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(54) ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

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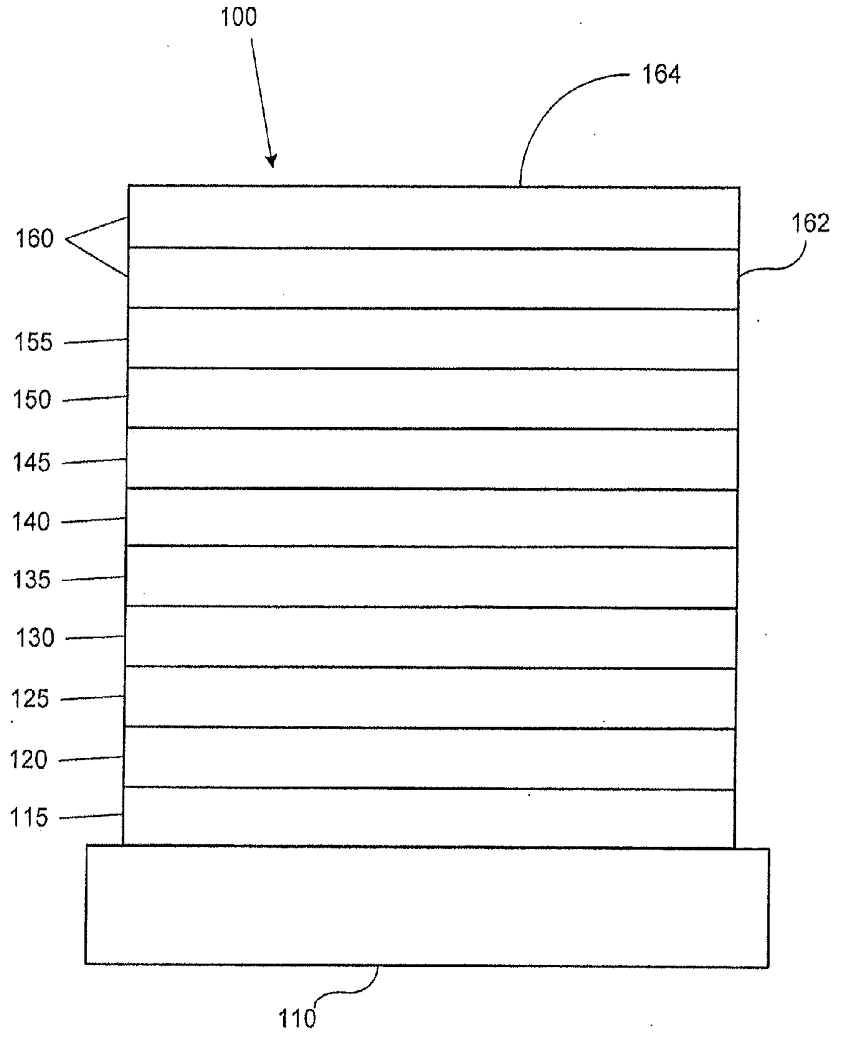
(57) ABSTRACT

Novel phosphorescent metal complexes containing 2-phenylisoquinoline ligands with at least two substituents on the isoquinoline ring are provided. The disclosed compounds have low sublimation temperatures that allow for ease of purification and fabrication into a variety of OLED devices.



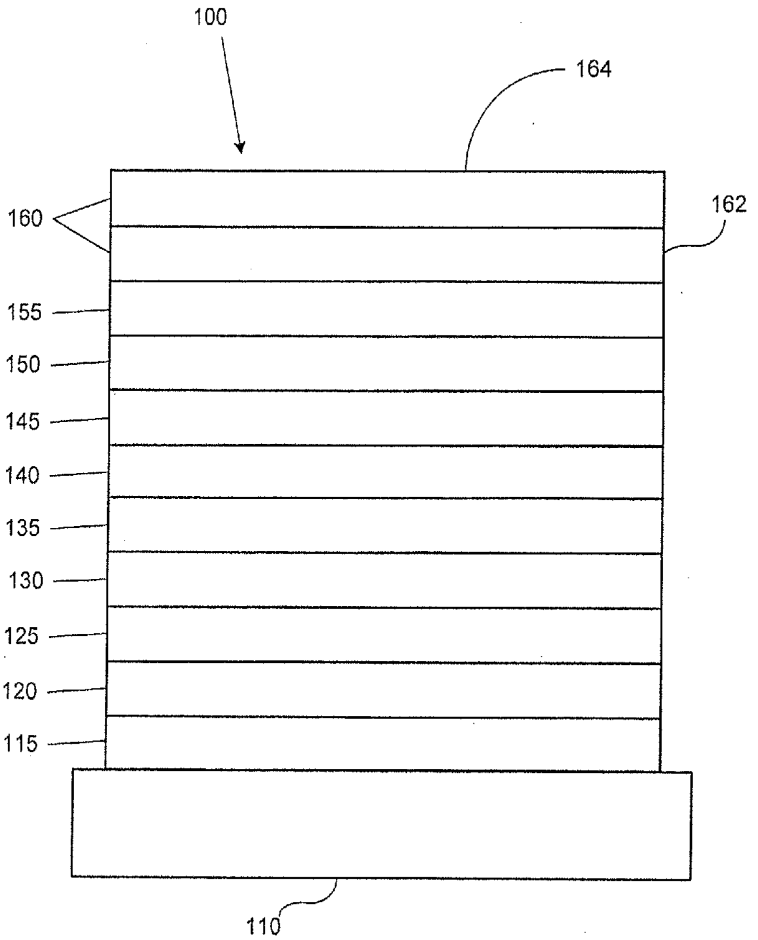


FIGURE 1

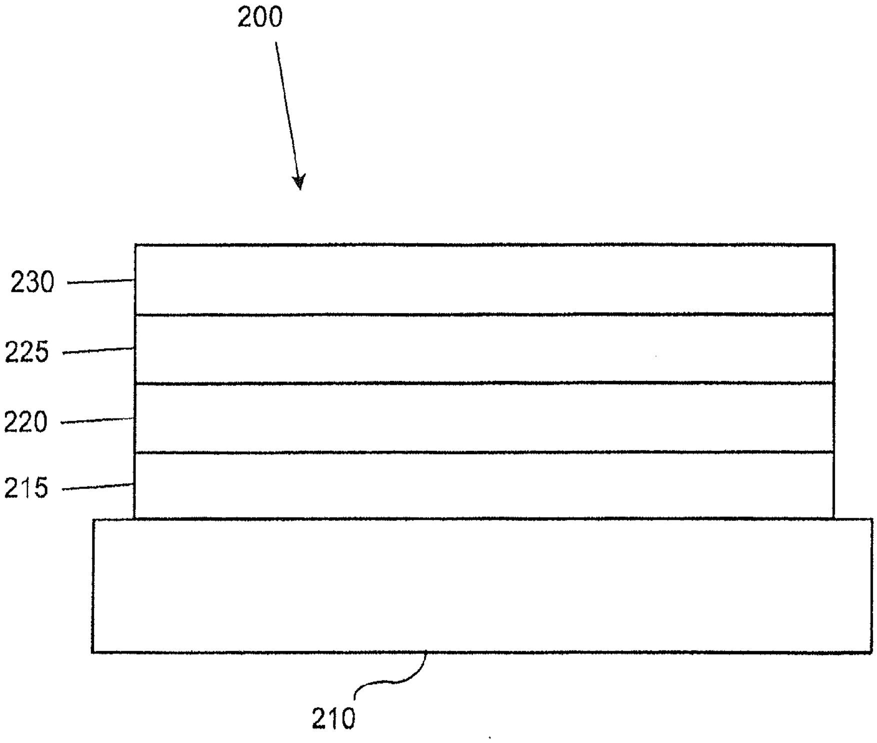
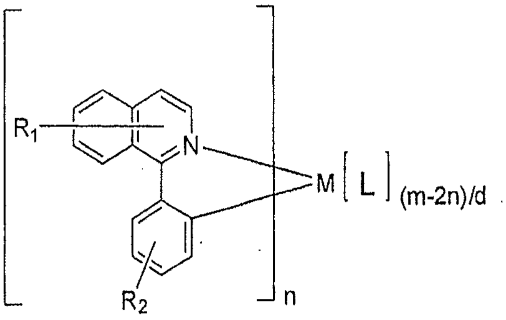


FIGURE 2



Formula I

FIGURE 3

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATION

[0001] This application is a continuation application of U.S. Non-Provisional application Ser. No. 13/316,162, filed Dec. 9, 2011, the entirety of which is incorporated herein by reference.

PARTIES TO A JOINT RESEARCH AGREEMENT

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

FIELD OF THE INVENTION

[0003] The present invention relates to metal complexes containing heterocyclic ligands with at least two substituents on the heterocyclic ligand. These metal complexes are suitable for use in OLED devices.

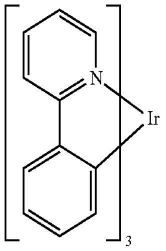
BACKGROUND

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

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

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

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



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

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

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

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

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

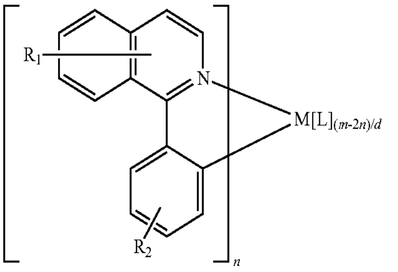
[0013] As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer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

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

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

SUMMARY OF THE INVENTION

[0016] In one aspect, a compound having the formula:



Formula I is provided.

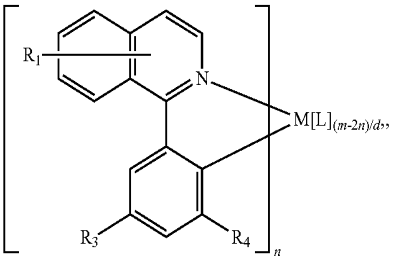
In the compound of Formula I, M is a metal having an atomic weight higher than 40, L is a second ligand, m is the maximum coordination number of the metal M, d is the denticity of L, and n is at least 1. R_1 is independently selected for each ligand and represents di, tri, tetra, penta substitutions, or no substitution. Each of R_1 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0017] At least two of R_1 is independently selected from two to six carbon containing alkyl, silyl, germyl, cycloalkyl, and combinations thereof. R_2 may represent mono, di, tri, tetra substitutions, or no substitution, and each of R_2 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.

[0018] In one aspect, R_1 represents di-substitution. In one aspect, R_1 represents di-alkyl substitution. In another aspect, R_1 represents silyl or germyl substitution.

[0019] In one aspect, the compound has the formula:

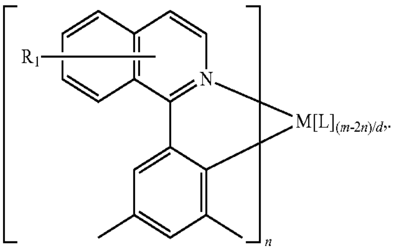
Formula II



wherein R_3 and R_4 are alkyl.

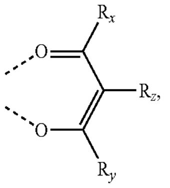
[0020] In one aspect, the compound has the formula:

Formula III



[0021] In one aspect, R_1 is independently selected from the group consisting of $CH(CH_3)_2$, $CH_2CH(CH_3)_2$, $CH_2C(CH_3)_3$, cyclopentyl, cyclohexyl, ethyl, trimethylsilyl, triethylsilyl, triisopropylsilyl, trimethylgermyl, triethylgermyl, and triisopropylgermyl.

[0022] In one aspect, n M is Ir. In one aspect, n is 2. In one aspect, L is a monoanionic bidentate ligand. In one aspect, L is



and

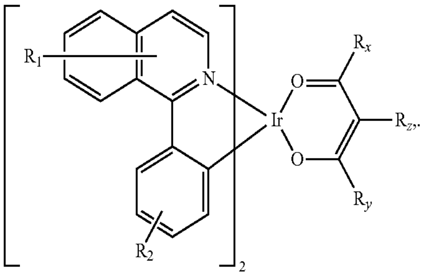
R_x, R_y, and R_z are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile,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

[0023] In one aspect, R_x, R_y, and R_z are independently selected from the group consisting of alkyl, hydrogen, deuterium, and combinations thereof.

[0024] In one aspect, R_z is hydrogen or deuterium, and R_x and R_y are independently selected from the group consisting of methyl, $CH(CH_3)_2$, and $CH_2CH(CH_3)_2$.

[0025] In one aspect, the compound has the formula:

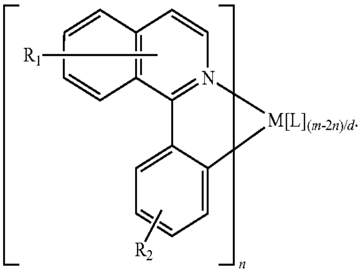
Formula IV



[0026] In one aspect, the compound is selected from Compound 1-Compound 50.

[0027] In one aspect, a first device is provided. The first device comprises a first organic light emitting device, further comprising an anode, a cathode, and an organic layer, disposed between the anode and the cathode, comprising a compound having the formula:

Formula I



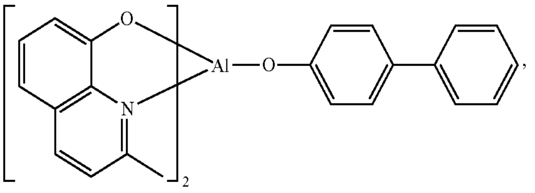
[0028] In the compound of Formula I, M is a metal having an atomic weight higher than 40, L is a second ligand, m is the maximum coordination number of the metal M, d is the denticity of L, and n is at least 1. R_1 is independently selected for each ligand and represents di, tri, tetra, penta substitutions, or no substitution. Each of R_1 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

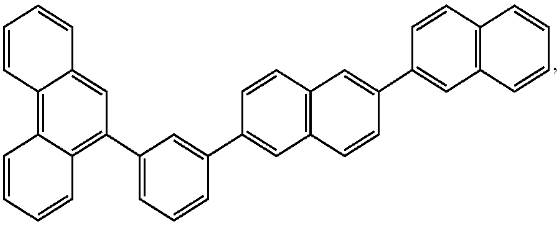
[0029] At least two of R_1 is independently selected from two to six carbon containing alkyl, silyl, germyl, cycloalkyl, and combinations thereof. R_2 may represent mono, di, tri, tetra substitutions, or no substitution, and each of R_2 is independently selected from the group consisting of hydrogen, 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.

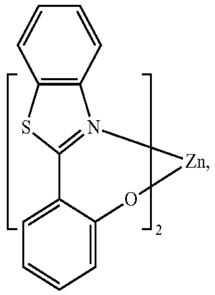
[0030] In one aspect, the first device is a consumer product. In one aspect, the first device is an organic light-emitting device. In one aspect, the organic layer is an emissive layer and the compound is a non-emissive dopant. In one aspect, the organic layer further comprises a host.

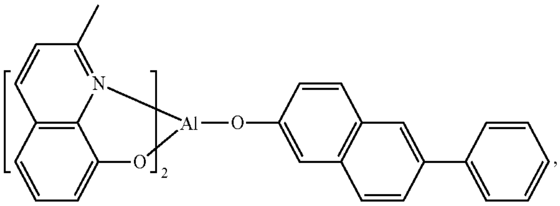
[0031] In one aspect, the host is a metal 8-hydroxyquinolate.

[0032] In one aspect, the host is selected from the group consisting of:









and combinations thereof.

BRIEF DESCRIPTION OF THE DRAWINGS

[0033] FIG. **1** shows an organic light emitting device.

[0034] FIG. **2** shows an inverted organic light emitting device that does not have a separate electron transport layer.

[0035] FIG. **3** shows a compound of Formula I.

DETAILED DESCRIPTION

[0036] 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.

[0037] 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.

[0038] 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.

[0039] FIG. **1** shows an organic light emitting device **100**. The figures are not necessarily drawn to scale. Device **100** may include a substrate **110**, an anode **115**, a hole injection layer **120**, a hole transport layer **125**, an electron blocking layer **130**, an emissive layer **135**, a hole blocking layer **140**, an electron transport layer **145**, an electron injection layer **150**, a protective layer **155**, and a cathode **160**. Cathode **160** is a compound cathode having a first conductive layer **162** and a second conductive layer **164**. Device **100** may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

[0040] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F.sub.4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

[0041] 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**.

[0042] 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**.

[0043] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. **1** and **2**. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

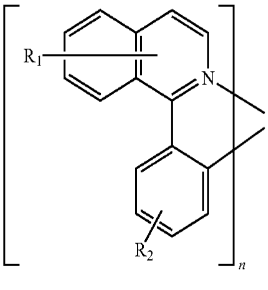
[0044] Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. patent application Ser. No. 10/233,470, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and 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 processability 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.

[0045] 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, 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.).

[0046] 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.

[0047] The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, arylkyl, heterocyclic group, aryl, aromatic group, and heteroaryl are known to the art, and are defined in U.S. Pat. No. 7,279,704 at cols. 31-32, which are incorporated herein by reference.

[0048] In one embodiment, a compound having the formula:



Formula I is provided.

In the compound of Formula I, M is a metal having an atomic weight higher than 40, L is a second ligand, m is the maximum coordination number of the metal M, d is the denticity of L, and n is at least 1. By "denticity" it is meant that d numerically represents the number of bonds a second ligand L makes with metal M. Thus, if L is a monodentate ligand, then d is 1, if L is a bidentate ligand, d is 2, etc. L can be one or more ligands, and when L represents more than one ligand, the ligands can be the same or different.

[0049] R_1 is independently selected for each ligand and represents di, tri, tetra, penta substitutions, or no substitution. Each of R_1 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

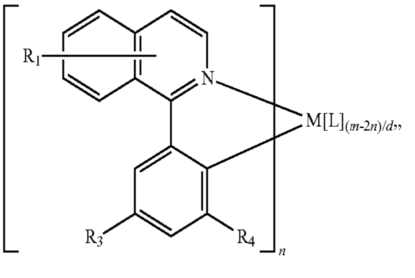
[0050] At least two of R_1 is independently selected from two to six carbon containing alkyl, silyl, germyl, cycloalkyl, and combinations thereof. R_2 may represent mono, di, tri, tetra substitutions, or no substitution, and each of R_2 is independently selected from the group consisting of hydrogen, 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.

[0051] It has been unexpectedly discovered that substitution at two or more of positions (i.e. R_1 represents at least di-substitution) on the heterocyclic ring in the compound of Formula I results in compounds with desirable properties. These properties enable OLED devices that incorporate compounds of Formula I to have improved properties such as higher efficiency and longer lifetime. Substitution of two or more positions as described above also results in compounds with lowered sublimation temperatures despite the fact that these compounds have higher molecular weights than unsubstituted or mono-substituted compounds, where the mono-substitution is on the heterocyclic ring. Without being bound by theory, it is believed that this decrease in sublimation temperature may be the result of decreased or less efficient molecular stacking in the solid state, thereby decreasing the energy required to disrupt the crystal lattice and resulting in decreased sublimation temperatures. Lower sublimation temperatures advantageously allow for easier purification of compounds of Formula I and better thermal stability in manufacturing.

[0052] In one embodiment, R_1 represents di-substitution. In one embodiment, R_1 represents di-alkyl substitution. In another embodiment, R_1 represents silyl or germyl substitution.

[0053] In one embodiment, the compound has the formula:

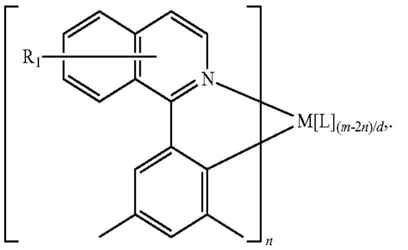
Formula II



wherein R_3 and R_4 are alkyl.

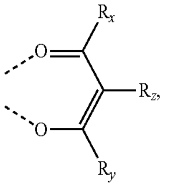
[0054] In one embodiment, the compound has the formula:

Formula III



[0055] In one embodiment, R_1 is independently selected from the group consisting of $CH(CH_3)_2$, $CH_2CH(CH_3)_2$, $CH_2C(CH_3)_3$, cyclopentyl, cyclohexyl, ethyl, trimethylsilyl, triethylsilyl, triisopropylsilyl, trimethylgermyl, triethylgermyl, and triisopropylgermyl.

[0056] In one embodiment, n M is Ir. In one embodiment, n is 2. In one embodiment, L is a monoanionic bidentate ligand. In one embodiment, L is



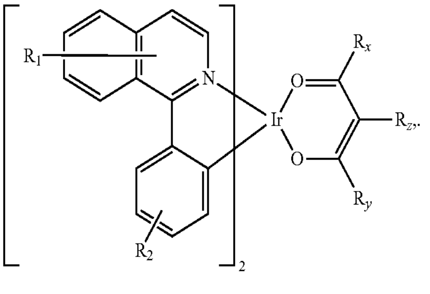
and R_x, R_y, and R_z are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile,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

[0057] In one embodiment, R_x, R_y, and R_z are independently selected from the group consisting of alkyl, hydrogen, deuterium, and combinations thereof.

[0058] In one embodiment, R_z is hydrogen or deuterium, and R_x and R_y are independently selected from the group consisting of methyl, $CH(CH_3)_2$, and $CH_2CH(CH_3)_2$.

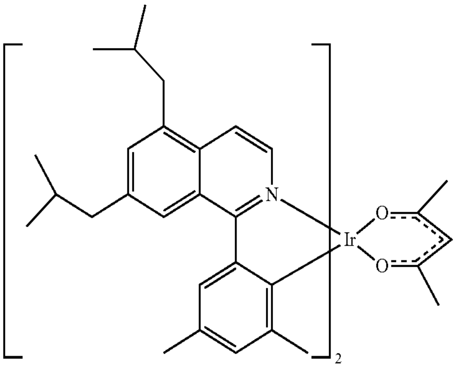
[0059] In one embodiment, the compound has the formula:

Formula IV



[0060] In one embodiment, the compound is selected from the group consisting of:

Compound 1



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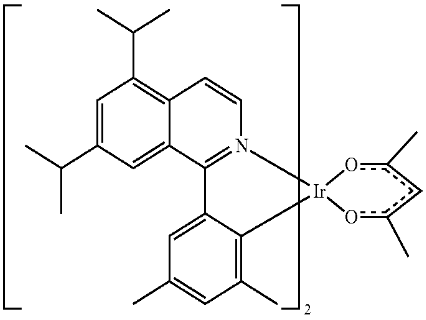
Compound 2



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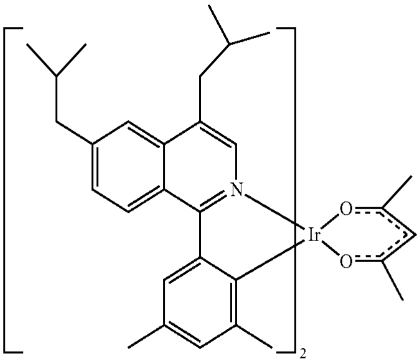
Compound 3



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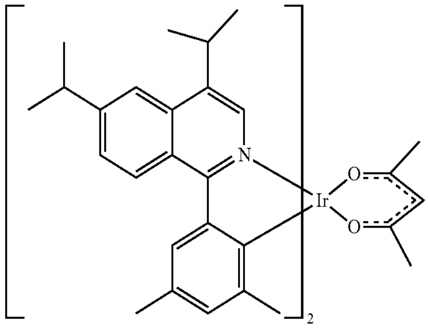
Compound 4



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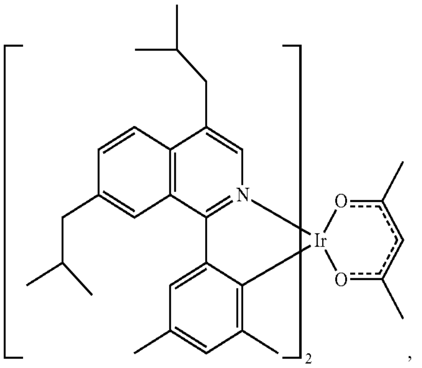
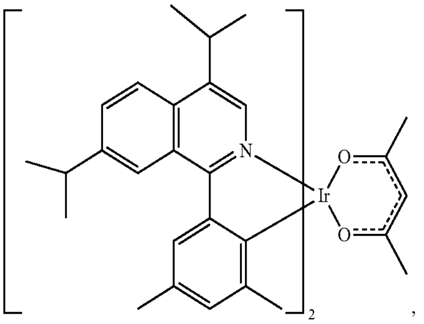
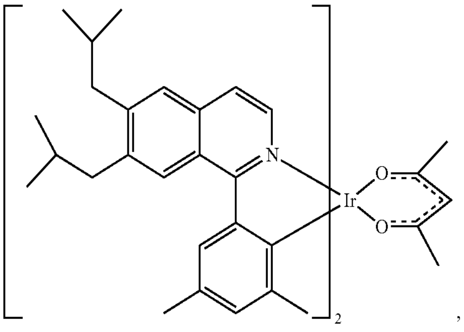
Compound 5



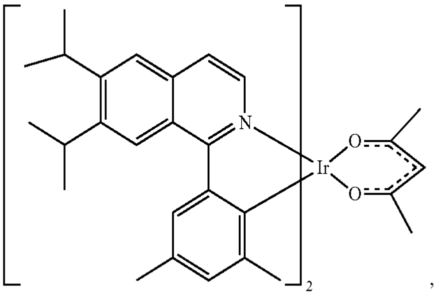
Compound 6



Compound 7



Compound 8



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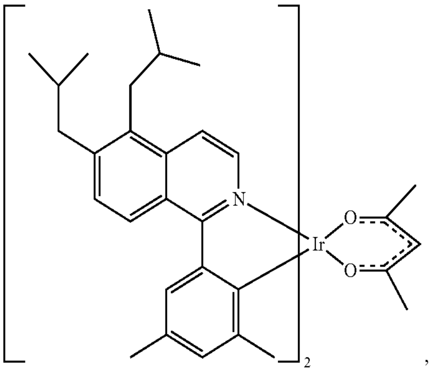
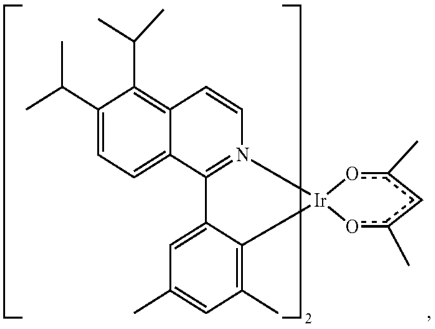
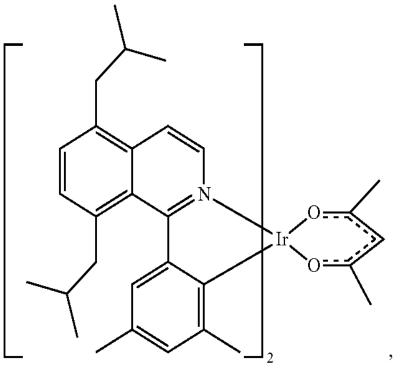
Compound 9



