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

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C09K 11/06	(2006.01)
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); ***C09K 11/06*** (2013.01); ***H01L 51/0052*** (2013.01); ***H01L 51/0054*** (2013.01); ***H01L 51/0058*** (2013.01); ***H01L 51/0067*** (2013.01); ***H01L 51/0072*** (2013.01); ***H01L 51/0074*** (2013.01); ***H01L 51/0094*** (2013.01); *C09K 2211/1029* (2013.01); *C09K 2211/185* (2013.01); *H01L 51/5016* (2013.01)

(58) **Field of Classification Search**

None

See application file for complete search history.

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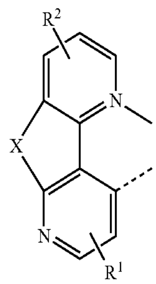
(57) **ABSTRACT**

A compound including a Ligand L of Formula I:

Formula I



as well as, a first device and a formulation containing the same, are disclosed. In the compound including the Ligand L of Formula I:

X is selected from the group consisting of S, Se, SiRR' and GeRR';

R^1, R^2, R, and R' are each 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;

any adjacent substitutions or substituents of R^1, R^2, R, and R' are optionally linked together to form a ring;

the Ligand L is coordinated to a metal M having an atomic number of 40 or greater; and

the Ligand L is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

20 Claims, 3 Drawing Sheets

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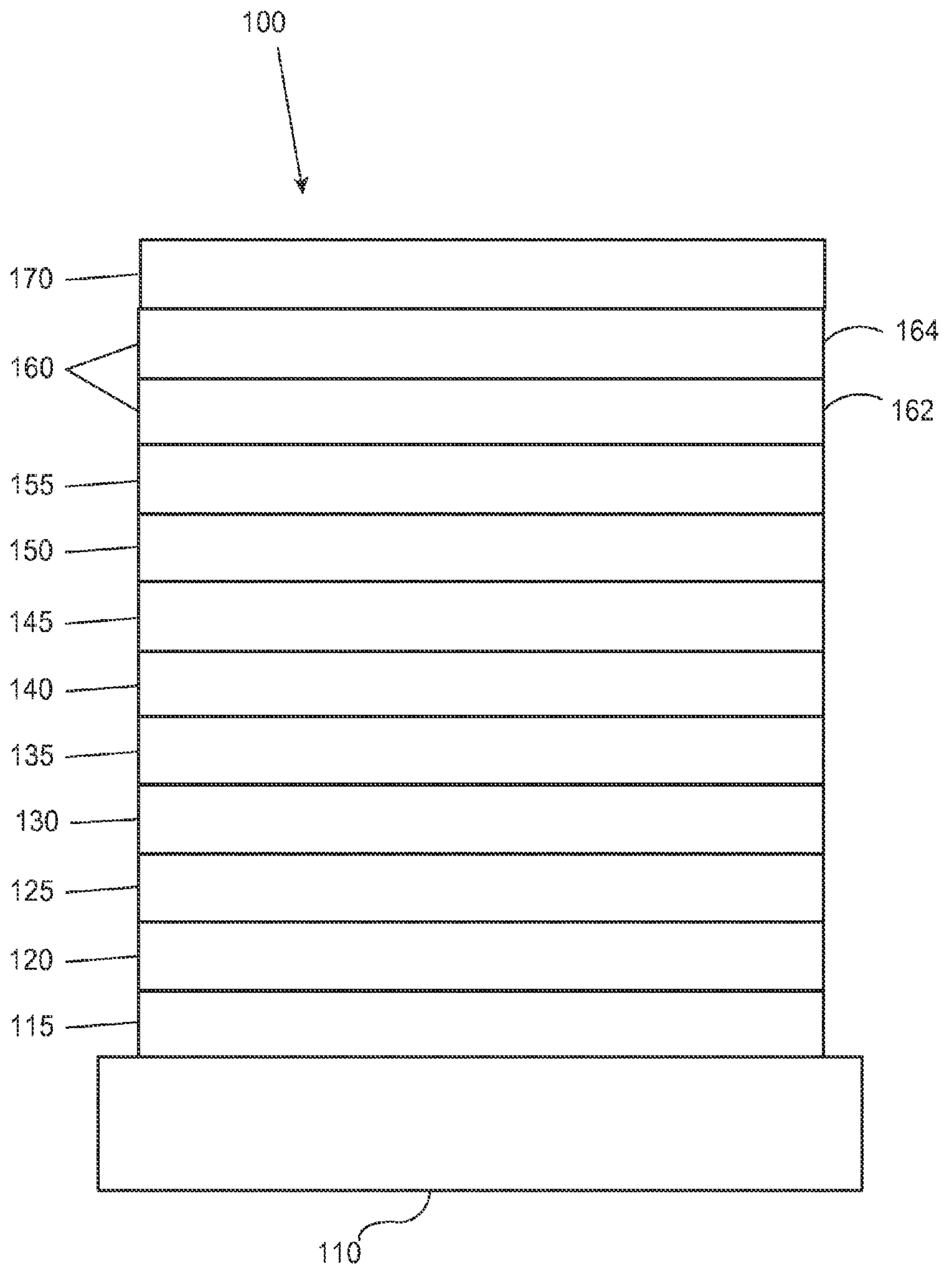


FIGURE 1

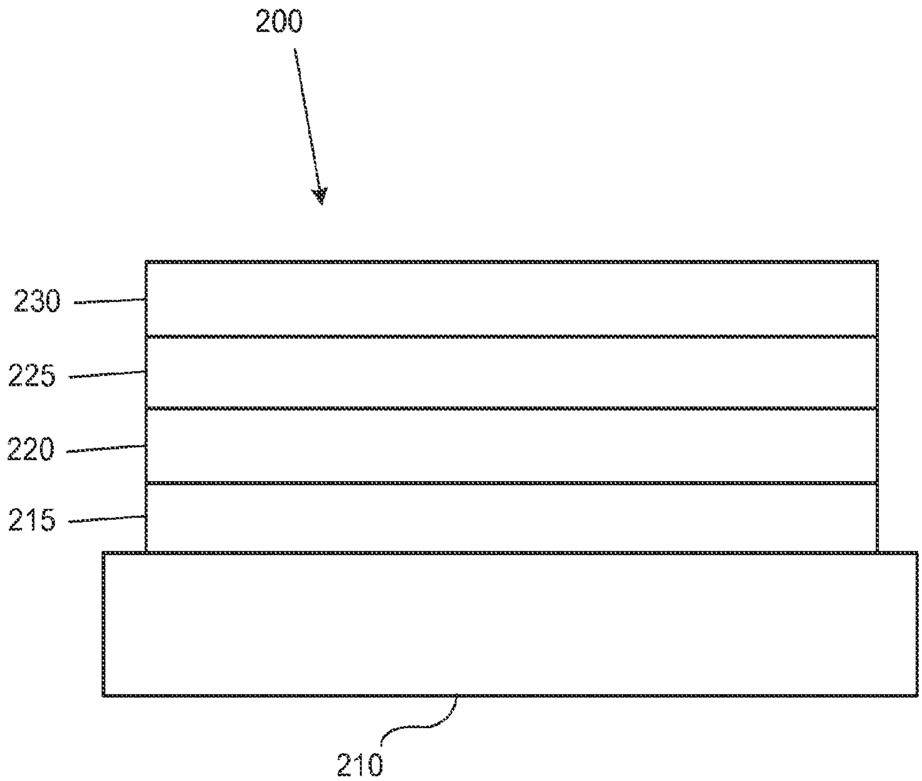


FIGURE 2

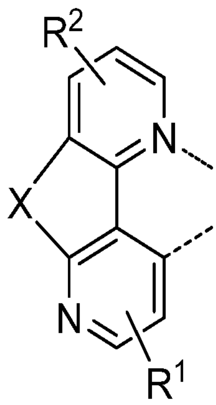


FIGURE 3

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.

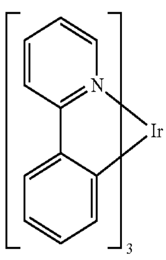
BACKGROUND

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.

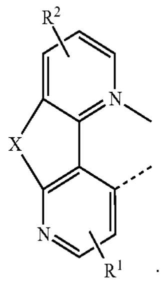
As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to 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 an embodiment, a compound is provided that includes a Ligand L of Formula I



In the compound including the Ligand L of Formula I:

R^1 represents mono, or di-substitution, or no substitution;

R^2 represents mono, di, or tri-substitution, or no substitution;

X is selected from the group consisting of S, Se, SiRR' and GeRR';

R^1, R^2, R, and R' are each 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;

any adjacent substitutions or substituents of R^1, R^2, R, and R' are optionally linked together to form a ring;

the Ligand L is coordinated to a metal M having an atomic number of 40 or greater, and

the Ligand L is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

In some embodiments, the metal M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt, Au, and Cu. In some embodiments, the metal M is Ir.

According to another embodiment, a first device comprising a first organic light emitting device is also provided. The first organic light emitting device can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer can include a compound including a Ligand L of Formula I. The first device can be a consumer product, an organic light-emitting device, and/or a lighting panel.

According to still another embodiment, a formulation the includes a compound having a Ligand L of Formula I is provided.

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 the Ligand L of Formula I 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 outcoupling, 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 polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a "mixture", the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a non-polymeric material consists essentially of polymeric silicon and inorganic silicon.

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 term "halo" or "halogen" as used herein includes fluorine, chlorine, bromine, and iodine.

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

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

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

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

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

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

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

The term "heteroaryl" as used herein contemplates single-ring hetero-aromatic groups that may include from one to three heteroatoms, for example, pyrrole, furan, thiophene, imidazole, oxazole, thiazole, triazole, pyrazole, pyridine, pyrazine and pyrimidine, and the like. The term heteroaryl also includes polycyclic hetero-aromatic systems having two or more rings in which two atoms are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Additionally, the heteroaryl group may be optionally substituted.

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

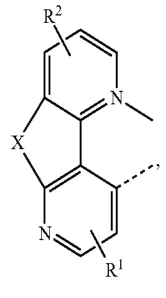
As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant position, such as carbon. Thus, for example, where R^1 is mono-substituted, then one R^1 must be other than H. Similarly, where R^1 is di-substituted, then two of R^1 must be other than H. Similarly, where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

The "aza" designation in the fragments described herein, 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.

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

Iridium tris pyridyl-pyridine complexes offer a platform for blue emission that does not require the use of electron withdrawing substituents. Intrinsically, the unfunctionalized compounds emit from a high energy triplet state with a peak maximum around 450 nm. However, at room temperature, the emission spectra is broadened significantly resulting in a decrease in the practical blue emission color. It has been shown that removing a sterically bulky ligation-directing substituent results in a substantial improvement of the practical emission color at room temperature. While not wishing to be bound by theory, it is believed that this effect is due to less distortion in the excited state. This disclosure describes a further improvement of pyridyl-pyridine complexes which provides ligation selectivity and rigidification of the ligand by tethering the pyridyl-pyridine ligands together with a single atom, such as silicon or sulfur, in order to enhance the emission color to give more blue emission at room temperature.

According to one embodiment, a compound including a Ligand L of Formula I:



Formula I is disclosed.

In the compound including the Ligand L of Formula I:

R^1 represents mono, or di-substitution, or no substitution;

R^2 represents mono, di, or tri-substitution, or no substitution;

X is selected from the group consisting of S, Se, SiRR' and GeRR';

R^1, R^2, R, and R' are each 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;

any adjacent substitutions or substituents of R^1, R^2, R, and R' are optionally linked together to form a ring;

the Ligand L is coordinated to a metal M having an atomic number of 40 or greater; and

the Ligand L is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

In some embodiments, the metal M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt, Au, and Cu. In some embodiments, the metal M is Ir.

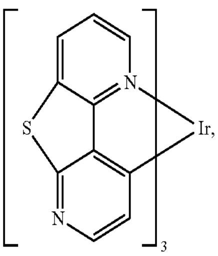
In some embodiments, the compound is homoleptic having formula of IrL_3. In some embodiments, the compound is a facial isomer, while the compound is a meridional isomer in other embodiments. In still other embodiments, the compound is heteroleptic.

In some embodiments, R^1 and R^2 are each independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof. In some embodiments, at least one of R^1 and R^2 comprises a moiety selected from the group consisting of phenyl, toluene, biphenyl and tetraphenyl. In some embodiments, both R^1 and R^2 comprises a moiety selected from the group consisting of phenyl, toluene, biphenyl and tetraphenyl. In some embodiments, R^1 is mono-substitution on the ortho position to N.

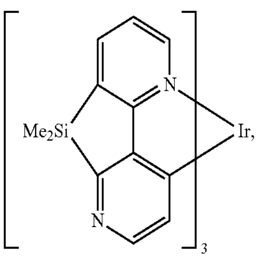
In some embodiments, R and R' are each independently selected from the group consisting of alkyl, aryl, heteroaryl, and combinations thereof.

In some more specific embodiments, the compound is selected from the group consisting of:

Compound 1



Compound 2



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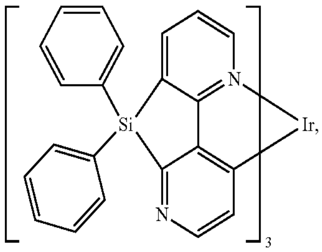
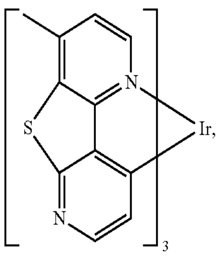
Compound 3



Compound 4



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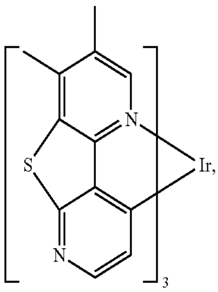

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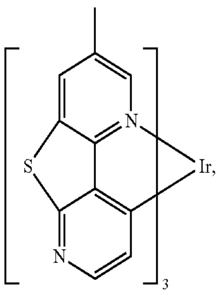
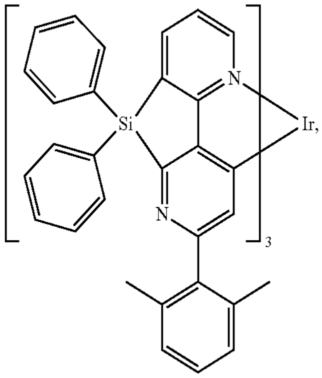


Compound 7



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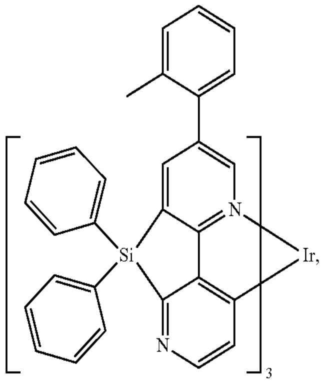
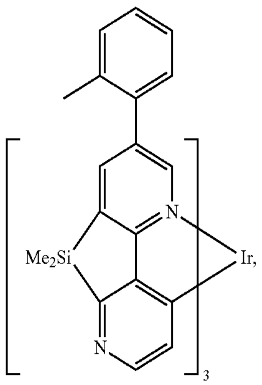
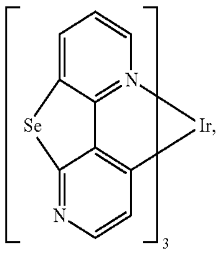
Compound 8



Compound 9



Compound 10



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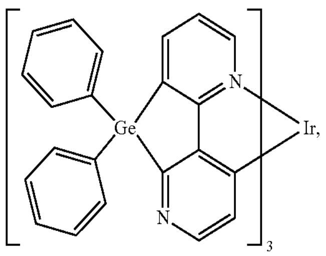

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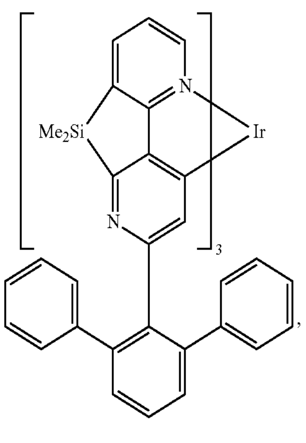

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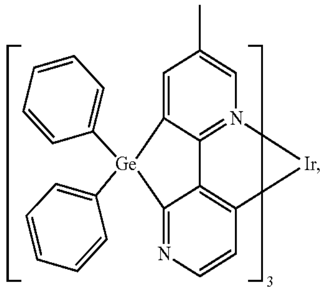
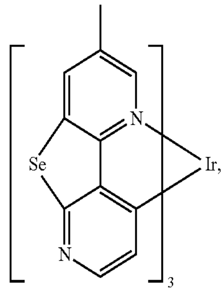
Compound 13



Compound 14



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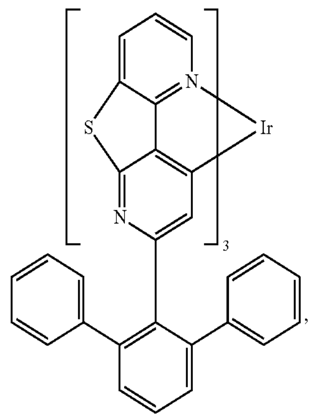
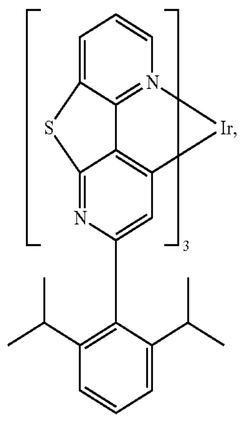


Compound 16



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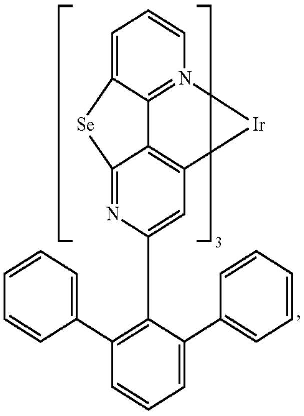
Compound 17



