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(12) United States Patent
Ma et al.**(10) Patent No.: US 9,130,177 B2**
(45) Date of Patent: Sep. 8, 2015**(54) 5-SUBSTITUTED 2 PHENYLQUINOLINE
COMPLEXES MATERIALS FOR LIGHT
EMITTING DIODE****(75) Inventors:** **Bin Ma**, Plainsboro, NJ (US); **Alan
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NJ (US)**(*) Notice:** Subject to any disclaimer, the term of this
patent is extended or adjusted under 35
U.S.C. 154(b) by 609 days.**(21) Appl. No.: 13/006,016****(22) Filed: Jan. 13, 2011****(65) Prior Publication Data**

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(51) Int. Cl.**H01L 51/54** (2006.01)**C09K 11/06** (2006.01)**H01L 51/00** (2006.01)**C07F 15/00** (2006.01)**H01L 51/50** (2006.01)**(52) U.S. Cl.**CPC **H01L 51/0085** (2013.01); **C07F 15/0033**
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2211/1029 (2013.01); **C09K 2211/185**
(2013.01); **H01L 51/5016** (2013.01)**(58) Field of Classification Search**CPC **C07F 15/0006**; **C07F 15/002**; **C07F**
15/0033; **C07F 15/0046**; **C07F 15/006**;
C07F 15/0073; **C07F 15/0086**; **C07F 7/006**;
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51/5012; **H01L 51/5016**; **C09K 11/06**; **C09K**
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See application file for complete search history.

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(57) ABSTRACTCompounds are provided that comprise a ligand having a
5-substituted 2-phenylquinoline. In particular, the 2-phe-
nylquinoline may be substituted with a bulky alkyl at the
5-position. These compounds may be used in organic light
emitting devices, in particular as red emitters in the emissive
layer of such devices, to provide devices having improved
properties.**26 Claims, 3 Drawing Sheets**

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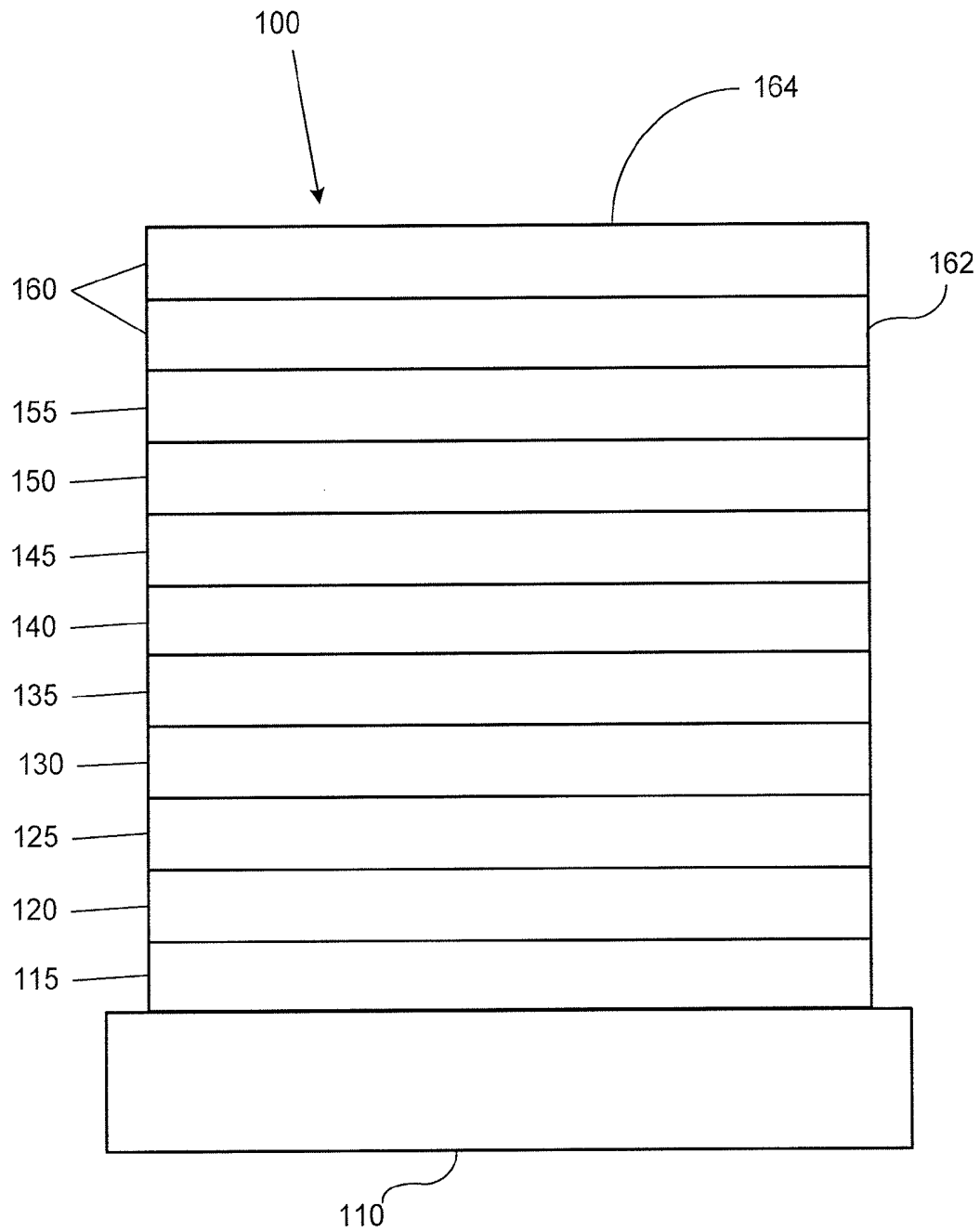


FIGURE 1

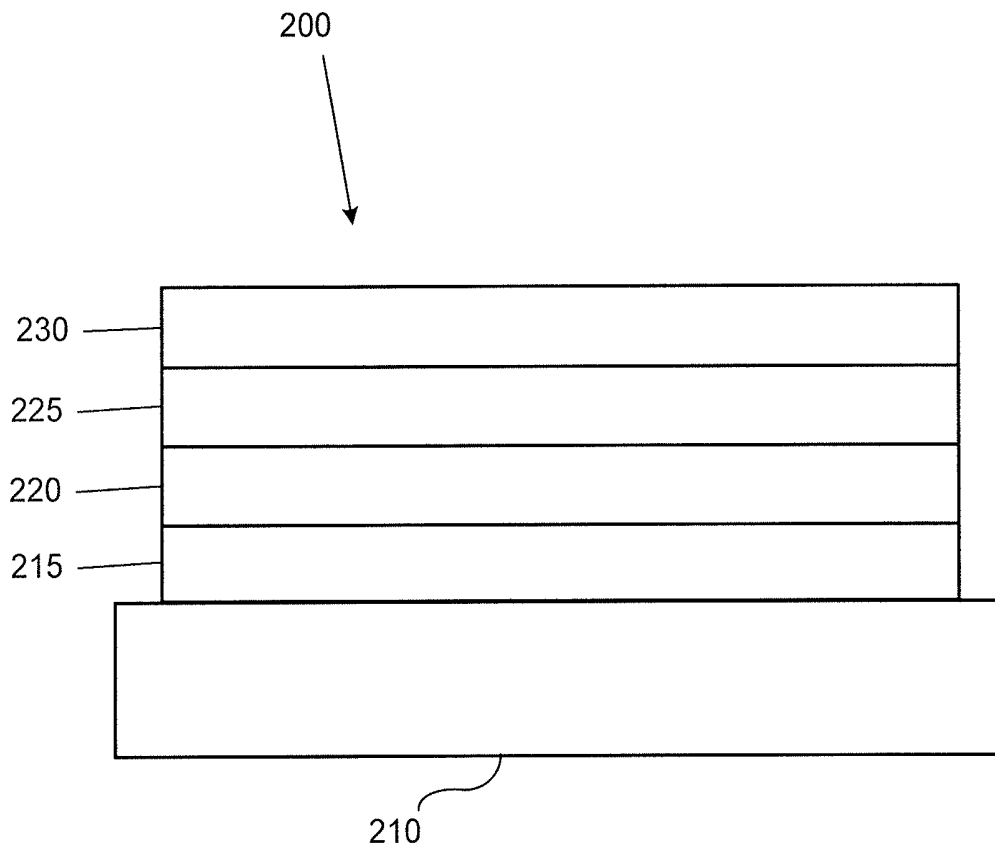


FIGURE 2

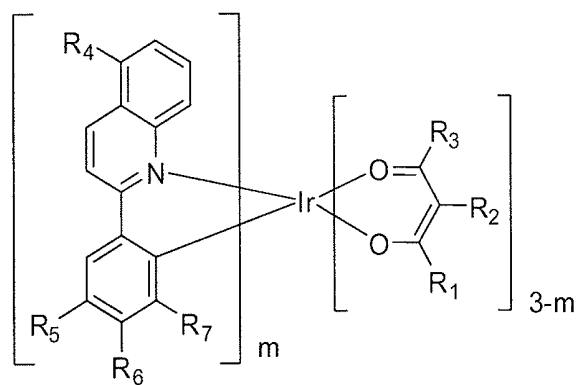
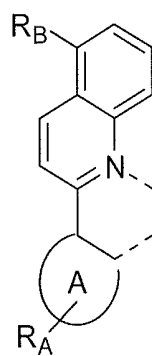


FIGURE 3

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5-SUBSTITUTED 2-PHENYLQUINOLINE COMPLEXES MATERIALS FOR LIGHT EMITTING DIODE

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

The present invention relates to organic light emitting devices (OLEDs). More specifically, the present invention is related to phosphorescent materials comprising a ligand having a 5-substituted 2-phenylquinoline. These materials may be used in OLEDs to provide devices having improved performance.

BACKGROUND

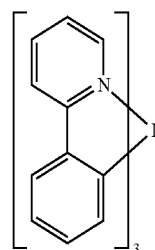
Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition,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

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

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

One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)₃, which has the structure:

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

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

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

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

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

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

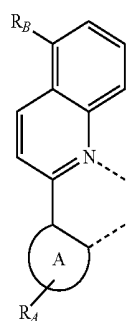
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As used herein, and as would be generally understood by one skilled in the art, a first work function is “greater than” or “higher than” a second work function if the first work function has a higher absolute value. Because work functions are generally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

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

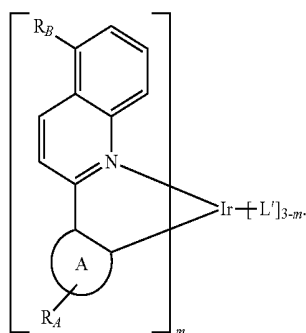
SUMMARY OF THE INVENTION

Compounds comprising a 5-substituted 2-phenylquinoline containing ligand are provided. The compounds comprise a ligand L having the formula:



A is a 5-membered or 6-membered carbocyclic or heterocyclic ring. Preferably, A is phenyl. R_A may represent mono, di, tri, or tetra substitutions. Each of R_A is independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. R_B is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. The ligand L is coordinated to a metal M having an atomic number greater than 40. Preferably, M is Ir.

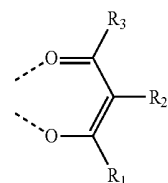
In one aspect, the compound has the formula:



L' is an ancillary ligand. m is 1, 2, or 3.

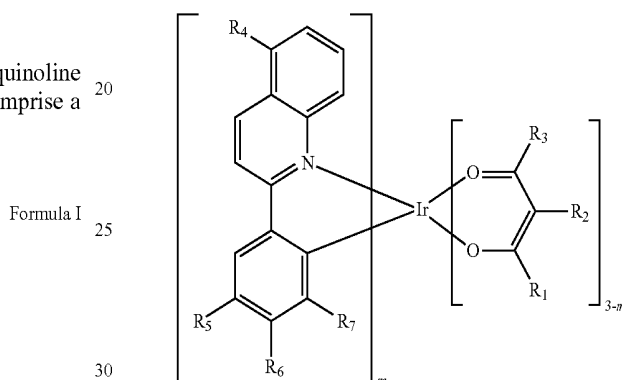
In another aspect, L' is a monoanionic bidentate ligand. In yet another aspect, L' is

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R_1 , R_2 , and R_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl.

In one aspect, the compound has the formula:



Formula III

R_1 , R_2 , R_3 , R_5 , R_6 and R_7 are independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. R_4 is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. m is 1, 2, or 3. Preferably, each of R_1 and R_3 are a branched alkyl with branching at a position further than the α position to the carbonyl group.

In one aspect, each of R_5 , R_6 and R_7 are independently selected from methyl and hydrogen, and at least one of R_5 , R_6 and R_7 is methyl. In another aspect, each of R_5 and R_7 are methyl, and R_6 is hydrogen. In yet another aspect, each of R_5 and R_6 are methyl, and R_7 is hydrogen. In a further aspect, each of R_5 , R_6 and R_7 are methyl.

In one aspect, R_4 is an alkyl group having at least 4 carbon atoms. In another aspect, R_4 is an alkyl group having at least 3 carbon atoms.

Specific, non-limiting examples of the 5-substituted 2-phenylquinoline containing compounds are provided. In one aspect, the compound is selected from the group consisting of Compound 1-Compound 50.

Additionally, a first device comprising an organic light emitting device is provided. The organic light emitting device further comprises an anode, a cathode; and an organic layer, disposed between the anode and the cathode. The organic layer comprises a compound comprising a ligand L having

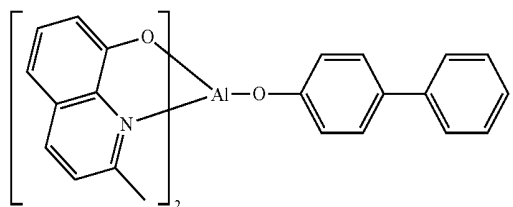
A is a 5-membered or 6-membered carbocyclic or heterocyclic ring. Preferably, A is phenyl. R_A may represent mono, di, tri, or tetra substitutions. Each of R_A is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. R_B is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. The

ligand L is coordinated to a metal M having an atomic number greater than 40. Preferably, M is Ir.

Specific, non-limiting examples of devices comprising the compounds are provided. In one aspect, the compound used in the first device is selected from the group consisting of Compound 1-Compound 50.

The various specific aspects discussed above for compounds comprising a ligand L having Formula I are also applicable to a compound comprising a ligand L having Formula I that is used in the first device. In particular, specific aspects of R_A , R_B , A, L', M, m, R_1 , R_2 , R_3 , R_4 , R_5 , R_6 , and R_7 of the compound comprising a ligand L having Formula I discussed above are also applicable to a compound comprising a ligand L having Formula I that is used in a first device.

In one aspect, the organic layer is an emissive layer and the compound is an emissive dopant. In another aspect, the organic layer further comprises a host. In yet another aspect, the host is a metal 8-hydroxyquinolate. Preferably, the host is:



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

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 shows an organic light emitting device.

