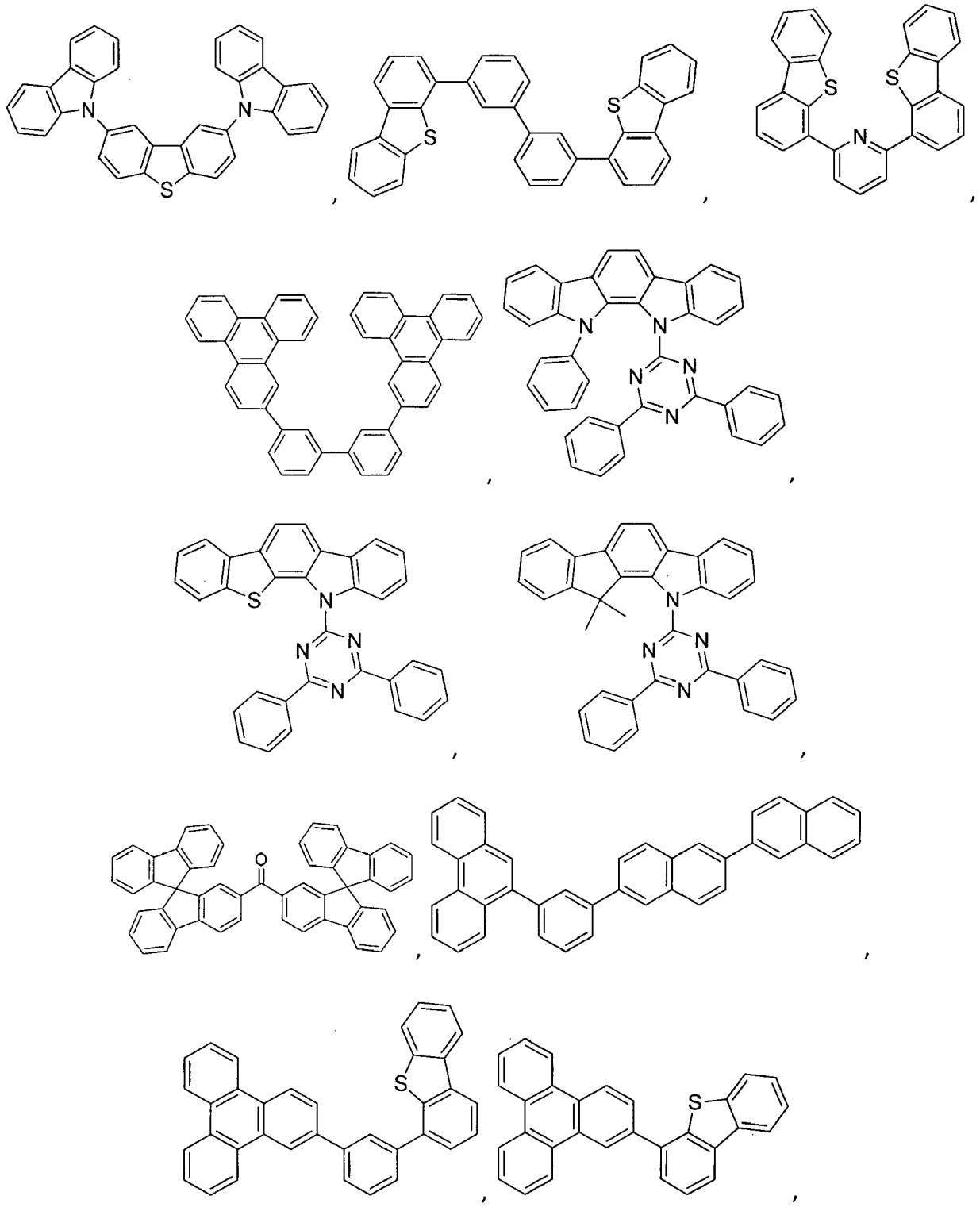
[0058] In some embodiments, the compound can be an emissive dopant. In some embodiments, the compound can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, *i.e.,* TADF (also referred to as E-type delayed fluorescence), triplet-triplet annihilation, or combinations of these processes.

[0059] According to another aspect of the present disclosure, a first device is also provided. The first device includes a first organic light emitting device, that includes an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer can include a compound according to Formula $Ir(L_A)_n(L_B)_{3-n}$, and its variants, as described herein. In some embodiments, the organic layer includes a host and a phosphorescent dopant.

[0060] The first device can be one or more of a a consumer product, an electronic component module, an organic light-emitting device, and a lighting panel. The organic layer can be an emissive layer and the compound can be an emissive dopant in some embodiments, while the compound can be a non-emissive dopant in other embodiments.

[0061] The organic layer can also include a host. In some embodiments, the host can include a metal complex. The host can be a triphenylene containing benzo-fused thiophene or benzo-fused furan. Any substituent in the host can be an unfused substituent independently selected from the group consisting of C_nH_{2n+1}, OC_nH_{2n+1}, OAr_1, $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH=CH-C_nH_{2n+1}$, $C\equiv C-C_nH_{2n+1}$, Ar_1, Ar_1-Ar_2, and $C_nH_{2n}-Ar_1$, or no substitution. In the preceding substituents n can range from 1 to 10; and Ar_1 and Ar_2 can be independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.

[0062] The host can be a compound comprising at least one chemical group selected from the group consisting of triphenylene, carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azatriphenylene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene. The host can include a metal complex. The host can be a specific compound selected from the group consisting of:



and combinations thereof.

[0063] In yet another aspect of the present disclsoure, a formulation that comprises a compound according to Formula $Ir(L_A)_n(L_B)_{3-n}$, and its variations described herein, is described. The formulation can include one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, and an electron transport layer material, disclosed herein.

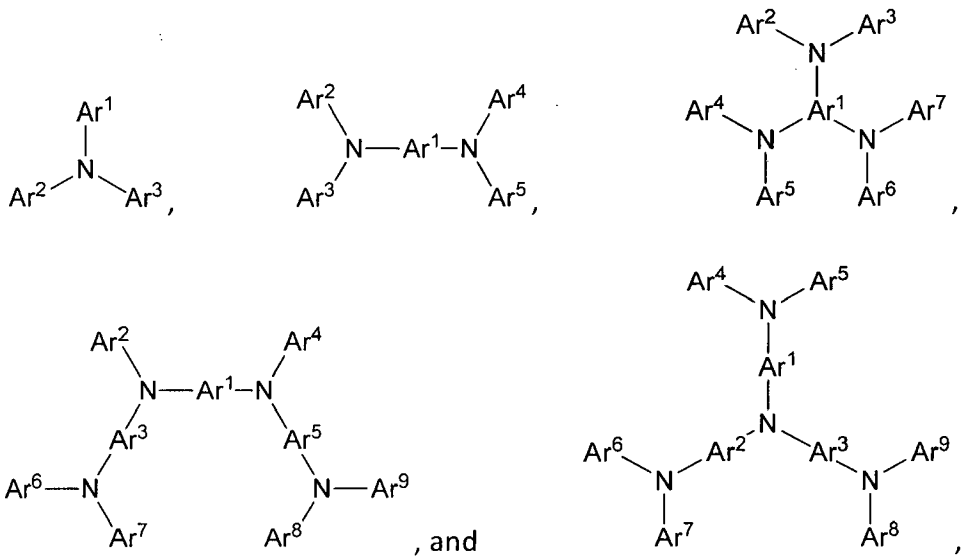
COMBINATION WITH OTHER MATERIALS

[0064] 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.

HIL/HTL:

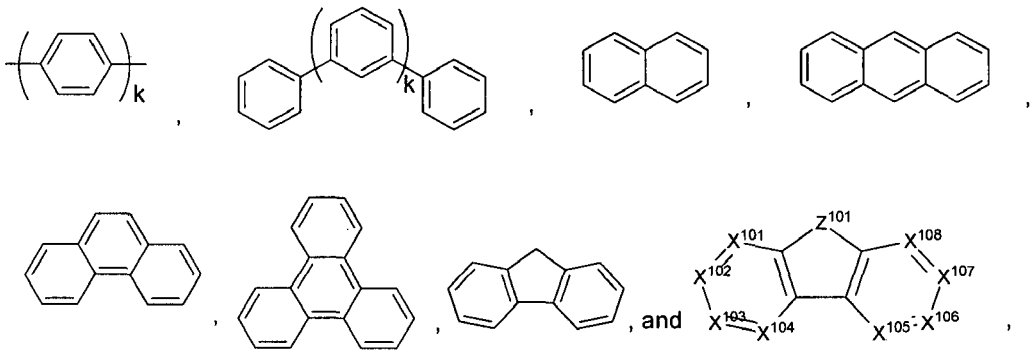
[0065] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphyrin 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 silane 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.

[0066] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:



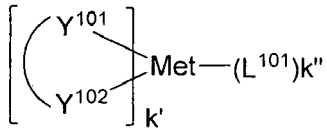
[0067] Each of Ar^1 to Ar^9 is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic 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 the group consisting of 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, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0068] In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:



wherein k is an integer from 1 to 20; X^{101} to X^{108} is C (including CH) or N; Z^{101} is NAr^1, O, or S; Ar^1 has the same group defined above.

[0069] Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:



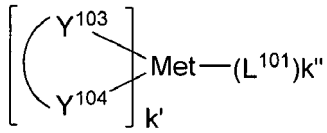
wherein Met is a metal, which can have an atomic weight greater than 40; (Y^{101}-Y^{102}) is a bidentate ligand, Y^{101} and Y^{102} are independently selected from C, N, O, P, and S; L^{101} is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

[0070] In one aspect, (Y^{101}-Y^{102}) is a 2-phenylpyridine derivative. In another aspect, (Y^{101}-Y^{102}) is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

[0071] Host:

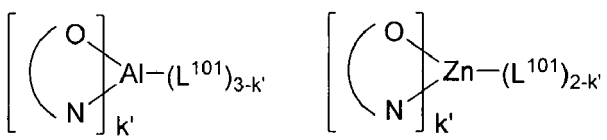
[0072] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. While the Table below categorizes host materials as preferred for devices that emit various colors, any host material may be used with any dopant so long as the triplet criteria is satisfied.

[0073] Examples of metal complexes used as host are preferred to have the following general formula:



wherein Met is a metal; (Y^{103}-Y^{104}) is a bidentate ligand, Y^{103} and Y^{104} are independently selected from C, N, O, P, and S; L^{101} is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

[0074] In one aspect, the metal complexes are:

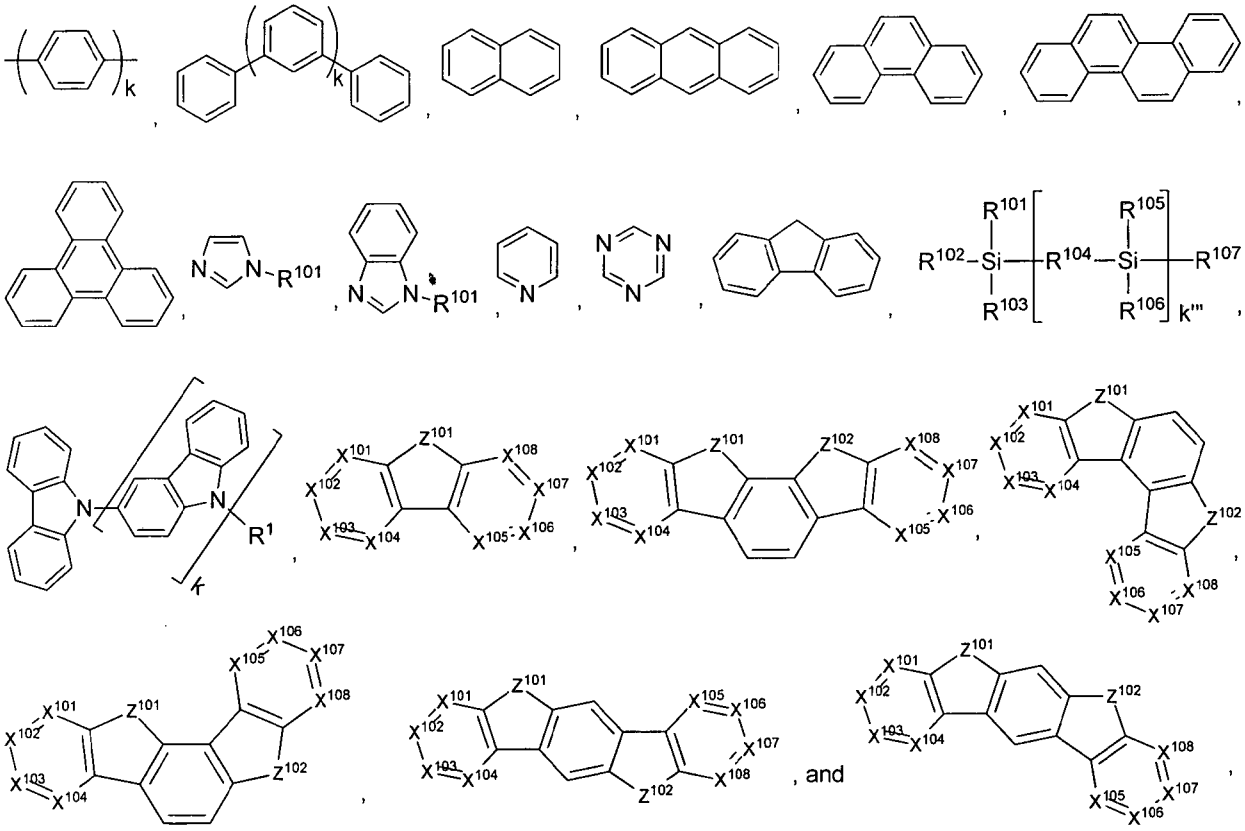


wherein (O-N) is a bidentate ligand, having metal coordinated to atoms O and N.

[0075] In another aspect, Met is selected from Ir and Pt. In a further aspect, (Y^{103}-Y^{104}) is a carbene ligand.

[0076] Examples of organic compounds used as host are selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of 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 the group consisting of 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, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0077] In one aspect, the host compound contains at least one of the following groups in the molecule:



wherein R^{101} to R^{107} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. k is an integer from 0 to 20 or 1 to 20; k''' is an integer from 0 to 20. X^{101} to X^{108} is selected from C (including CH) or N.
Z^{101} and Z^{102} is selected from NR^{101}, O, or S.

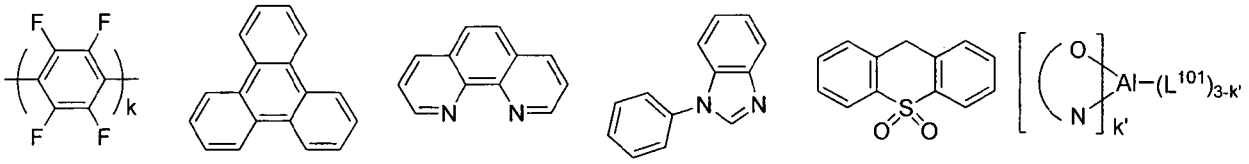
HBL:

[0078] 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.

[0079] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

[0080] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

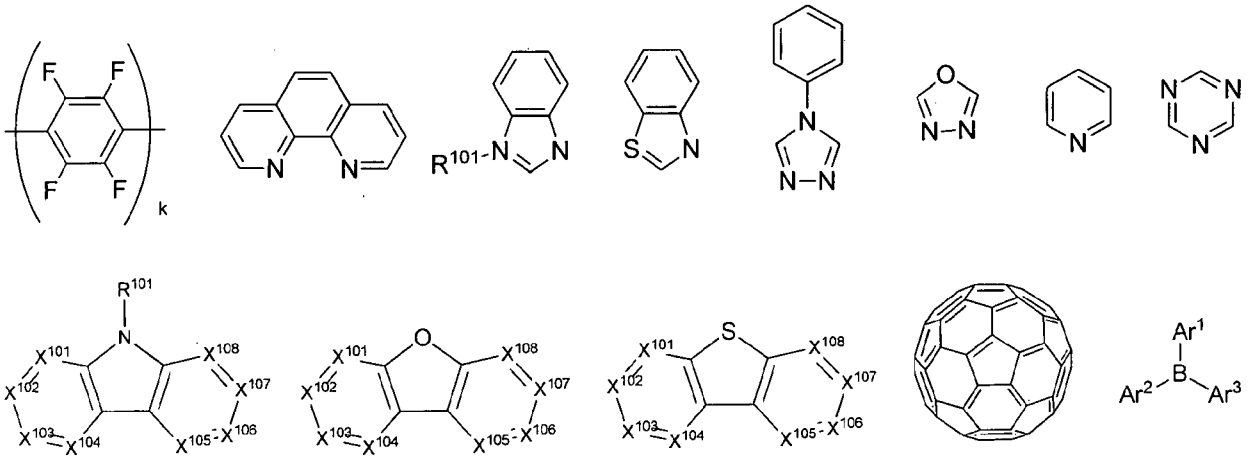


wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

ETL:

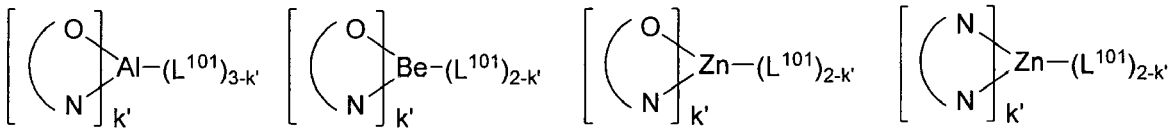
[0081] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

[0082] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:



wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. Ar^1 to Ar^3 has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X^{101} to X^{108} is selected from C (including CH) or N.

[0083] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

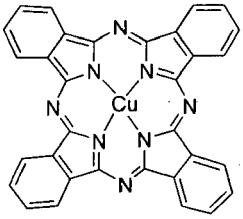
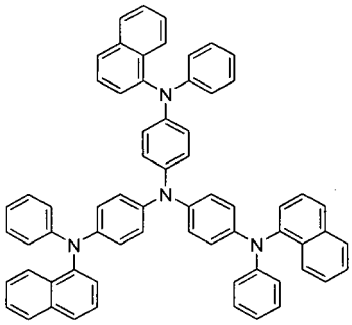
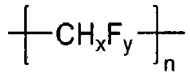
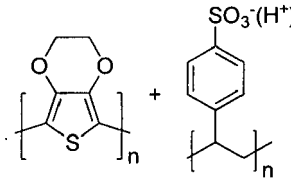
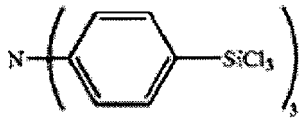
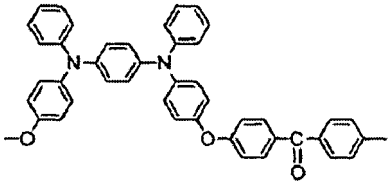


wherein (O-N) or (N-N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L^{101} is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

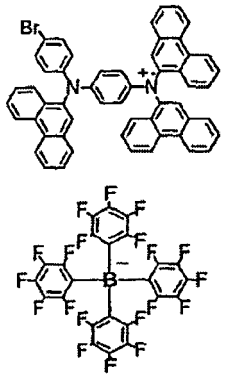
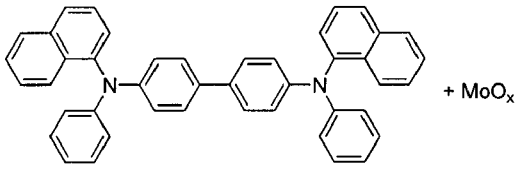
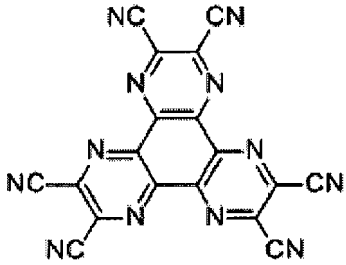
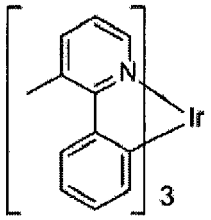
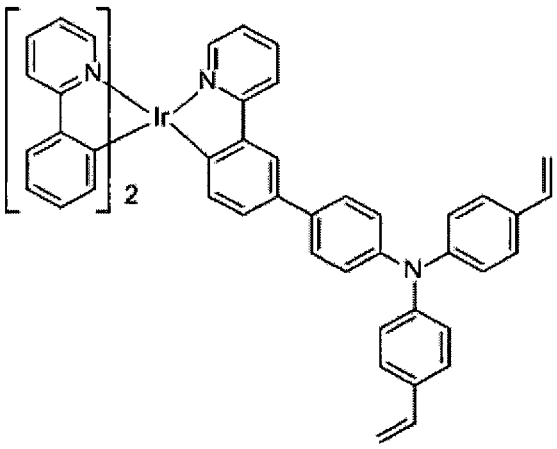
[0084] In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated. Thus, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. encompasses undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also encompass undeuterated, partially deuterated, and fully deuterated versions thereof.