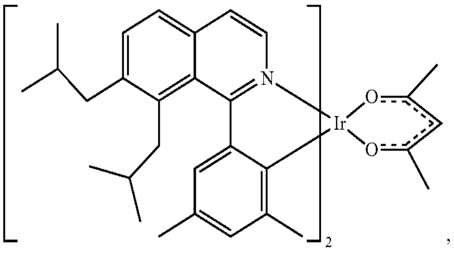
Compound 10



Compound 11



Compound 12



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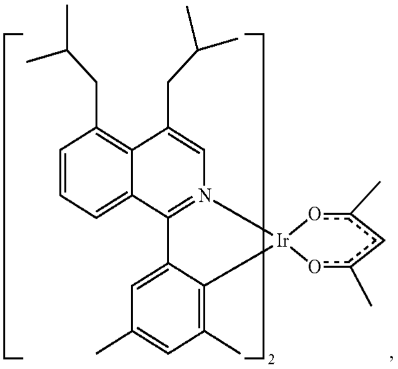
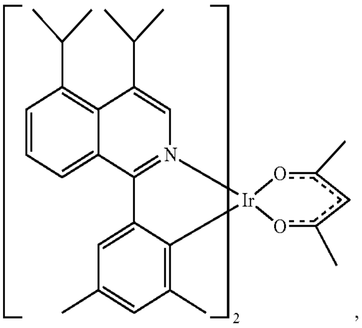
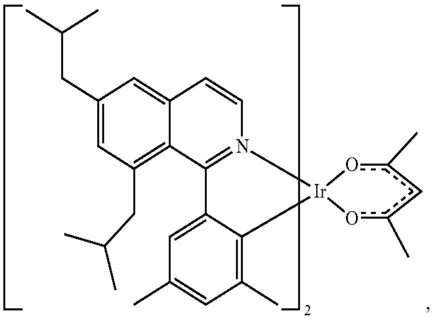
Compound 13



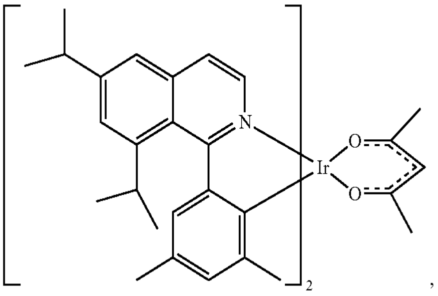
Compound 14



Compound 15



Compound 16



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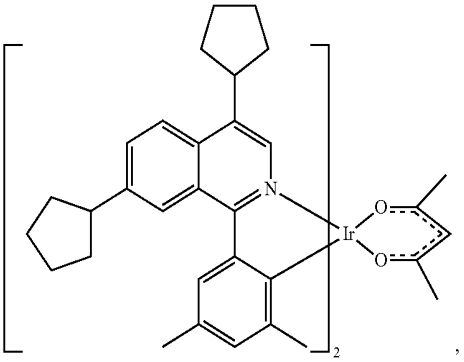
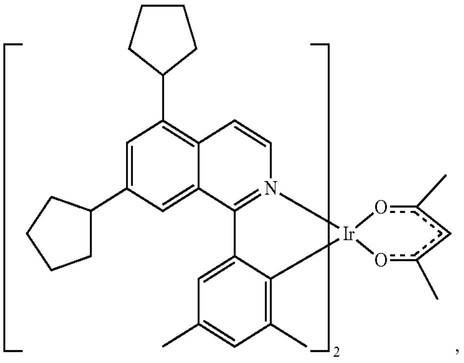
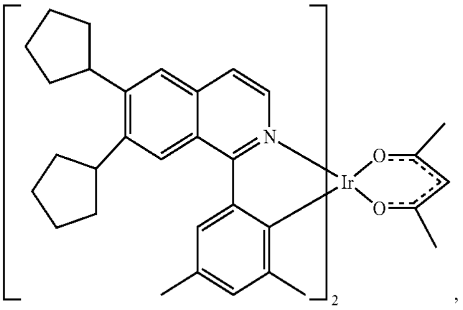
Compound 17



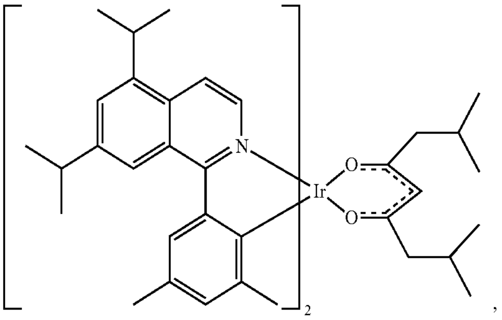
Compound 18



Compound 19



Compound 20



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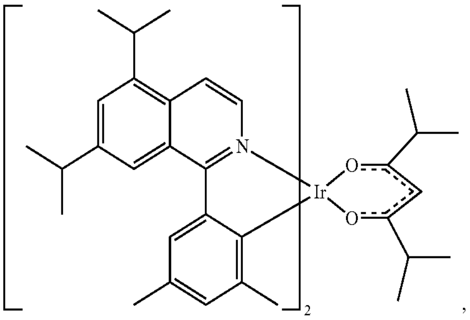
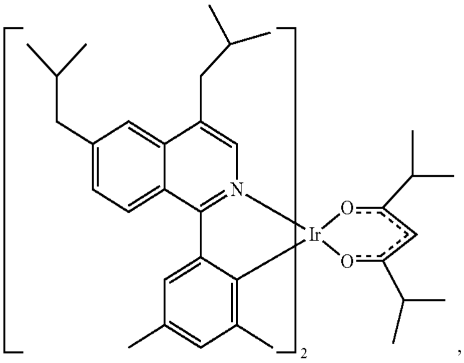
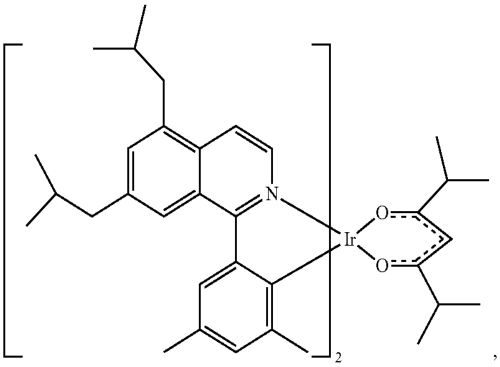
Compound 21



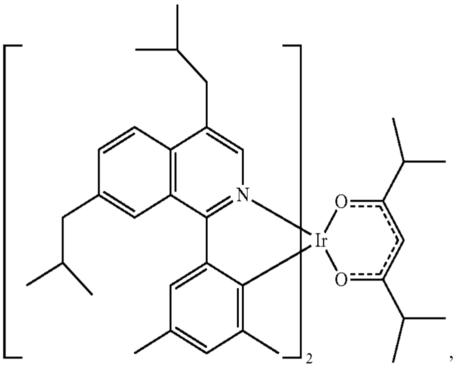
Compound 22



Compound 23



Compound 24



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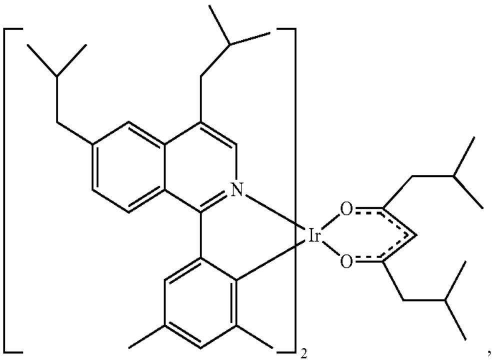
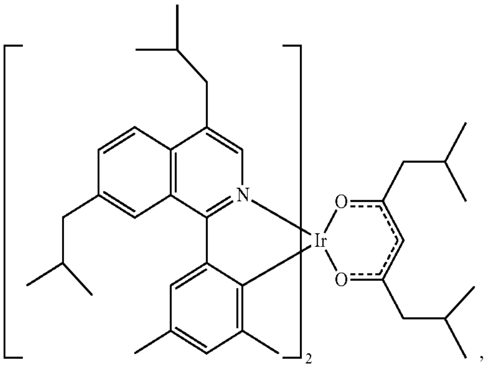
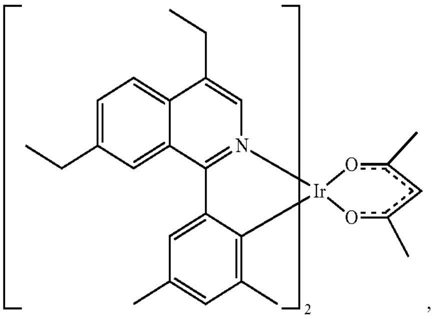
Compound 25



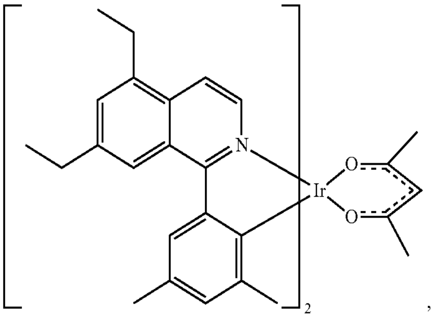
Compound 26



Compound 27



Compound 28



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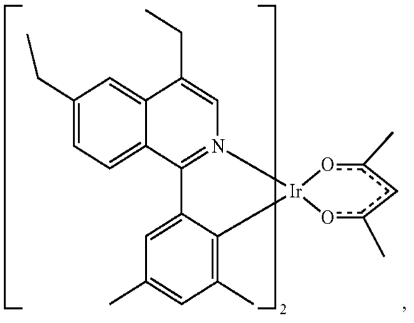
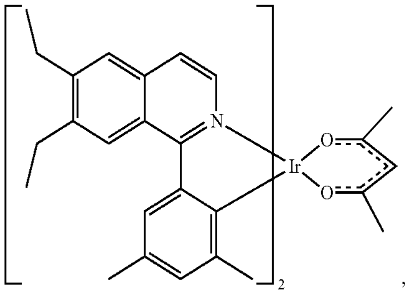
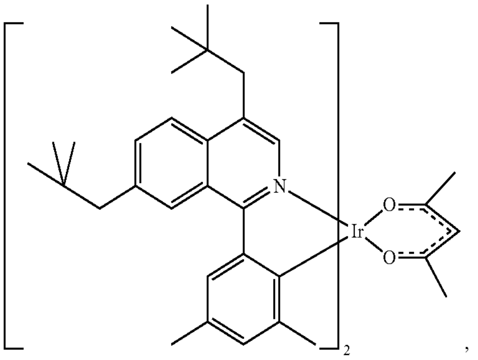
Compound 29



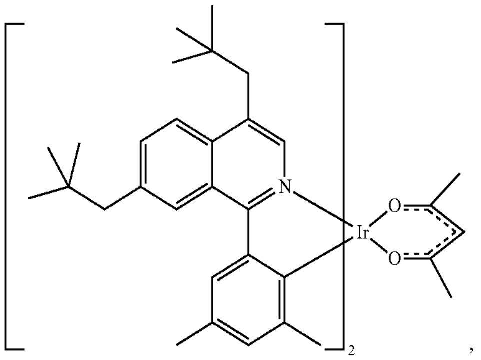
Compound 30



Compound 31



Compound 32



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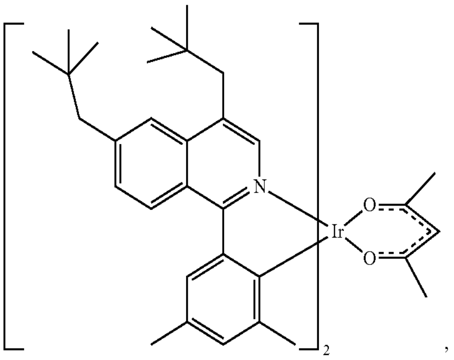
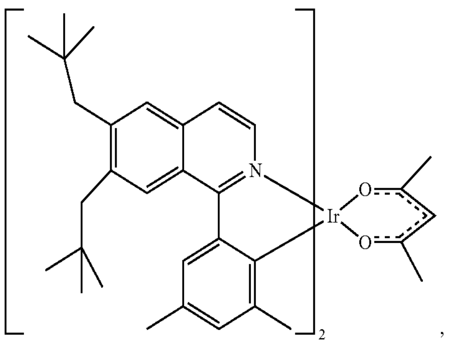
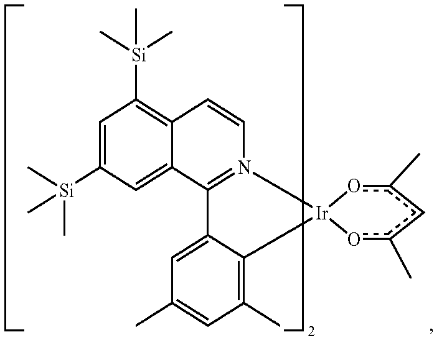
Compound 33



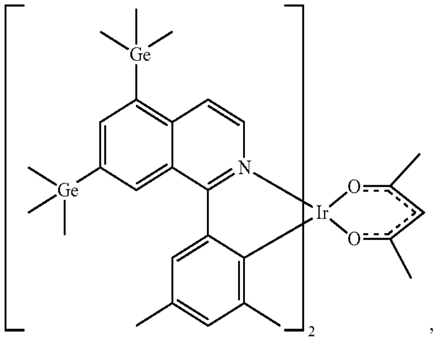
Compound 34



Compound 34



Compound 36



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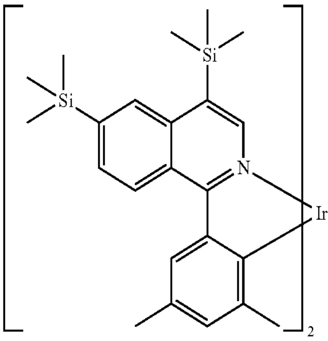
Compound 37



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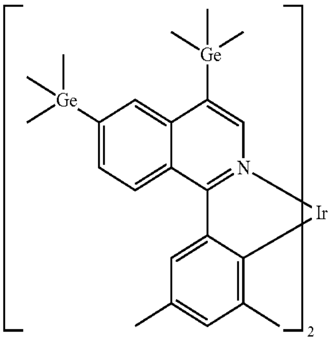
Compound 38



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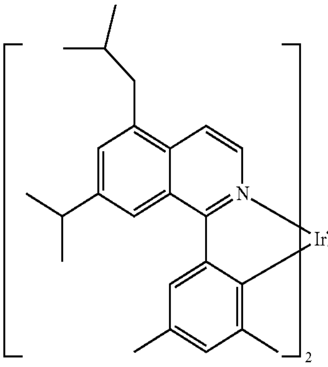
Compound 39



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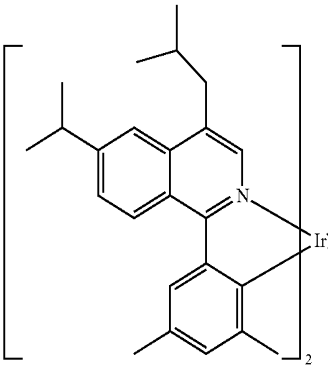
Compound 40



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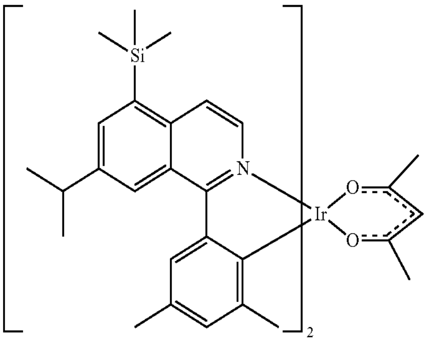
Compound 41



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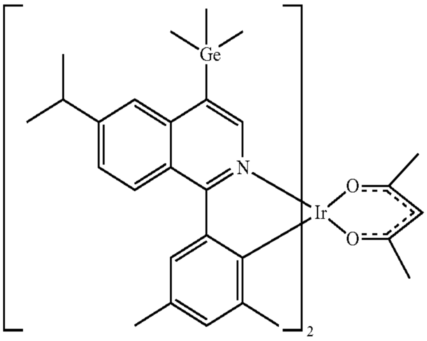
Compound 42



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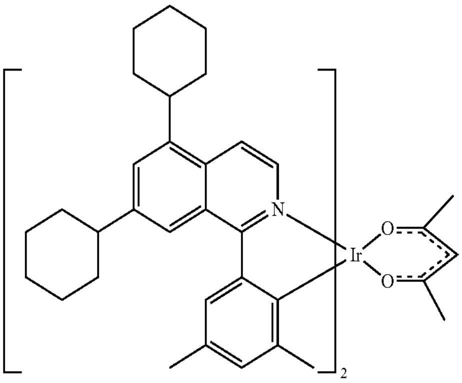
Compound 43



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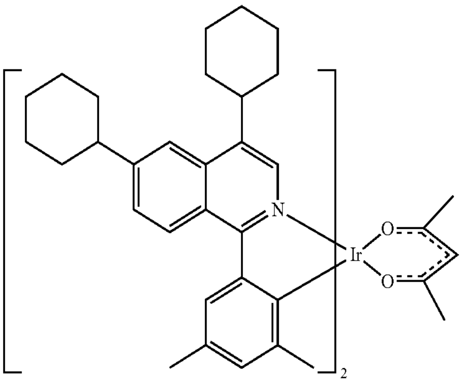
Compound 44



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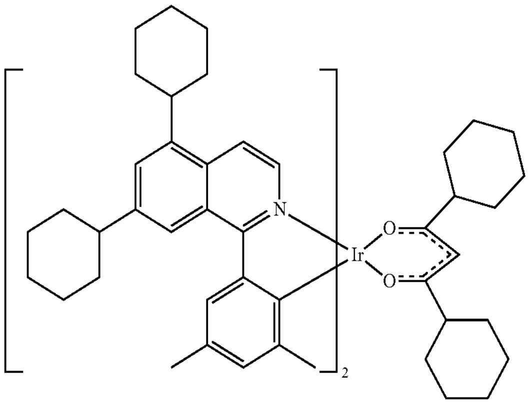
Compound 45



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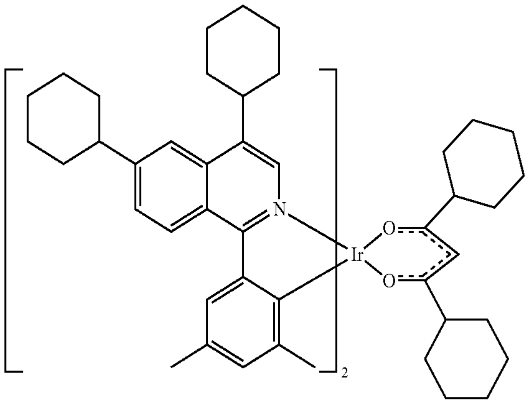
Compound 46



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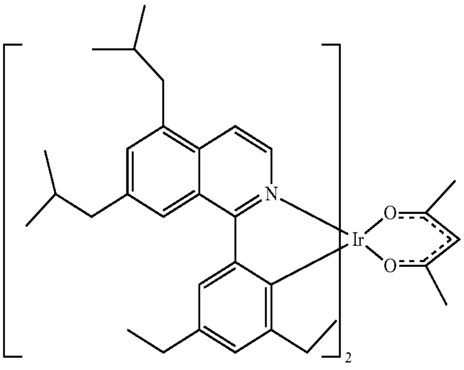
Compound 47



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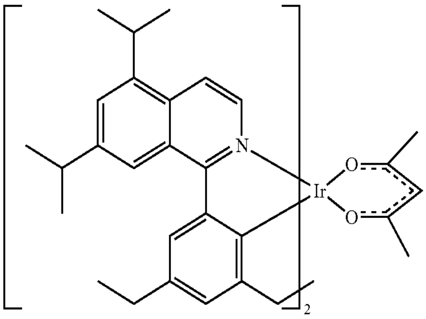
Compound 48



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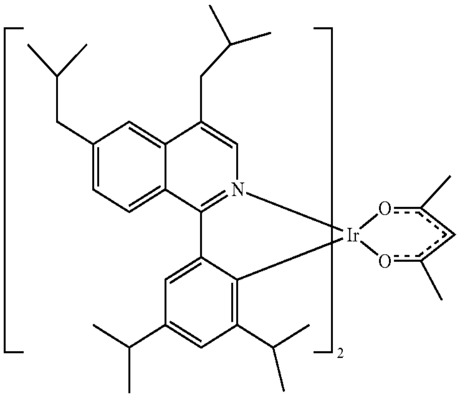
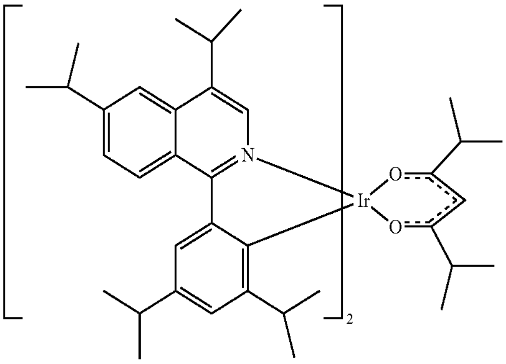
Compound 49



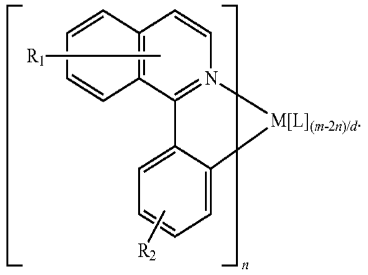
, and

Compound 50



[0061] In one embodiment, a first device is provided. The first device comprises a first organic light emitting device, further comprising an anode, a cathode, and an organic layer, disposed between the anode and the cathode, comprising a compound having the formula:

Formula I



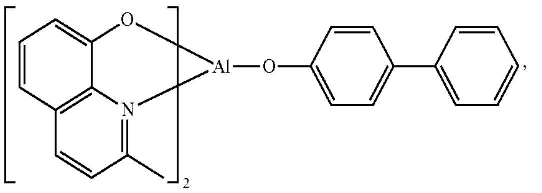
In the compound of Formula I, M is a metal having an atomic weight higher than 40, L is a second ligand, m is the maximum coordination number of the metal M, d is the denticity of L, and n is at least 1. R_1 is independently selected for each ligand and represents di, tri, tetra, penta substitutions, or no substitution. Each of R_1 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

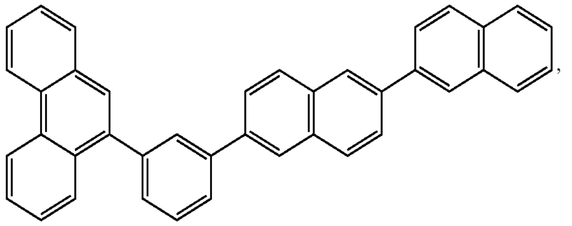
[0062] At least two of R_1 is independently selected from two to six carbon containing alkyl, silyl, germyl, cycloalkyl, and combinations thereof. R_2 may represent mono, di, tri, tetra substitutions, or no substitution, and each of R_2 is independently selected from the group consisting of hydrogen, 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.

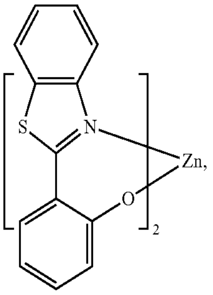
[0063] In one embodiment, the first device is a consumer product. In one embodiment, the first device is an organic light-emitting device. In one embodiment, the organic layer is an emissive layer and the compound is a non-emissive dopant. In one embodiment, the organic layer further comprises a host.

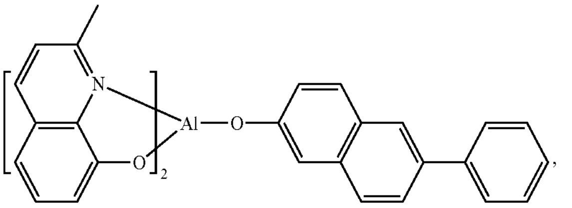
[0064] In one embodiment, the host is a metal 8-hydroxyquinolate.

[0065] In one embodiment, the host is selected from the group consisting of:









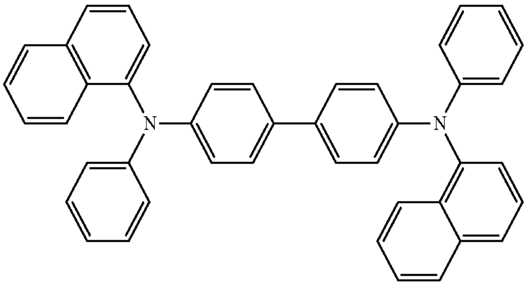
and combinations thereof.

[0066] Device Examples

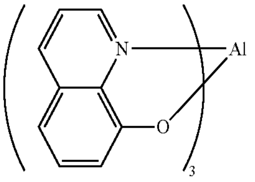
[0067] All example devices were fabricated by high vacuum ($<10^{-7}$ Torr) thermal evaporation (VTE). The anode electrode is 1200 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1000 Å of Al. All devices are encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H_2O and O_2) immediately after fabrication, and a moisture getter was incorporated inside the package.