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

FIG. 3 shows an exemplary compound comprising a 5-substituted 2-phenylquinoline ligand (top) and a preferred embodiment of the 5-substituted 2-phenylquinolone compound (bottom).

DETAILED DESCRIPTION

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

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

More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent

Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

FIG. 1 shows an organic light emitting device 100. The figures are not necessarily drawn to scale. Device 100 may include a substrate 110, an anode 115, a hole injection layer 120, a hole transport layer 125, an electron blocking layer 130, an emissive layer 135, a hole blocking layer 140, an electron transport layer 145, an electron injection layer 150, a protective layer 155, 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.

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.

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

The simple layered structure illustrated in FIGS. 1 and 2 is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various

layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device **200**, hole transport layer **225** transports holes and injects holes into emissive layer **220**, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.

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

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. 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.

Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of con-

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

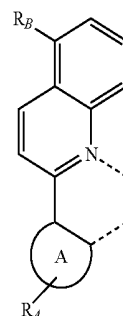
The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may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

The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, 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.

Novel organometallic 2-phenylquinoline Ir complexes are provided. In particular, the compounds comprise an alkyl having at least 2 carbon atoms. It is believed that compounds containing a bulky alkyl at the 5-position on the phenylquinoline is novel. In addition, it is believed that the presence of a bulky alkyl at the 5-position may increase efficiency by preventing self-quenching. Notably, placing the bulky alkyl at the 5-position on the 2-phenylquinoline does not shift the emission wavelength or change the color. Therefore, these compounds may provide improved efficiency and maintain saturated red emission. These compounds may be useful in organic light emitting devices, in particular as red emitters in the emissive layer of such devices.

Compounds comprising a 5-substituted 2-phenylquinoline containing ligand are provided. The compounds comprise a ligand L having the formula:

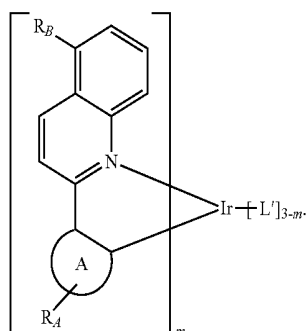
Formula I



A is a 5-membered or 6-membered carbocyclic or heterocyclic ring. Preferably, A is phenyl. R_A may represent mono, di, tri, or tetra substitutions. Each of R_A is independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. These compounds may be fully or partially deuterated. R_B is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. The ligand L is coordinated to a metal M having an atomic number greater than 40. Preferably, M is Ir.

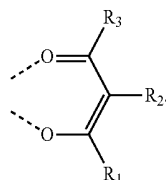
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In one aspect, the compound has the formula:



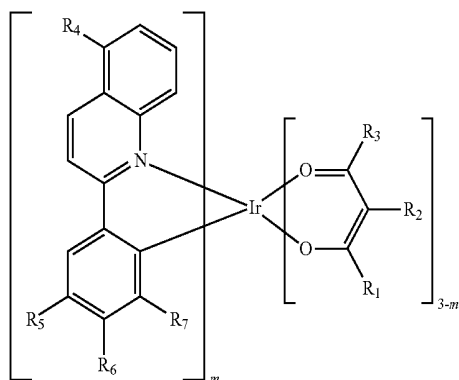
L' is an ancillary ligand. m is 1, 2, or 3.

In another aspect, L' is a monoanionic bidentate ligand. In yet another aspect, L' is



R₁, R₂, and R₃ are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl.

In one aspect, the compound has the formula:



R₁, R₂, R₃, R₅, R₆ and R₇ are independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. R₄ is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. m is 1, 2, or 3.

Preferably, each of R₁ and R₃ are a branched alkyl with branching at a position further than the α position to the carbonyl group. Without being bound by theory, it is believed that a branched alkyl substituent at R₁ and R₃ may provide high device efficiency and stability, and a very narrow emission spectrum.

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The placement of substituents on the compound having Formula III may improve efficiency while maintaining a desirable spectrum. In particular, it is believed that substitution on the position ortho to the R₅ next to quinoline with a substituent other than hydrogen, as shown in Formula III, may result in broadening the compound's spectrum. In addition, alkyl substitution on quinoline at the 3-position may broaden the emission spectrum. Alkyl substitution at the 4, 6, or 7-position may slightly blue shift the emission spectrum, thereby making the emission less saturated. Therefore, the substitution pattern of the 5-substituted 2-phenylquinoline compounds described herein may provide highly desirable compound and device characteristics.

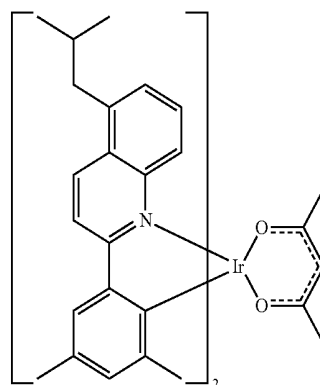
In one aspect, each of R₅, R₆ and R₇ are independently selected from methyl and hydrogen, and at least one of R₅, R₆ and R₇ is methyl. In another aspect, each of R₅ and R₇ are methyl, and R₆ is hydrogen. In yet another aspect, each of R₅ and R₆ are methyl, and R₇ is hydrogen. In a further aspect, each of R₅, R₆ and R₇ are methyl.

In one aspect, R₄ is an alkyl group having at least 4 carbon atoms. In another aspect, R₄ is an alkyl group having at least 3 carbon atoms.

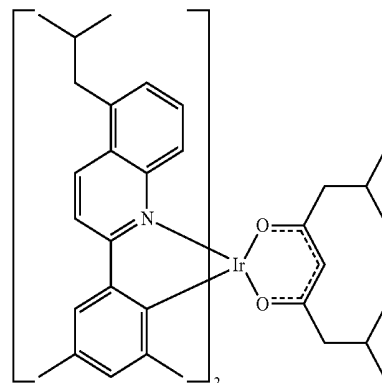
Alkyl substitutions may be particularly important because they offer a wide range of tunability in terms of evaporation temperature, solubility, energy levels, device efficiency and narrowness of the emission spectrum. Additionally, alkyl groups can be stable functional groups chemically and in device operation.

Specific, non-limiting examples of the 5-substituted 2-phenylquinoline containing compounds are provided. In one aspect, the compound is selected from the group consisting of:

Compound 1

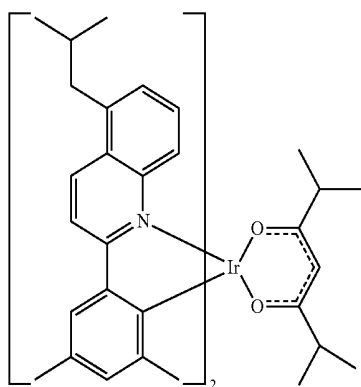


Compound 2



11

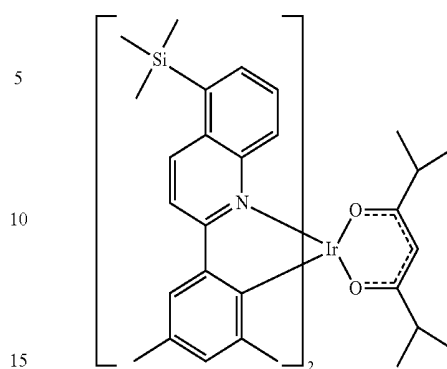
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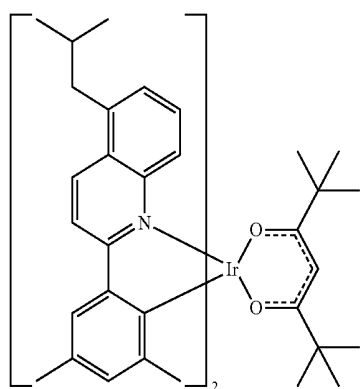
Compound 3

12

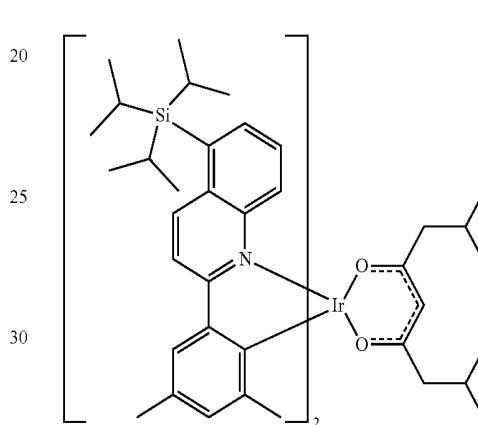
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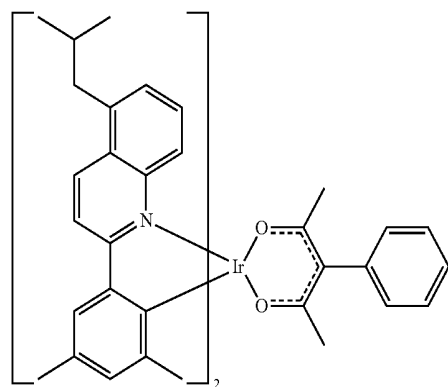
Compound 7



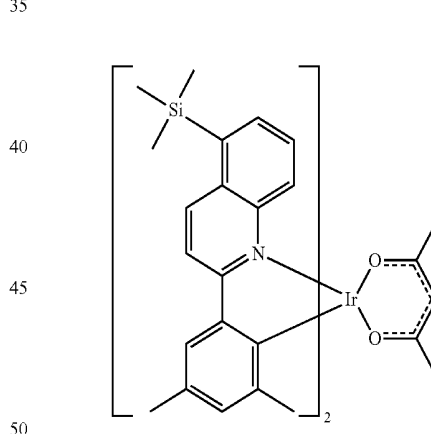
Compound 4



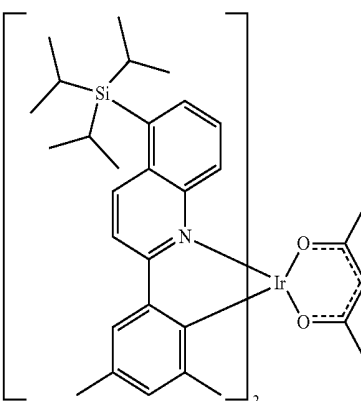
Compound 8



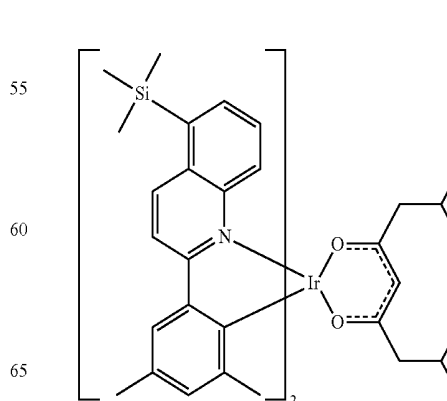
Compound 5



Compound 9



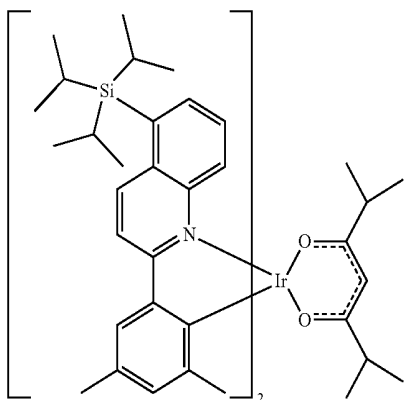
Compound 6



Compound 10

13

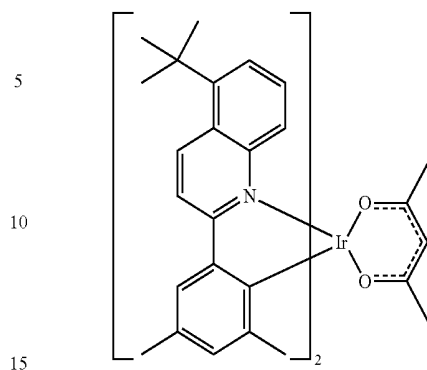
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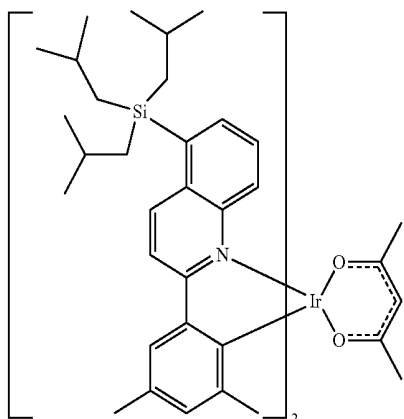
Compound 11

14

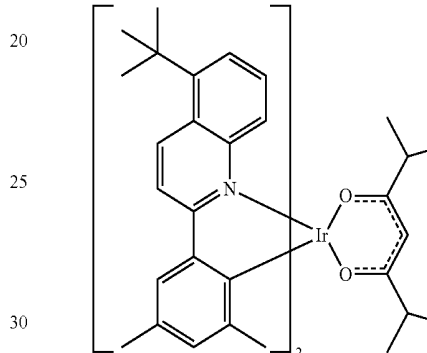
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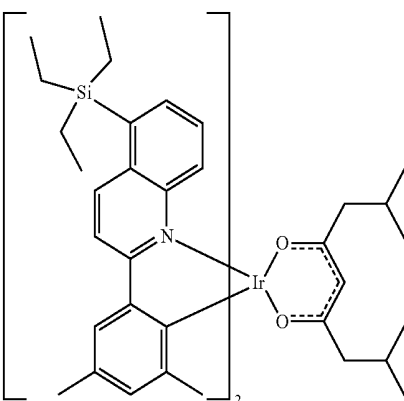
Compound 15