[0085] 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 A below. Table A lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE A

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Phthalocyanine and porphyrin compounds		Appl. Phys. Lett. 69, 2160(1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydrocarbon polymer		Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and silane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants	 and	EP1725079A1

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
		
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides		US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009
n-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265

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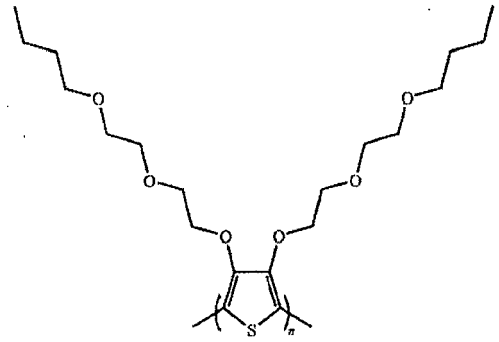
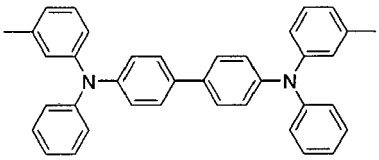
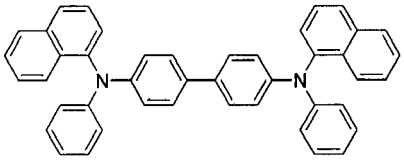
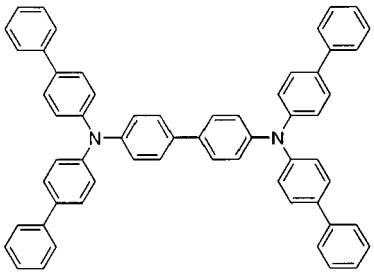
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216
Hole transporting materials		
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		US5061569
		EP650955

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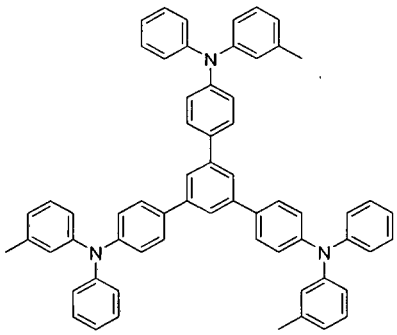
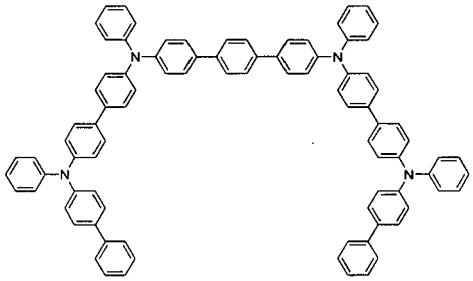
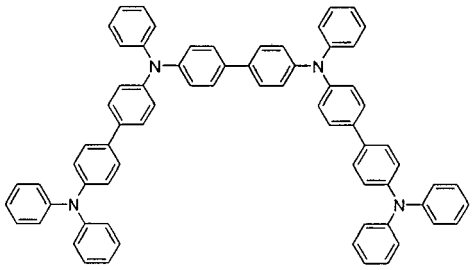
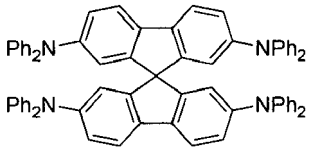
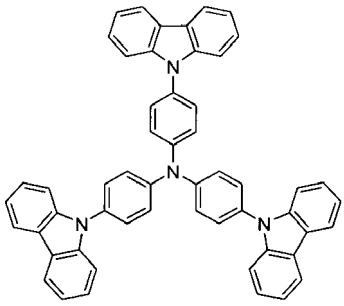
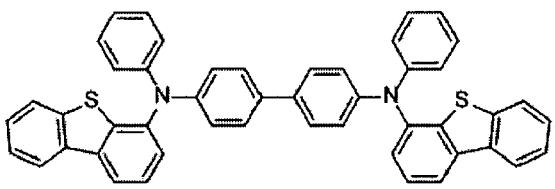
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)
Triarylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/(di)benzofuran		US20070278938, US20080106190 US20110163302

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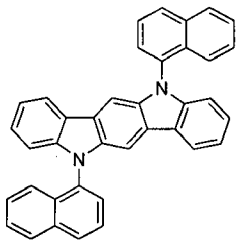
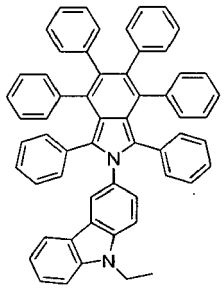
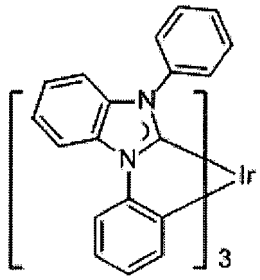
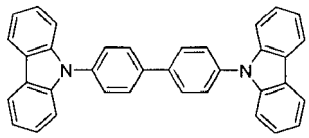
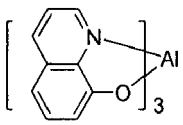
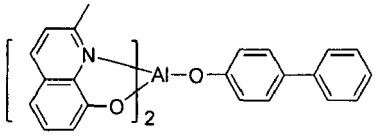
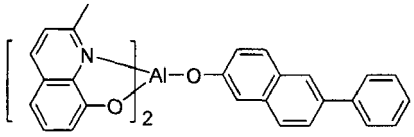
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials		
Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551

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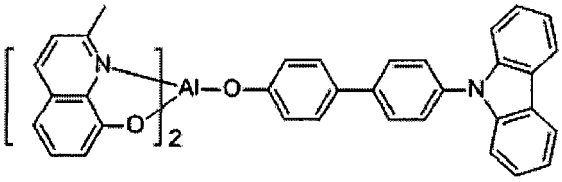
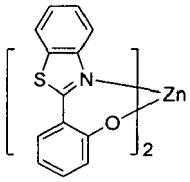
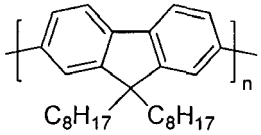
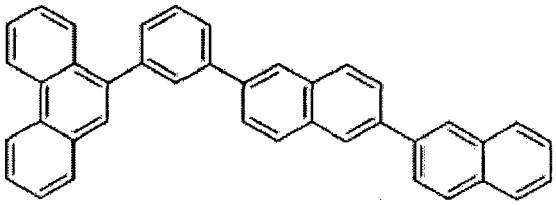
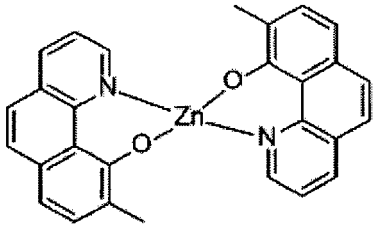
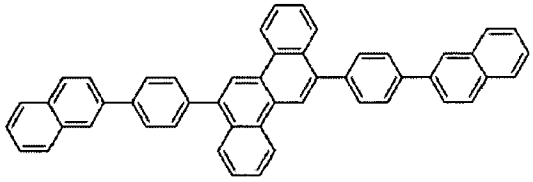
Phosphorescent OLED host materials		
Red hosts		
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
MATERIAL	**EXAMPLES OF MATERIAL**	**PUBLICATIONS**
Zinc complexes		WO2010056066
Chrysene based compounds		WO2011086863

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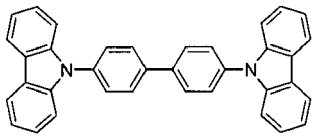
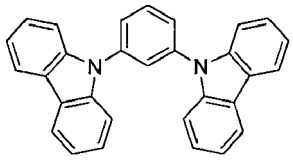
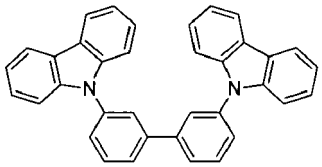
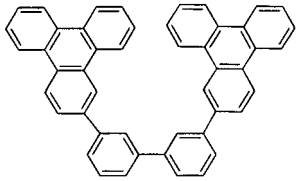
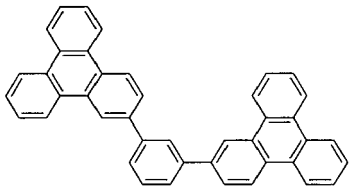
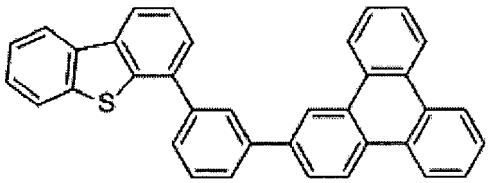
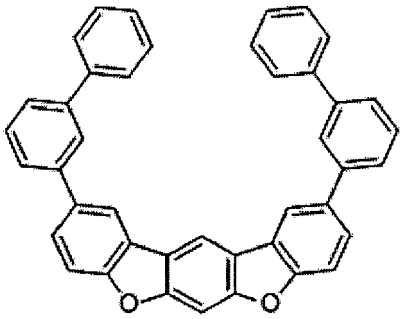
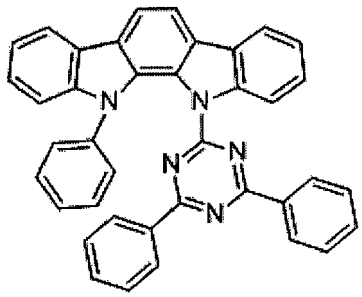
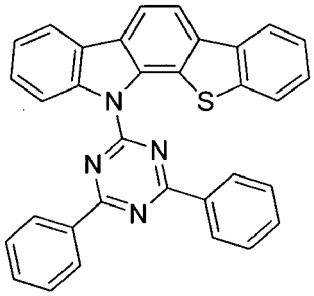
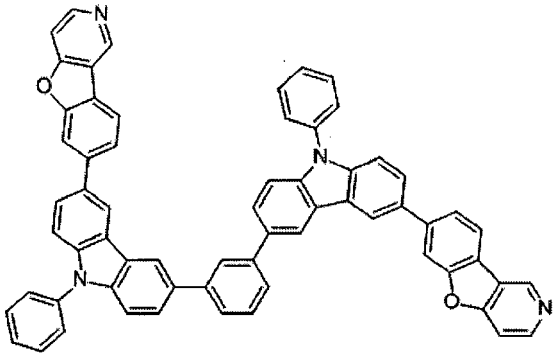
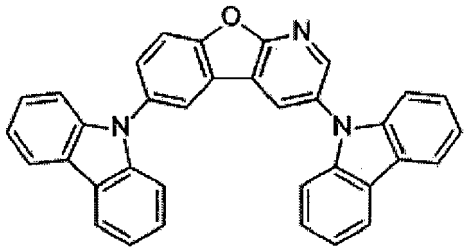
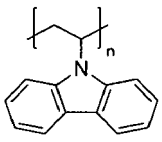
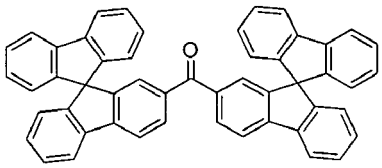
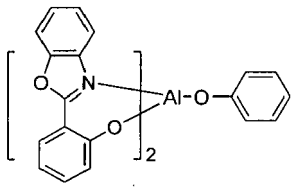
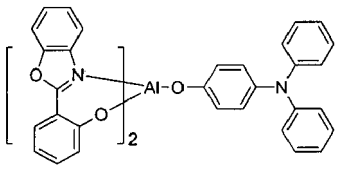
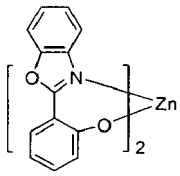
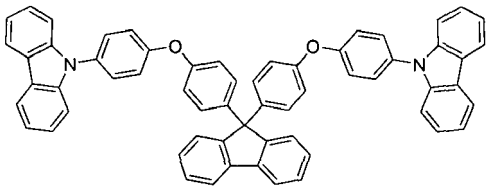
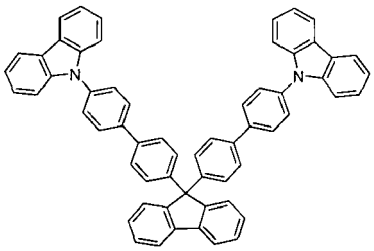
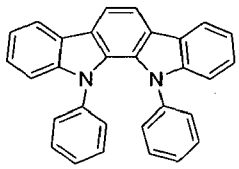
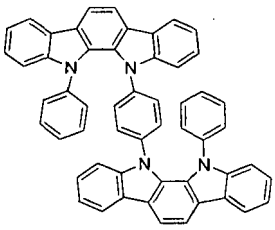
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965
		US20060280965
MATERIAL	**EXAMPLES OF MATERIAL**	**PUBLICATIONS**
		WO2009021126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931

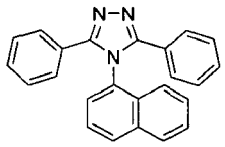
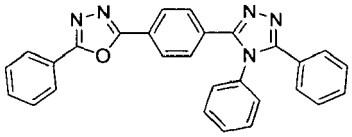
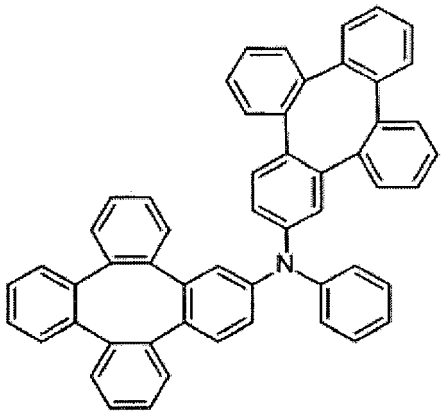
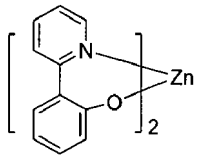
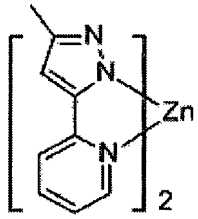
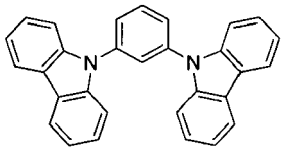
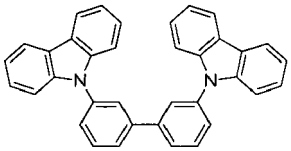
(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Donor acceptor type molecules		WO2008056746
		WO2010107244
Aza-carbazole/DBT/DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280(2000)
Spirofluorene compounds		WO2004093207

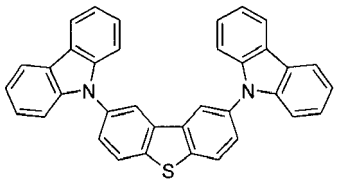
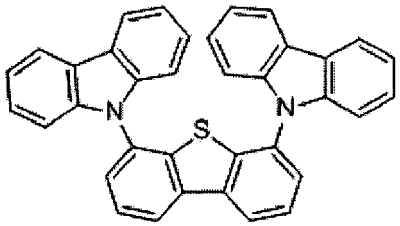
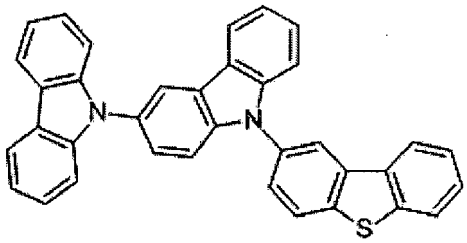
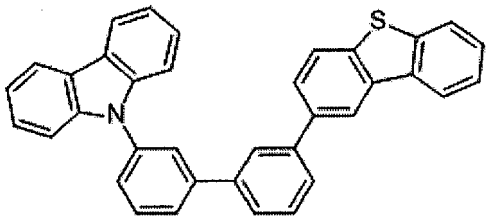
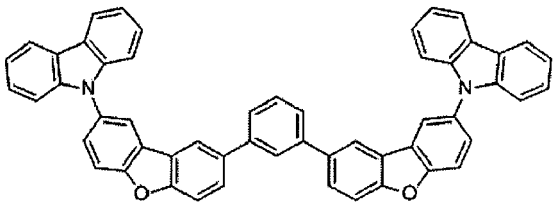
(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal phenoxybenzooxazole compounds		WO2005089025
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297
Indolocarbazoles		WO2007063796
		WO2007063754

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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

(continued)

Blue hosts		
Dibenzothiophene/Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
MATERIAL	**EXAMPLES OF MATERIAL**	**PUBLICATIONS**
		US20090167162
		WO2009086028
		US20090030202, US20090017330
		US20100084966

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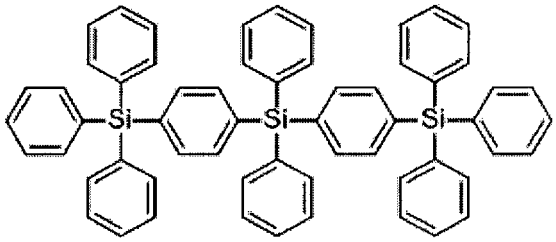
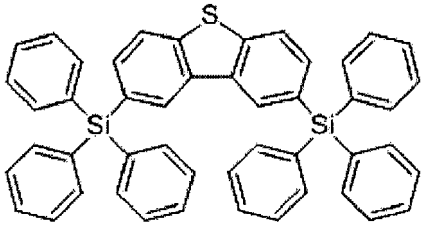
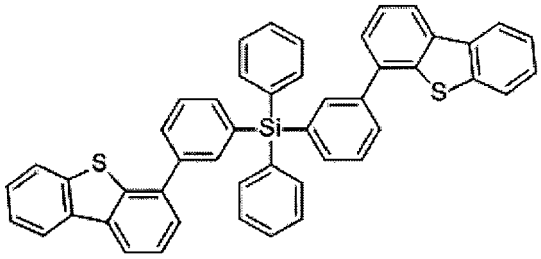
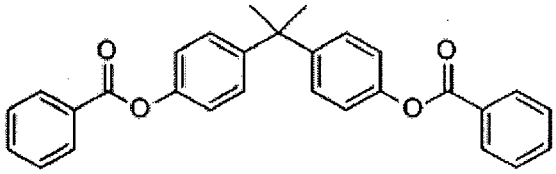
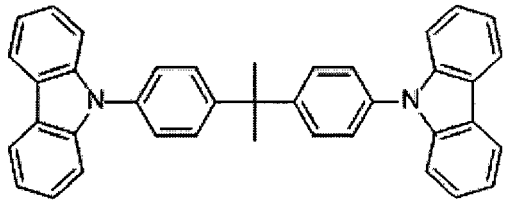
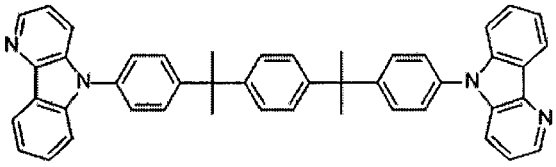
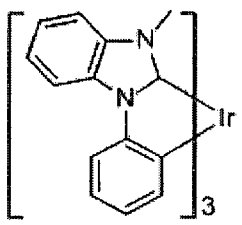
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon aryl compounds		US20050238919
		WO2009003898
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
Carbazole linked by nonconjugated groups		US20040115476
Aza-carbazoles		US20060121308
High triplet metal organometallic complex		US7154114

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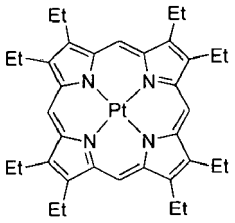
Phosphorescent dopants		
Red dopants		
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)

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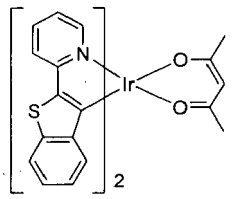
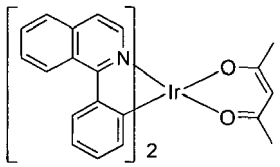
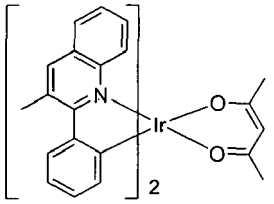
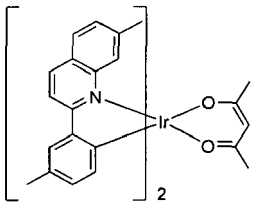
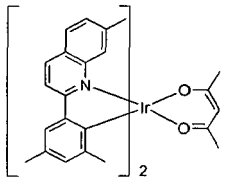
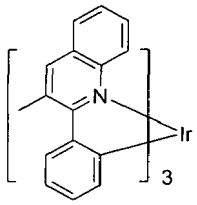
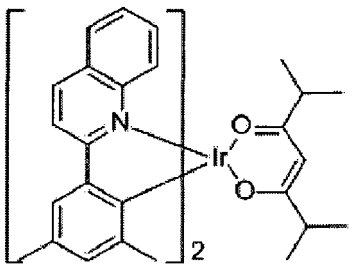
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US20030072964
		US20030072964
		US20060202194
		US20060202194
		US20070087321
		US20080261076 US20100090591

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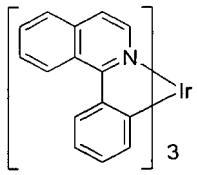
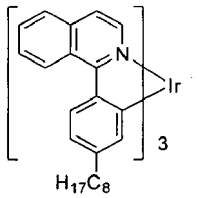
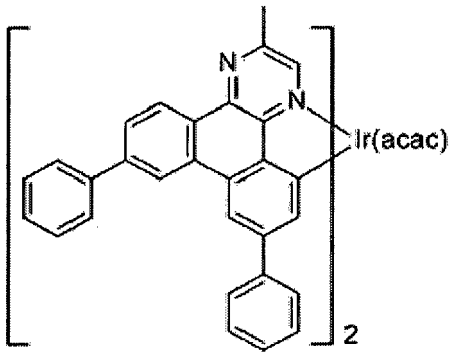
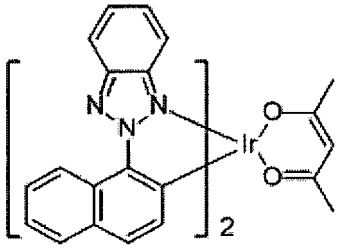
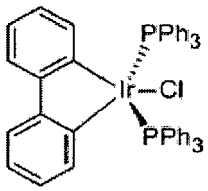
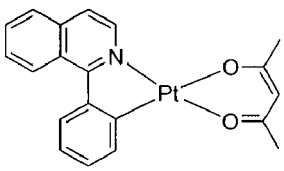
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
		US7232618
Platinum(II) organometallic complexes		WO2003040257

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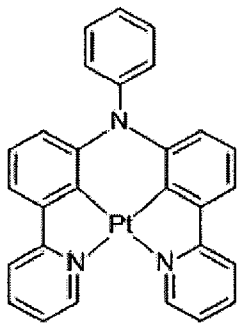
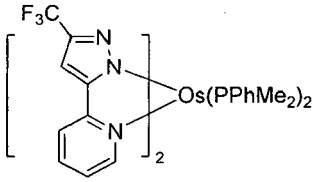
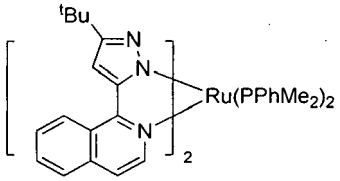
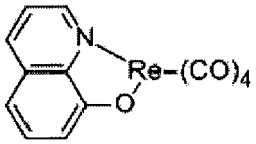
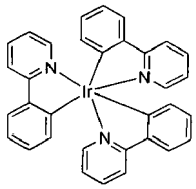
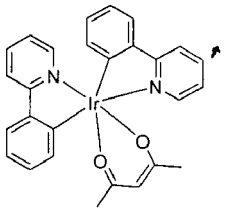
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070103060
Osmium(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
Green dopants		
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656