[0068] The organic stack of the device examples consisted of sequentially, from the ITO surface, 100 Å of Compound A as the hole injection layer (HIL), 400 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (NPD) as the hole transporting layer (HTL), 300 Å of the compound of Formula I doped in with BAlq as host with from 4 to 12 wt % of an iridium-containing phosphorescent compound as the emissive layer (EML), 450 or 550 Å of Alq_3 (tris-8-hydroxyquinoline aluminum) as the electron transport layer (ETL). Comparative Examples with Compound B and C were fabricated similarly to the Device Examples except that the Compound B and C were used as the emitters in the EML.

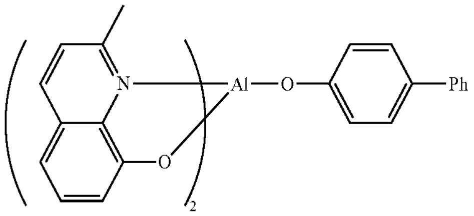
[0069] The device results and data are summarized in Tables 1, 2, and 3 from those devices. As used herein, Compounds A, B, and C have the following structures:



NPD

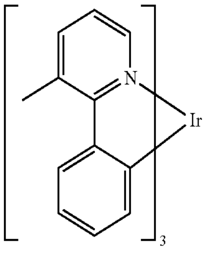


Alq



BAlq

Compound A



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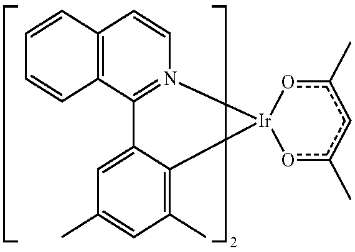
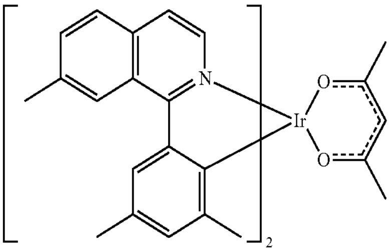


Compound B



Compound C

TABLE 1

Device structures of invention compounds and comparative compounds

Example	HIL	HTL	EML (300 Å, doping %)	BL	ETL
Comparative Example 1	Compound A 100 Å	NPD 400 Å	BAlq Compound B 6%	None	Alq 550 Å
Comparative Example 2	Compound A 100 Å	NPD 400 Å	BAlq Compound B 9%	None	Alq 550 Å
Comparative Example 3	Compound A 100 Å	NPD 400 Å	BAlq Compound B 12%	None	Alq 550 Å
Comparative Example 4	Compound A 100 Å	NPD 400 Å	BAlq Compound C 6%	None	Alq 550 Å
Comparative Example 5	Compound A 100 Å	NPD 400 Å	BAlq Compound C 9%	None	Alq 550 Å
Comparative Example 6	Compound A 100 Å	NPD 400 Å	BAlq Compound C 12%	None	Alq 550 Å
Example 1	Compound A 100 Å	NPD 400 Å	BAlq Compound 1 4%	None	Alq 550 Å
Example 2	Compound A 100 Å	NPD 400 Å	BAlq Compound 1 6%	None	Alq 550 Å
Example 3	Compound A 100 Å	NPD 400 Å	BAlq Compound 1 8%	None	Alq 550 Å
Example 4	Compound A 100 Å	NPD 400 Å	BAlq Compound 1 6%	BAlq 100 Å	Alq 450 Å
Example 5	Compound A 100 Å	NPD 400 Å	BAlq Compound 2 5%	None	Alq 550 Å
Example 6	Compound A 100 Å	NPD 400 Å	BAlq Compound 2 7%	None	Alq 550 Å
Example 7	Compound A 100 Å	NPD 400 Å	BAlq Compound 2 10%	None	Alq 550 Å
Example 8	Compound A 100 Å	NPD 400 Å	BAlq Compound 2 7%	BAlq 100 Å	Alq 450 Å
Example 9	Compound A 100 Å	NPD 400 Å	BAlq Compound 3 5%	None	Alq 550 Å
Example 10	Compound A 100 Å	NPD 400 Å	BAlq Compound 3 7%	None	Alq 550 Å
Example 11	Compound A 100 Å	NPD 400 Å	BAlq Compound 3 10%	None	Alq 550 Å
Example 12	Compound A 100 Å	NPD 400 Å	BAlq Compound 3 7%	BAlq 100 Å	Alq7 450 Å
Example 13	Compound A 100 Å	NPD 400 Å	BAlq Compound 22 4%	None	Alq 550 Å
Example 14	Compound A 100 Å	NPD 400 Å	BAlq Compound 22 6%	None	Alq 550 Å
Example 15	Compound A 100 Å	NPD 400 Å	BAlq Compound 22 8%	None	Alq 550 Å
Example 16	Compound A 100 Å	NPD 400 Å	BAlq Compound 22 6%	BAlq 100 Å	Alq 450 Å

TABLE 2

VTE device results

	x	y	λ_{max} (nm)	FWHM (nm)	Voltage (V)	LE (Cd/A)	EQE (%)	PE (lm/W)	LT80 % (h)
Comparative Example 1 Compound B	0.693	0.304	635	63	10	10.8	18.3	3.4	606
Comparative Example 2 Compound B	0.695	0.303	637	66	9.9	10.5	18.5	3.3	799
Comparative Example 3 Compound B	0.693	0.304	637	66	9.5	10.0	17.7	3.3	948
Comparative Example 4 Compound C	0.690	0.306	633	63	10.3	12.2	19.1	3.7	650
Comparative Example 5 Compound C	0.692	0.306	635	65	9.4	11.8	19.3	3.9	475
Comparative Example 6 Compound C	0.691	0.306	635	66	8.9	11.5	19.0	4.1	700
Example 1 Compound 1	0.687	0.309	628	52	10.1	12.5	17.8	3.9	178
Example 2 Compound 1	0.689	0.307	630	56	9.9	12.6	18.7	4.0	174
Example 3 Compound 1	0.691	0.306	632	56	9.5	12.4	19.0	4.1	171

TABLE 2-continued

VTE device results

	x	y	λ_{max} (nm)	FWHM (nm)	Voltage (V)	LE (Cd/A)	EQE (%)	PE (lm/W)	LT80 % (h)
Example 4 Compound 1	0.690	0.307	630	56	10.9	12.5	18.6	3.6	160
Example 5 Compound 2	0.687	0.311	630	58	9.5	13.8	19.6	4.6	350
Example 6 Compound 2	0.688	0.310	630	60	9.5	13.8	19.9	4.5	360
Example 7 Compound 2	0.688	0.310	632	62	8.8	13.1	19.4	4.7	400
Example 8 Compound 2	0.687	0.309	630	58	10.5	12.9	18.7	3.9	360
Example 9 Compound 3	0.685	0.313	626	58	9.5	14.8	19.8	4.9	232
Example 10 Compound 3	0.687	0.311	628	62	8.9	14.5	20.5	5.1	260
Example 11 Compound 3	0.688	0.310	630	64	8.1	14.0	20.3	5.4	235
Example 12 Compound 3	0.687	0.311	628	60	9.7	14.5	20.2	4.7	280
Example 13 Compound 22	0.684	0.313	626	48	9.3	14.8	18.8	5.0	192
Example 14 Compound 22	0.686	0.311	626	52	8.8	14.3	19.1	5.1	170
Example 15 Compound 22	0.686	0.311	628	52	8.2	14.2	19.2	5.4	122
Example 16 Compound 22	0.686	0.312	626	50	9.3	14.8	19.6	5.0	210

[0070] Table 2 is a summary of the device data. The luminous efficiency (LE), external quantum efficiency (EQE) and power efficiency (PE) were measured at 1000 nits, while the lifetime ($LT_{80\%}$) was defined as the time required for the device to decay to 80% of its initial luminance under a constant current density of 40 mA/cm^2.

[0071] From Table 2, it can be seen that the EQE, LE and PE of Compounds 1, 2, 3, and 22, which are compounds of Formula I, at three different doping concentrations (without a hole blocking layer) are all higher than those of Comparative Compounds B and C. For example, when the device has the same 6% emitter doping concentration without the hole blocking layer, Compound 22 has EQE of 19.1%, LE of 14.3 Cd/A, and PE of 5.1 lm/W, respectively. This compares to Comparative Compounds B and C which have EQE of 18.3 and 19.1%, LE of 10.8 and 12.2 Cd/A, and PE of 3.4 and 3.7 lm/W, respectively. The device results indicate that, surprisingly, the di-alkyl substituted Compounds 1, 2, 3 and 22 are more efficient than comparative compound B and mono-substituted compound C. It can also been seen from Table 2 that the FWHM (full width at half maximum) values of Compound 1, 2, 3, and 22 under different device structures are in the range of 48-64 nm, which is significantly narrower than those of Compounds B and C, which are in the range of 63-66 nm. Smaller FWHM values are often desirable in display applications. Thus, the use of compounds of Formula I, which are at least di-substituted on the heterocyclic ring contained therein can improve device performance, because these compounds have high EQE, LE, PE values and low FWHM values.

TABLE 3

Comparison of Sublimation Temperatures

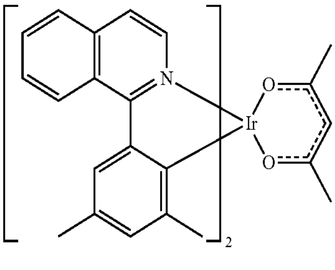
Compounds	Sublimation Temperature (° C.)	Temperature Difference Relative to Compound B
 Compound B	210	

TABLE 3-continued

Comparison of Sublimation Temperatures

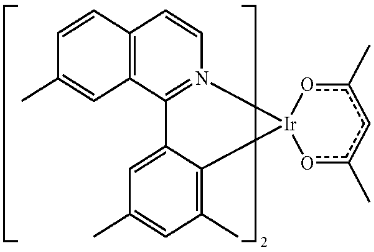
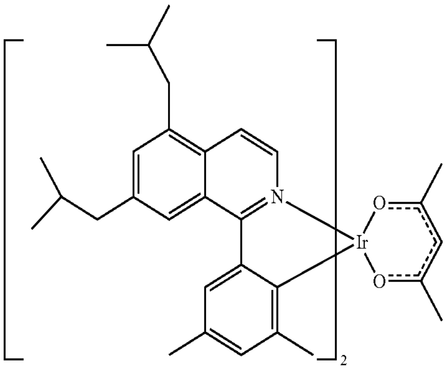
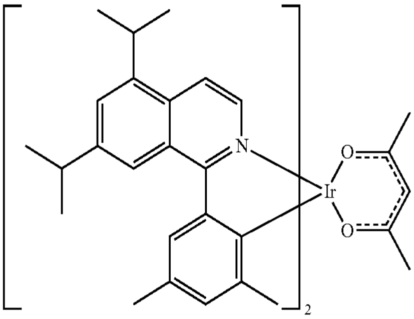
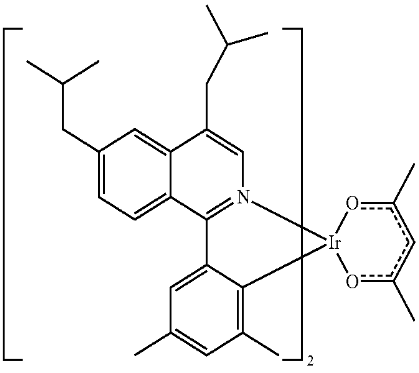
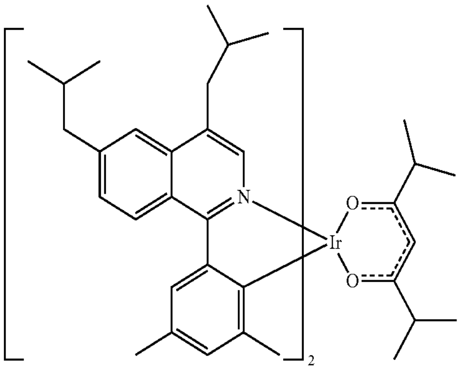
Compounds	Sublimation Temperature (° C.)	Temperature Difference Relative to Compound B
 Compound C	218	−8
 Compound 1	197	13
 Compound 2	202	8
 Compound 3	204	6

TABLE 3-continued

Comparison of Sublimation Temperatures

Compounds	Sublimation Temperature (° C.)	Temperature Difference Relative to Compound B
 Compound 22	194	16

[0072] It can be seen that di-substitution on the heteroaromatic ring in compounds of Formula I can decreases the sublimation temperature of complex as shown in Table 3. It was surprisingly discovered that di-substituted compounds of Formula I had lower sublimation temperatures than un-substituted or mono-substituted compounds. For example, Compound 22 had a significantly lower sublimation temperature than Comparative Compound B (194° C. vs 210° C.) despite the fact that Compound 22 has a higher molecular weight than Comparative Compound B.

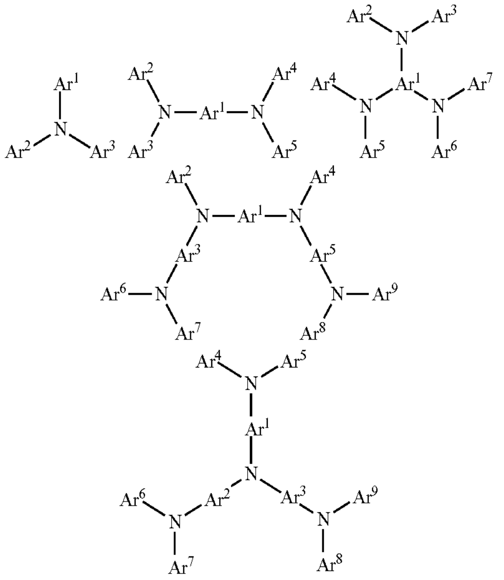
Combination with Other Materials

[0073] 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:

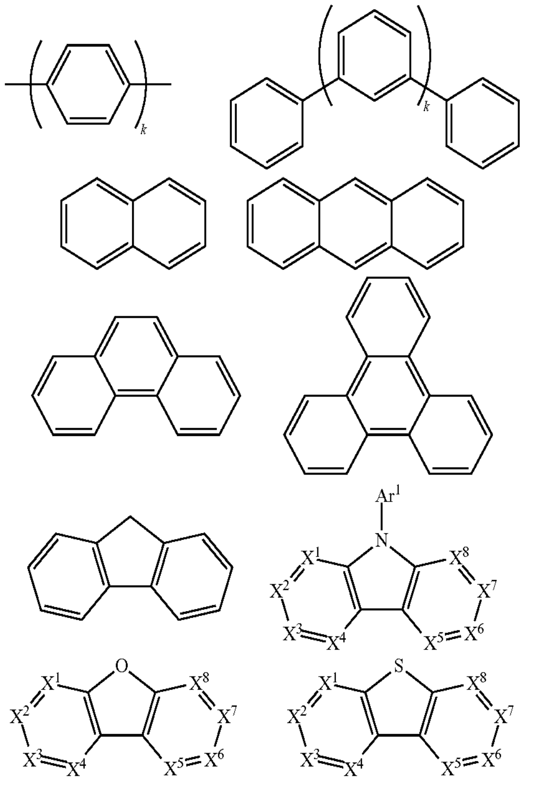
[0074] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphryin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and sliane derivatives; a metal oxide derivative, such as MoO_x; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

[0075] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:



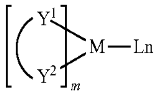
[0076] Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds 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.

[0077] In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:



[0078] k is an integer from 1 to 20; X^1 to X^8 is C (including CH) or N; Ar^1 has the same group defined above.

[0079] Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:



[0080] M is a metal, having an atomic weight greater than 40; (Y^1-Y^2) is a bidentate ligand, Y^1 and Y^2 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

[0081] In one aspect, (Y^1-Y^2) is a 2-phenylpyridine derivative.

[0082] In another aspect, (Y^1-Y^2) is a carbene ligand.

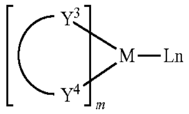
[0083] In another aspect, M is selected from Ir, Pt, Os, and Zn.

[0084] 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:

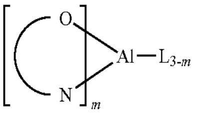
[0085] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any 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.

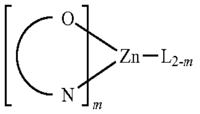
[0086] Examples of metal complexes used as host are preferred to have the following general formula:



[0087] M is a metal; (Y^3-Y^4) is a bidentate ligand, Y^3 and Y^4 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

[0088] In one aspect, the metal complexes are:





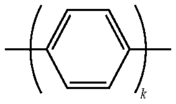
[0089] (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

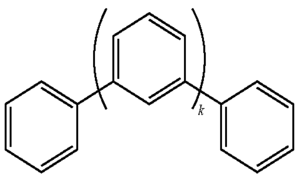
[0090] In another aspect, M is selected from Ir and Pt.

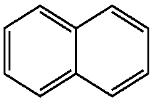
[0091] In a further aspect, (Y^3-Y^4) is a carbene ligand.

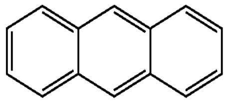
[0092] Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atome, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

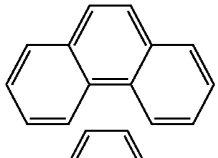
[0093] In one aspect, host compound contains at least one of the following groups in the molecule:

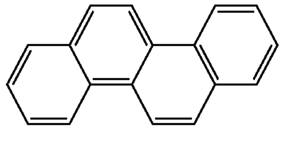


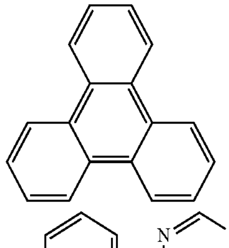


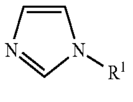


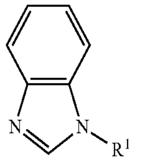


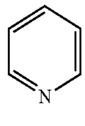


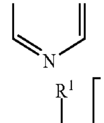


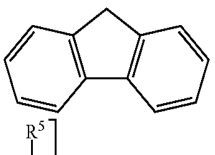


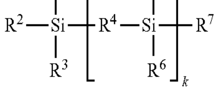


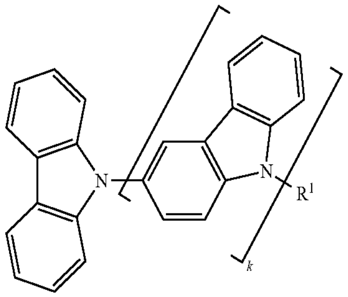












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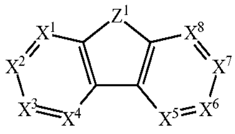
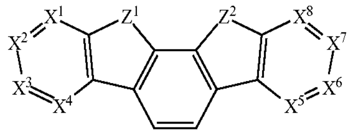
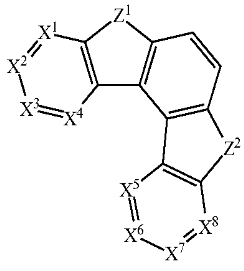
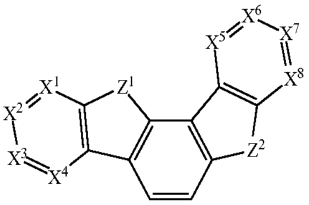
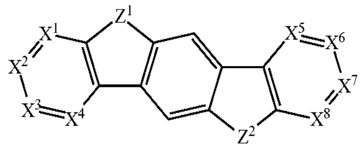
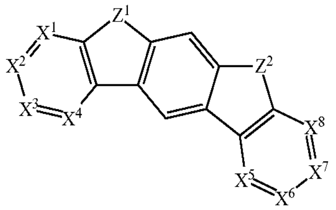












[0094] R^1 to R^7 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

[0095] k is an integer from 0 to 20.

[0096] X^1 to X^8 is selected from C (including CH) or N.

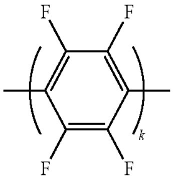
[0097] Z^1 and Z^2 is selected from NR^1, O, or S.

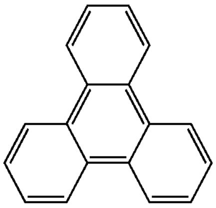
HBL:

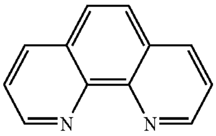
[0098] A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED.

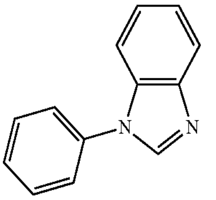
[0099] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

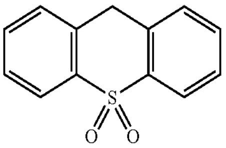
[0100] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

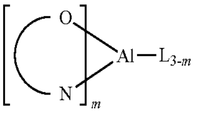










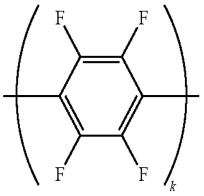


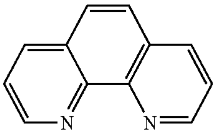
[0101] k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

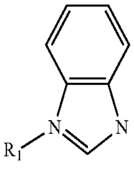
ETL:

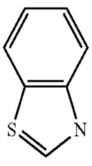
[0102] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

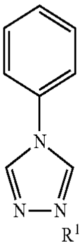
[0103] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

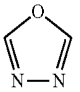


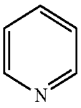


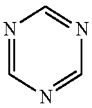


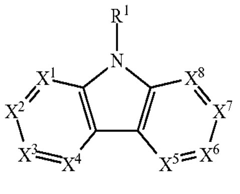












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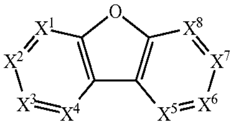
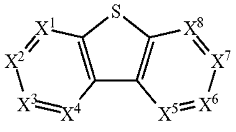
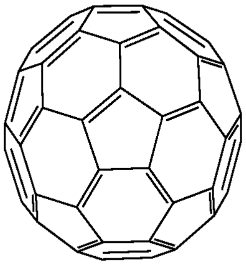
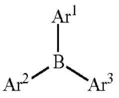








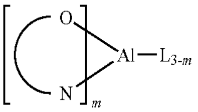
[0104] R^1 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

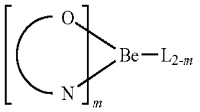
[0105] Ar^1 to Ar^3 has the similar definition as Ar's mentioned above.

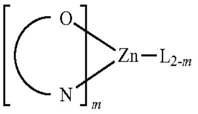
[0106] k is an integer from 0 to 20.

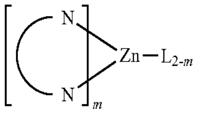
[0107] X^1 to X^8 is selected from C (including CH) or N.

[0108] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:









[0109] (O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

[0110] In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated.