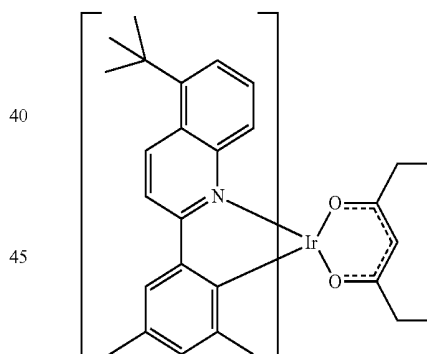
Compound 12



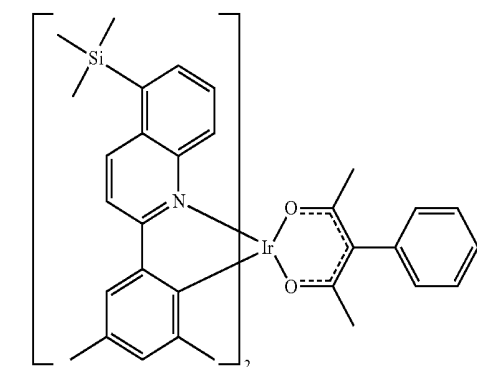
Compound 16



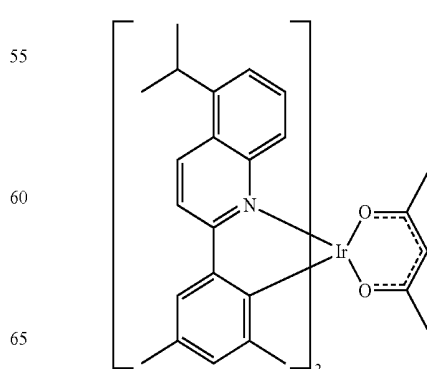
Compound 13



Compound 17



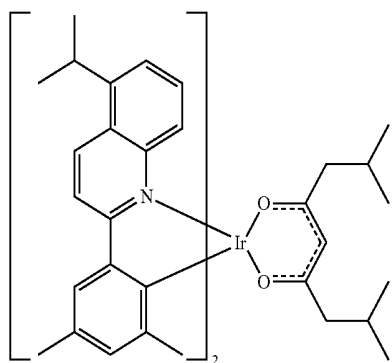
Compound 14



Compound 18

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-continued



Compound 19

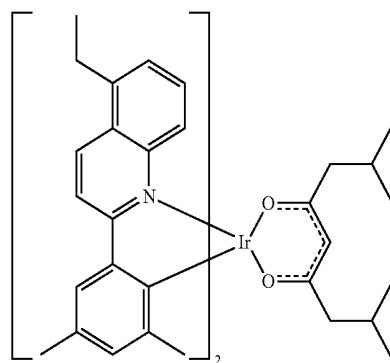
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16

-continued



Compound 23

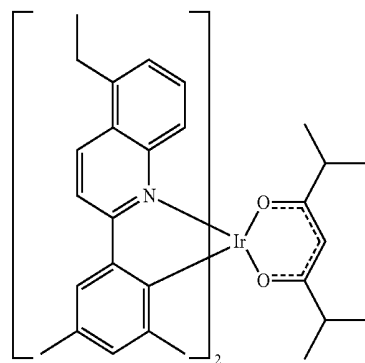
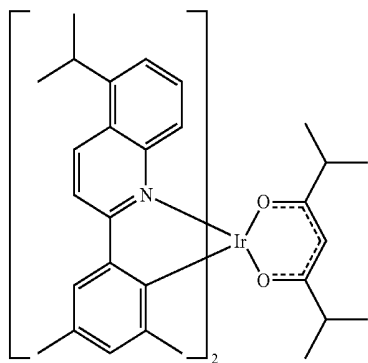
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Compound 20



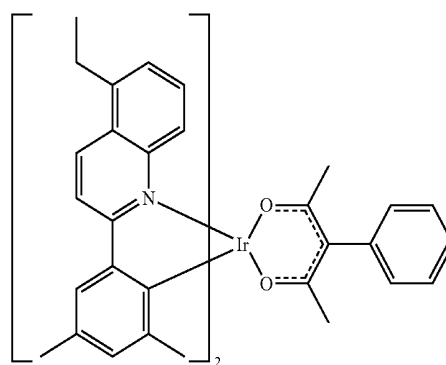
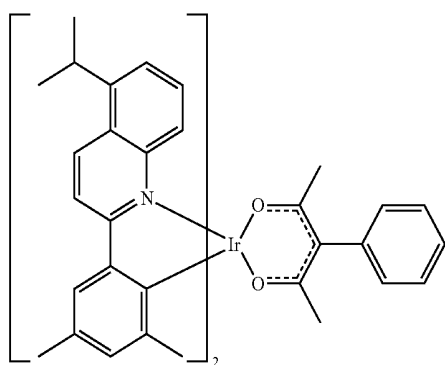
Compound 24

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Compound 21



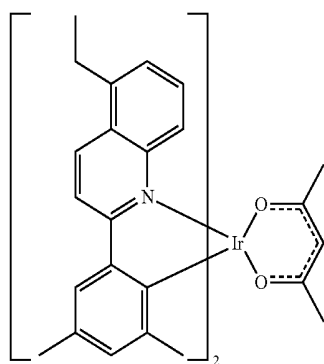
Compound 25

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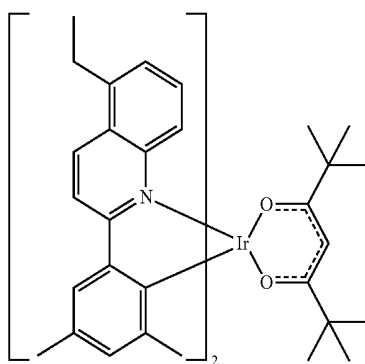
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Compound 22

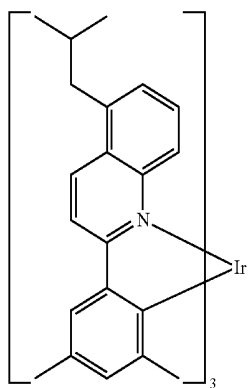


Compound 26



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-continued



Compound 27

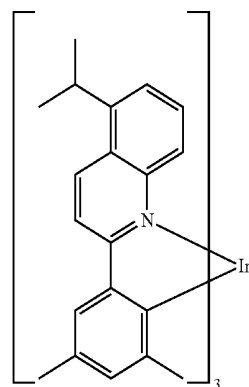
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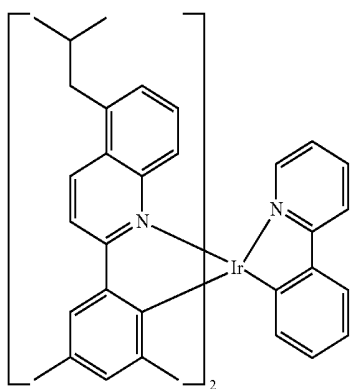
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Compound 31

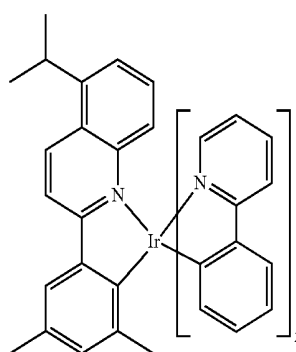


Compound 28

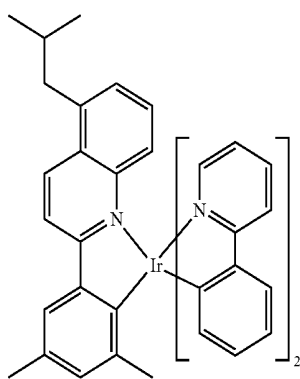
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Compound 32



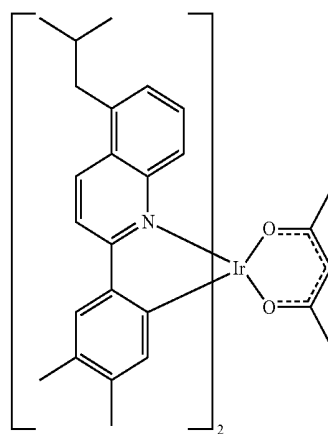
Compound 29

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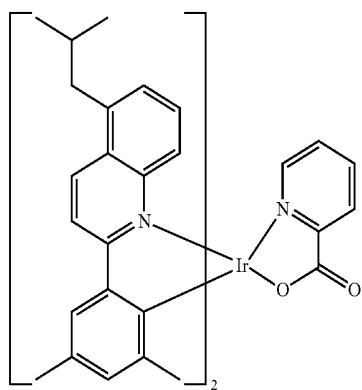
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Compound 33

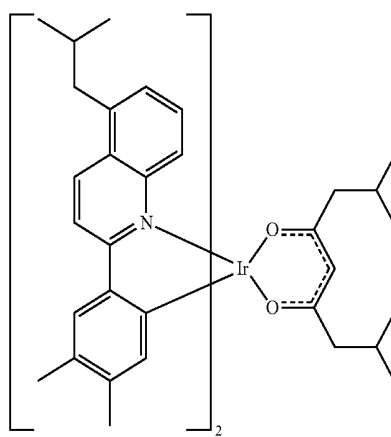


Compound 30

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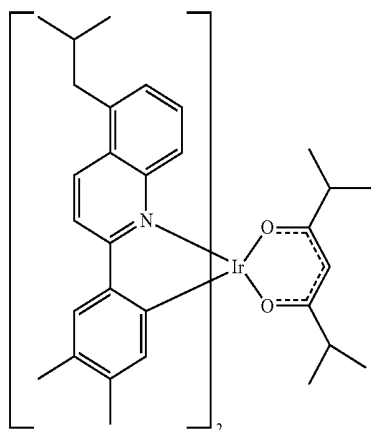
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Compound 34

19

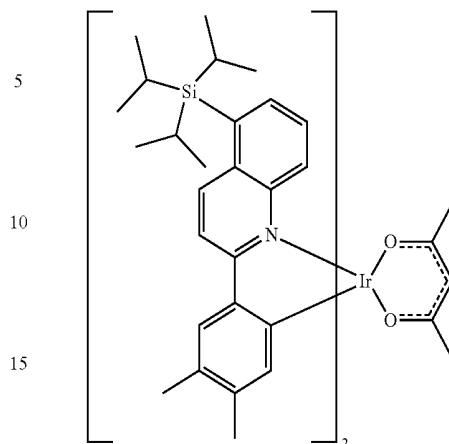
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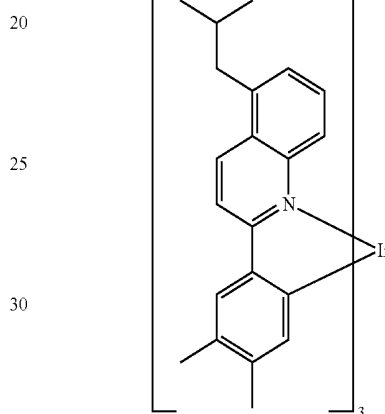
Compound 35

20

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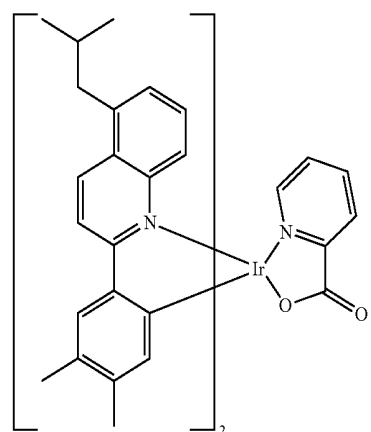


Compound 38

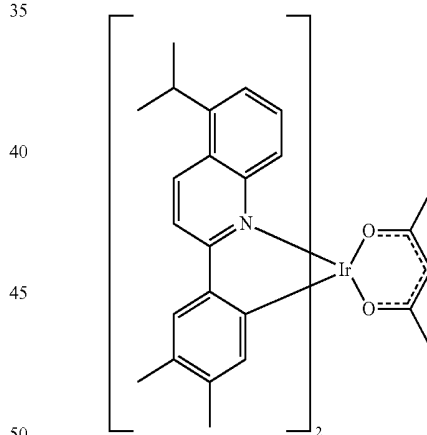
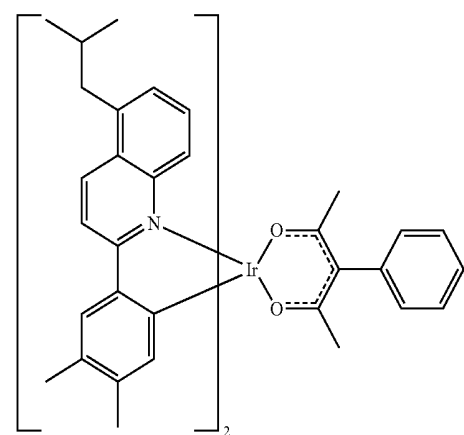


Compound 39

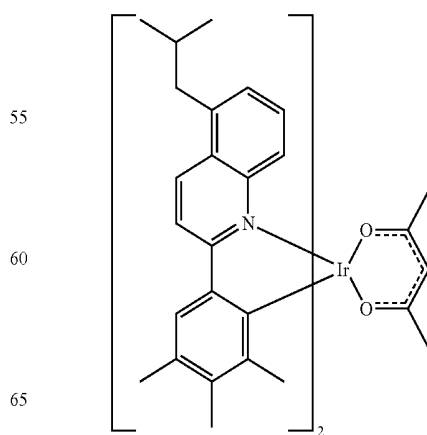
Compound 36



Compound 37



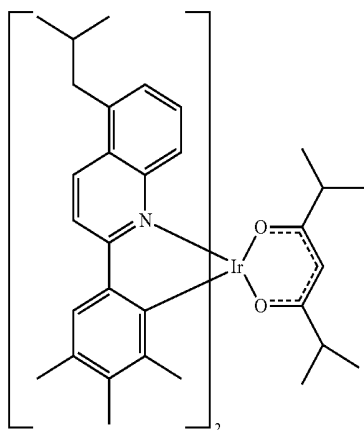
Compound 40



Compound 41

21

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Compound 42

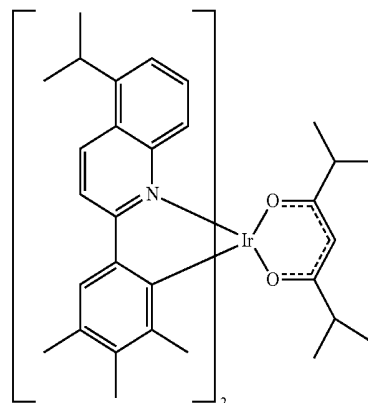
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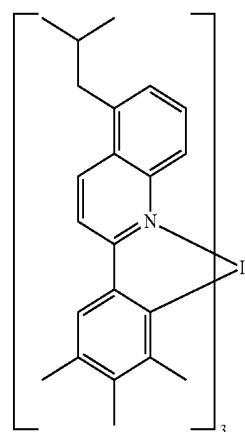
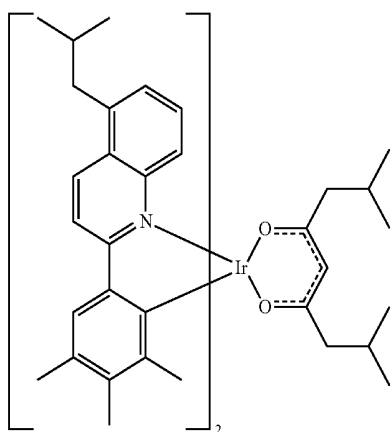
Compound 46

Compound 43

20

25

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Compound 47

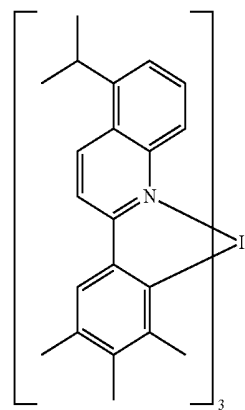
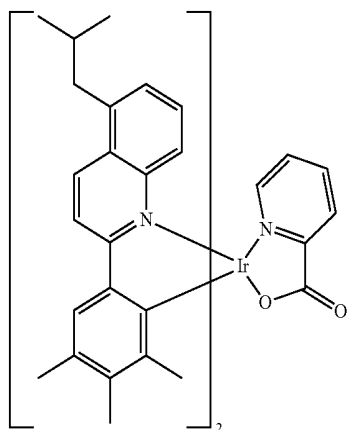
Compound 44

