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(54) **ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES**

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H01L 51/00 (2006.01)
C07F 15/00 (2006.01)
H01L 51/50 (2006.01)

(52) **U.S. Cl.**
CPC ***H01L 51/0085*** (2013.01); ***C07F 15/0033*** (2013.01); *H01L 51/5016* (2013.01)

(58) **Field of Classification Search**
CPC H01L 51/0085; C07F 15/0033
See application file for complete search history.

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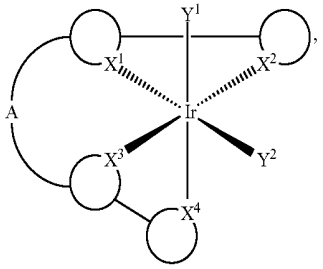
(57) **ABSTRACT**

Iridium complexes comprising a tetradentate ligand and two monodentate ligands, devices containing the same and formulations containing the same are described. The iriium complexes can have a structure according to Formula (I)

Formula (I)



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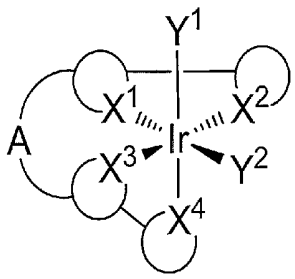
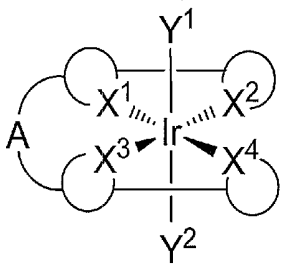


Formula (I)



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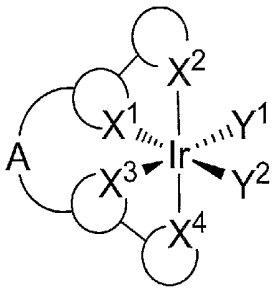
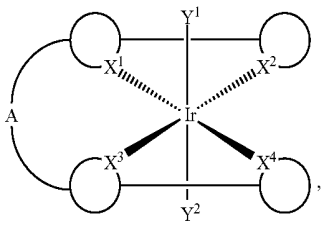


Formula (III)

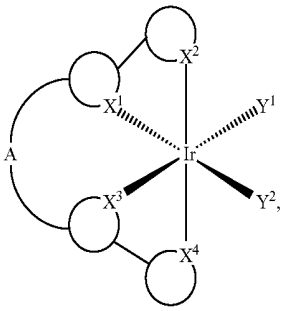
Formula (II)



Formula (II)

or

Formula (III)



Formula (III)

where the iridium complex includes:

a tetradentate ligand coordinated to an iridium core by coordinating atoms X^1, X^2, X^3 and X^4; a first monodentate ligand coordinated to the iridium core by coordinating atom Y^1; and a second monodentate ligand coordinated to the iridium core by coordinating atom Y^2, wherein X^1, X^2, X^3 and X^4 are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom, wherein Y^1 and Y^2 are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom, and A is a linker.

19 Claims, 3 Drawing Sheets

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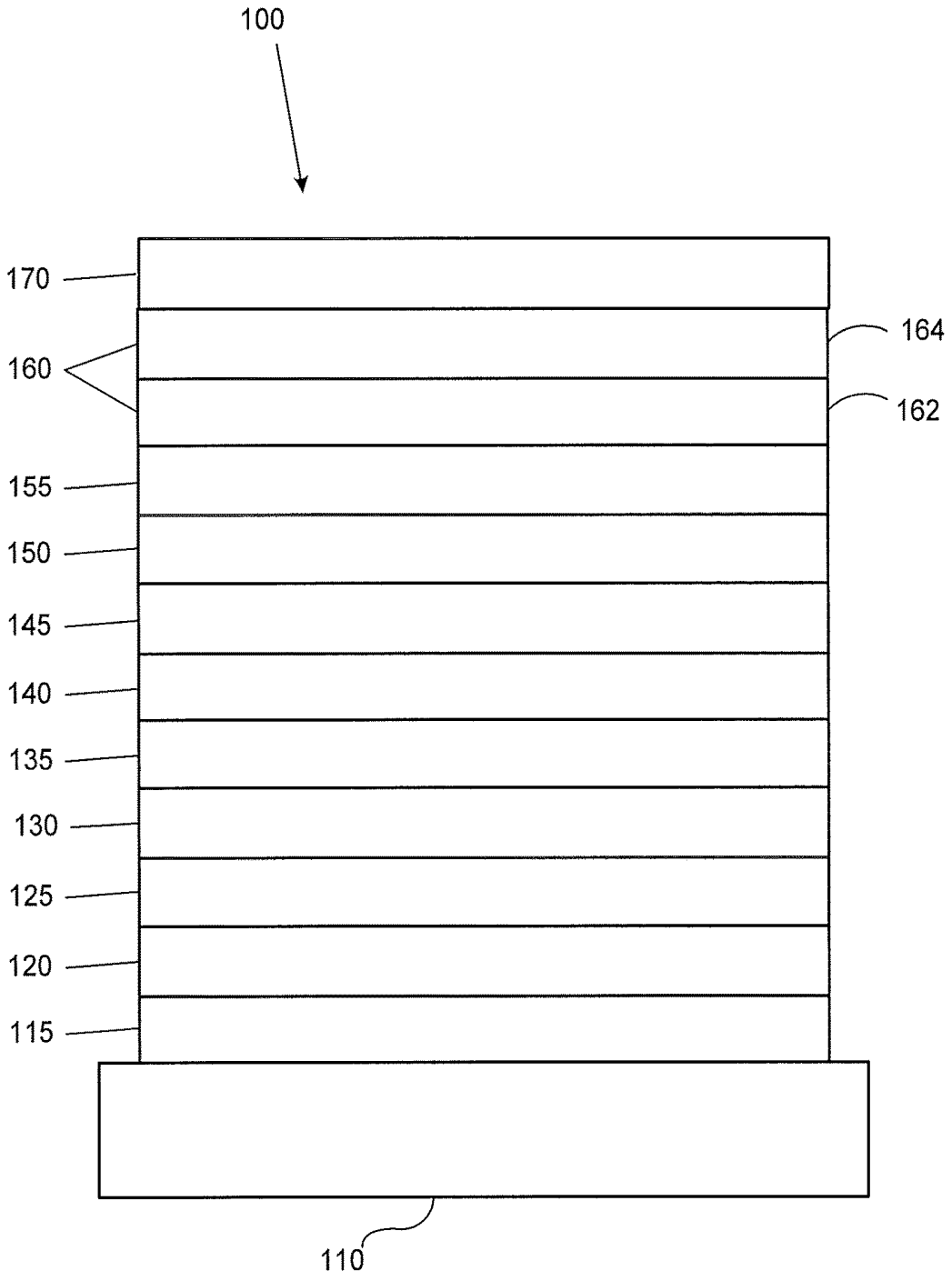


FIGURE 1

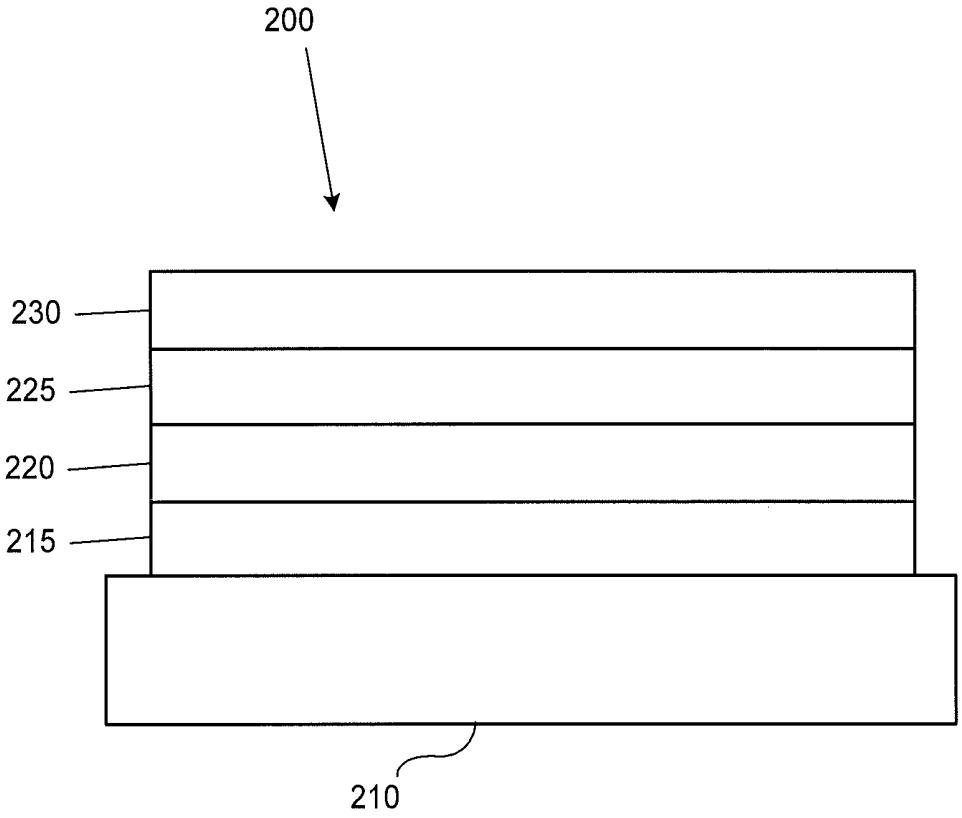
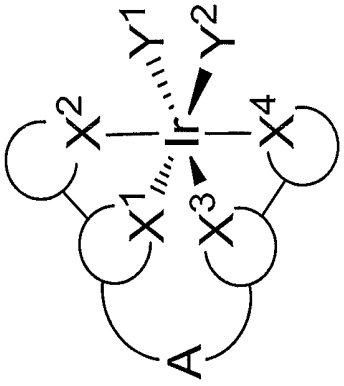


FIGURE 2



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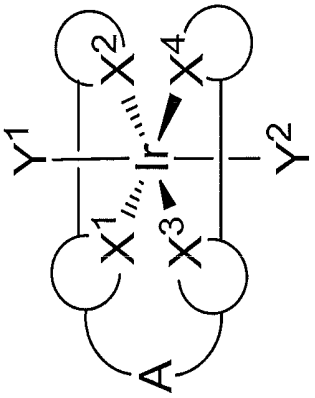

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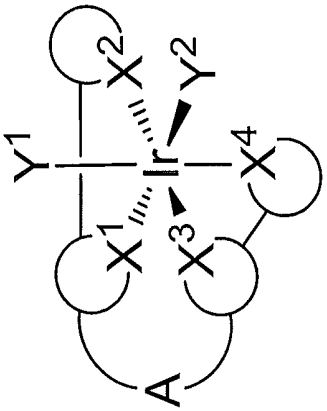


Formula (I)

FIG. 3

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

PARTIES TO A JOINT RESEARCH AGREEMENT

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

The present invention relates to compounds for use as emitters and devices, such as organic light emitting diodes, including the same.

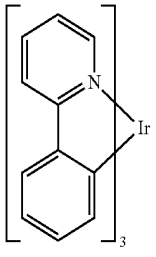
BACKGROUND

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.

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.

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.

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



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

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.

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.

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.

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.

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.

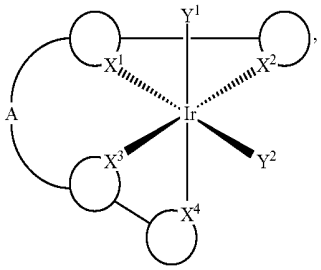
As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum 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.

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

SUMMARY OF THE INVENTION

According to one embodiment, an iridium complex having a structure according to Formula (I)

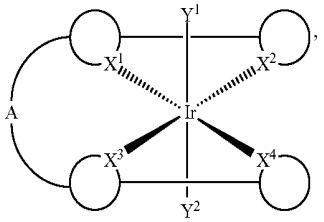
Formula (I)



or

Formula (II)

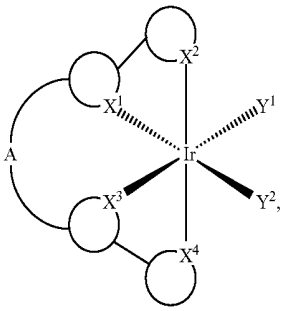
Formula (II)



or

Formula (III)

Formula (III)



comprising:

a tetradentate ligand coordinated to an iridium core by coordinating atoms X^1, X^2, X^3 and X^4;

a first monodentate ligand coordinated to the iridium core by coordinating atom Y^1; and

a second monodentate ligand coordinated to the iridium core by coordinating atom Y^2,

wherein X^1, X^2, X^3 and X^4 are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom;

wherein Y^1 and Y^2 are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom; and

wherein A is a linker.

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 emissive layer may include a host and a phosphorescent dopant. The emissive layer can include a compound according to one of Formula (I), Formula (II), and Formula (III), and the variations thereof as described herein.

In yet another aspect of the present disclsoure, a formulation that comprises a compound according to Formula (I), Formula (II) or Formula (III), and the variations thereof as described herein. 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.

BRIEF DESCRIPTION OF THE DRAWINGS

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), Formula (II), and Formula (III) as disclosed herein.

DETAILED DESCRIPTION

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.

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.

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 U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

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 U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

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.

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**.

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**.

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.

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.

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 poly-

meric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCMS2009/042829, 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.

Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, 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.

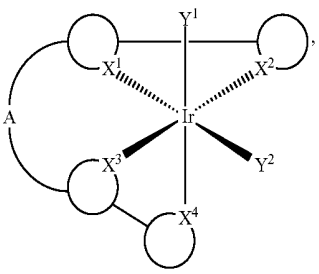
The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may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

The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, heterocyclic group, aryl, aromatic group, and heteroaryl are known to the art, and are defined in U.S. Pat. No 7,279,704 at cols. 31-32, which are incorporated herein by reference.

As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant carbon. Thus, where R^2 is monosubstituted, then one R^2 must be other than H. Similarly, where R^3 is disubstituted, then two of R^3 must be other than H. Similarly, where R^2 is unsubstituted R^2 is hydrogen for all available positions.

According to one embodiment, an iridium complex having a structure according to Formula (I):

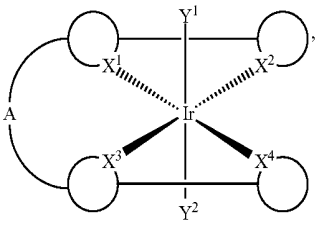
Formula (I)



or

Formula (II):

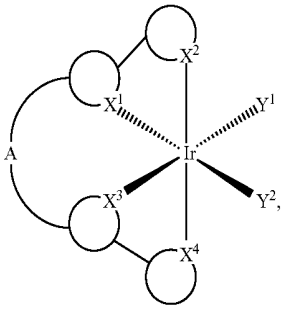
Formula (II)



or

Formula (III):

Formula (III)



comprising:

a tetradentate ligand coordinated to an iridium core by coordinating atoms X^1, X^2, X^3 and X^4;

a first monodentate ligand coordinated to the iridium core by coordinating atom Y^1; and

a second monodentate ligand coordinated to the iridium core by coordinating atom Y^2,

wherein X^1, X^2, X^3 and X^4 are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom;

wherein Y^1 and Y^2 are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom; and

wherein A is a linker.

In some embodiments, at least one coordinating atom selected from the group consisting of X^1, X^2, X^3 and X^4, is other than nitrogen. As used herein, "halides" can include any or all of fluorine, chlorine, bromide, iodide, and astinide.

In some embodiments, X^1, X^2, X^3 and X^4 are independently selected from the group consisting of an anionic coordinating atom selected from the group consisting of carbon and nitrogen, and a neutral coordinating atom selected from the group consisting of nitrogen, oxygen, phosphorus, and carbene carbon.

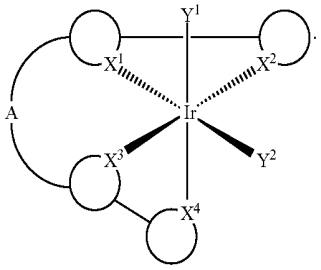
In some embodiments, Y^1 and Y^2 are independently selected from the group consisting of an anionic coordinating atom selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen, and a neutral coordinating atom selected from the group consisting of nitrogen, phosphorus, arsenic, carbene carbon, and oxygen.

In some embodiments, the compound is neutral, while the compound is ionic in other embodiments.

In some embodiments, the tetradentate ligand has a square-planar coordinate geometry.

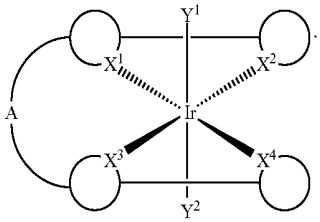
In some embodiments, the iridium complex has a structure according to Formula (I):

Formula (I)



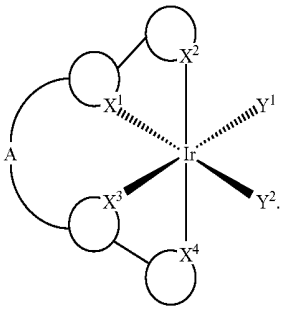
In some embodiments, the iridium complex has a structure according to Formula (II):

Formula (II)

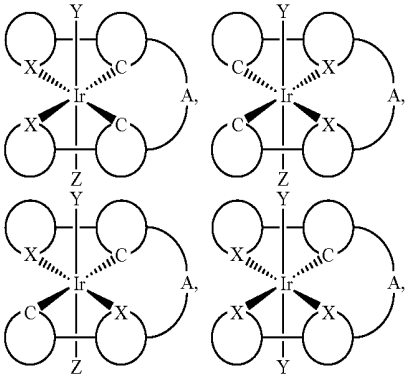


In some embodiments, the iridium complex has a structure according to Formula (III):

Formula (III)



In some more specific embodiments, the iridium complex has a structure selected from the group consisting of:



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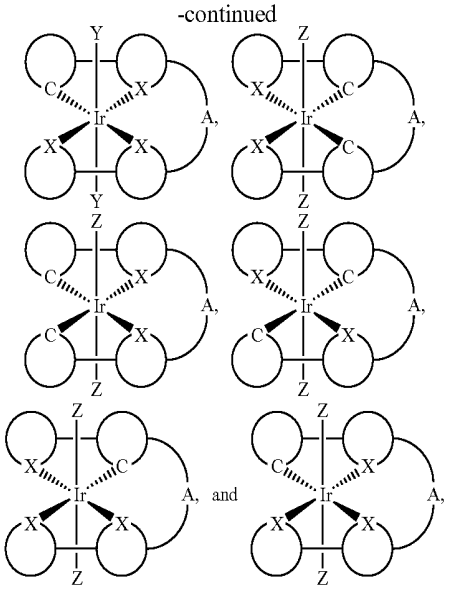


wherein each C, X, Y and Z can be same or different;

wherein each C is independently an anionic coordinating carbon atom,

wherein each X is independently a coordinating atom other than anionic carbon atom,

wherein each Y is independently an anionic coordinating atom,

wherein each Z is independently a neutral coordinating atom, and

A is a linker.

In some embodiments, the iridium complex has the structure of Formula (I), where one of X_1, X_2, X_3, and X_4 is C, and three of X_1, X_2, X_3, and X_4 are X. In other embodiments, the iridium complex has the structure of Formula (II), where one of X_1, X_2, X_3, and X_4 is C, and three of X_1, X_2, X_3, and X_4 are X. In still other embodiments, the iridium complex has the structure of Formula (III), where one of X_1, X_2, X_3, and X_4 is C, and three of X_1, X_2, X_3, and X_4 are X.

In some embodiments, the iridium complex has the structure of Formula (I), where two of X_1, X_2, X_3, and X_4 are C, and two of X_1, X_2, X_3, and X_4 are X. In other embodiments, the iridium complex has the structure of Formula (II), where two of X_1, X_2, X_3, and X_4 are C, and two of X_1, X_2, X_3, and X_4 are X. In still other embodiments, the iridium complex has the structure of Formula (III), where two of X_1, X_2, X_3, and X_4 are C, and two of X_1, X_2, X_3, and X_4 are X.

In some embodiments, the iridium complex has the structure of Formula (I), where three of X_1, X_2, X_3, and X_4 are C, and one of X_1, X_2, X_3, and X_4 is X. In other embodiments, the iridium complex has the structure of Formula (II), where three of X_1, X_2, X_3, and X_4 are C, and one of X_1, X_2, X_3, and X_4 are X. In still other embodiments, the iridium complex has the structure of Formula (III), where three of X_1, X_2, X_3, and X_4 are C, and one of X_1, X_2, X_3, and X_4 is X.

In some embodiments, X can be a neutral coordinating atom.

In some embodiments, X is a coordinating atom independently selected from the group consisting of nitrogen, oxygen, phosphorus, and carbene carbon; Y is an anionic coordinating atom independently selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen; and Z is a neutral coordinating atom independently selected from the group consisting of nitrogen, carbon, phosphorus, arsenic, and oxygen carbene carbon.

In some embodiments, X^1, X^2, X^3, and X^4 are each part of a 5- or 6-membered aryl or heteroaryl ring. In some embodiments, X^1, X^2, X^3, and X^4 can be part of fused ring systems. Examples of such fused ring systems include, but are not limited to, carbazole, dibenzothiophene, dibenzofuran, aza-carbazole, aza-dibenzothiophene, aza-dibenzofuran, triphenylene, aza-triphenylene, fluorene, aza-fluorene, benzimidazole, aza-benzimidazole and imidazo[1,2-f] phenanthridine.

In some embodiments, adjacent rings containing coordinating atoms X^1, X^2, X^3, and X^4 can be part of fused ring systems. For example, adjacent rings containing coordinating atoms X^1, X^2, X^3, and X^4 can be part of a phenanthroline or a benzoquinoline moiety.

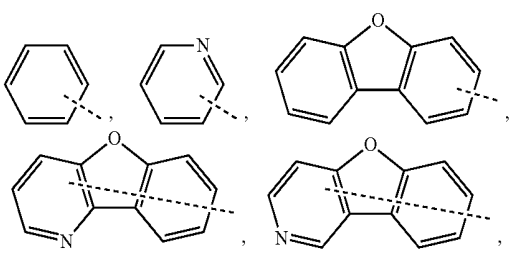
In some embodiments, at least one of X^1, X^2, X^3, and X^4 is a sp^2 carbon atom from a benzene ring.

In some embodiments, at least one of X^1, X^2, X^3, and X^4 is an anionic coordinating nitrogen that is part of a N-heterocyclic ring. Examples of N-heterocyclic rings include, but are not limited to, imidazole, benzoimidazole, pyrazole, and triazole.

In some embodiments, at least one of X^1, X^2, X^3, and X^4 is a selected from the group consisting of a neutral carbene that is part of a N-heterocyclic carbene, a neutral phosphorus that is part of a phosphorus atom of a trisubstituted phosphine, and a neutral nitrogen that is part of a N-heterocyclic ring. Examples of N-heterocyclic rings comprising neutral carbene coordinating atoms or neutral nitrogen coordinating atoms include, but are not limited to, imidazole, benzoimidazole, pyrazole, and triazole.

In some embodiments, linker A is a single bond or a bivalent functional group comprising a moiety selected from the group consisting of, BR_1, NR_1, PR_1, O, S, Se, C═O, S═O, SO_2, CR_1R_2, SiR_1R_2, GeR_1R_2, and combinations thereof, wherein R_1 and R_2 are 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, wherein R_1, R_2 are optionally joined to form a ring. The linker and substituents R_1 and R_2 can be linear or branched. In some embodiments, linker A is a bivalent functional group comprising at least two moieties selected from the group consisting of, BR_1, NR_1, PR_1, O, S, Se, C═O, S═O, SO_2, CR_1R_2, SiR_1R_2, GeR_1R_2, and combinations thereof.