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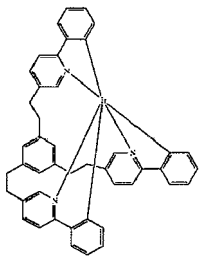
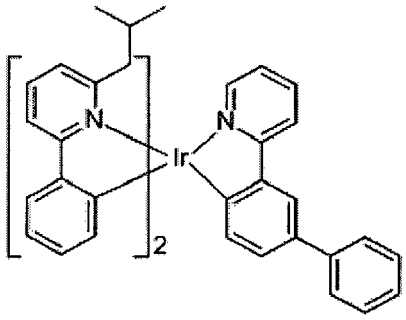
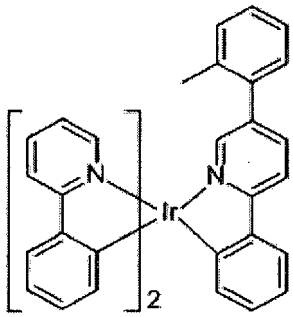
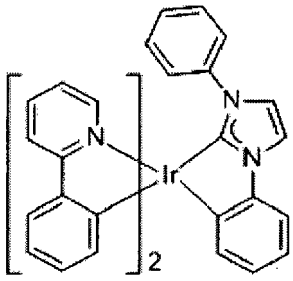
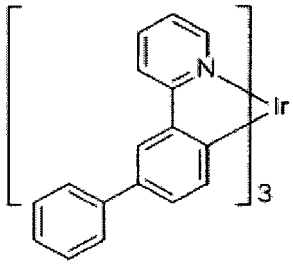
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7332232
		US20090108737
		WO2010028151
		EP1841834B
		US20060127696

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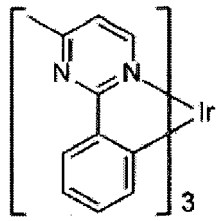
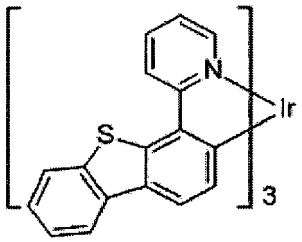
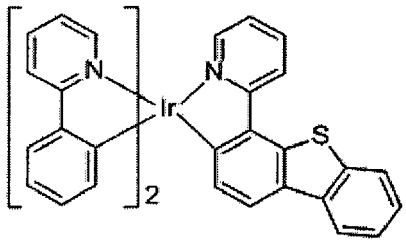
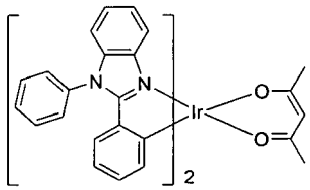
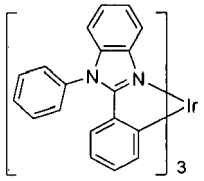
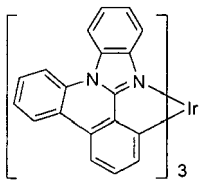
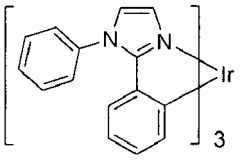
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090039776
		US6921915
		US20100244004
		US6687266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US 20060008670 JP2007123392

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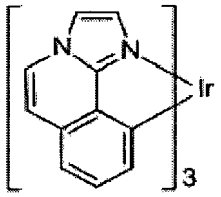
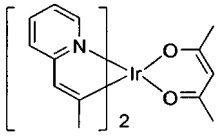
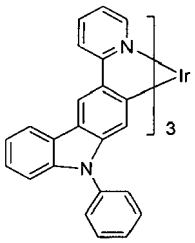
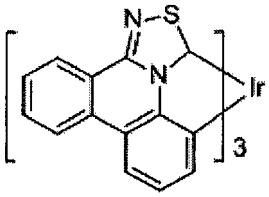
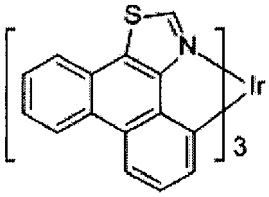
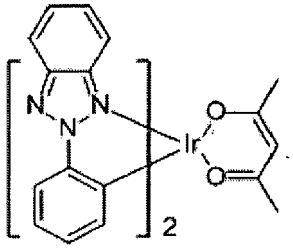
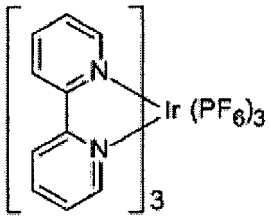
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006,45,7800
		WO2009050290
		US20090165846
		US20080015355
		US20010015432

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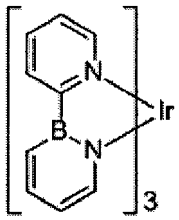
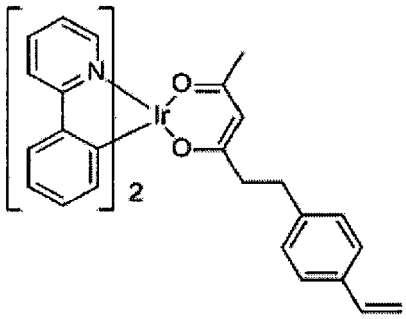
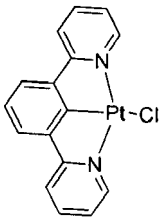
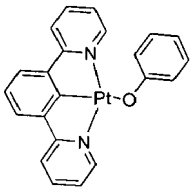
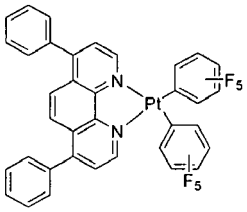
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20100295032
Monomer for polymeric metal organometallic compounds		US7250226, US7396598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)

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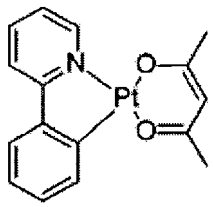
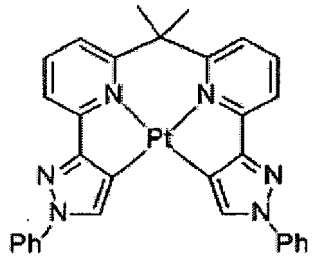
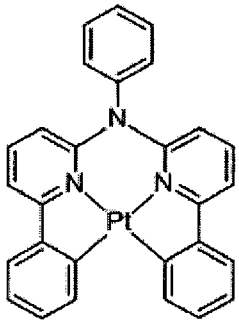
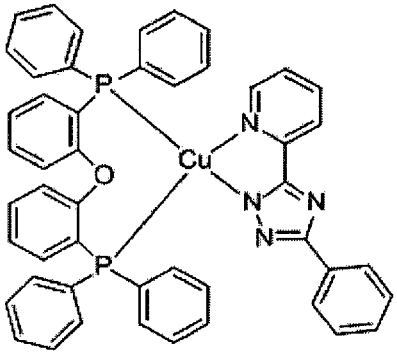
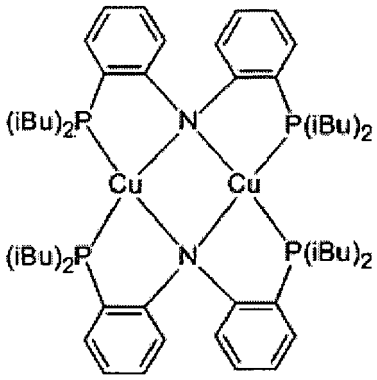
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2002015645
		US20060263635
		US20060182992 US20070103060
Cu complexes		WO2009000673
		US20070111026

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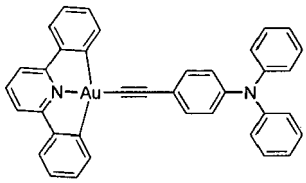
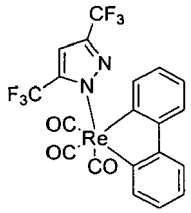
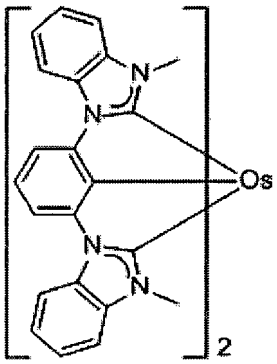
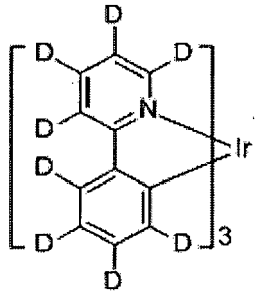
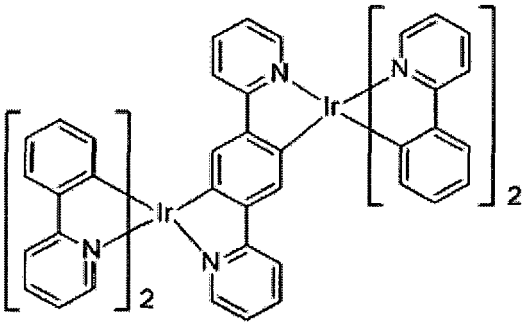
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)
Osmium(II) complexes		US7279704
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802

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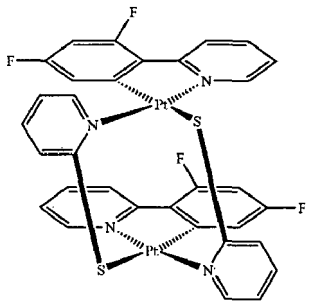
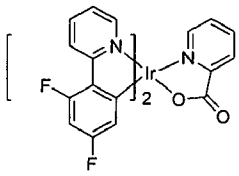
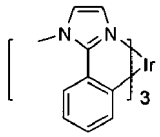
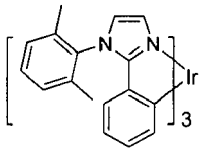
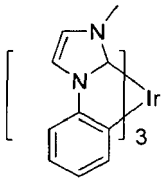
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7090928
Blue dopants		
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		US7393599, WO2006056418, US20050260441, WO2005019373

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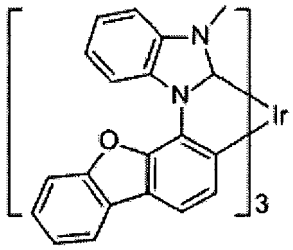
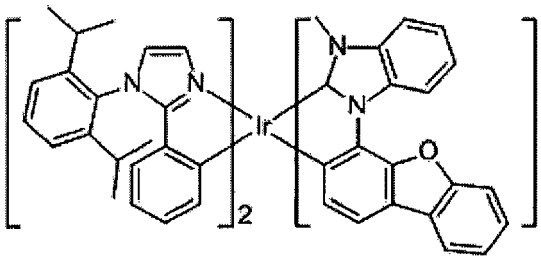
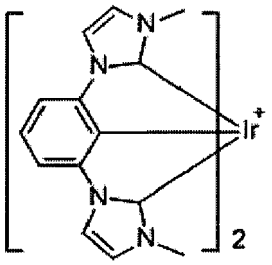
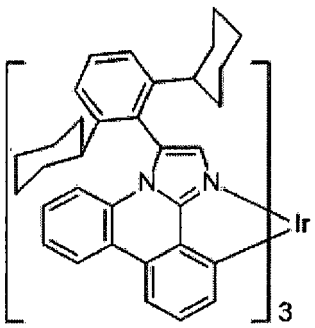
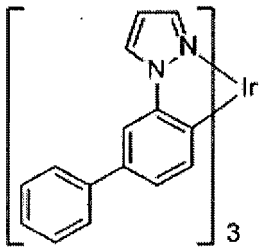
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7534505
		WO2011051404
		US7445855
		US20070190359, US20080297033 US20100148663
		US7338722

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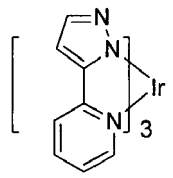
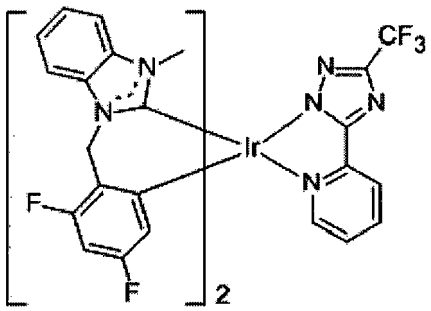
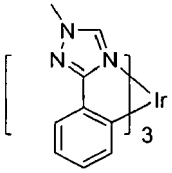
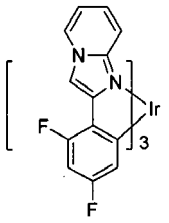
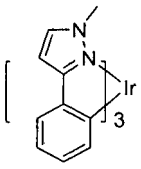
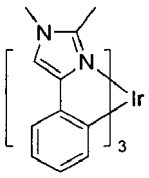
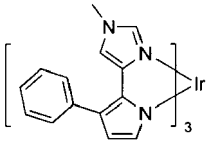
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20020134984
		Angew. Chem. Int. Ed. 47, 4542 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380

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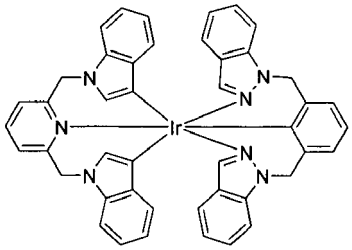
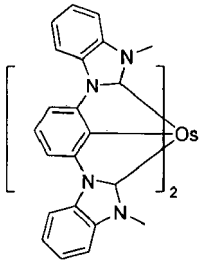
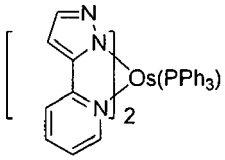
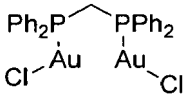
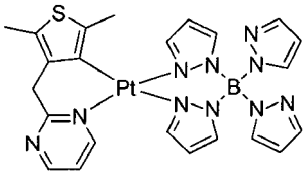
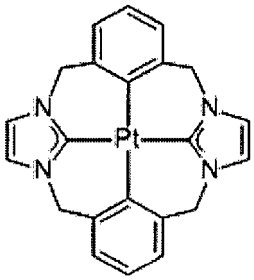
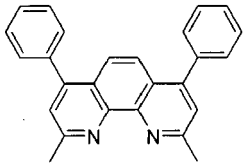
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006082742
Osmium(II) complexes		US7279704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett.74,1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874
Pt tetradentate complexes with at least one metal-carbene bond		US7655323
Exciton/hole blocking layer materials		
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)

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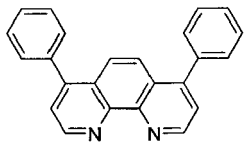
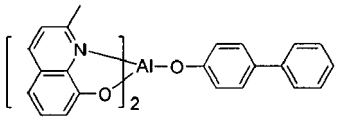
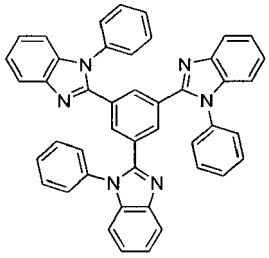
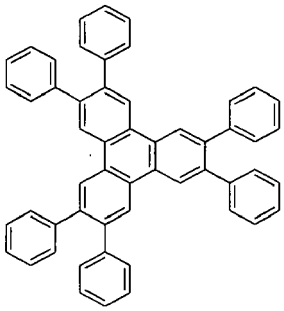
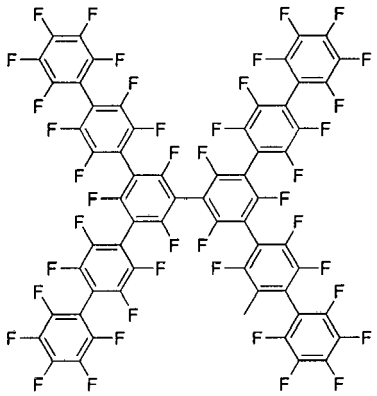
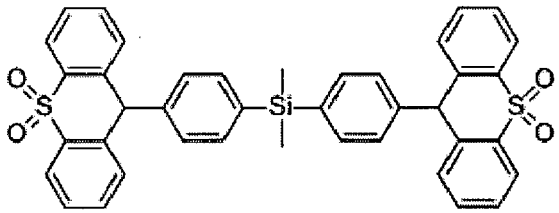
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085

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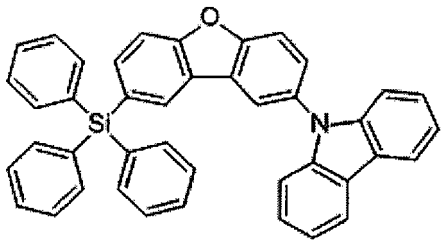
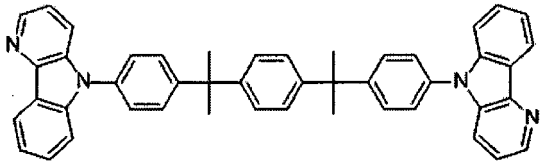
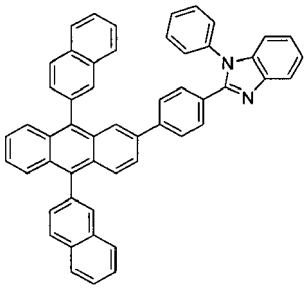
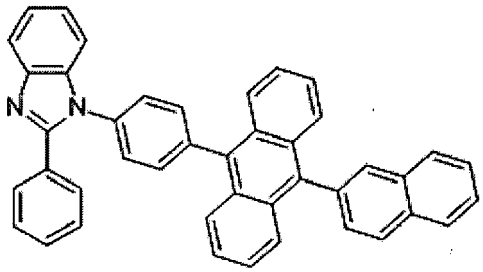
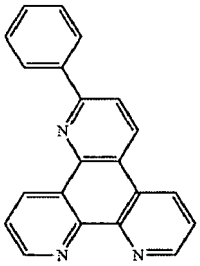
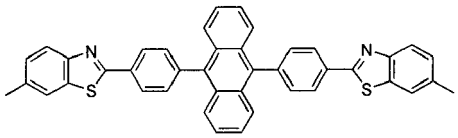
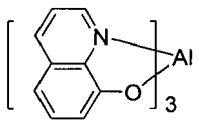
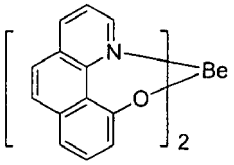
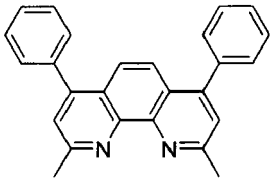
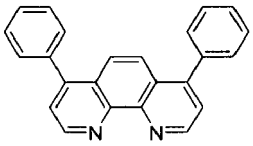
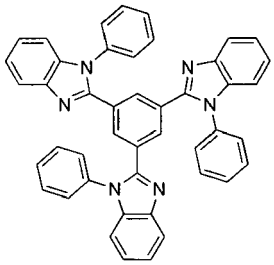
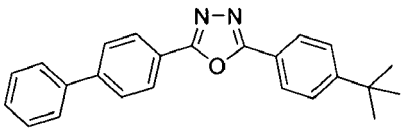
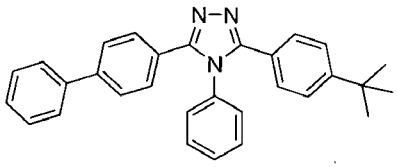
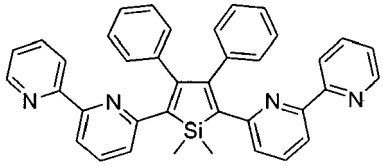
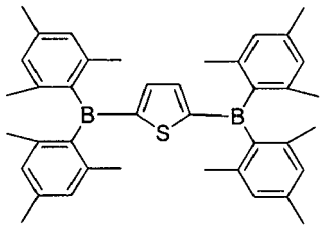
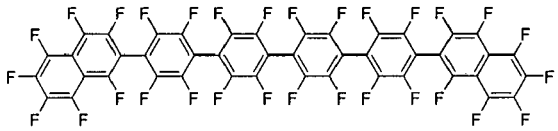
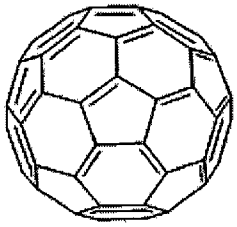
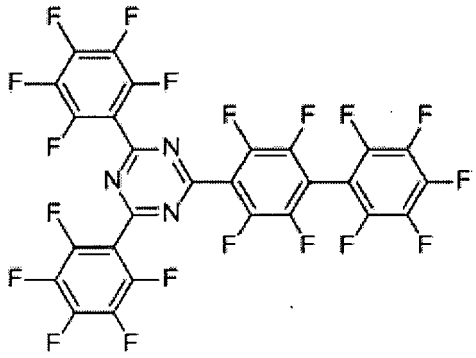
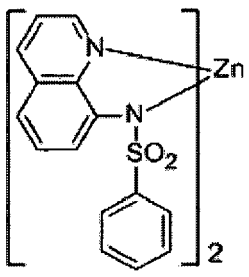
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051
Aza-carbazoles		US20060121308
Electron transporting materials		
Anthracenebenzoimidazole compounds		WO2003060956
		US20090179554
MATERIAL	**EXAMPLES OF MATERIAL**	**PUBLICATIONS**
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) US7230107
Metal hydroxybenzoquinolates		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)

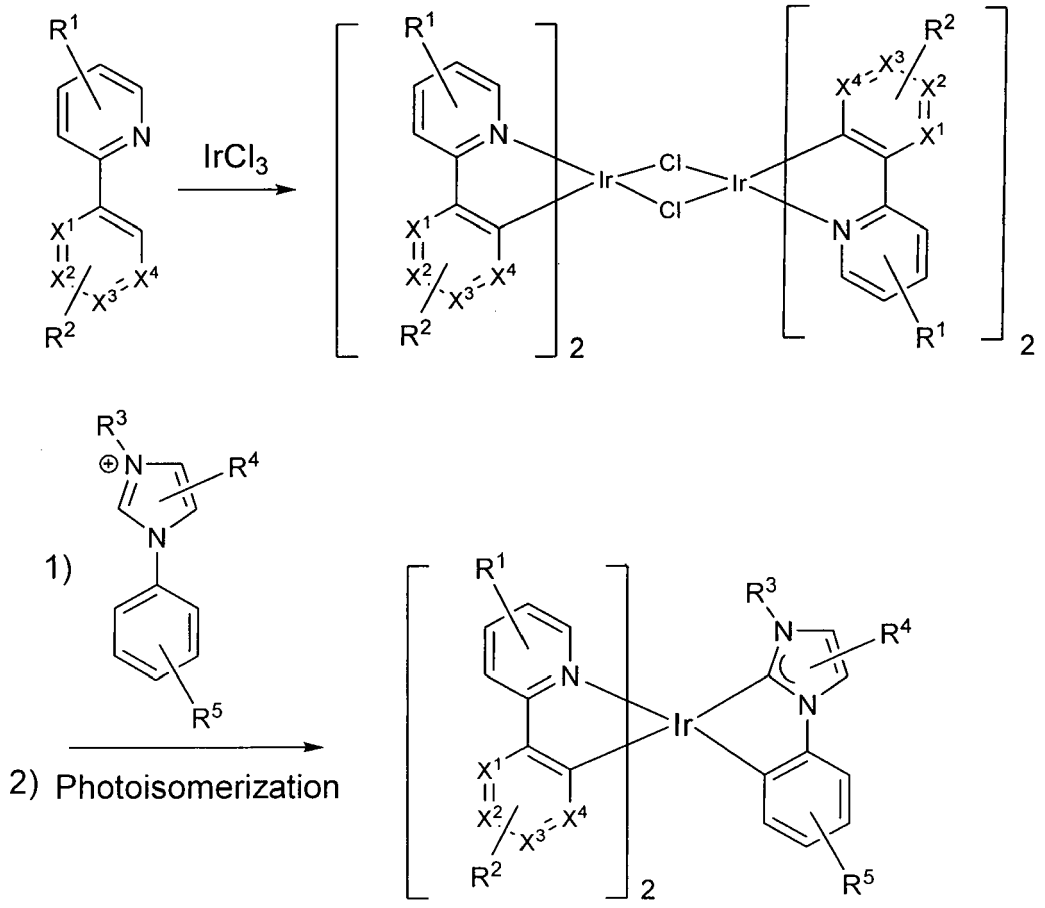
(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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

Example 1 - Compound Synthesis

[0086] The compounds of formula I can be made by any suitable method. In some embodiments, such compounds can be made in a manner consistent with the reaction scheme shown on the following:

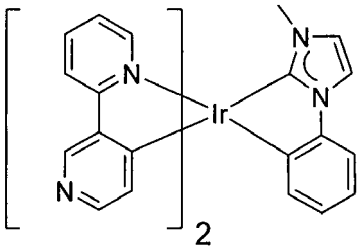


[0087] Such methods may be modified as applied to the synthesis of any particular compound, based on the knowledge of persons of skill in the art.