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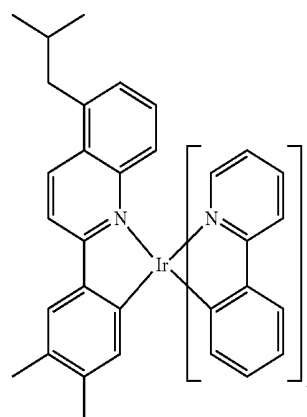
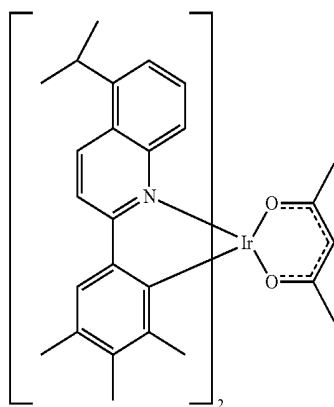
Compound 48

Compound 45

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60

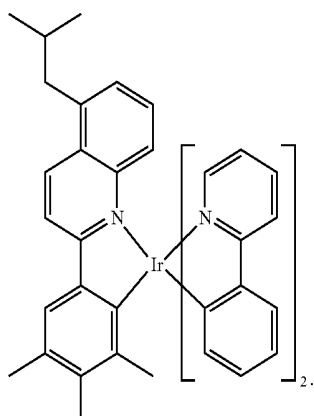
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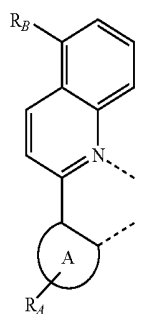
Compound 49

23

-continued

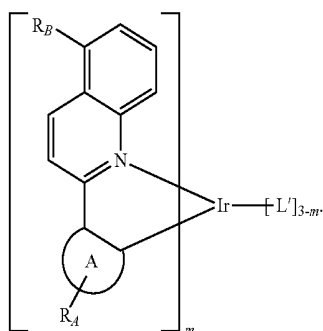


Additionally, a first device comprising an organic light emitting device is provided. The organic light emitting device further comprises an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer comprises a compound comprising a ligand L having the formula:



A is a 5-membered or 6-membered carbocyclic or heterocyclic ring. Preferably, A is phenyl. R_A may represent mono, di, tri, or tetra substitutions. Each of R_A is independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. R_B is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. The ligand L is coordinated to a metal M having an atomic number greater than 40. Preferably, M is Ir.

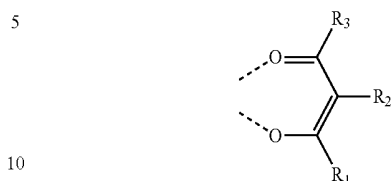
In one aspect, the compound has the formula:



L' is an ancillary ligand. m is 1, 2, or 3.

24

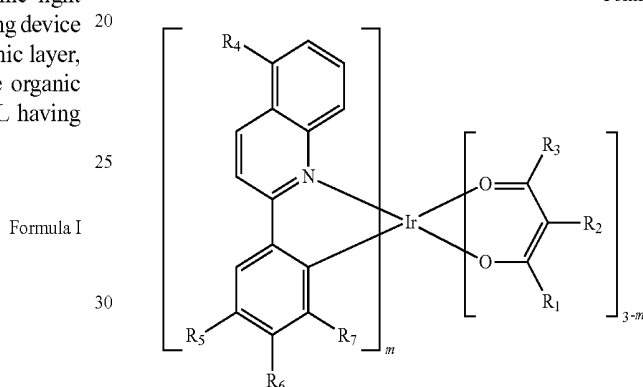
In one aspect, L' is a monoanionic bidentate ligand. In another aspect, L' is



R_1 , R_2 , and R_3 are independently selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl.

In one aspect, the compound has the formula:

Formula III



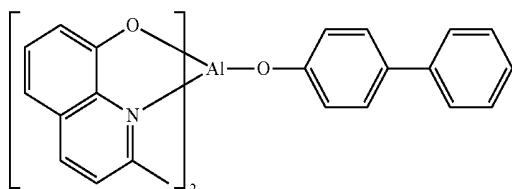
Formula I

R_1 , R_2 , R_3 , R_5 , R_6 and R_7 are independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl. R_4 is selected from the group consisting of alkyl having at least 2 carbon atoms, amino, alkenyl, alkynyl, arylkyl, and silyl. m is 1, 2, or 3.

Specific, non-limiting examples of devices comprising the compounds are provided. In one aspect, the first device comprises a compound selected from the group consisting of Compound 1-Compound 50.

In one aspect, the organic layer is an emissive layer and the compound is an emissive dopant. In another aspect, the organic layer further comprises a host. In yet another aspect, the host is a metal 8-hydroxyquinolate. Preferably, the host is:

Formula II



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

Combination with Other Materials

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

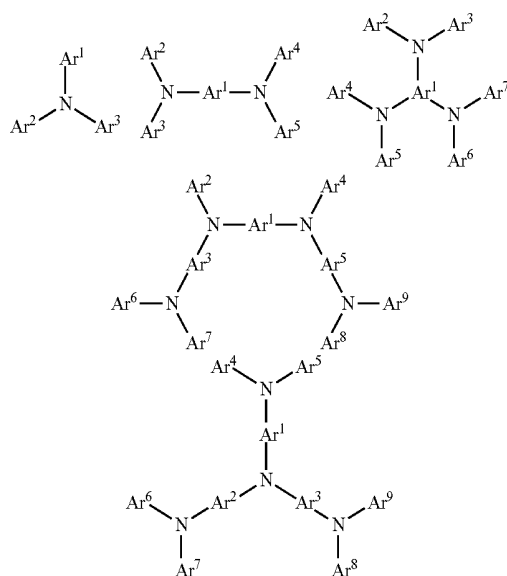
25

may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

HIL/HTL:

A hole injecting/transporting material to be used in embodiments of 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 are not limited to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as MoO_3 ; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

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

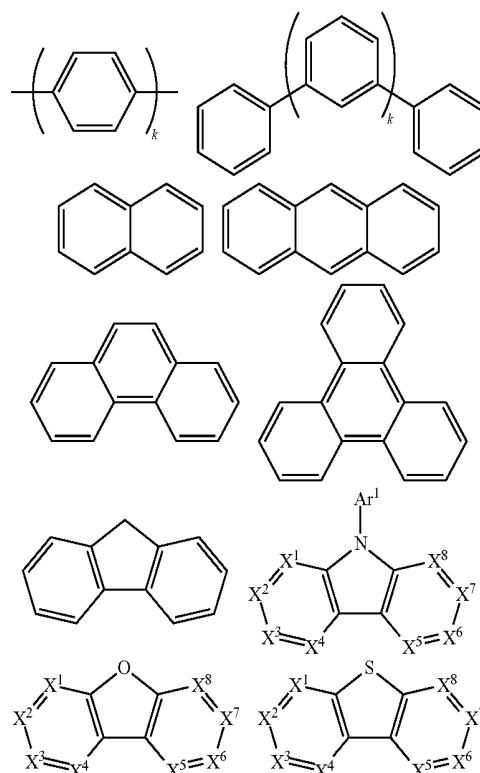


Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, benzoselenophene, 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, benzofuro-
pyridine, furodipyridine, benzothienopyridine, thienodipyri-

26

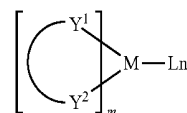
dine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at 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, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

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



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

Examples of metal complexes used in the HIL or HTL include, but are not limited to, the following general formula:



M is a metal, having an atomic weight greater than 40; ($\text{Y}^1\text{-Y}^2$) 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.

In one aspect, ($\text{Y}^1\text{-Y}^2$) is a 2-phenylpyridine derivative.

In another aspect, ($\text{Y}^1\text{-Y}^2$) is a carbene ligand.

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

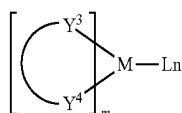
In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

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Host:

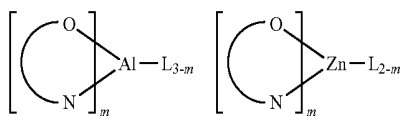
The light emitting layer of the organic EL device in some embodiments the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited,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

Examples of metal complexes used as hosts are preferred to have the following general formula:



M is a metal; (Y³-Y⁴) is a bidentate ligand, Y³ and Y⁴ 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.

In one aspect, the metal complexes are:



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

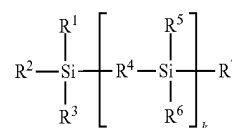
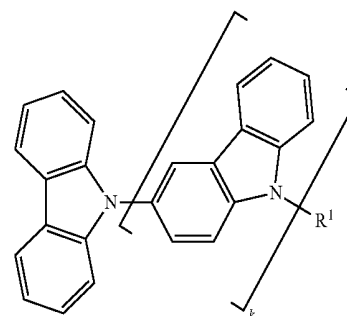
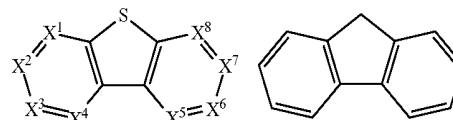
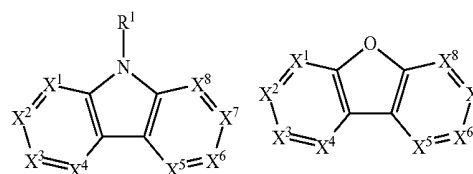
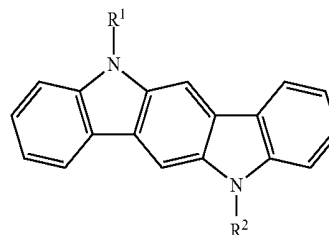
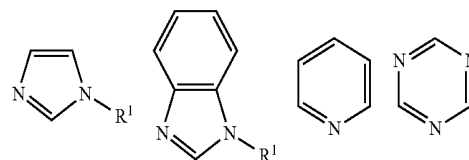
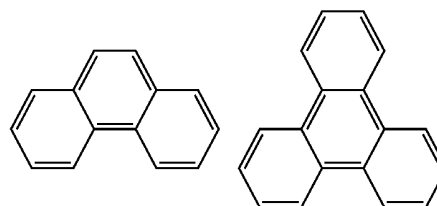
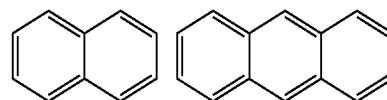
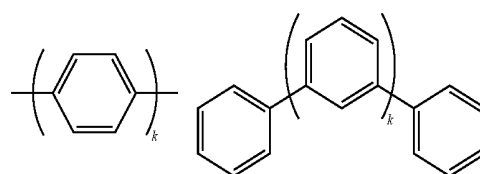
In another aspect, M is selected from Ir and Pt.

In a further aspect, (Y³-Y⁴) is a carbene ligand.

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

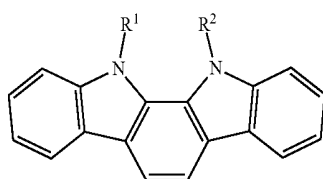
28

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



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-continued



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

k is an integer from 0 to 20.

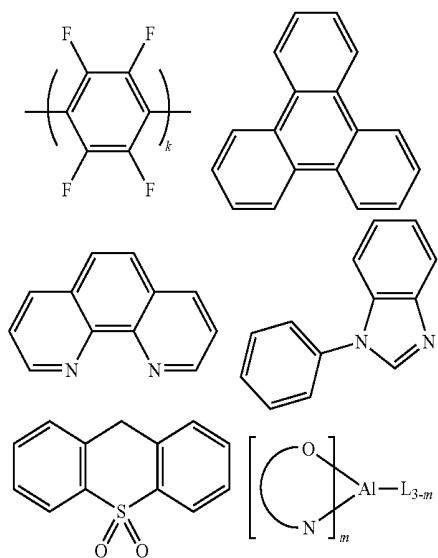
X^1 to X^8 is selected from CH or N.

HBL:

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

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

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



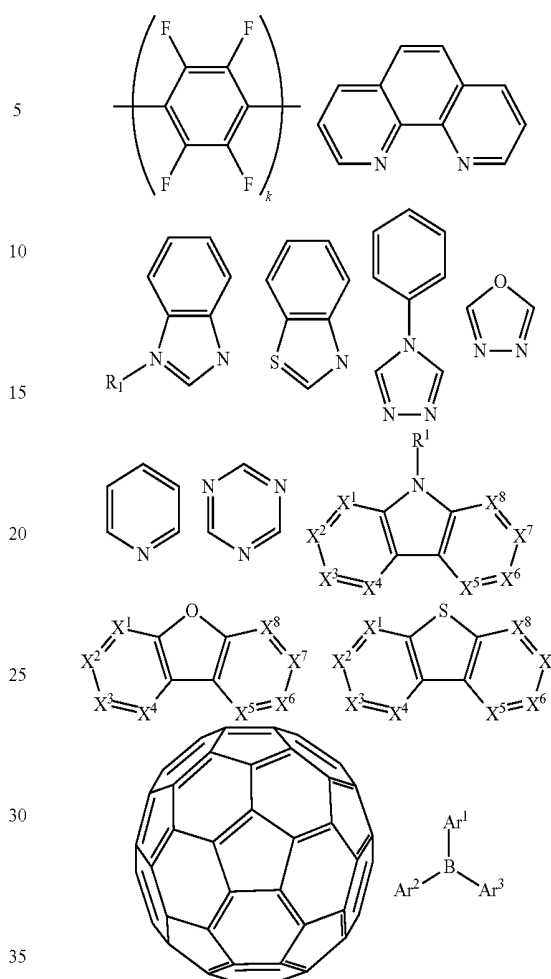
k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

ETL:

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

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

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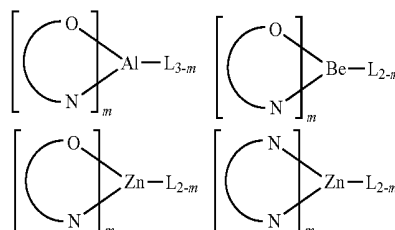
R^1 is selected from the group consisting of hydrogen, deuterium, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

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

k is an integer from 0 to 20.

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

In another aspect, the metal complexes used in the ETL contain, but are not limited to, the following general formula:



(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.