[0111] 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 4 below. Table 4 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 4

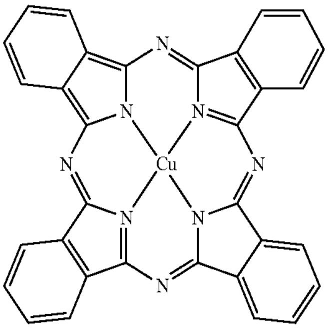
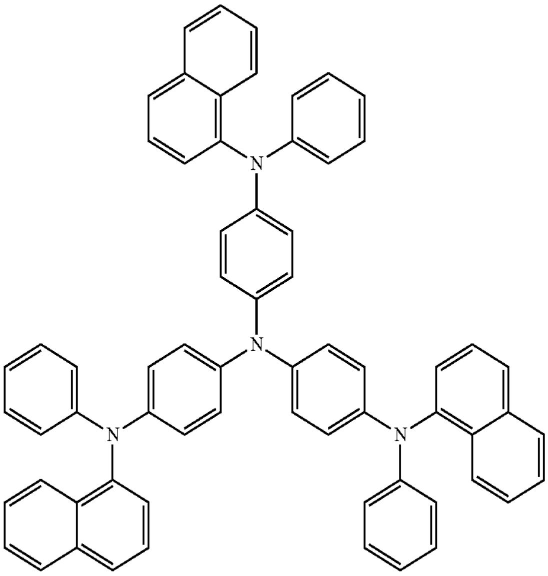
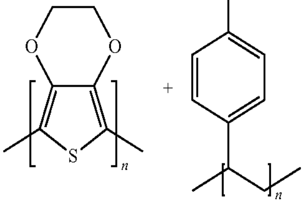
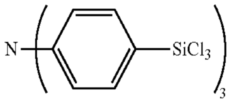
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydrocarbon polymer	$-\!\!\left[CH_xF_y \right]_n\!\!-$	Appl. Phys. Lett. 78, 673 (2001)
Conducting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

TABLE 4-continued

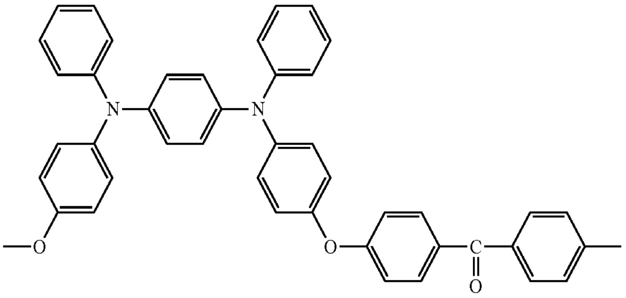
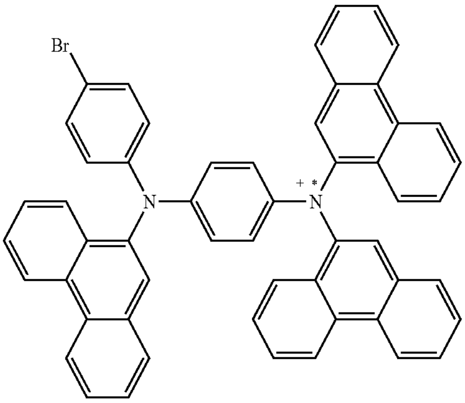
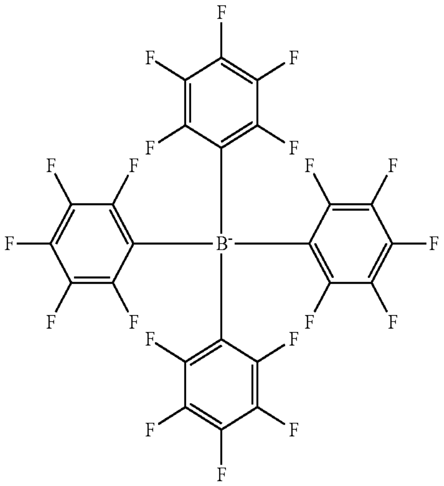
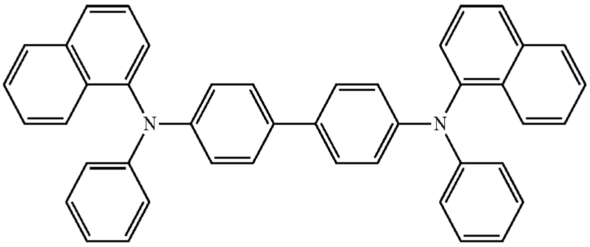
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine or polythiophene polymers with conductivity dopants	 and  	EP1725079A1
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides	 + MoO_x	US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 4-continued

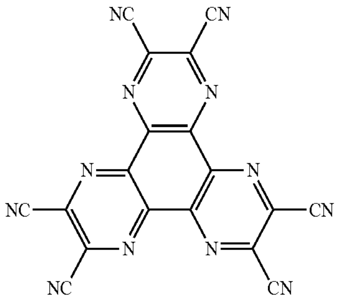
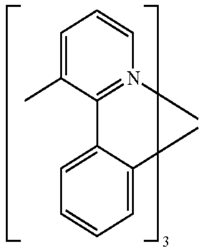
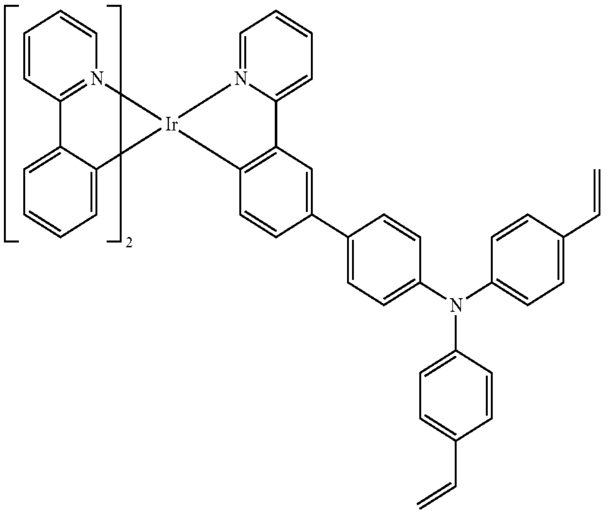
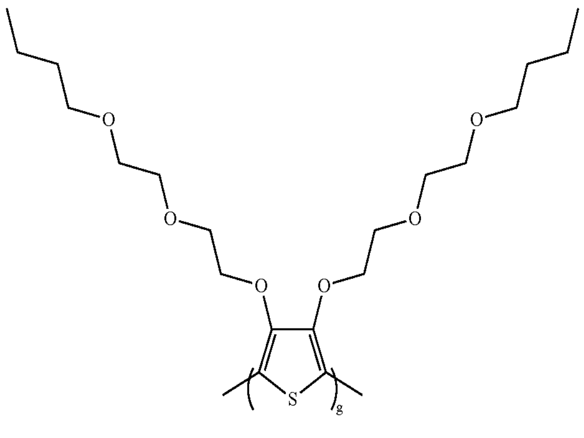
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
n-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216

TABLE 4-continued

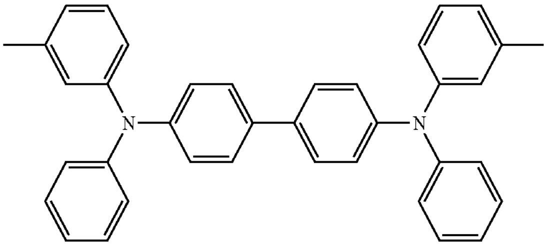
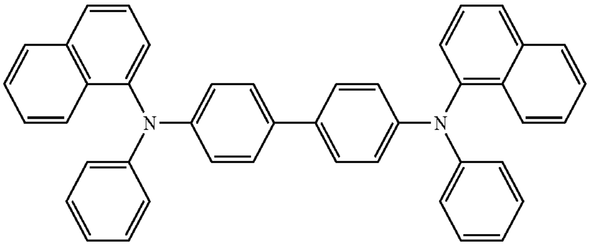
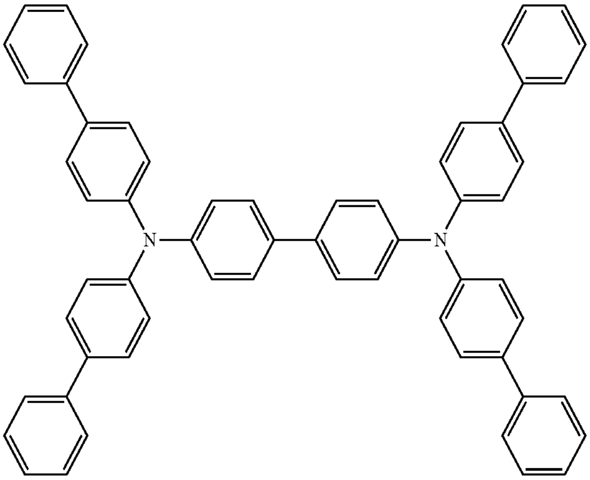
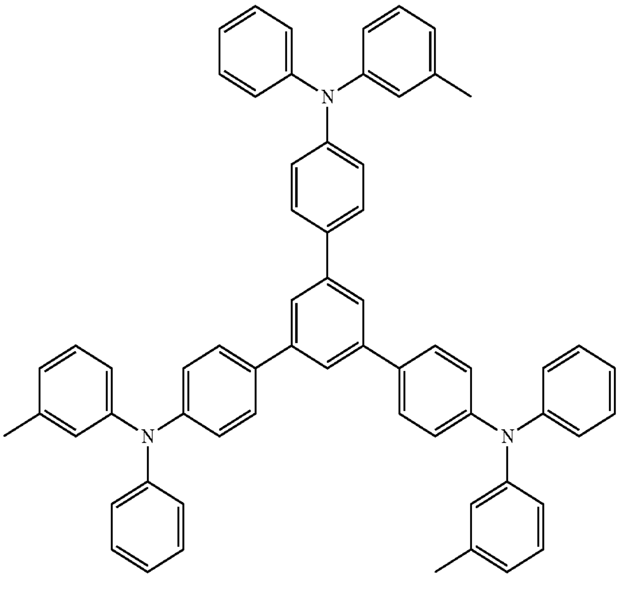
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole transporting materials		
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5,061,569
		EP650955
		J. Mater. Chem. 3, 319 (1993)

TABLE 4-continued

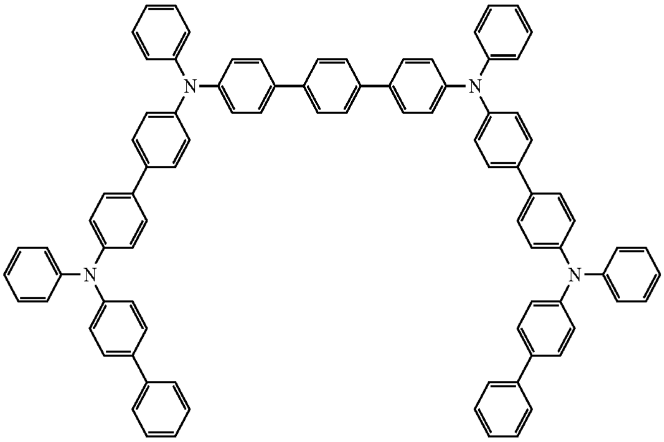
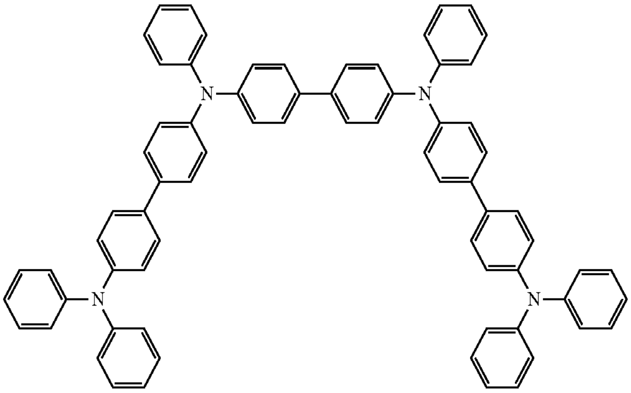
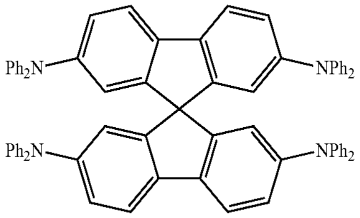
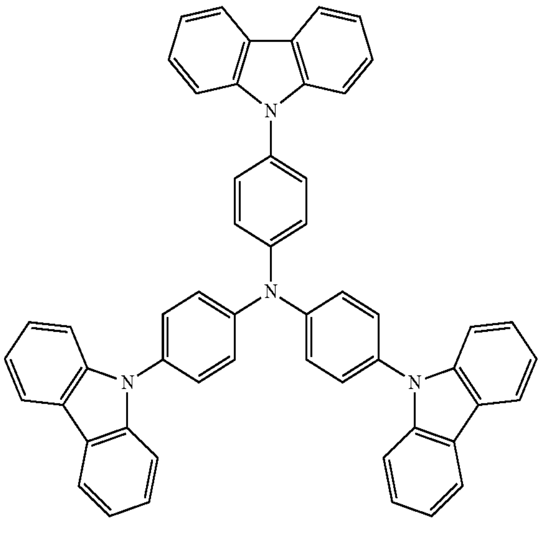
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572

TABLE 4-continued

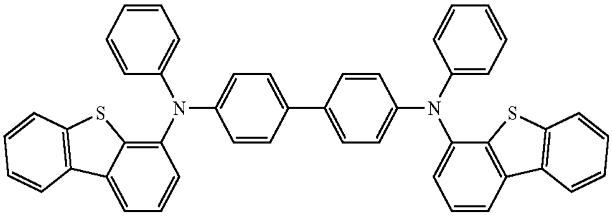
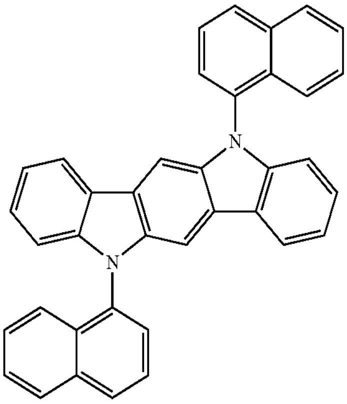
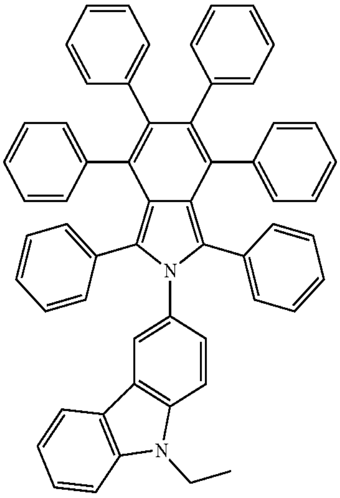
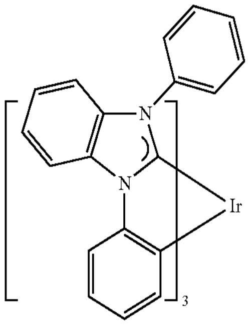
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine with (di)benzothiophene/(di) benzofuran		US20070278938, US20080106190 US20110163302
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221

TABLE 4-continued

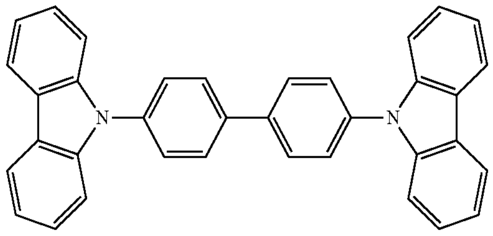
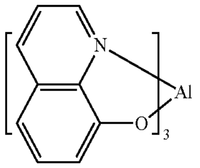
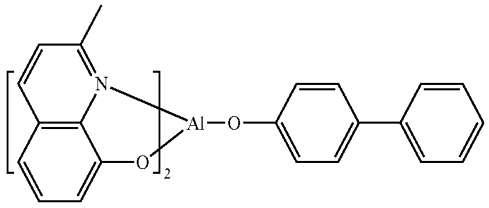
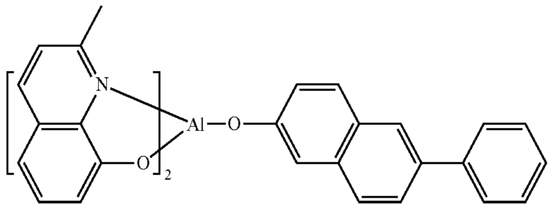
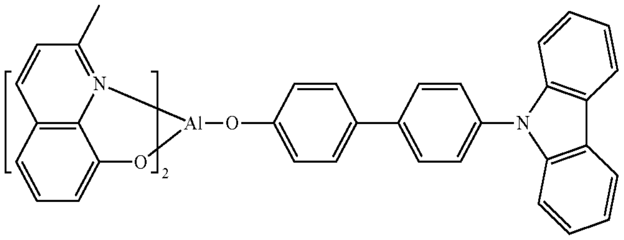
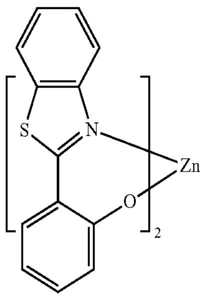
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Phosphorescent OLED host materials Red hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)

TABLE 4-continued

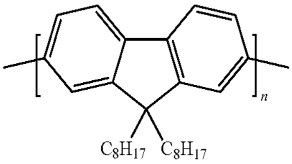
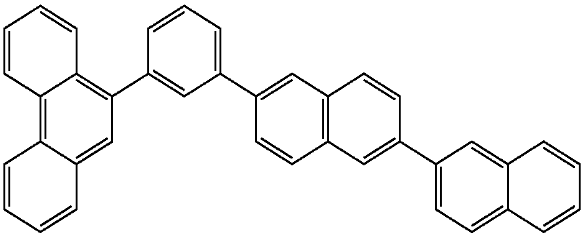
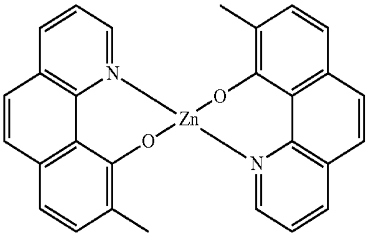
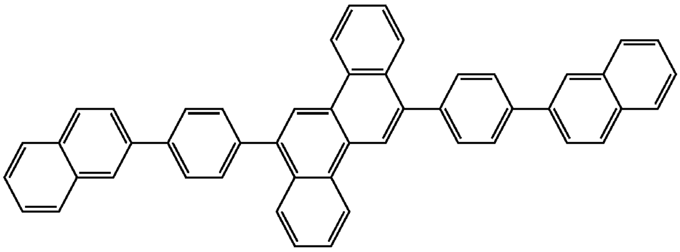
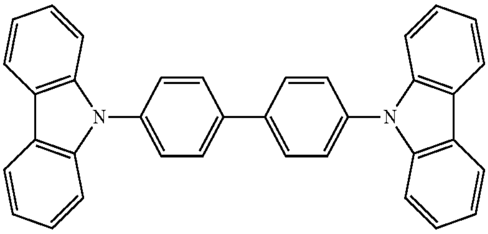
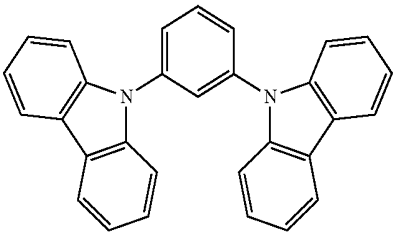
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2010056066
Chrysene based compounds		WO2011086863
	Green hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553

TABLE 4-continued

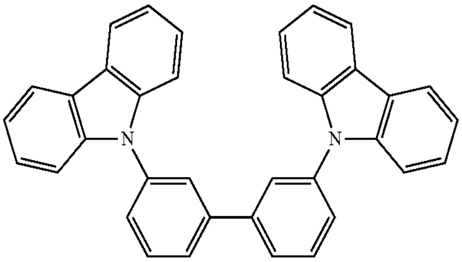
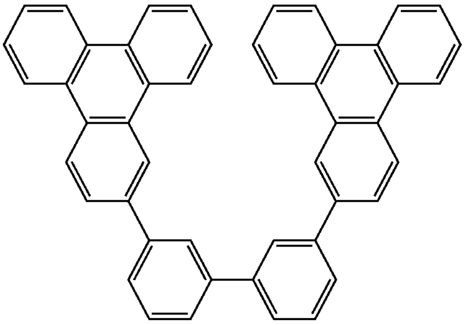
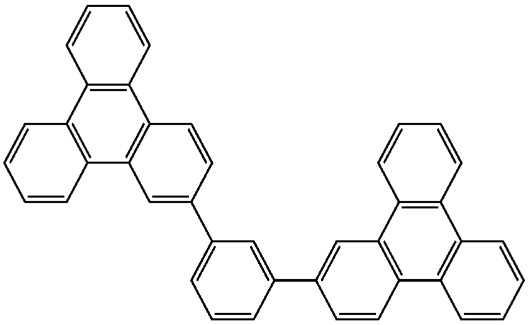
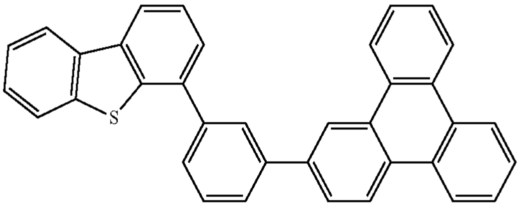
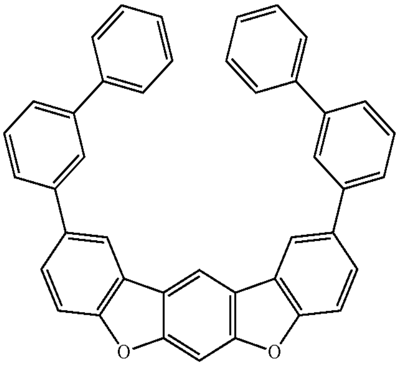
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2001039234
Aryltriphenylene compounds		US20060280965
		US20060280965
		WO2009021 126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931

TABLE 4-continued

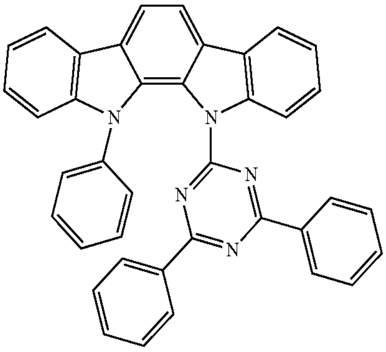
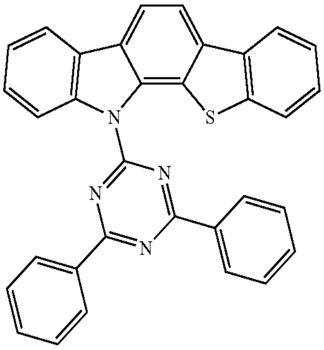
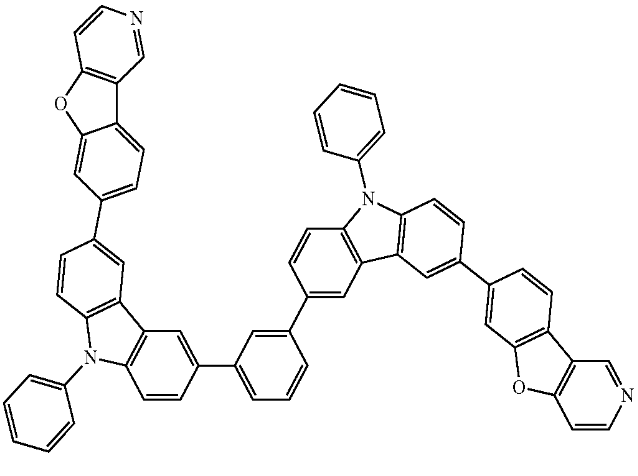
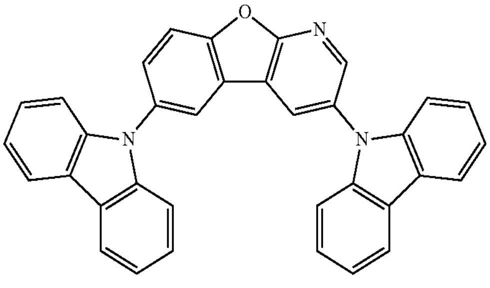
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Donor acceptor type molecules		WO2008056746
		WO2010107244
Aza-carbazole/DBT/DBF		JP2008074939
		US20100187984

TABLE 4-continued

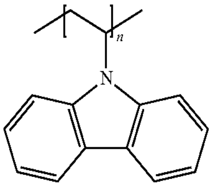
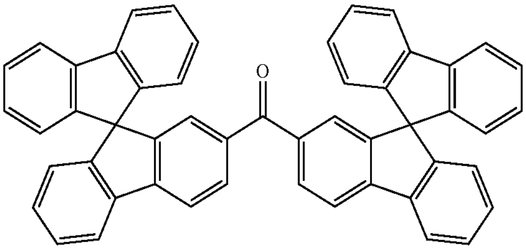
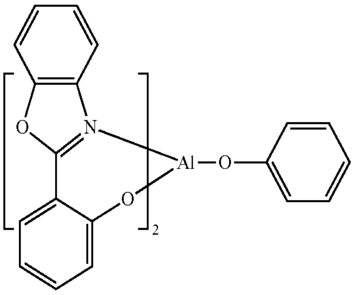
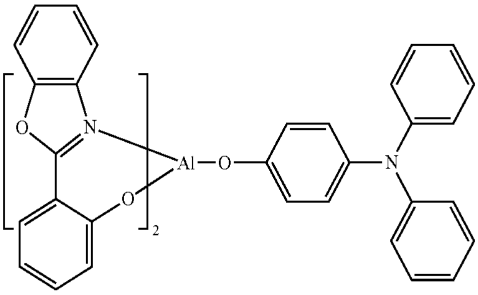
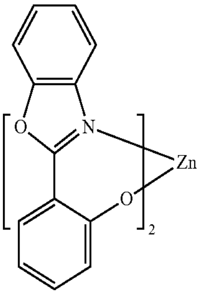
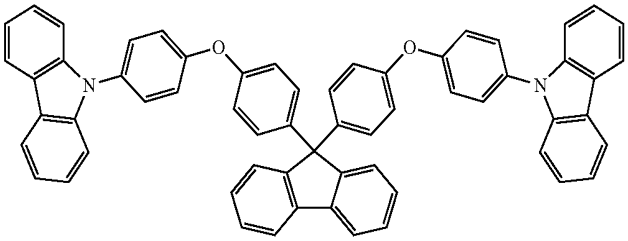
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207
Metal phenoxybenzooxazole compounds		WO2005089025
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297

TABLE 4-continued

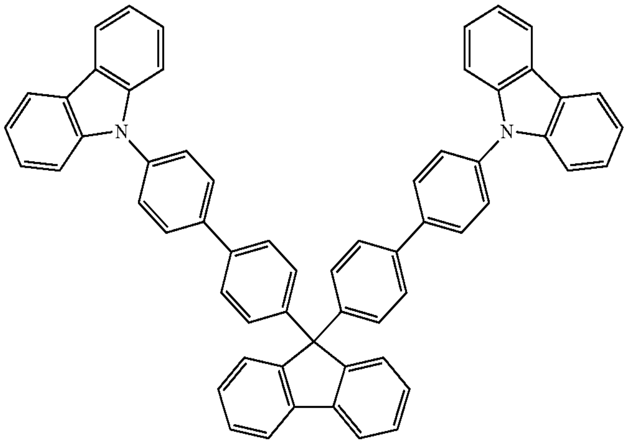
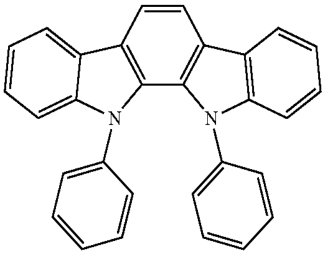
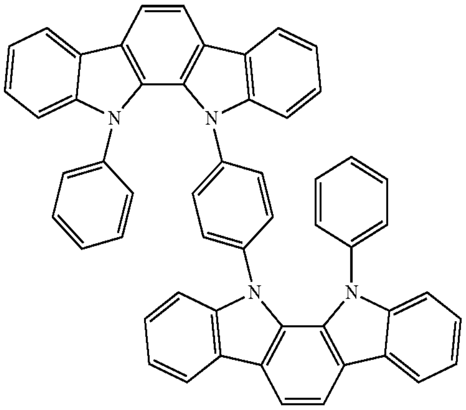
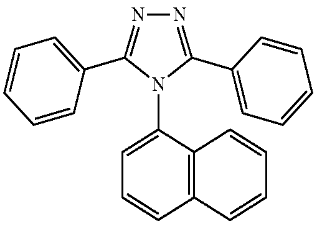
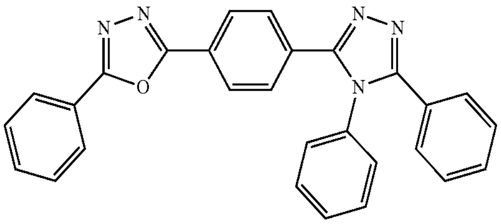
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		JP2007254297
Indolocabazoles		WO2007063796
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822