In some embodiments, the first monodentate ligand, the second monodentate ligand, or both, are anionic moieties coordinated to the iridium (III) atom by an atom selected from the group consisting of carbon, nitrogen, halide, sulfur, oxygen, and carbene carbon. In some such embodiments, the anionic moiety is selected from the group consisting of:



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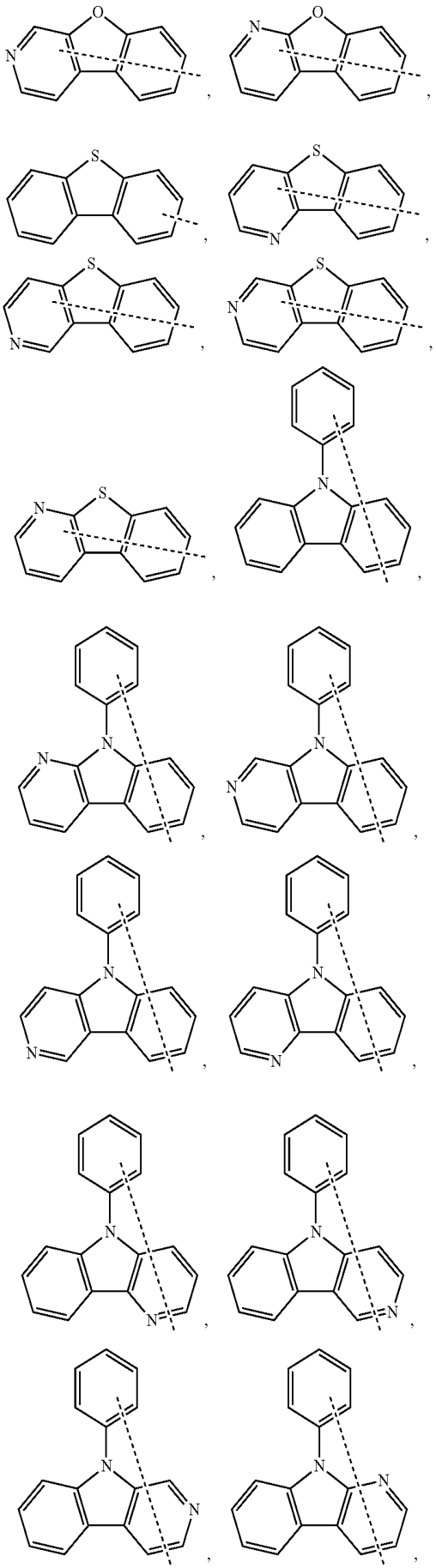

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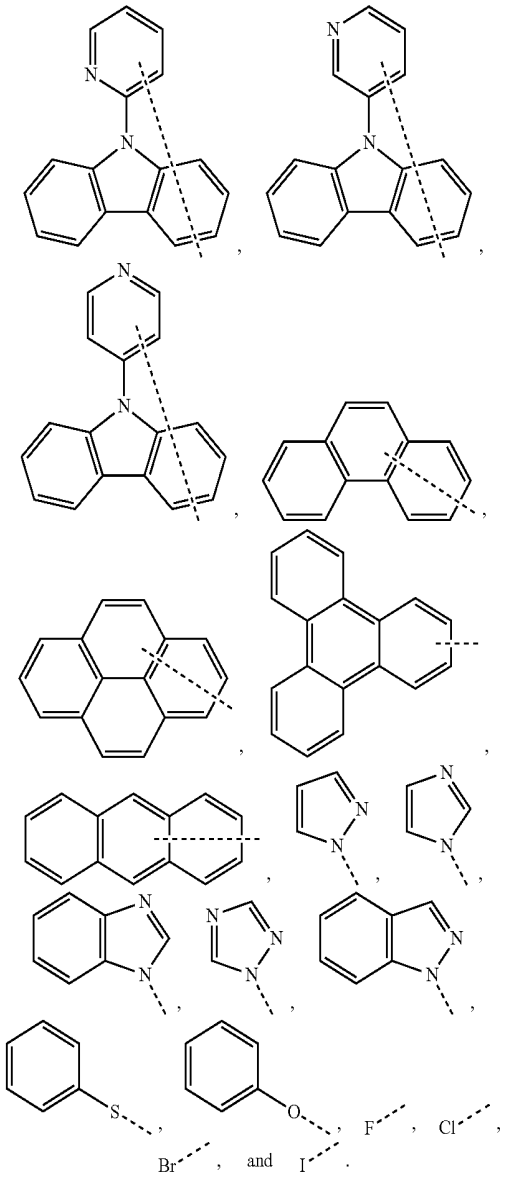
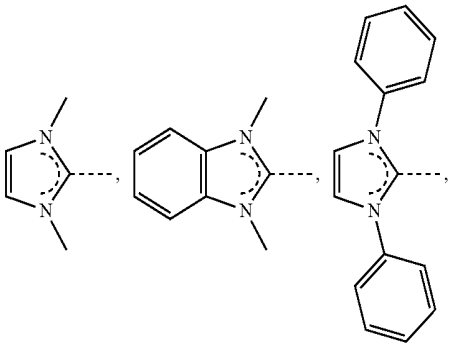


In some embodiments, the first monodentate ligand, the second monodentate ligand, or both are neutral moieties coordinated to the iridium (III) atom by an atom selected from the group consisting of nitrogen, carbene carbon, phosphorus, arsenic, and oxygen. In some of such embodiments, the neutral moiety is selected from the group consisting of:



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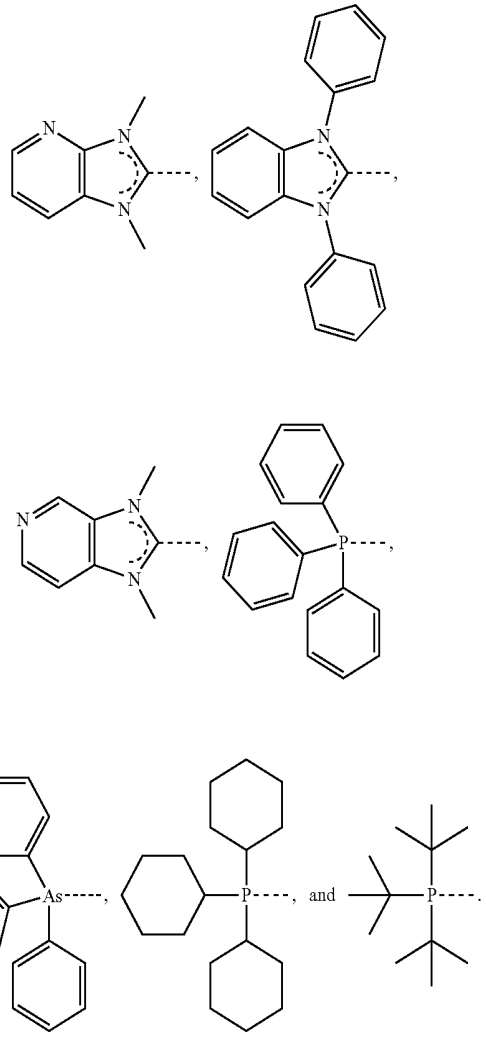
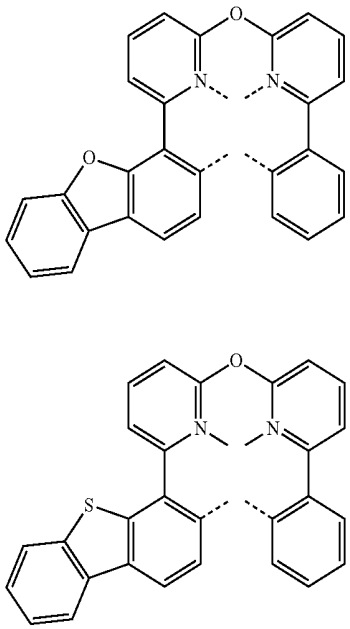


In some embodiments, the tetradentate ligand is selected from the group consisting of:



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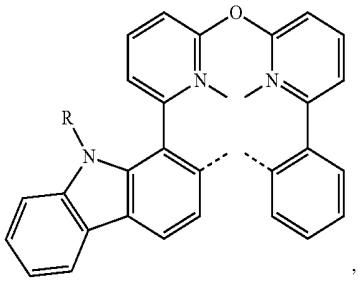

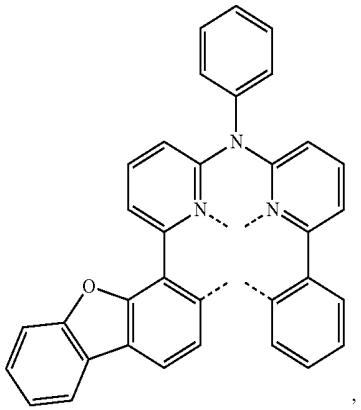

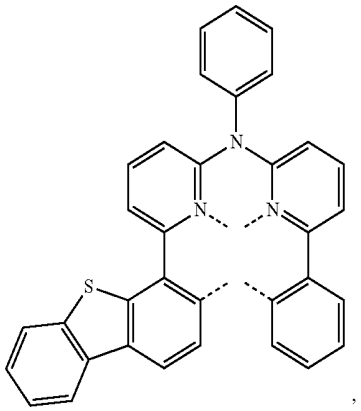

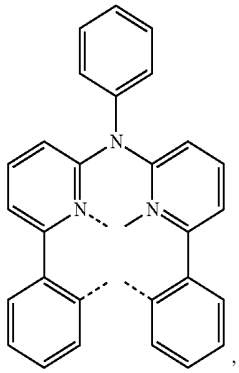

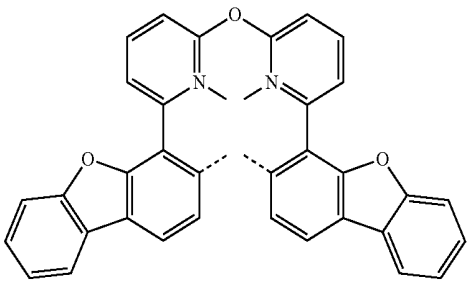

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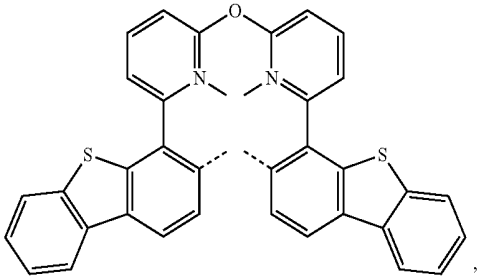

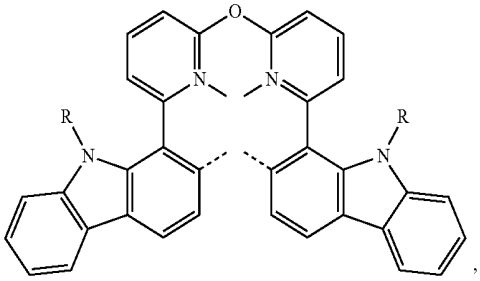

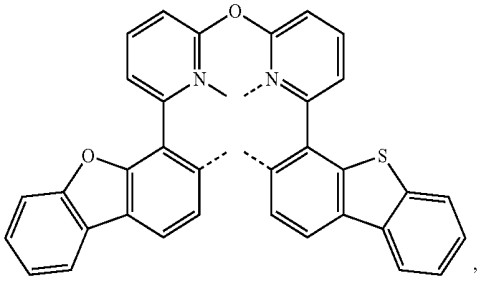

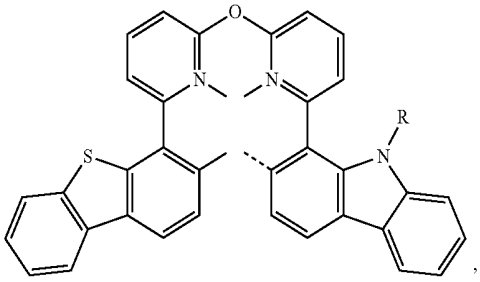

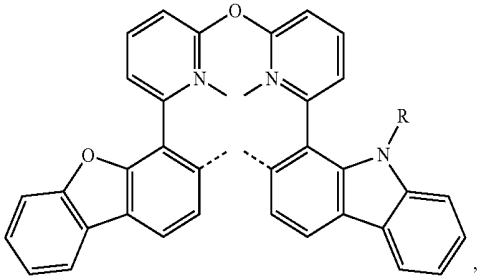

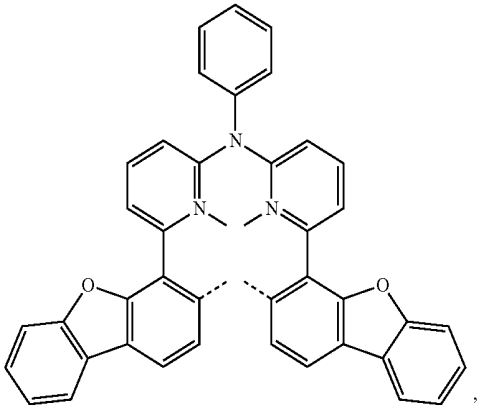

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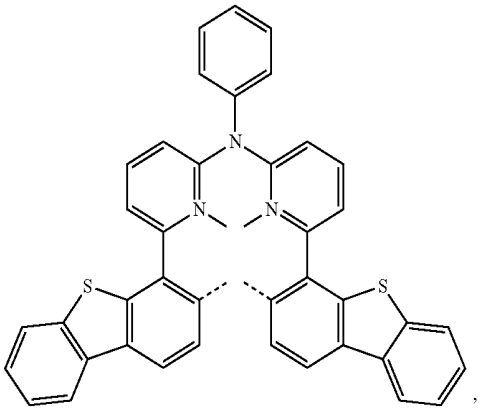

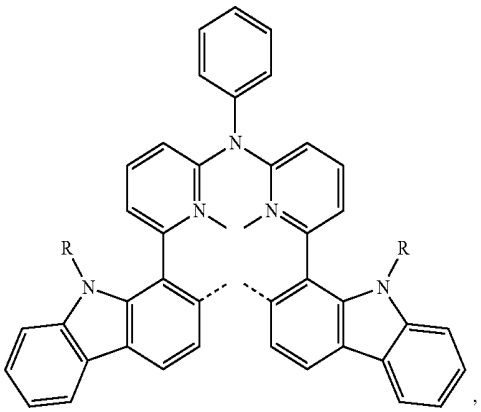

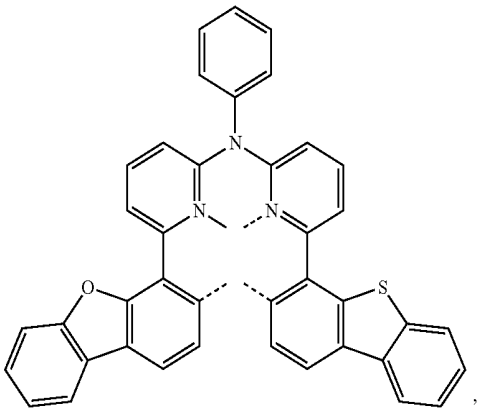

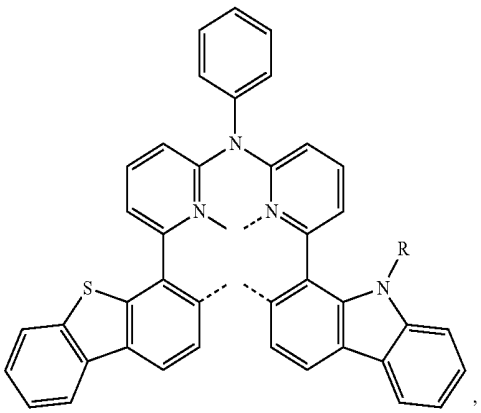

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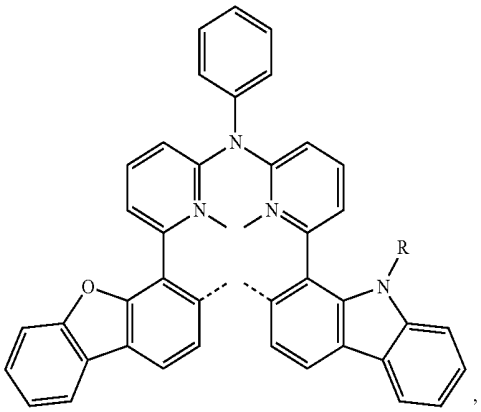

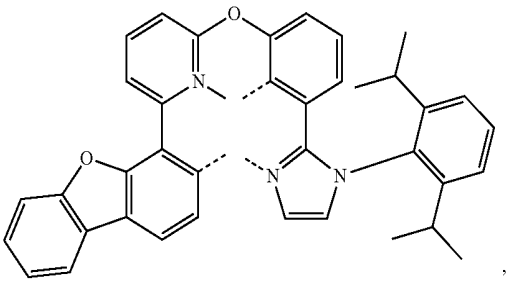

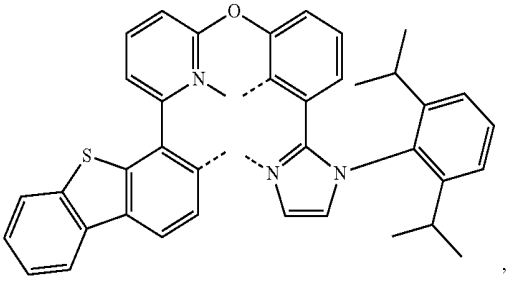

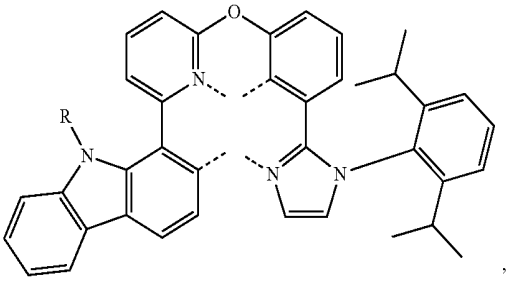

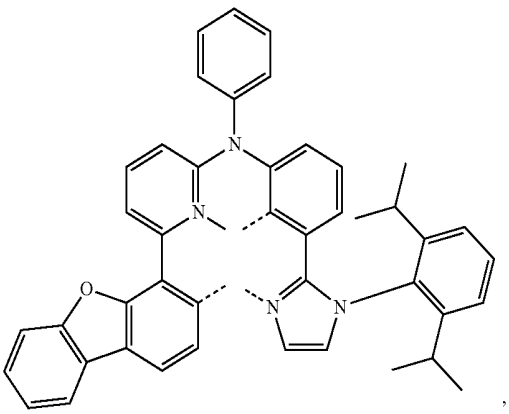

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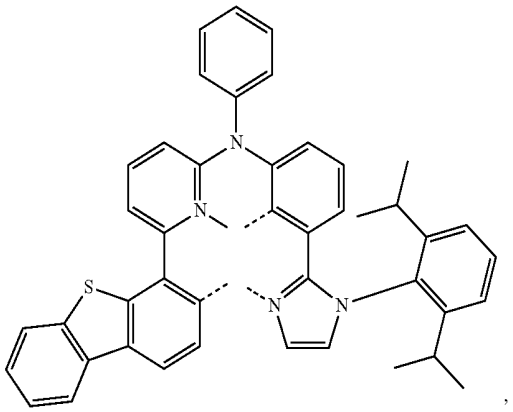

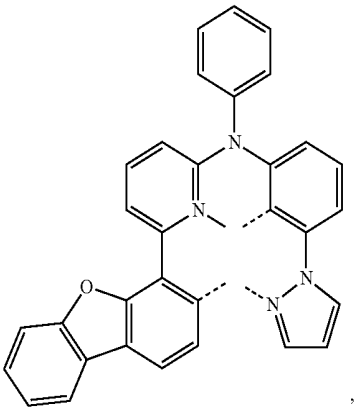

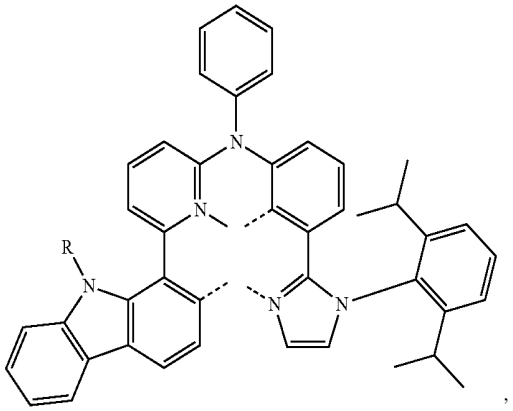

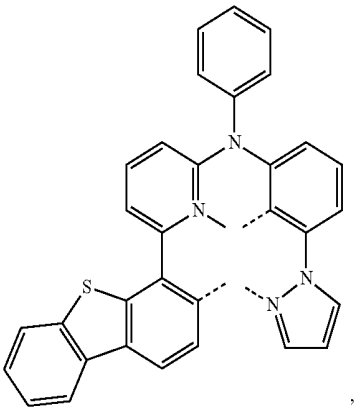

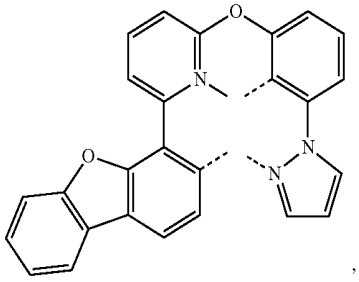

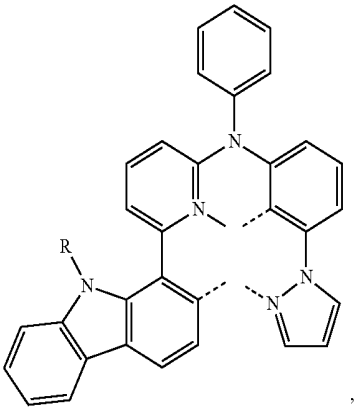

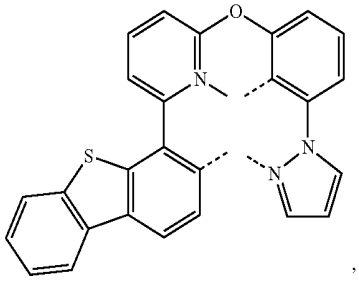

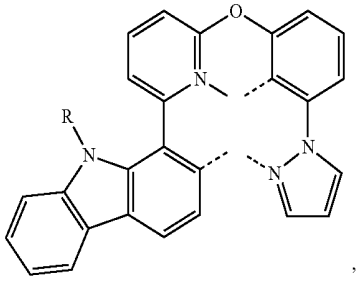

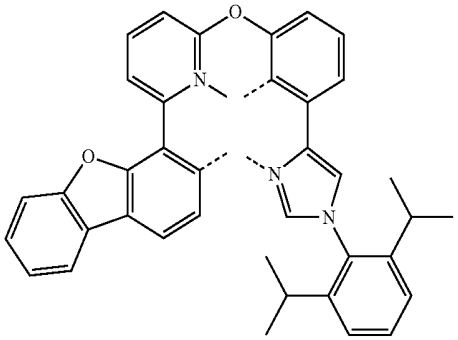

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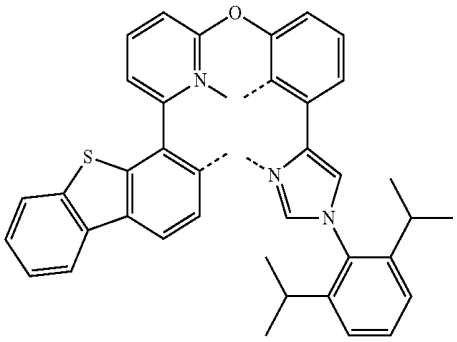

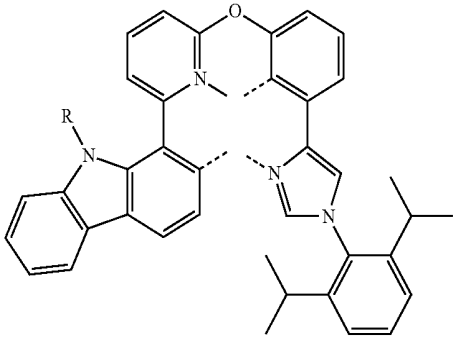

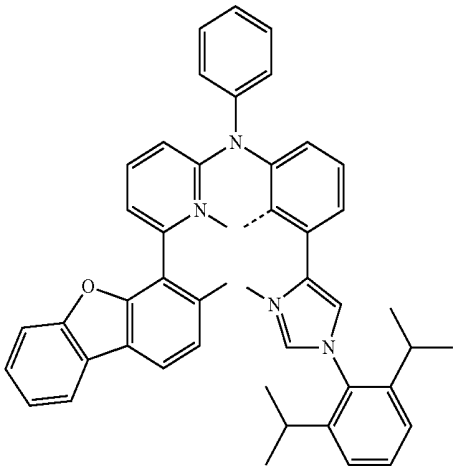

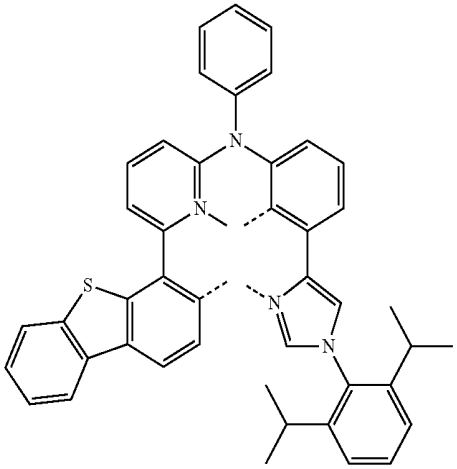

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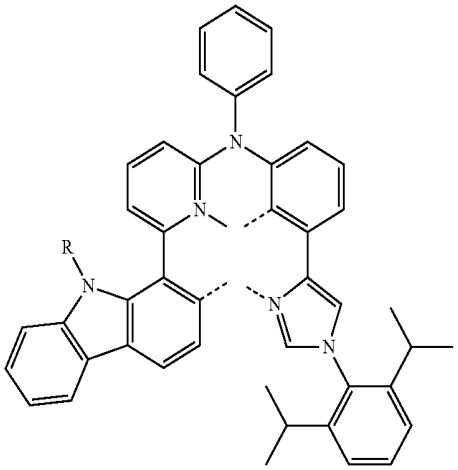