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

In addition to and/or in combination with the materials disclosed herein, many hole injection materials, hole trans-

porting materials, host materials, dopant materials, exciton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an

OLED in combination with materials disclosed herein are listed in Table 1 below. Table 1 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 1

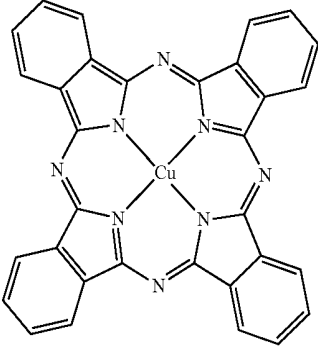
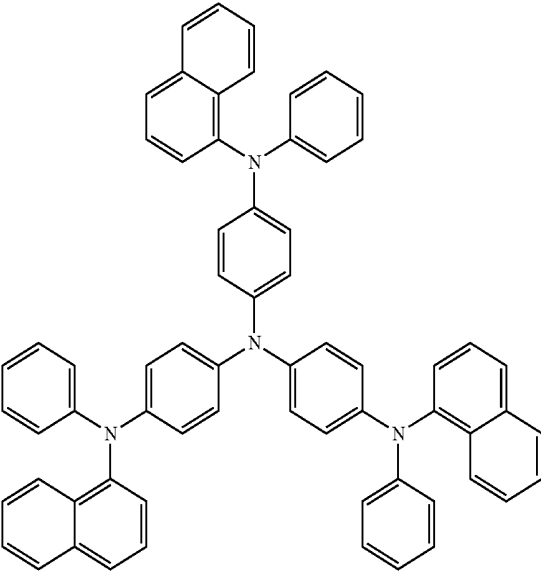
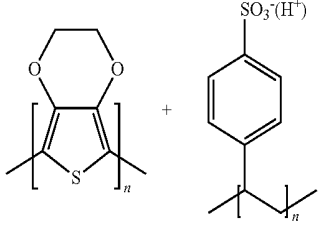
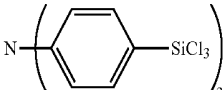
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Phthalocyanine and porphyrin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylaminates		J. Lumin. 72-74, 985 (1997)
CF _x Fluorohydrocarbon polymer	$\text{---}[\text{CH}_x\text{F}_y]_n\text{---}$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and silane SAMs		US20030162053

TABLE 1-continued

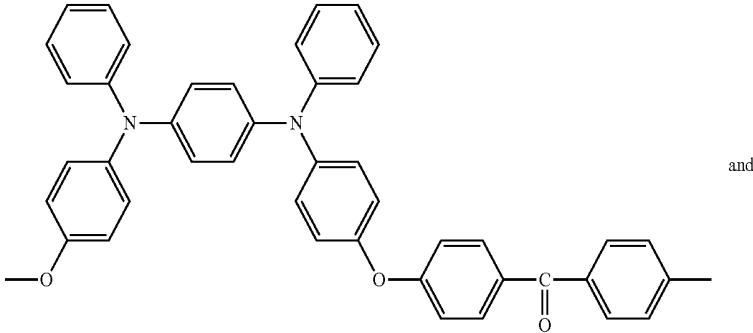
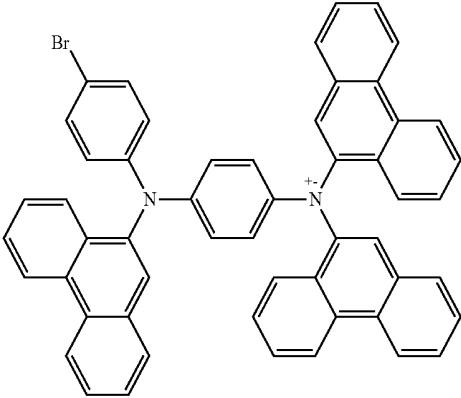
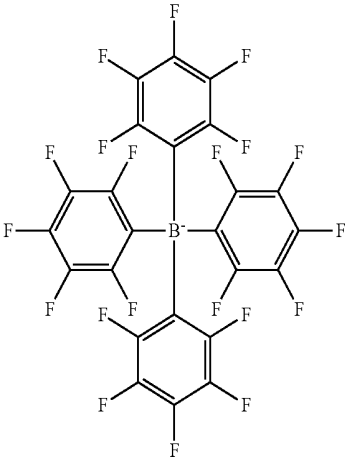
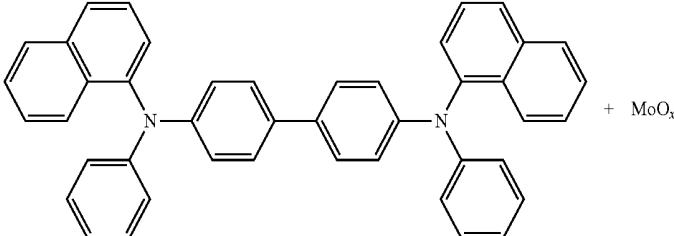
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine or polythiophene polymers with conductivity dopants		EA01725079A1
	and	
		
		
Arylamines complexed with metal oxides such as molybdenum and tungsten oxides		SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 1-continued

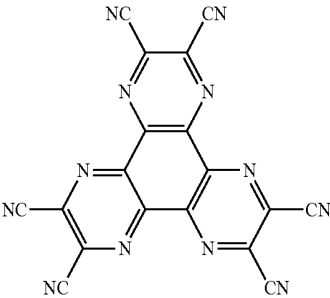
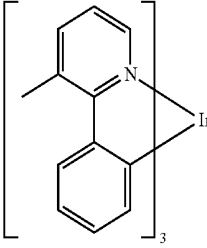
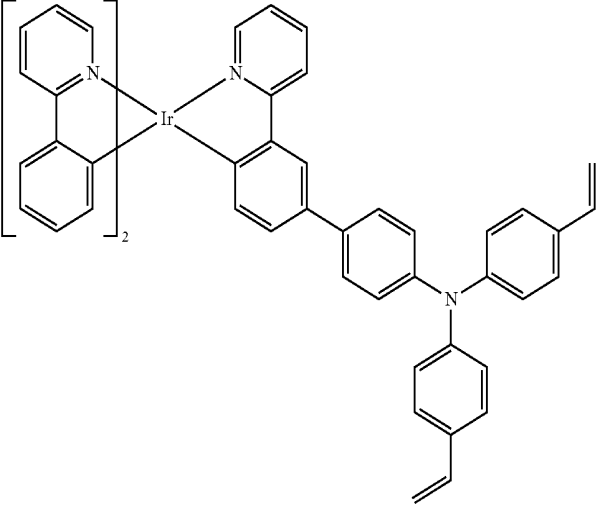
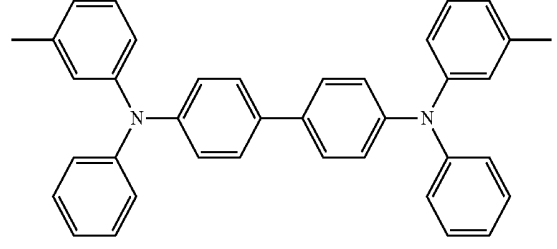
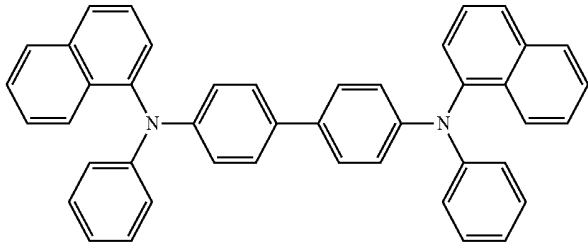
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Hole transporting materials		
Triarylamines (e.g., TPD, α -NPD)		Appl. Phys. Lett. 51, 913 (1987)
		US5061569

TABLE 1-continued

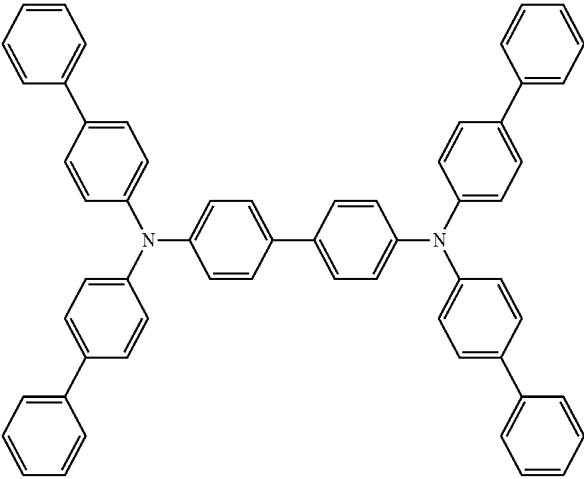
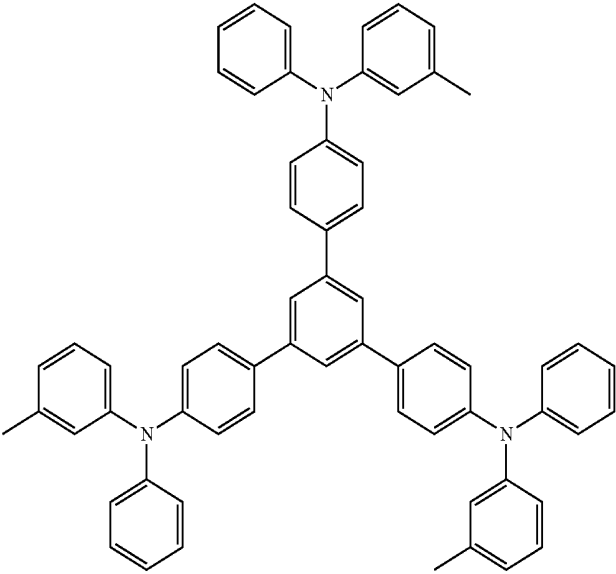
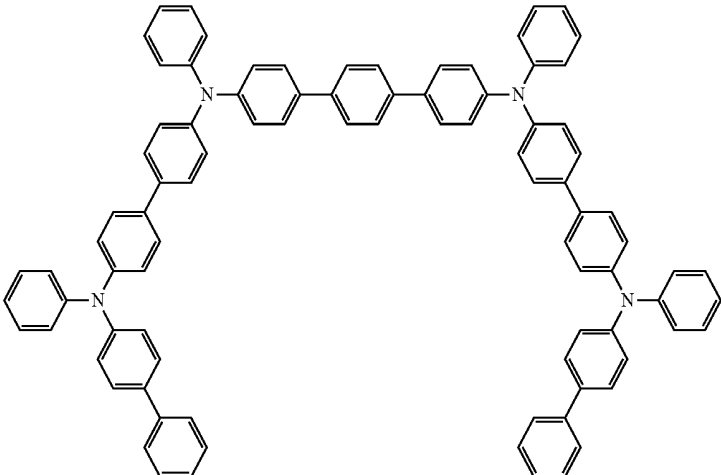
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		J. Mater. Chem., 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE 1-continued

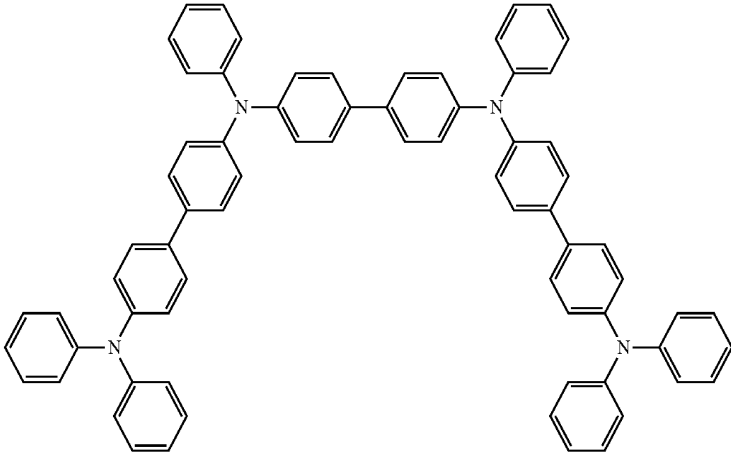
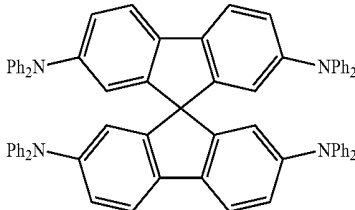
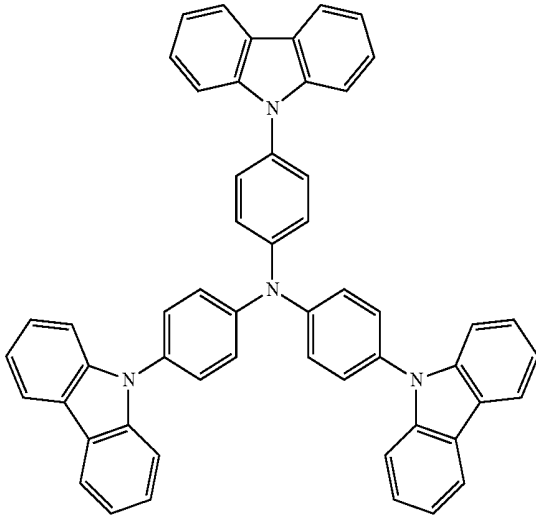
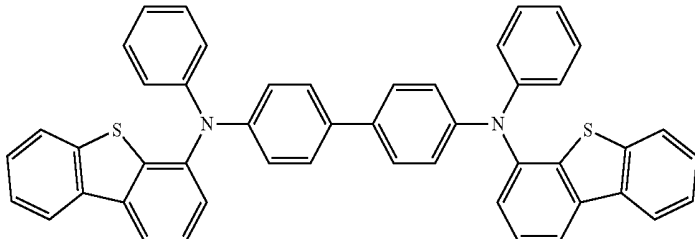
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
Triarylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190

TABLE 1-continued

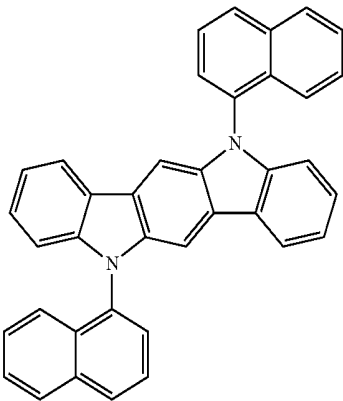
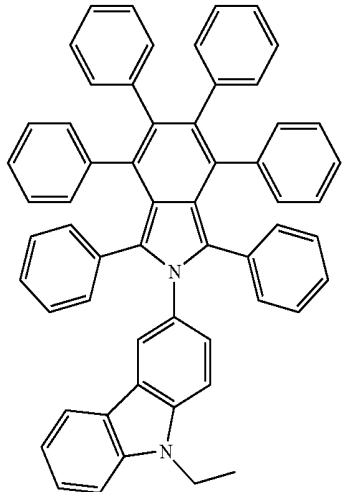
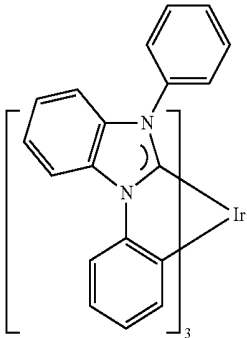
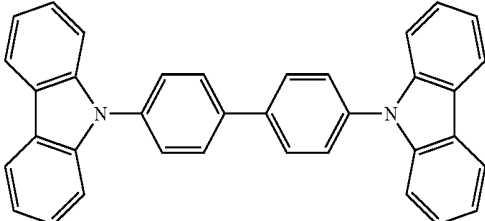
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