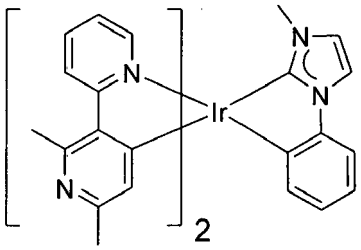
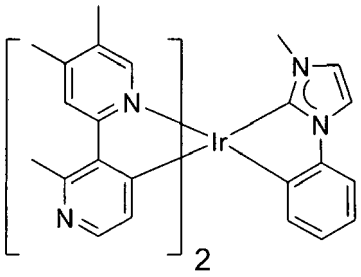
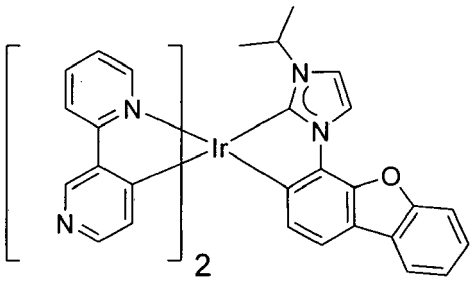
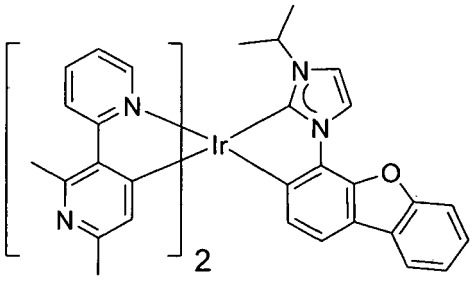
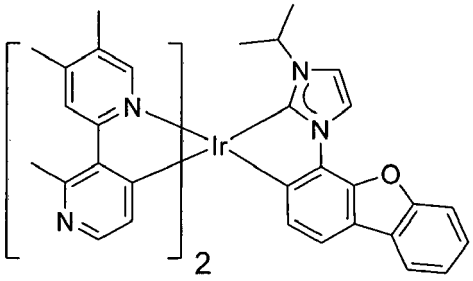
Example 2 - Computational Examples

[0088] Density Functional Theory (DFT) calculations were performed for certain example compounds and comparative compounds. The results are shown in Table 1, below. Geometry optimization calculations were performed using the Gaussian 09 software package using the B3LYP hybrid functional and CEP-31g effective core potential basis set.

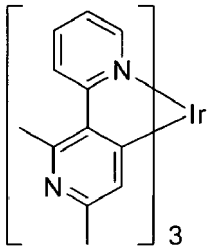
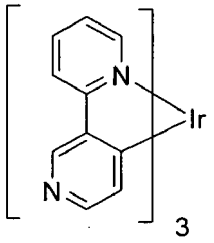
Table 1 Calculation results of selected compounds of formula I and comparative compounds

Compound	HOMO (eV)	LUMO (eV)	Gap (eV)	S1 (nm)	T1 (nm)
 Compound 1	-5.43	-1.75	3.67	419	469

(continued)

Compound	HOMO (eV)	LUMO (eV)	Gap (eV)	S1 (nm)	T1 (nm)
 Compound 4	-5.33	-1.62	3.72	415	470
 Compound 14	-5.29	-1.51	3.78	407	467
 Compound 441	-5.38	-1.78	3.61	422	468
 Compound 444	-5.31	-1.64	3.66	417	469
 Compound 454	-5.27	-1.54	3.73	407	465

(continued)

Compound	HOMO (eV)	LUMO (eV)	Gap (eV)	S1 (nm)	T1 (nm)
 Comparative Compound 1	-5.61	-1.74	3.88	399	464
 Comparative Compound 2	-5.81	-1.89	3.91	395	462

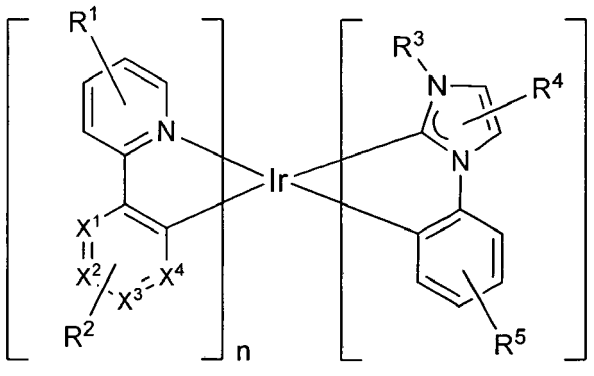
[0089] The selected compounds of formula I were compared against Comparative Compounds 1 and 2. A carbene ligand is present in the compounds of formula I. From the calculation results, the compounds of formual I have slightly red-shifted color compared to the comparative compounds. However, the calculated emission maximum of the compounds of formula I remains blue.

[0090] Another noticeable difference is the HOMO of the compounds of formula I. The comparative compounds have a HOMO level deeper than -5.60 eV, while the HOMO level of the compounds of Formula I is significantly shallower. The deep HOMO of the comparative compounds makes them inefficient hole traps. As a result, devices using the comparative compounds as emitters usually need highly confined structures, which can reduce the device stability. The shallow HOMO energy level of the inventive compounds makes them efficient hole traps in devices. It will in turn enable stable devices.

[0091] 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 include 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.

[0092] Preferred embodiments of the invention are as follows:

1. A compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



, Formula I;

wherein R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;

wherein R^2 represents up to tri-substitution, or no substitution;

wherein R^4 represents mono, or di-substitution, or no substitution;

wherein X^1, X^2, X^3, and X^4 are each independently C or N;

wherein at least one of X^1, X^2, X^3, and X^4 is N;

wherein any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;

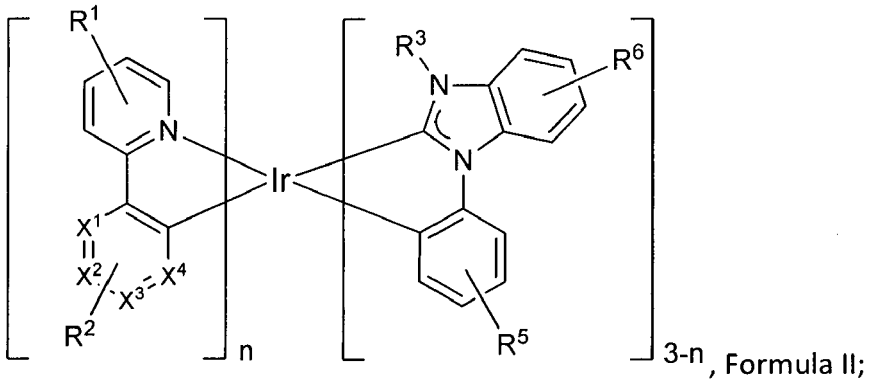
wherein each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein n is either 1 or 2.

2. The compound of paragraph 1, wherein n is 1.

3. The compound of paragraph 1, wherein n is 2.

4. The compound of any one of paragraphs 1 to 3, wherein the compound has the formula:



, Formula II;

wherein R^6 represents mono, di, tri, or tetra-substitution, or no substitution;

wherein any adjacent substitutions of R^6 are optionally linked together to form a ring; and

wherein each R^6 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

5. The compound of paragraph 4, wherein only one of X^1, X^2, X^3, and X^4 is N.

6. The compound of paragraph 5, wherein X^2 is N.

7. The compound of any one of paragraphs 1 to 6, wherein R^1 is selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, and combinations thereof.

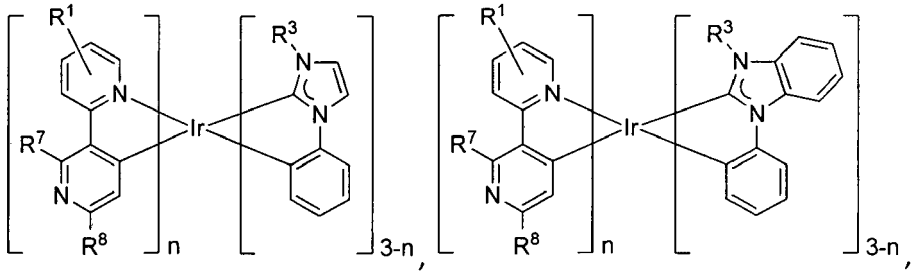
8. The compound of any one of paragraphs 1 to 7, wherein R^2 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, nitrile, and combinations thereof.

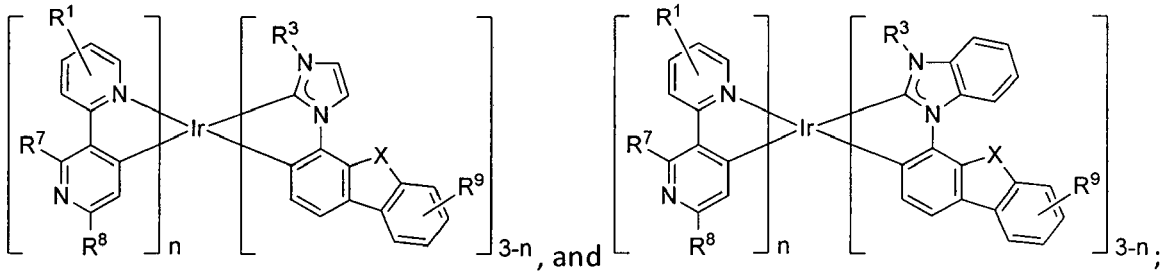
9. The compound of any one of paragraphs 1 to 8, wherein R^3 is alkyl or cycloalkyl.

10. The compound of any one of paragraphs 1 to 8, wherein R^3 is aryl or substituted aryl.

11. The compound of any one of paragraphs 1 to 8, wherein R^3 is selected from the group consisting of: ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, cyclopentyl, and cyclohexyl, wherein each group is optionally partially or fully deuterated.

12. The compound of paragraph 1, wherein the compound is selected from the group consisting of:



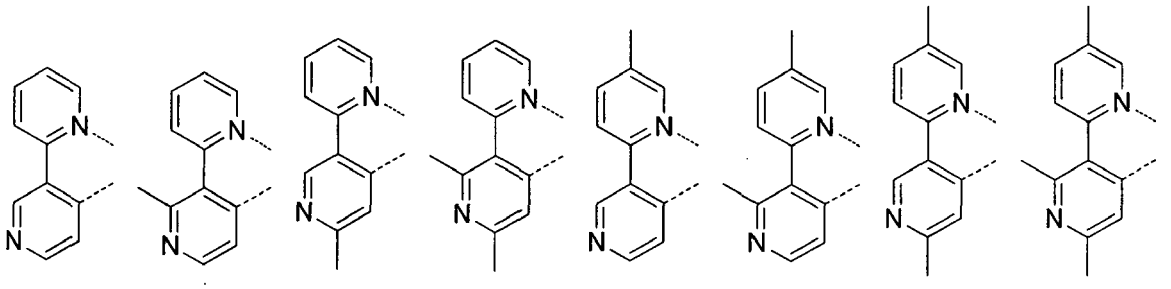


wherein R^9 represents mono, di, tri, or tetra-substitution, or no substitution;

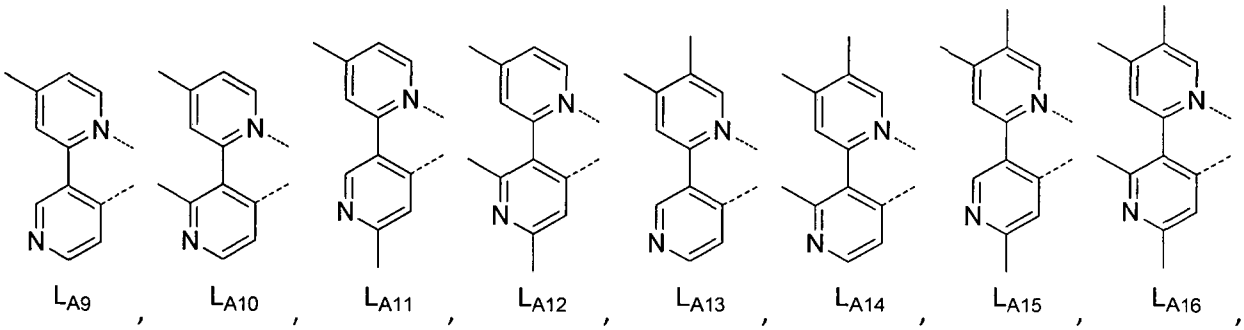
wherein each R^7, R^8, and R^9 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein X is O or S.

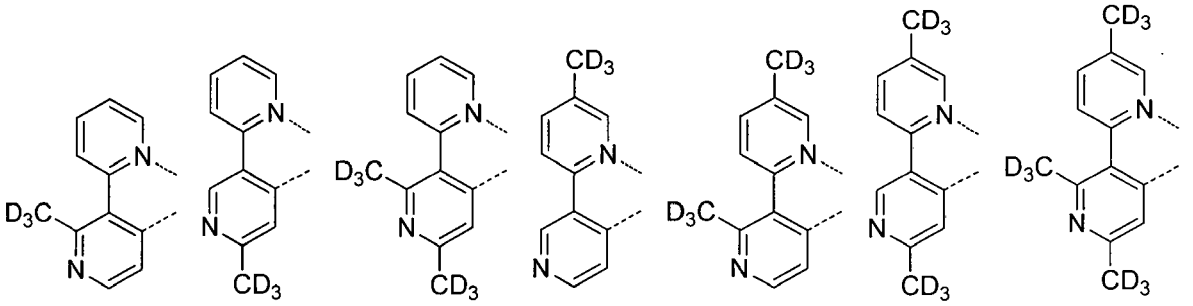
13. The compound of any one of paragraphs 1 to 4 and 9 to 11, wherein L_A is selected from the group consisting of:



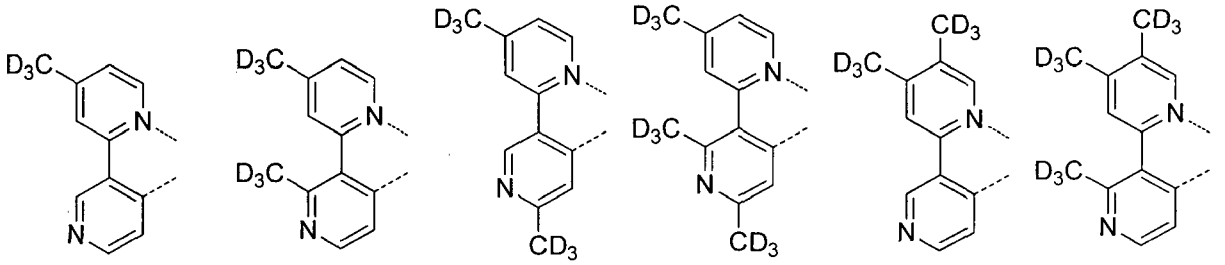
L_{A1}, L_{A2}, L_{A3}, L_{A4}, L_{A5}, L_{A6}, L_{A7}, L_{A8},



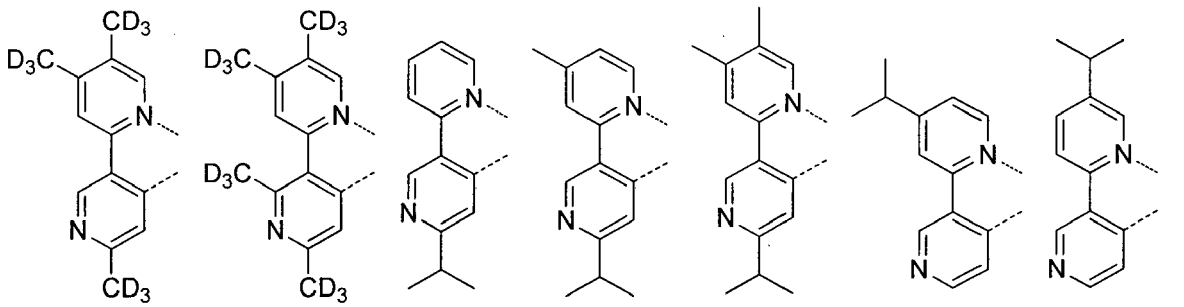
L_{A9}, L_{A10}, L_{A11}, L_{A12}, L_{A13}, L_{A14}, L_{A15}, L_{A16},



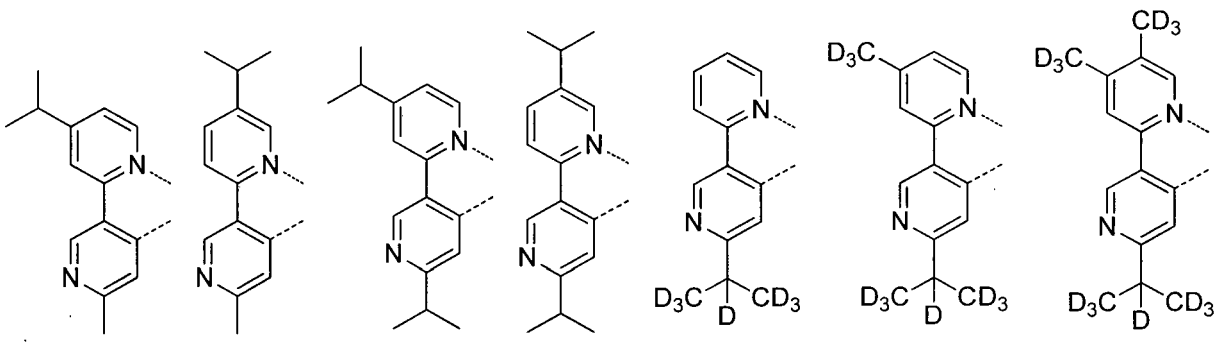
L_{A17}, L_{A18}, L_{A19}, L_{A20}, L_{A21}, L_{A22}, L_{A23},



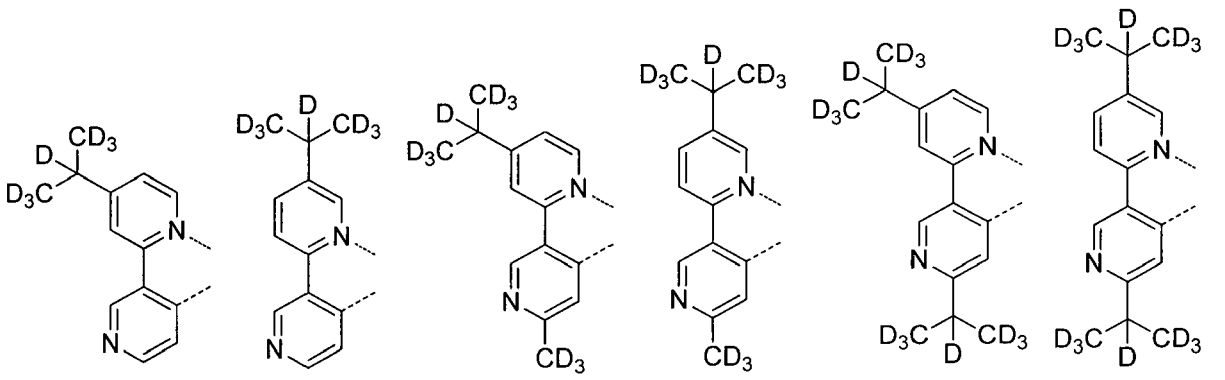
L_{A24}, L_{A25}, L_{A26}, L_{A27}, L_{A28}, L_{A29},



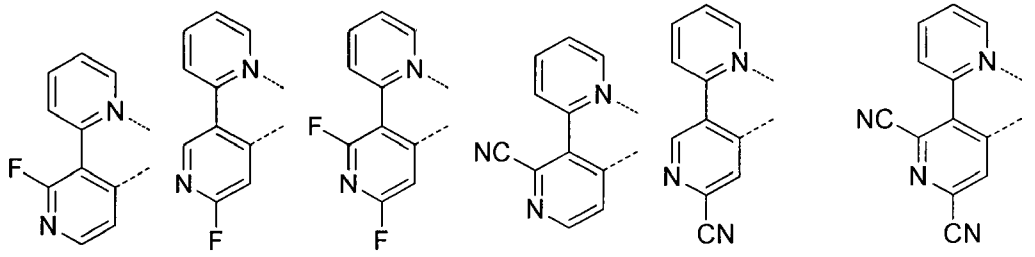
L_{A30}, L_{A31}, L_{A32}, L_{A33}, L_{A34}, L_{A35}, L_{A36},



L_{A37}, L_{A38}, L_{A39}, L_{A40}, L_{A41}, L_{A42}, L_{A43},

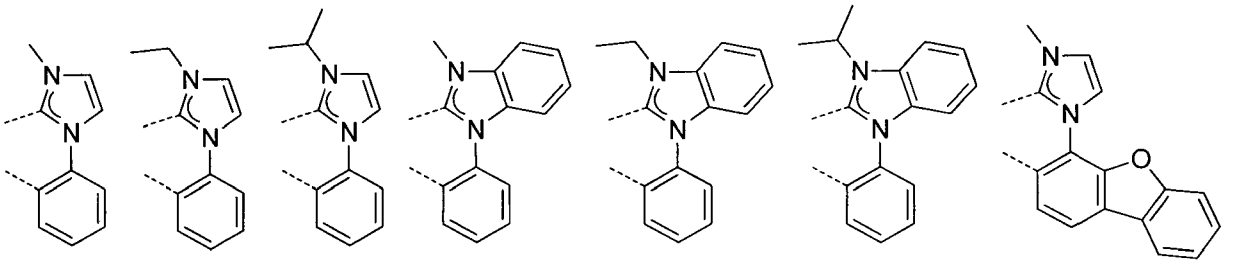


L_{A44}, L_{A45}, L_{A46}, L_{A47}, L_{A48}, L_{A49},

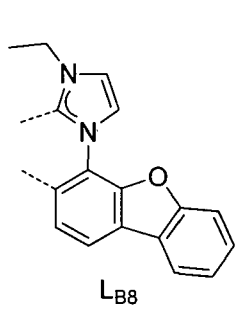


L_{A50}, L_{A51}, L_{A52}, L_{A53}, L_{A54}, and L_{A55}.