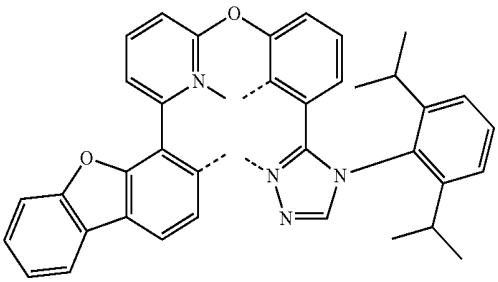

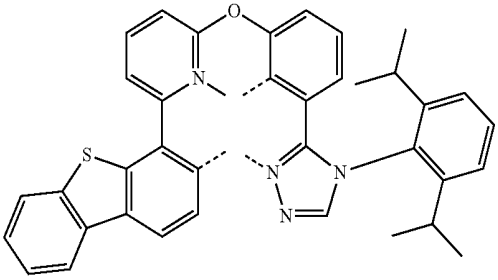

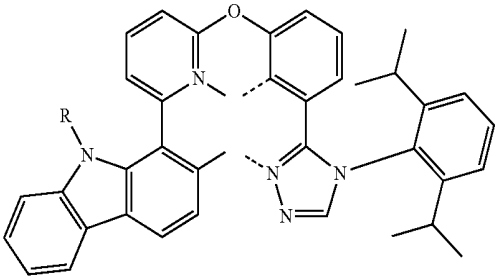

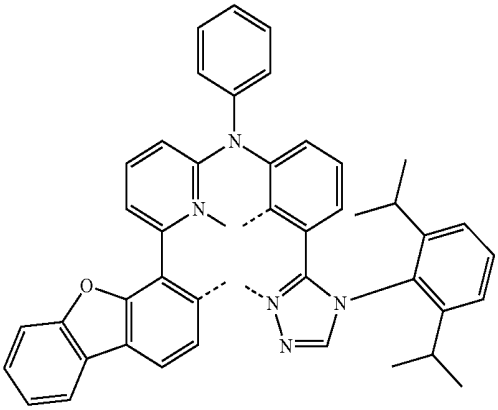

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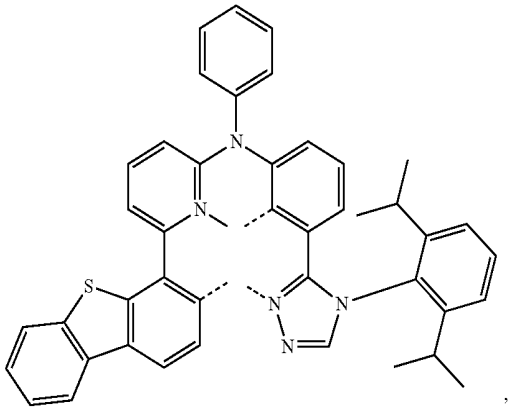

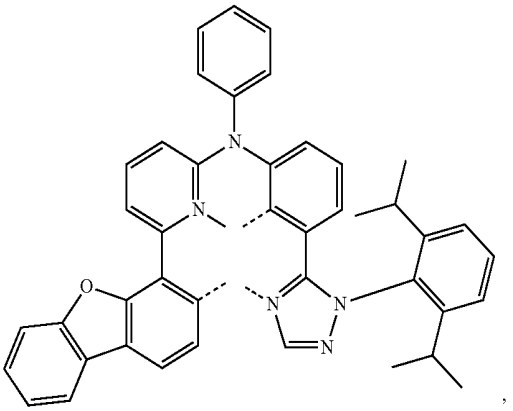

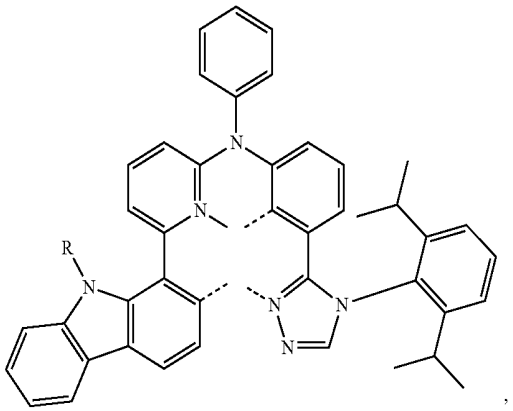

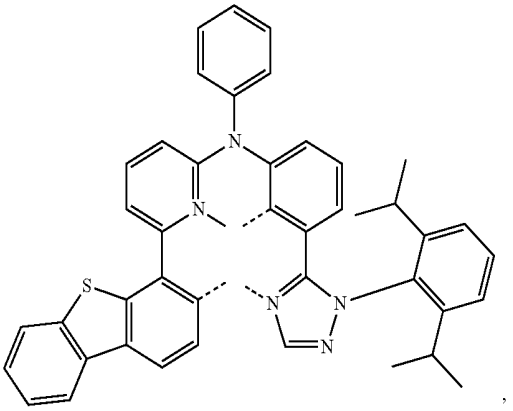

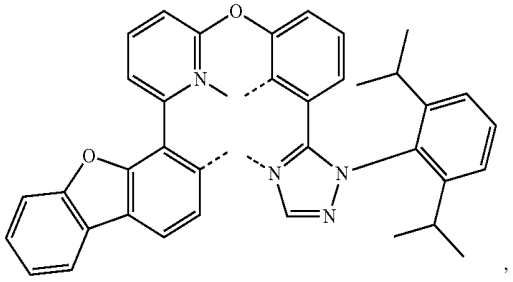

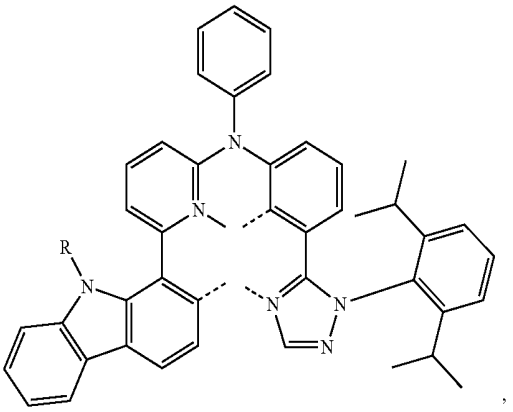

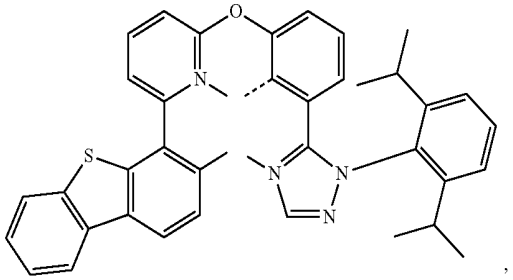

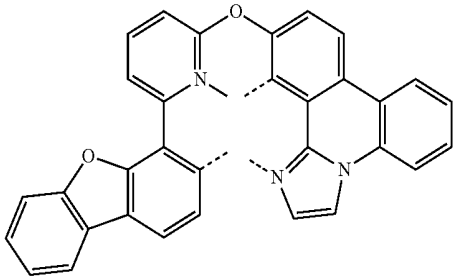

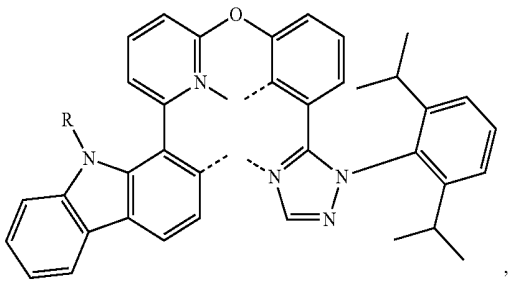

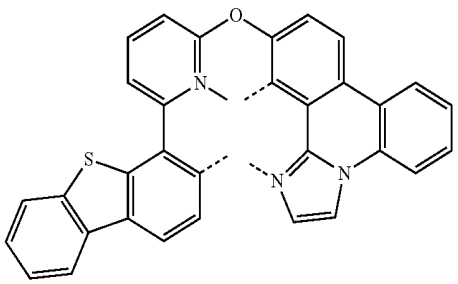

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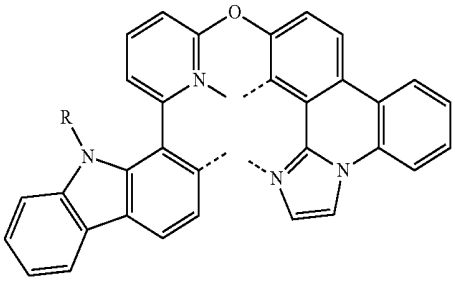

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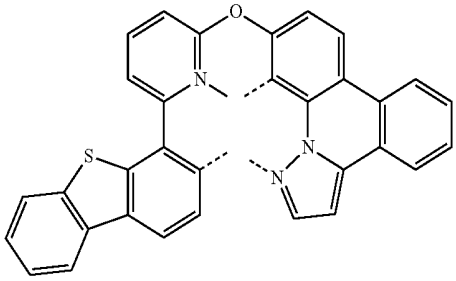

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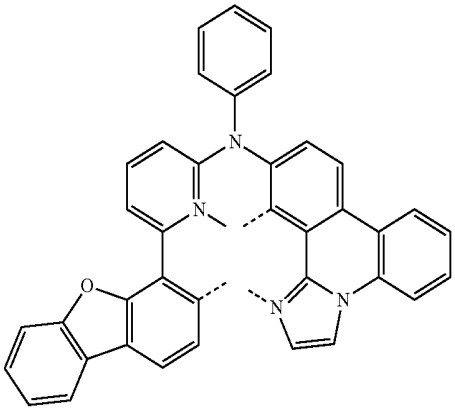

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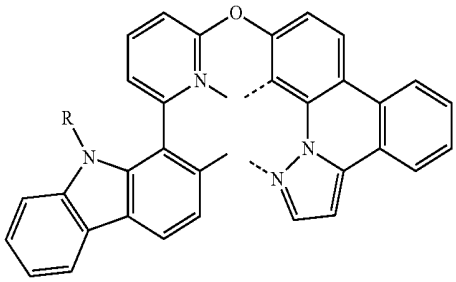

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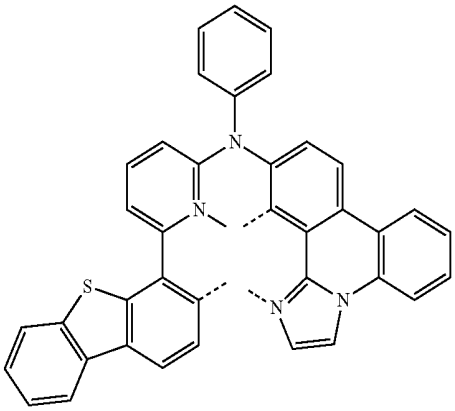

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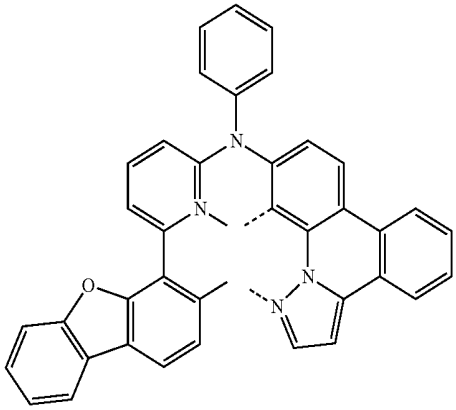

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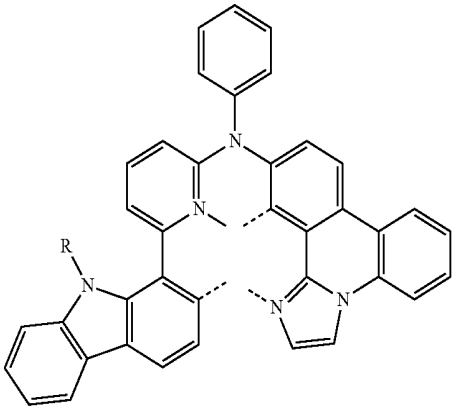

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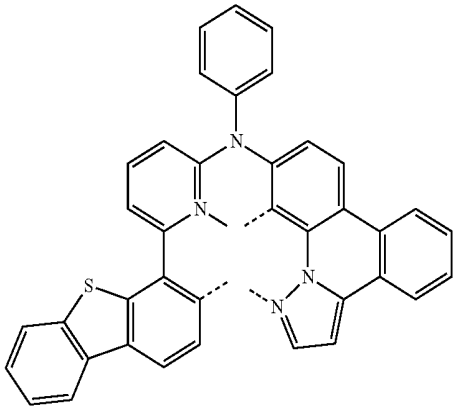

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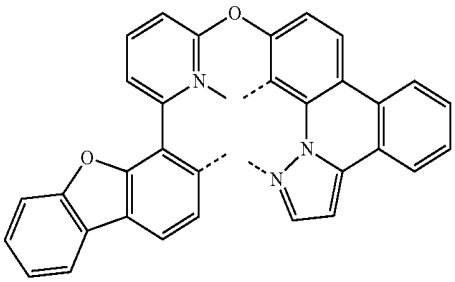

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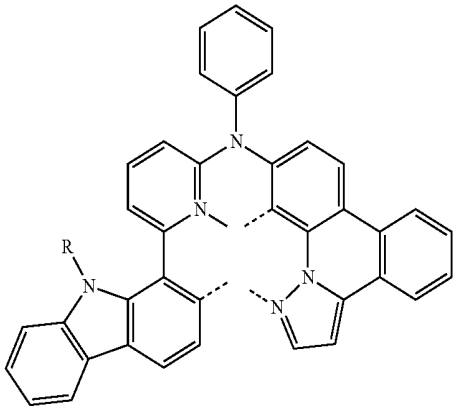

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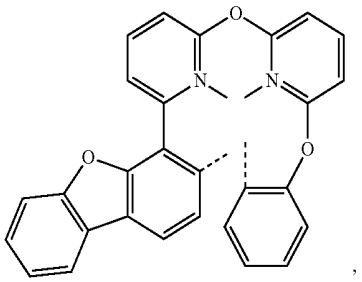

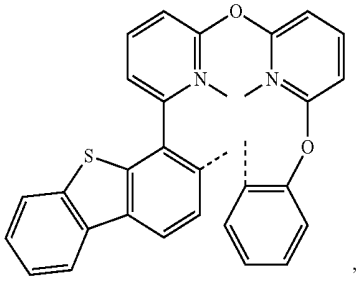

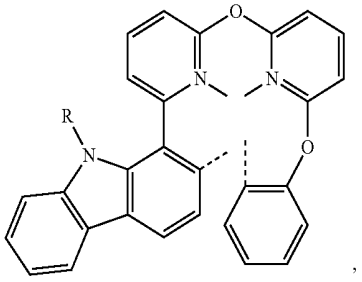

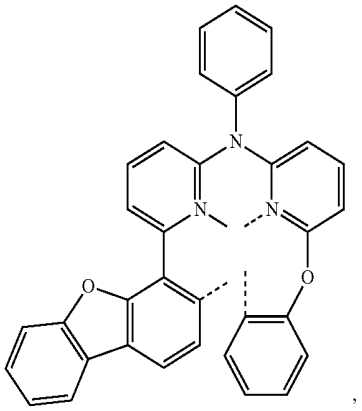

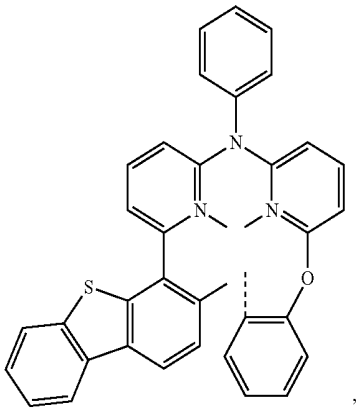

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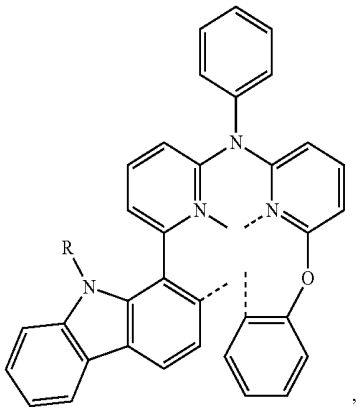

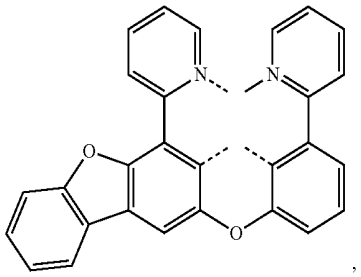

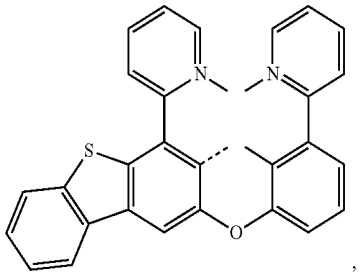

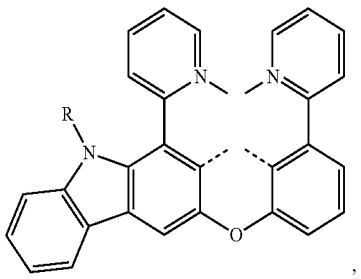

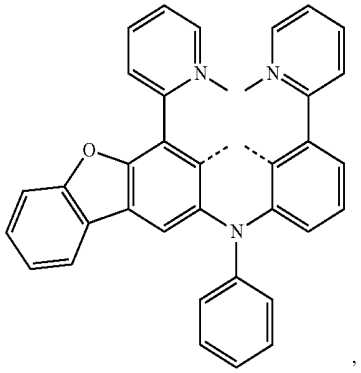

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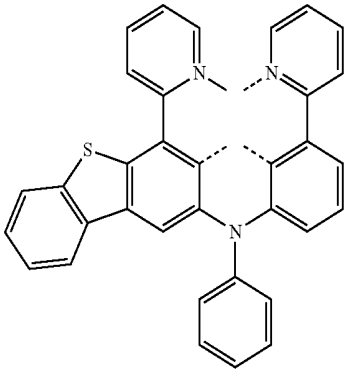

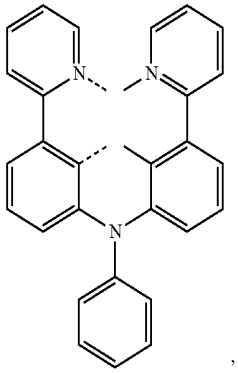

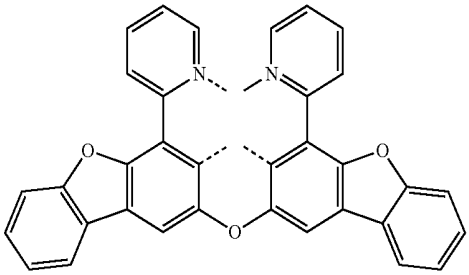

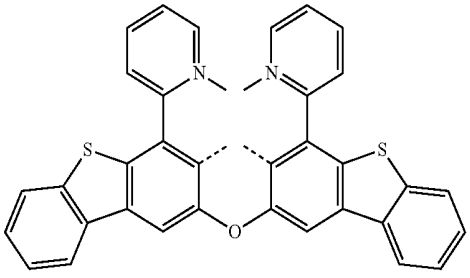

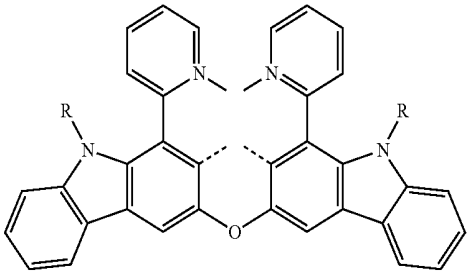

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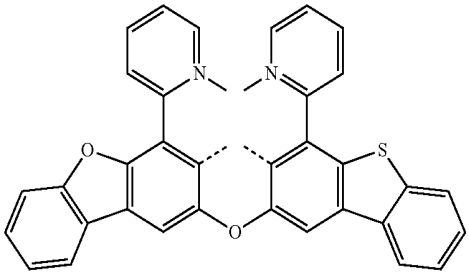

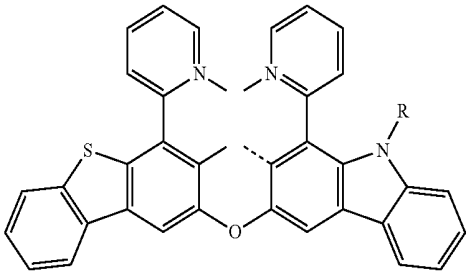

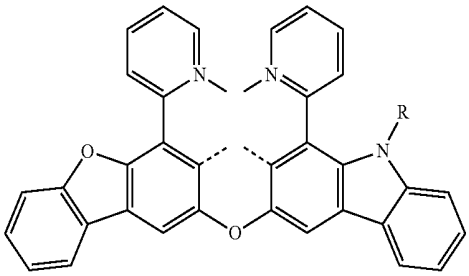

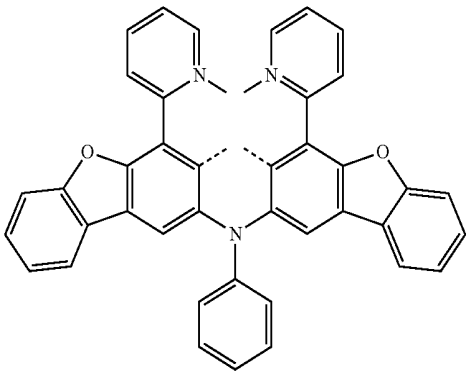

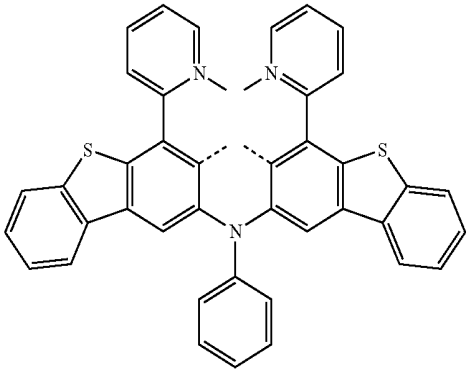

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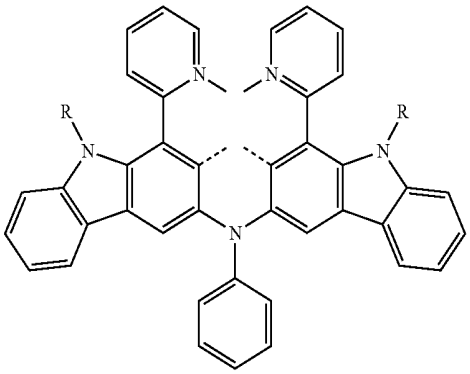

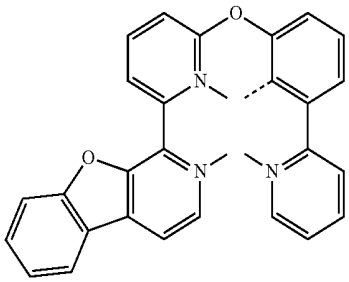

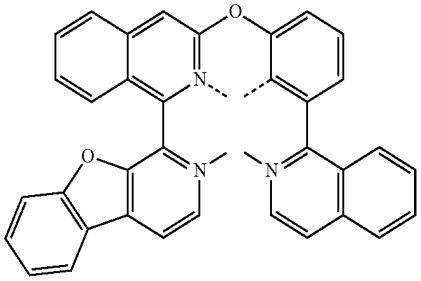

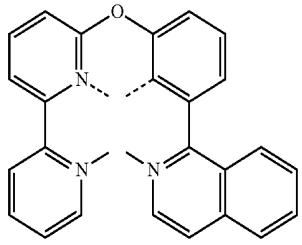

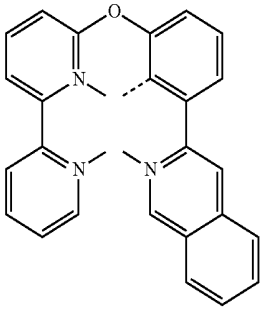

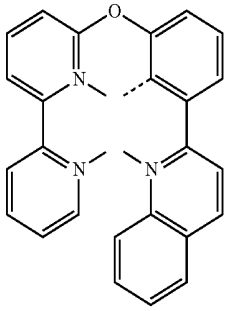

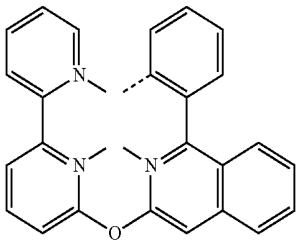

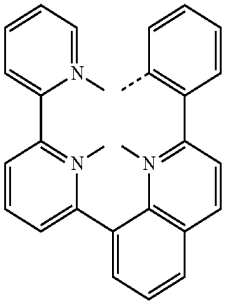

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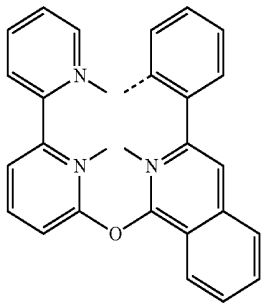