TABLE 4-continued

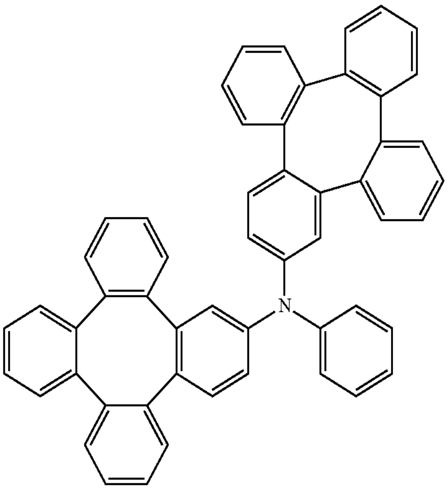
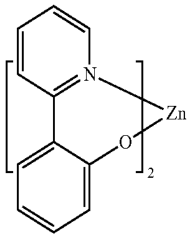
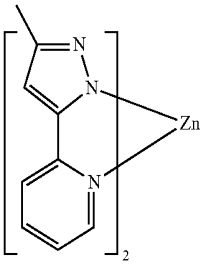
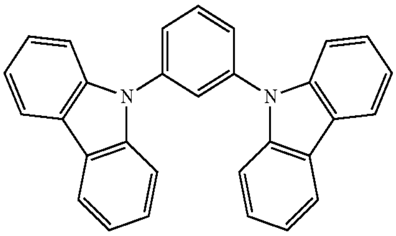
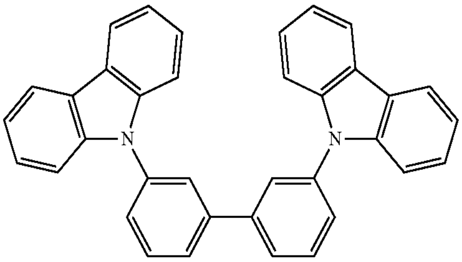
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359

TABLE 4-continued

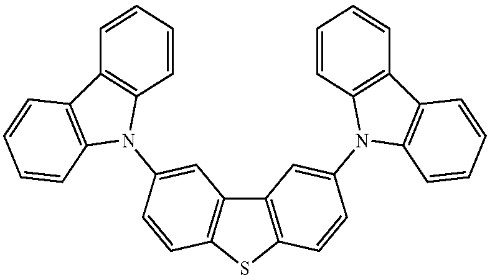
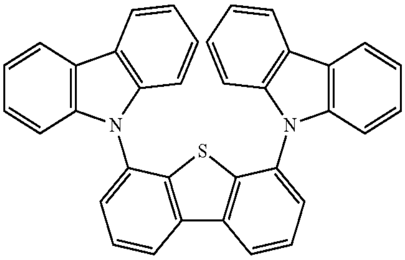
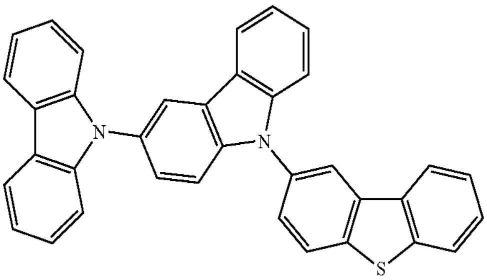
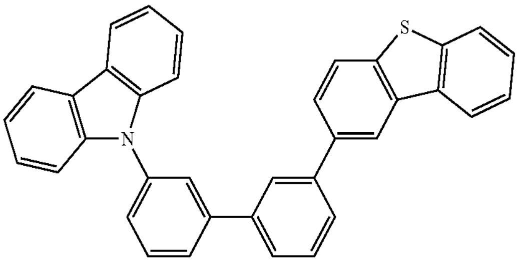
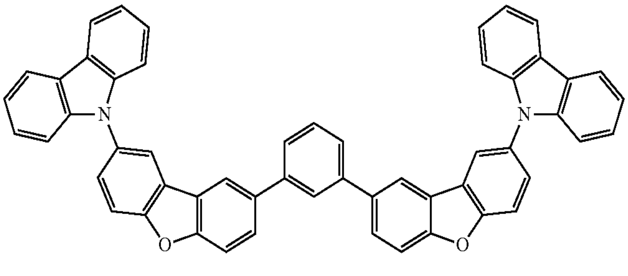
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzothiophene/ Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162
		WO2009086028
		US20090030202, US20090017330
		US20100084966

TABLE 4-continued

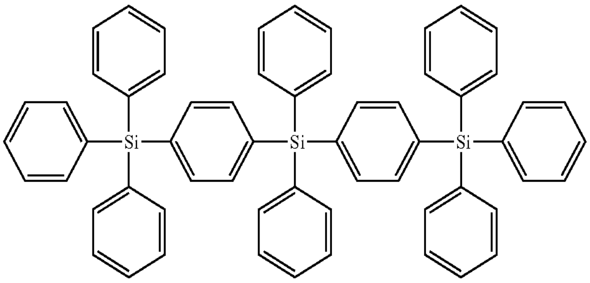
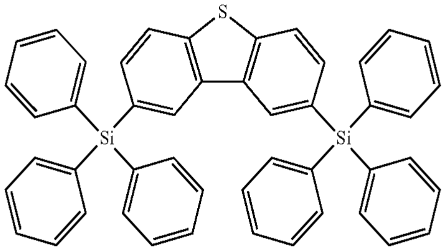
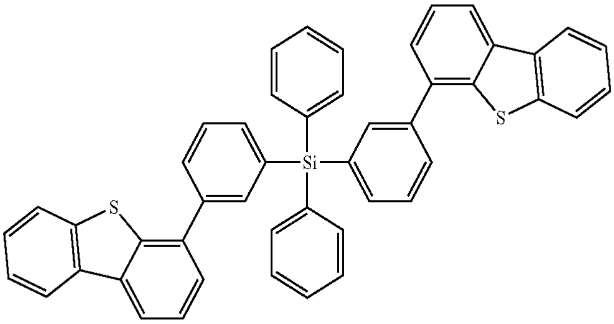
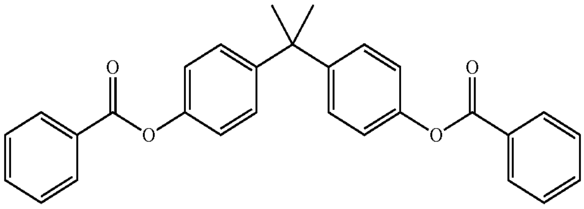
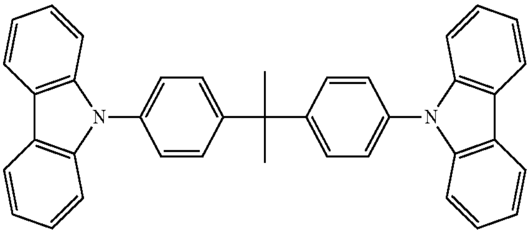
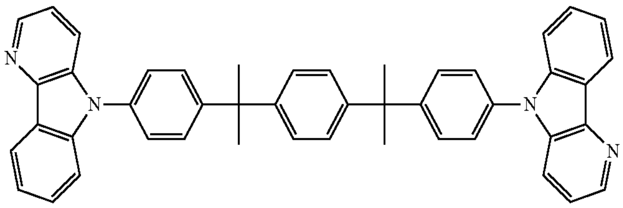
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon aryl compounds		US20050238919
		WO2009003898
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308

TABLE 4-continued

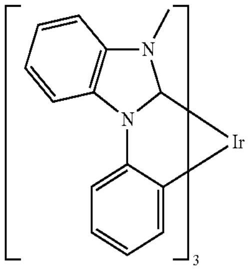
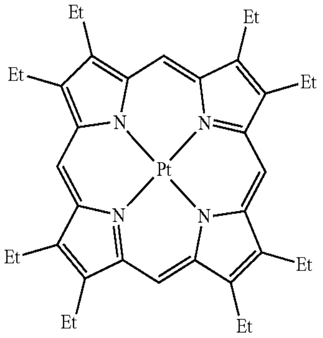
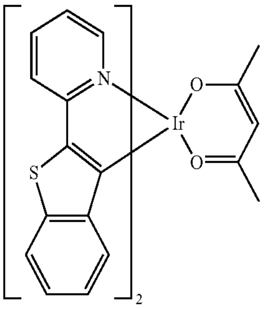
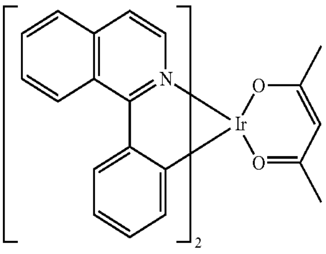
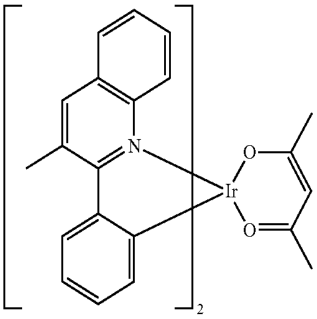
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114
	Phosphorescent dopants Red dopants	
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US2006835469
		US2006835469

TABLE 4-continued

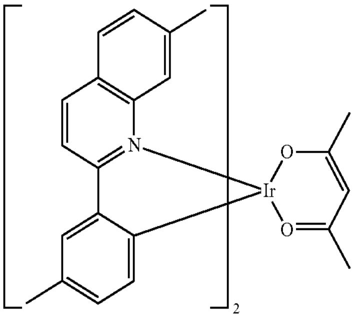
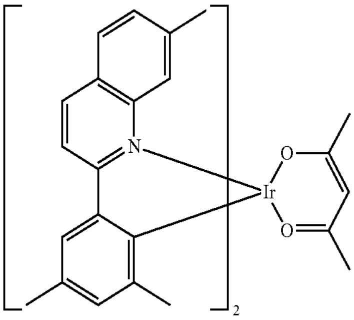
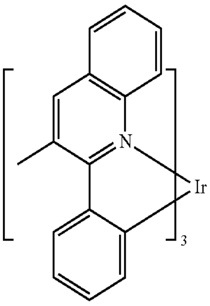
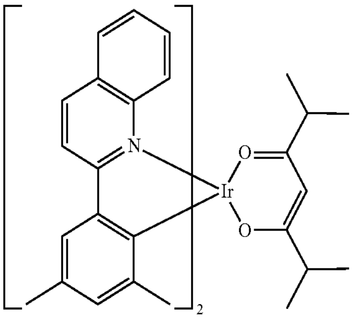
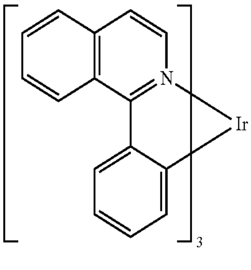
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060202194
		US20060202194
		US20070087321
		US20080261076 US20100090591
		US20070087321

TABLE 4-continued

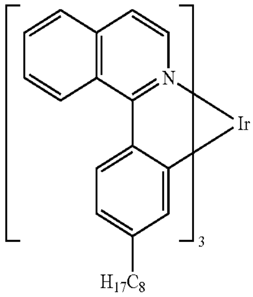
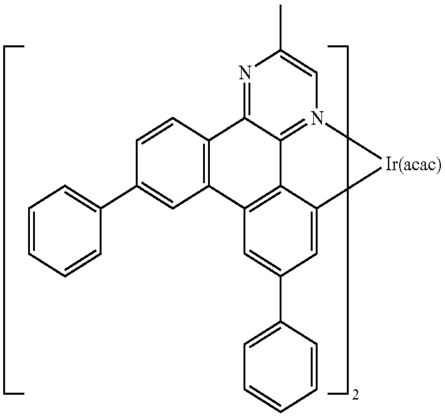
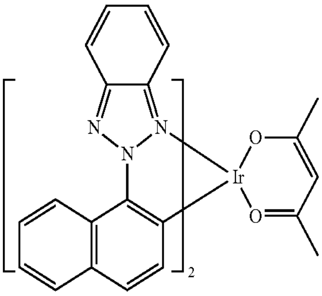
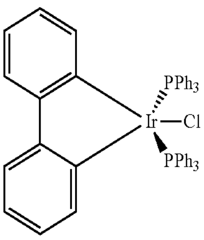
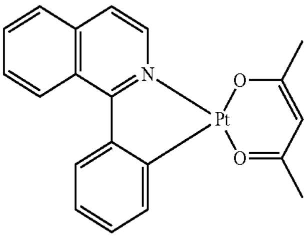
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
		U.S. Pat. No. 7,232,618
Platinum(II) organometallic complexes		WO2003040257

TABLE 4-continued

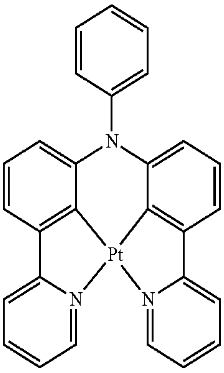
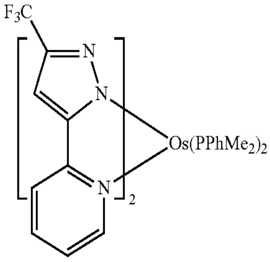
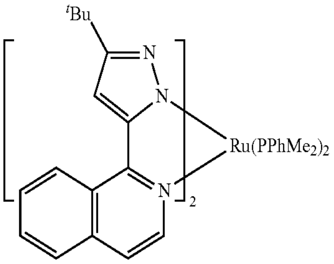
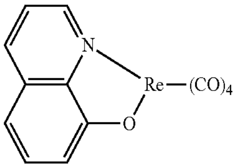
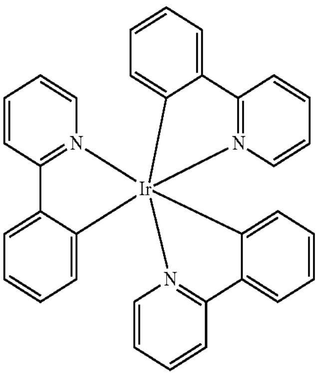
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070103060
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
	Green dopants	
Iridium(III) organometallic complexes	 and its derivatives	Inorg.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

TABLE 4-continued

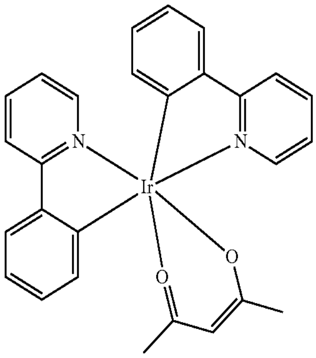
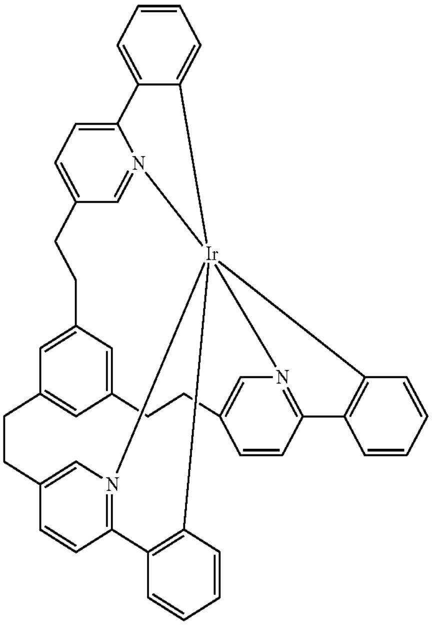
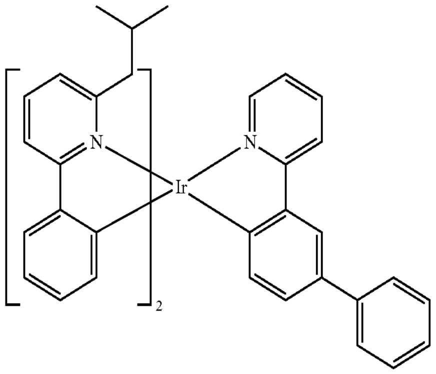
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20020034656
		U.S. Pat. No. 7,332,232
		US20090108737

TABLE 4-continued

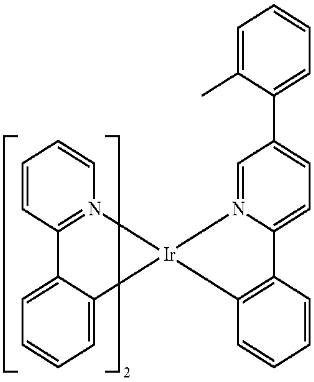
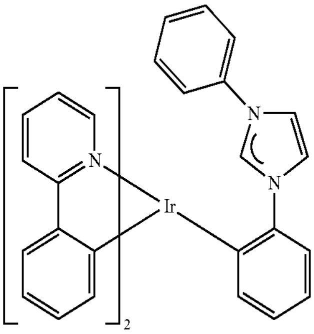
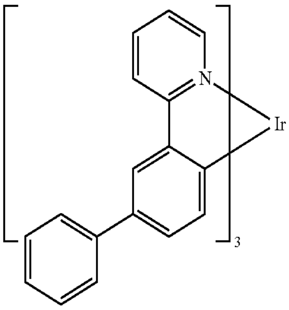
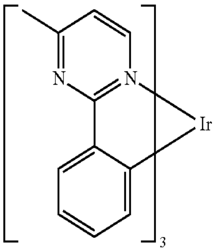
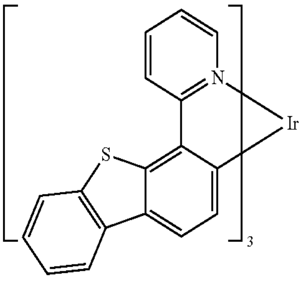
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2010028151
		EP1841834B
		US20060127696
		US20090039776
		U.S. Pat. No. 6,921,915

TABLE 4-continued

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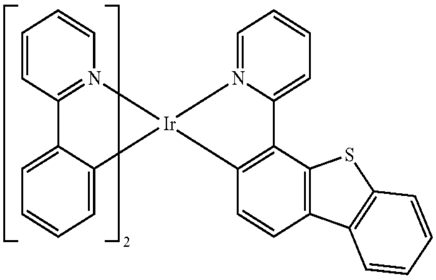
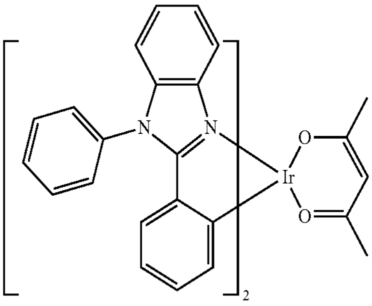
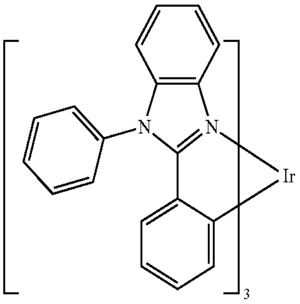
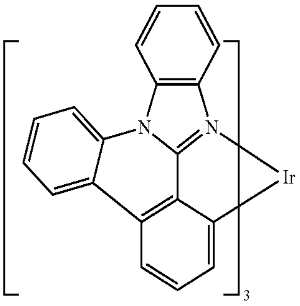
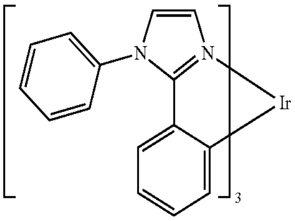
		US20100244004
		U.S. Pat. No. 6,687,266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US 20060008670 JP2007123392

TABLE 4-continued

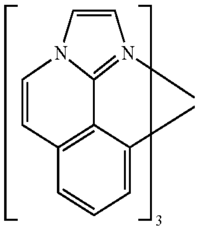
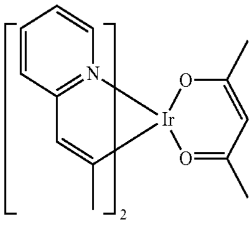
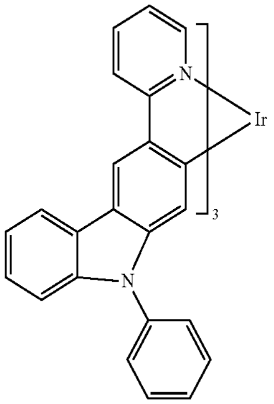
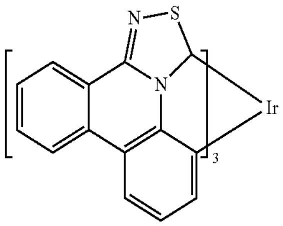
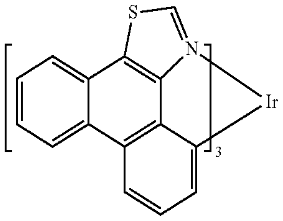
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846

TABLE 4-continued

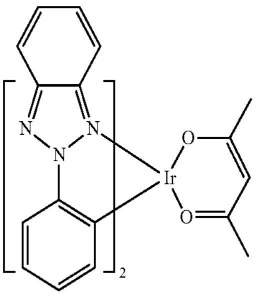
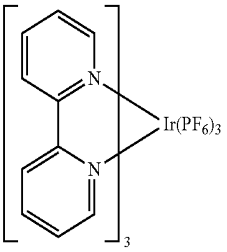
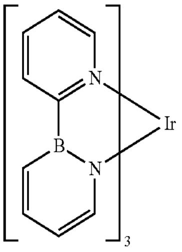
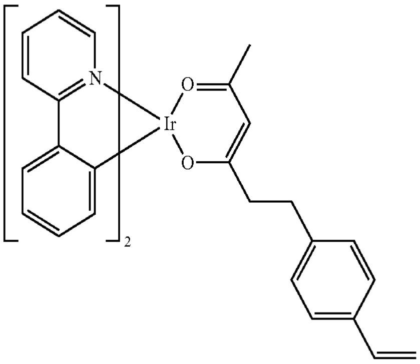
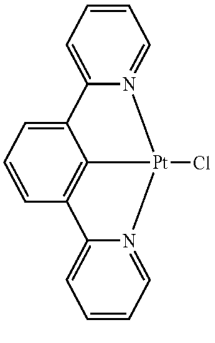
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20080015355
		US20010015432
		US20100295032
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)

TABLE 4-continued

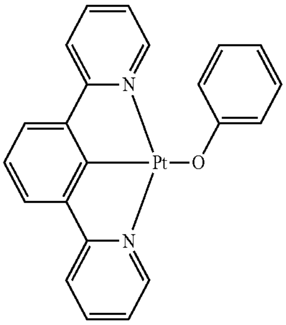
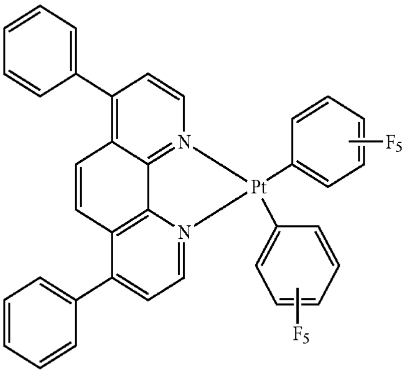
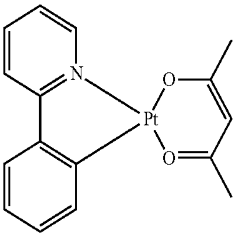
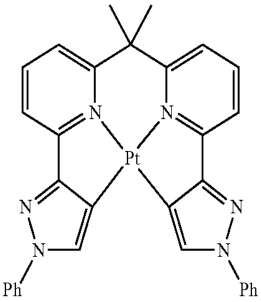
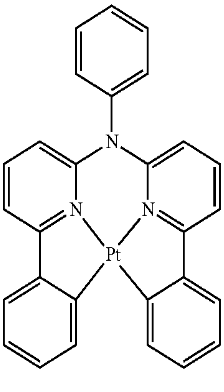
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635
		US20060182992 US20070103060

TABLE 4-continued

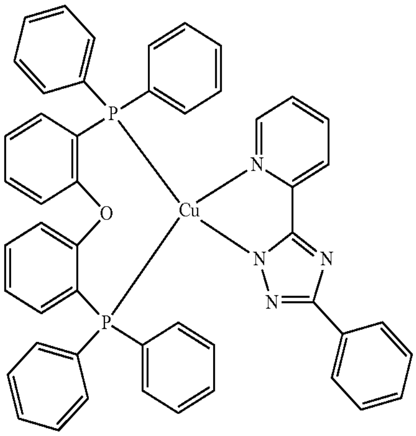
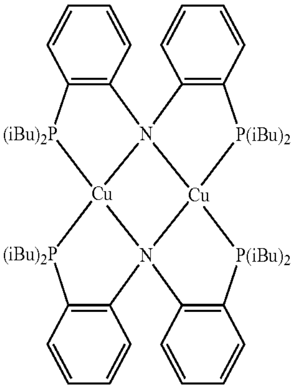
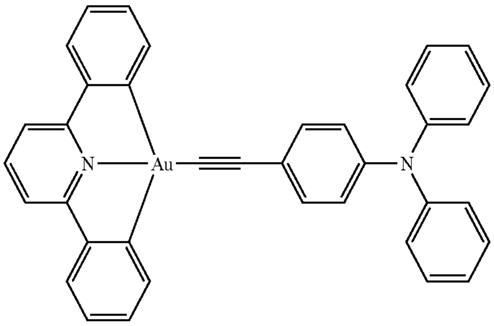
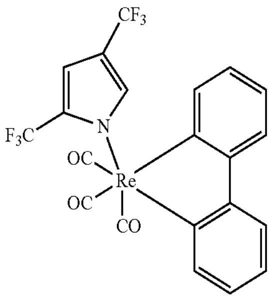
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
		US20070111026
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE 4-continued

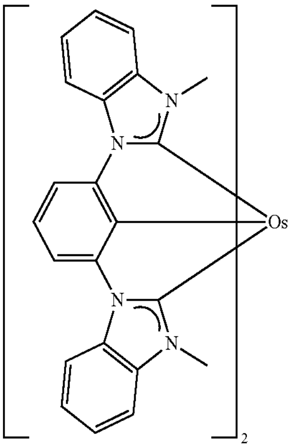
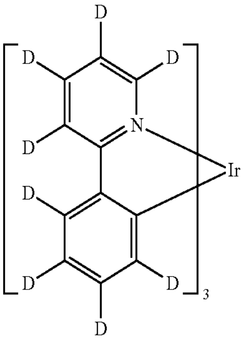
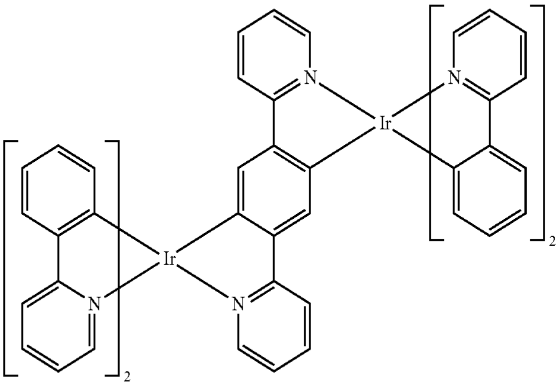
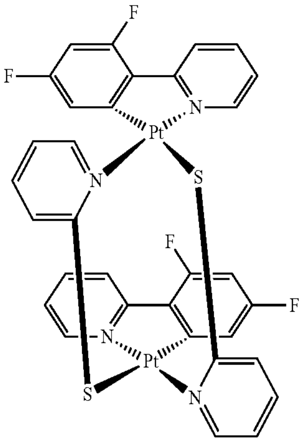
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(II) complexes		U.S. Pat. No. 7,279,704
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928