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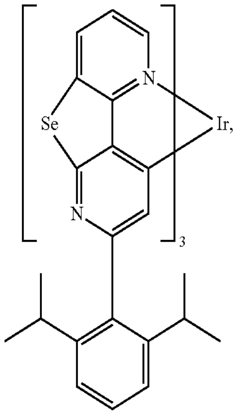
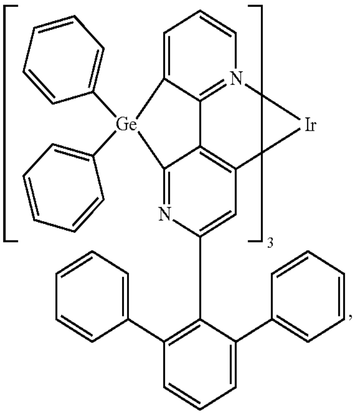
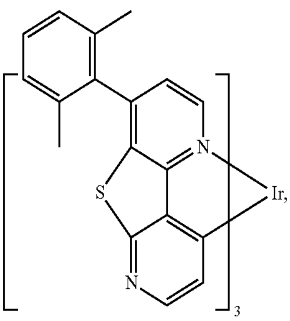


Compound 19



Compound 20



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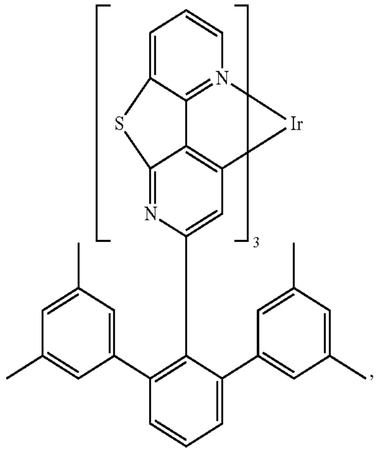
Compound 21



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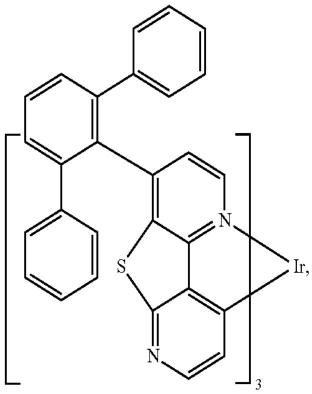

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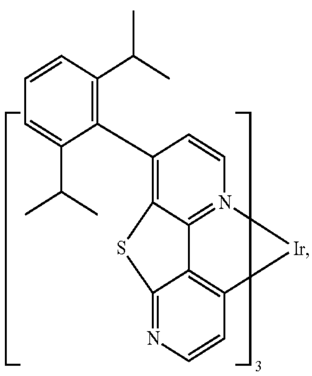
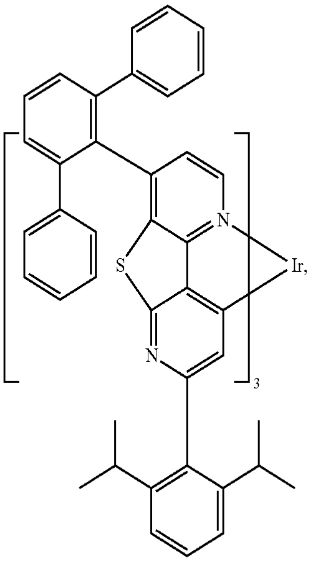
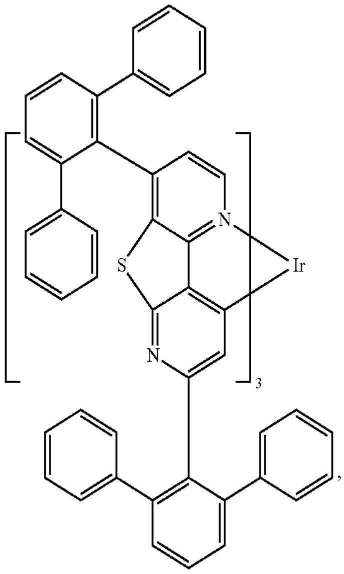


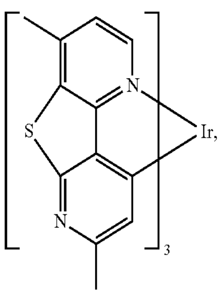
Compound 24



Compound 25



Compound 26



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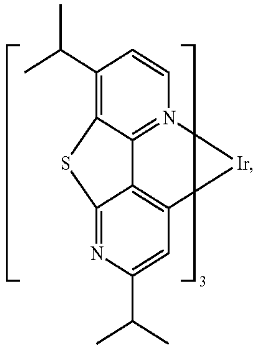

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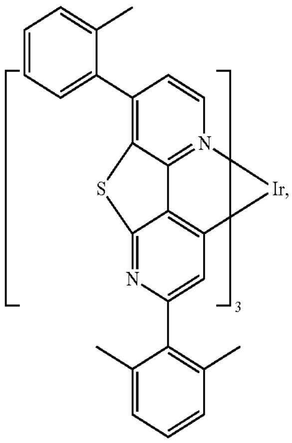
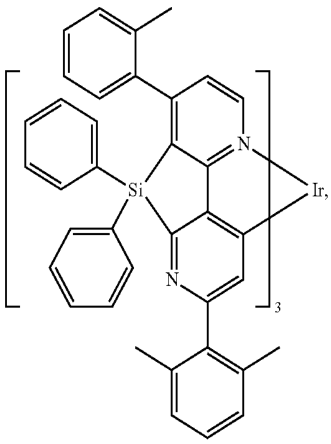
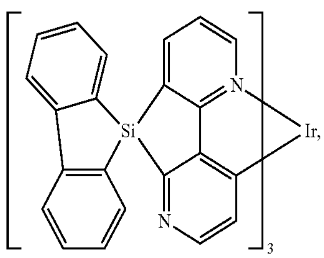


Compound 29



Compound 30



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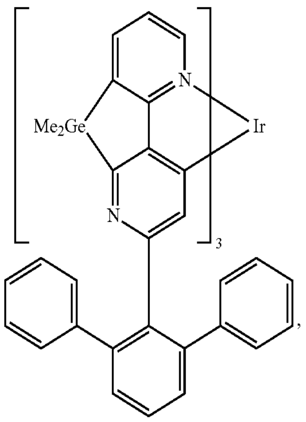
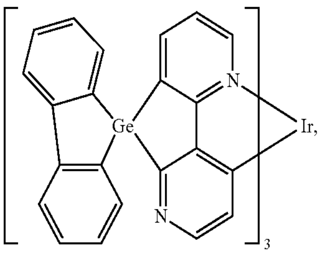
Compound 31



Compound 32



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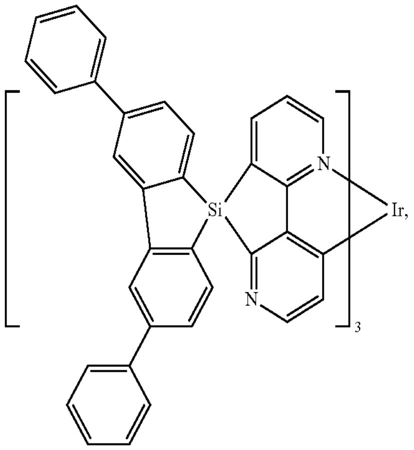
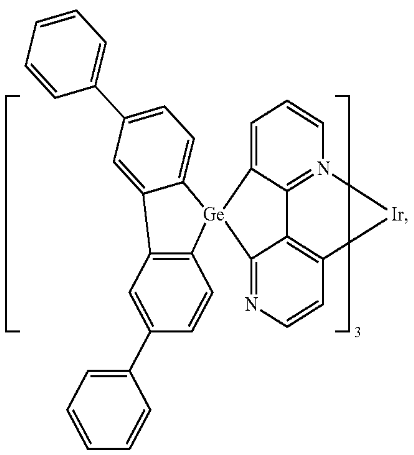


Compound 34



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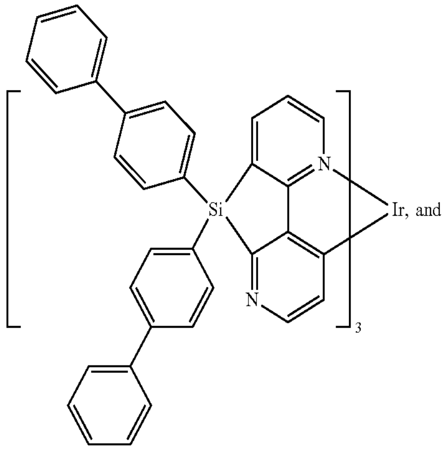
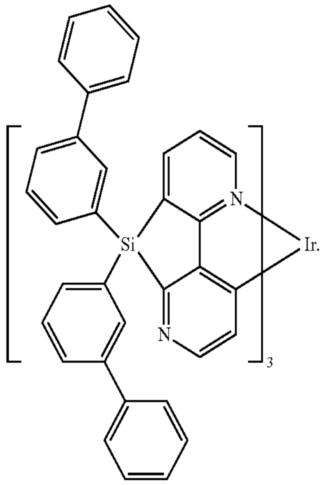
Compound 35



Compound 36

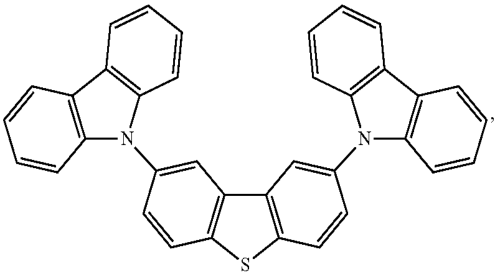


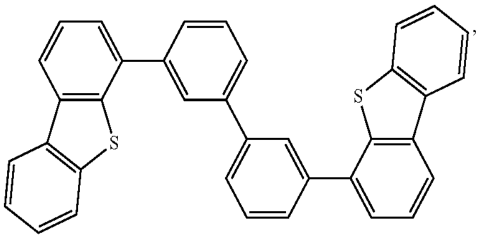
According to another aspect of the present disclosure, a first device is also provided. The first device includes a first organic light emitting device, that includes an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer can include a host and a phosphorescent dopant. The organic layer can include a compound comprising a Ligand L of Formula I and any variations of the compound as described herein.

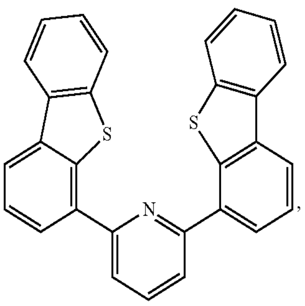
The first device can be one or more of a consumer product, an organic light-emitting device and a lighting panel. The organic layer can be an emissive layer and the compound can be an emissive dopant in some embodiments, while the compound can be a non-emissive dopant in other embodiments.

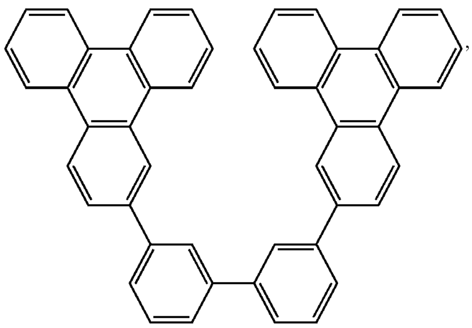
The organic layer can also include a host. In some embodiments, the host can include a metal complex. The host can be a triphenylene containing benzo-fused thiophene or benzo-fused furan. Any substituent in the host can be an unfused substituent independently selected from the group consisting of C_nH_{2n+1},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

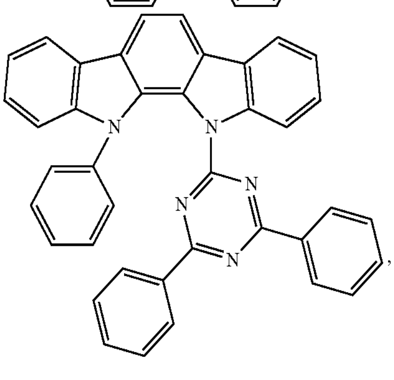
The host can be a compound selected from the group consisting of carbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene. The host can include a metal complex. The host can be a specific compound selected from the group consisting of:











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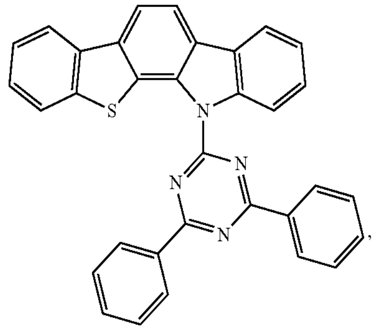
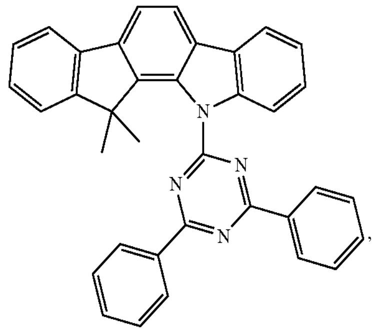
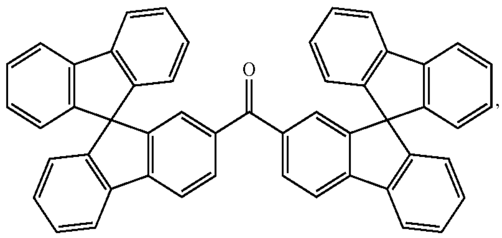
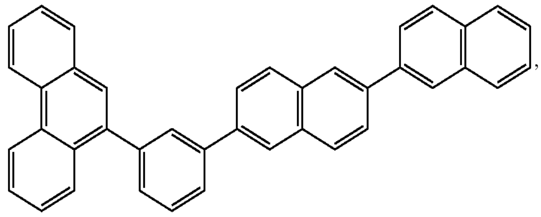
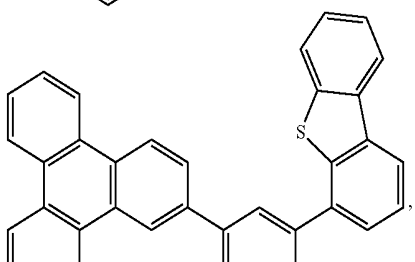
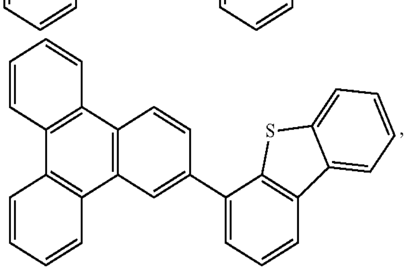












and combinations thereof.

In yet another aspect of the present disclosure, a formulation that comprises a compound comprising a Ligand L of Formula I and any variations of the compound 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.

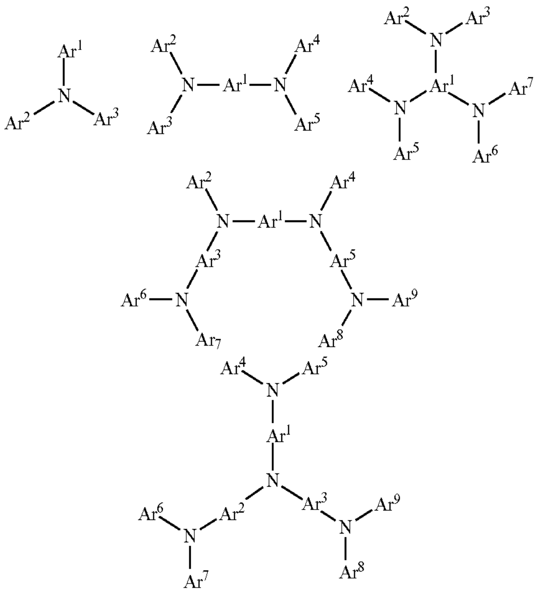
Combination with Other Materials

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:

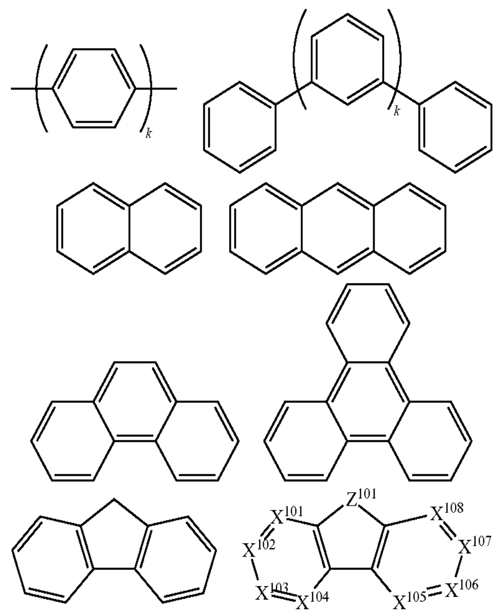
A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphyrin derivative;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

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



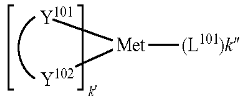
Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as 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:



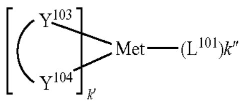
wherein Met is a metal, which can have an atomic weight greater than 40; (Y^{101}-Y^{102}) is a bidentate ligand, Y^{101} and Y^{102} are independently selected from C, N, O, P, and S; L^{101} is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached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

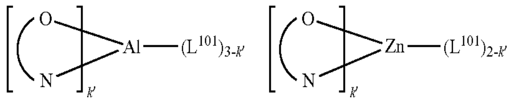
The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes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



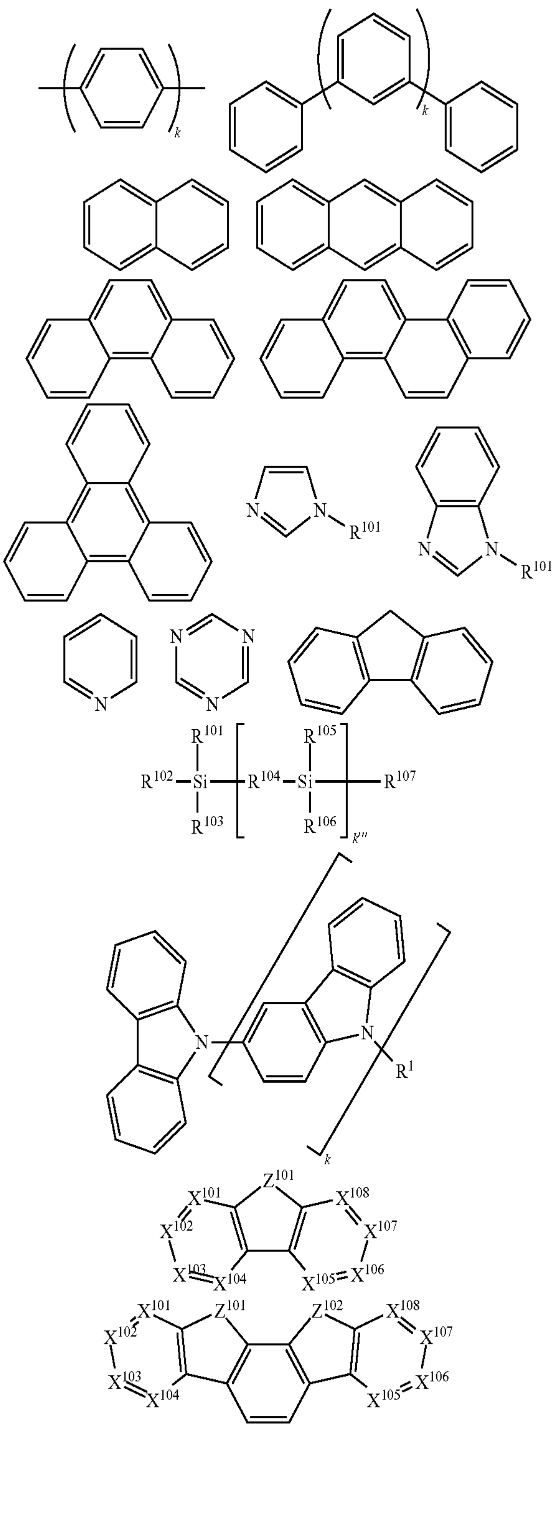
wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