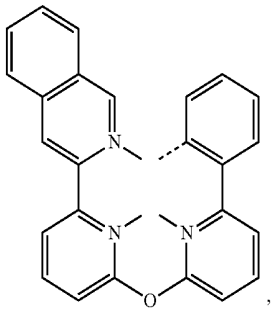

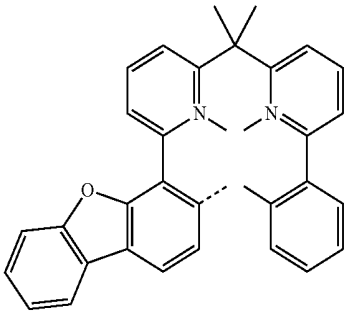

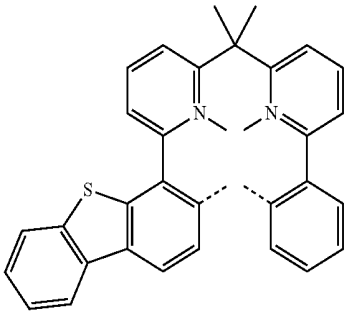

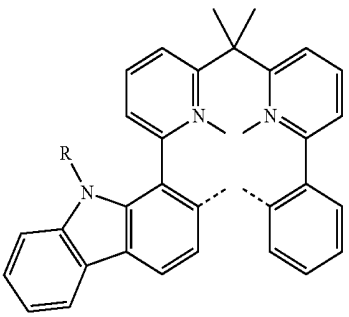

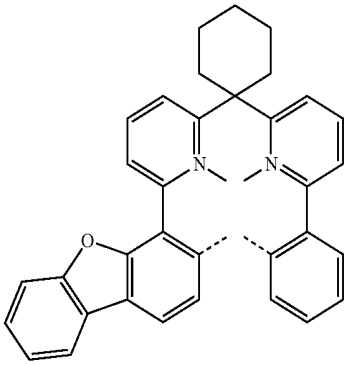

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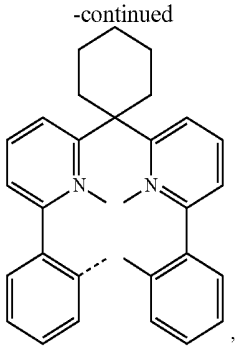

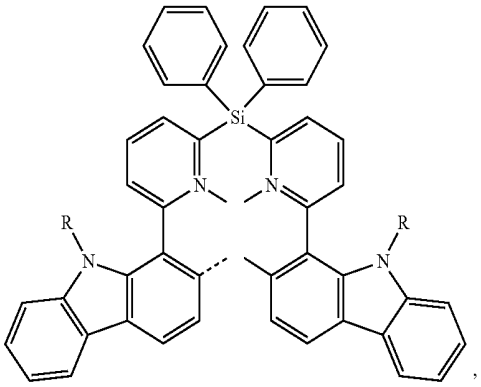

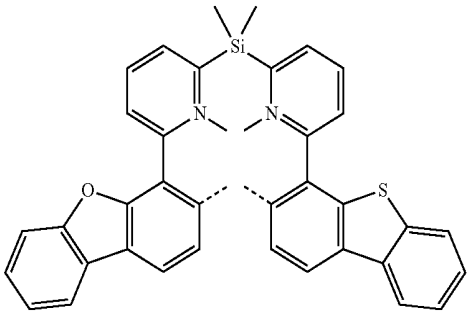

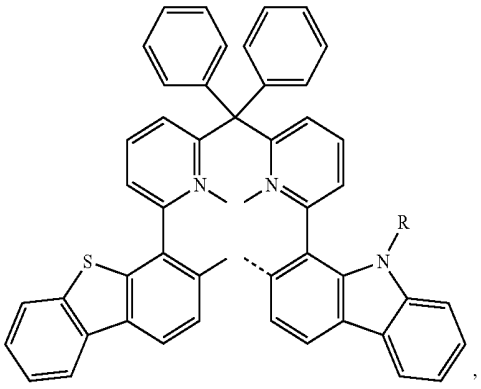

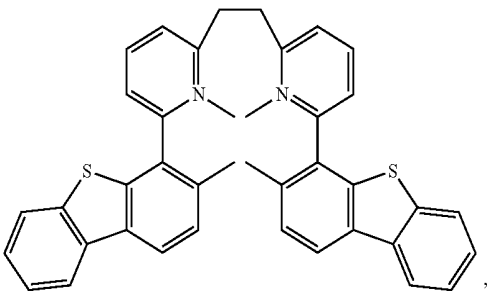

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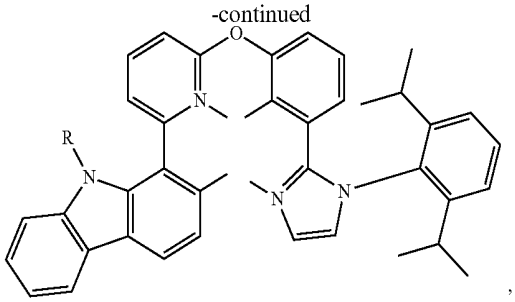

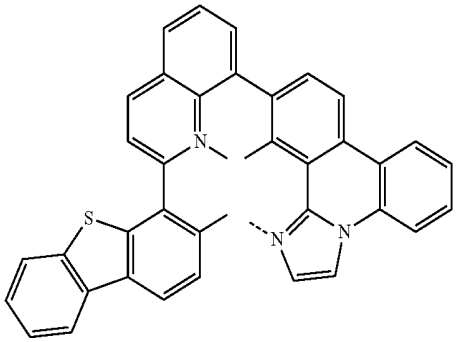

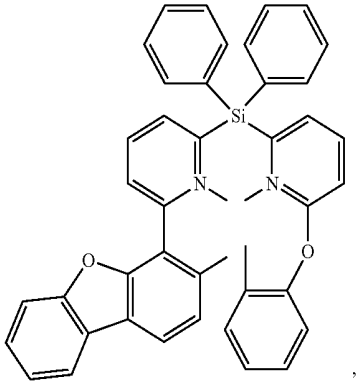

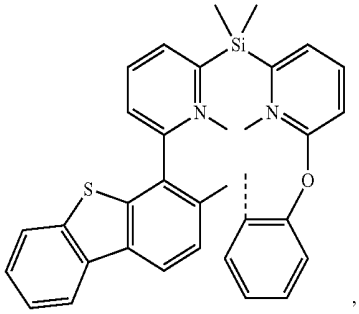

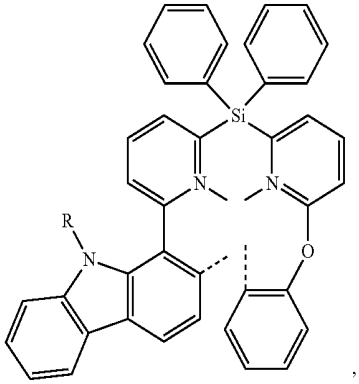

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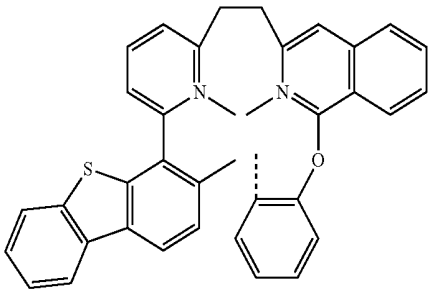

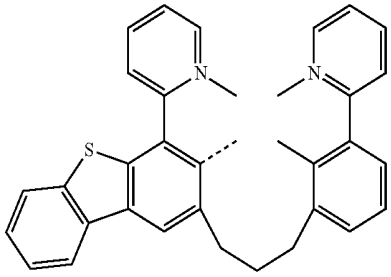

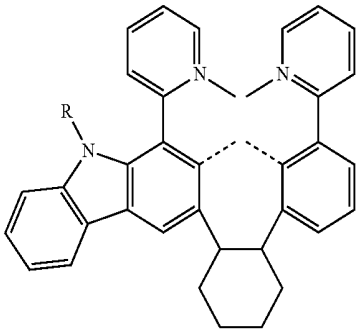

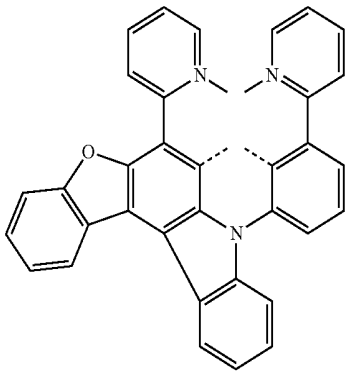

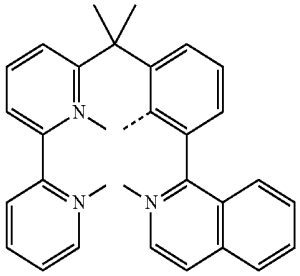

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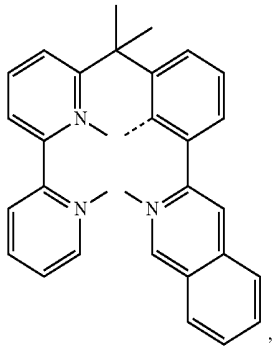


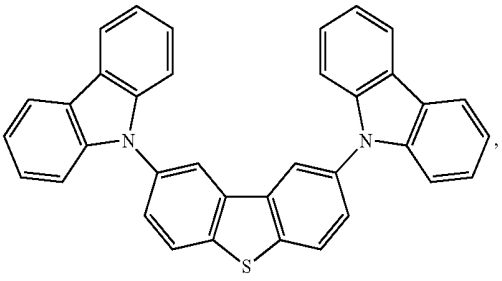
wherein R is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl,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

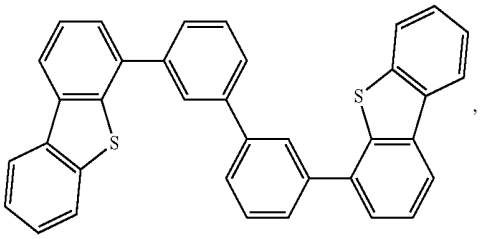
According to another aspect of the present disclosure, a first device is also provided. The first device includes a first organic light emitting device, that includes an anode, a cathode, and an organic layer disposed between the anode and the cathode. The emissive layer may include a host and a phosphorescent dopant. The emissive layer can include a compound according to one of Formula (I), Formula (II), and Formula (III), and the variations thereof as described herein.

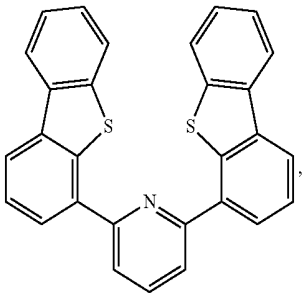
The first device can be one or more of a consumer product, an organic light-emitting device and a lighting panel. The organic layer can be an emissive layer and the compound can be an emissive dopant in some embodiments, while the compound can be a non-emissive dopant in other embodiments.

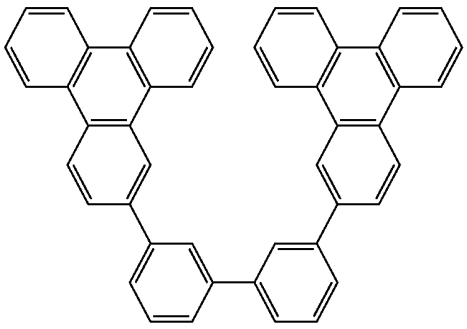
The organic layer can also include a host. In some embodiments, the host can include a metal complex. The host can be a triphenylene containing benzo-fused thiophene or benzo-fused furan. Any substituent in the host can be an unfused substituent independently selected from the group consisting of C_nH_{2n+1}, 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, $Ar_1{-}Ar_2$, $C_nH_{2n}{-}Ar_1$, 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.

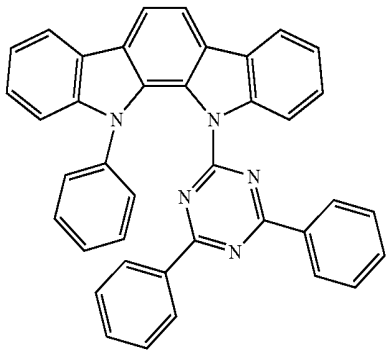
The host can be a compound selected from the group consisting of carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene. The "aza" designation in the fragments described above, i.e., aza-dibenzofuran, aza-dibenzonethiophene, 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. The host can include a metal complex. The host can be a specific compound selected from the group consisting of:











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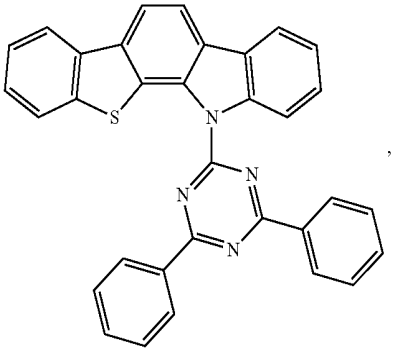
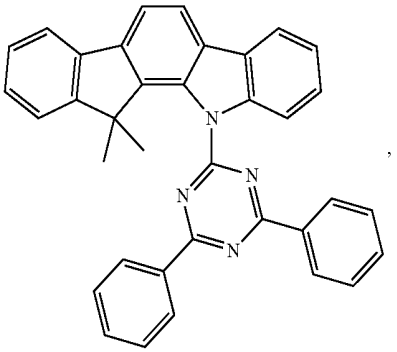
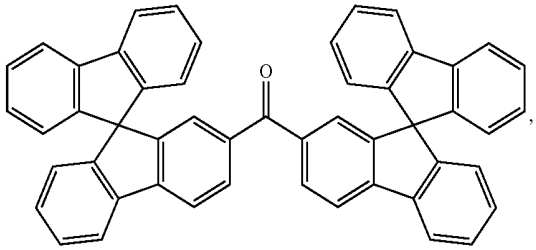
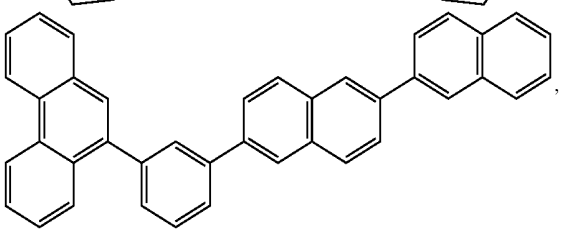
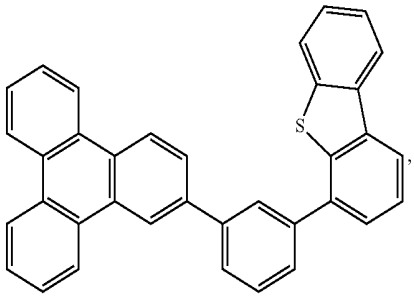
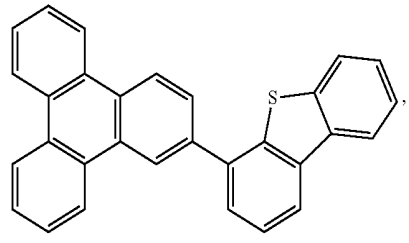












and combinations thereof.

In yet another aspect of the present disclsoure, a formulation that comprises a compound according to Formula (I), Formula (II) or Formula (III), and the variants thereof as

described herein. 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.

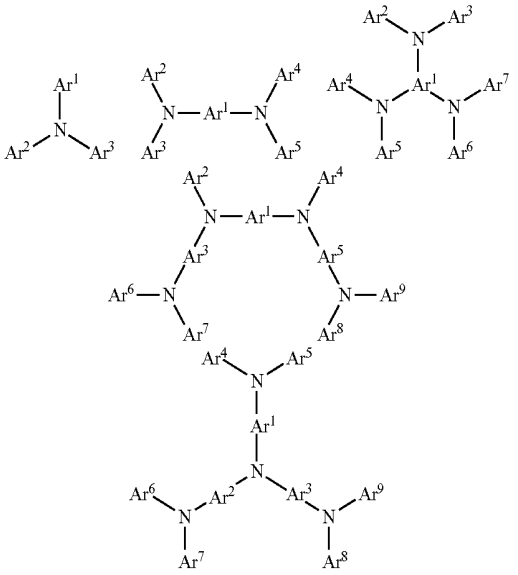
Combination with Other Materials

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:

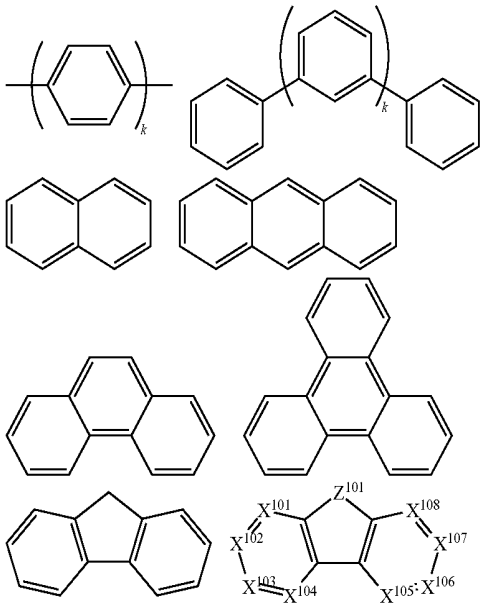
A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphryin derivative;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

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



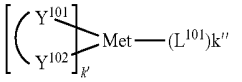
Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as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

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.

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

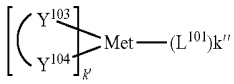
maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

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.

Host:

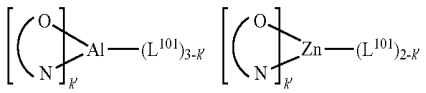
The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes 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.

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.

In one aspect, the metal complexes are:

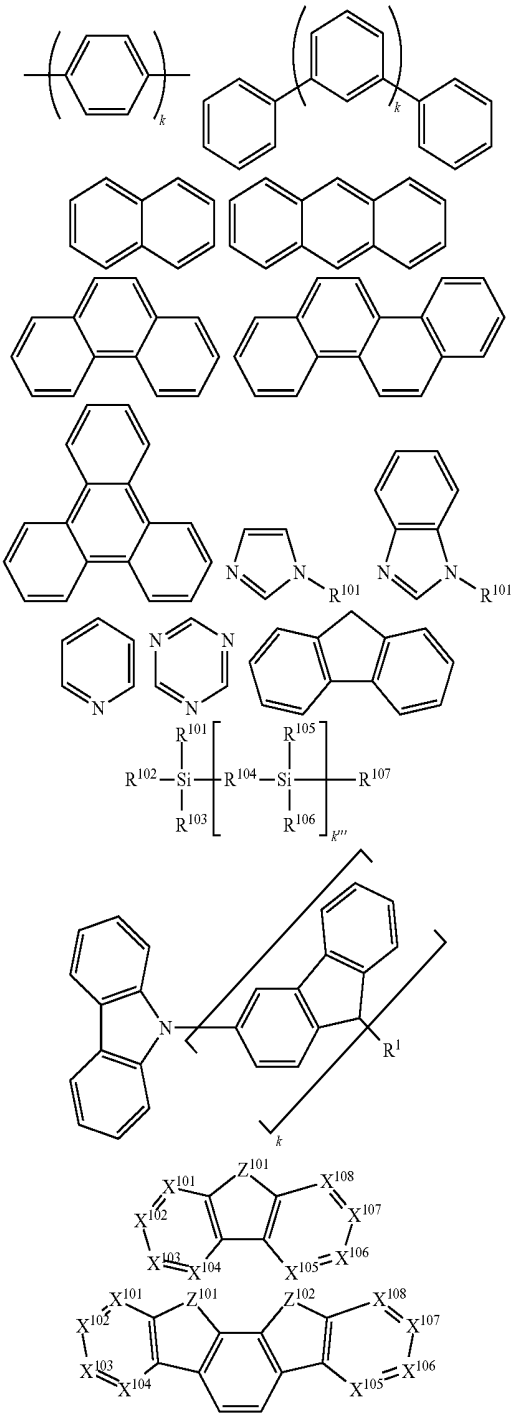


wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

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

Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atome, 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, sulfanyl, sulfonyl, phosphino, and combinations thereof.

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



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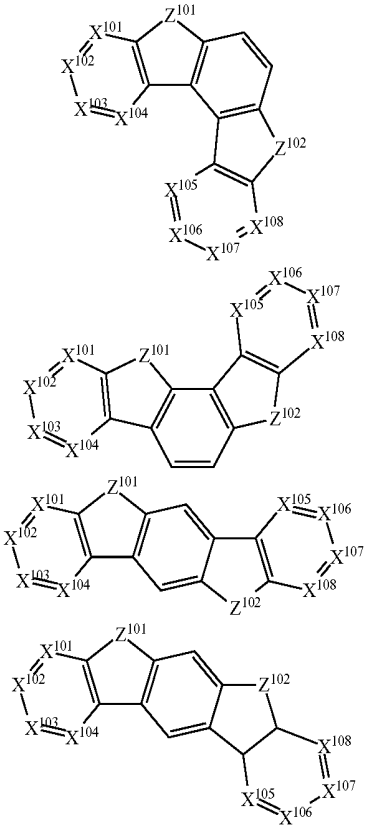


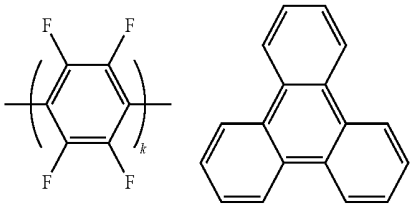
wherein R^{101} to R^{107} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, 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:

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.

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

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



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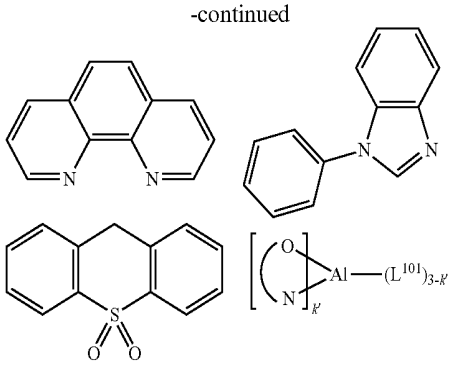
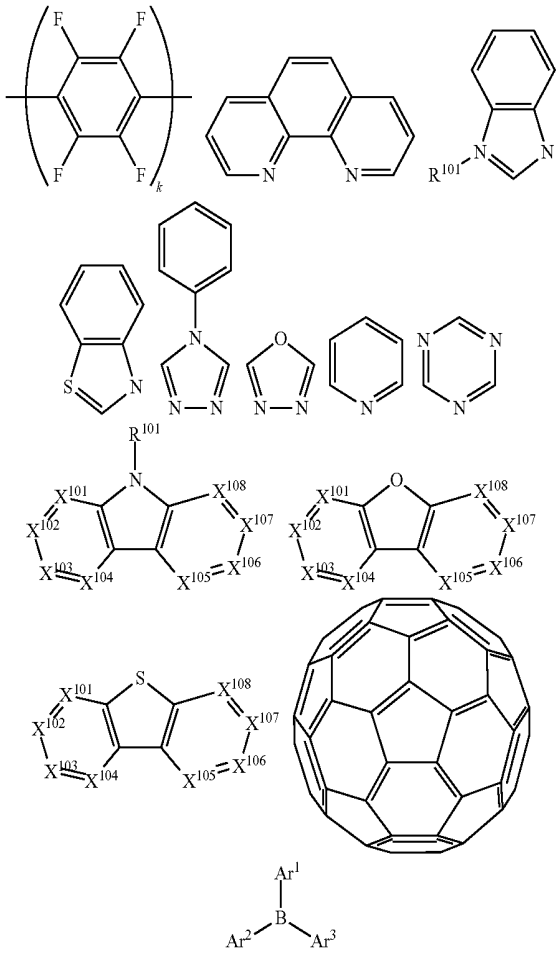


wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

ETL:

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.

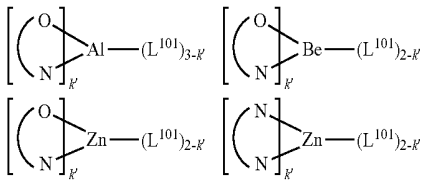
In one aspect, compound used in ETL contains at least one of the following groups in the molecule:



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.

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.

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.