TABLE 4-continued

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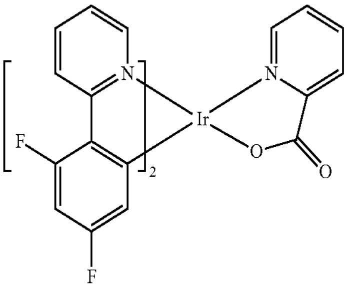
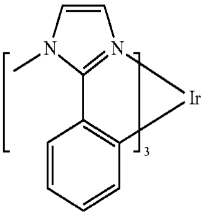
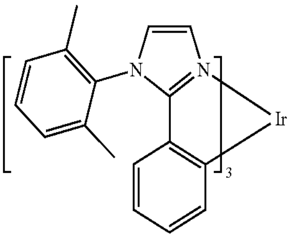
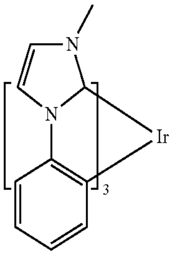
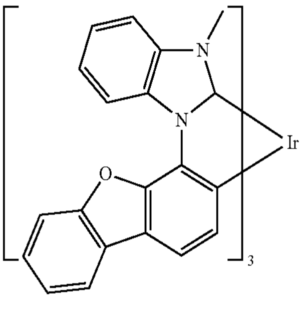
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		U.S. Pat. No. 7,393,599, WO2006056418, US20050260441, WO2005019373
		U.S. Pat. No. 7,534,505

TABLE 4-continued

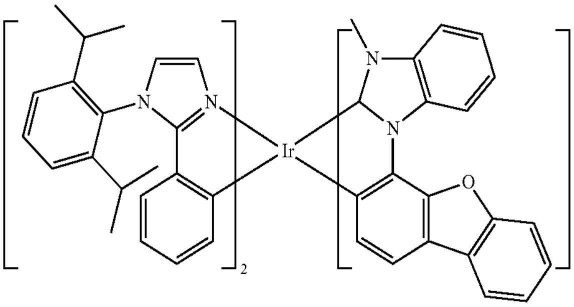
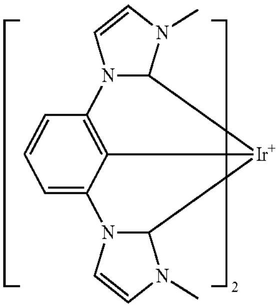
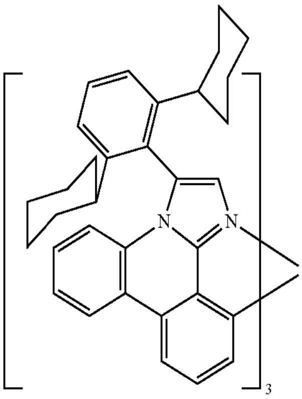
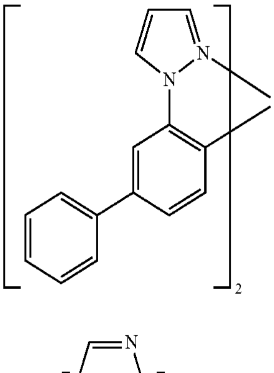
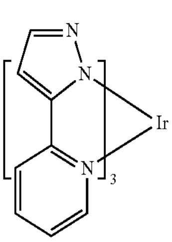
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2011051404
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033 US20100148663
		U.S. Pat. No. 7,338,722
		US20020134984

TABLE 4-continued

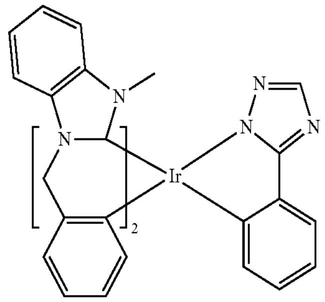
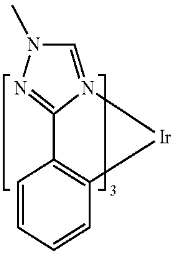
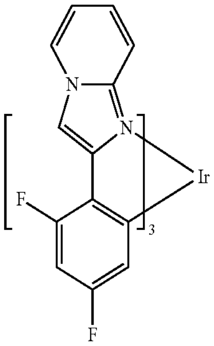
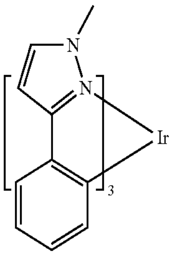
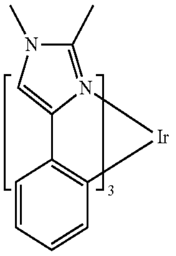
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873

TABLE 4-continued

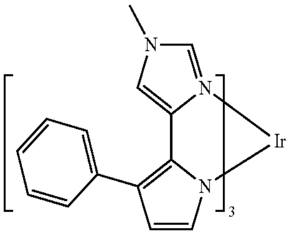
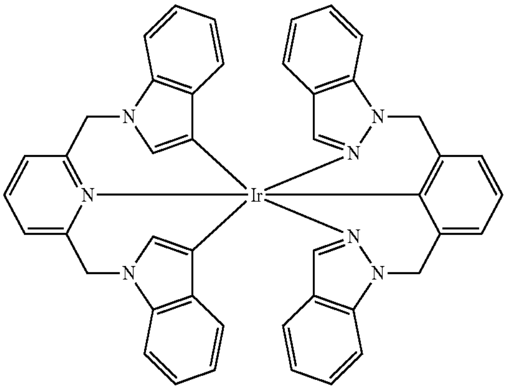
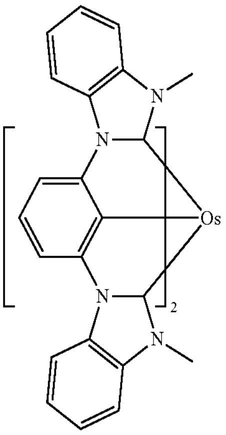
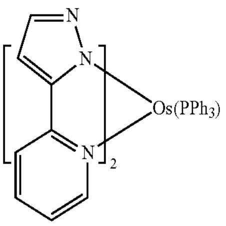
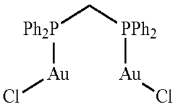
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2007004380
		WO2006082742
Osmium(II) complexes		U.S. Pat. No. 7,279,704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)

TABLE 4-continued

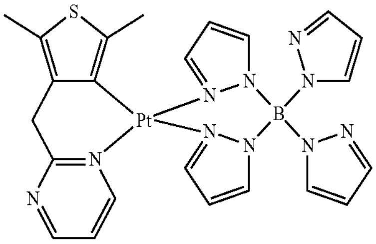
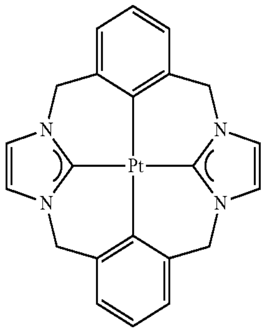
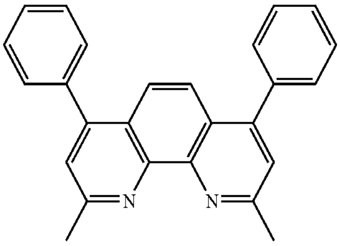
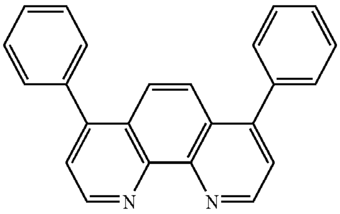
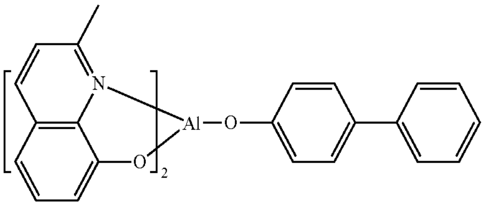
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Platinum(II) complexes		WO2006098120, WO2006103874
Pt tetradentate complexes with at least one metal-carbene bond		U.S. Pat. No. 7,655,323
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl.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

TABLE 4-continued

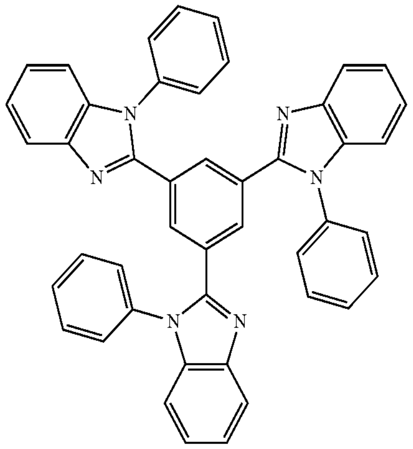
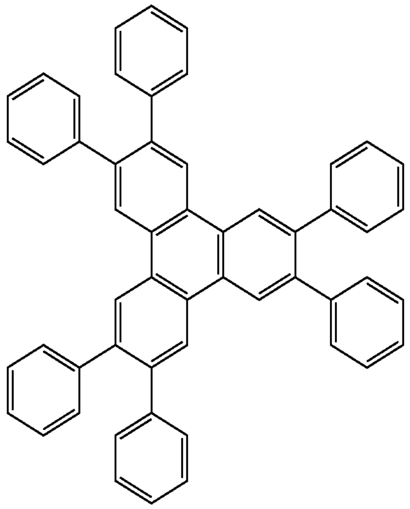
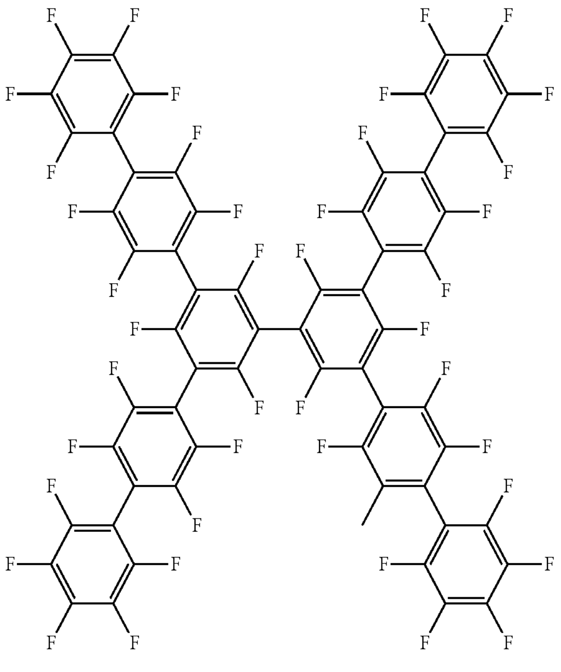
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)

TABLE 4-continued

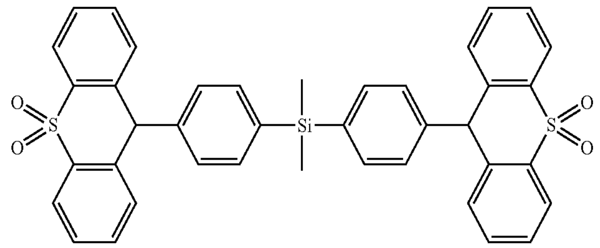
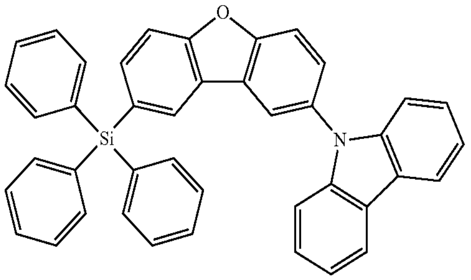
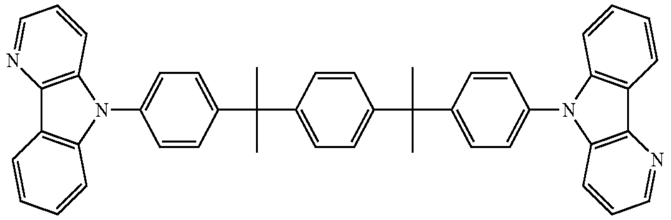
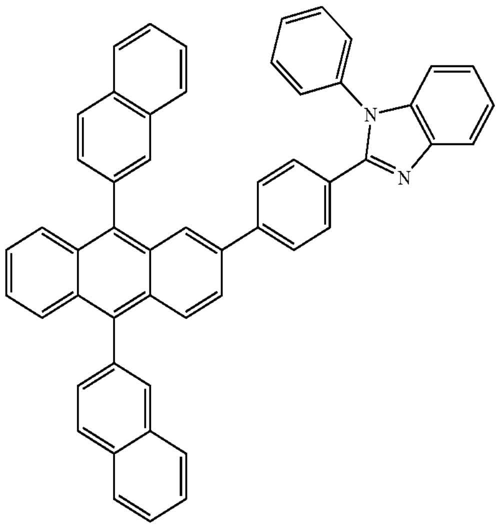
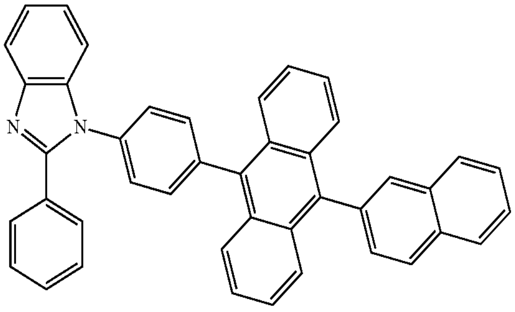
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051
Aza-carbazoles		US20060121308
	Electron transporting materials	
Anthracene-benzoimidazole compounds		WO2003060956
		US20090179554

TABLE 4-continued

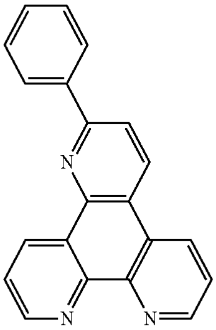
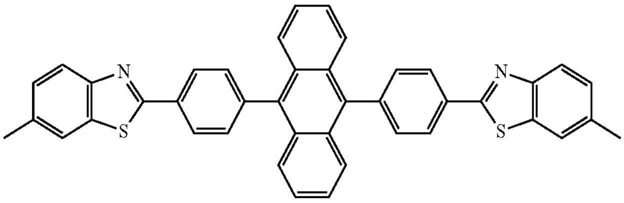
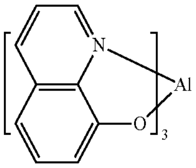
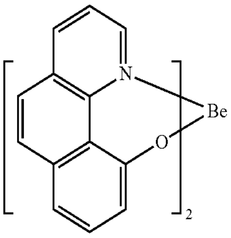
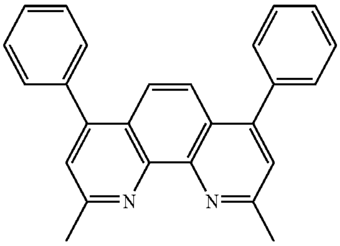
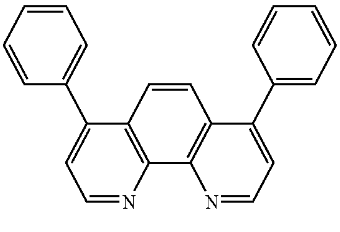
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7,230,107
Metal hydroxybenoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
		Appl. Phys. Lett. 79, 449 (2001)

TABLE 4-continued

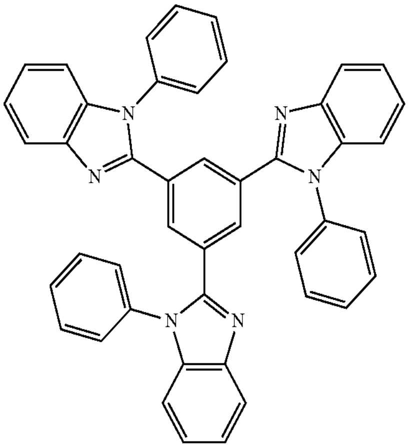
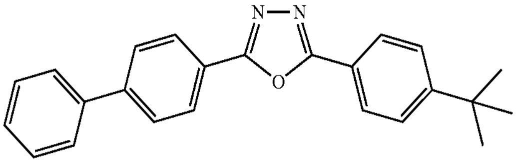
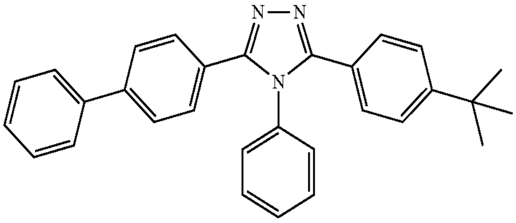
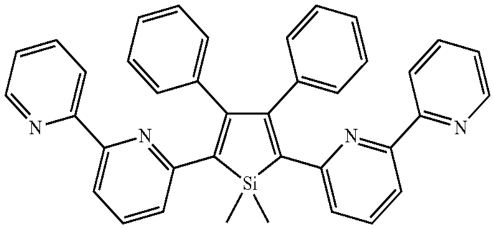
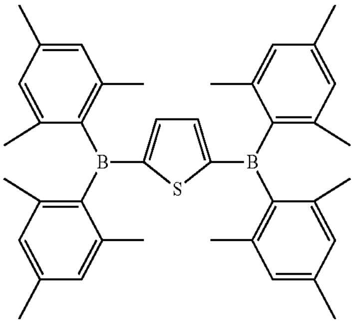
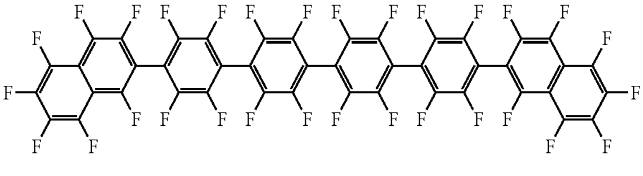
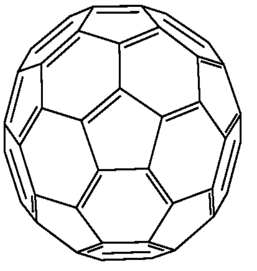
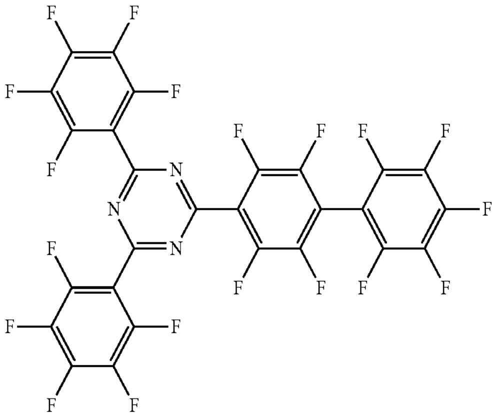
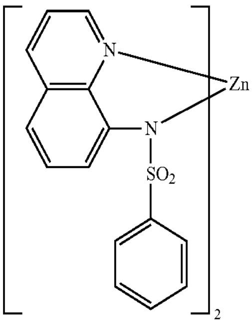
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)

TABLE 4-continued

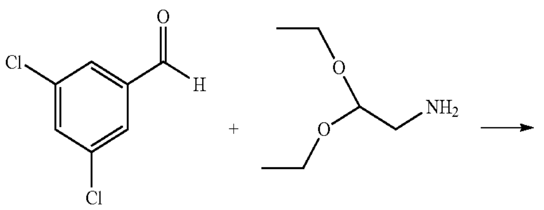
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fullerene (e.g., C60)		US20090101870
Triazine complexes		US20040036077
Zn (N^N) complexes		U.S. Pat. No. 6,528,187

EXPERIMENTAL

[0112] Chemical abbreviations used throughout this document are as follows: Cy is cyclohexyl, dba is dibenzylideneacetone, EtOAc is ethyl acetate, DME is dimethoxyethane, dppe is 1,2-bis(diphenylphosphino)ethane, THF is tetrahydrofuran, DCM is dichloromethane, DMF is dimethylformamide, S-Phos is dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine.

Synthesis of Compound 1

[0113]



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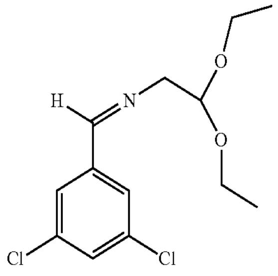
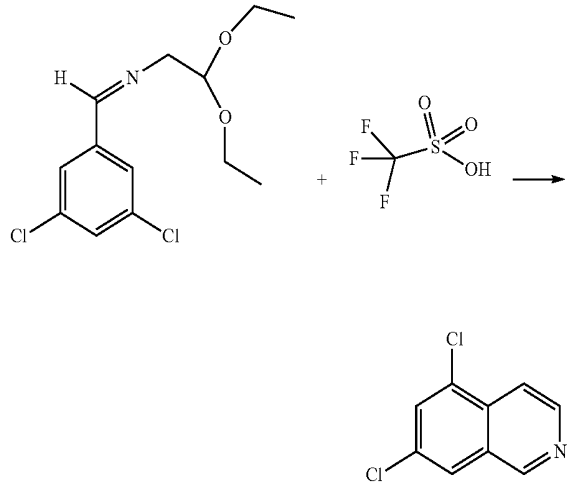


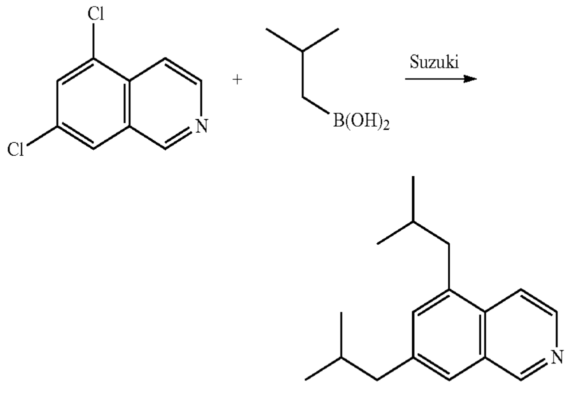
Synthesis of N-(3,5-dichlorobenzylidene)-2,2-diethoxyethanamine

[0114] 3,5-dichlorobenzaldehyde (51.2 g, 284 mmol), 2,2-diethoxyethanamine (38.6 g, 284 mmol) and 270 mL toluene were charged in a 500 mL three-necked flask. The mixture was heated to reflux for 24 hours under N_2 with Dean-Stark apparatus to collect water by-product. 86 g (100%) light yellow liquid was obtained after evaporated solvent. The product was confirmed by GC-MS and NMR and taken on to the next step without further purification.



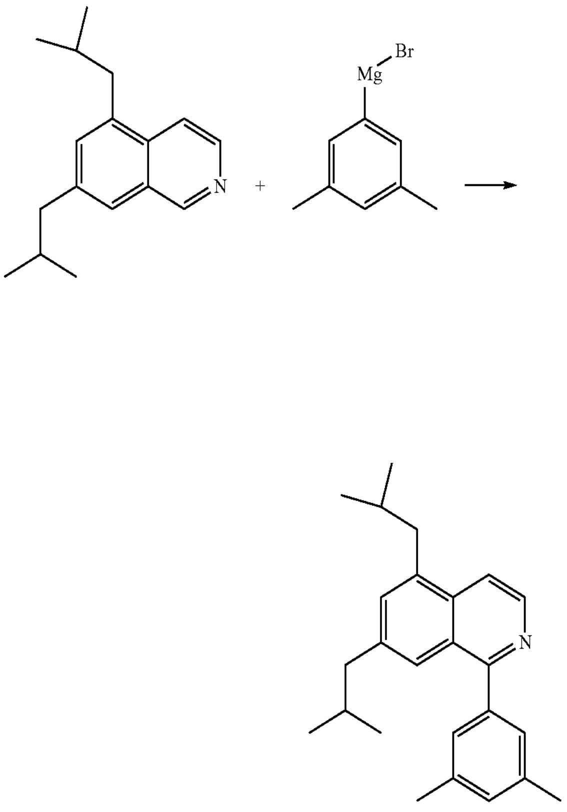
Synthesis of 5, 7-dichloroisoquinoline

[0115] Trifluoromethanesulfonic acid (15.83 g, 103 mmol) was charged in a three-necked 100 mL flask which was equipped with a Dean-Stark apparatus and and addition funnel. The trifluoromethanesulfonic acid was first heated to 120° C. and to the acid, N-(3,5-dichlorobenzylidene)-2,2-diethoxyethanamine (4 g, 13.78 mmol) dissolved in 4 mL DCM was added dropwise. After addition, the mixture was heated for another 2 hours at 120° C., then cooled to room temperature, and 8 mL of MeOH was added to quench the reaction. The reaction mixture was poured into aqueous ammonium hydroxide (120 mmol) solution, made basic with additional aqueous ammonium hydroxide, and stirred and filtered. A white solid (2.1 g, 77%) was obtained after distillation. The identity of the product was confirmed by GC and HPLC. A larger scale reaction with 32.2 g of N-(3,5-dichlorobenzylidene)-2,2-diethoxyethanamine was conducted in a same way and 16.5 g (75%) of the product was obtained for next step.