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 atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

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



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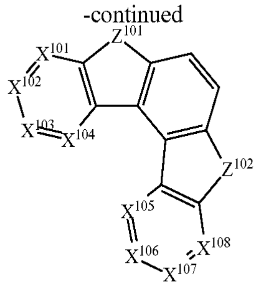
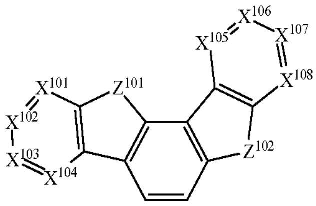
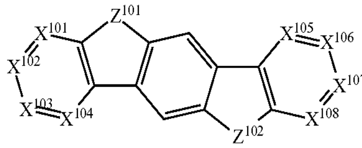
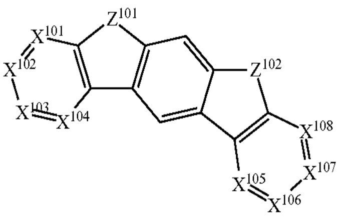





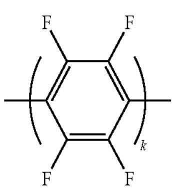
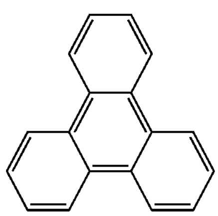
wherein R^{101} to R^{107} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile,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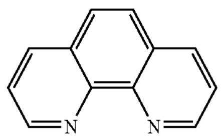
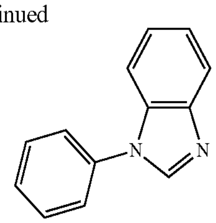
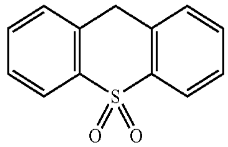
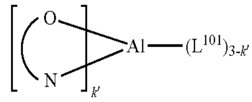
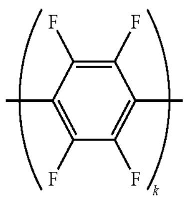
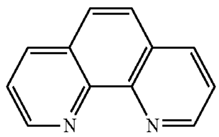
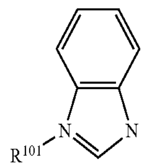
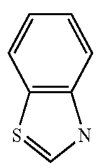
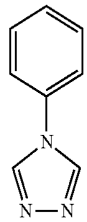
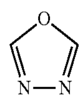
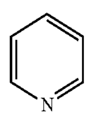
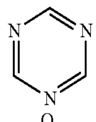
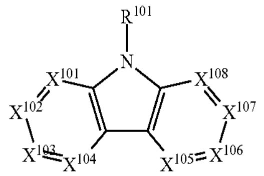
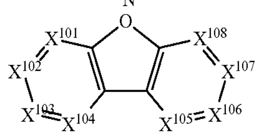
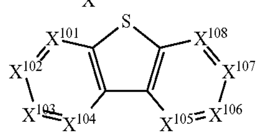
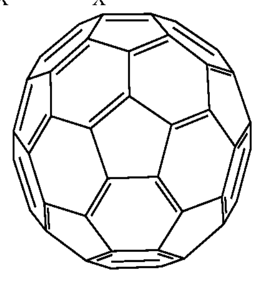
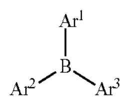





wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

ETL:

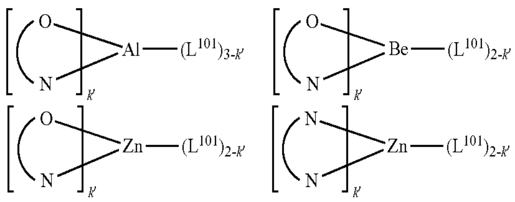
Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may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

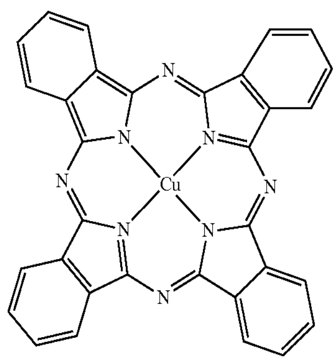
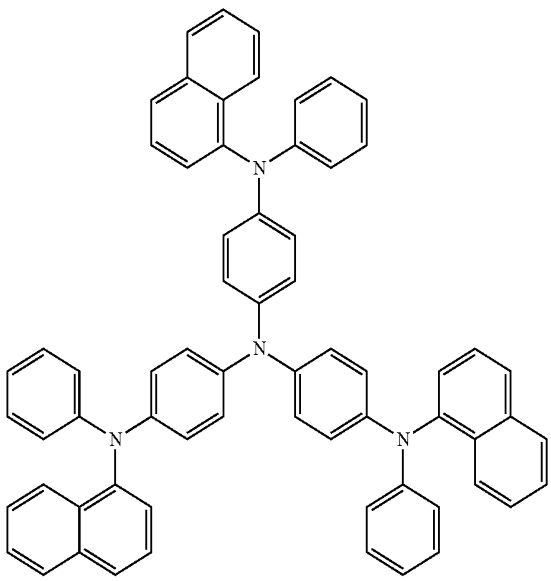
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)

TABLE 1-continued

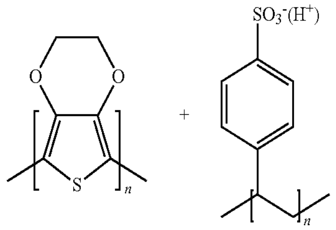
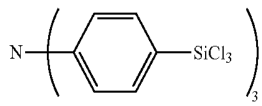
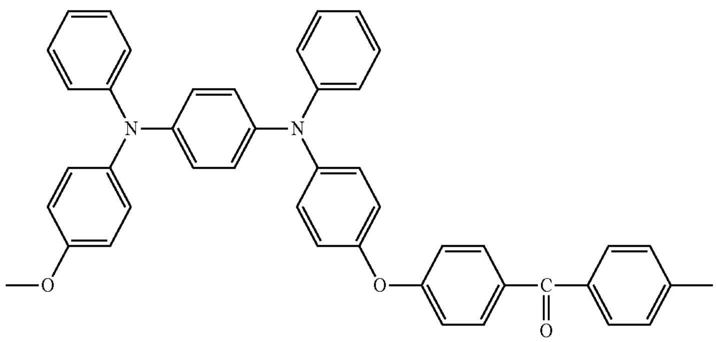
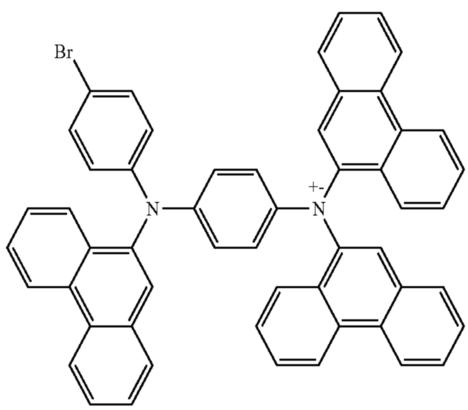
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
CFx Fluoro-hydro-carbon polymer	$-[CH_xF_y]_n-$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT: PSS, poly-aniline poly-thio-phene)		Synth. Met. 87, 171 (1997) WO2007002683
Phos-phonic acid and silane SAMs		US20030162053
Triaryl-amine or poly-thio-phene polymers with con-ductivity dopants	 and	EP1725079A1
		

TABLE 1-continued

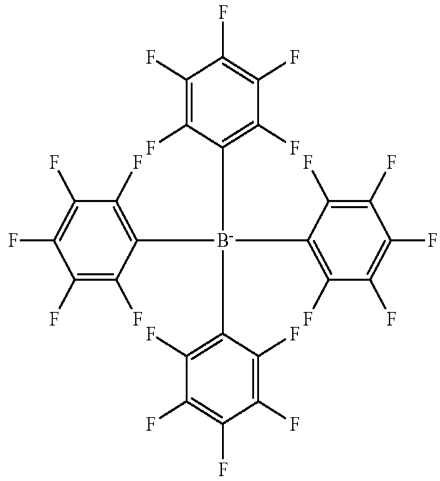
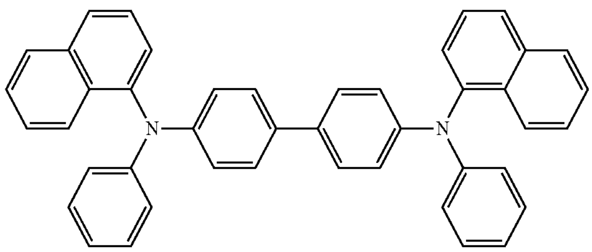
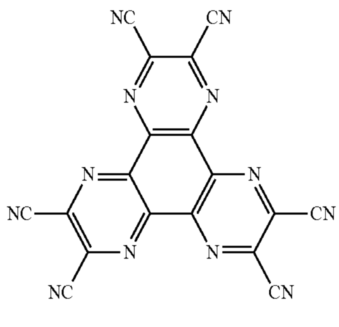
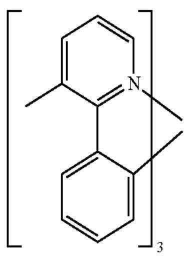
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides	 + MoO_x	US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009
n-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279

TABLE 1-continued

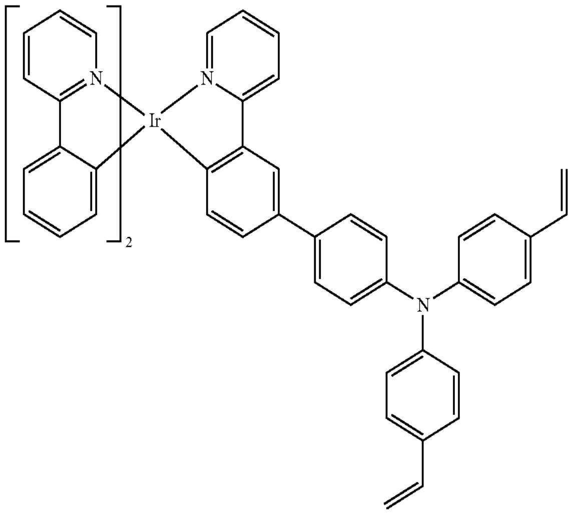
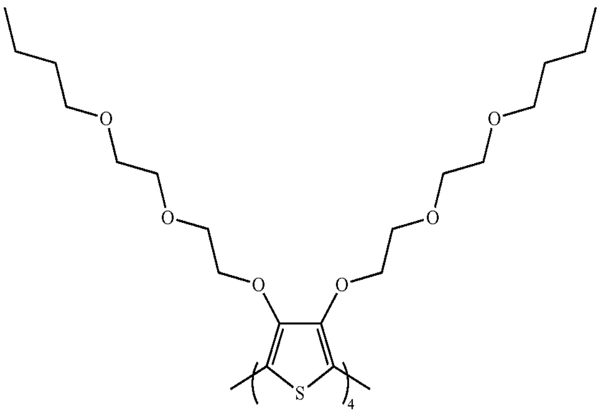
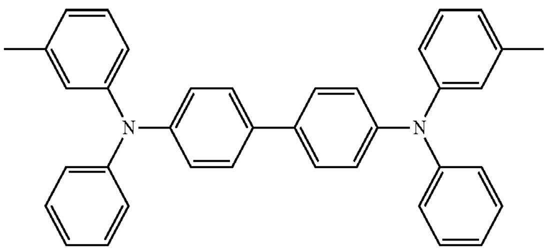
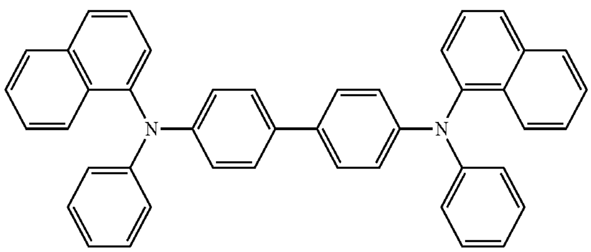
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cross-linkable compounds		US20080220265
Polythiophene based polymers and co-polymers		WO2011075644 EP2350216
	Hole transporting materials	
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5,061,569

TABLE 1-continued

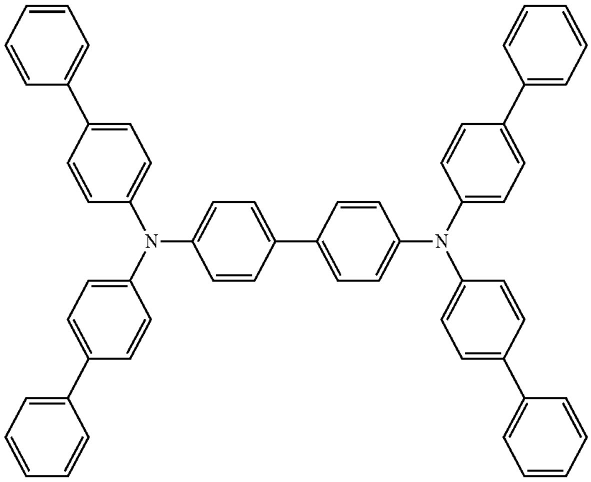
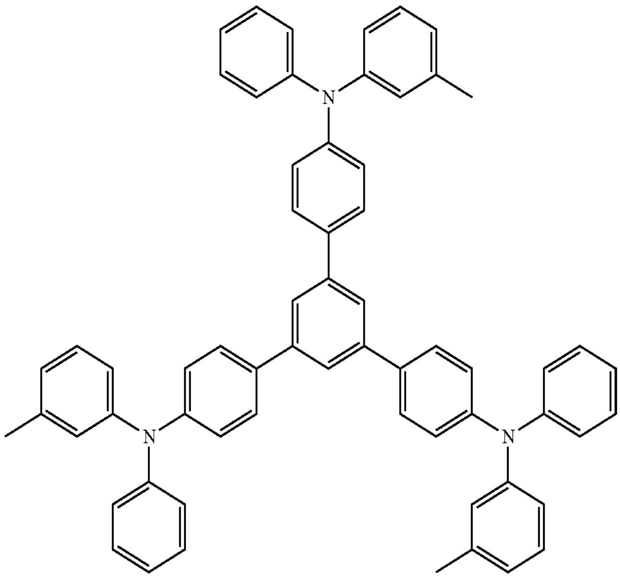
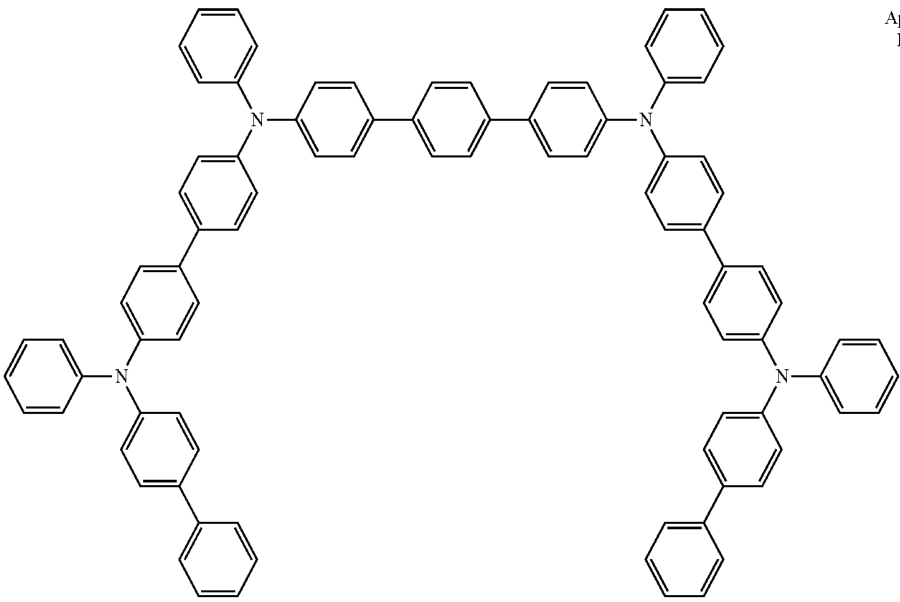
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		EP650955
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE 1-continued