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

TABLE 1

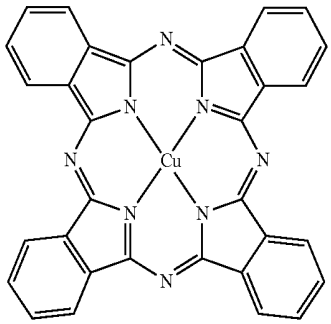
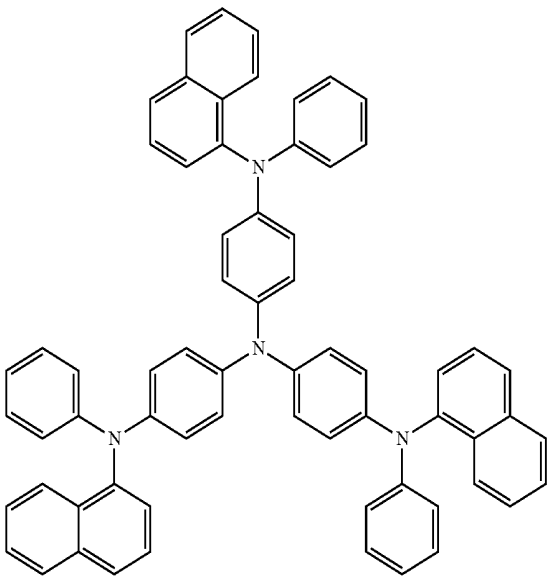
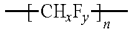
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydrocarbon polymer		Appl. Phys. Lett. 78, 673 (2001)

TABLE 1-continued

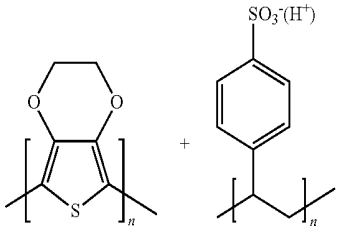
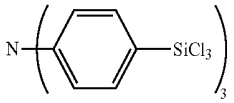
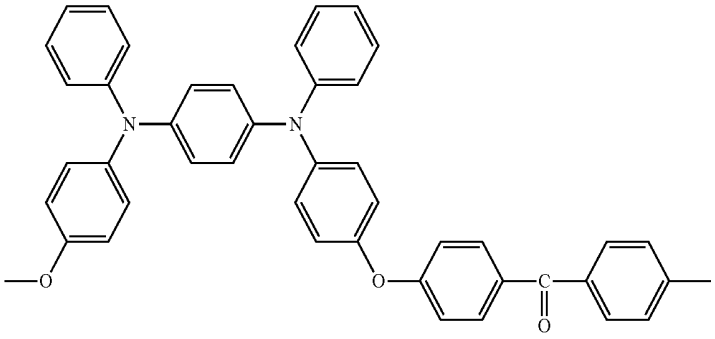
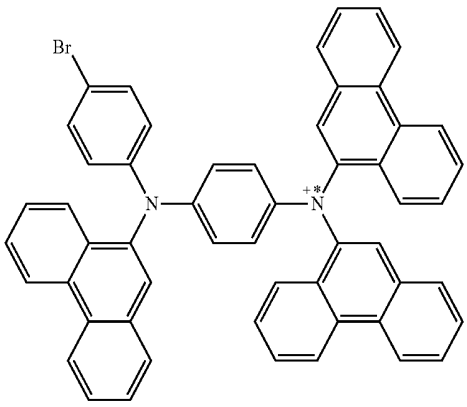
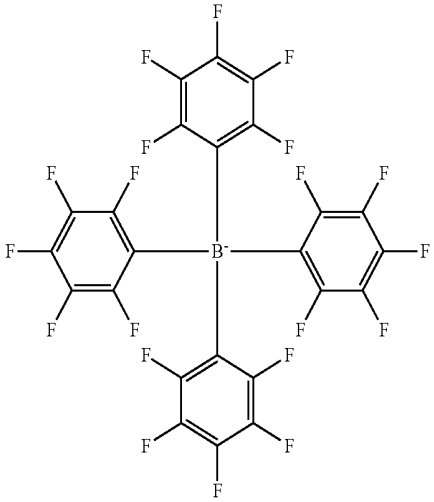
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and sliane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants	 and  	EP1725079A1

TABLE 1-continued

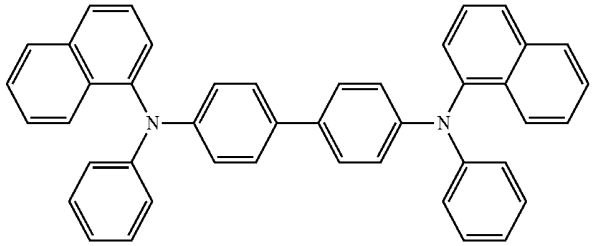
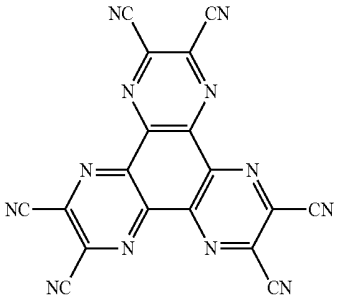
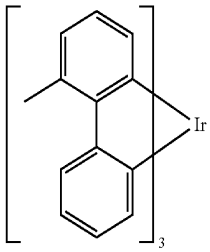
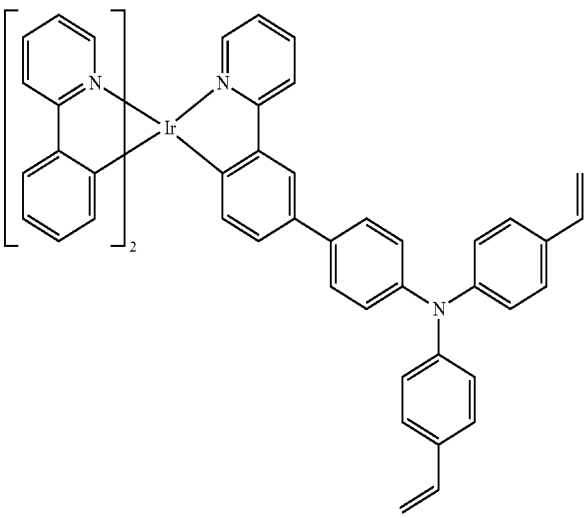
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides	 + MoO_x	US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009
n-type semi-conducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279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

TABLE 1-continued

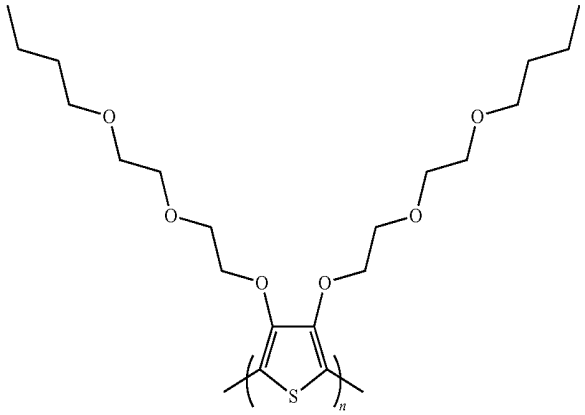
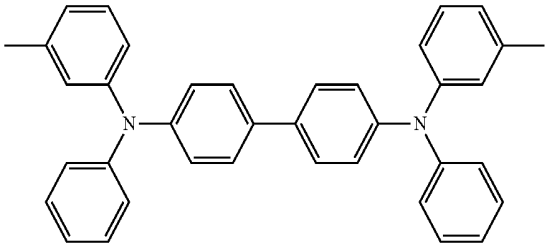
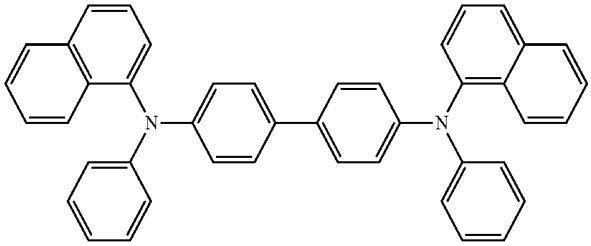
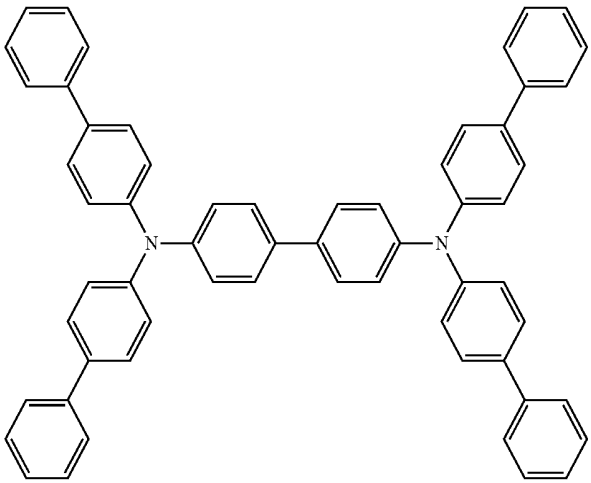
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216
	Hole transporting materials	
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5,061,569
		EP650955

TABLE 1-continued

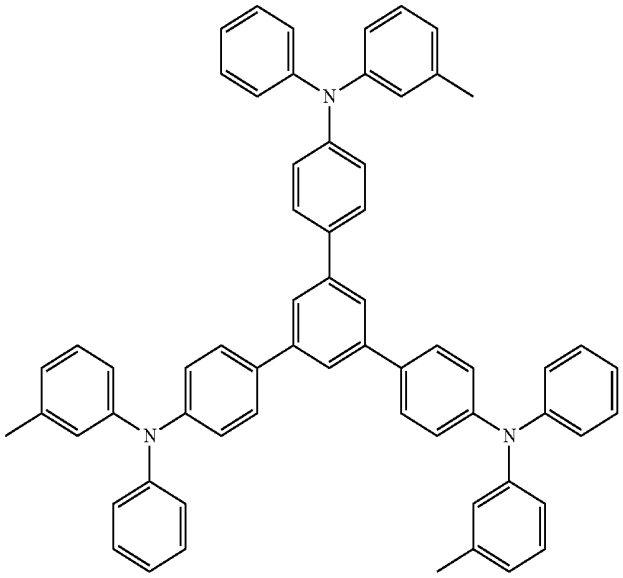
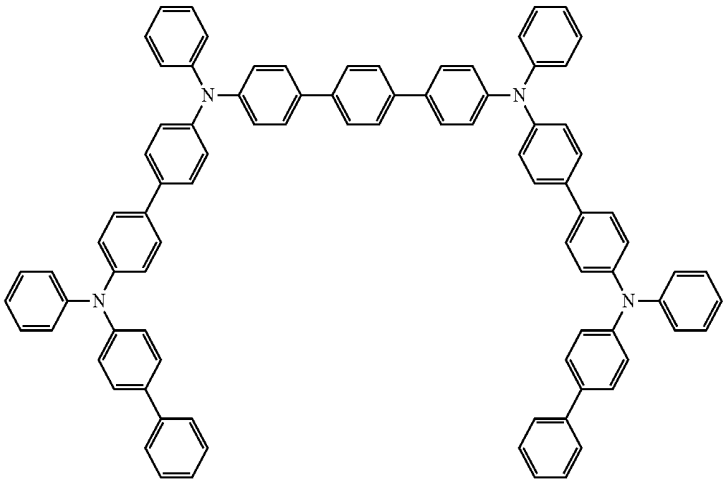
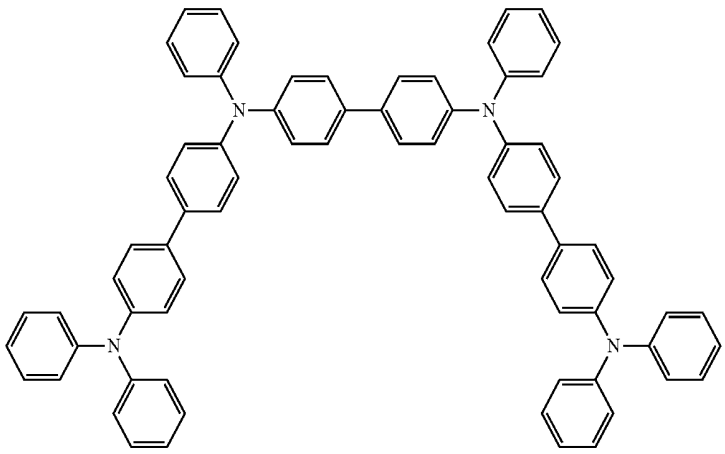
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE 1-continued

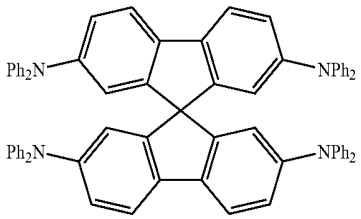
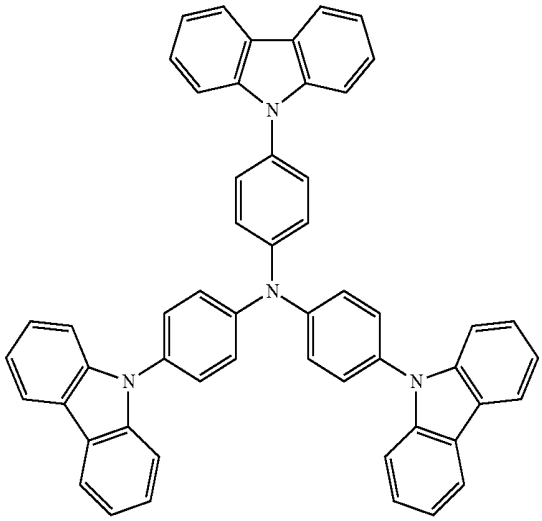
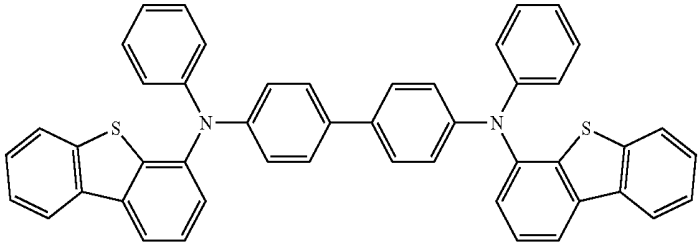
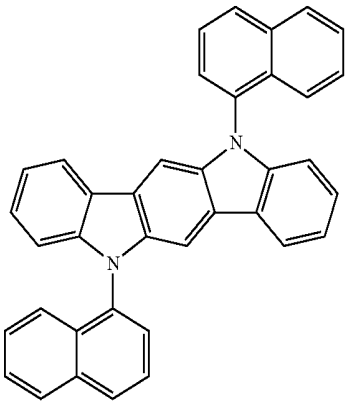
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190 US20110163302
Indolocarbazoles		Synth. Met. 111, 421 (2000)

TABLE 1-continued

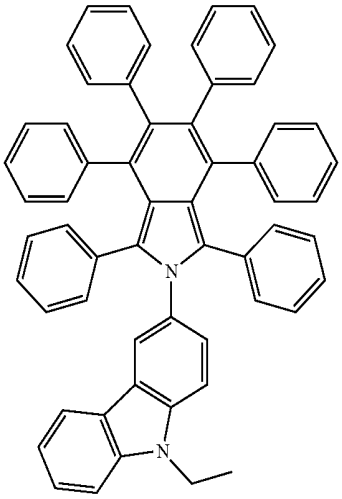
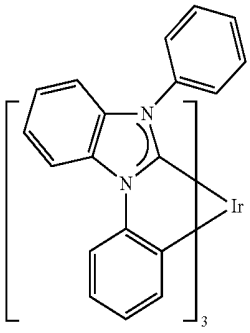
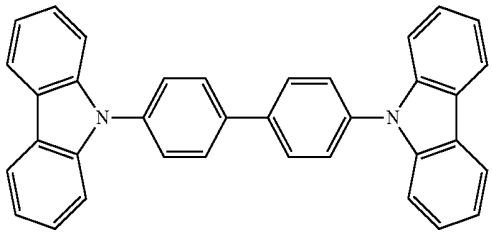
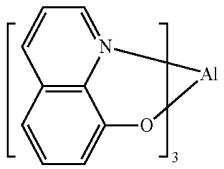
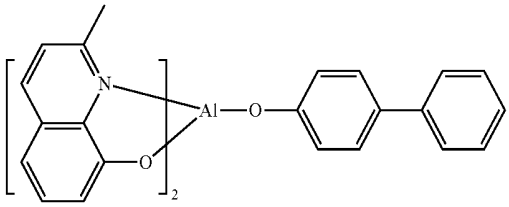
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials		
Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxy-quinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)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

TABLE 1-continued

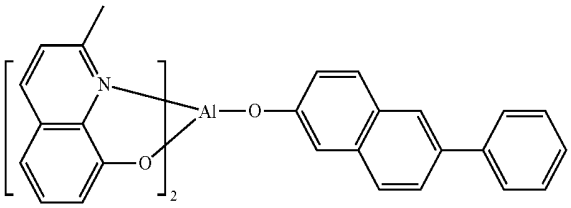
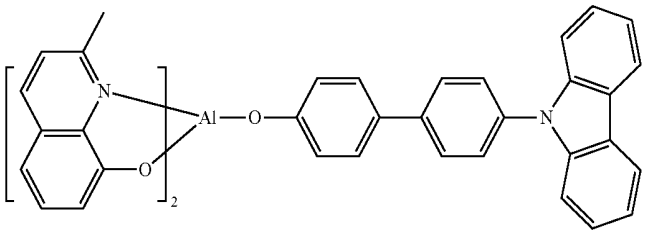
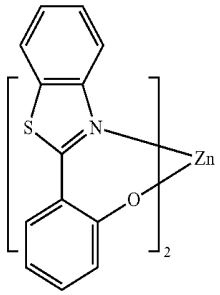
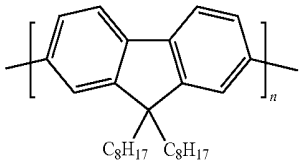
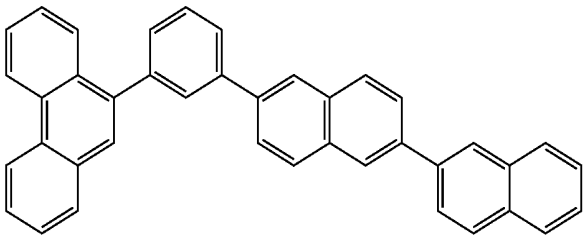
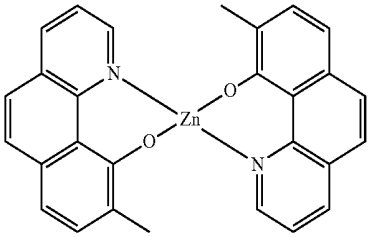
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2005014551
		WO2006072002
Metal phenoxy-benzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2010056066

TABLE 1-continued

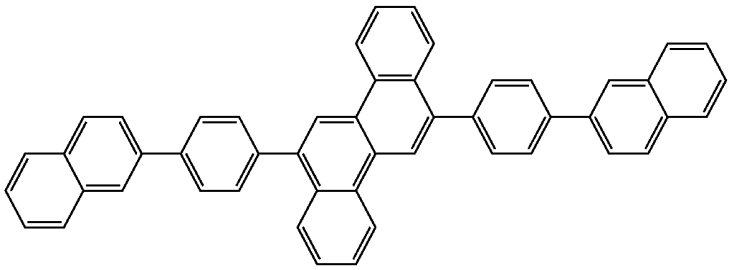
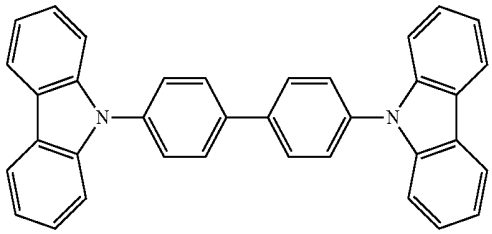
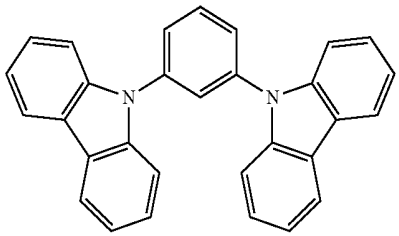
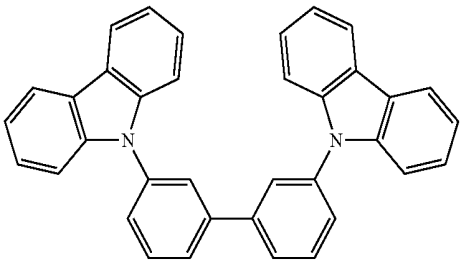
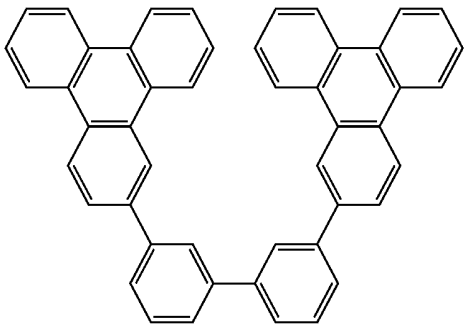
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Chrysene based compounds		WO2011086863
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE 1-continued

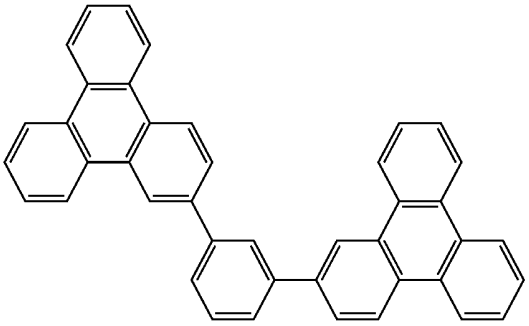
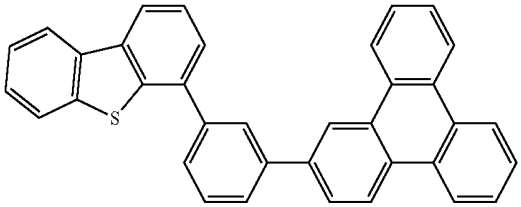
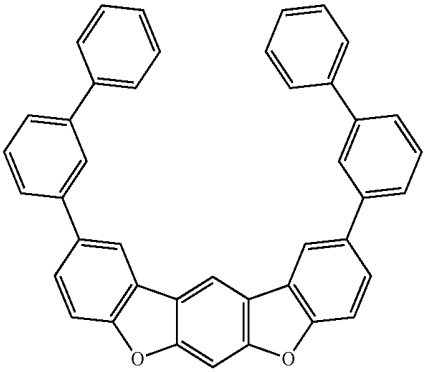
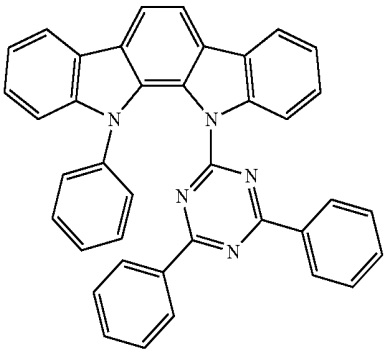
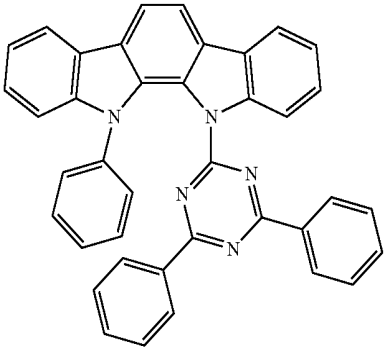
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060280965
		WO2009021126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931
Donor acceptor type molecules		WO2008056746
		WO2010107244

TABLE 1-continued

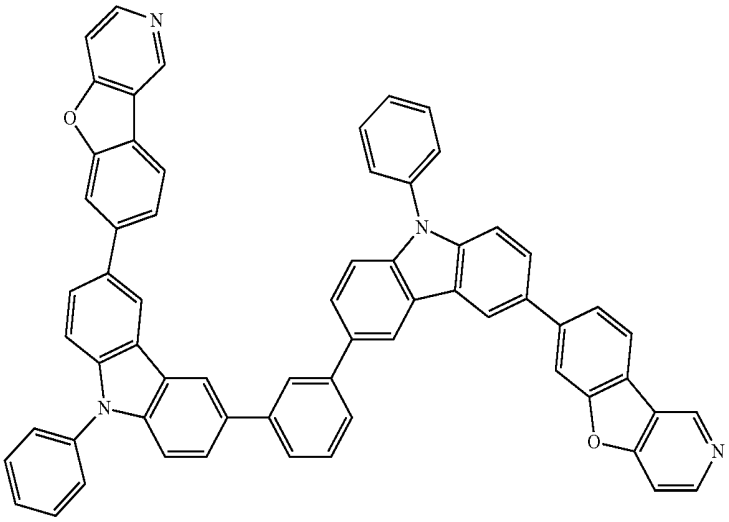
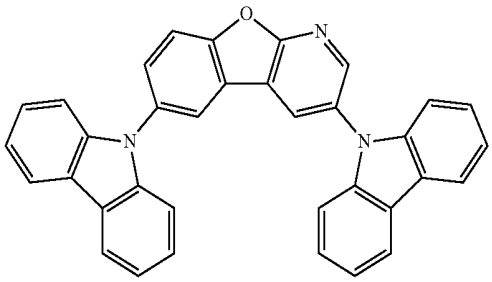
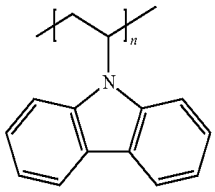
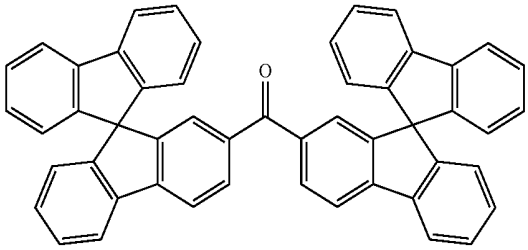
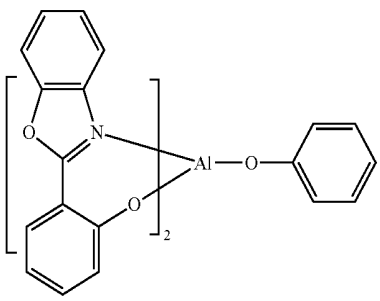
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza-carbazole/ DBT/DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207
Metal phenoxy-benzooxazole compounds		WO2005089025