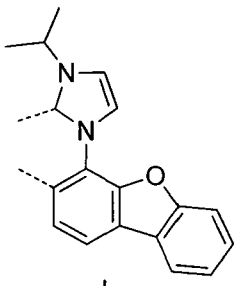
14. The compound of any one of paragraphs 1 to 8, wherein L_B is selected from the group consisting of:



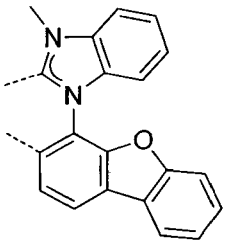
L_{B1}, L_{B2}, L_{B3}, L_{B4}, L_{B5}, L_{B6}, L_{B7},



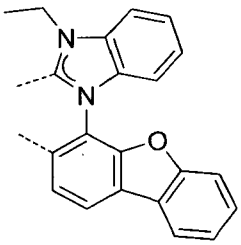
L_{B8} ,



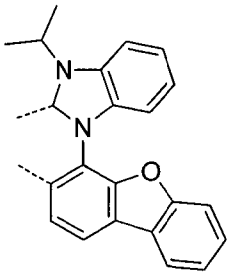
L_{B9} ,



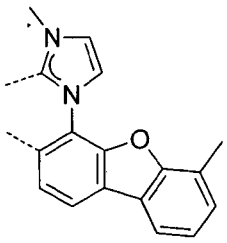
L_{B10} ,



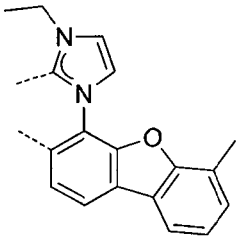
L_{B11} ,



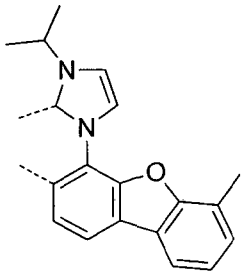
L_{B12} ,



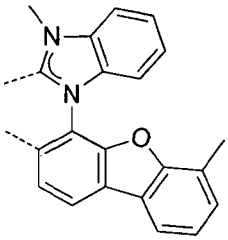
L_{B13} ,



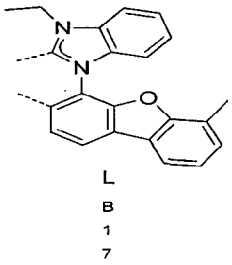
L_{B14} ,



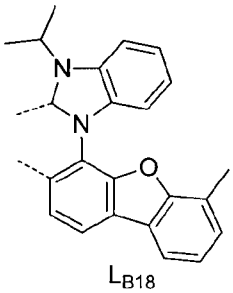
L_{B15} ,



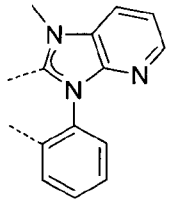
L_{B16} ,



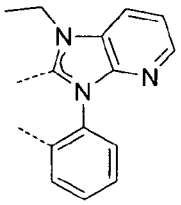
L_{B17} ,



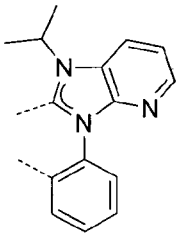
L_{B18} ,



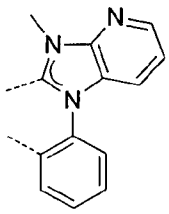
L_{B19} ,



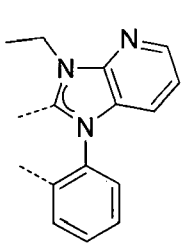
L_{B20} ,



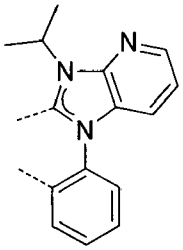
L_{B21} ,



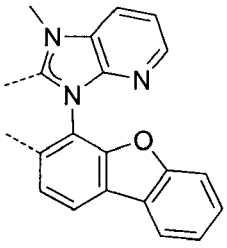
L_{B22} ,



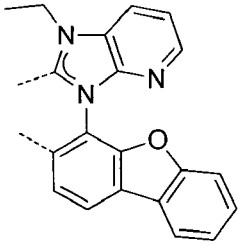
L_{B23} ,



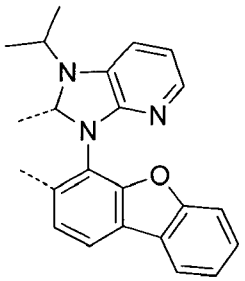
L_{B24} ,



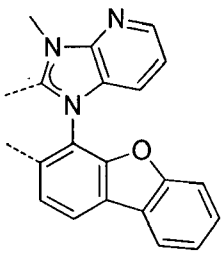
L_{B25} ,



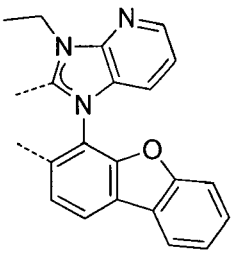
L_{B26} ,



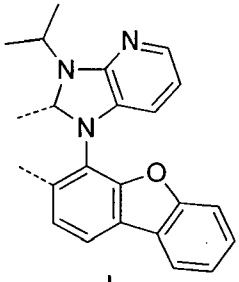
L_{B27} ,



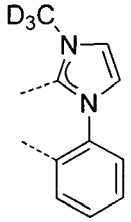
L_{B28} ,



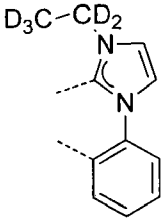
L_{B28} ,



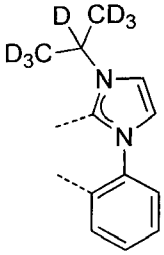
L_{B30} ,



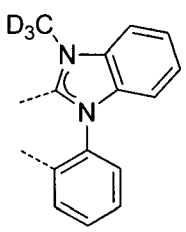
L_{B31} ,



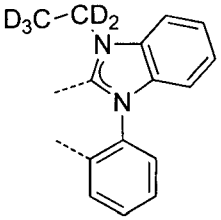
L_{B32} ,



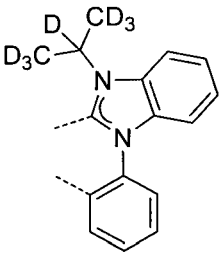
L_{B33} ,



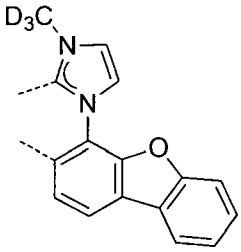
L_{B34} ,



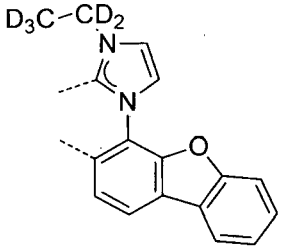
L_{B35} ,



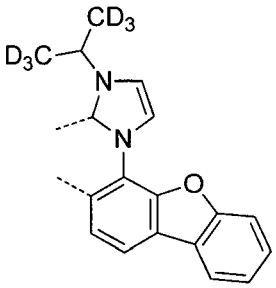
L_{B36} ,



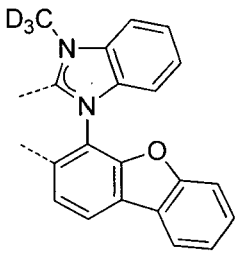
L_{B37} ,



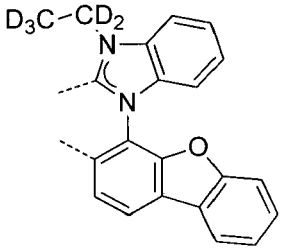
L_{B38} ,



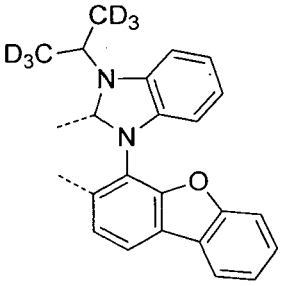
L_{B39} ,



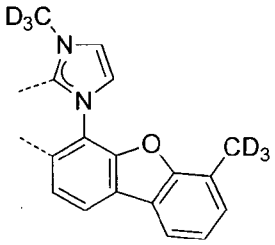
L_{B40} ,



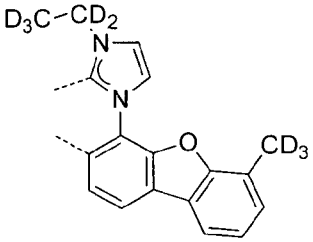
L_{B41} ,



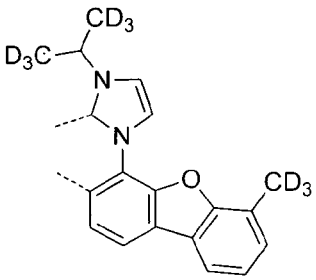
L_{B42} ,



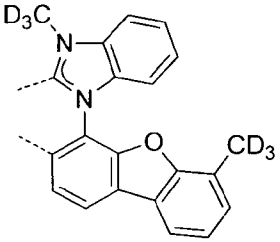
L_{B43} ,



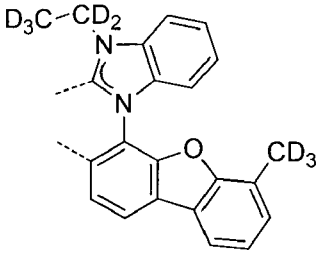
L_{B44} ,



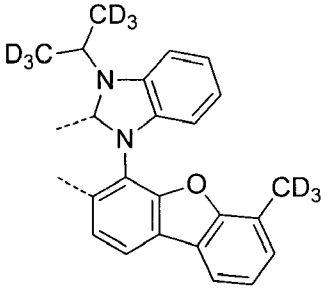
L_{B45} ,



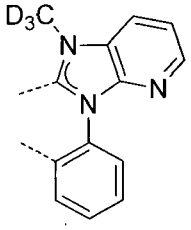
L_{B46} ,



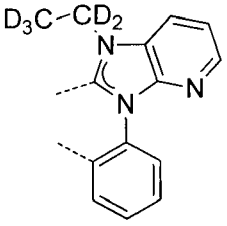
L_{B47} ,



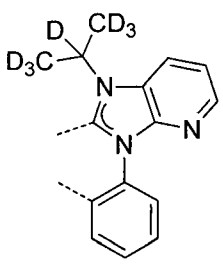
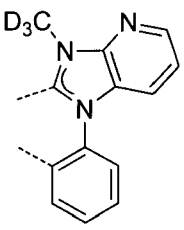
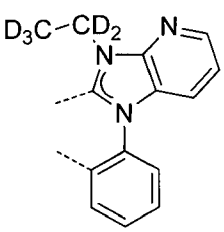
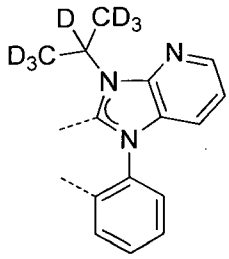
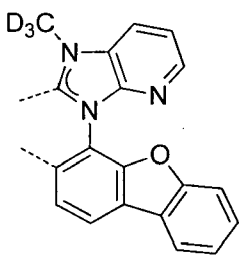
L_{B48} ,

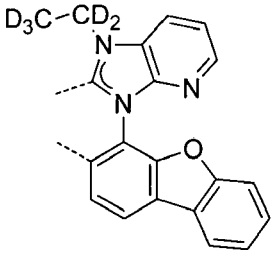
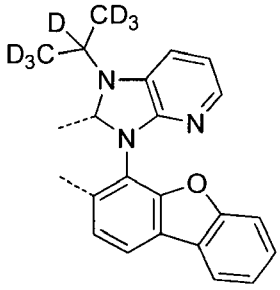
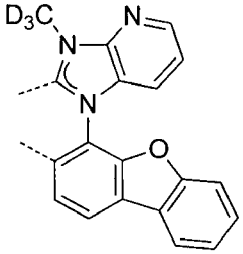
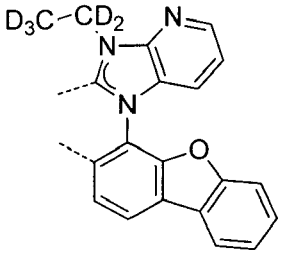


L_{B49} ,

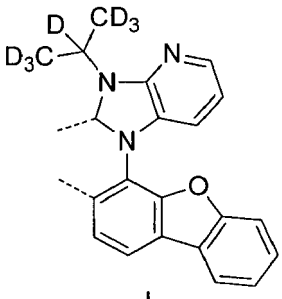


L_{B50} ,

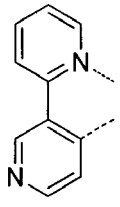
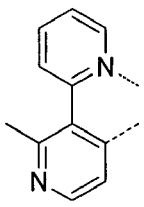
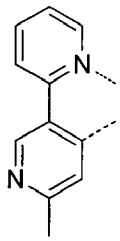
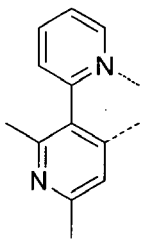
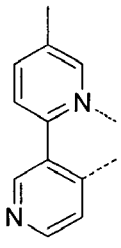
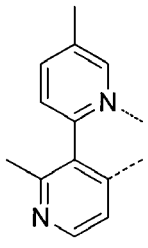
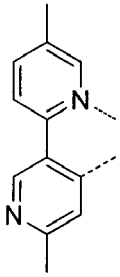
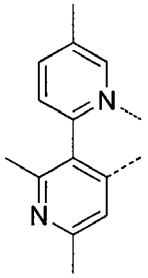

L_{B51} ,

L_{B52} ,

L_{B53} ,

L_{B54} ,

L_{B55} ,

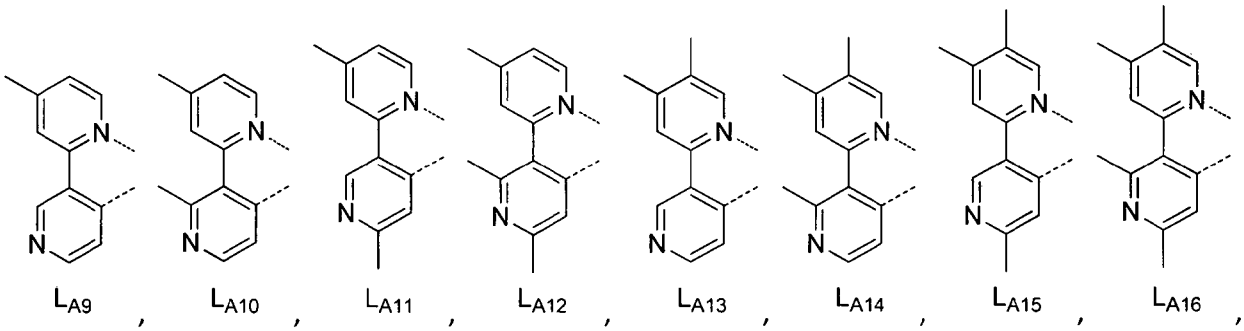

L_{B56} ,

L_{B57} ,

L_{B58} ,

L_{B59} ,

and

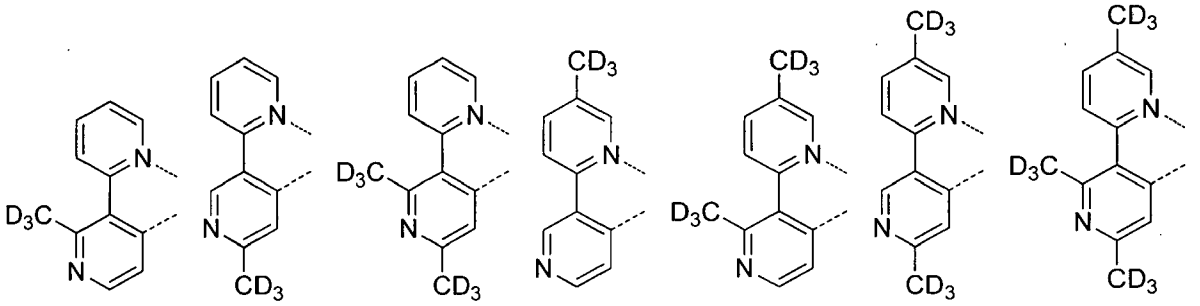

L_{B60} .