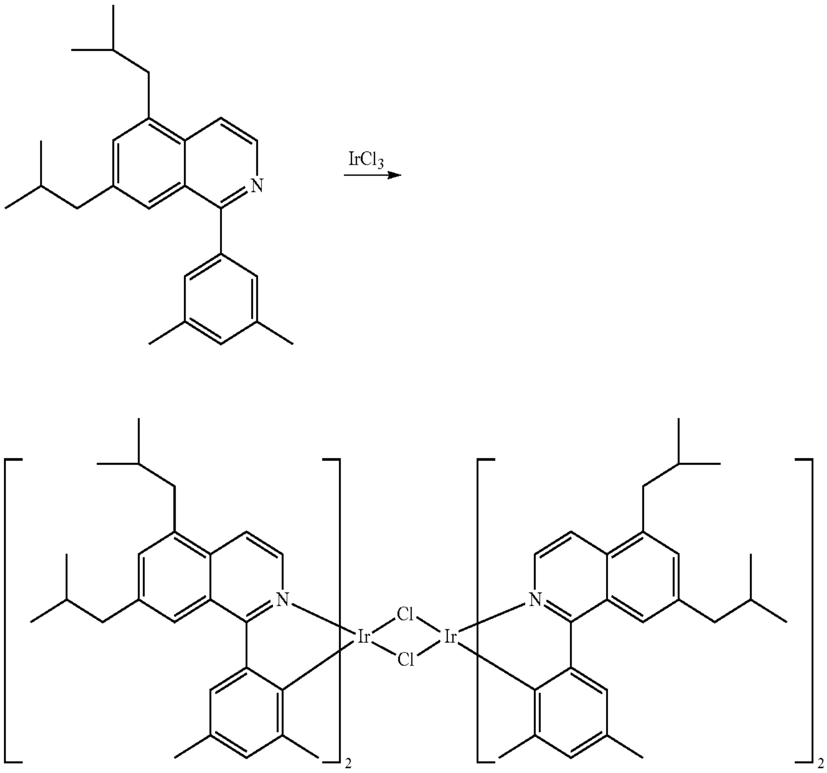
Synthesis of 5,7-diisobutylisoquinoline

[0116] 5,7-Dichloroisoquinoline (5.8 g, 29.3 mmol), isobutylboronic acid (8.96 g, 88 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.962 g, 2.34 mmol), $Pd_2(dba)_3$ (0.536 g, 0.586 mmol), K_3PO_4 (21.8 g, 103 mmol), 150 mL toluene and 15 mL water were charged in a flask. The reaction mixture was purged by bubbling N_2 for 30 minutes then heated to reflux overnight. GC-MS analysis showed that the reaction was complete. Silica gel chromatography with 15% ethyl acetate in hexane (v/v) as elutent resulted in 6.7 g (95%) of the product.



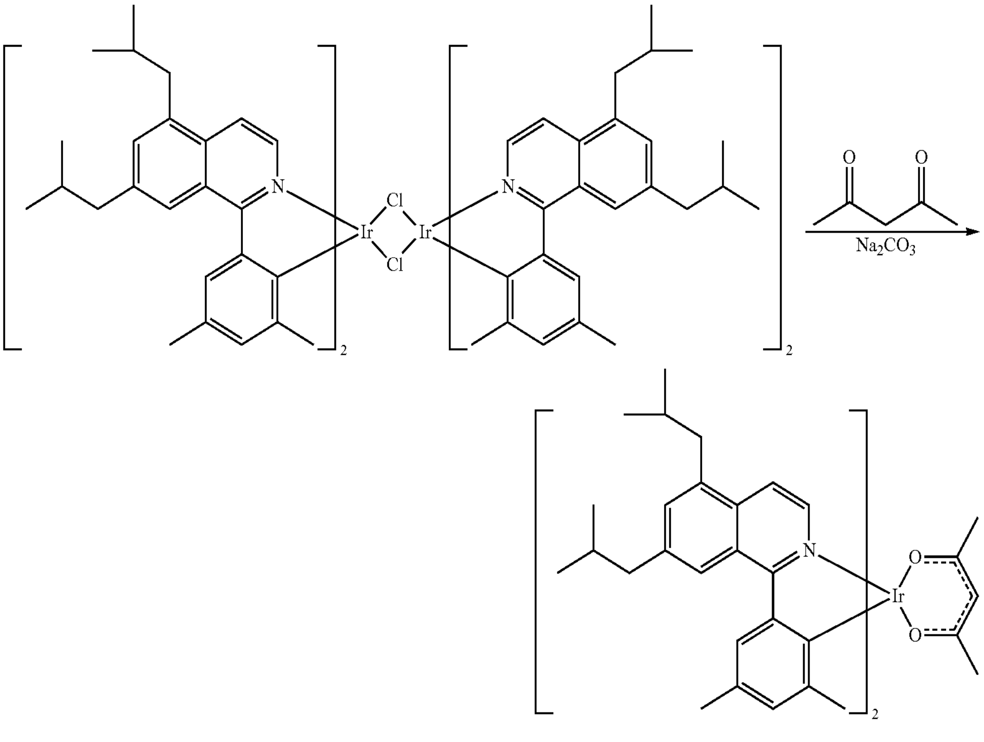
Synthesis of 1-(3,5-dimethylphenyl)-5,7-diisobutylisoquinoline

[0117] 5,7-Diisobutylisoquinoline (7.4 g, 30.7 mmol) in 50 mL dry THF and was added to (3,5-dimethylphenyl) magnesium bromide (100 mL, 50.0 mmol) dropwise at room temperature and allowed to stir for 16 hours, after which the reaction mixture was heated to reflux for 5 hours. GC and HPLC analysis indicated the reaction was complete, but contained a small amount of reduced byproducts which were converted to the desired product by treatment with DDQ in THF for few minutes. After aqueous workup, 6.5 g (61.4%) of product was obtained.



Synthesis of Iridium Dimer

[0118] 1-(3,5-dimethylphenyl)-5,7-diisobutylisoquinoline (6.0 g, 17.37 mmol) and $IrCl_3.H_2O$ (2.57 g, 6.95 mmol), 90 mL 2-ethoxylethanol and 30 mL water were charged in a 250 mL flask. The reaction mixture was heated to reflux under nitrogen for 19 hours. 3.1 g (24.3%) of dimer was obtained after filtration and washing with methanol, which was used for next step without further purification.

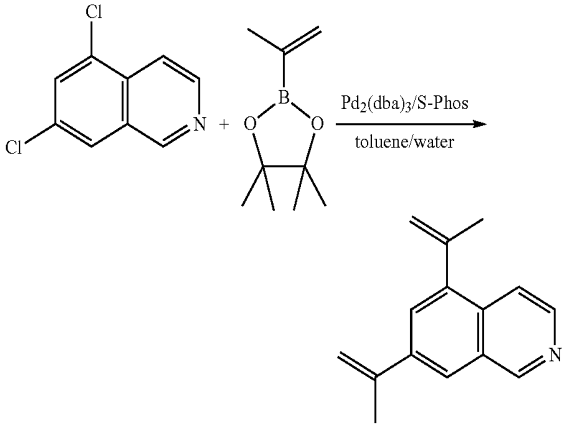


Synthesis of Compound 1

[0119] 2-(3,5-dimethylphenyl)-5,7-diisobutylquinoline iridium dimer (1.5 g, 0.82 mmol), 2,4-pentanedione (1.63 g, 16.36 mmol), Na_2CO_3 (1.73 g, 16.36 mmol) and 2-ethoxyethanol (60 mL) were charged in a 250 flask and stirred at room temperature for 72 hours. The resulting precipitate was filtered and washed with methanol. The solid was further purified by passing it through a silica gel plug (that was pretreated with 15% triethylamine in hexanes). 0.55 g (34.3%) of product was obtained after workup. The identity of the product was confirmed by LC-MS.

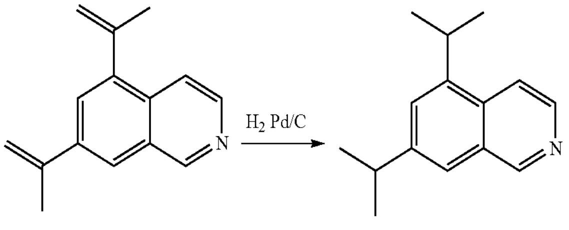
Synthesis of Compound 2

[0120]



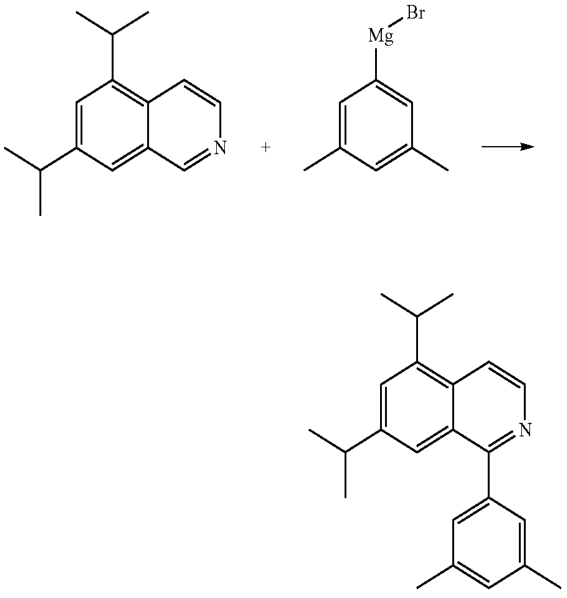
Synthesis of 5,7-di(prop-1-en-2-yl)isoquinoline

[0121] 5,7-Dichloroisoquinoline (5.1 g, 25.8 mmol), 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane (9.95 g, 59.2 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.846 g, 2.06 mmol), $Pd_2(dba)_3$ (0.472 g, 0.515 mmol), K_3PO_4 (19.13 g, 90 mmol), 100 mL toluene and 10 mL water were charged in a flask. The reaction mixture was purged by bubbling N_2 for 30 minutes then heated to reflux overnight. GC-MS analysis showed that the reaction was complete. 5.1 g (91%) of product was obtained after silica gel column chromatography and confirmed by GC-MS.



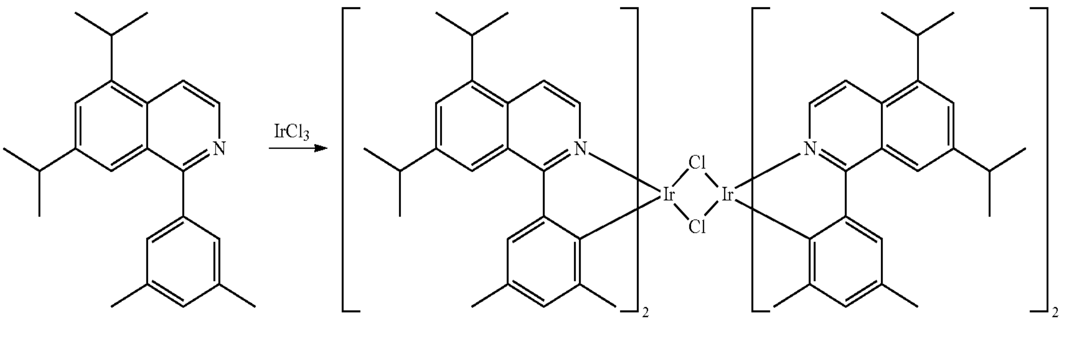
Synthesis of 5,7-diisopropyl)isoquinoline

[0122] 5,7-Di(prop-1-en-2-yl)isoquinoline (5.1 g, 24.37 mmol) was dissolved in 50 mL EtOH in a glass bottle and purged with N_2 for 30 minutes. To the solution, 10% Pd/C (1.3 g, 1.218 mmol) was added into the bottle under nitrogen. Hydrogenation was conducted for 4 hours, after which GC-MS analysis indicated the reaction was complete.



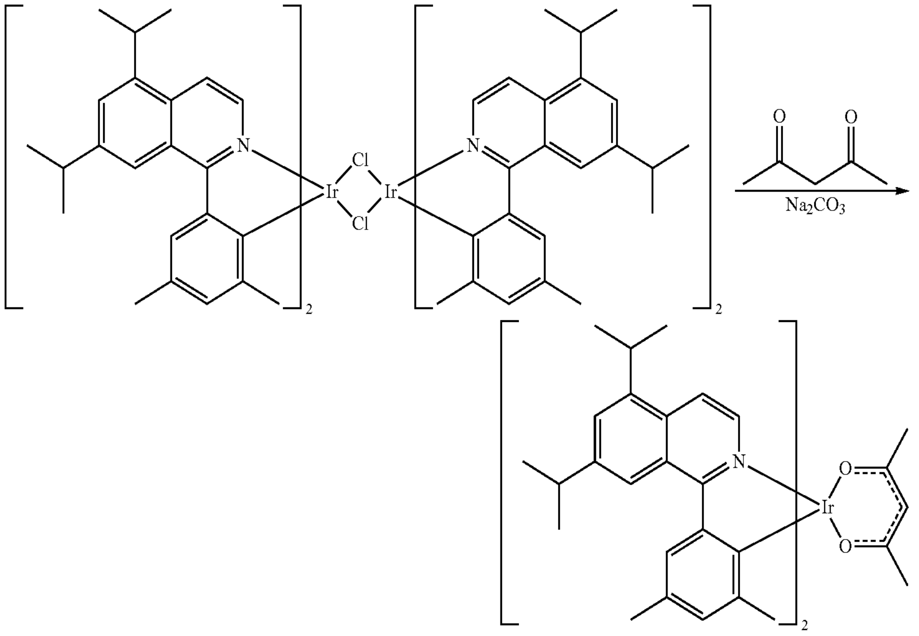
Synthesis of 1-(3,5-dimethylphenyl)-5,7-diisopropylisoquinoline

[0123] 5,7-diisopropylisoquinoline (3.1 g, 14.5 mmol) in 50 mL dry THF and was added with 0.5 M (3,5-dimethylphenyl)magnesium bromide THF solution (50 mL, 25.0 mmol) dropwise at room temperature and allowed to stir for 16 hours, after which the reaction mixture was heated to reflux for 5 hours. GC and HPLC analysis indicated the reaction was complete, but contained a small amount of reduced byproducts which were converted to the desired product by treatment with DDQ in THF for few minutes. After aqueous workup, 2.4 g (52%) of product was obtained.



Synthesis of Iridium Dimer

[0124] 1-(3,5-Dimethylphenyl)-5,7-diisopropylisoquinoline (2.4 g, 7.56 mmol) and $IrCl_3.H_2O$ (1.167 g, 3.15 mmol), 45 mL 2-ethoxylethanol and 15 mL water were charged in a 250 mL flask. The reaction mixture was heated to reflux under nitrogen for 19 hours. After cooling the reaction, filtration, and washing with methanol, 1.2 g (44.2%) of dimer was obtained, which was used for next step without further purification.

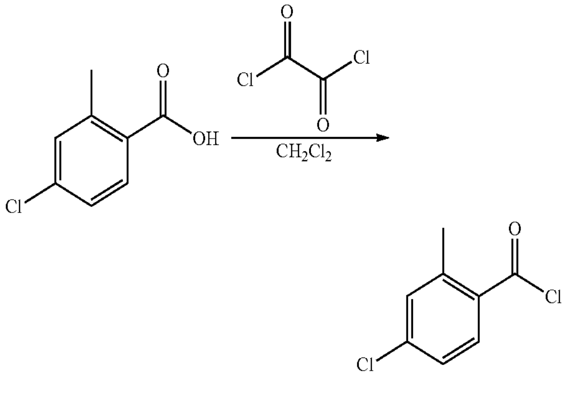


Synthesis of Compound 2

[0125] 2-(3,5-Dimethylphenyl)-5,7-diisopropylquinoline iridium dimer (1.2 g, 0.697 mmol), 2,4-pentanedione (0.697 g, 6.97 mmol), Na_2CO_3 (0.739 g, 6.97 mmol) and 2-ethoxyethanol (40 mL) were stirred at room temperature for 48 hours. The precipitate was filtered and washed with methanol. The solid was further purified by passing it through a silica gel plug (pretreated with 15% tryethylamine in hexanes). After workup of the reaction 0.68 g (52.8%) of product was obtained, which was confirmed by LC-MS.

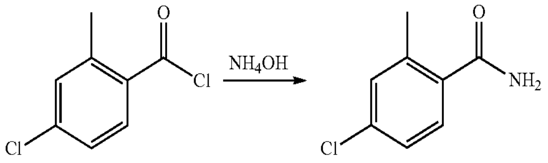
Synthesis of Compound 3

[0126]



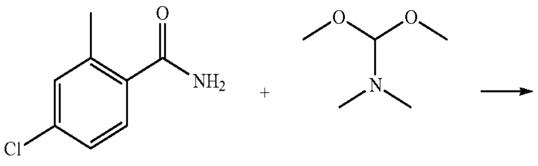
Synthesis of 4-Chloro-2-methylbenzoyl chloride

[0127] To a mixture of 4-chloro-2-methylbenzoic acid (24.0 g, 141 mmol) in dichloromethane (20 mL) and dimethylformamide (4 mL) at room temperature was added dropwise oxalyl chloride (26.8 g, 258 mmol). The reaction was stirred room temperature for 2 hours. Hexanes were added and the reaction mass was concentrated to give 4-chloro-2-methylbenzoyl chloride (26.6 g, quantitative) and used in the next step without purification.



Synthesis of 4-Chloro-2-methylbenzamide

[0128] 30% Ammonium hydroxide (300 mL, 4.76 mol) was cooled in a salt ice bath. 4-chloro-2-methylbenzoyl chloride (26.4 g, 140 mmol) in tetrahydrofuran (150 mL) added and stirred for 1 hr. Water was added. Crystals were filtered off and washed with water and dried under vacuum to give 4-chloro-2-methylbenzamide (20.0 g, 84% yield).



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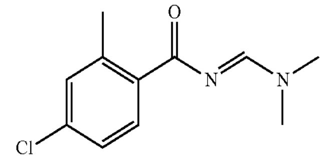
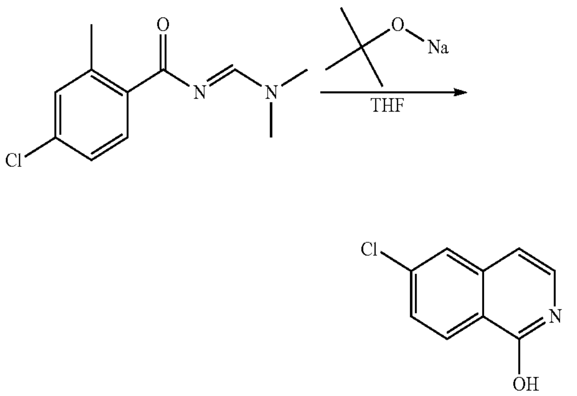


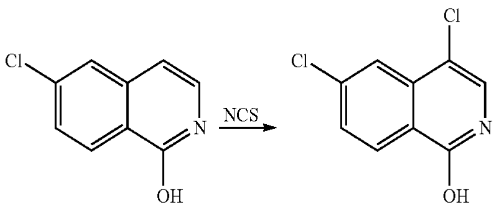
Synthesis of 4-Chloro-N-((dimethylamino)methylene)-2-methylbenzamide

[0129] A mixture of 4-chloro-2-methylbenzamide (20.8 g, 123 mmol) and 1,1-dimethylmethaneamine (17.5 g, 147 mmol) in tetrahydrofuran (250 mL) was refluxed for 2.5 hours and then concentrated. The resulting crystals were triturated in hexanes and filtered to give 4-chloro-N-((dimethylamino)methylene)-2-methylbenzamide (25.7 g, 93% yield).



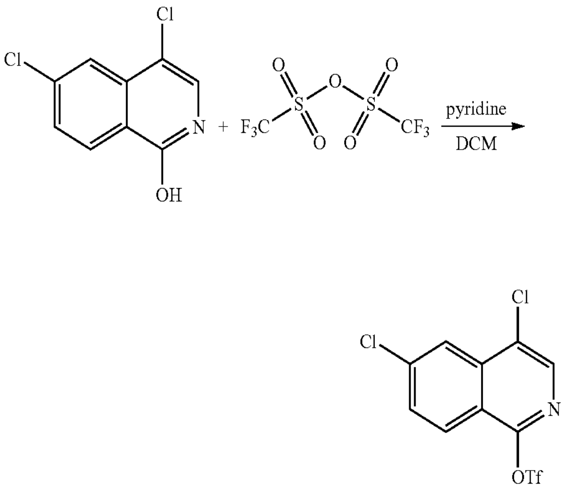
Synthesis of 6-Chloroisoquinolin-1-ol

[0130] A mixture of 4-chloro-N-((dimethylamino)methylene)-2-methylbenzamide (25.7 g, 114 mmol), sodium tert-butoxide (25.7 g, 267 mmol) and tetrahydrofuran (450 mL) was refluxed under N_2 for 3 hours and then poured into water (1 L). The pH was adjusted to 4 with aqueous HCl. The solids were filtered off and washed with water and dried under vacuum to give 6-chloroisoquinolin-1-ol (14.7 g, 71.6% yield).

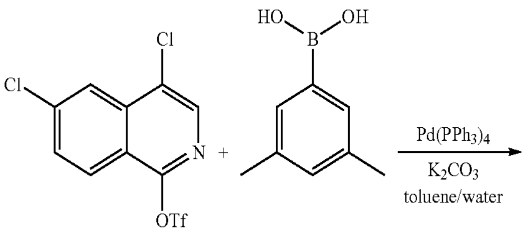


Synthesis of 4,6-Dichloroisoquinolin-1-ol

[0131] A mixture of 6-chloroisoquinolin-1-ol (13.5 g, 75 mmol) and acetonitrile (400 mL) was heated to reflux. N-Chlorosuccinimide (10.57 g, 79 mmol) in acetonitrile (110 mL) was added dropwise. The mixture was refluxed overnight. Crystals were filtered off. The filtrate was concentrated and the resulting crystals were washed with water and combined with the above crystals and dried under vacuum to give 4,6-dichloroisoquinolin-1-ol (14.2 g, 88% yield). It was taken on without analysis to the next step.



[0132] Synthesis of 4,6-Dichloroisoquinolin-1-yl trifluoromethanedsulfonate. A mixture of 4, 6-dichloroisoquinolin-1-ol (14.2 g, 66.5 mmol), pyridine (10.8 mL, 133 mmol) and dichloromethane (200 mL) was cooled in an ice bath. Trifluoromethanesulfonic anhydride (22.4 mL, 133 mmol) was added dropwise. The mixture was stirred overnight at room temperature. Water was added and $NaHCO_3$ (20 g) was added slowly. The organic layer was dried over Na_2SO_4, concentrated and flash chromatographed using silica gel chromatography (4:1 hexanes: dichloromethane, v/v) to give 4,6-dichloroisoquinolin-1-yl trifluoromethanedsulfonate (3.7 g, 16% yield).



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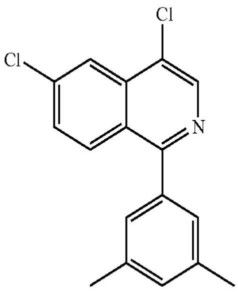
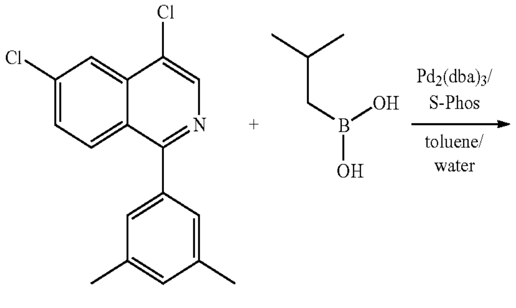


Synthesis of 4,6-Dichloro-1-(3,5-dimethylphenyl)isoquinoline

[0133] A mixture of 4,6-dichloroisoquinolin-1-yl trifluoromethanesulfonate (4.0 g, 11.6 mmol), 3,5-dimthylphenyl) boronic acid (1.6 g, 10.8 g), Pd(PPh$_3$)$_4$ (0.67 g, 0.58 mmol), potassium carbonate (4.79, 34.7 mmol), toluene (100 mL) and water (10 mL) was purged with nitrogen and refluxed overnight. The concentrated toluene layer was chromatographed using silica gel chromatography (2:1 hexanes:dichloromethane, v/v) to give 4,6-dichloro-1-(3,5-dimethylphenyl)isoquinoline (3.0 g, 92% yield).