TABLE 1-continued

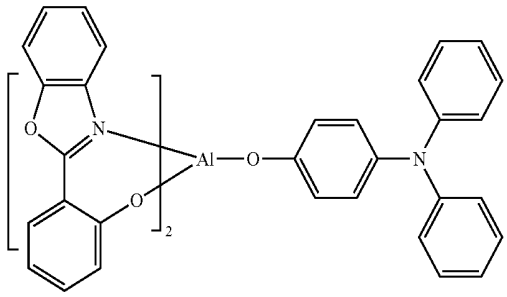
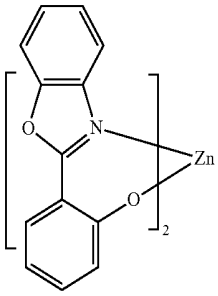
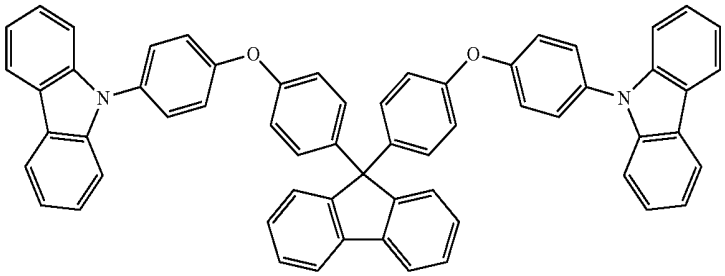
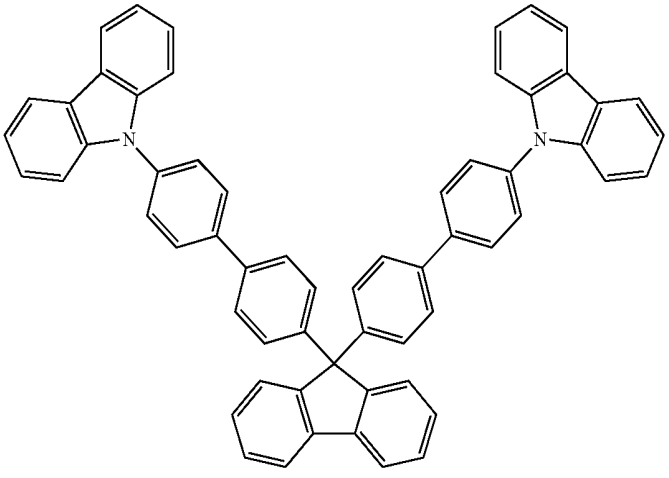
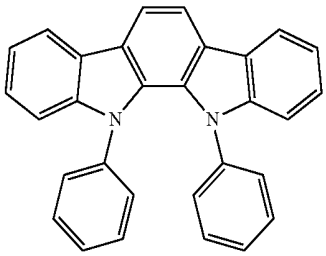
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297
Indolocabazoles		WO2007063796

TABLE 1-continued

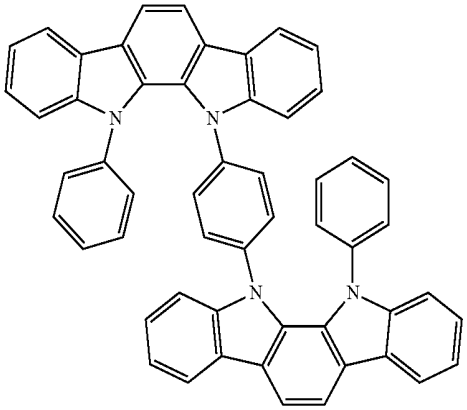
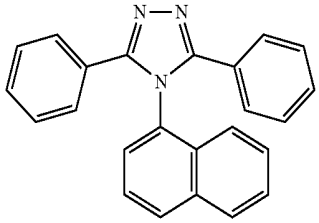
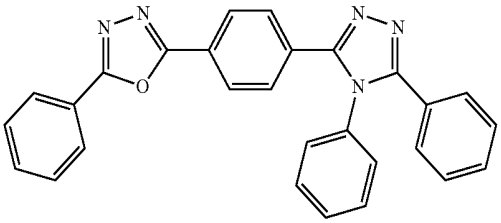
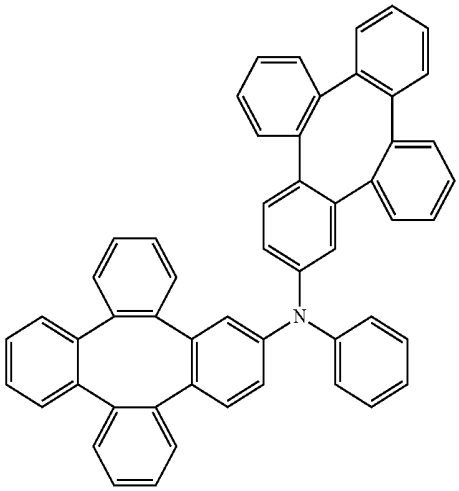
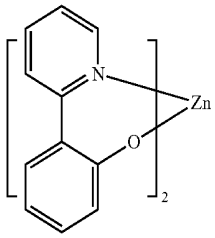
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900

TABLE 1-continued

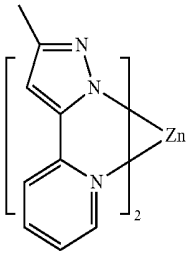
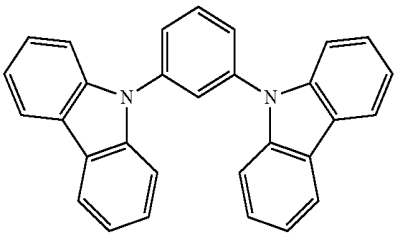
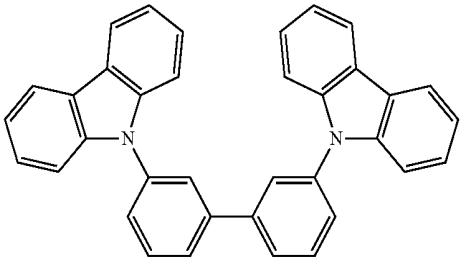
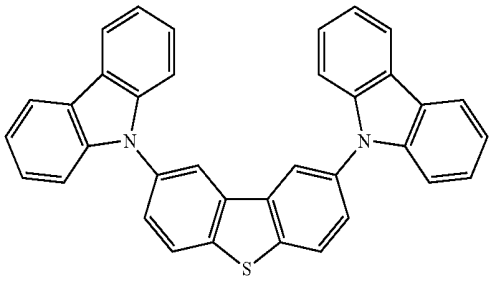
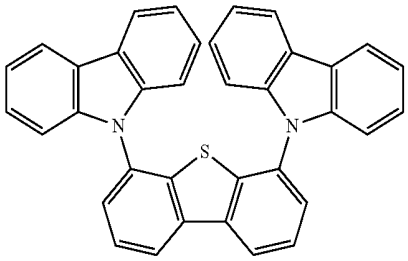
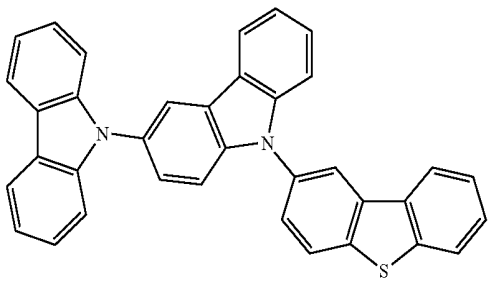
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/ Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162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

TABLE 1-continued

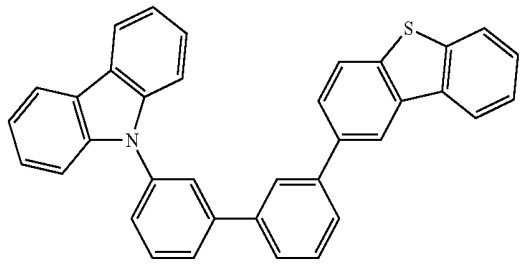
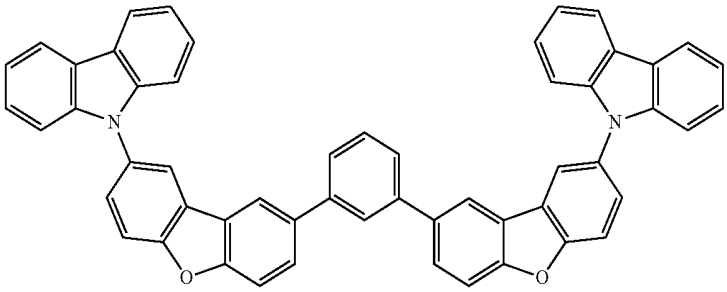
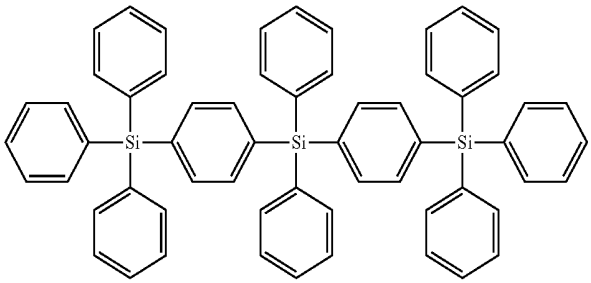
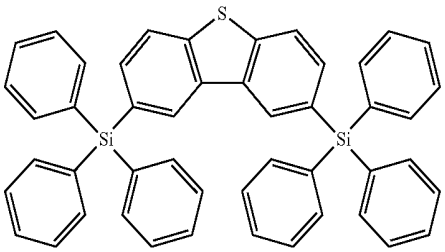
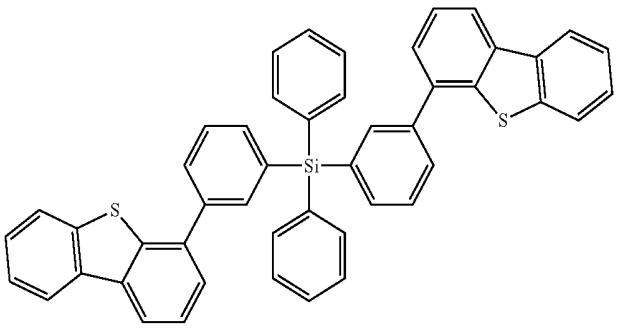
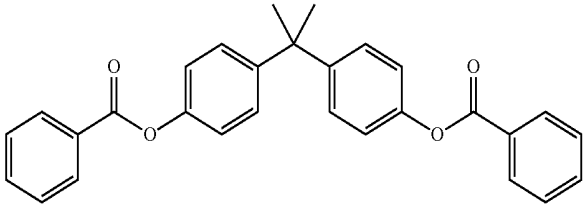
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090030202, US20090017330
		US20100084966
Silicon aryl compounds		US20050238919
		WO2009003898
Silicon/ Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298

TABLE 1-continued

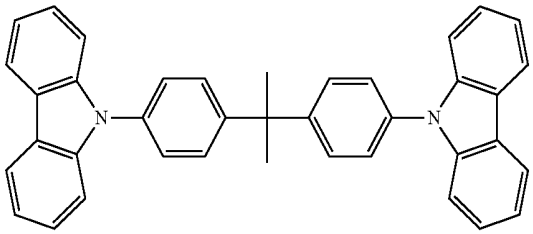
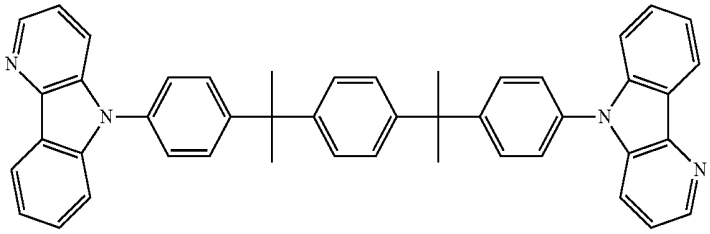
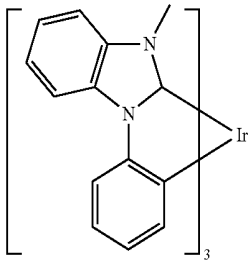
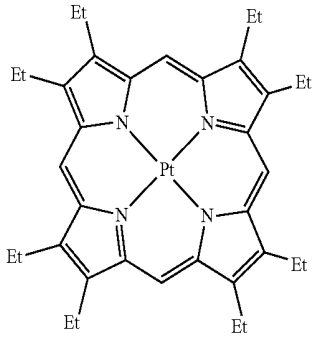
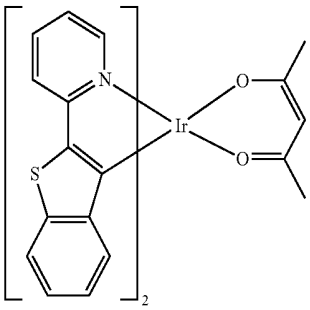
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114
Phosphorescent dopants Red dopants		
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

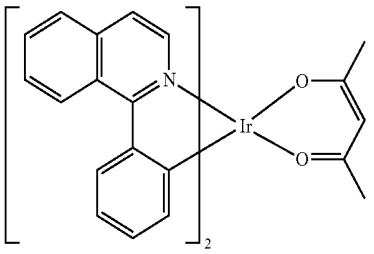
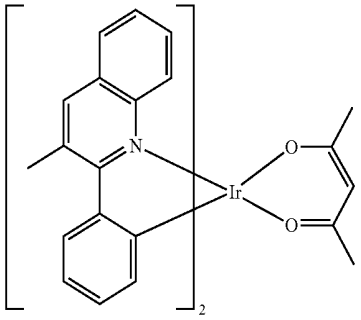
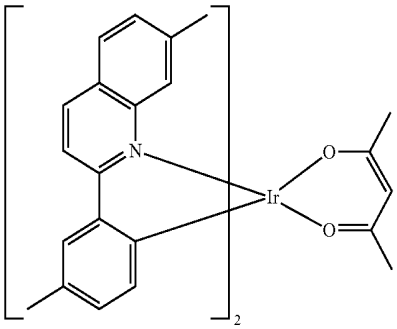
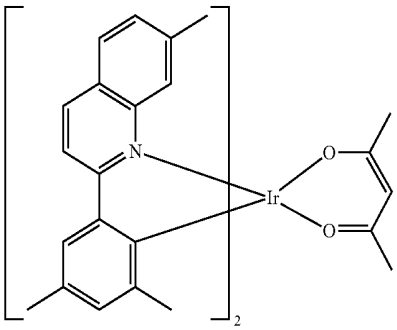
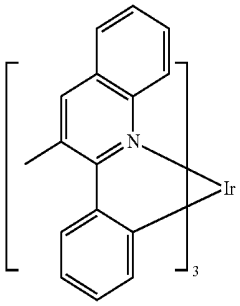
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US2006835469
		US2006835469
		US20060202194
		US20060202194
		US20070087321

TABLE 1-continued

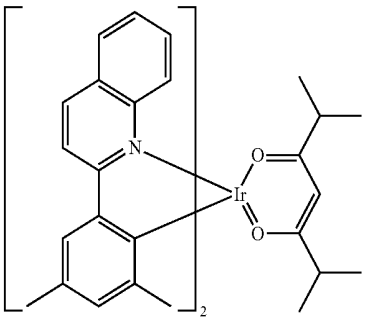
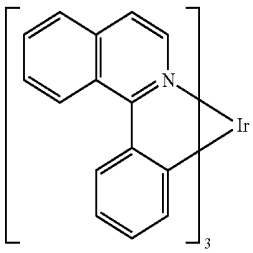
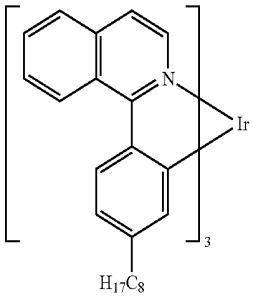
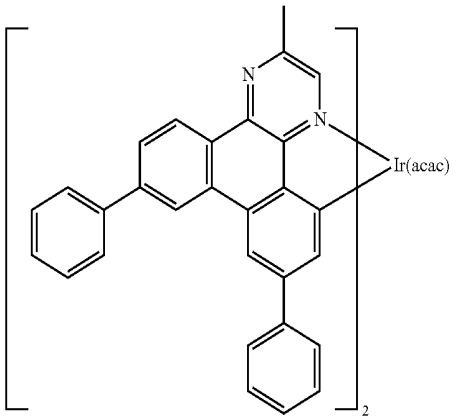
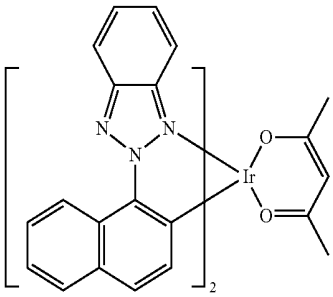
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20080261076 US20100090591
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842

TABLE 1-continued

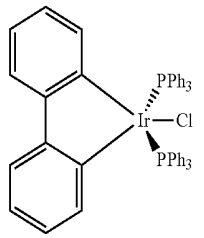
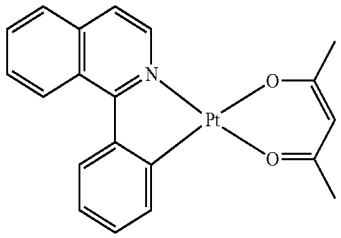
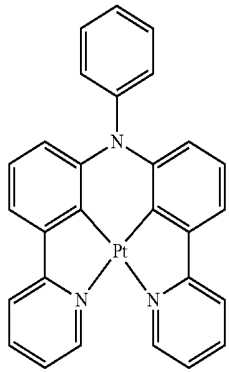
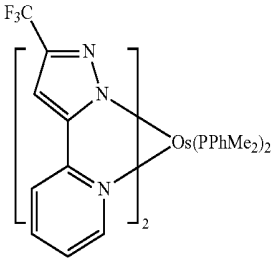
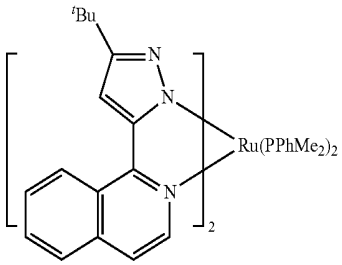
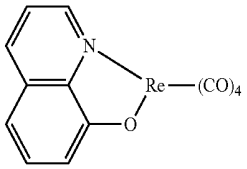
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,232,618
Platinum(II) organometallic complexes		WO2003040257
		US20070103060
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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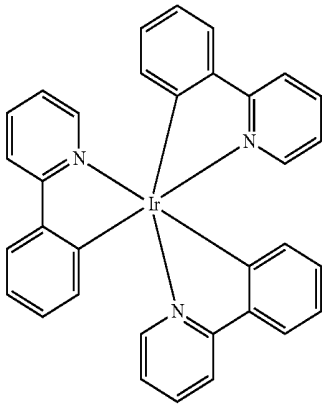
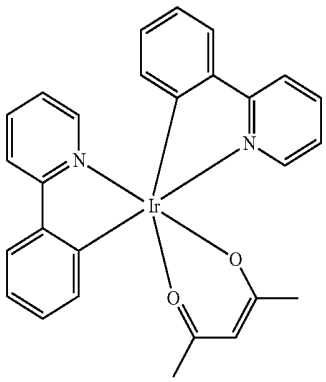
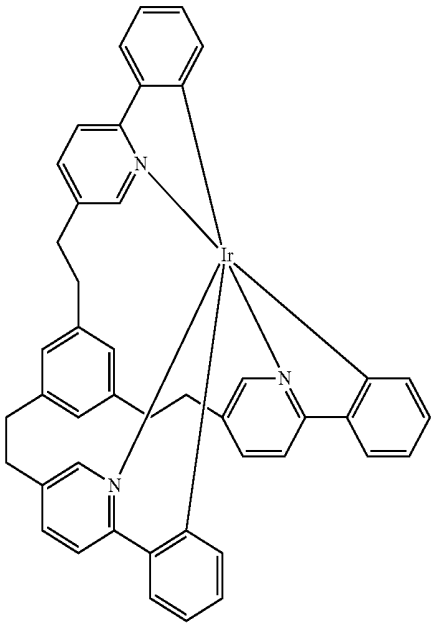
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656
		U.S. Pat. No. 7,332,232

TABLE 1-continued

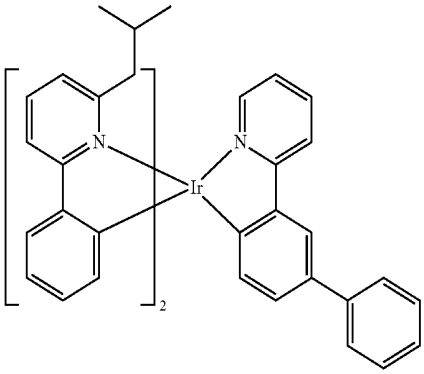
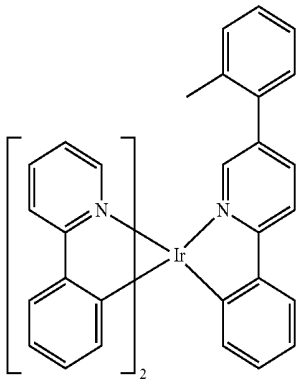
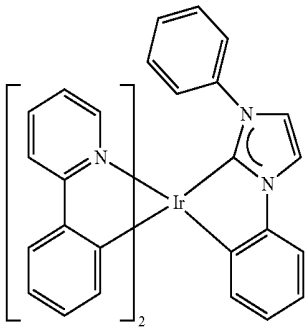
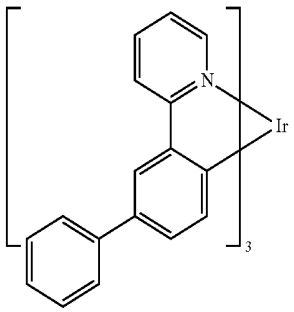
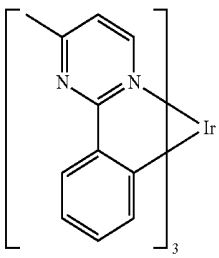
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090108737
		WO2010028151
		EP1841834B
		US20060127696
		US20090039776

TABLE 1-continued

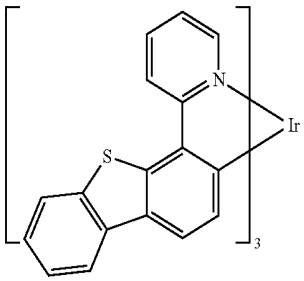
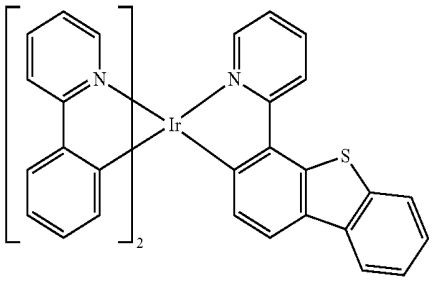
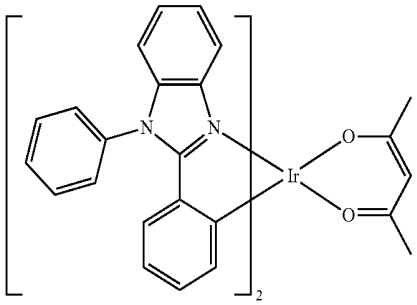
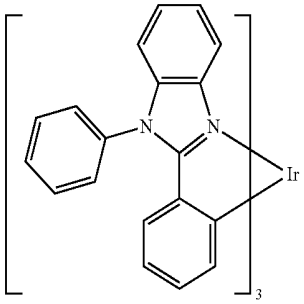
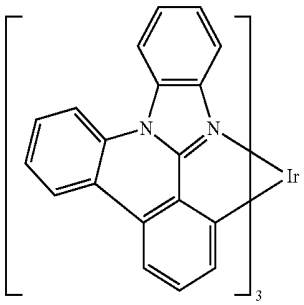
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 6,921,915
		US20100244004
		U.S. Pat. No. 6,687,266
		Chem. Mater. 16, 2480 (2004)
		US20070190359

TABLE 1-continued

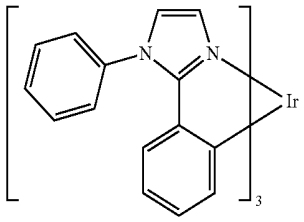
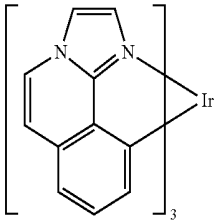
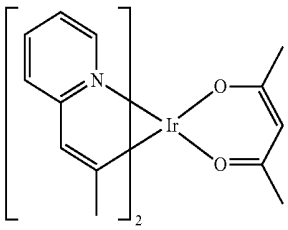
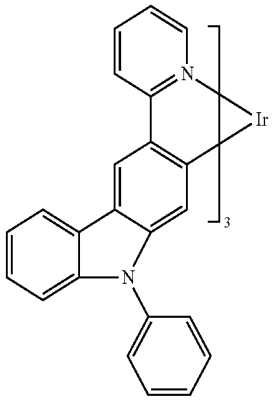
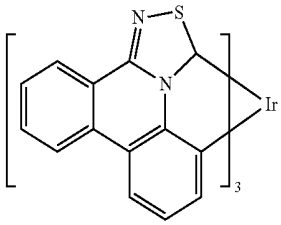
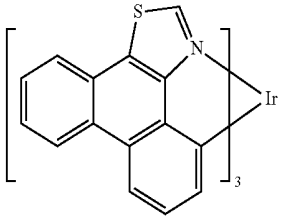
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US 20060008670 JP2007123392
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846

TABLE 1-continued

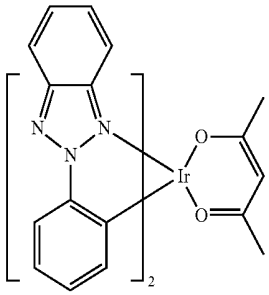
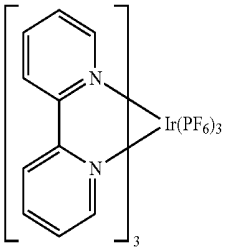
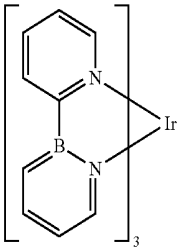
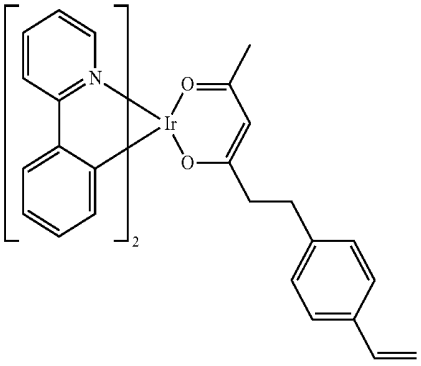
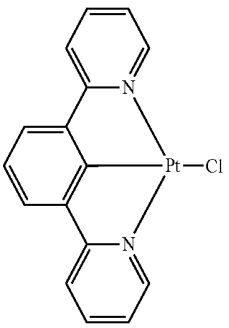
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20080015355
		US20010015432
		US20100295032
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)