15. The compound of paragraph 14, wherein L_A is selected from the group consisting of:

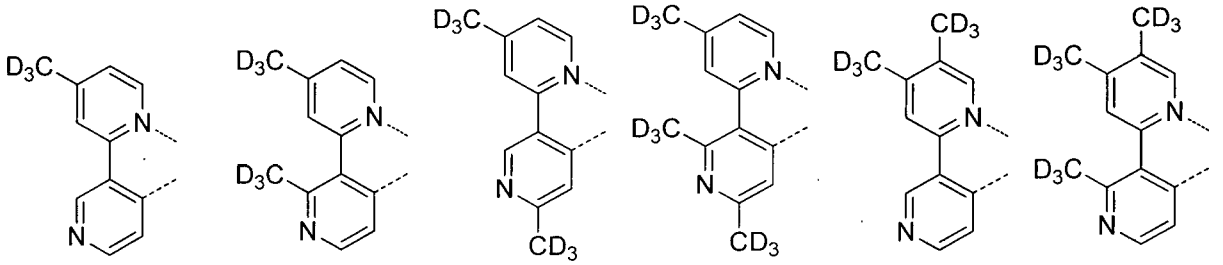

L_{A1} ,

L_{A2} ,

L_{A3} ,

L_{A4} ,

L_{A5} ,

L_{A6} ,

L_{A7} ,

L_{A8} ,



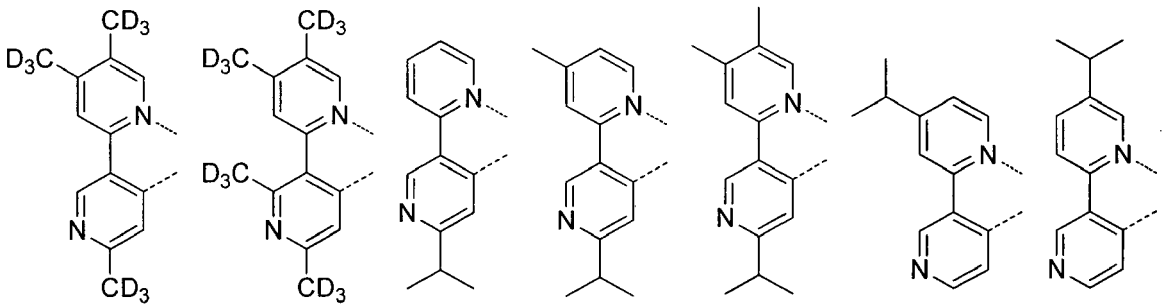
L_{A9}, L_{A10}, L_{A11}, L_{A12}, L_{A13}, L_{A14}, L_{A15}, L_{A16},



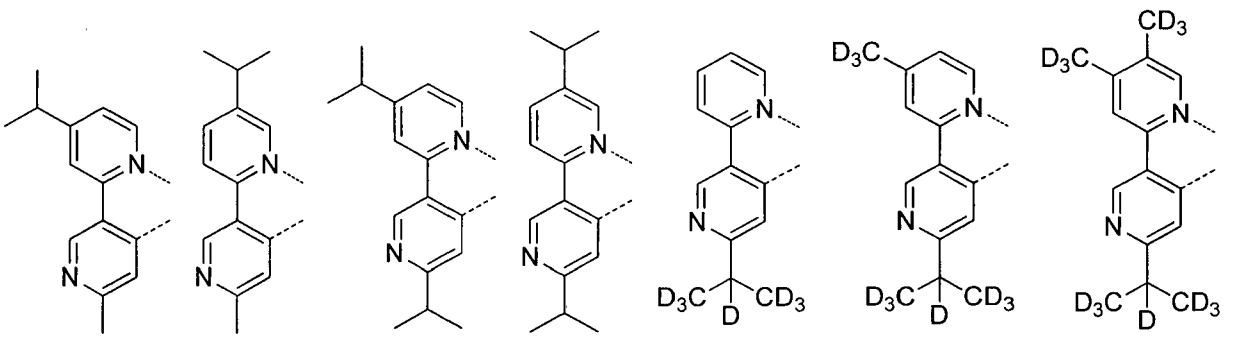
L_{A17}, L_{A18}, L_{A19}, L_{A20}, L_{A21}, L_{A22}, L_{A23},



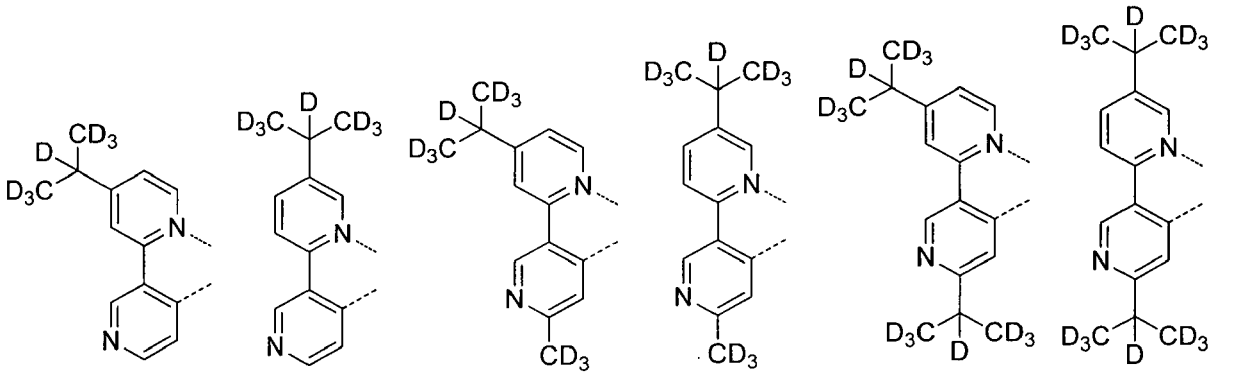
L_{A24}, L_{A25}, L_{A26}, L_{A27}, L_{A28}, L_{A29},



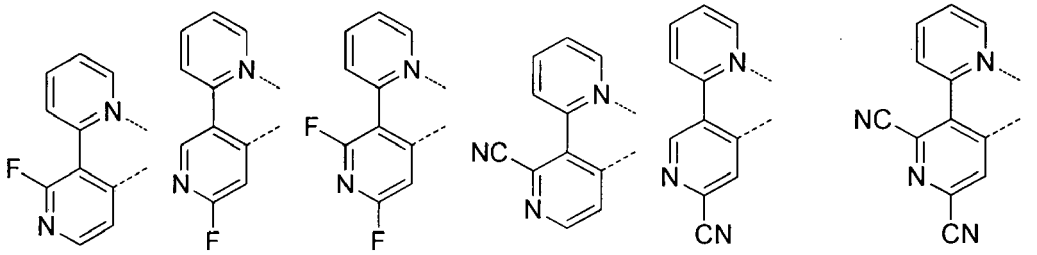
L_{A30}, L_{A31}, L_{A32}, L_{A33}, L_{A34}, L_{A35}, L_{A36},



L_{A37} , L_{A38} , L_{A39} , L_{A40} , L_{A41} , L_{A42} , L_{A43} ,



L_{A44} , L_{A45} , L_{A46} , L_{A47} , L_{A48} , L_{A49} ,



L_{A50} , L_{A51} , L_{A52} , L_{A53} , L_{A54} , and L_{A55} ;

wherein n is 2; and

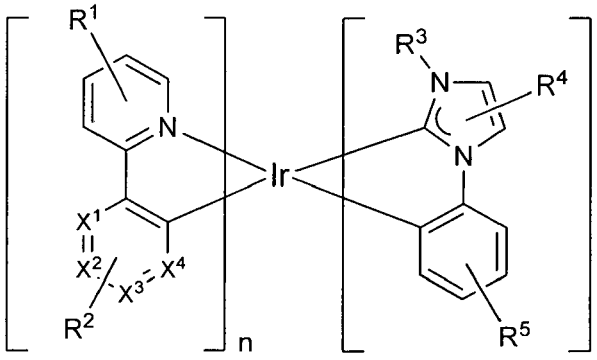
wherein the compound is selected from the group consisting of compound 1 to compound 3300, wherein each Compound x has the formula $Ir(L_{Ak})_2(L_{Bj})$, wherein x = 55*j* + *k* - 55, wherein *k* is an integer from 1 to 55, and *j* is an integer from 1 to 60.

16. A first device comprising a first organic light emitting device, the first organic light emitting device comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



, Formula I;

wherein R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;

wherein R^2 represents up to tri-substitution, or no substitution;

wherein R^4 represents mono, or di-substitution, or no substitution;

wherein X^1, X^2, X^3, and X^4 are each independently C or N;

wherein at least one of X^1, X^2, X^3, and X^4 is N;

wherein any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;

wherein each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, cyano, and combinations thereof; and

wherein n is either 1 or 2.

17. The first device of paragraph 16, wherein the first device is selected from the group consisting of a consumer product, an electronic component module, an organic light-emitting device, and a lighting panel.

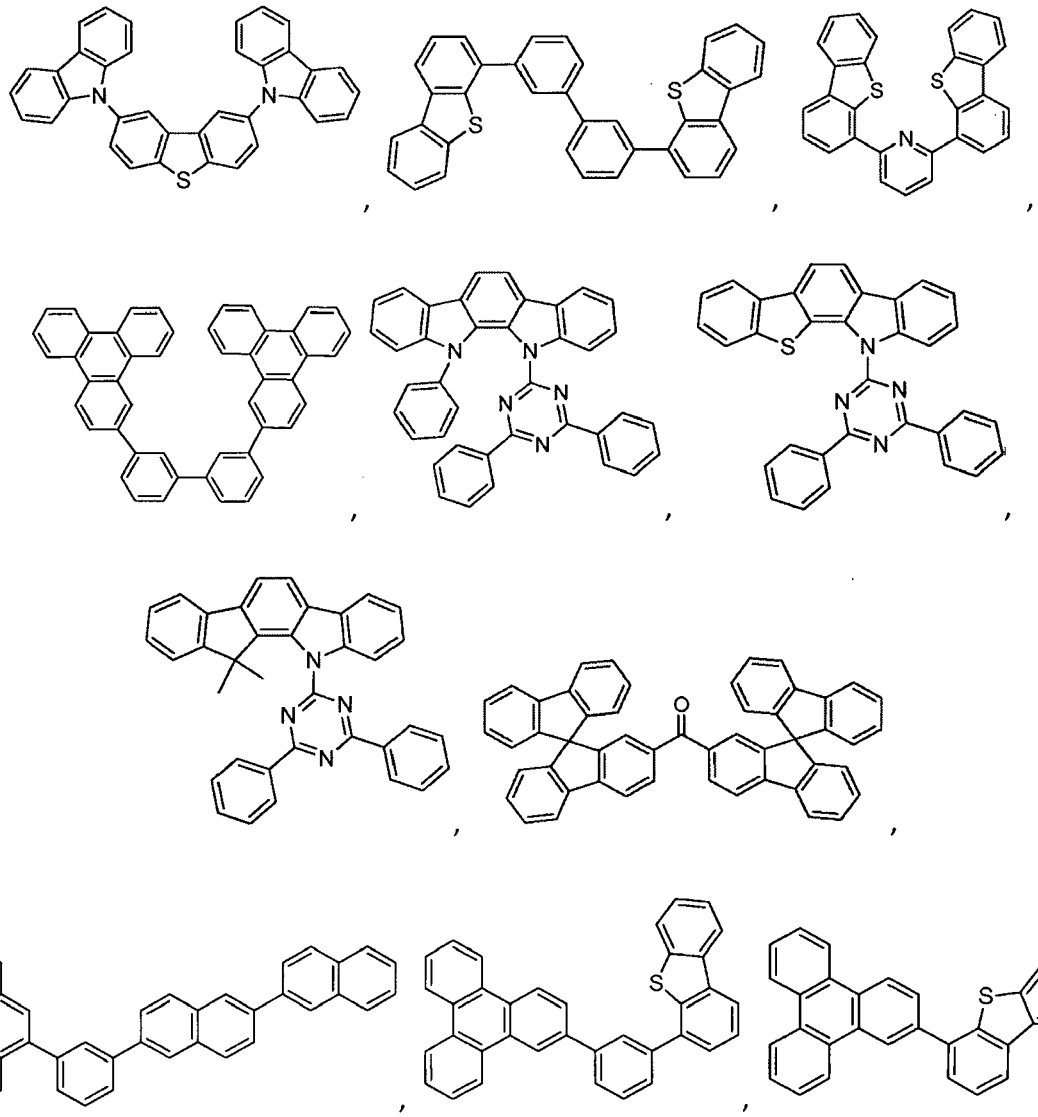
18. The first device of paragraph 16 or 17, wherein the organic layer is an emissive layer and the compound is an emissive dopant or a non-emissive dopant.

19. The first device of any one of paragraphs 16 to 18, wherein the organic layer further comprises a host, wherein the host comprises a triphenylene containing benzo-fused thiophene or benzo-fused furan;

wherein any substituent in the host is an unfused substituent independently selected from the group consisting of C_nH_{2n+1}, OC_nH_{2n+1}, OAr_1, $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH=CH-C_nH_{2n+1}$, $C\equiv CC_nH_{2n+1}$, Ar_1, Ar_1-Ar_2, C_nH_{2n}-Ar_1, or no substitution;
wherein n is from 1 to 10; and
wherein Ar_1 and Ar_2 are independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.

20. The first device of any one of paragraphs 16 to 19, wherein the organic layer further comprises a host, wherein the host comprises at least one chemical group selected from the group consisting of triphenylene, carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azatriphenylene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene.

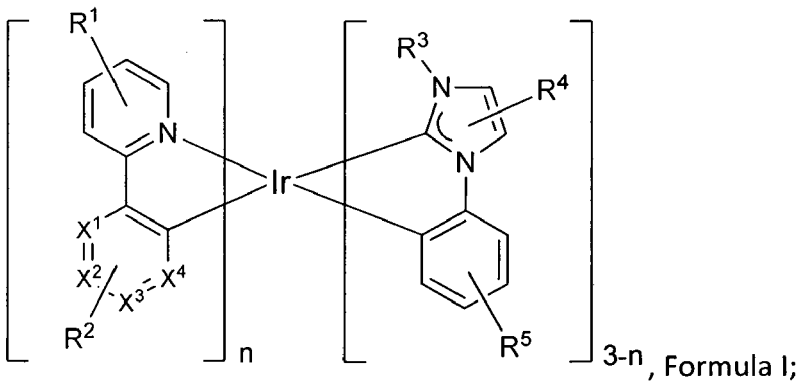
21. The first device of any one of paragraphs 16 to 20, wherein the organic layer further comprises a host and the host is selected from the group consisting of :



and combinations thereof.

22. The first device of any one of paragraphs 16 to 21, wherein the organic layer further comprises a host and the host comprises a metal complex.

23. A formulation comprising a compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



, Formula I;

wherein R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;

wherein R^2 represents up to tri-substitution, or no substitution;

wherein R^4 represents mono, or di-substitution, or no substitution;

wherein X^1, X^2, X^3, and X^4 are each independently C or N;

wherein at least one of X^1, X^2, X^3, and X^4 is N;

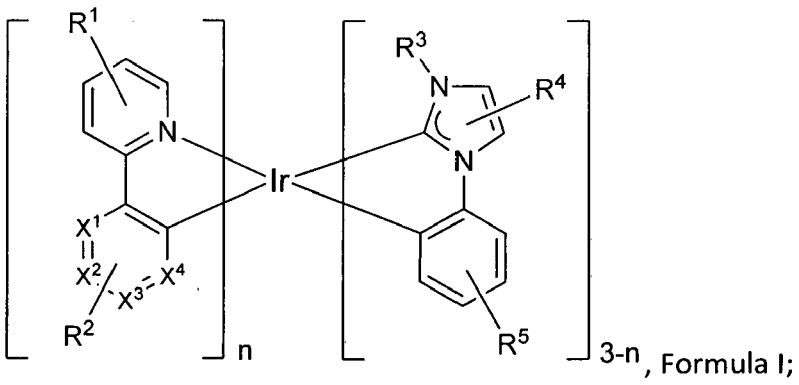
wherein any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;

wherein each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, cyano, and combinations thereof; and

wherein n is either 1 or 2.

Claims

1. A compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



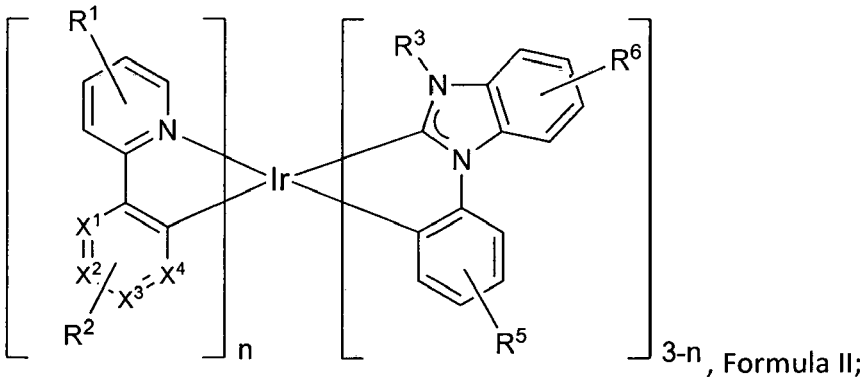
, Formula I;

wherein R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;
wherein R^2 represents up to tri-substitution, or no substitution;
wherein R^4 represents mono, or di-substitution, or no substitution;
wherein X^1, X^2, X^3, and X^4 are each independently C or N;
wherein at least one of X^1, X^2, X^3, and X^4 is N;
wherein any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;
wherein each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and
wherein n is either 1 or 2.

2. The compound of claim 1, wherein n is 1.

3. The compound of claim 1, wherein n is 2.

4. The compound of any one of claims 1 to 3, wherein the compound has the formula:



, Formula II;

wherein R^6 represents mono, di, tri, or tetra-substitution, or no substitution;
wherein any adjacent substitutions of R^6 are optionally linked together to form a ring; and
wherein each R^6 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

5. The compound of claim 4, wherein only one of X^1, X^2, X^3, and X^4 is N.

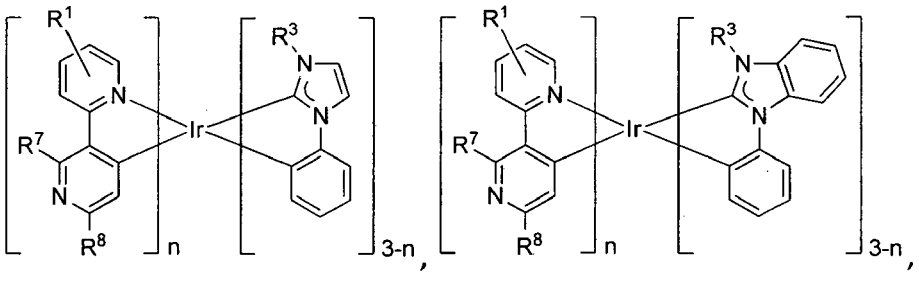
6. The compound of any one of claims 1 to 5, wherein R^1 is selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, and combinations thereof.

7. The compound of any one of claims 1 to 6, wherein R^2 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, nitrile, and combinations thereof.

8. The compound of any one of claims 1 to 7, wherein R^3 is alkyl or cycloalkyl.

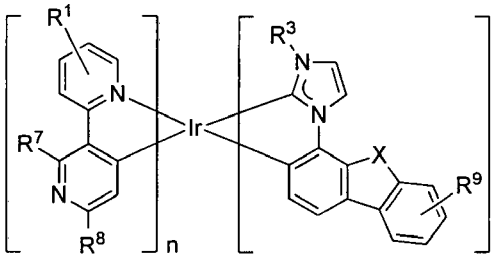
9. The compound of any one of claims 1 to 7, wherein R^3 is aryl or substituted aryl.

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

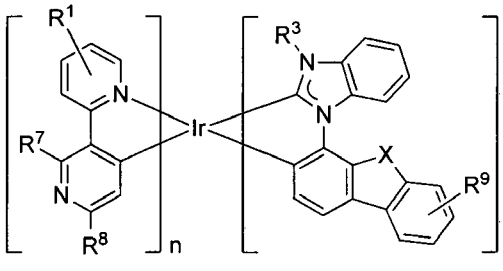


,

,



, and



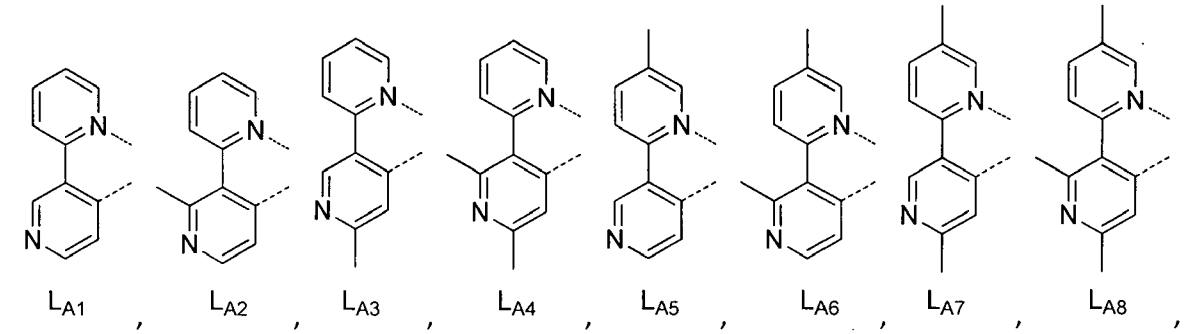
;

wherein R^9 represents mono, di, tri, or tetra-substitution, or no substitution;

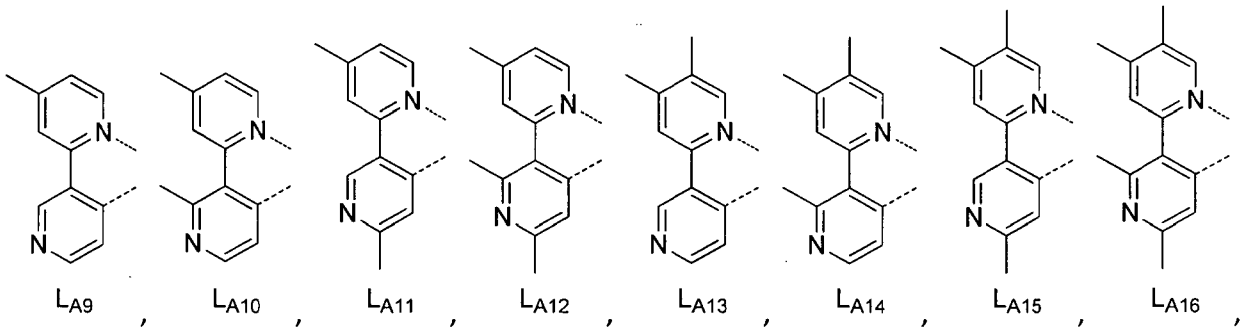
wherein each R^7, R^8, and R^9 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein X is O or S.