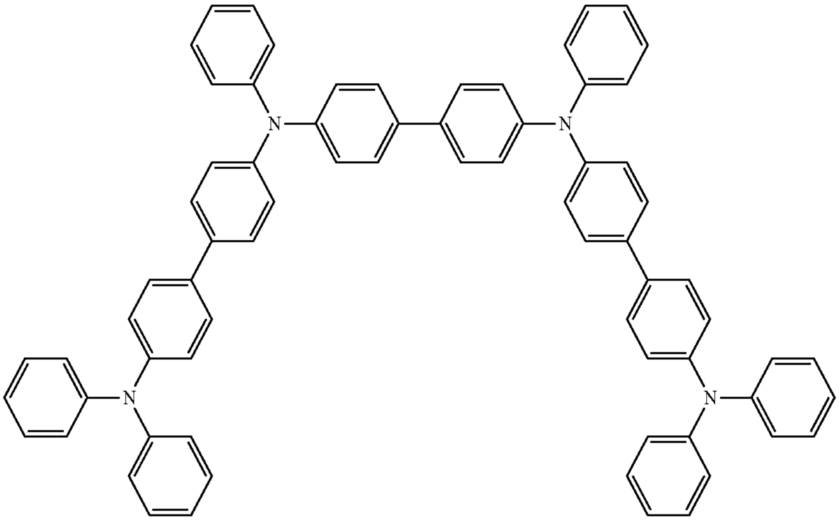
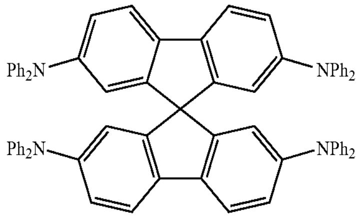
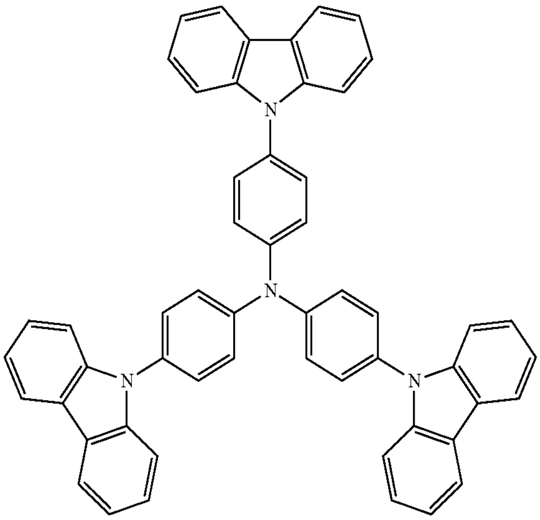
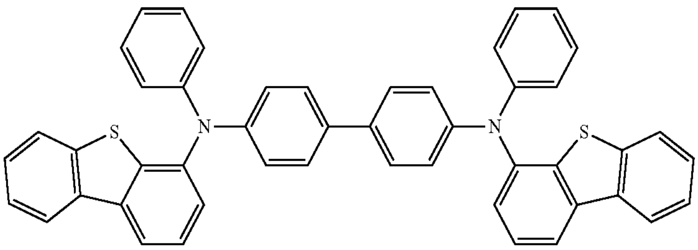
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
Triarylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/(di)benzofuran		US20070278938, US20080106190 US20110163302

TABLE 1-continued

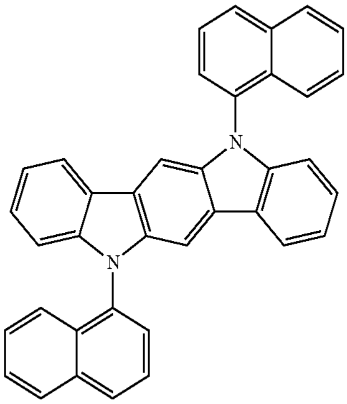
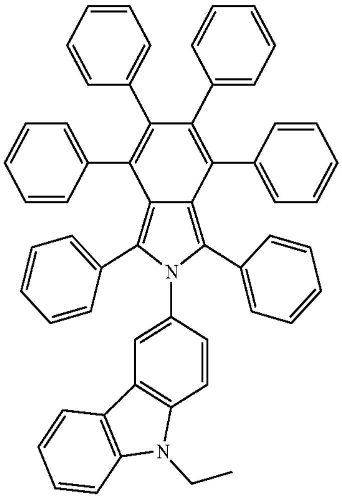
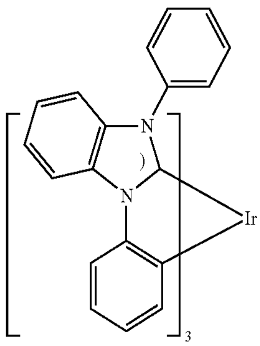
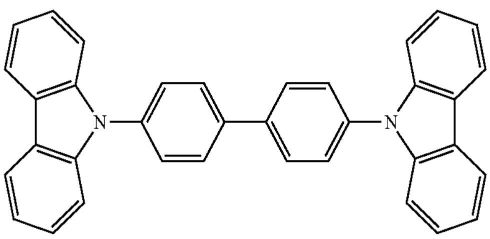
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

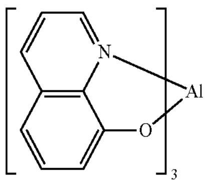
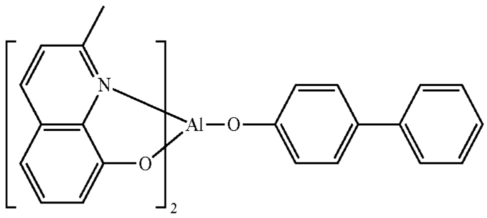
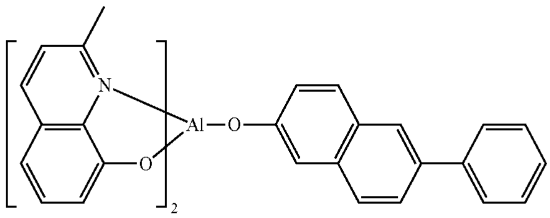
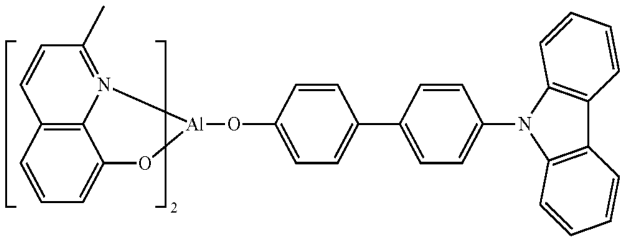
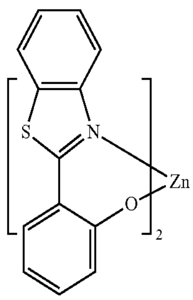
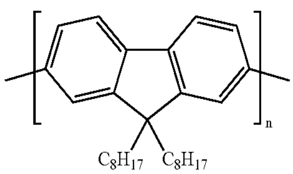
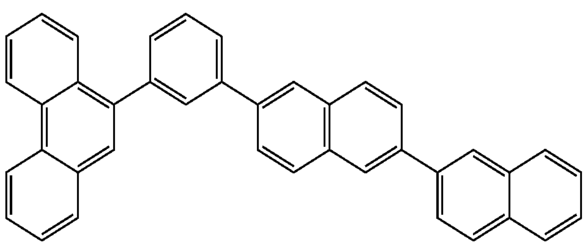
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and ploymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065

TABLE 1-continued

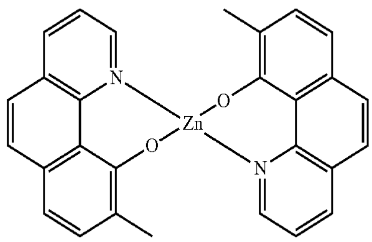
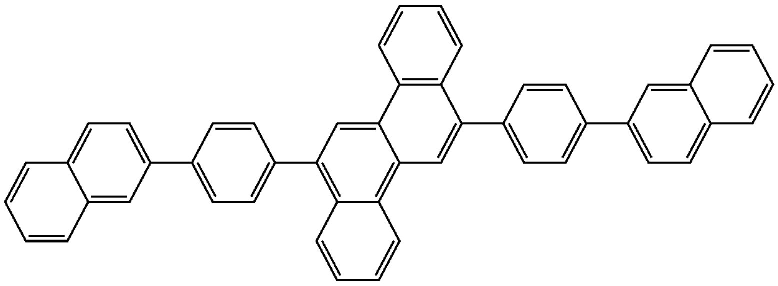
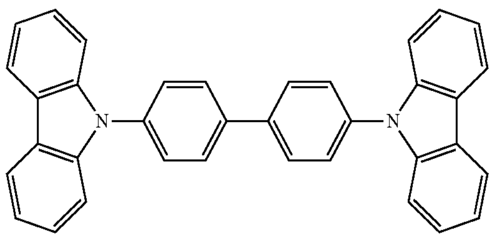
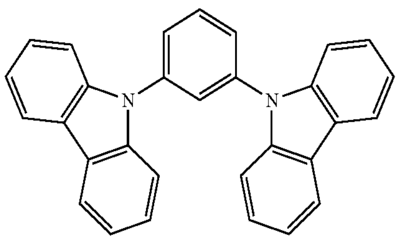
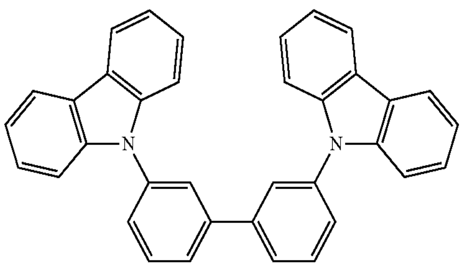
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
Zinc com-plexes		WO2010056066
Chrysene based com-pounds		WO20110866863
Green hosts		
Aryl-carba-zoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234

TABLE 1-continued

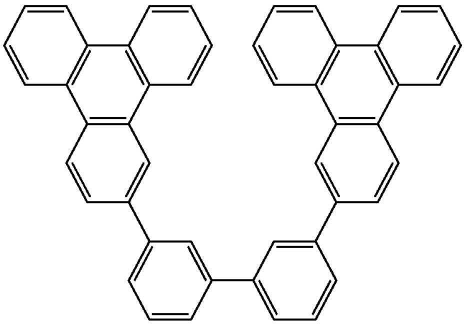
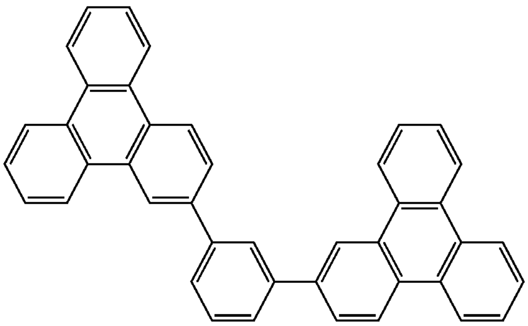
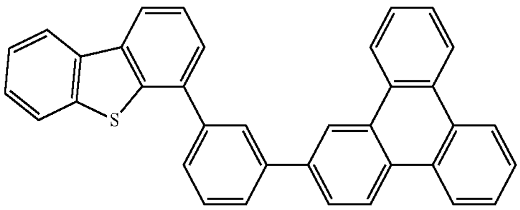
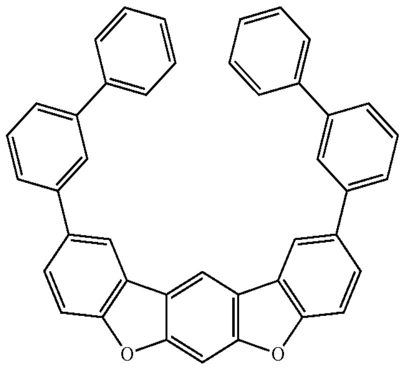
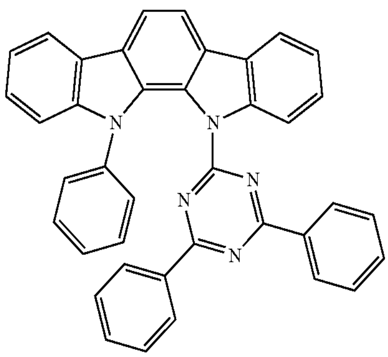
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aryltriphenylene compounds		US20060280965
		US20060280965
		WO2009021126
Polyfused heteroaryl compounds		US20090309488 US20090302743 US20100012931
Donor acceptor type molecules		WO2008056746

TABLE 1-continued

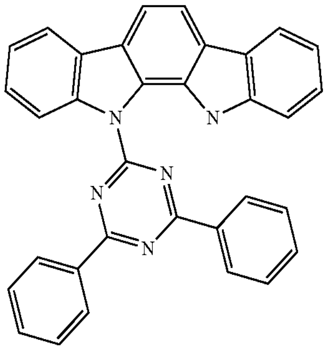
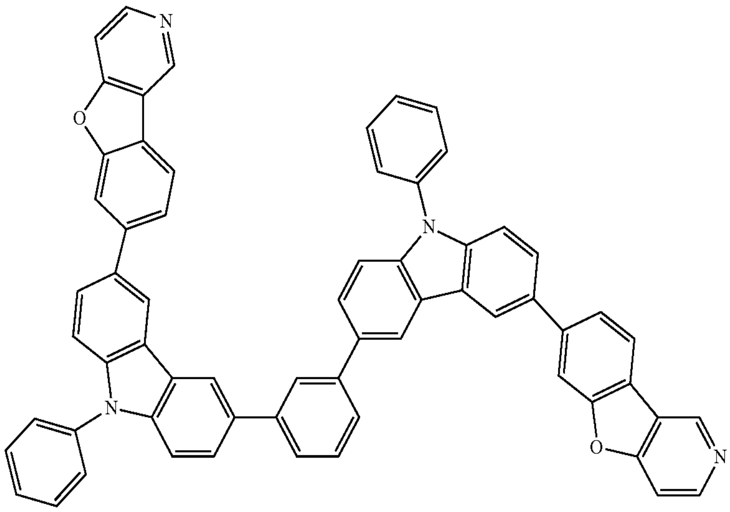
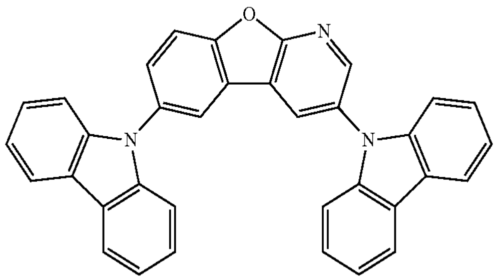
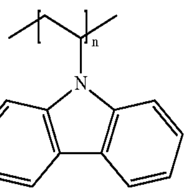
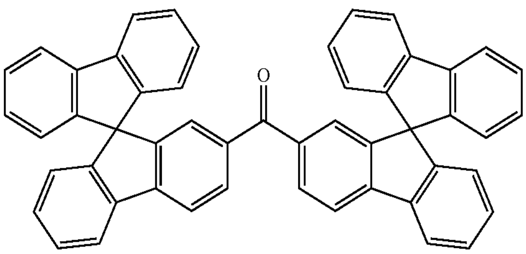
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2010107244
Aza-carbazole/ DBT/ DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spiro-fluorene compounds		WO2004093207

TABLE 1-continued

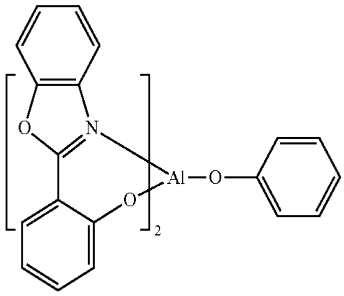
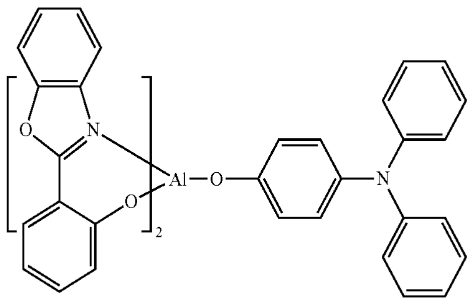
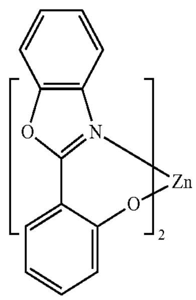
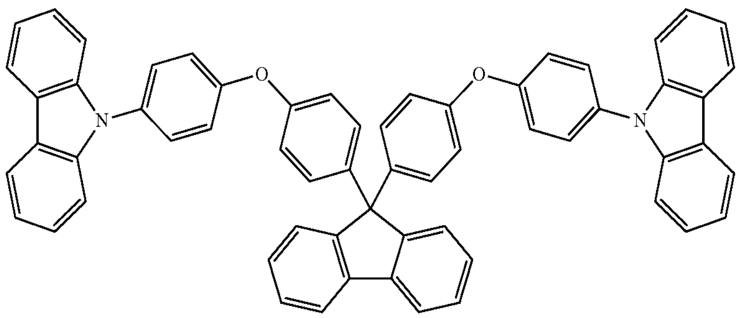
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal phenoxybenzooxazole compounds		WO2005089025
		WO2006132173
		JP200511610
Spirofluorenecarbazole compounds		JP2007254297

TABLE 1-continued

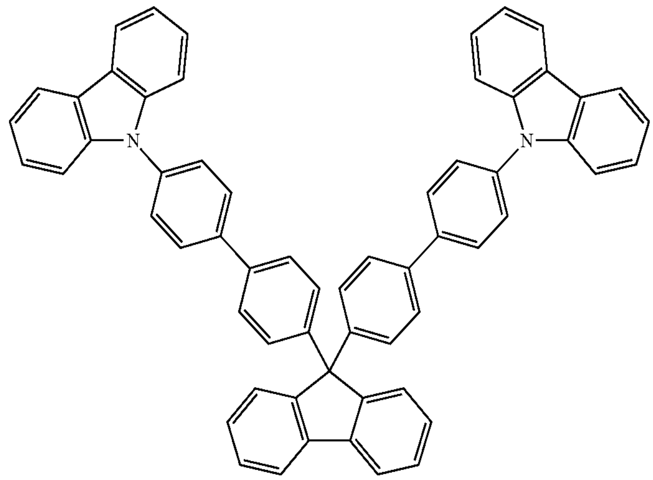
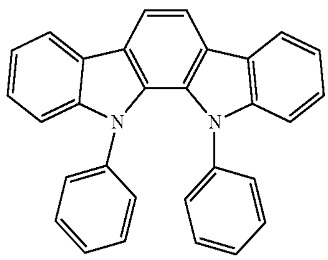
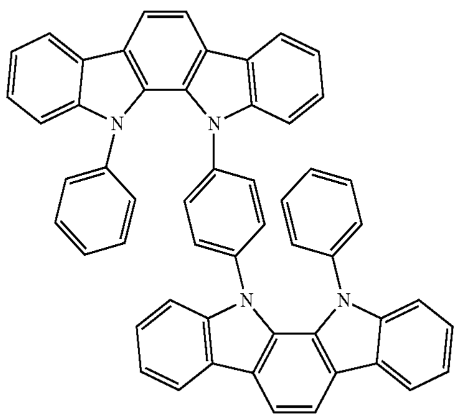
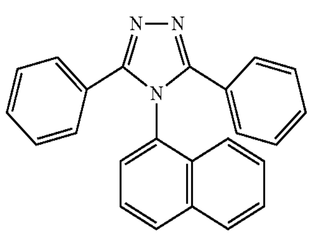
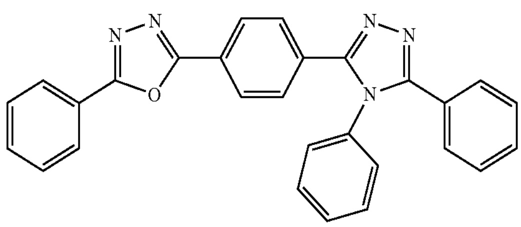
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		JP2007254297
Indolo-carba-zoles		WO2007063796
		WO2007063754
5-member ring electron deficient hetero-cycles (e.g., triazole, oxadi-azole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822