TABLE 1-continued

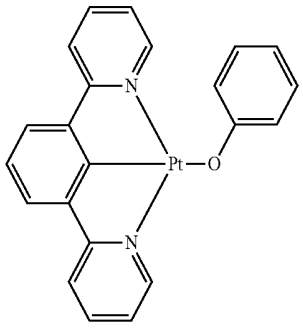
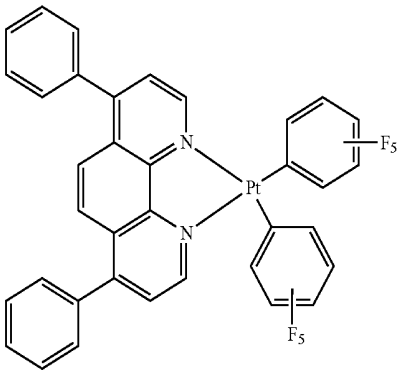
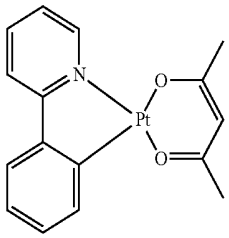
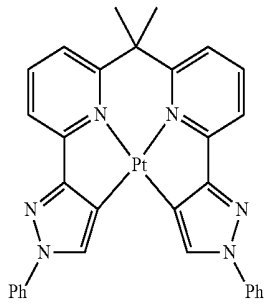
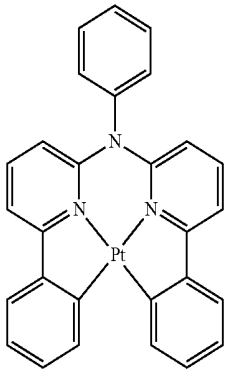
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635
		US20060182992 US20070103060

TABLE 1-continued

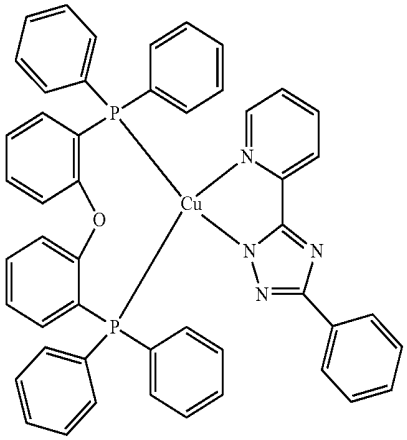
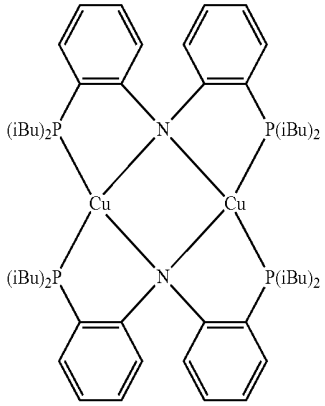
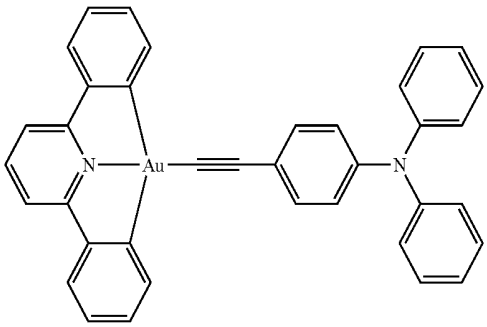
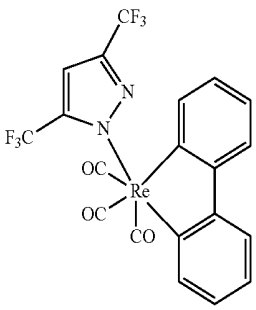
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
		US20070111026
Gold complexes		Chem, Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE 1-continued

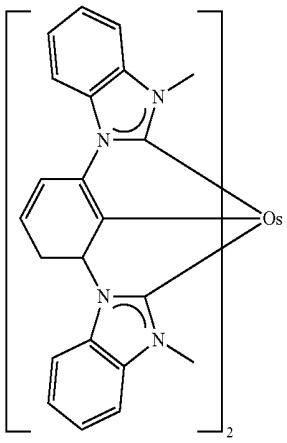
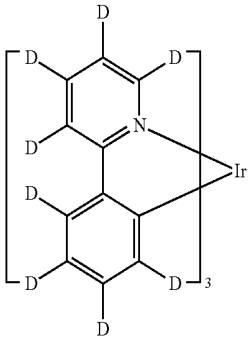
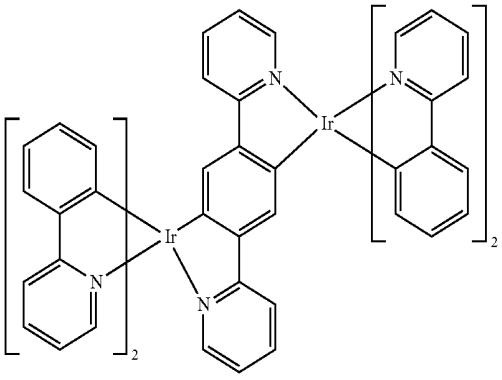
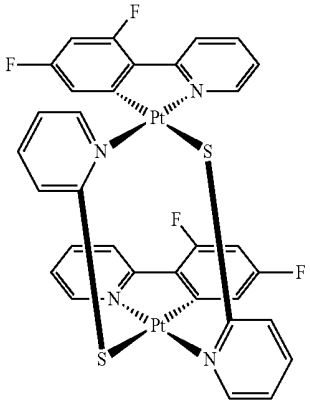
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(II) complexes		U.S. Pat. No. 7,279,704
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928

TABLE 1-continued

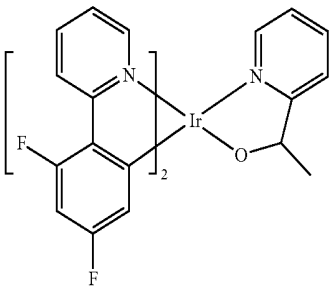
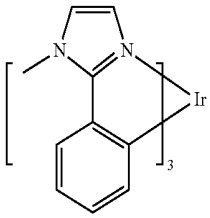
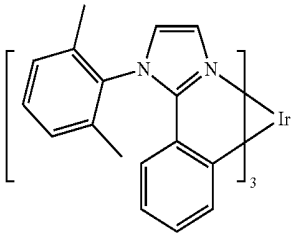
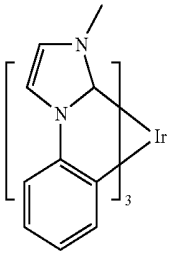
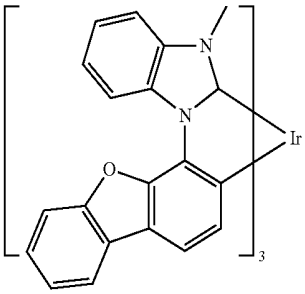
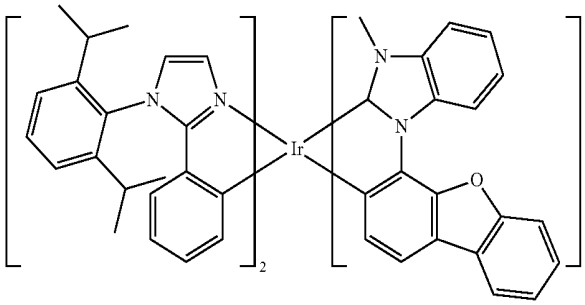
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Blue dopants	
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		U.S. Pat. No. 7,393,599, WO2006056418, US20050260441, WO2005019373
		U.S. Pat. No. 7,534,505
		WO2011051404

TABLE 1-continued

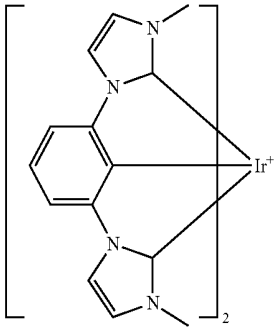
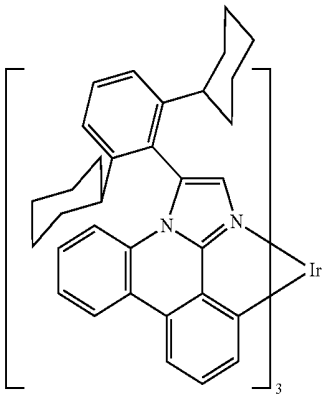
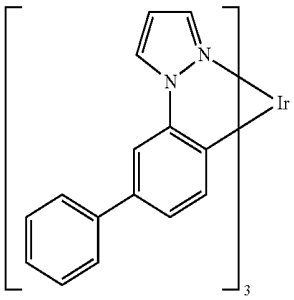
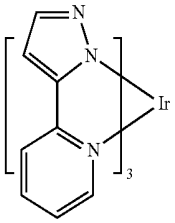
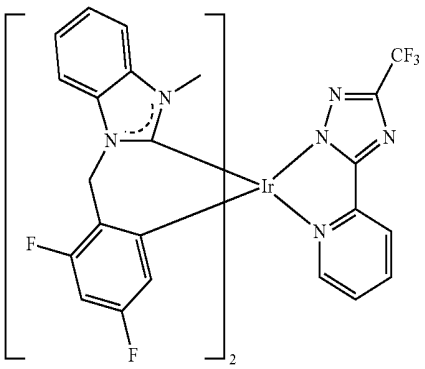
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033 US20100148663
		U.S. Pat. No. 7,338,722
		US20020134984
		Angew. Chem. Int. Ed. 47, 4542 (2008)

TABLE 1-continued

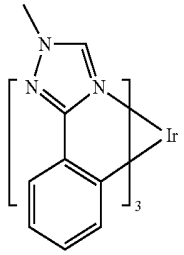
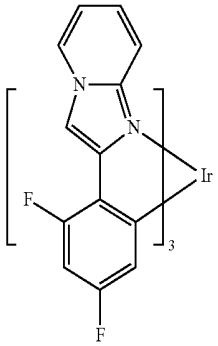
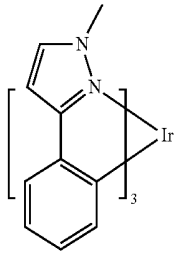
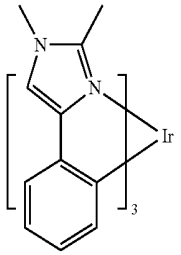
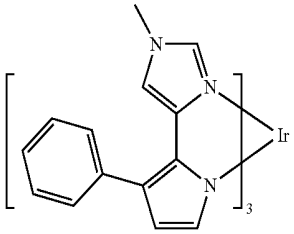
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380

TABLE 1-continued

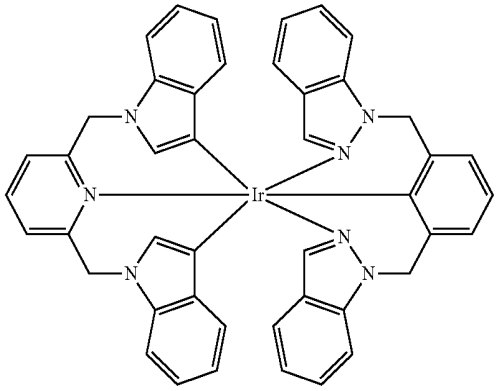
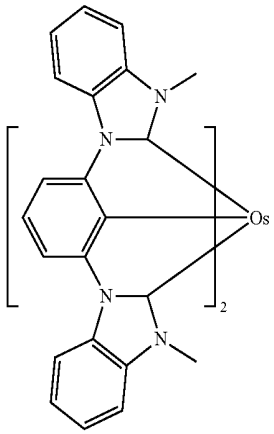
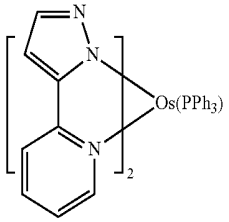
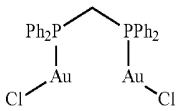
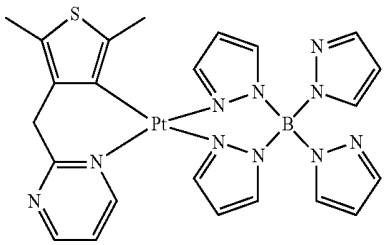
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006082742
Osmium(II) complexes		U.S. Pat. No. 7,279,704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874

TABLE 1-continued

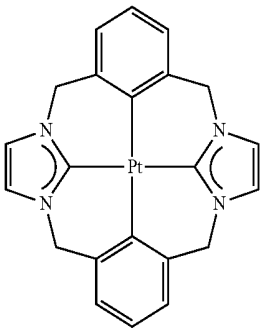
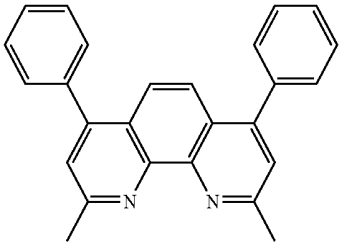
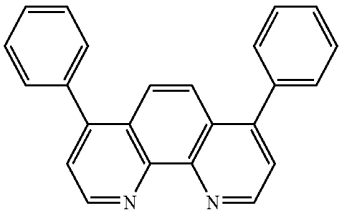
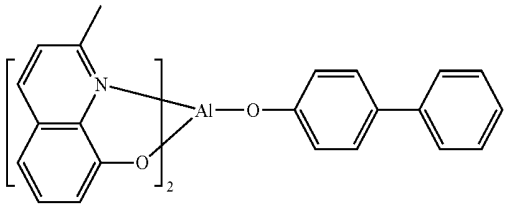
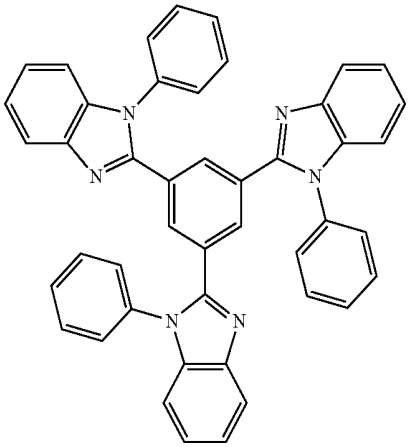
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Pt tetradentate complexes with at least one metal-carbene bond		U.S. Pat. No. 7,655,323
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxy-quinolates (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)

TABLE 1-continued

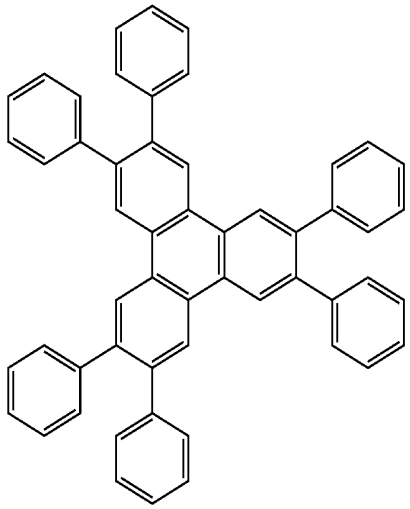
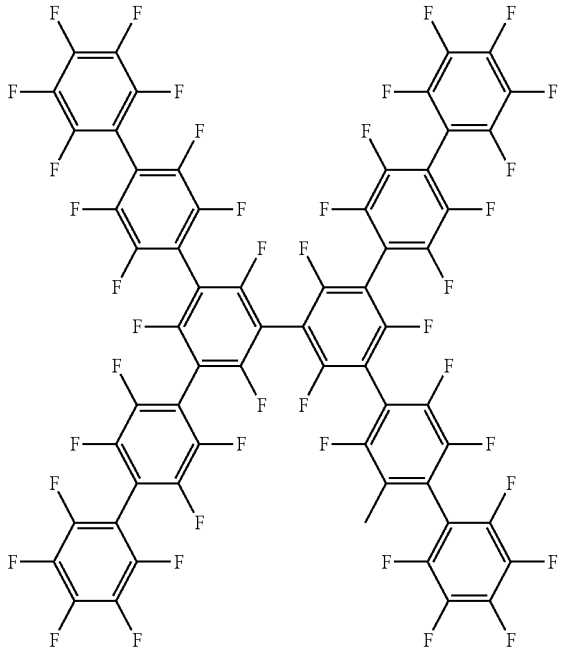
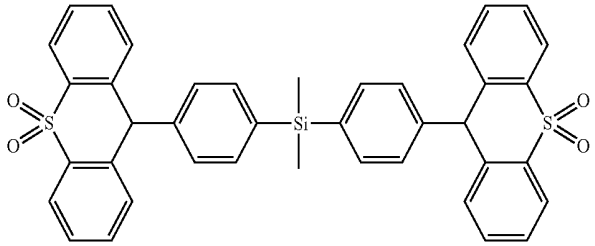
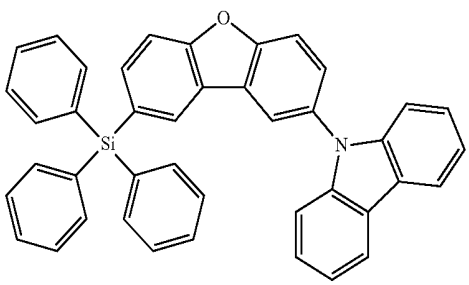
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzo-heterocycles		WO2010079051

TABLE 1-continued

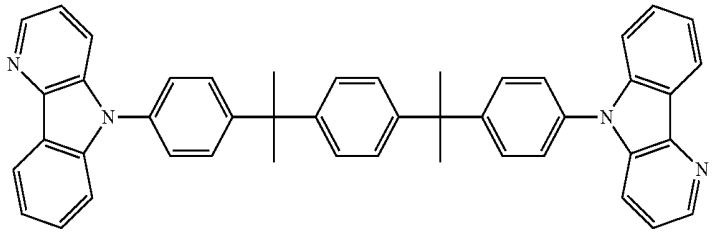
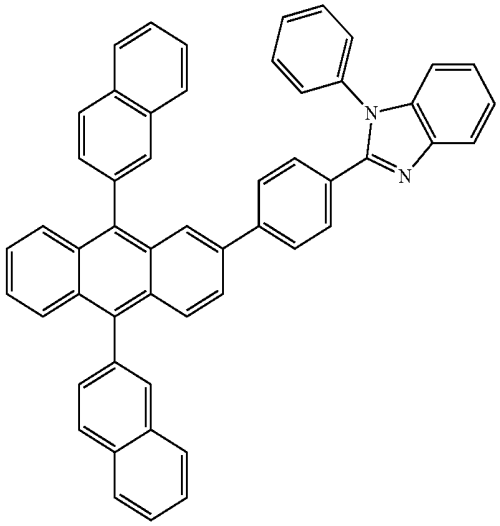
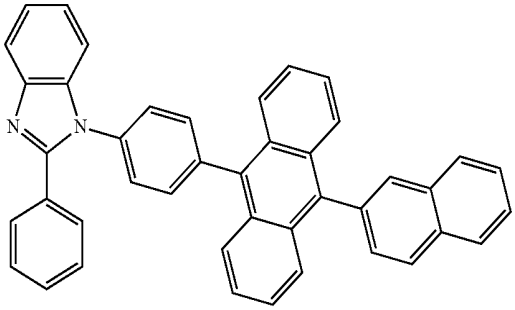
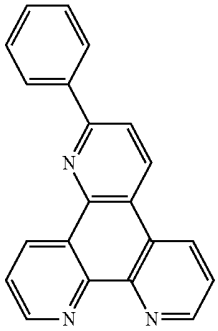
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza-carbazoles		US20060121308
	Electron transporting materials	
Anthracene-benzoimidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives		US20090115316

TABLE 1-continued

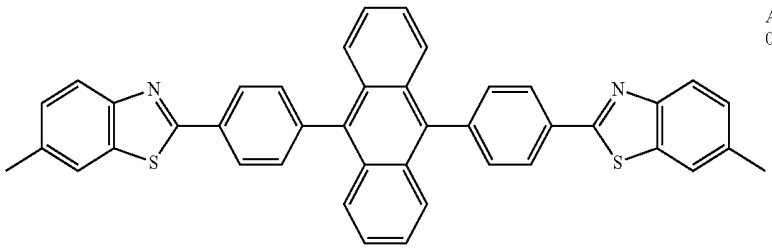
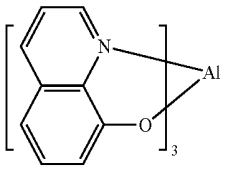
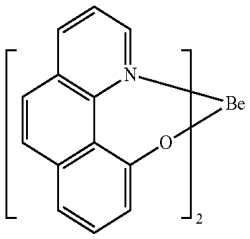
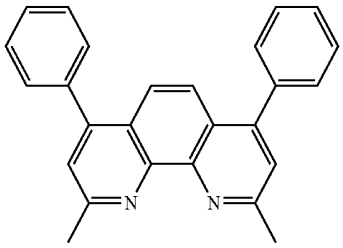
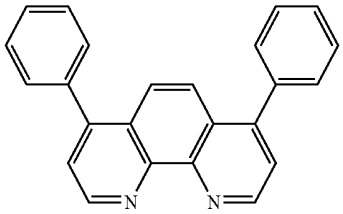
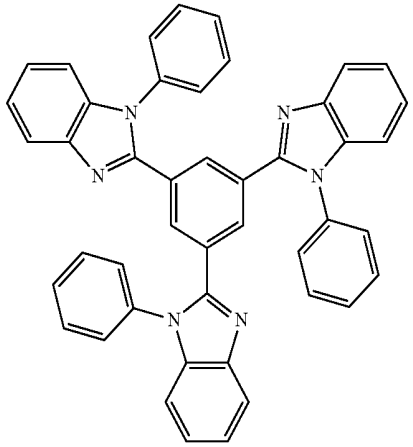
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxy-quinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7,230,107
Metal hydroxy-benoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such 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)

TABLE 1-continued

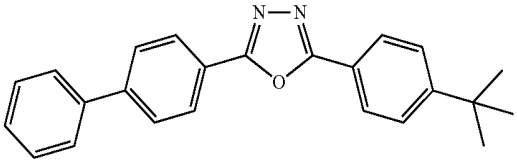
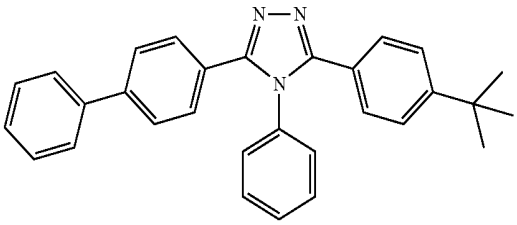
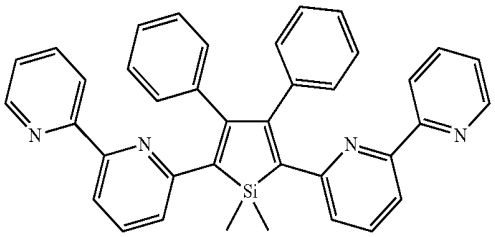
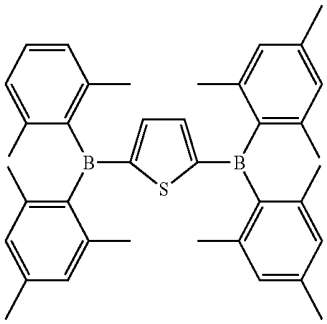
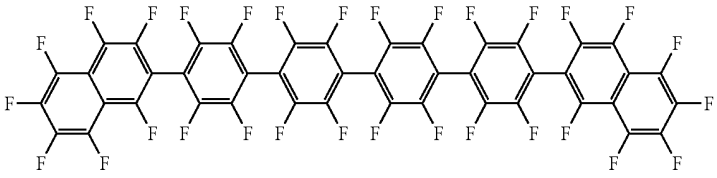
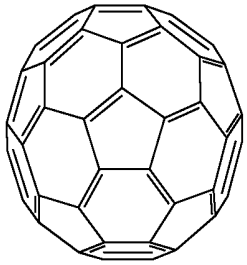
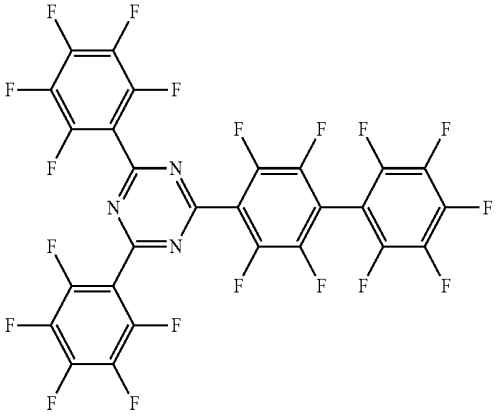
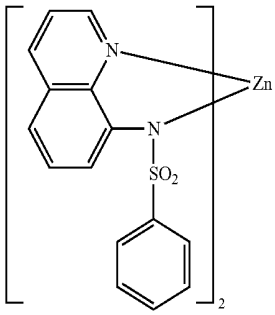
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870