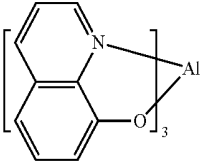
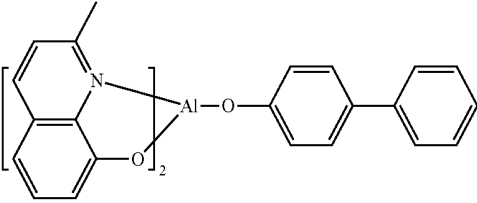
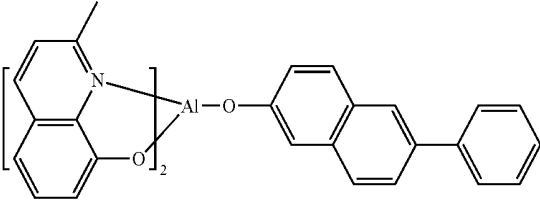
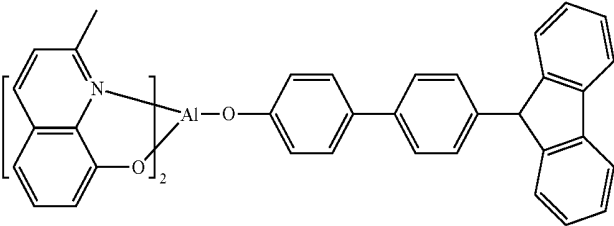
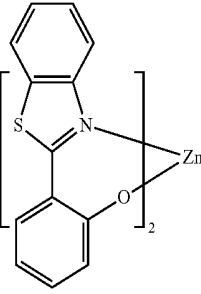
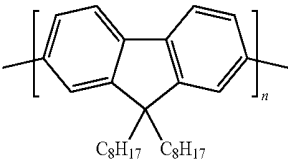
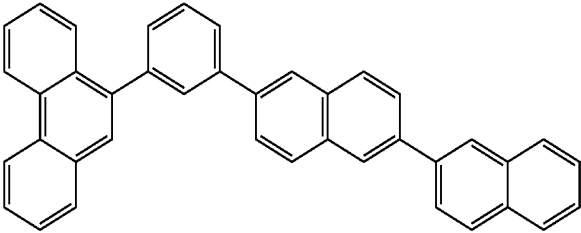
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal 8-hydroxyquinolates (e.g., Alq ₃ , BA1q)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065

TABLE 1-continued

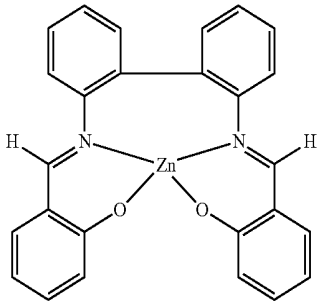
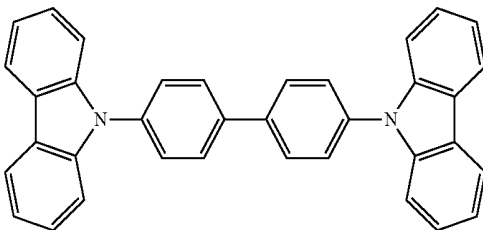
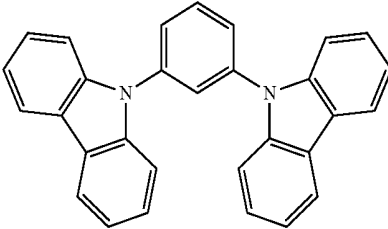
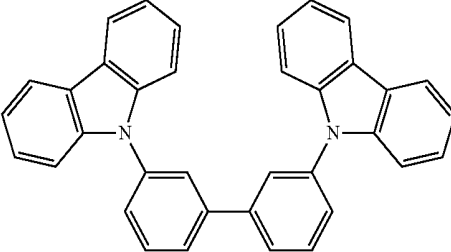
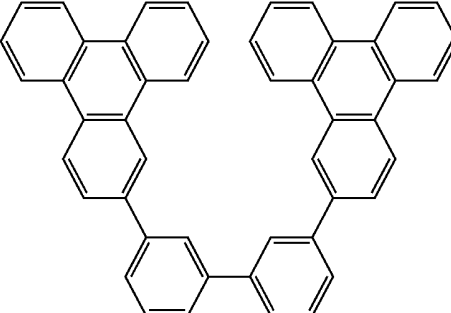
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Zinc complexes		WO2009062578
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Arylcarbazoles		US20030175553
Arylcarbazoles		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE 1-continued

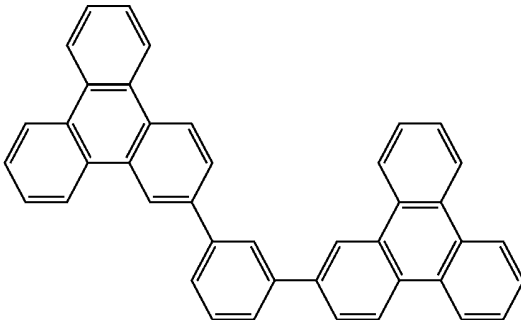
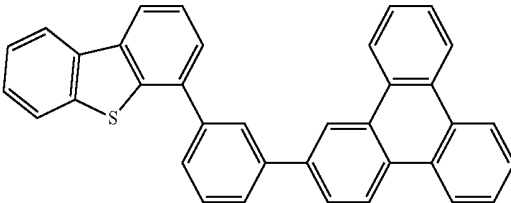
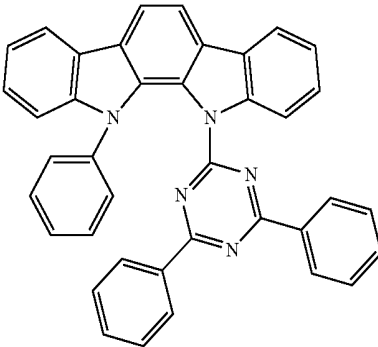
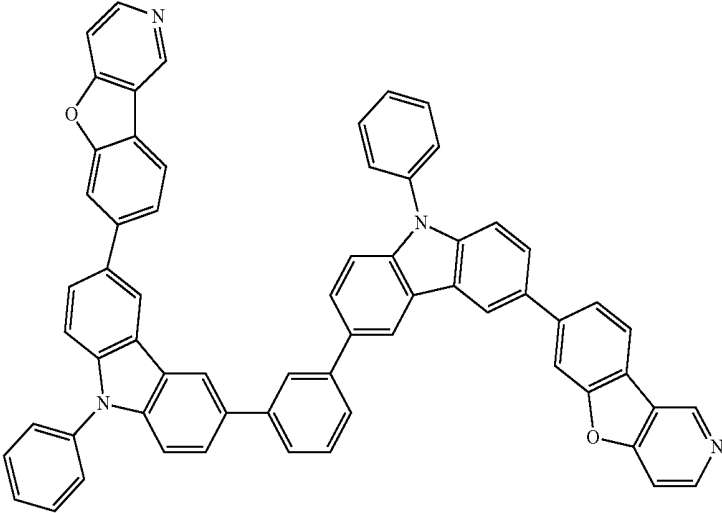
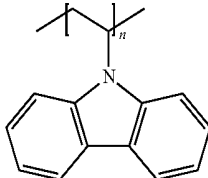
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Donor acceptor type molecules		US20060280965
		WO2009021126
		WO2008056746
Aza-carbazole/ DBT/DBF		JP2008074939
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)

TABLE 1-continued

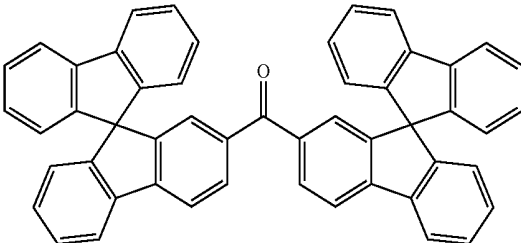
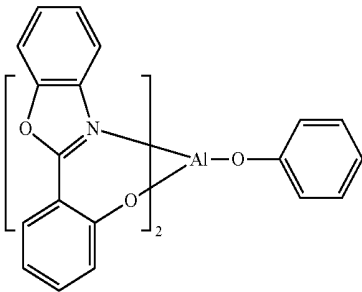
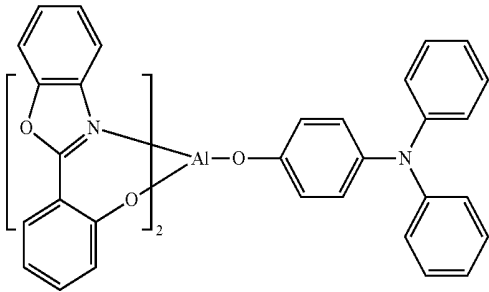
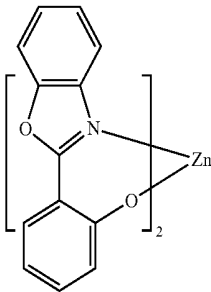
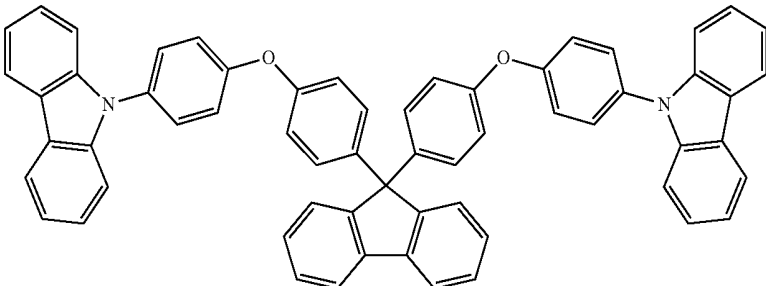
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Spirofluorene compounds		WO2004093207
Metal phenoxy-benzoxazole compounds		WO2005089025
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		JP200511610
Spirofluorene-carbazole compounds		JP2007254297

TABLE 1-continued

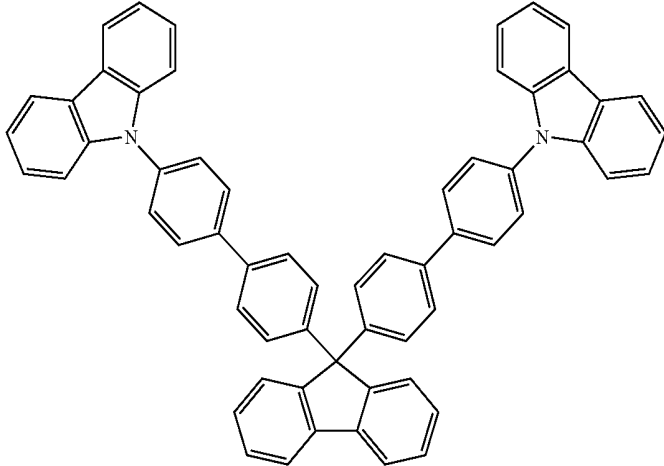
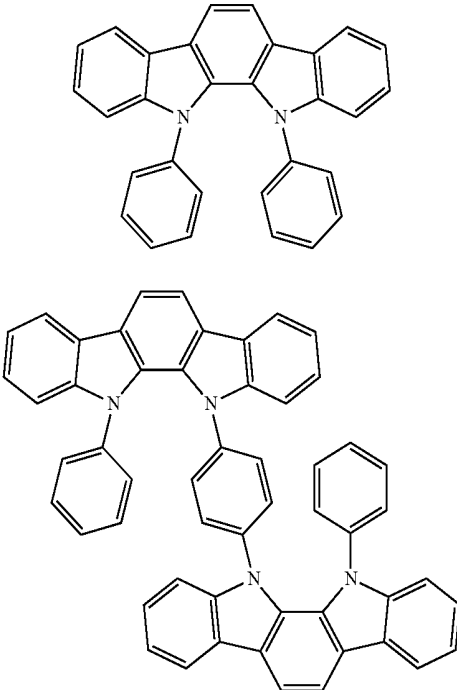
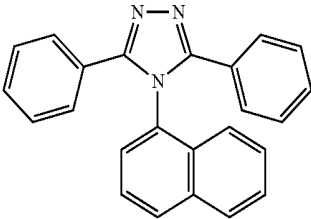
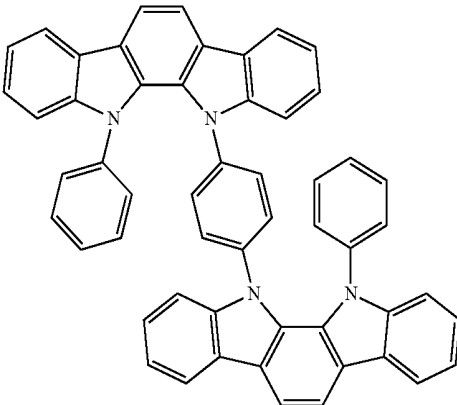
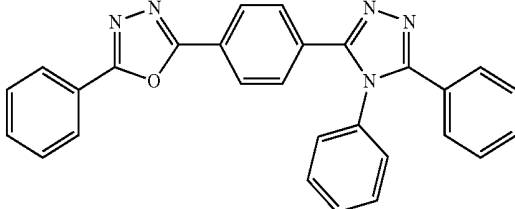
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocabazoles		JP2007254297
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)	 	WO2007063796
		WO2007063754
		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822

TABLE 1-continued

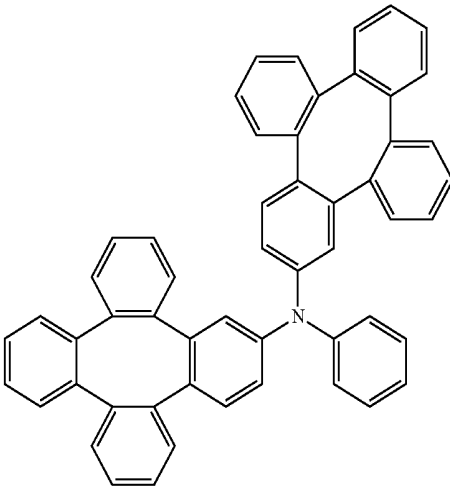
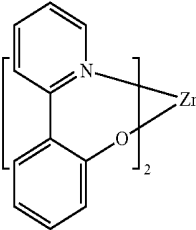
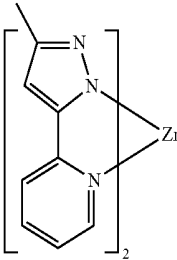
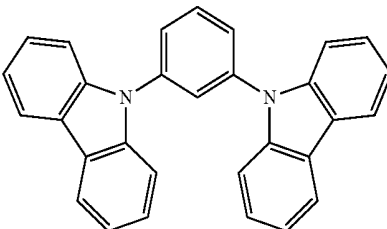
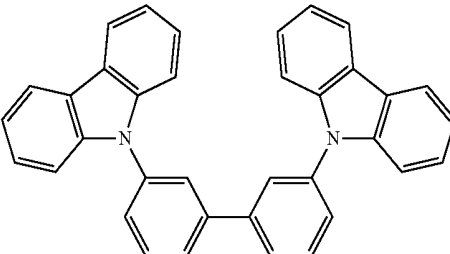
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		US20050112407
Metal phenoxy-pyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N-N ligands)		US20040137268, US20040137267
Blue hosts		
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359