TABLE 1-continued

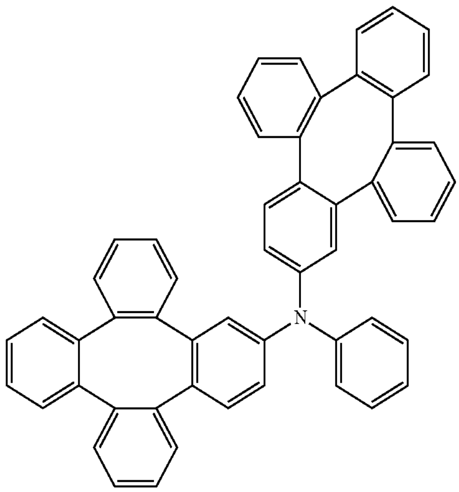
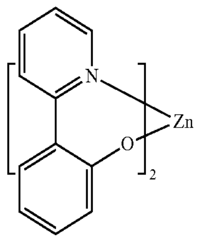
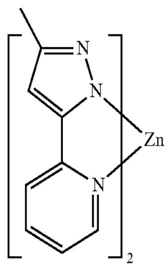
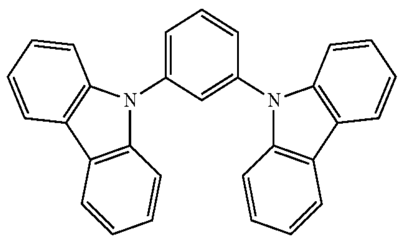
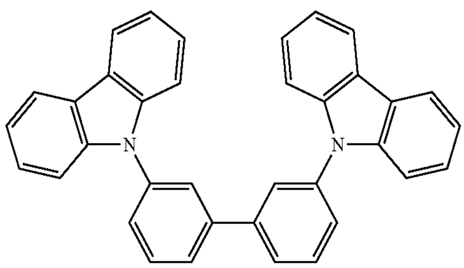
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett. 82, 2422 (2003)
		US20070190359

TABLE 1-continued

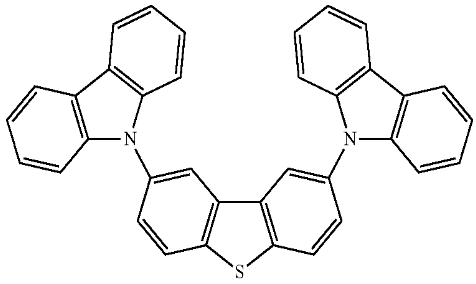
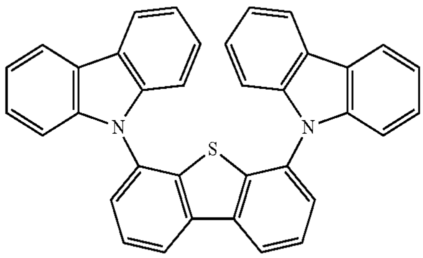
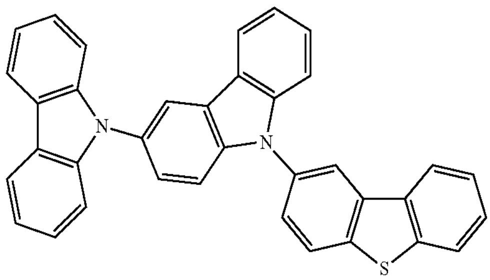
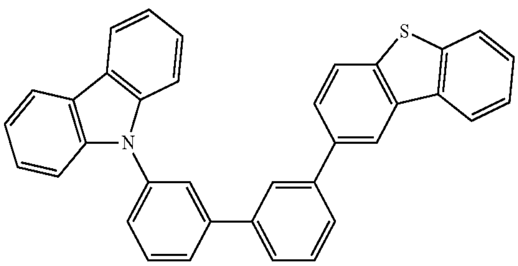
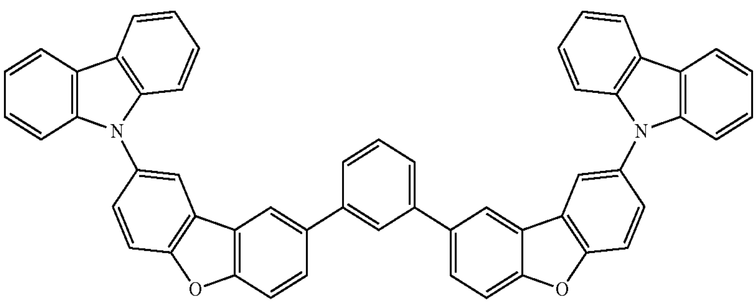
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzothiophene/Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162
		WO2009086028
		US20090030202, US20090017330
		US20100084966

TABLE 1-continued

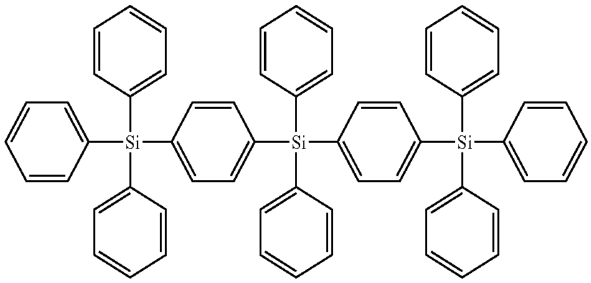
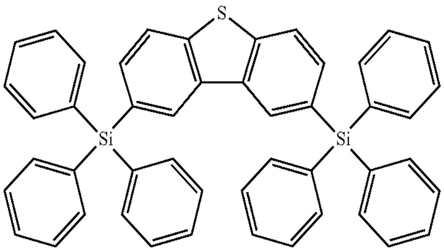
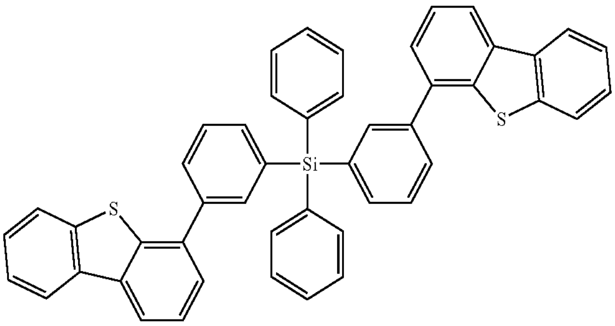
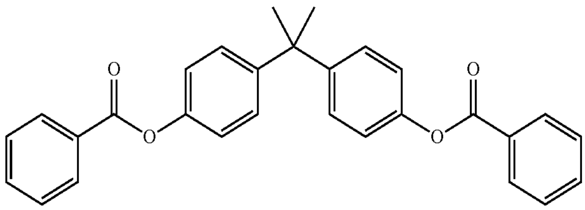
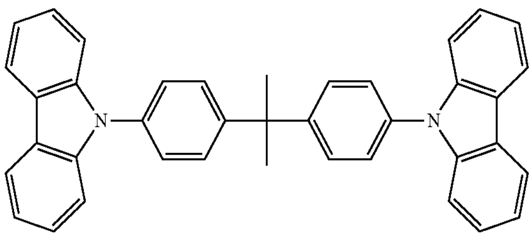
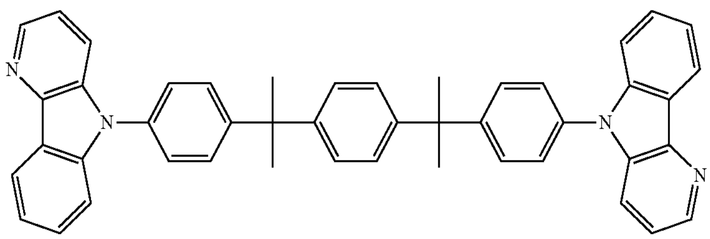
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon aryl compounds		US20050238919
		WO2009003898
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308

TABLE 1-continued

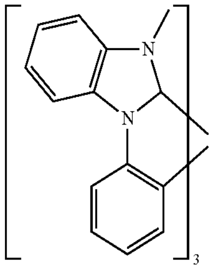
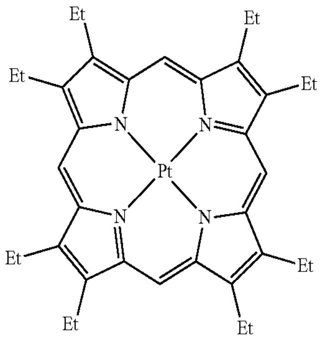
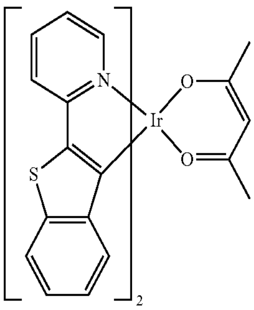
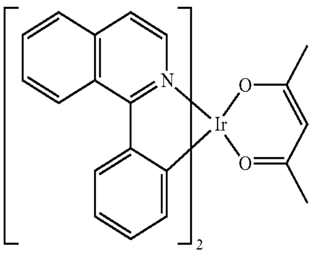
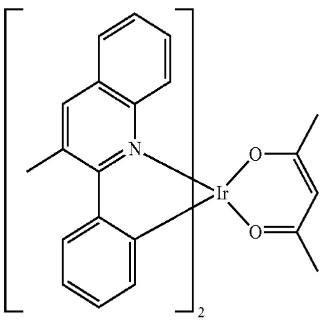
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114
	Phosphorescent dopants Red dopants	
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium (III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US2006835469
		US2006835469

TABLE 1-continued

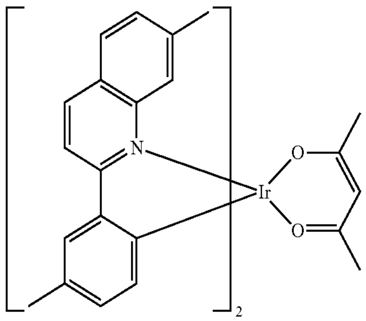
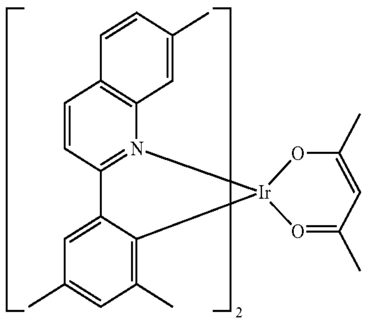
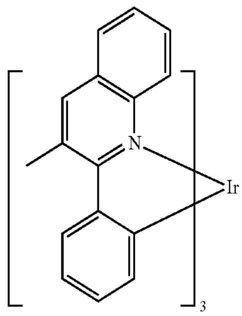
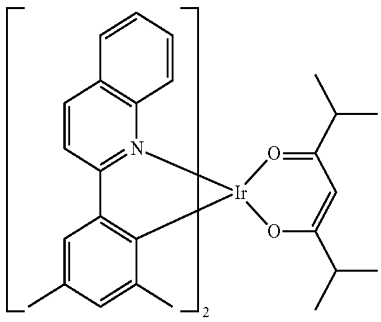
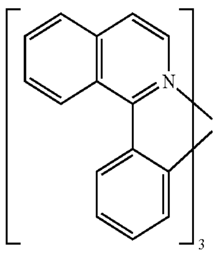
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		US20060202194
		US20060202194
		US20070087321
		US20080261076 US20100090591
		US20070087321

TABLE 1-continued

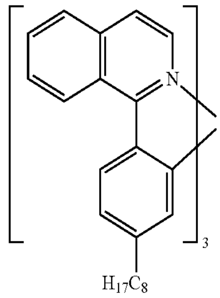
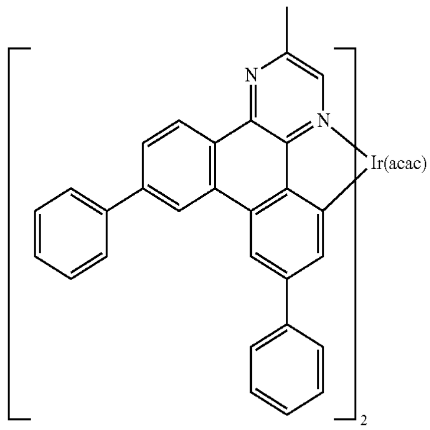
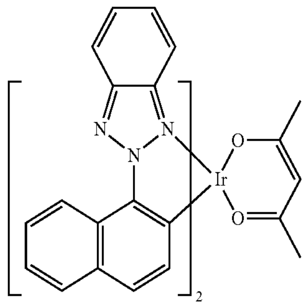
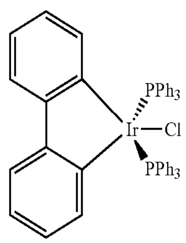
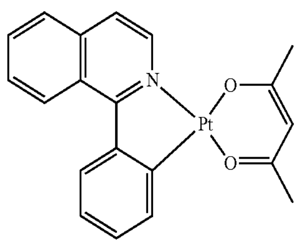
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
		U.S. Pat. No. 7,232,618
Platinum (II) organometallic complexes		WO2003040257

TABLE 1-continued

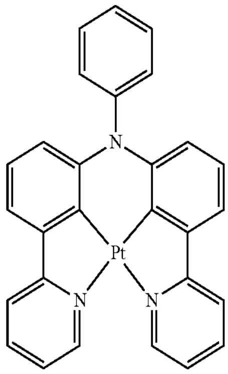
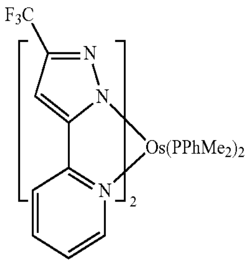
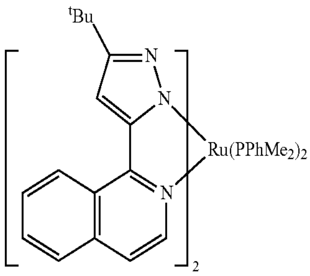
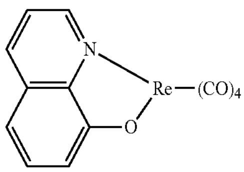
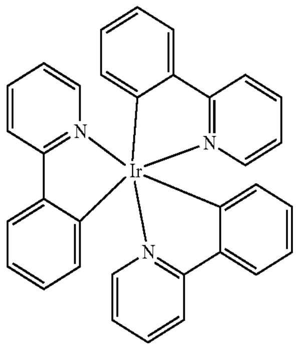
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070103060
Osminum (III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium (II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
	Green dopants	
Iridium (III) organometallic complexes	 and its derivatives	Inorg.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

TABLE 1-continued

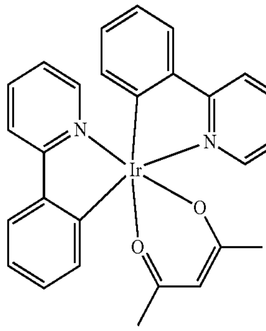
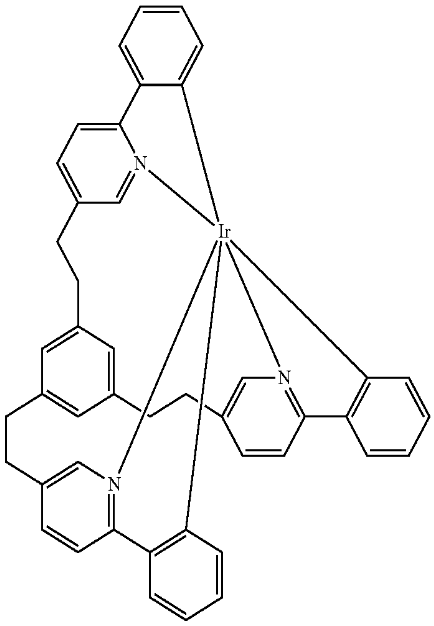
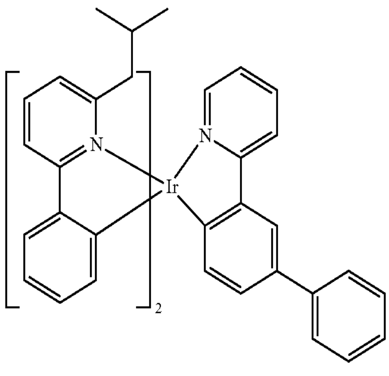
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20020034656
		U.S. Pat. No. 7,332,232
		US20090108737

TABLE 1-continued

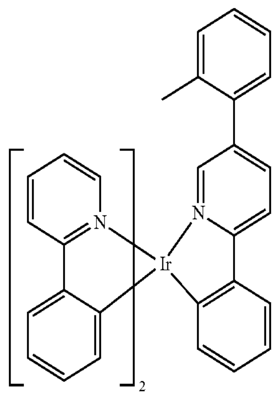
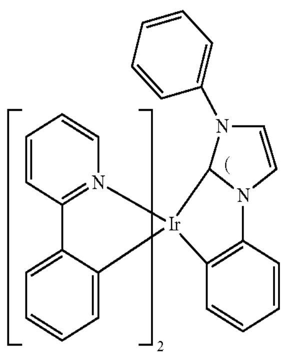
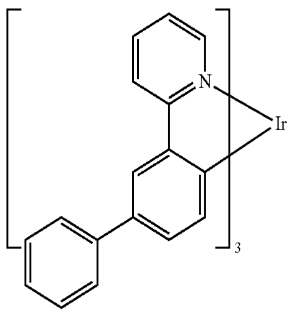
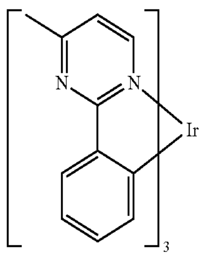
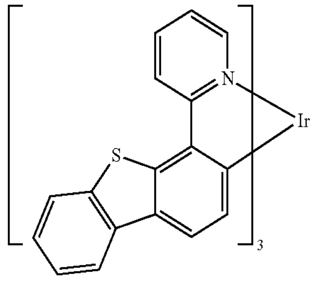
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		WO2010028151
		EP1841834B
		US20060127696
		US20090039776
		U.S. Pat. No. 6,921,915