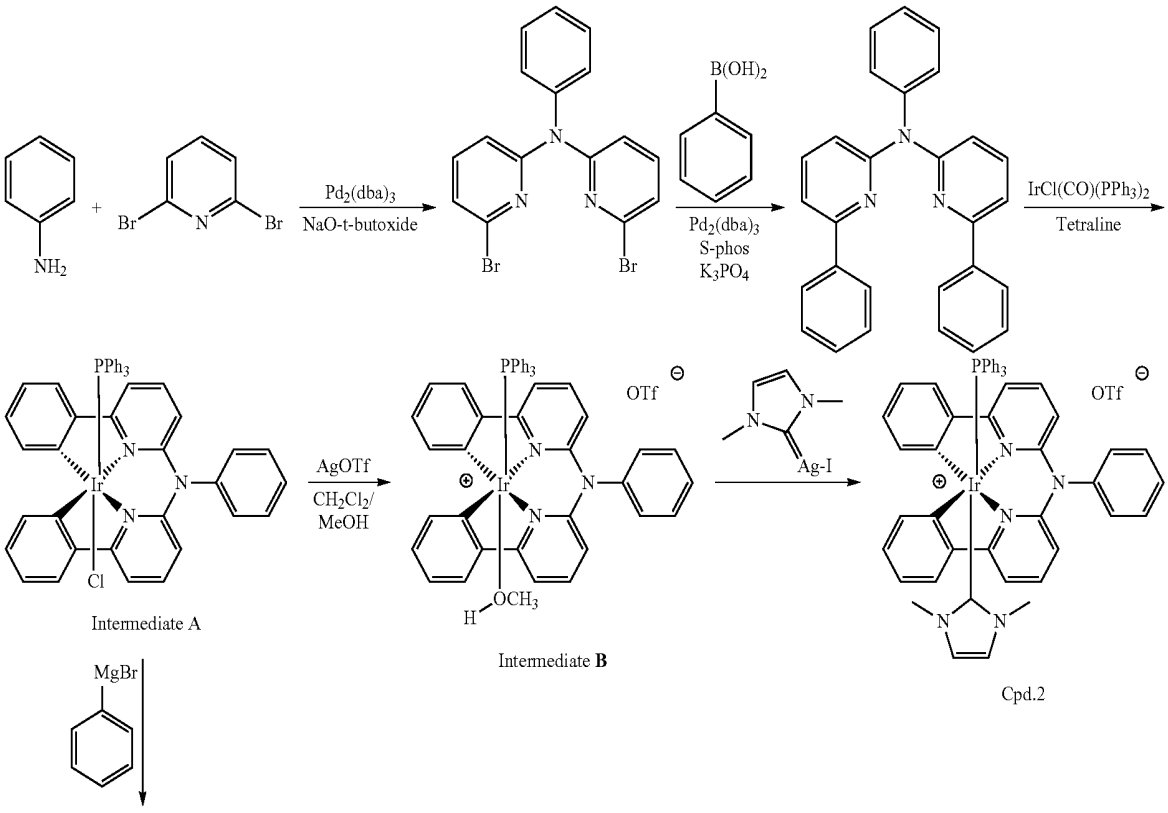
TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triazine complexes		US20040036077
Zn (N^N) complexes		U.S. Pat. No. 6,528,187

EXPERIMENTAL

Synthesis of Compounds 1 and 2

Compounds 1 and 2 were synthesized using the following pathway:



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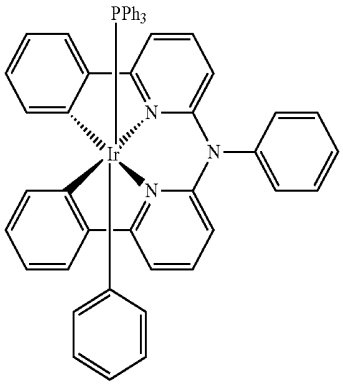


Cpd. 1

Synthesis of 6-bromo-N-(6-bromopyridin-2-yl)-N-phenylpyridin-2-amine

The following were added to a 500 ml three-necked round-bottomed flask: 2,6-dibromopyridine (20 g, 84 mmol), aniline (3.08 ml, 33.8 mmol), ((S)-5-(diphenylphosphino)cyclopenta-1,3-dien-1-yl)((R)-3-(diphenylphosphino)cyclopenta-2,4-dien-1-yl)iron (0.749 g, 1.351 mmol), $Pd_2(dba)_3$ (0.618 g, 0.675 mmol), and sodium 2-methylpropan-2-olate (8.11 g, 84 mmol) with Toluene (Volume: 250 ml). The reaction mixture was refluxed at 90° C. in an oil bath for 18 h. The reaction mixture was diluted with EtOAc and passed through a tightly packed celite plug followed by EtOAc and DCM wash. The solvent was concentrated and the crude mixture was subjected to column chromatography (50% dichloromethane in hexanes) to yield desired compound (5.22 g, 38%).

Synthesis of N,6-diphenyl-N-(6-phenylpyridin-2-yl) pyridin-2-amine

The following were added to a 500 ml round-bottomed flask: 6-bromo-N-(6-bromopyridin-2-yl)-N-phenylpyridin-2-amine (5.22 g, 12.89 mmol), phenylboronic acid (3.93 g, 32.2 mmol), $Pd_2(dba)_3$ (0.236 g, 0.258 mmol), dicyclohexyl (2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.423 g, 1.031 mmol), potassium phosphate tribasic monohydrate (8.90 g, 38.7 mmol), toluene (200 ml) and water (20 ml). The reaction mixture was heated and refluxed overnight. The reaction mixture was then diluted with water and extracted with ETOAC. The combined organic portion was washed with brine and dried over $MgSO_4$. The solvent was evaporated and the residue was purified by column chromatograph (8/1/1 heptane/EtOAc/dcm) to yield desired product (4.76 g, 92%).

Synthesis of intermediate A

A 50 mL round-bottomed flask was charged with N,6-diphenyl-N-(6-phenylpyridin-2-yl)pyridin-2-amine (0.3 g, 0.751 mmol), Vaska's complex, $IrCl(CO)[P(C_6H_5)_3]_2$, (0.195 g, 0.250 mmol) and tridecane (10 drops). The reaction mixture was heated to 240° C. for 46 h. The reaction mixture was subjected to column chromatography (SiO2, 50% EtOAc to 90% EtOAc in heptane) to yield the desired product (76 mg, 34%).

Synthesis of Compound 1

A 100 mL round-bottomed flask was charged with intermediate A (130 mg, 0.146 mmol), phenylmagnesium bromide (200 μl, 0.600 mmol) and dioxane (3 ml) to give a yellow suspension. The reaction was then refluxed for 16 hrs. The solvent was evaporated and the residue was subjected to column chromatography (SiO2, 50% EtOAc in heptane, then 100% DCM) to yield desired product (136 mg, 100%).

Synthesis of Intermediate B

A 100 mL round-bottomed flask was charged with intermediate A and (trifluoromethyl)sulfonyl)oxy)silver (29.0 mg, 0.113 mmol) in DCM/MeOH (5 ml/5 ml) to give a yellow suspension. The suspension was then stirred overnight at room temperature. The reaction mixture was filtered to remove the salt. The filtrate was concentrated to dryness and used for next step without purification.

Synthesis of Compound 2

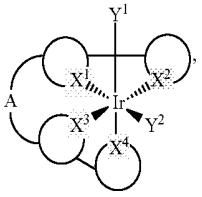
A 50 mL round-bottomed flask was charged with intermediate B (100 mg, 0.097 mmol), N,N-dimethyl imidazole silver carbene complex (48 mg, 0.145 mmol) and dichloroethane (8 ml) to give a brown suspension. The suspension was refluxed for 19 h. The reaction mixture was filtered and the filtrate was subjected to column (SiO_2, 20% acetone in DCM) to yield compound 2 (19 mg, 20%).

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.

We claim:

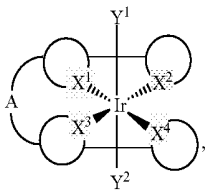
1. A compound having a structure according to Formula (I)

Formula (I)



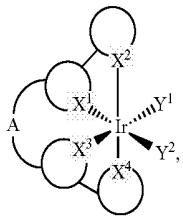
or

Formula (II)



or

Formula (III)



comprising:

a tetradentate ligand coordinated to an iridium core by coordinating atoms X^1, X^2, X^3 and X^4;

a first monodentate ligand coordinated to the iridium core by coordinating atom Y^1; and

a second monodentate ligand coordinated to the iridium core by coordinating atom Y^2,

wherein X^1, X^2, $X^3$and $X^4$are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom;

wherein at least one of X^1, X^2, $X^3$and $X^4$is a neutral carbene that is part of a N-heterocyclic carbene;

wherein X^1, X^2, X^3 and X^4 are each part of a 5- or 6-membered aryl or heteroaryl ring;

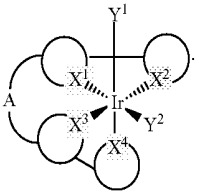
wherein $Y^1$and $Y^2$are independently selected from the group consisting of an anionic coordinating atom selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen and a neutral coordinating atom selected from the group consisting of nitrogen, phosphorus, arsenic, carbene carbon and oxygen; and

A is a linker.

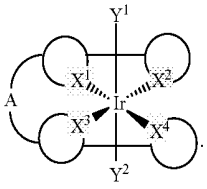
2. The compound of claim **1**, wherein X^1, X^2, X^3 and X^4 are independently selected from the group consisting of an anionic coordinating atom selected from the group consisting of carbon and nitrogen, and a neutral coordinating atom selected from the group consisting of nitrogen, oxygen, phosphorus, and carbene carbon.

3. The compound of claim **1**, having a structure according to Formula (I):

Formula (I)



Formula (II)

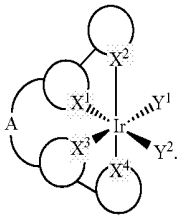


4. The compound of claim **1**, having a structure according to Formula (II):

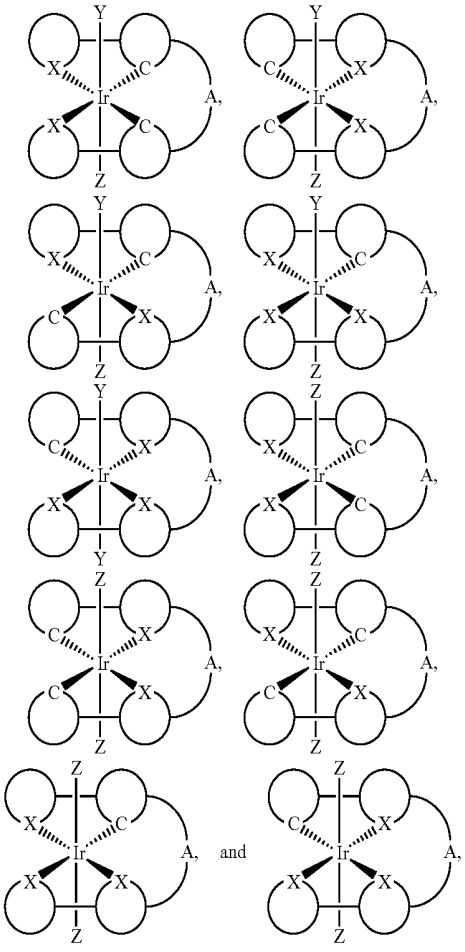
Formula (II)

5. The compound of claim **1**, having a structure according to Formula (III):

Formula (III)



6. The compound of claim **1**, having a structure selected from the group consisting of:



wherein each C, X, Y, and Z can be same or different;

wherein each C is independently an anionic coordinating carbon atom,

wherein each Y is independently an anionic coordinating atom,

wherein each Z is independently a neutral coordinating atom, and

A is a linker.

7. The compound of claim **6**,

wherein X is a coordinating atom independently selected from the group consisting of nitrogen, oxygen, phosphorus, and carbene carbon,

wherein Y is an anionic coordinating atom independently selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen, and

wherein Z is a neutral coordinating atom independently selected from the group consisting of nitrogen, phosphorus, arsenic, carbene carbon and oxygen.

8. The compound of claim **1**, wherein at least one of X^1, X^2, X^3 and X^4 is a sp^2carbon atom from a benzene ring.

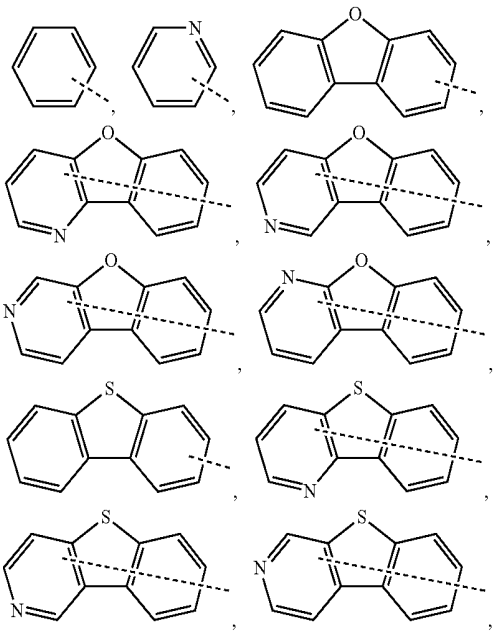
9. The compound of claim **1**, wherein at least one of X^1, X^2, X^3 and X^4 is an anionic coordinating nitrogen that is part of a N-heterocyclic ring.

10. The compound of claim **1**, wherein at least one of X^1, X^2, $X^3$and $X^4$is a neutral carbene that is part of an imidazole.

11. The compound of claim **1**, wherein A is a single bond or a bivalent functional group comprising a moiety selected from the group consisting of, BR_1, NR_1, PR_1, **0**, S, Se, C═O, S═O, SO_2, CR_1IR_2, Si R_iR_2, Ge R_1R_2, and combinations thereof, wherein $R_1$and R_2 are 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, wherein R_1, $R_2$are optionally joined to form a ring.

12. The compound of claim **1**, wherein the first monodentate ligand, the second monodentate ligand, or both, are anionic moieties coordinated to the iridium (III) atom by an atom selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen.

13. The compound of claim **12**, wherein the anionic moiety is selected from the group consisting of:



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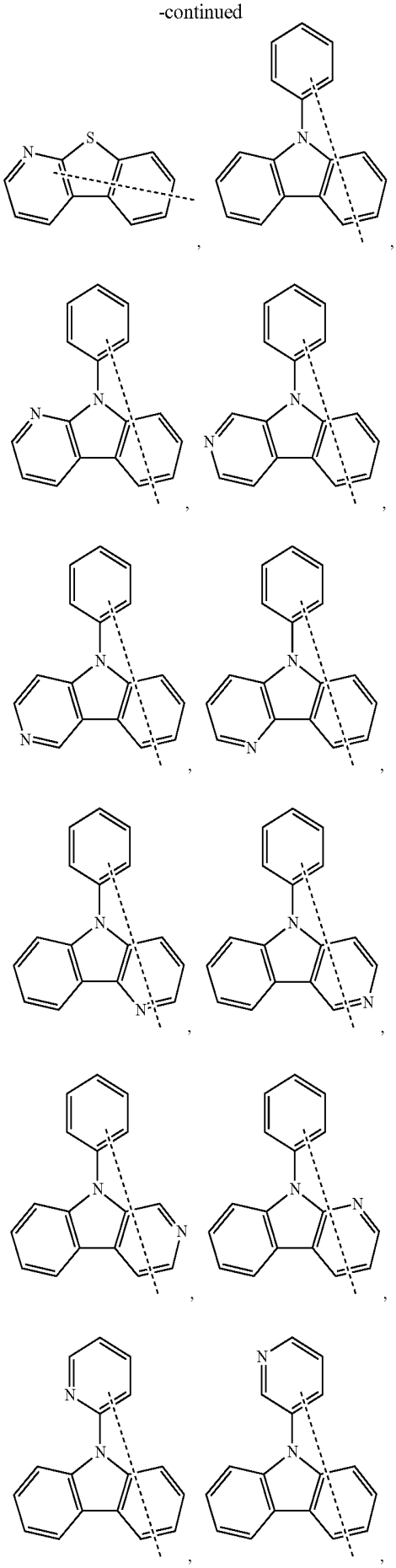

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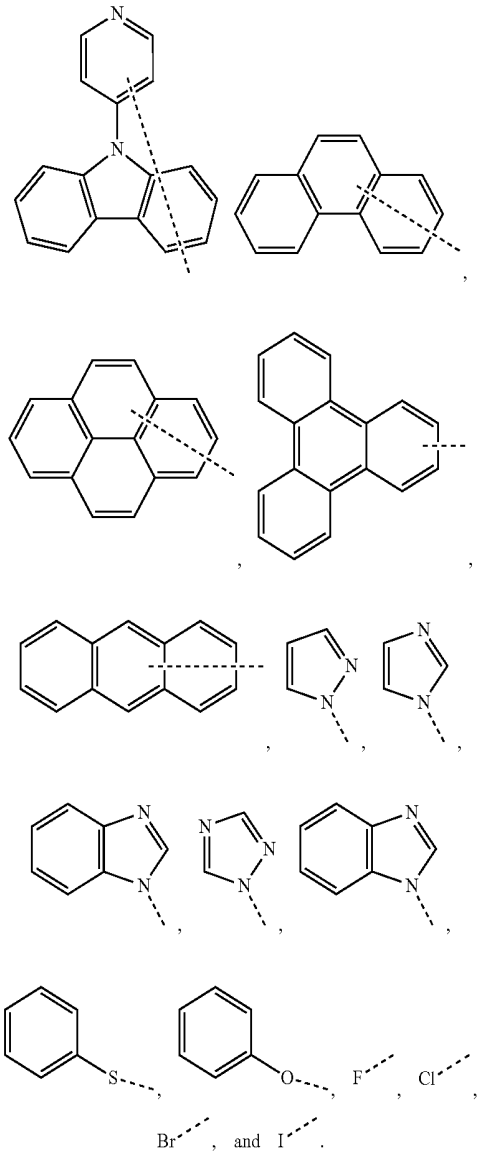
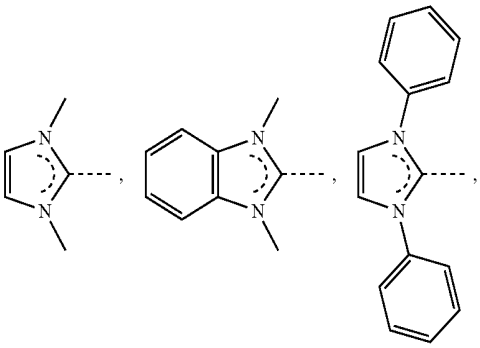


Br , and I .

14. The compound of claim 1, wherein the first monodentate ligand, the second monodentate ligand, or both are neutral moieties coordinated to the iridium (III) atom by an atom selected from the group consisting of nitrogen, carbene carbon, phosphorus, arsenic, and oxygen.

15. The compound of claim 14, wherein the neutral moiety is selected from the group consisting of:



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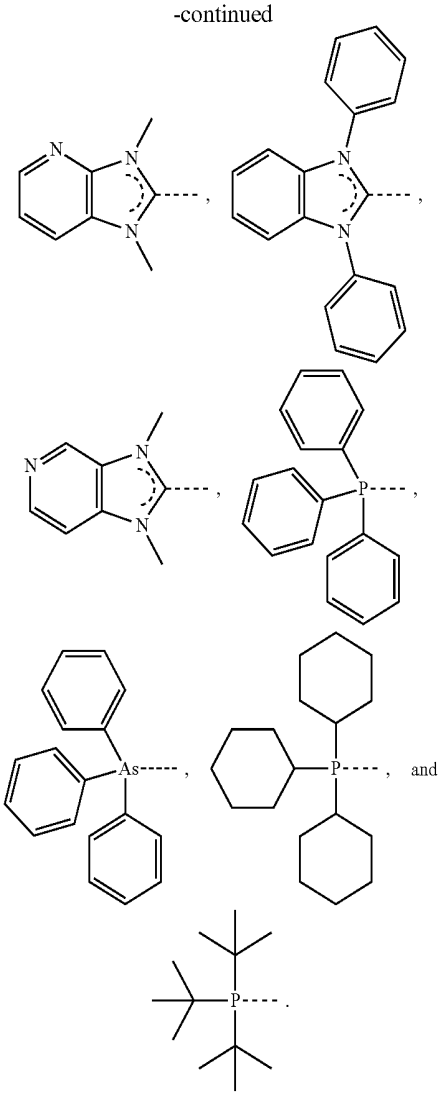


and

16. The compound of claim 1, wherein the first monodentate ligand, the second monodentate ligand, or both are neutral moieties coordinated to the iridium (III) atom by a carbene carbon.

17. The compound of claim 1, wherein at least two of X^1, X^2, $X^3$and $X^4$are neutral carbenes that are part of a N-heterocyclic carbene.

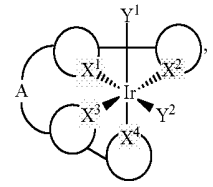
18. A first device comprising a first organic light emitting device, the first organic light emitting device comprising:

an anode;

a cathode; and

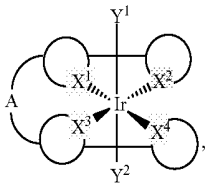
an organic layer, disposed between the anode and the cathode, comprising a compound having a structure according to Formula (I)

Formula (I)



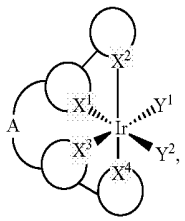
or

Formula (II)



or

Formula (III)



comprising:

a tetradentate ligand coordinated to an iridium core by coordinating atoms X^1, X^2, $X^3$and X^4;

a first monodentate ligand coordinated to the iridium core by coordinating atom Y^1; and

a second monodentate ligand coordinated to the iridium core by coordinating atom Y^2,

wherein X^1, X^2, $X^3$and $X^4$are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom;

wherein at least one of X^1, X^2, $X^3$and $X^4$is a neutral carbene that is part of a N-heterocyclic carbene;

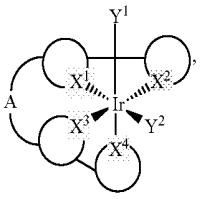
wherein X^1, X^2, X^3 and X^4 are each part of a 5- or 6-membered aryl or heteroaryl ring;

wherein $Y^1$and $Y^2$are independently selected from the group consisting of an anionic coordinating atom selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen and a neutral coordinating atom selected from the group consisting of nitrogen, phosphorus, arsenic, carbene carbon and oxygen; and

A is a linker.

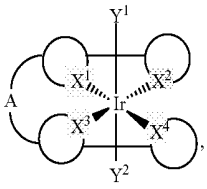
19. A formulation comprising a compound having a structure according to Formula (I)

Formula (I)



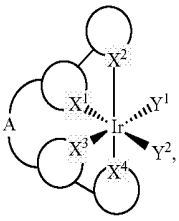
or

Formula (II)



or

Formula (III)



comprising:

a tetradentate ligand coordinated to an iridium core by coordinating atoms X^1, X^2, $X^3$and X^4;

a first monodentate ligand coordinated to the iridium core by coordinating atom Y^1; and

a second monodentate ligand coordinated to the iridium core by coordinating atom Y^2,

wherein X^1, X^2, $X^3$and $X^4$are independently selected from the group consisting of an anionic coordinating atom and a neutral coordinating atom;

wherein at least one of X^1, X^2, $X^3$and $X^4$is a neutral carbene that is part of a N-heterocyclic carbene;

wherein X^1, X^2, $X^3$and $X^4$are each part of a 5- or 6-membered aryl or heteroaryl ring;

wherein $Y^1$and $Y^2$are independently selected from the group consisting of an anionic coordinating atom selected from the group consisting of carbon, nitrogen, halide, sulfur, and oxygen and a neutral coordinating atom selected from the group consisting of nitrogen, phosphorus, arsenic, carbene carbon and oxygen; and

A is a linker.

* * * * *

专利名称(译)	有机电致发光材料和器件		
公开(公告)号	US10056565	公开(公告)日	2018-08-21
申请号	US14/085459	申请日	2013-11-20
[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	TSAI JUI YI KOTTAS GREGG		
发明人	TSAI, JUI-YI KOTTAS, GREGG		
IPC分类号	H01L51/00 C07F15/00 H01L51/50		
CPC分类号	H01L51/0085 C07F15/0033 H01L51/5016		
代理机构(译)	DUANE MORRIS LLP		
其他公开文献	US20150137080A1		

摘要(译)

描述了包含四齿配体和两个单齿配体的铱络合物，含有它们的装置和含有它们的配方。铱络合物可具有根据式（I）的结构 或 公式（II） 或 公式（III） 铱络合物包括： 四齿通过配位原子X I ，X 2 ，X 3 和X 4 ，配体与铱核配位;第一个单齿配体通过配位原子Y 1 与铱核配位;和第二单齿配体通过配位原子Y 2 与铱核配位，其中X 1 ，X 2 ，X 3 和X 4 独立地选自阴离子配位原子和中性配位原子，其中Y 1 和Y 2 独立地选自阴离子配位原子和中性配位原子，A是连接基。