TABLE 1-continued

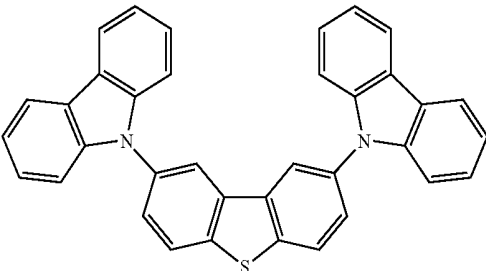
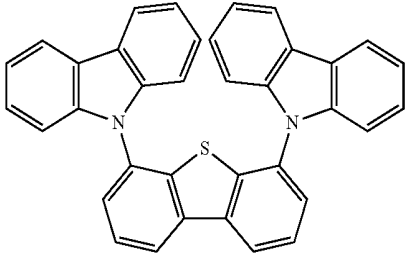
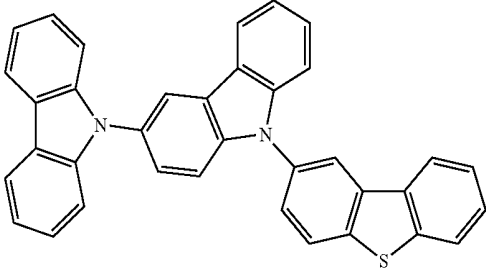
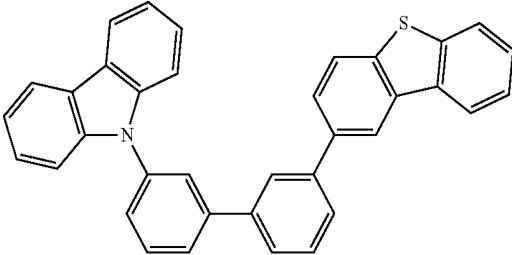
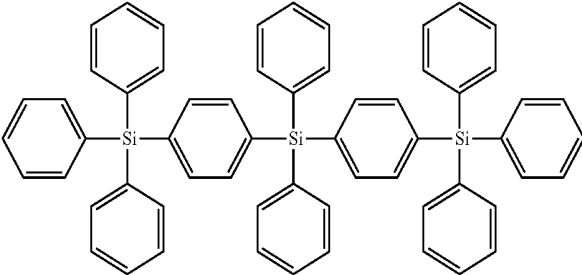
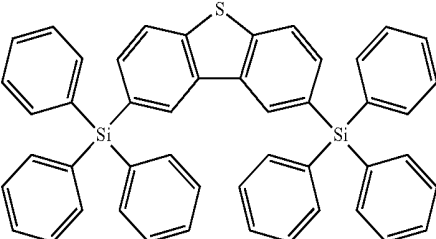
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzothiophene/ Dibenzofuran- carbazole compounds		WO2006114966, US20090167162
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Silicon aryl compounds		US20050238919
		WO2009003898

TABLE 1-continued

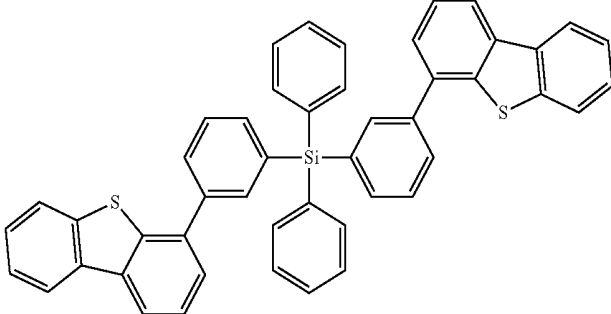
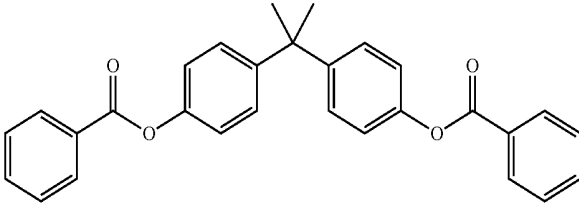
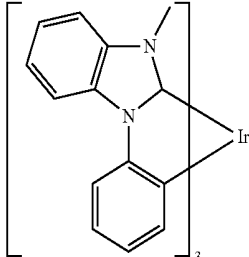
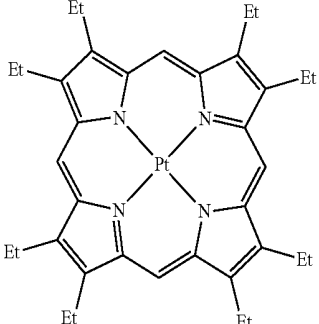
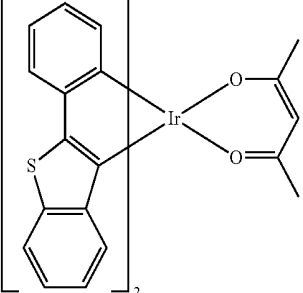
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex		US7154114
	Phosphorescent dopants Red dopants	
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium (III) organometallic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

TABLE 1-continued

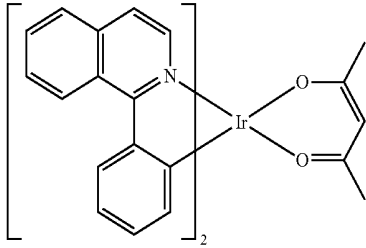
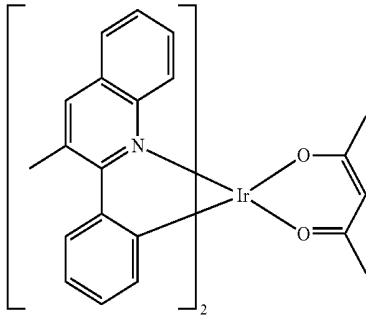
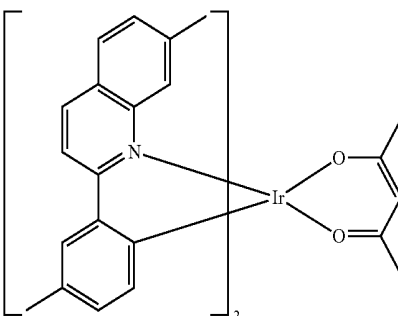
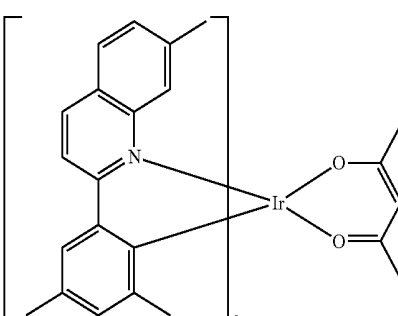
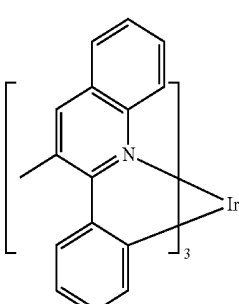
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		US20070087321

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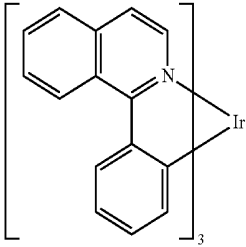
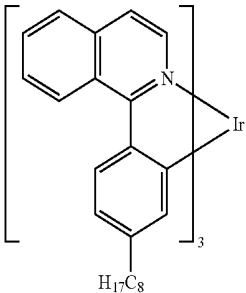
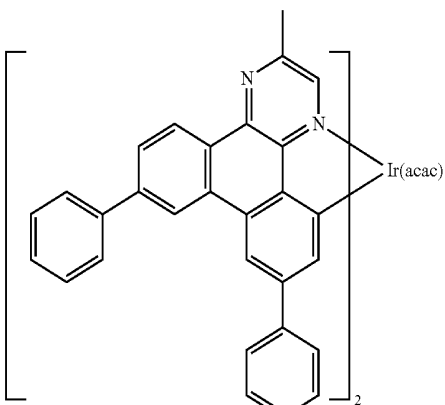
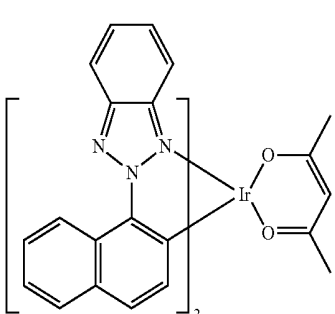
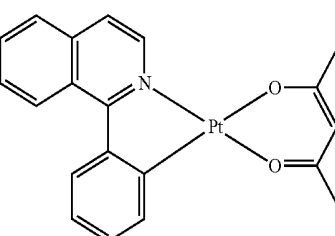
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842
Platinum (II) organometallic complexes		WO2003040257

TABLE 1-continued

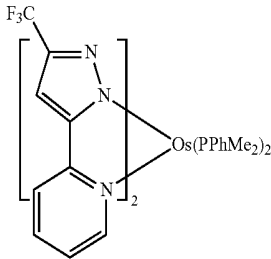
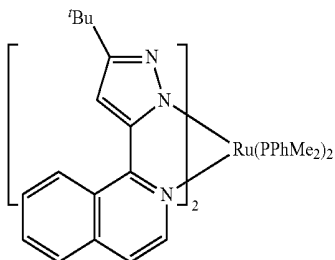
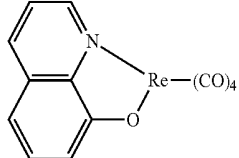
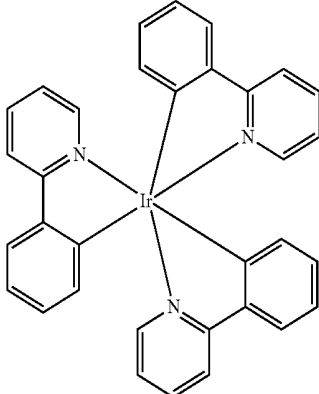
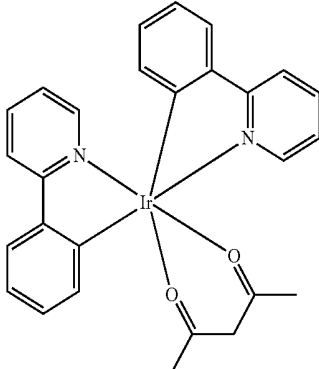
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium (III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium (II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
Green dopants		
Iridium (III) organometallic complexes	 <p>and its derivatives</p> 	Inorg. Chem.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

TABLE 1-continued

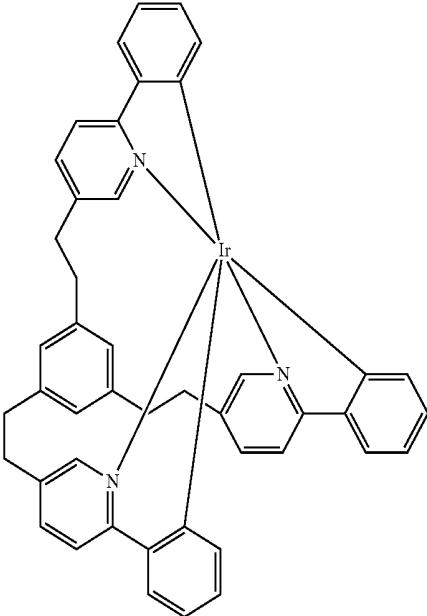
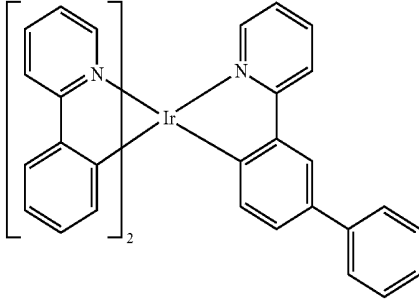
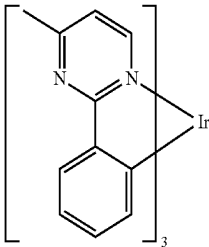
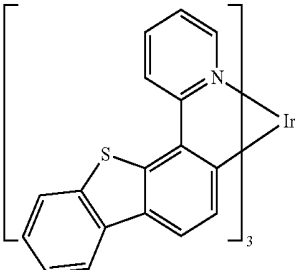
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		US20090108737
		US20090039776
		US6921915

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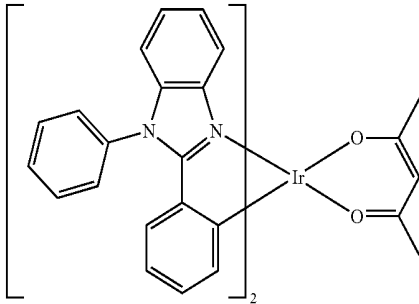
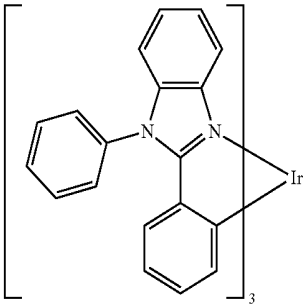
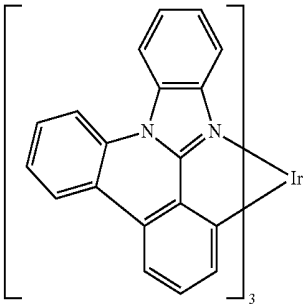
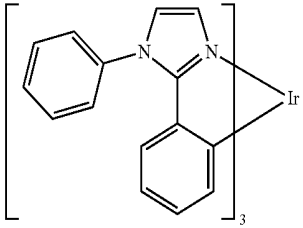
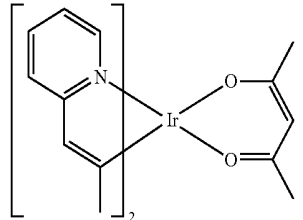
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US6687266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US 20060008670 JP2007123392
		Adv. Mater. 16, 2003 (2004)