TABLE 1-continued

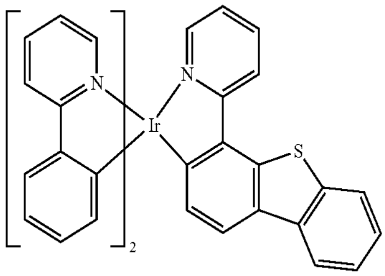
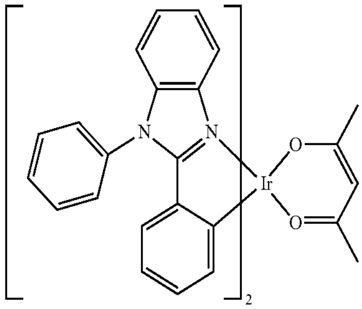
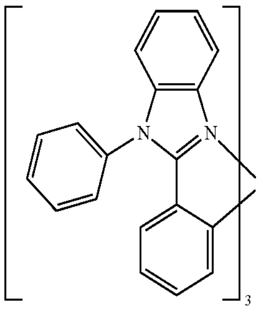
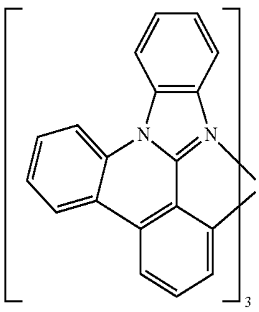
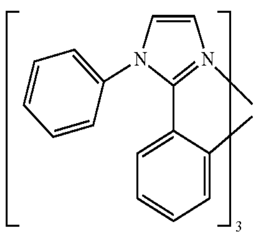
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		US20100244004
		U.S. Pat. No. 6,687,266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US 20060008670 JP2007123392

TABLE 1-continued

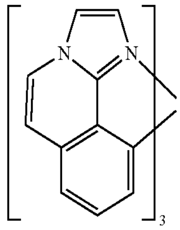
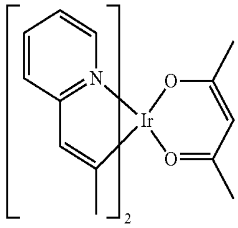
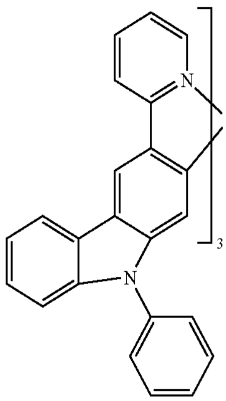
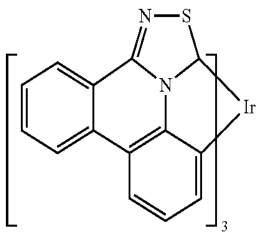
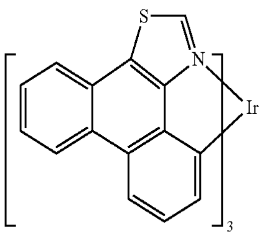
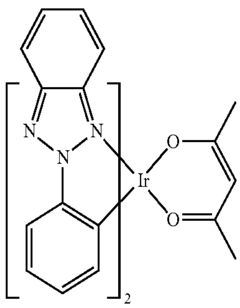
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846
		US20080015355

TABLE 1-continued

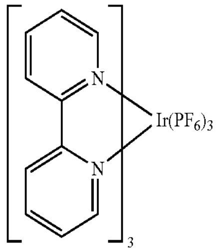
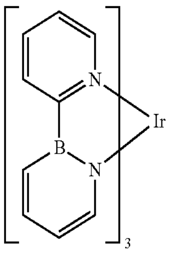
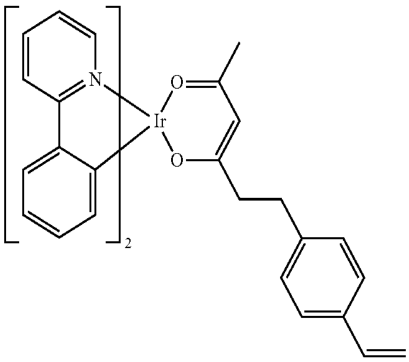
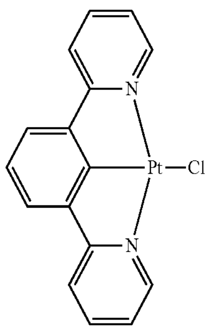
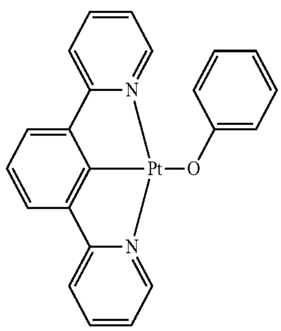
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		US20010015432
		US20100295032
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett.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

TABLE 1-continued

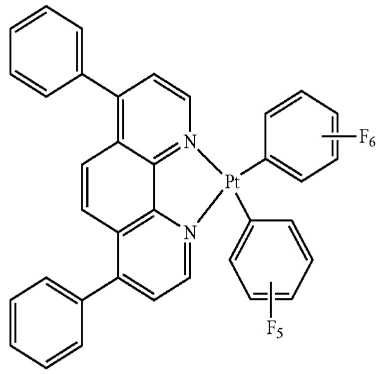
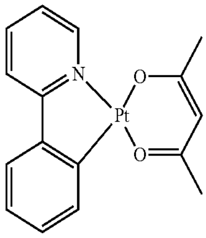
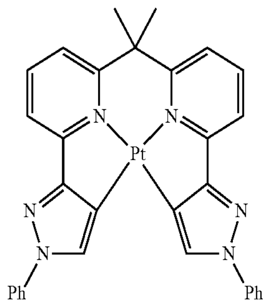
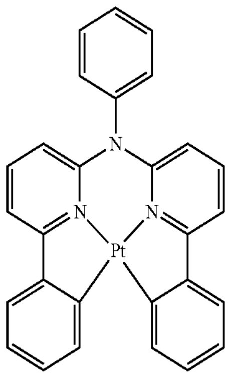
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635
		US20060182992 US20070103060

TABLE 1-continued

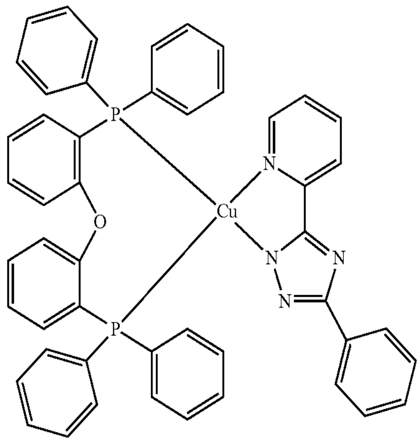
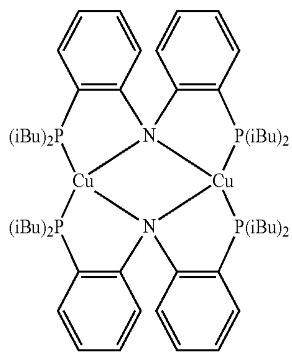
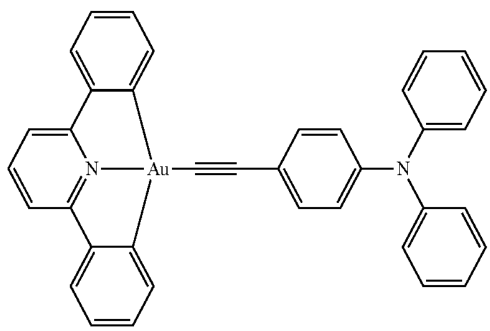
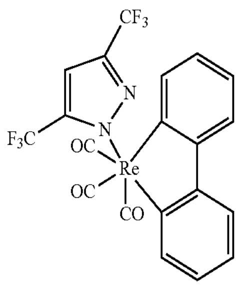
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
		US20070111026
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE 1-continued

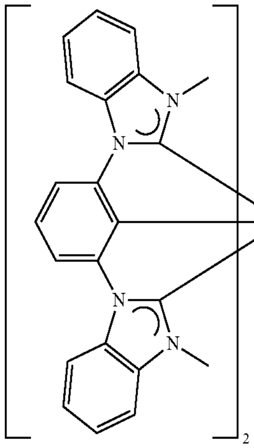
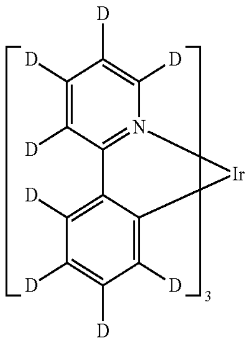
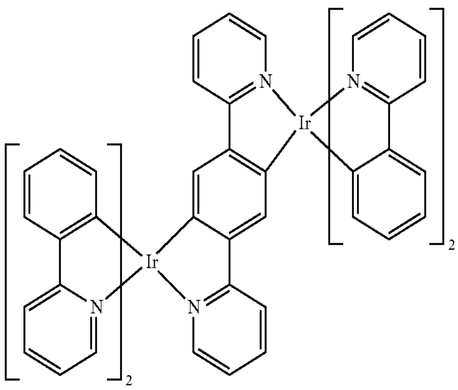
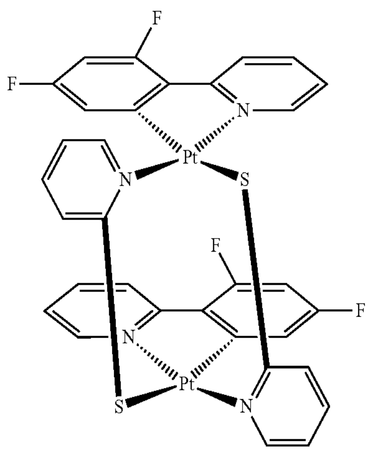
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium (II) complexes		U.S. Pat. No. 7,279,704
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928

TABLE 1-continued

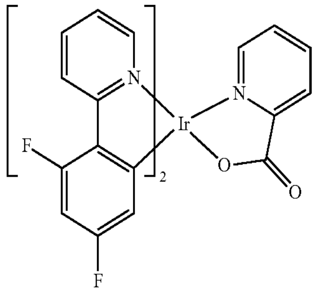
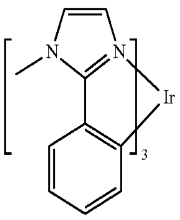
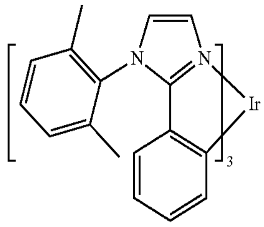
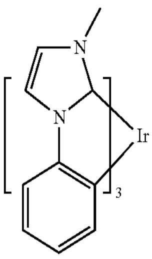
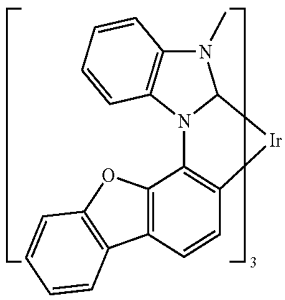
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Blue dopants	
Iridium (III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		U.S. Pat. No. 7,393,599, WO2006056418, US20050260441, WO2005019373
		U.S. Pat. No. 7,534,505

TABLE 1-continued

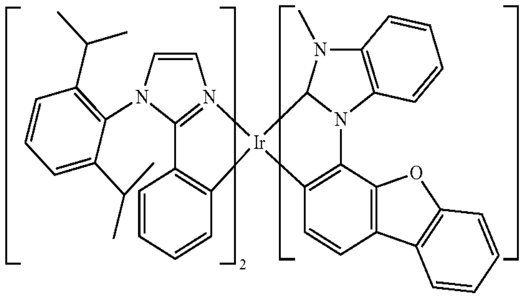
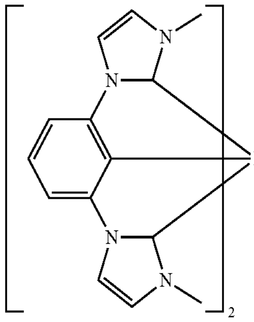
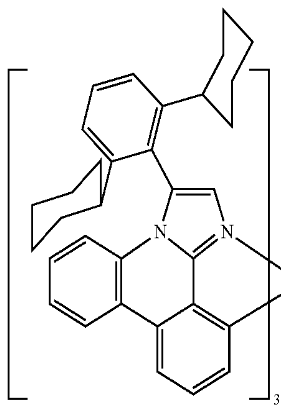
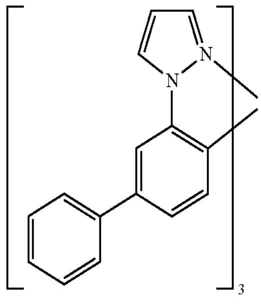
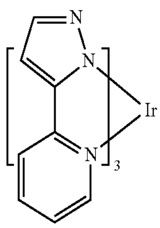
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		WO2011051404
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033 US20100148663
		U.S. Pat. No. 7,338,722
		US20020134984

TABLE 1-continued

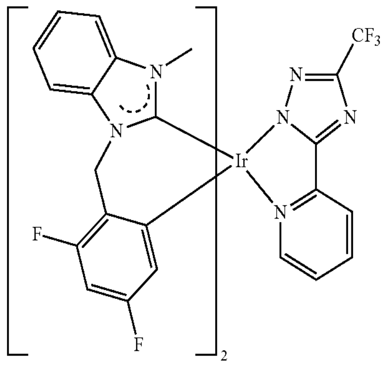
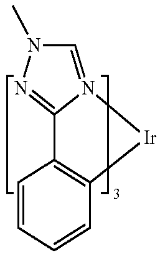
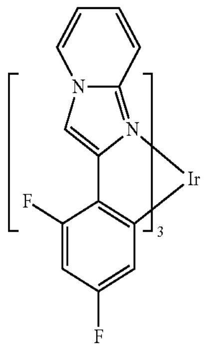
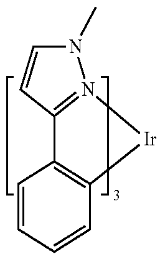
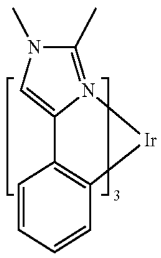
MATE-RIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		Angew. Chem. Int. Ed. 47, 4542 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873

TABLE 1-continued

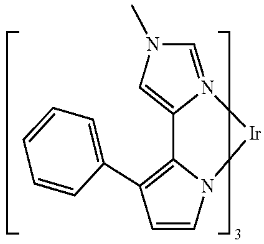
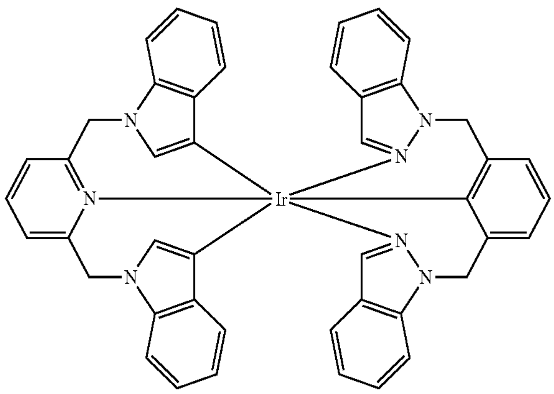
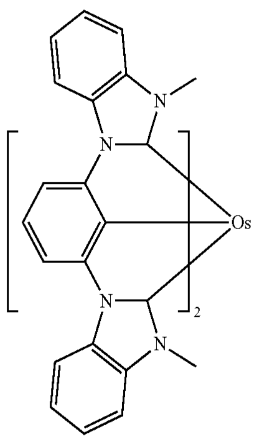
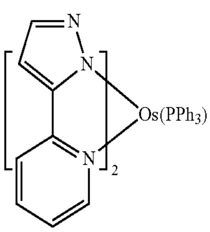
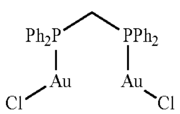
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2007004380
		WO2006082742
Osmium (II) complexes		U.S. Pat. No. 7,279,704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)

TABLE 1-continued

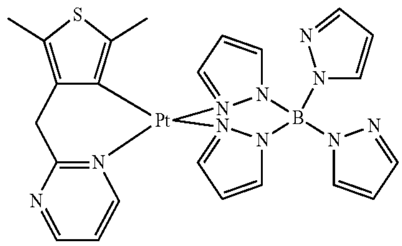
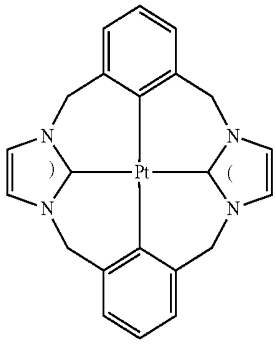
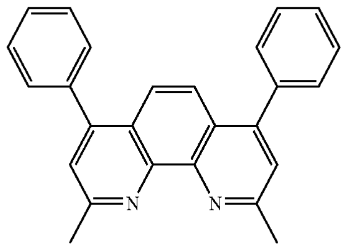
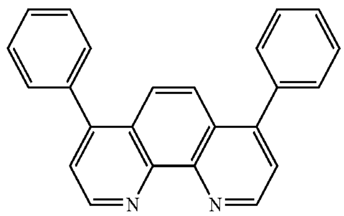
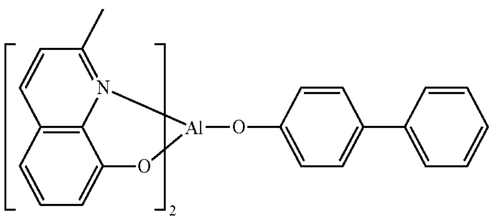
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Platinum (II) complexes		WO2006098120, WO2006103874
Pt tetradentate complexes with at least one metal-carbene bond		U.S. Pat. No. 7,655,323
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)