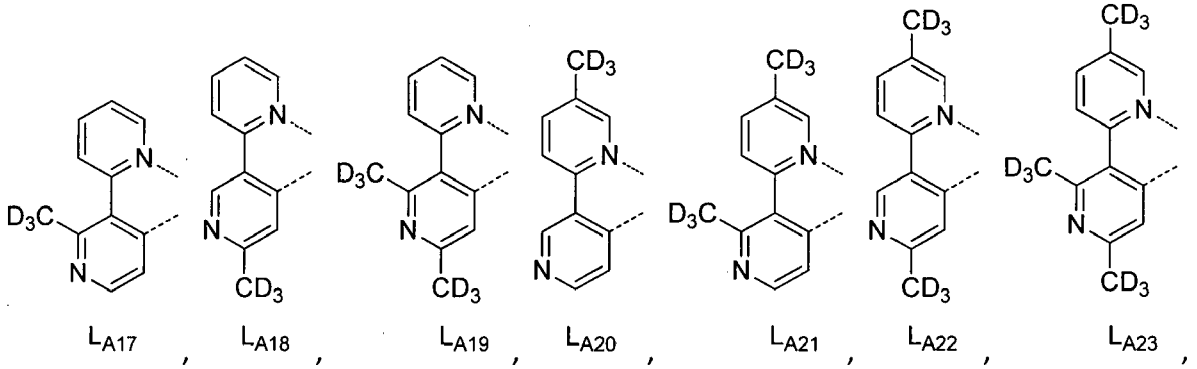
11. The compound of any one of claims 1 to 3, and 8 or 9, wherein L_A is selected from the group consisting of:



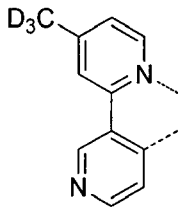
L_{A1}, L_{A2}, L_{A3}, L_{A4}, L_{A5}, L_{A6}, L_{A7}, L_{A8},



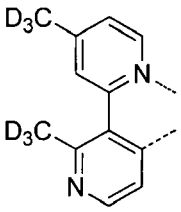
L_{A9}, L_{A10}, L_{A11}, L_{A12}, L_{A13}, L_{A14}, L_{A15}, L_{A16},



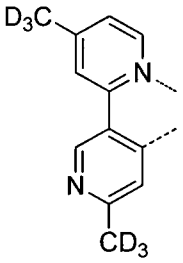
L_{A17}, L_{A18}, L_{A19}, L_{A20}, L_{A21}, L_{A22}, L_{A23},



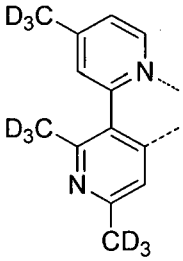
L_{A24} ,



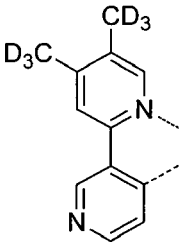
L_{A25} ,



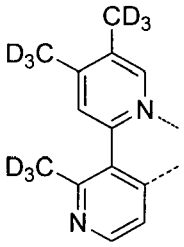
L_{A26} ,



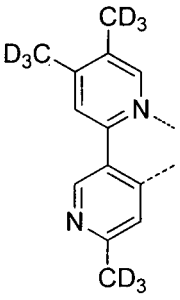
L_{A27} ,



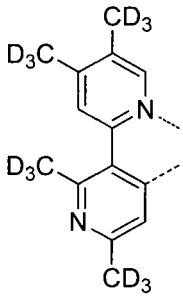
L_{A28} ,



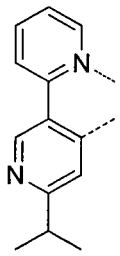
L_{A29} ,



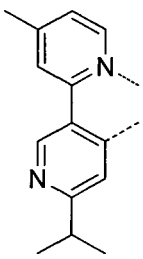
L_{A30} ,



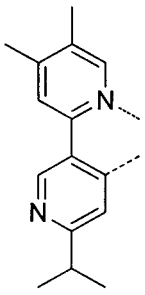
L_{A31} ,



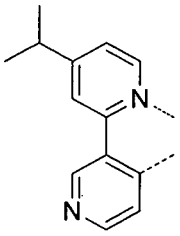
L_{A32} ,



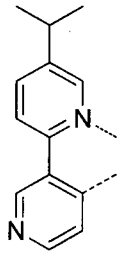
L_{A33} ,



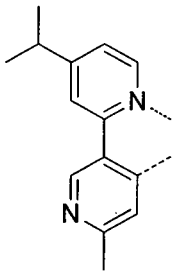
L_{A34} ,



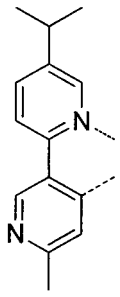
L_{A35} ,



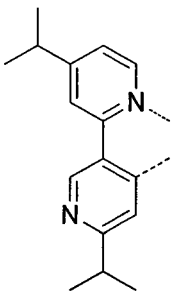
L_{A36} ,



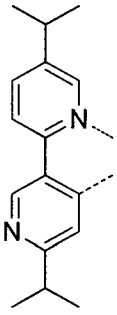
L_{A37} ,



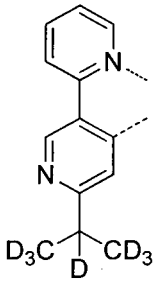
L_{A38} ,



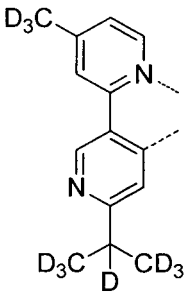
L_{A39} ,



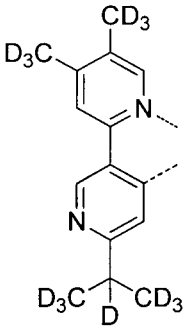
L_{A40} ,



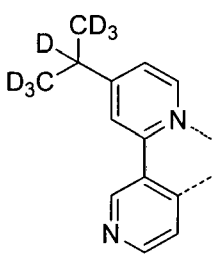
L_{A41} ,



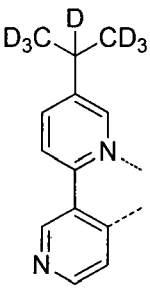
L_{A42} ,



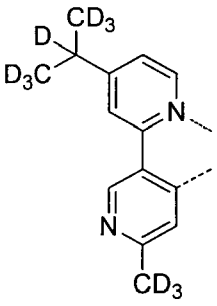
L_{A43} ,



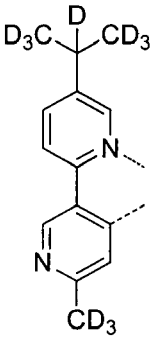
L_{A44} ,



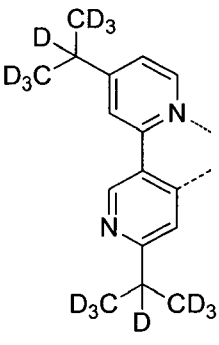
L_{A45} ,



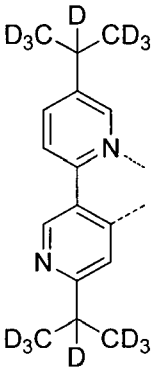
L_{A46} ,



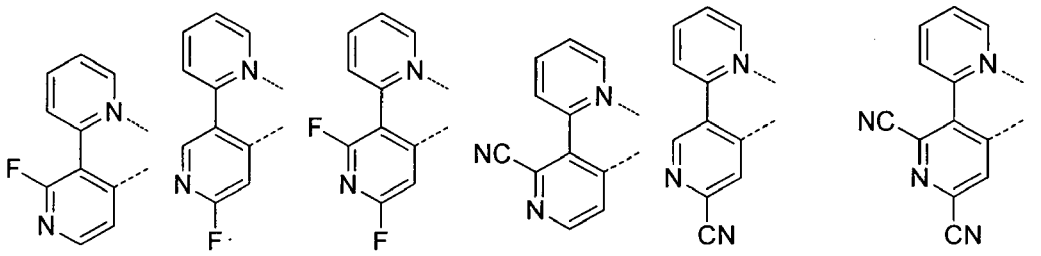
L_{A47} ,



L_{A48} ,

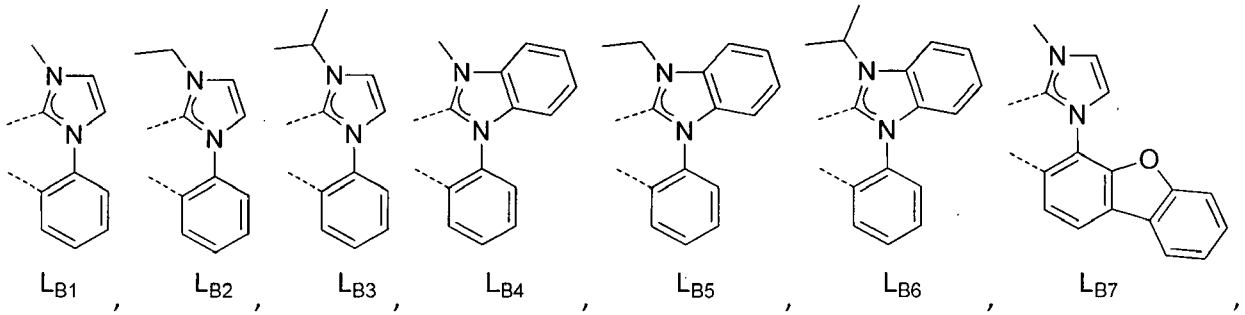


L_{A49} ,

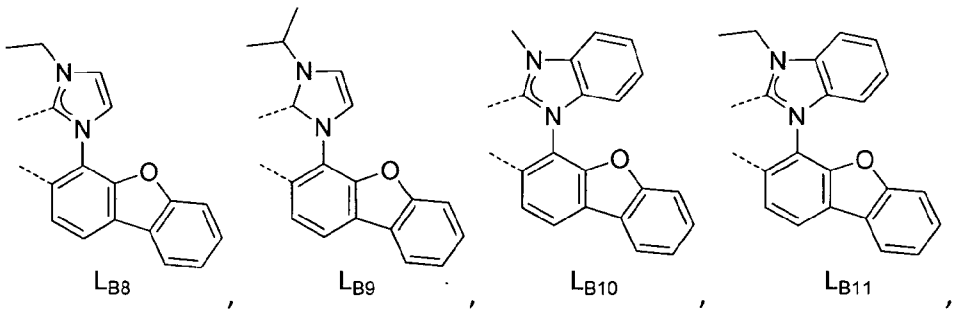


L_{A50}, L_{A51}, L_{A52}, L_{A53}, L_{A54}, and L_{A55}.

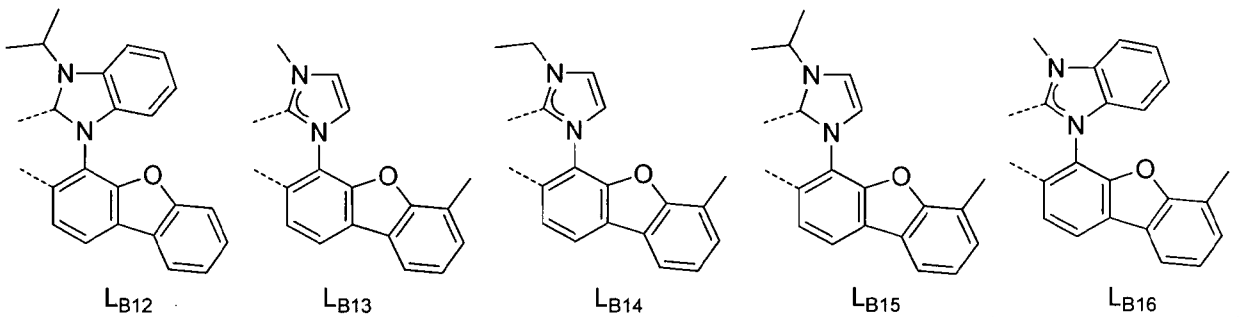
12. The compound of any one of claims 1 to 7, wherein L_B is selected from the group consisting of:



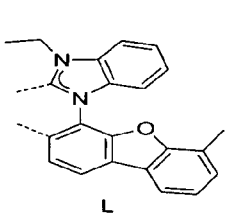
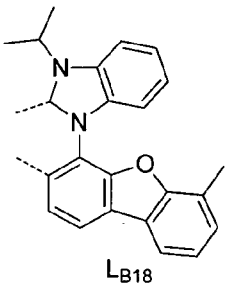
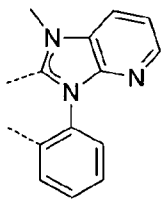
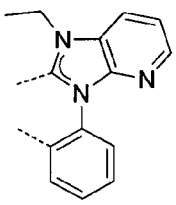
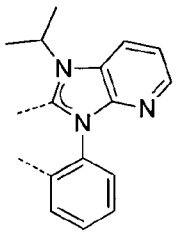
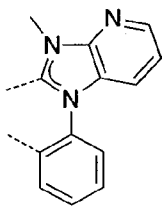
L_{B1}, L_{B2}, L_{B3}, L_{B4}, L_{B5}, L_{B6}, L_{B7},

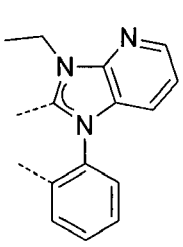
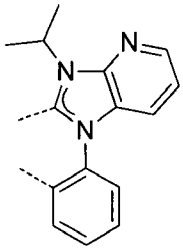
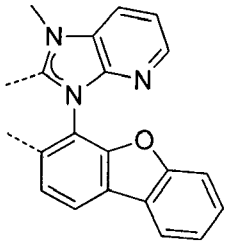
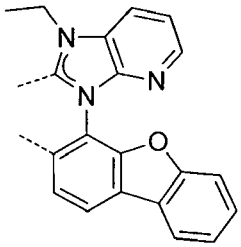
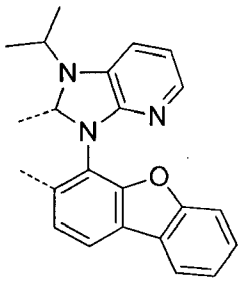


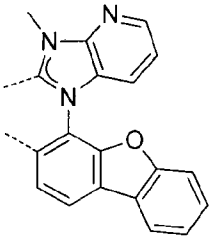
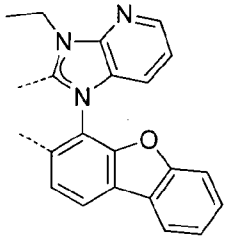
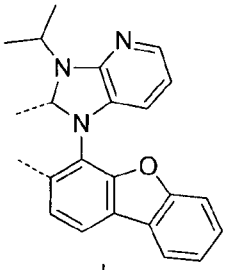
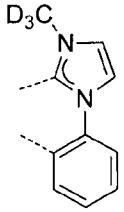
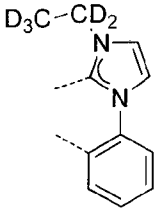
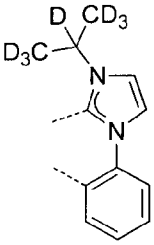
L_{B8}, L_{B9}, L_{B10}, L_{B11},

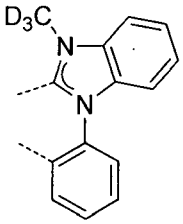
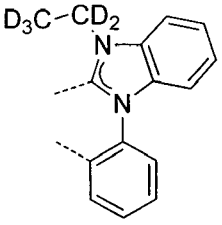
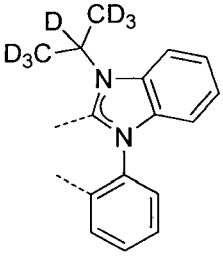
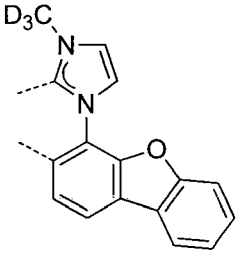
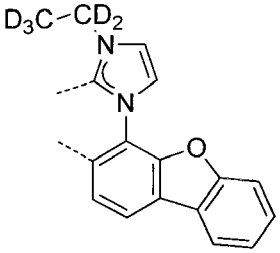


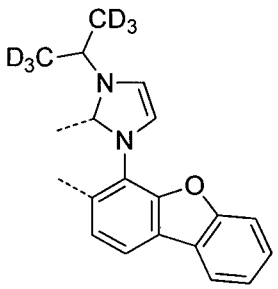
L_{B12}, L_{B13}, L_{B14}, L_{B15}, L_{B16},


L_{B17},

L_{B18},

L_{B19},

L_{B20},

L_{B21},

L_{B22},

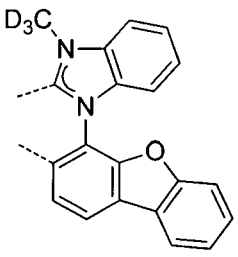

L_{B23},

L_{B24},

L_{B25},

L_{B26},

L_{B27},


L_{B28},

L_{B28},

L_{B30},

L_{B31},

L_{B32},

L_{B33},

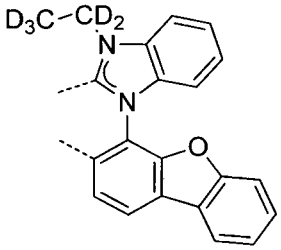

L_{B34},

L_{B35},

L_{B36},

L_{B37},

L_{B38},



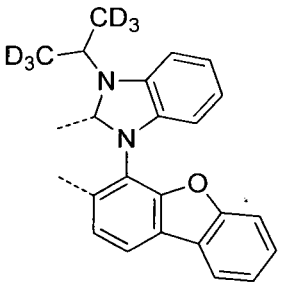
L_{B39} ,



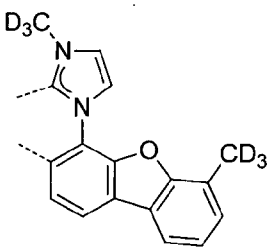
L_{B40} ,



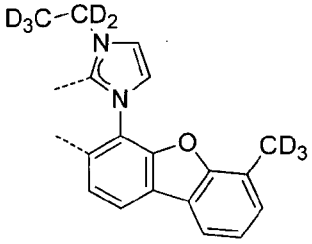
L_{B41} ,



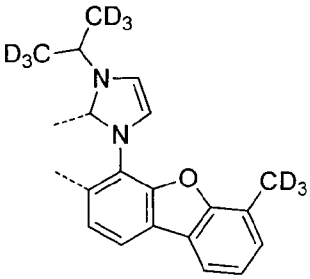
L_{B42} ,



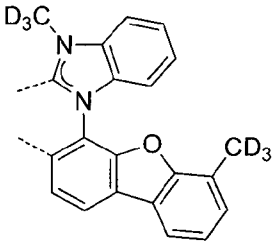
L_{B43} ,



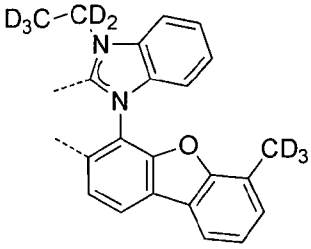
L_{B44} ,



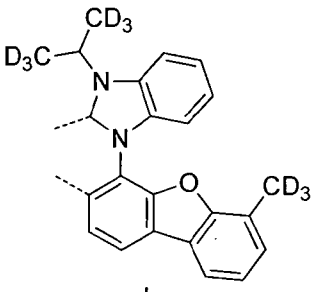
L_{B45} ,



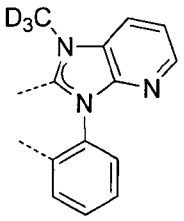
L_{B46} ,



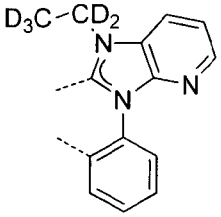
L_{B47} ,



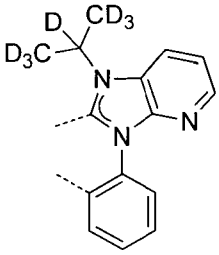
L_{B48} ,



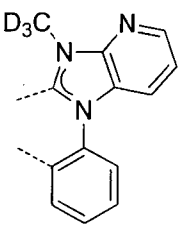
L_{B49} ,



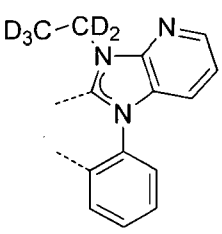
L_{B50} ,



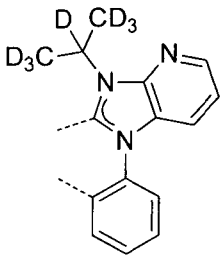
L_{B51} ,



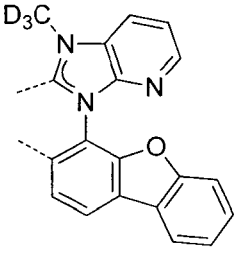
L_{B52} ,



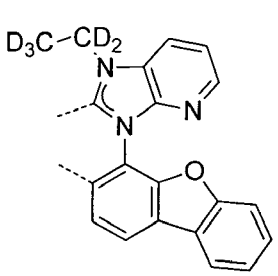
L_{B53} ,

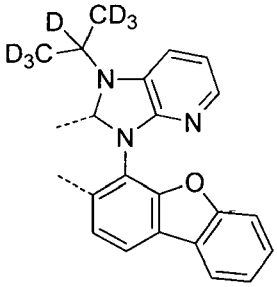


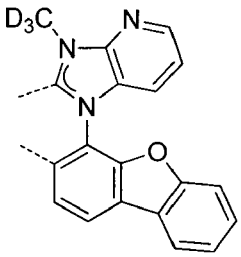
L_{B54} ,

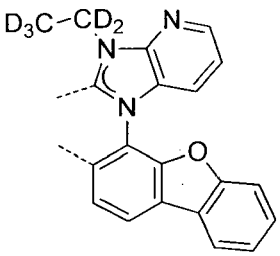


L_{B55} ,

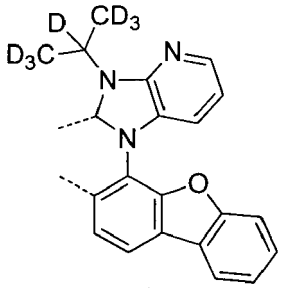

L_{B56} ,


L_{B57} ,

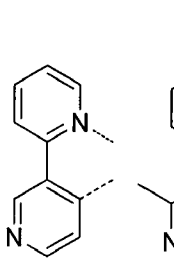

L_{B58} ,

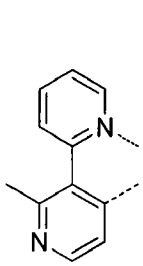

L_{B59} ,

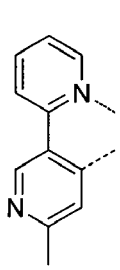
and

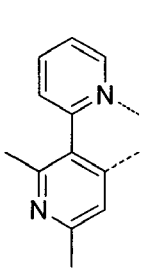

L_{B60} .