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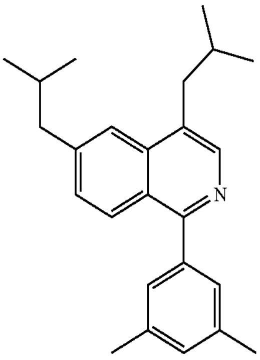
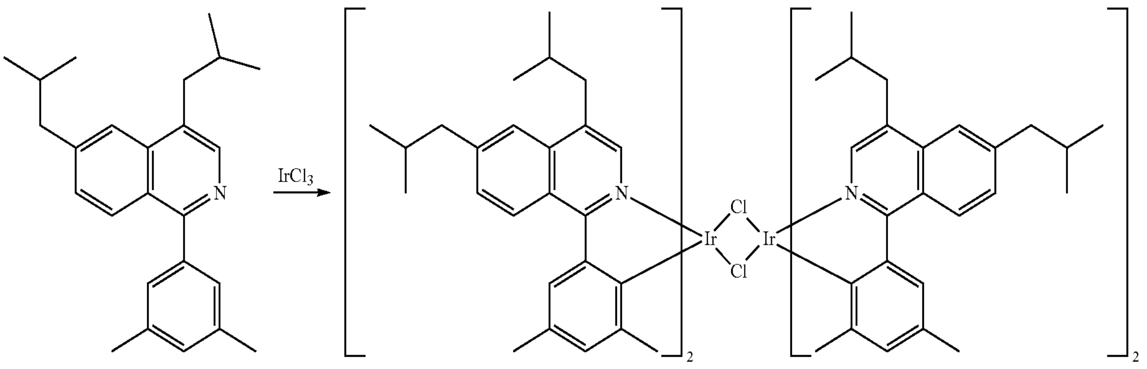


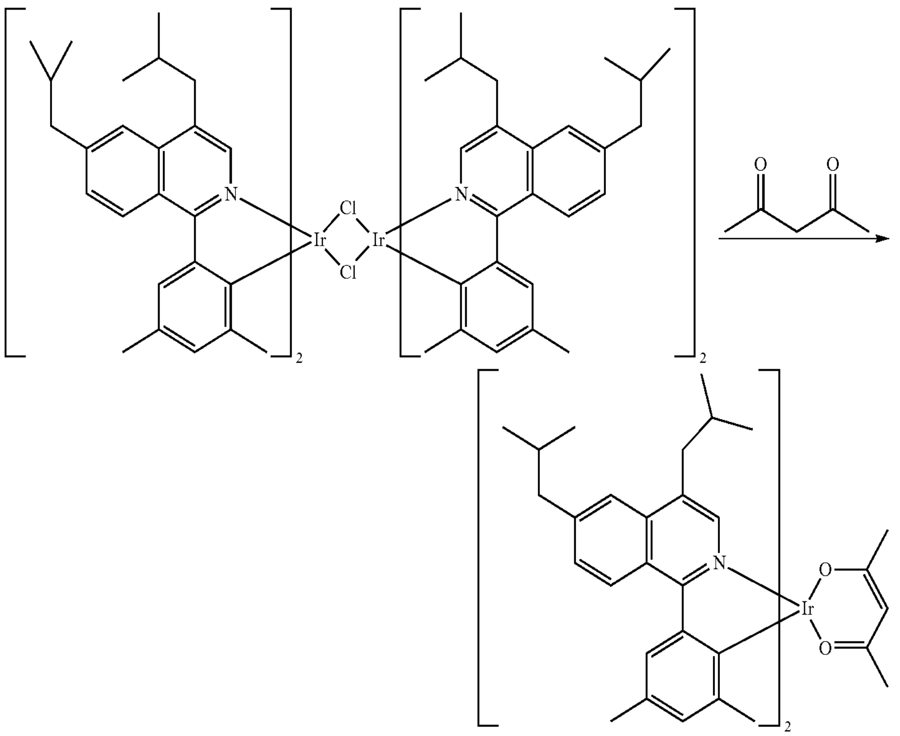
Synthesis of 1-(3,5-Dimethylphenyl)isoquinoline

[0134] A mixture of 4,6-dichloro-1-(3,5-dimethylphenyl) isoquinoline (3.2 g, 10.59 mmol), isobutylboronic acid (4.32 g, 42.4 mmol), PdAdba)$_3$ (0.388 g, 0.424 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.696 g, 1.694 mmol), K$_3$PO$_4$.H$_2$O (24.38 g, 106 mmol), toluene (133 mL) and water (11 mL) were purged with nitrogen for 30 minutes and refluxed overnight. The toluene layer was chromatographed using silica gel chromatography (100% dichloromethane to 4:1 dichloromethane:ethyl acetate, v/v) to give 1-(3,5-dimethylphenyl)isoquinoline (3.3 g, 90% yield).



Synthesis of 1-(3,5-Dimethylphenyl)isoquinoline Iridium dimer

[0135] A mixture of 1-(3,5-dimethylphenyl)-4,6-diisobutylisoquinoline (3.3 g, 9.55 mmol), $IrCl_3.3H_2O$ (1.475 g, 3.98 mmol), 2-ethoxyethanol (45 mL) and water (15 mL) were refluxed overnight and then filtered and washed with methanol to give 1-(3,5-dimethylphenyl)isoquinoline iridium dimer (2.0 g, 54.8% yield).

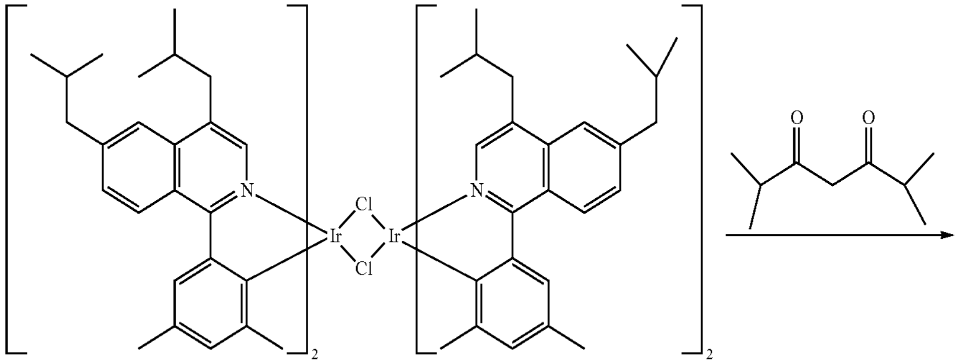


Synthesis of Compound 3

[0136] A mixture of 1-(3,5-dimethylphenyl)isoquinoline iridium dimer (1.2 g, 0.655 mmol), pentane-2,4-dione (0.655 g, 6.55 mmol), potassium carbonate (0.905 g, 6.55 mmol) and 2-ethoxyethanol (60 mL) was stirred at room temperature overnight and filtered, washed with methanol and chromaographed using silica gel chromatography (4:1 hexanes:dichloromethane, v/v, silica gel pre-treated with triethylamine). The residue was dissolved in dichloromethane and 2-propanol. The dichloromethane was removed on a rotoevaporator and 0.68 g of crystals were filtered off and then sublimed at 230° C. to give Compound 3 (0.32 g, 24.9%), which was confirmed by LC-MS.

Synthesis of Compound 22

[0137]



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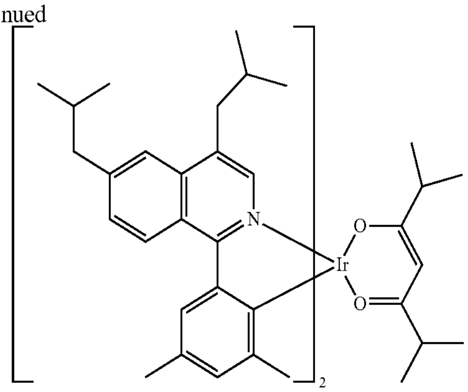


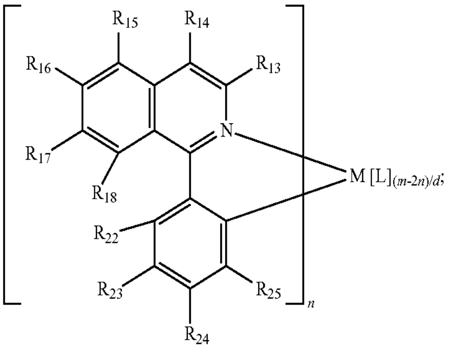
Synthesis of Compound 22

[0138] A mixture of 1-(3,5-dimethylphenyl)isoquinoline iridium dimer (0.8 g, 0.436 mmol), 2,6-dimethylheptane-3,5-dione (0.682 g, 4.36 mmol), potassium carbonate (0.603 g, 4.36 mmol) and 2-ethoxyethanol (60 mL) were stirred at room temperature overnight and filtered, washed with methanol and chromaographed on silica gel (4:1 hexanes: dichloromethane, v/v, silica gel pre-treated with triethylamine). The residue was dissolved in dichloromethane and 2-propanol. The dichloromethane was removed on a roto-evaporator and 0.60 g of crystals were obtained after filtration. It was confirmed by LC-MS.

[0139] 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.

1. A compound having the formula:

Formula I



wherein M is a metal having an atomic weight higher than 40;

wherein L is a second ligand;

wherein m is the maximum coordination number of the metal M;

wherein d is the denticity of L;

wherein n is at least 1;

wherein each of R_{13}, R_{14}, R_{15}, R_{16}, R_{17}, and R_{18} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

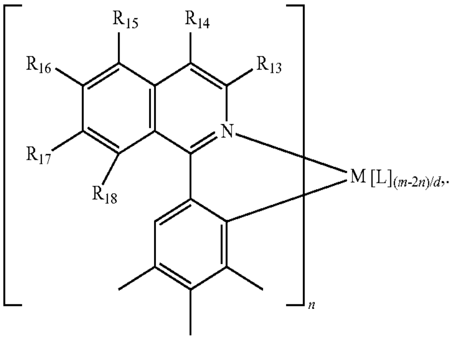
wherein at least two of R_{13}, R_{14}, R_{15}, R_{16}, R_{17}, and R_{18} are independently selected from alkyl with two to three carbon atoms;

wherein each of R_{22}, R_{23}, R_{24}, and R_{25} 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.

2. The compound of claim **1**, wherein R_{23} and R_{25} are alkyl, and R_{24} is hydrogen.

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

Formula III



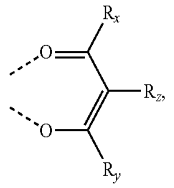
4. The compound of claim **1**, wherein at least one of R_{13}, R_{15}, R_{16}, and R_{18} is selected from the group consisting of ethyl and $CH(CH_3)_2$.

5. The compound of claim **1**, wherein M is Jr.

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

7. The compound of claim **1**, wherein L is a monoanionic bidentate ligand.

8. The compound of claim **7**, wherein L is



and

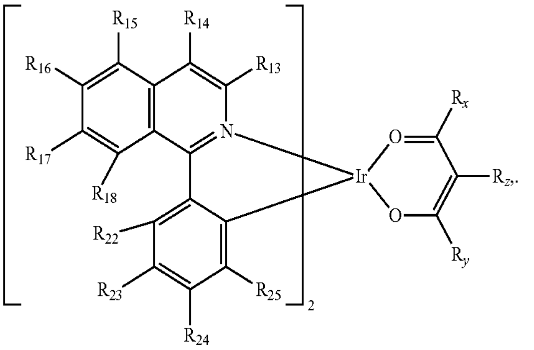
wherein R_x, R_y, and R_z are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile,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

9. The compound of claim **8**, wherein R_x, R_y, and R_z are independently selected from the group consisting of alkyl, hydrogen, deuterium, and combinations thereof.

10. The compound of claim **9**, wherein R_z is hydrogen or deuterium, and R_x and R_y are independently selected from the group consisting of methyl, $CH(CH_3)_2$, and $CH_2CH(CH_3)_2$.

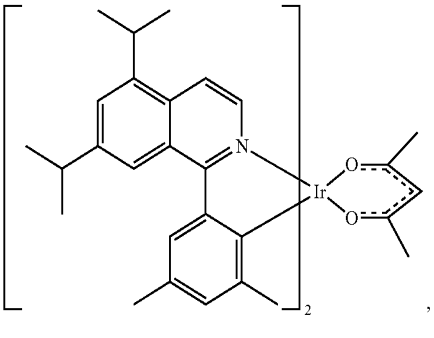
11. The compound of claim **8**, wherein the compound has the formula:

Formula IV



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

Compound 2



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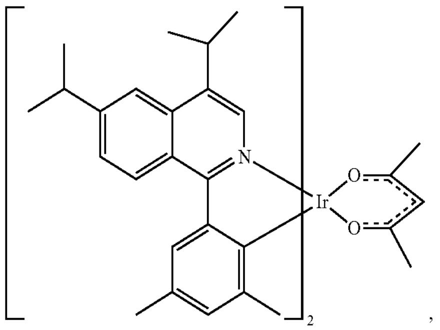
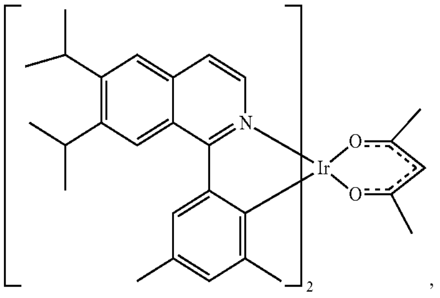
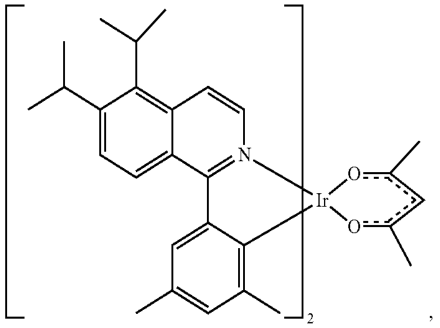
Compound 4



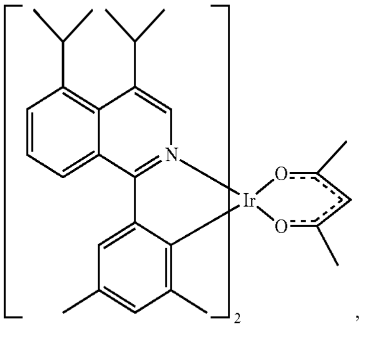
Compound 8



Compound 10



Compound 14



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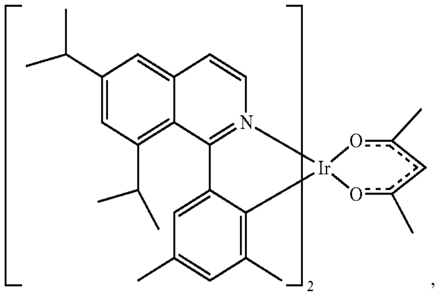
Compound 16



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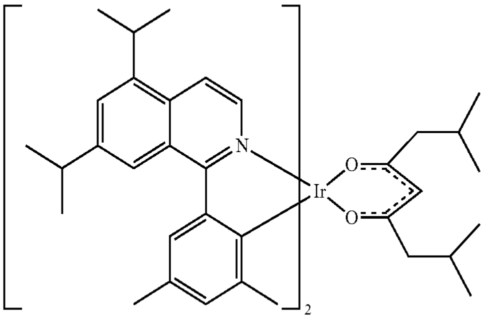
Compound 20



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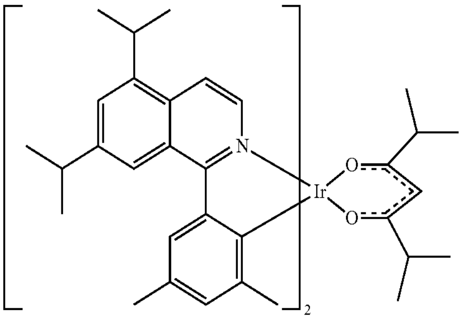
Compound 21



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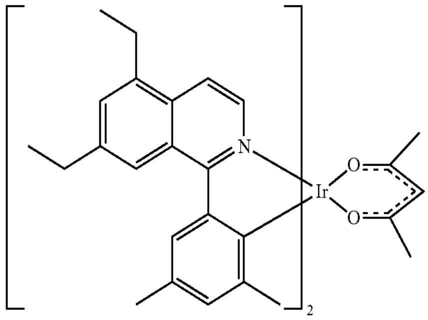
Compound 28



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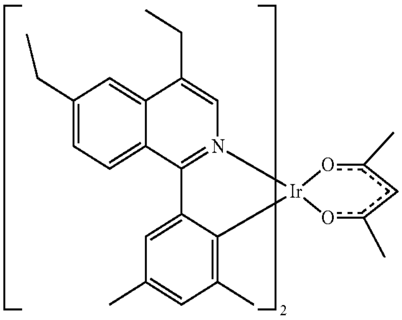
Compound 29



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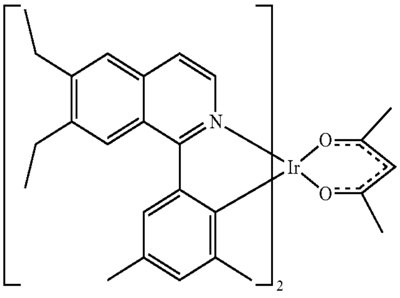
Compound 30



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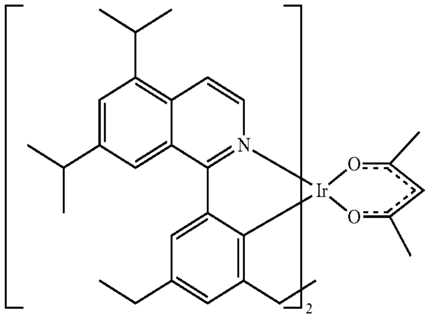
Compound 48



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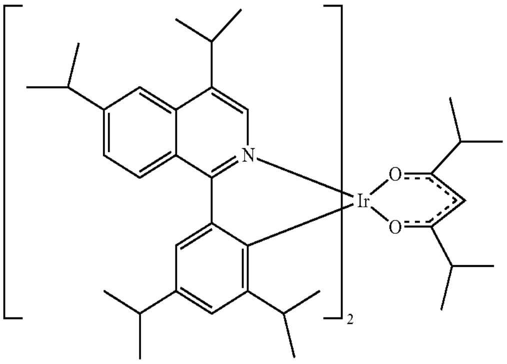
Compound 50



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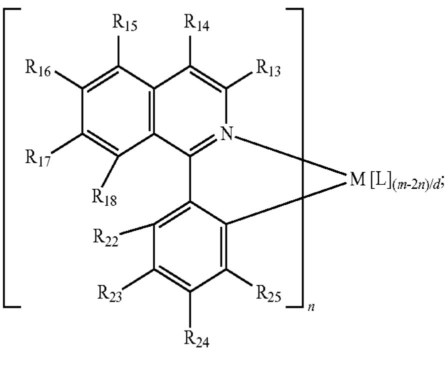
13. A first device comprising a first organic light emitting device, comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound having the formula:

Formula I



wherein M is a metal having an atomic weight higher than 40;

wherein L is a second ligand;

wherein m is the maximum coordination number of the metal M;

wherein d is the denticity of L;

wherein n is at least 1;

wherein each of R_{13}, R_{14}, R_{15}, R_{16}, R_{17}, and R_{18} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

wherein at least two of R_{13}, R_{14}, R_{15}, R_{16}, R_{17}, and R_{18} are independently selected from alkyl with two to three carbon atoms; and

wherein each of R_{22}, R_{23}, R_{24}, and R_{25} 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.

14. The first device of claim **13**, wherein the first device is a consumer product.

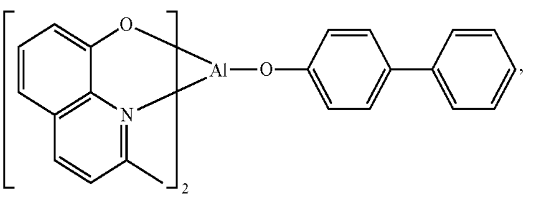
15. The first device of claim **13**, wherein the first device is an organic light-emitting device.

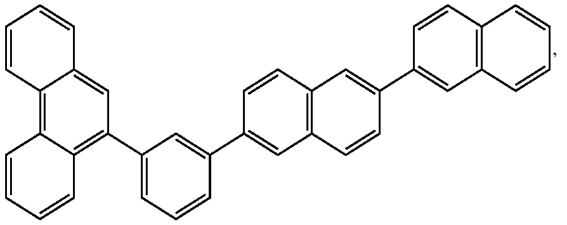
16. The first device of claim **13**, wherein the organic layer is an emissive layer and the compound is a non-emissive dopant.

17. The first device of claim **13**, wherein the organic layer further comprises a host.

18. The first device of claim **17**, wherein the host is a metal 8-hydroxyquinolate.

19. The first device of claim **17**, wherein the host is selected from the group consisting of:





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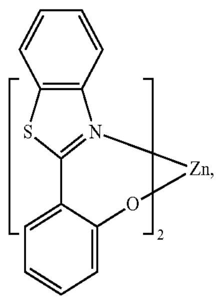
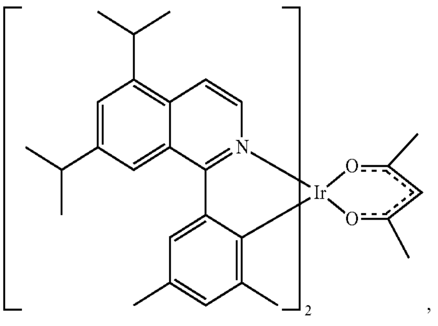


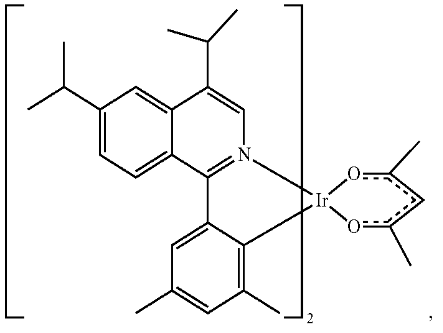
and combinations thereof.

20. The first device of claim **13**, wherein the compound is selected from the group consisting of:

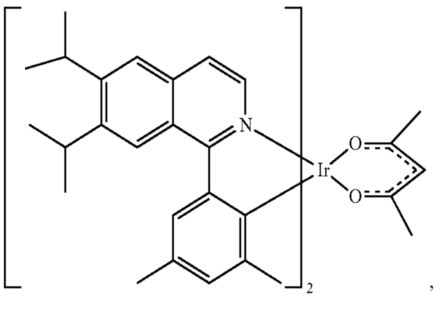
Compound 2



Compound 4



Compound 8



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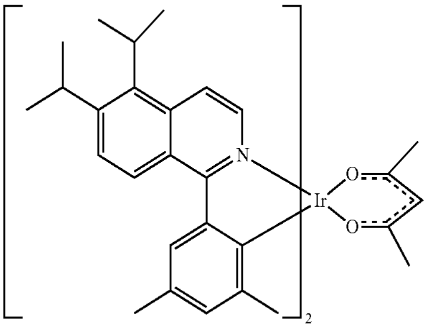
Compound 10



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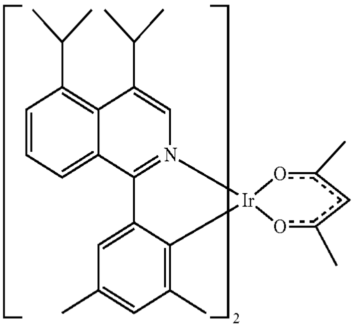
Compound 14



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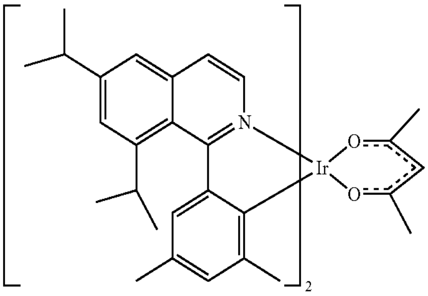
Compound 16



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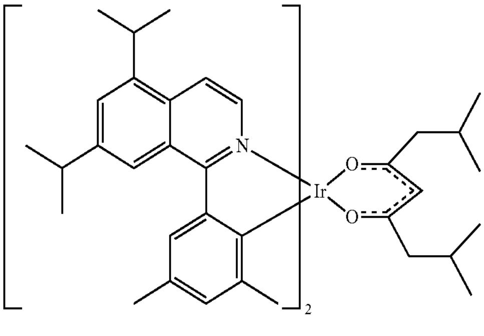
Compound 20



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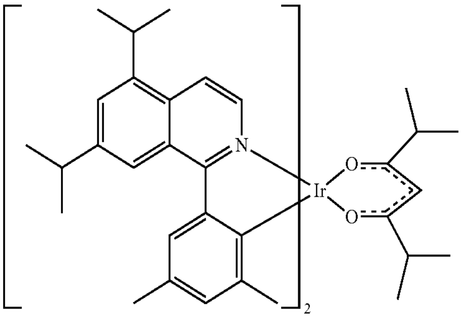
Compound 21



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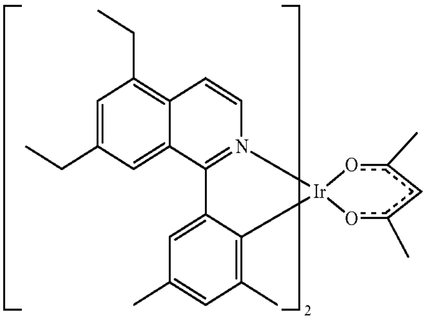
Compound 28



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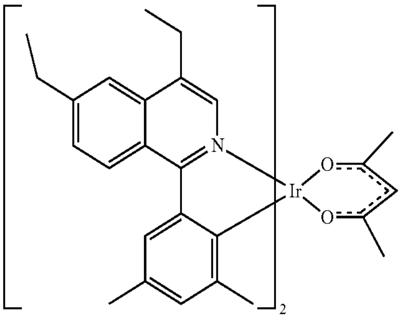
Compound 29



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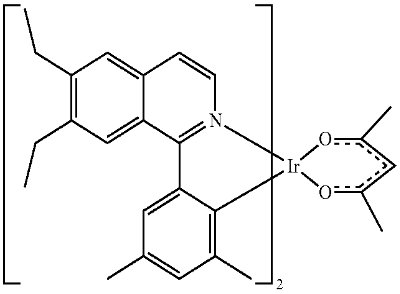
Compound 30



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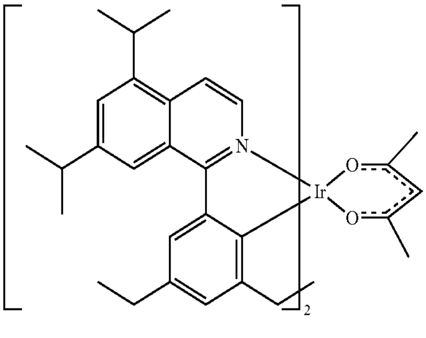
Compound 48



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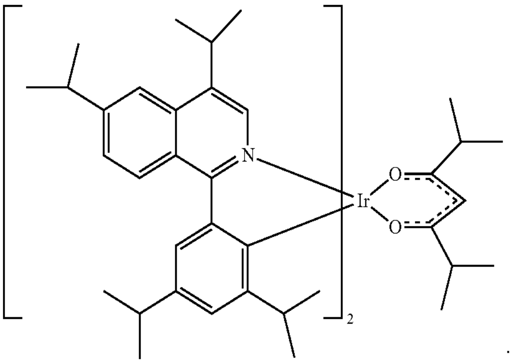
Compound 50



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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	US15/336201	申请日	2016-10-27
[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	MA BIN DEANGELIS ALAN XIA CHUANJUN		
发明人	MA, BIN DEANGELIS, ALAN XIA, CHUANJUN		
IPC分类号	H01L51/00 C09K11/06 C09K11/02 C07F15/00		
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其他公开文献	US10454046		
外部链接	Espacenet USPTO		

摘要(译)

提供了含有2-苯基异喹啉配体的新型磷光金属配合物，其在异喹啉环上具有至少两个取代基。所公开的化合物具有低升华温度，其允许易于纯化和制造成各种OLED装置。