TABLE 1-continued

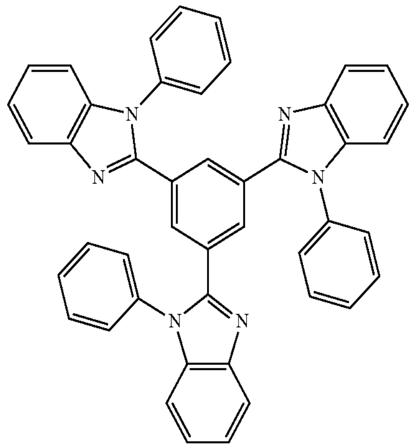
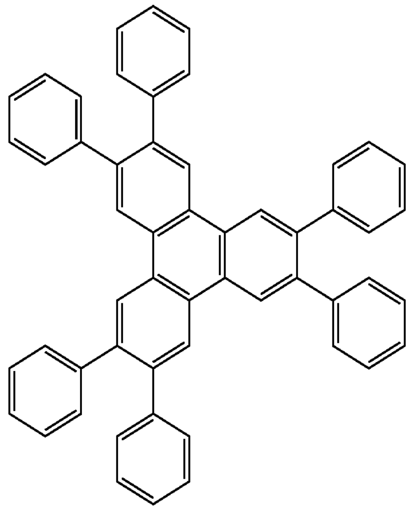
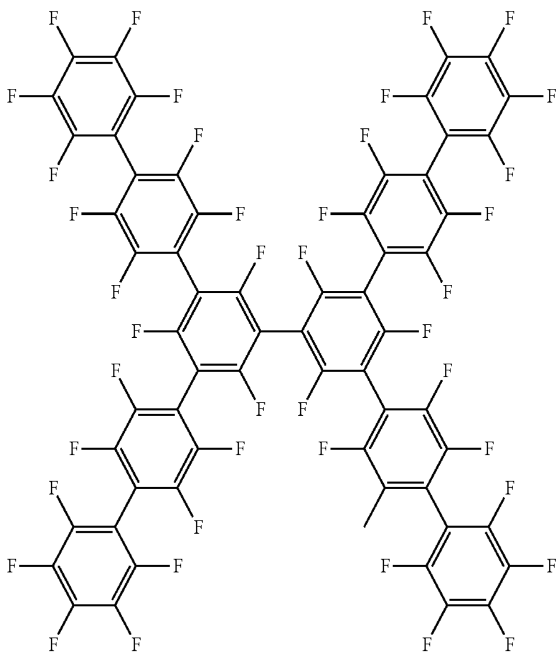
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)

TABLE 1-continued

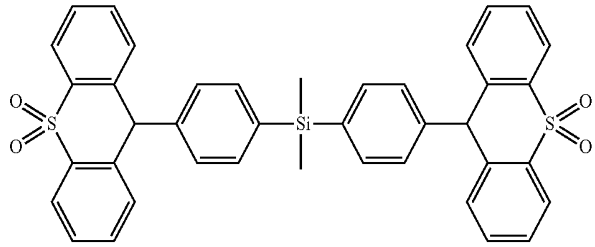
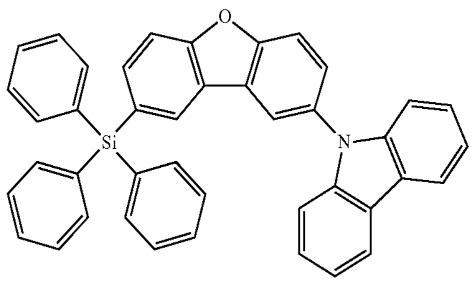
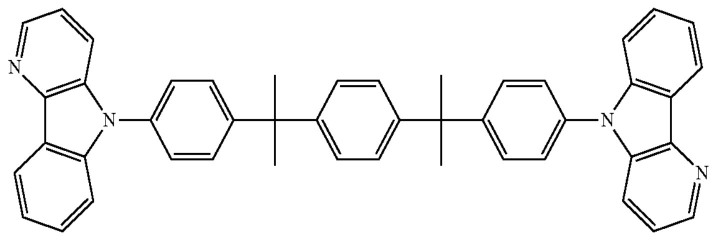
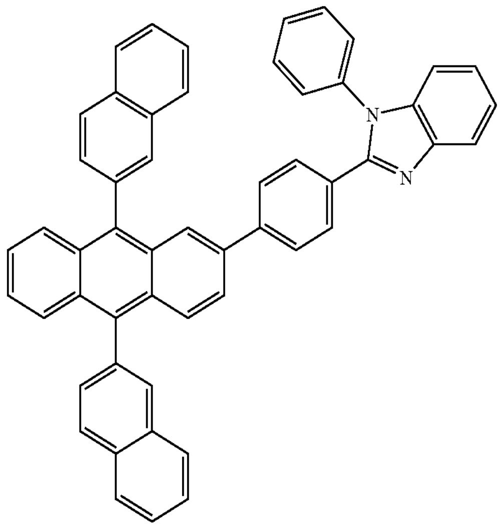
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051
Azacarbazoles		US20060121308
	Electron transporting materials	
Anthracene-benzoimidazole compounds		WO2003060956

TABLE 1-continued

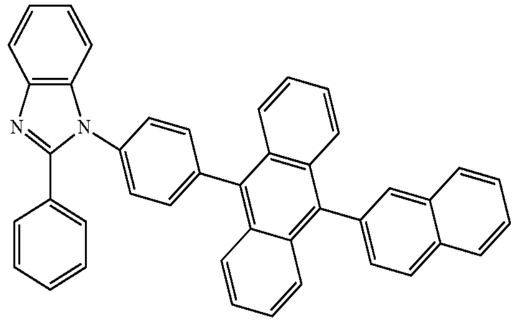
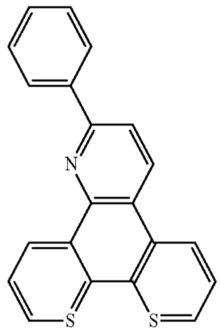
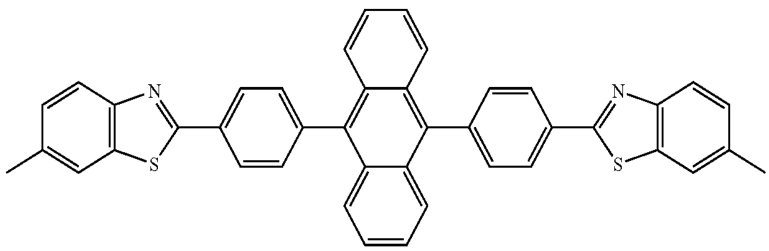
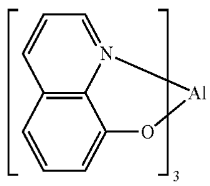
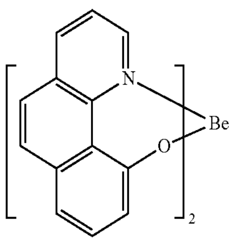
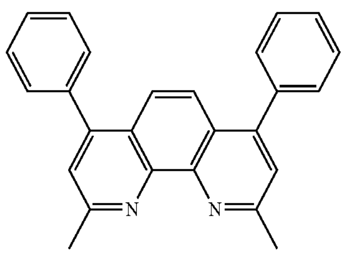
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090179554
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) US7230107
Metal hydroxybenoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)

TABLE 1-continued

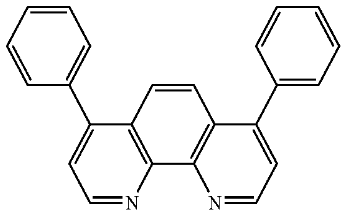
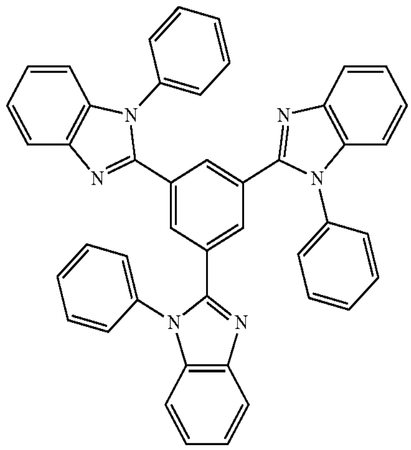
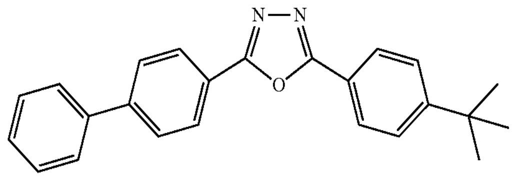
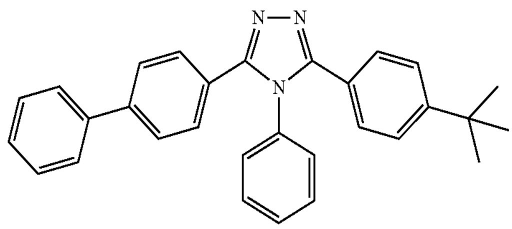
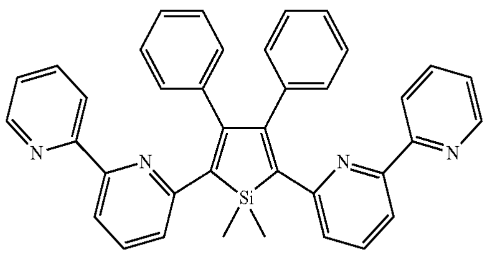
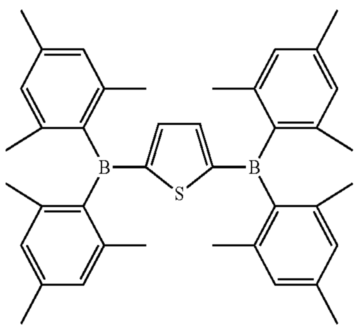
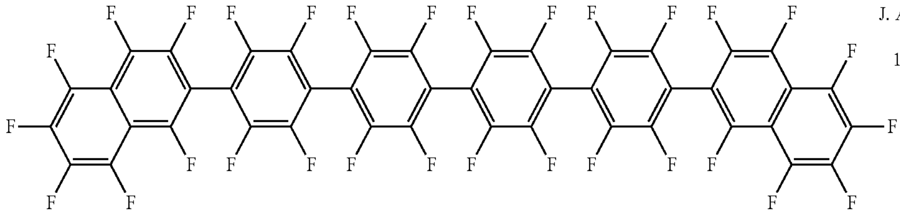
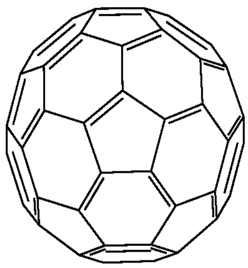
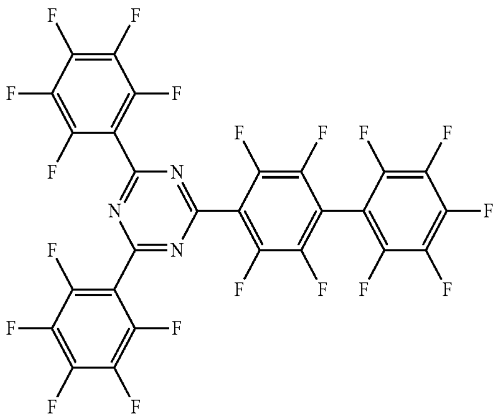
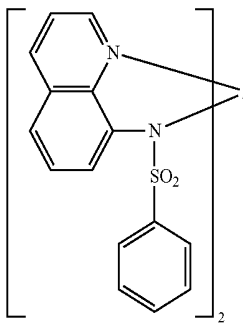
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 79, 449 (2001)
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)

TABLE 1-continued

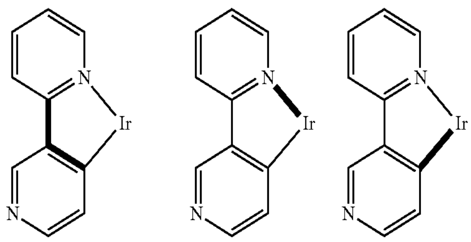
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870
Triazine compounds		US20040036077
Zn (N^N) complexes		U.S. Pat. No. 6,528,187

EXPERIMENTAL

Facial-tris Iridium pyridyl-pyridine complexes offer a unique platform that enables blue emitting phosphorescent complexes without the use of electronic substituents attached to the aromatic rings. It is discovered that the position of the nitrogen is an important factor determining the color of the compound as with the unsubstituted parent ligand there are two possible ligation sites. Hence site blocking/directing substituents, often fluoro or alkyl, can be used to direct ligation to the desired isomer. While the use of site directing substituents is desirable from a synthetic yield and isolation standpoint, it can compromise other properties of the complex. For example, fluorine often blue-shifts the emission energy; however, blue phosphorescent complexes that have fluorine substituted in analogous positions for a phenylpyridine ligand, such as the well-studied FIrpic complex (iridium (III) bis(4,6-difluorophenylpyridinato) picolinate), have been shown to be unstable in electroluminescent devices. Furthermore, bulky alkyl substituents, such as methyl groups, can have steric influences on the plane of the bidentate ligand, resulting in a significant red-shifting effect at room temperature. This effect is observed when comparing methyl blocked pyridyl-pyridine emitters to analogous non-blocked complexes.

The invention described here is a modification to the pyridyl-pyridine ligand that provides both a site direction for synthesis of the desired tris isomer in high yield as well as a rigidifying effect on the ligand in order to provide more a saturated blue emission at room temperature. Both of these effects can be accomplished by bridging the pyridyl pyridine ligand with a single non-conjugating atom linker, such as silicon or sulfur. Silicon or sulfur, or larger atoms, may be preferred over oxygen due to the effect of the atom's size on the ligand bite angle for complexation.

Density functional theory was used to minimize the ground state geometry of the complexes. Calculations were performed using the B3LYP/cep-31g/THF functional, basis set and solvent polarization, respectively. The relavent bond angles and bond lengths for the C—C—C, Ir—N and Ir—C bonds are defined in bold:



C—C—C Bond Angle Ir—N Bond Ir—C Bond

TABLE 2

Bond angles and bond lengths for invention compounds and comparative examples.

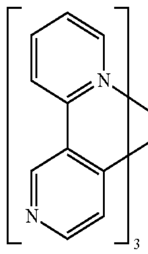
	Structure	Bond angle (°)	Ir-N (Å)	Ir-C (Å)
Comparative Example 1		116.3	2.17	2.03

TABLE 2-continued

Bond angles and bond lengths for invention compounds and comparative examples.

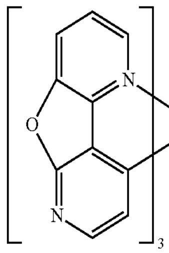
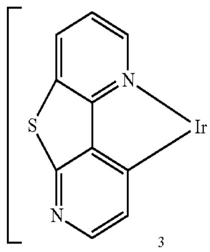
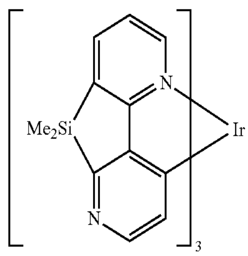
	Structure	Bond angle (°)	Ir-N (Å)	Ir-C (Å)
Comparative Example 2		125.6	2.41	2.03
Compound 1		121.4	2.25	2.04
Compound 2		119.3	2.21	2.04

Table 2 shows the preferred structures where the bridging atom is large enough to bridge the two pyridine rings without significant distortion around the metal. The data shows that where the bridging atom is oxygen, the bond angle (125.6°) and Ir—N bond length (2.41 Å) are significantly distorted compared to Comparative Example 1 and the invention compounds. For a non-strained ring system, the bond angle should be close to an ideal 120° as is the case for Compound 1 and 2.

Table 3 shows the energy level calculations for bridged and unbridged pyridyl-pyridine ligands.

TABLE 3

Energy level calculations

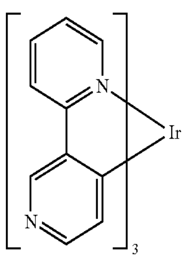
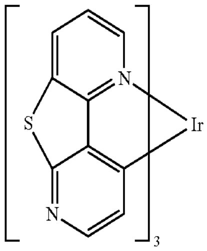
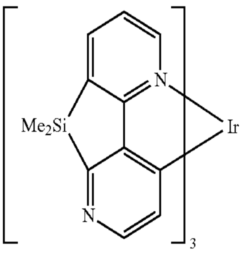
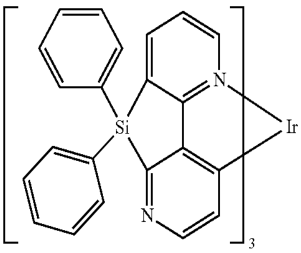
	Structure	HOMO (eV)	LUMO (eV)	Gap (eV)	Dipole (Debye)	$S1_{gas}$ (nm)	$T1_{gas}$ (nm)
Comparative Example 1		−5.87	−1.89	−3.91	16.22	395	462

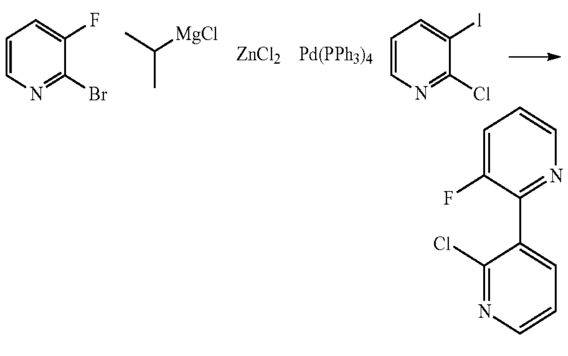
TABLE 3-continued

Energy level calculations							
	Structure	HOMO (eV)	LUMO (eV)	Gap (eV)	Dipole (Debye)	$S1_{gas}$ (nm)	$T1_{gas}$ (nm)
Compound 1		−6.11	−2.07	−4.04	14.44	390	445
Compound 2		−5.71	−1.74	−3.97	14.74	386	463
Compound 3		−5.79	−1.83	−3.96	14.29	386	465