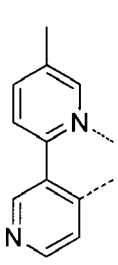
13. The compound of claim 14, wherein L_A is selected from the group consisting of:

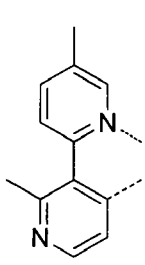

L_{A1} ,

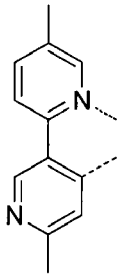

L_{A2} ,

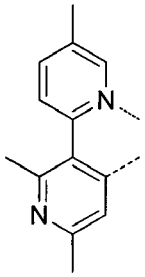

L_{A3} ,

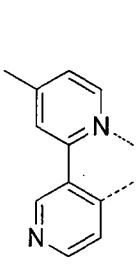

L_{A4} ,

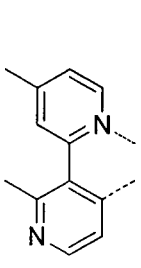

L_{A5} ,

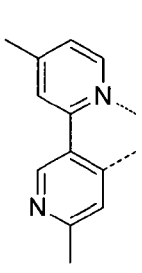

L_{A6} ,

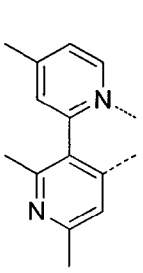

L_{A7} ,

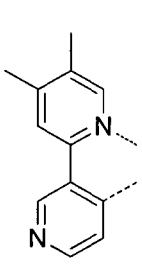

L_{A8} ,

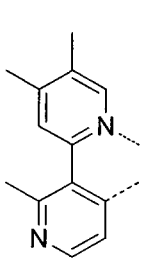

L_{A9} ,

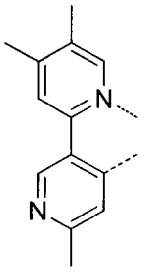

L_{A10} ,

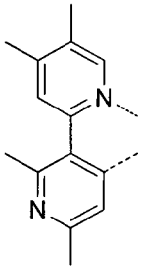

L_{A11} ,

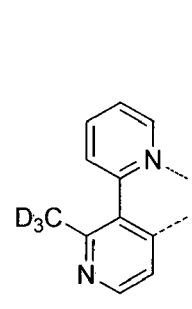

L_{A12} ,


L_{A13} ,

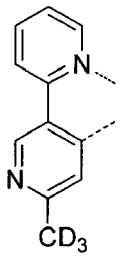

L_{A14} ,


L_{A15} ,

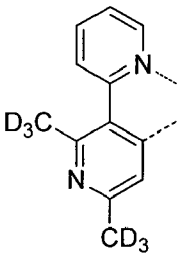

L_{A16} ,



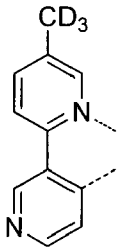
L_{A17} ,



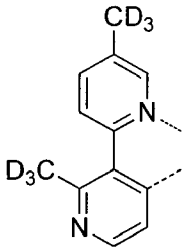
L_{A18} ,



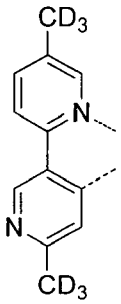
L_{A19} ,



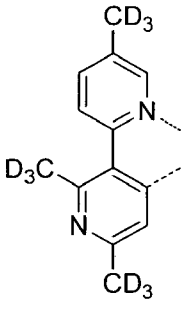
L_{A20} ,



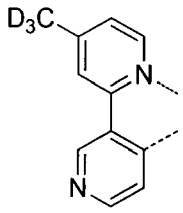
L_{A21} ,



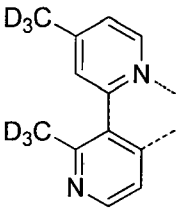
L_{A22} ,



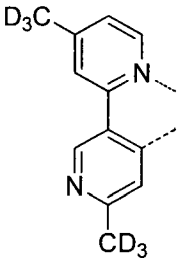
L_{A23} ,



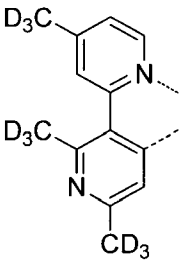
L_{A24} ,



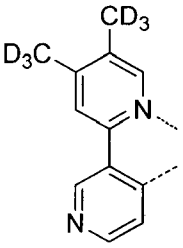
L_{A25} ,



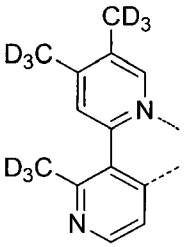
L_{A26} ,



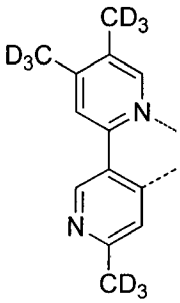
L_{A27} ,



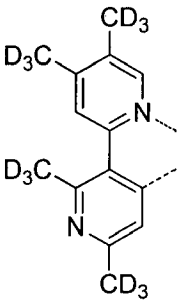
L_{A28} ,



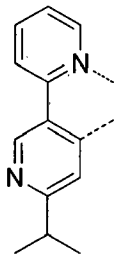
L_{A29} ,



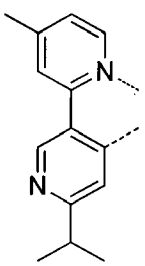
L_{A30} ,



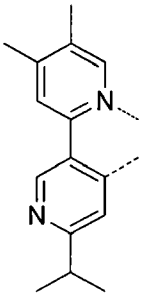
L_{A31} ,



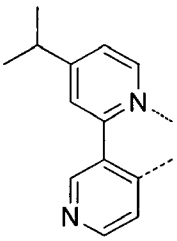
L_{A32} ,



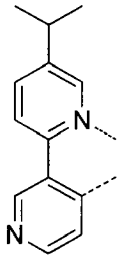
L_{A33} ,



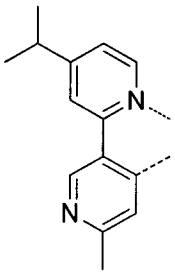
L_{A34} ,



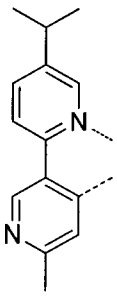
L_{A35} ,



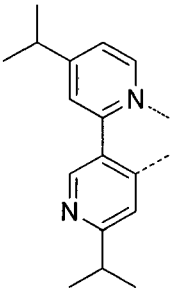
L_{A36} ,



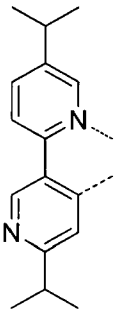
L_{A37} ,



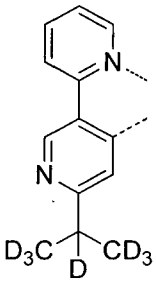
L_{A38} ,



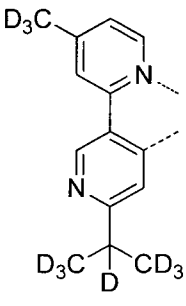
L_{A39} ,



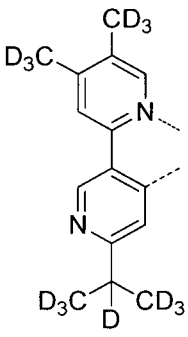
L_{A40} ,



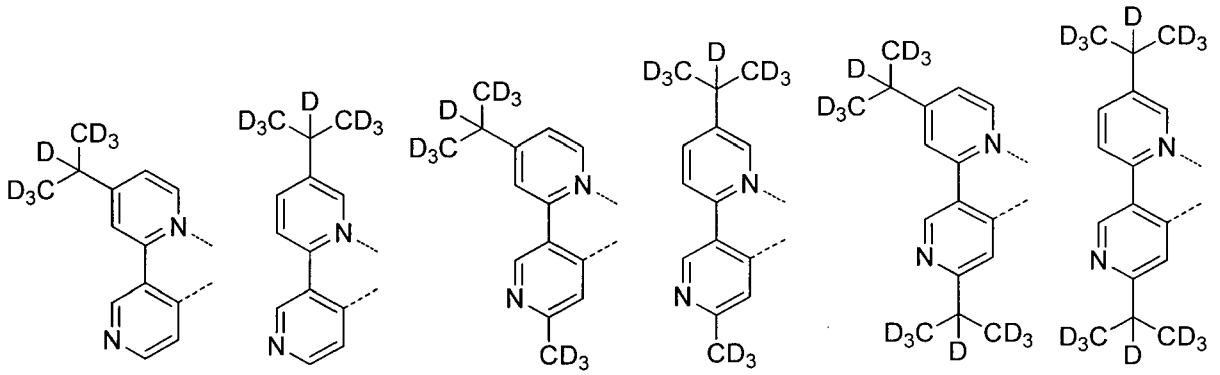
L_{A41} ,



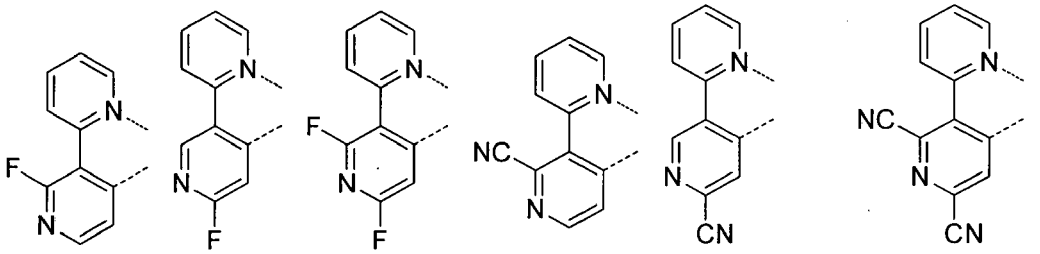
L_{A42} ,



L_{A43} ,



L_{A44} , L_{A45} , L_{A46} , L_{A47} , L_{A48} , L_{A49} ,



L_{A50} , L_{A51} , L_{A52} , L_{A53} , L_{A54} , and L_{A55} ;

wherein n is 2; and

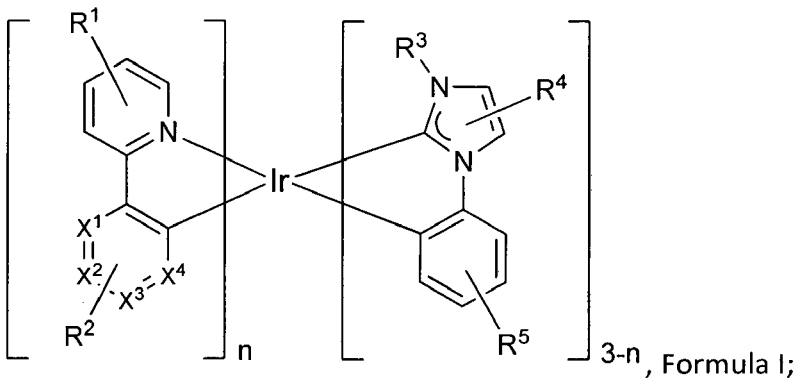
wherein the compound is selected from the group consisting of compound 1 to compound 3300, wherein for each Compound x has the formula $Ir(L_{Ak})_2(L_{Bj})$, x = 55j + *k* - 55, wherein *k* is an integer from 1 to 55, and j is an integer from 1 to 60.

14. A first device comprising a first organic light emitting device, the first organic light emitting device comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



, Formula I;

wherein R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;

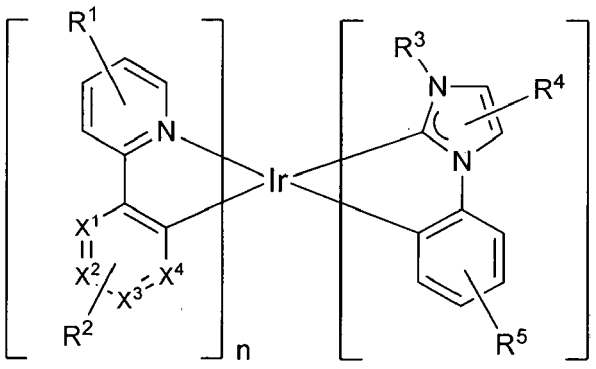
wherein R^2 represents up to tri-substitution, or no substitution;

wherein R^4 represents mono, or di-substitution, or no substitution;

wherein X^1, X^2, X^3, and X^4 are each independently C or N;

wherein at least one of X^1, X^2, X^3, and X^4 is N;
wherein any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;
wherein each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, cyano, and combinations thereof; and
wherein n is either 1 or 2.

15. A formulation comprising a compound having the formula $Ir(L_A)_n(L_B)_{3-n}$, having the structure:



, Formula I;

wherein R^1 and R^5 each independently represent mono, di, tri, or tetra-substitution, or no substitution;
wherein R^2 represents up to tri-substitution, or no substitution;
wherein R^4 represents mono, or di-substitution, or no substitution;
wherein X^1, X^2, X^3, and X^4 are each independently C or N;
wherein at least one of X^1, X^2, X^3, and X^4 is N;
wherein any adjacent substituents of R^1, R^2, R^3, R^4, and R^5 are optionally linked together to form a ring;
wherein each R^1, R^2, R^3, R^4, and R^5 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, cyano, and combinations thereof; and
wherein n is either 1 or 2.

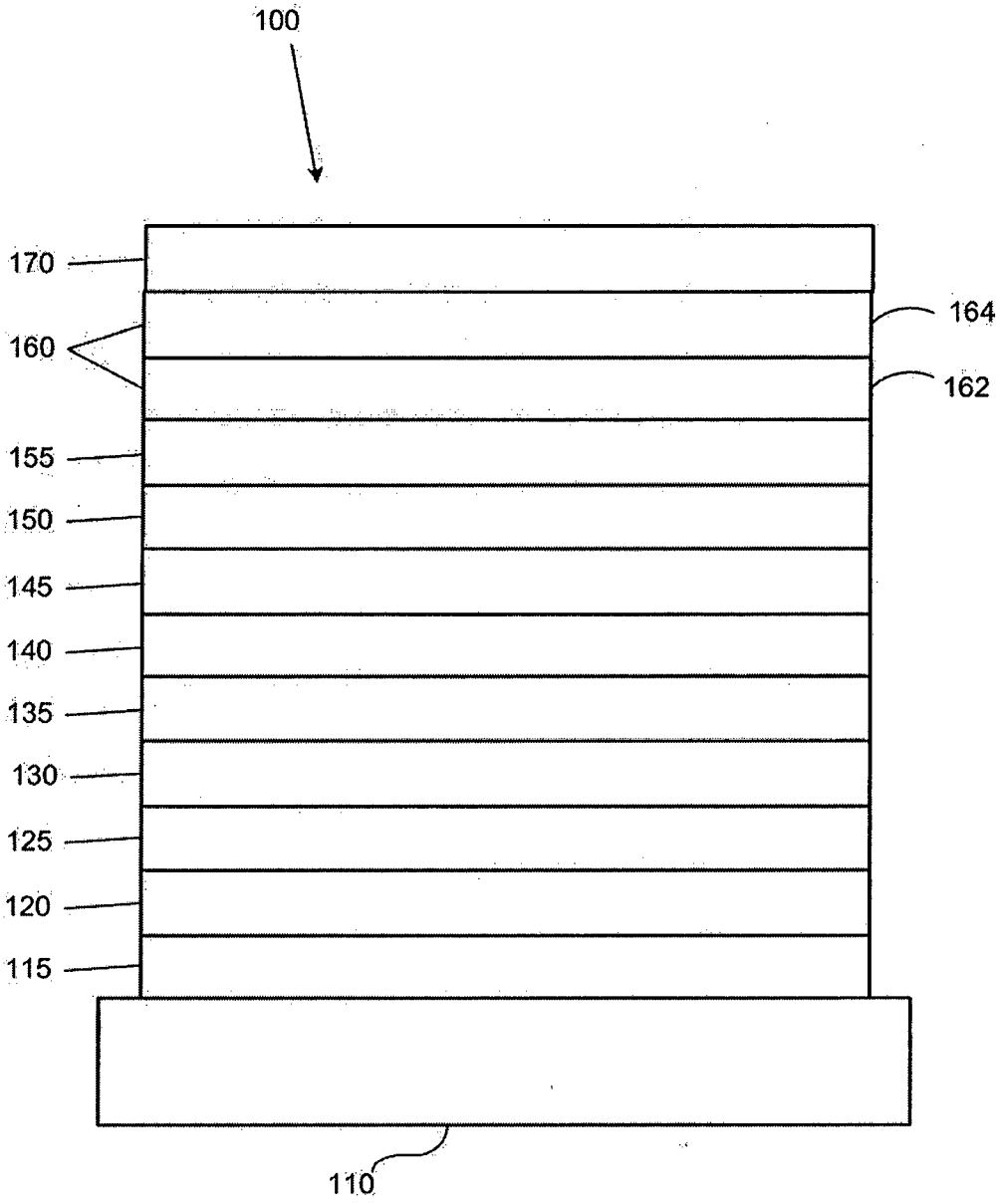


FIGURE 1

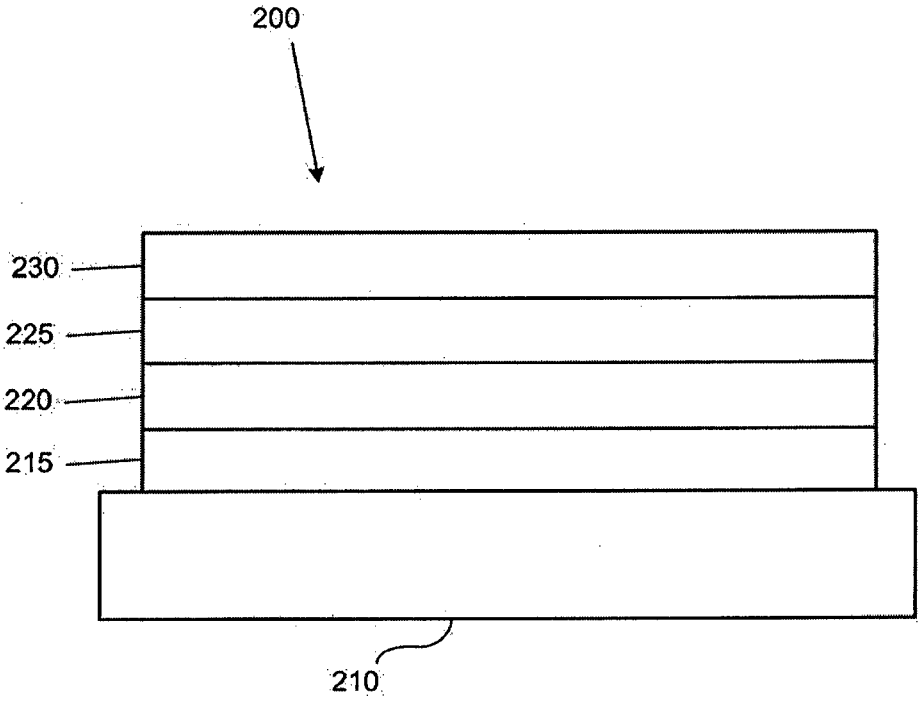


FIGURE 2

Formula I

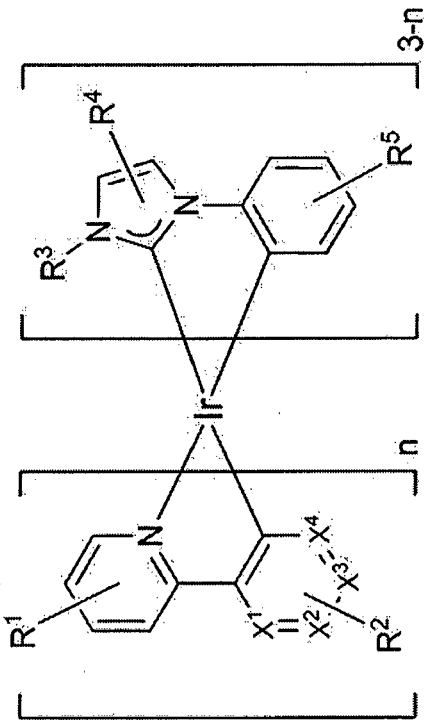


Figure 3

Formula II

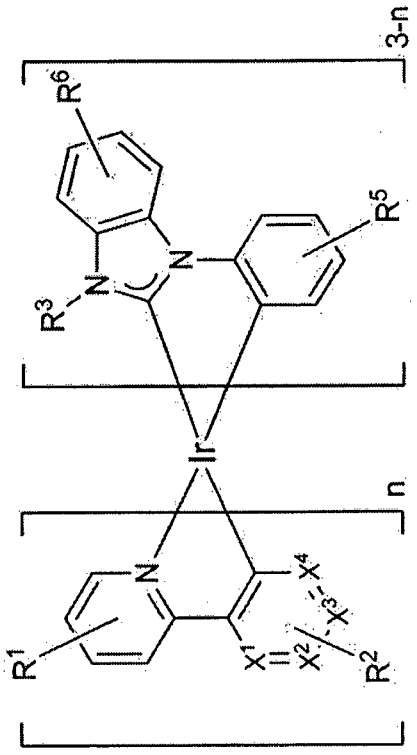


Figure 4

REFERENCES CITED IN THE DESCRIPTION

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专利名称(译)	有机电致发光材料和器件		
公开(公告)号	EP2874195A2	公开(公告)日	2015-05-20
申请号	EP2014003725	申请日	2014-11-05
[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 LIN CHUN		
发明人	XIA, CHUANJUN LIN, CHUN		
IPC分类号	H01L51/54 H01L51/50		
CPC分类号	C07F15/0033 C09B57/10 C09K11/06 C09K2211/185 H01L51/0054 H01L51/0067 H01L51/0071 H01L51/0072 H01L51/0074 H01L51/0085 H01L51/5016		
优先权	61/904530 2013-11-15 US 61/907450 2013-11-22 US 14/521257 2014-10-22 US 14/521281 2014-10-22 US		
其他公开文献	EP2874195A3 EP2874195B1		
外部链接	Espacenet		

摘要(译)

描述具有式I的结构式Ir（LA）n（LB）3-n的化合物。在式Ir（LA）n（LB）3-n中，n为1或2; R1，R2，R4和R5各自独立地表示最多取代数或不取代; X1，X2，X3和X4各自独立地为C或N; X1，X2，X3和X4中的至少一个是N.此外，R1，R2，R3，R4和R5的任何相邻取代基任选地连接在一起形成环，并且每个R1，R2，R3， R4和R5独立地选自氢，氘，卤化物，烷基，环烷基，杂烷基，芳烷基，烷氧基，芳氧基，氨基，甲硅烷基，烯基，环烯基，杂烯基，炔基，芳基，杂芳基，酰基，羰基，羧酸，酯，腈，异腈，硫烷基，亚磺酰基，磺酰基，膦基及其组合。还描述了包含式Ir（LA）n（LB）3-n的化合物的制剂和装置，例如OLED。

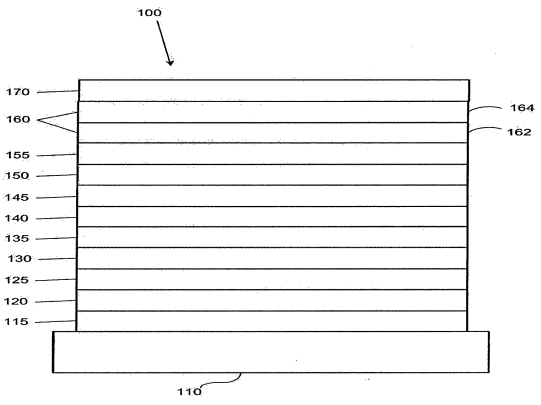

FIGURE 1