Synthetic Examples

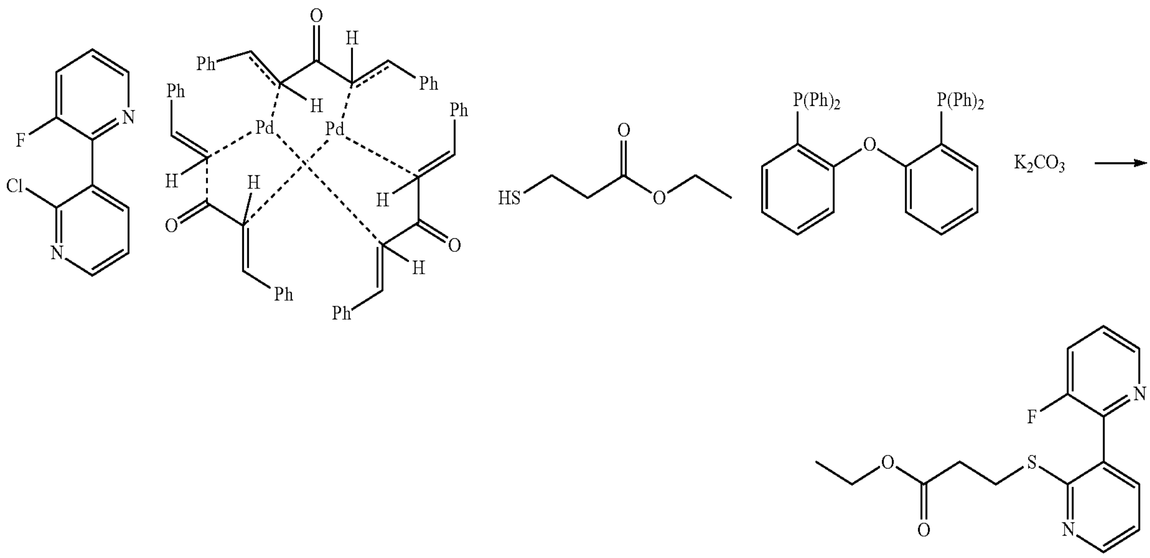
Synthesis of Ligand 1

Synthesis of 2'-chloro-3-fluoro-2,3'-bipyridine



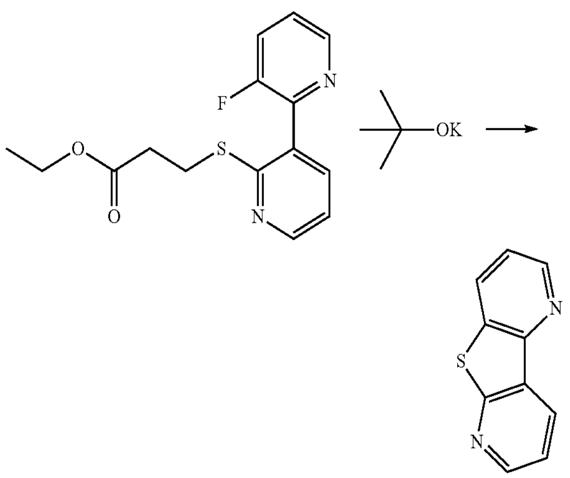
A solution of isopropylmagnesium chloride in THF (2.0 M, 20.05 ml, 40.1 mmol) was dissolved in THF (25 ml) and cooled in ice/water bath, before 2-bromo-3-fluoropyridine (3.72 ml, 36.8 mmol) was slowly added via syringe. The resulting solution in stirred at room temperature for 1 hour, then a zinc(II) chloride solution in THF (0.5 M, 80 ml, 40.1 mmol) was added via syringe and stirred at room temperature overnight, forming a nearly colorless, heterogeneous mixture. Separately, a flask containing 2-chloro-3-iodopyridine (8 g, 33.4 mmol) and $Pd(PPh_3)_4$ (1.930 g, 1.671 mmol) was degassed, then THF (100 ml) was added and the resulting solution was warmed to near reflux. The zinc chloride suspension was added via cannula to the 2-chloro-3iodopyridine solution and the resulting yellow mixture was stirred at reflux over the weekend, cooled to room temperature, and then filtered through celite. Solvent removal from the filtrates was followed by partitioning between EtOAc and basic water. The aqueous layer was extracted with EtOAc three times, the combined organics were washed with brine, dried, and the solvent as removed. After coating on celite, the product was eluted on a 200 g silica column using 10-25% EtOAc in DCM, collecting pale yellow R_f~0.45 fractions, yielding a pale yellow solid, 5.29 g (76%).

Synthesis of ethyl 3-((3-fluoro-[2,3'-bipyridin]-2'-yl)thio)propanoate



2'-chloro-3-fluoro-2,3'-bipyridine (4.96 g, 23.78 mmol), $Pd_2(dba)_3$ (0.544 g, 0.594 mmol), (oxybis(2,1-phenylene))bis(diphenylphosphine) (0.640 g, 1.189 mmol), and potassium carbonate (8.21 g, 59.4 mmol) were combined in a 3-neck flask, vacuum/backfilled three times with nitrogen, and degassed. Toluene (120 ml) was added and heated to a gentle reflux, which produced a light orange mixture. Ethyl 3-mercaptopropanoate (3.31 ml, 26.2 mmol) was added and the reaction mixture was heated at reflux overnight. The reaction mixture was cooled to room temperature, diluted with EtOAc and filtered through celite. After solvent removal from the filtrate, the residue was coated on celite and eluted on a 120 g silica column using 25% EtOAc/DCM, then 50% EtOAc/DCM. The resulting very pale yellow fractions with R_f~0.6 (50% EtOAc/DCM) was collected yielding a yellow-stained oil containing ethyl 3-((3-fluoro-[2,3'-bipyridin]-2'-yl)thio)propanoate, 6.95 g (95%).

Synthesis of thieno[2,3-b:4,5-b']dipyridine



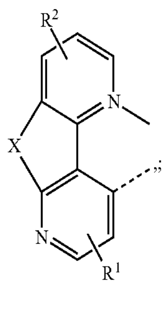
A solution of ethyl 3-((3-fluoro-[2,3'-bipyridin]-2'-yl)thio)propanoate (6.20 g, 20.24 mmol) in dioxane (120 ml) was added via cannula to a nitrogen-purged flask containing potassium tert-butoxide (3.41 g, 30.4 mmol) and the mixture was heated at reflux overnight with efficient stirring. The mixture first became a sludge, then a more fluid suspension. The reaction mixture was cooled to room temperature, partitioned between EtOAc and water/brine, separated, and the aqueous layer was extracted three more times with EtOAc. The combined organics were washed with brine, dried, and the solvent was removed. The residue was coated on celite and eluted on a 120 g silica column using 1:1 EtOAc/DCM, collecting R_f~0.35 fractions, yielding 3.44 g of yellowish solid that was distilled on a kugelrohr (170-205° C.) to yield a nearly colorless oil containing thieno[2,3-b:4,5-b']dipyridine that crystallizes at room temperature, 3.37 g (89%).

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 comprising a Ligand L of Formula I:

Formula I



wherein R^1 represents mono, or di-substitution, or no substitution;

wherein R^2 represents mono, di, or tri-substitution, or no substitution;

wherein X is GeRR';

wherein R^1, R^2, R, and R' are each 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 any adjacent substitutions are optionally linked together to form a ring;

wherein the Ligand L is coordinated to a metal M having an atomic number of 40 or greater; and

wherein the Ligand L is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

2. The compound of claim **1**, wherein M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt, Au, and Cu.

3. The compound of claim **1**, wherein M is Ir.

4. The compound of claim **1**, wherein the compound is homoleptic having formula of IrL_3.

5. The compound of claim **4**, wherein said compound is a facial isomer.

6. The compound of claim **4**, wherein said compound is a meridional isomer.

7. The compound of claim **1**, wherein the compound is heteroleptic.

8. The compound of claim **1**, wherein R^1, and R^2 are each independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

9. The compound of claim **1**, wherein at least one of R^1 and R^2 is a moiety selected from the group consisting of phenyl, toluene, biphenyl and tetraphenyl.

10. The compound of claim **1**, wherein X is GeRR', and R and R' are each independently selected from the group consisting of alkyl, aryl, heteroaryl, and combinations thereof.

11. The compound of claim **1**, wherein R^1 is mono-substitution on the ortho position to N, and R^1 is selected from the group consisting of 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.

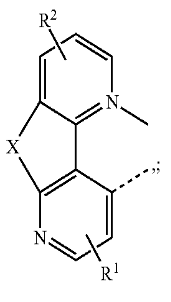
12. A first device comprising a first organic light emitting device, the first organic light emitting device comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound comprising a Ligand L of Formula I:

Formula I



wherein R^1 represents mono, or di-substitution, or no substitution;

wherein R^2 represents mono, di, or tri-substitution, or no substitution;

wherein X is GeRR';

wherein R^1, R^2, R, and R' are each 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 any adjacent substitutions are optionally linked together to form a ring;

wherein the Ligand L is coordinated to a metal M having an atomic number of 40 or greater; and

wherein the Ligand L is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

13. The first device of claim **12**, wherein the organic layer is an emissive layer and the compound is an emissive dopant.

14. The first device of claim **12**, wherein the organic layer is an emissive layer and the compound is a non-emissive dopant.

15. The first device of claim **12**, wherein the organic layer further comprises a host material.

16. The first device of claim **15**, wherein the host material comprises a triphenylene containing benzo-fused thiophene or benzo-fused furan;

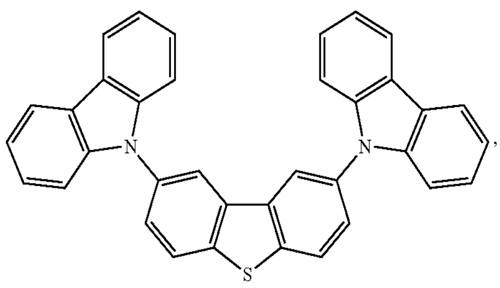
wherein any substituent in the host material is an unfused substituent independently selected from the group consisting of C_nH_{2n+1}, OAr_1, $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH{=}CH{-}C_nH_{2n+1}$, $C{\equiv}C{-}C_nH_{2n+1}$, Ar_1, $Ar_1{-}Ar_2$, and $C_nH_{2n}{-}Ar_1$;

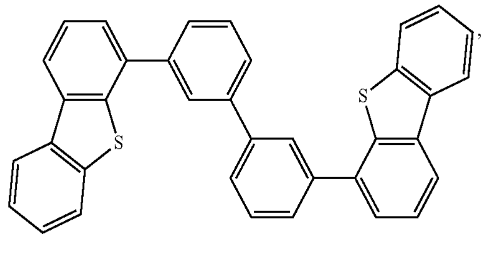
wherein n is from 1 to 10; and

wherein Ar_1 and Ar_2 are independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.

17. The first device of claim **15**, wherein the host material comprises at least one chemical group selected from the group consisting of carbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene.

18. The first device of claim **15**, wherein the host material is selected from the group consisting of:





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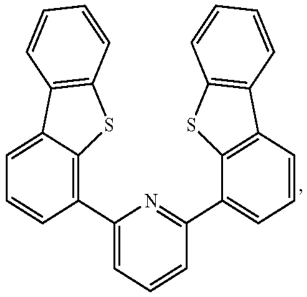

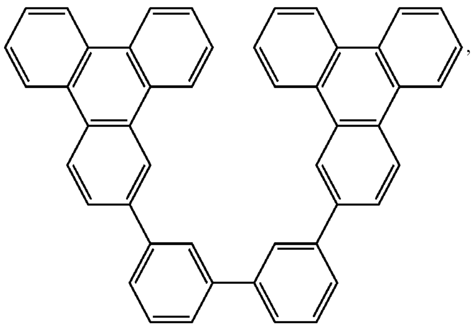

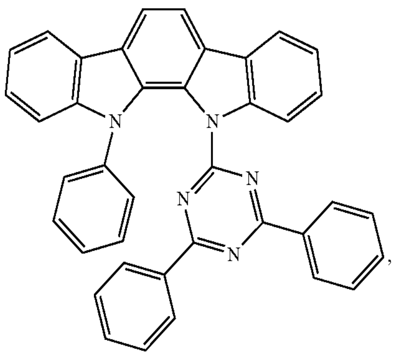

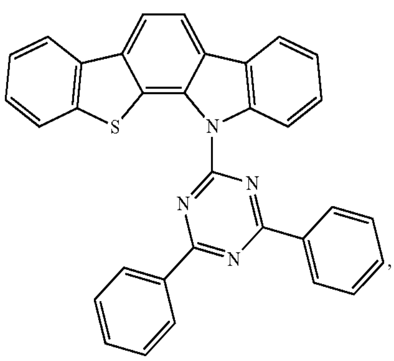

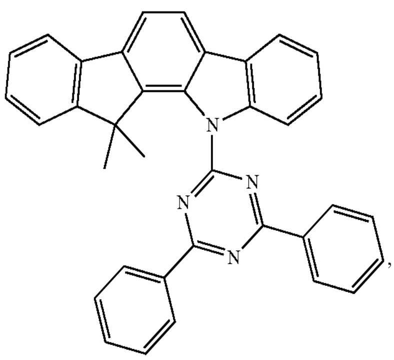

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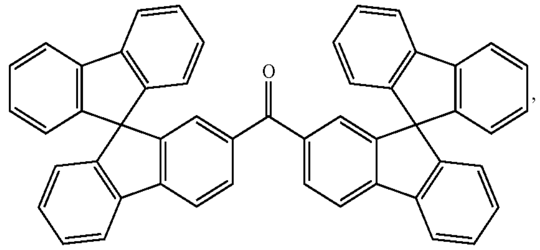
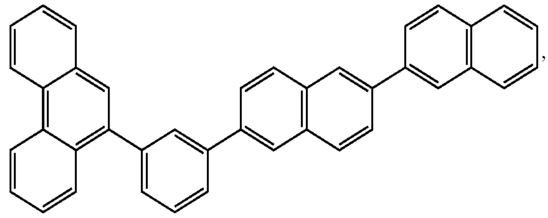
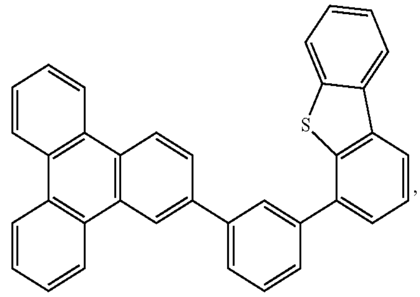
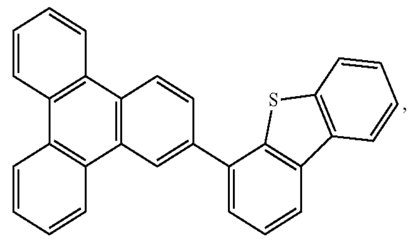




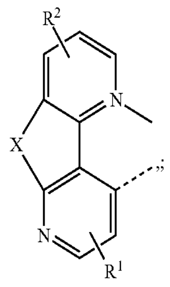




and combinations thereof.

19. A formulation comprising a compound comprising a Ligand L of Formula I:

Formula I



wherein R^1 represents mono, or di-substitution, or no substitution;

wherein R^2 represents mono, di, or tri-substitution, or no substitution;

wherein X is GeRR';

wherein R^1, R^2, R, and R' are each 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;

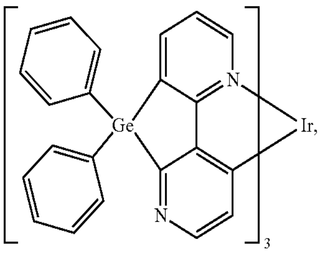
wherein any adjacent substitutions are optionally linked together to form a ring;

wherein the Ligand L is coordinated to a metal M having an atomic number of 40 or greater; and

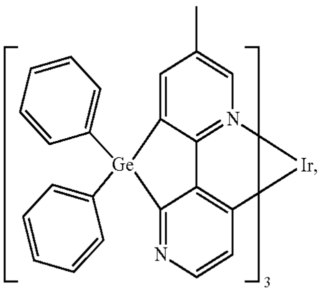
wherein the Ligand L is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

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

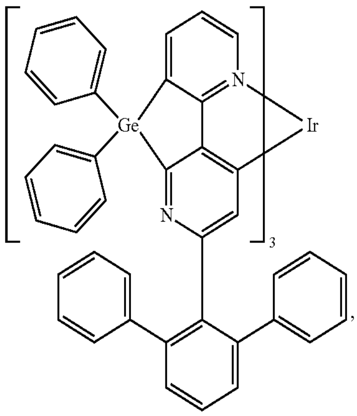
Compound 11



Compound 13



Compound 19



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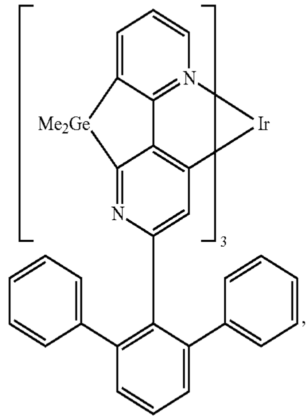
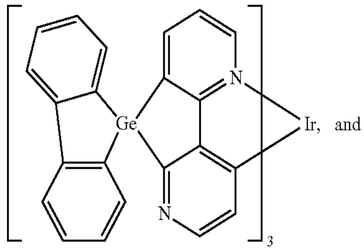
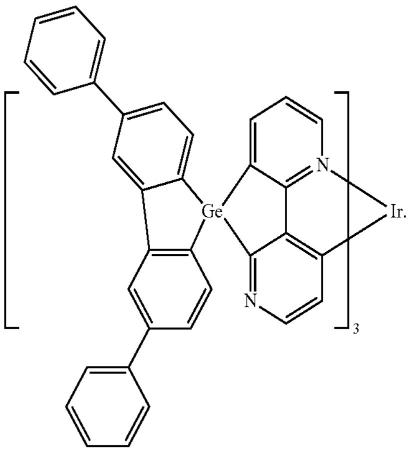
Compound 31



Compound 32



Compound 34



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专利名称(译)	有机电致发光材料和器件		
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申请号	US14/194311	申请日	2014-02-28
[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	SZIGETHY GEZA BROOKS JASON		
发明人	SZIGETHY, GEZA BROOKS, JASON		
IPC分类号	H01L51/54 C07F15/00 C09K11/06 H01L51/00 H01L51/50		
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代理机构(译)	DUANE MORRIS LLP		
其他公开文献	US20150249223A1		
外部链接	Espacenet USPTO		

摘要(译)

包含式I的配体L的化合物： 以及第一装置和含有它的制剂公开了。在包含式I的配体L的化合物中： X选自S，Se，SiRR'和GeRR'; R 1 ，R 2 ，R和R'各自独立地选自氢，氘，卤化物，烷基，环烷基，杂烷基，芳烷基，烷氧基，芳氧基，氨基，甲硅烷基，烯基，环烯基，杂烯基，炔基，芳基，杂芳基，酰基，羰基，羧酸，酯，腈，异腈，硫烷基，亚磺酰基，磺酰基，膦基及其组合; 任何R 1 ，R 2 ，R和R'的相邻取代基或取代基任选地连接在一起形成环; 配体L与原子序数为40或更大的金属M配位;并且 配体L任选地与其他配体连接以包含三齿，四齿，五齿或十齿配体。

Formula I