TABLE 1-continued

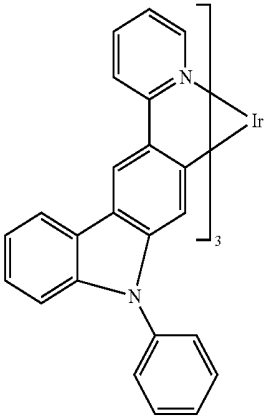
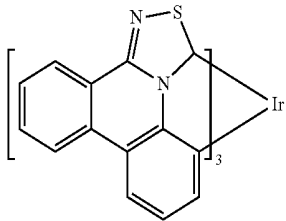
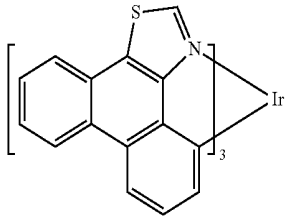
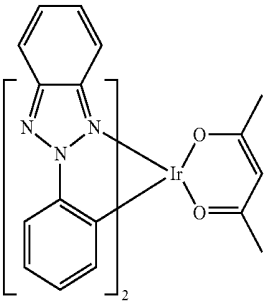
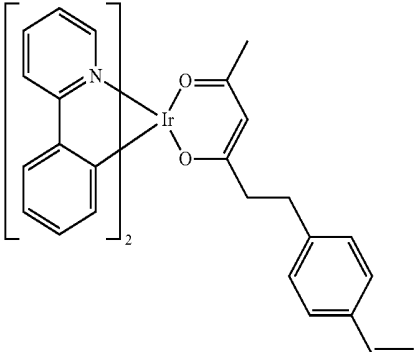
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846
		US20080015355
Monomer for polymeric metal organometallic compounds		US7250226, US7396598

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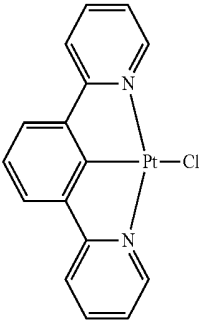
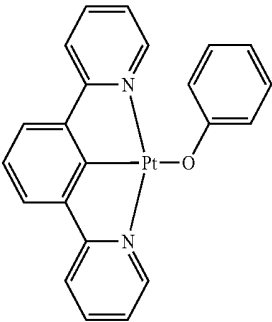
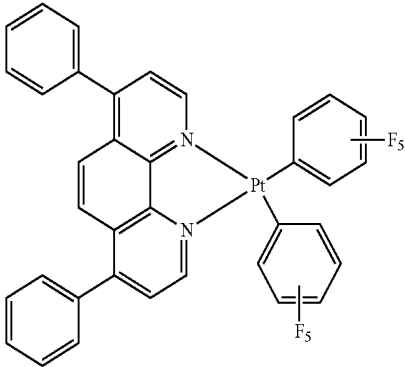
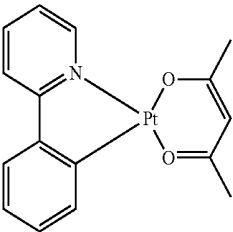
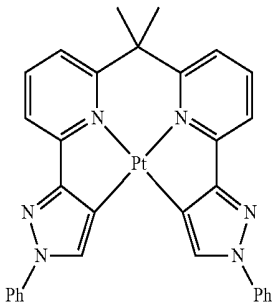
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Pt (II) organometallic complexes, including polydentate ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635

TABLE 1-continued

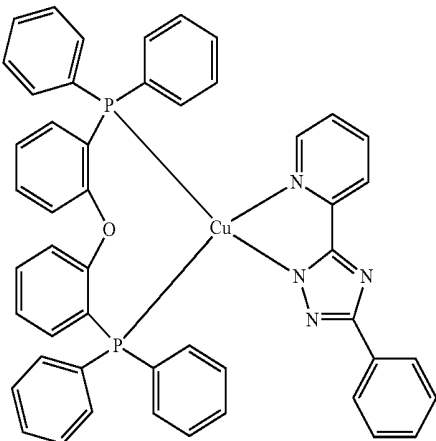
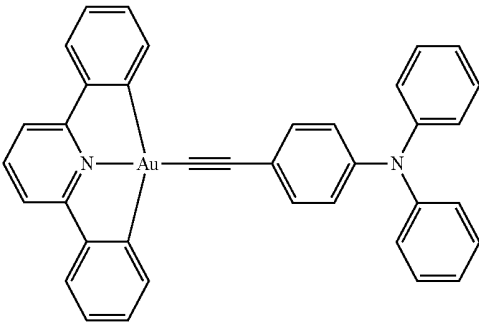
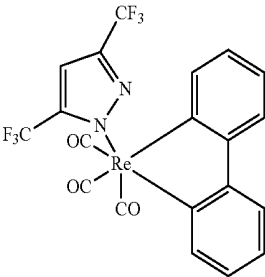
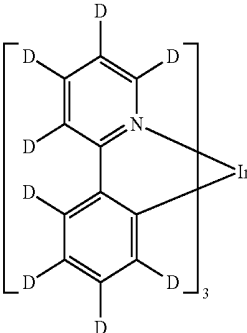
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium (III) complexes		Inorg. Chem. 42, 1248 (2003)
Deuterated organometallic complexes		US20030138657

TABLE 1-continued

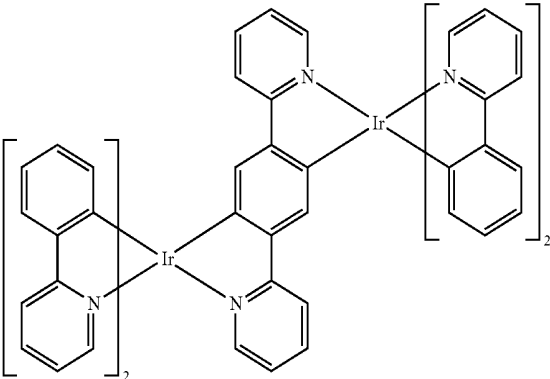
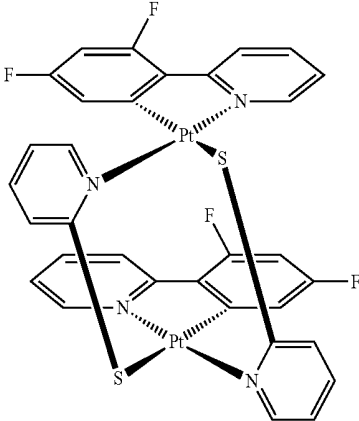
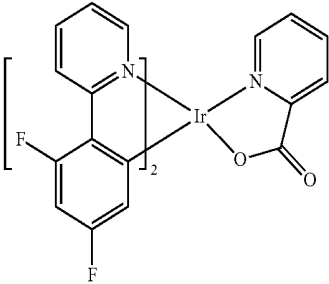
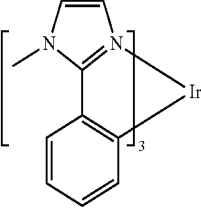
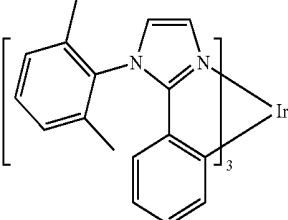
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Organometallic complexes with two or more metal centers		US20030152802
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	Blue dopants	
Iridium (III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923

TABLE 1-continued

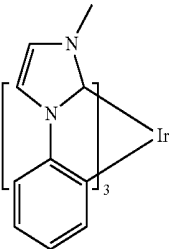
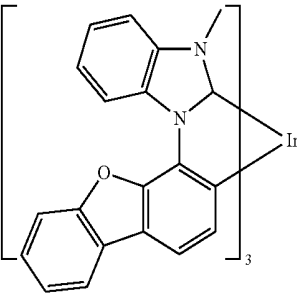
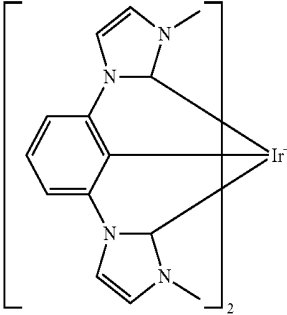
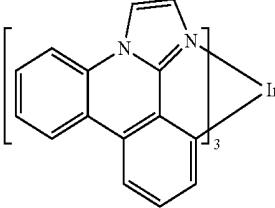
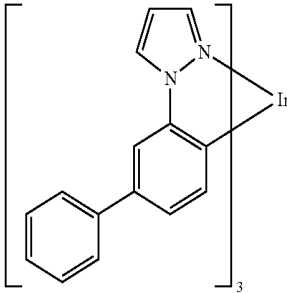
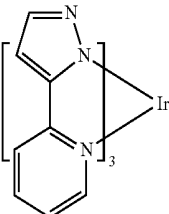
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		US20070190359, US20080297033
		US7338722
		US20020134984

TABLE 1-continued

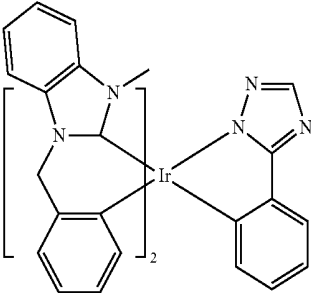
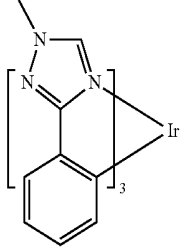
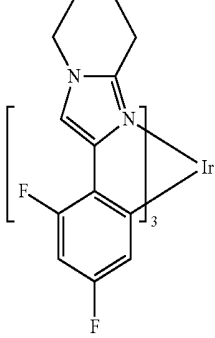
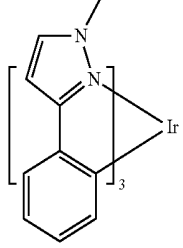
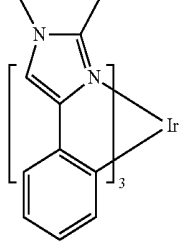
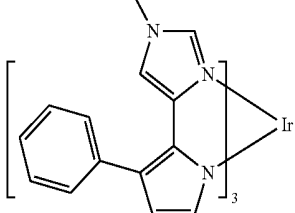
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		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380

TABLE 1-continued

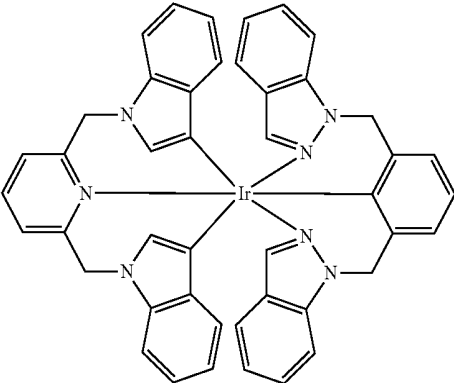
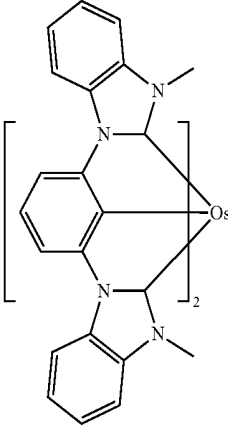
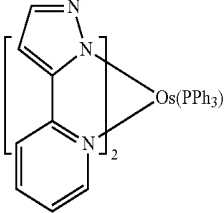
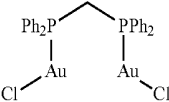
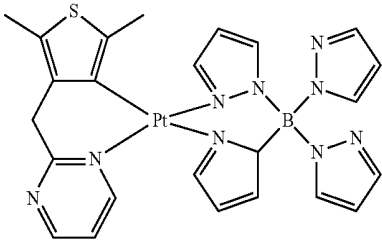
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium (II) complexes		WO2006082742
		US7279704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum (II) complexes		WO2006098120, WO2006103874
Exciton/hole blocking layer materials		

TABLE 1-continued

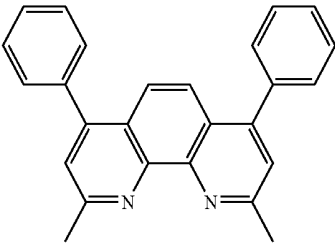
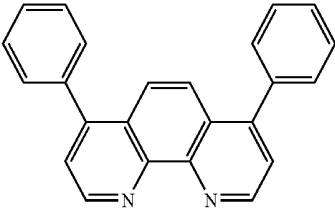
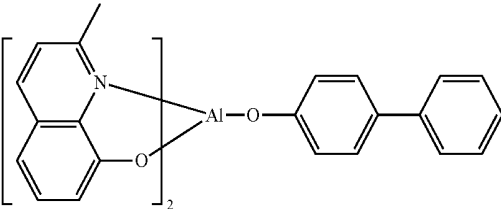
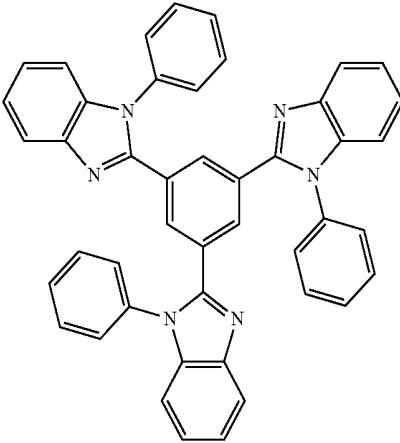
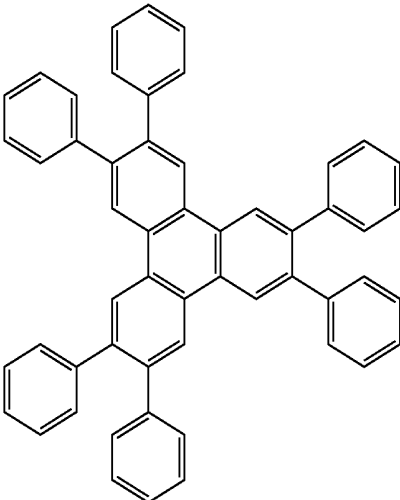
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Bathocuprine compounds (e.g., BCP BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993

TABLE 1-continued

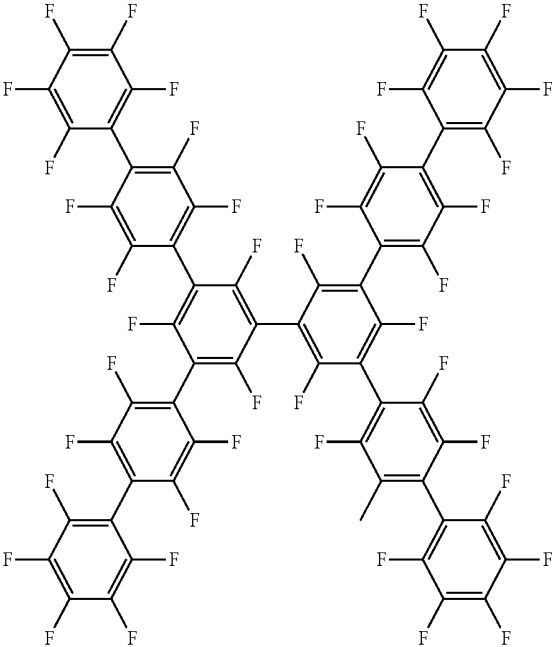
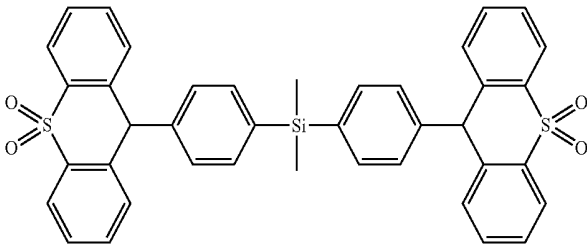
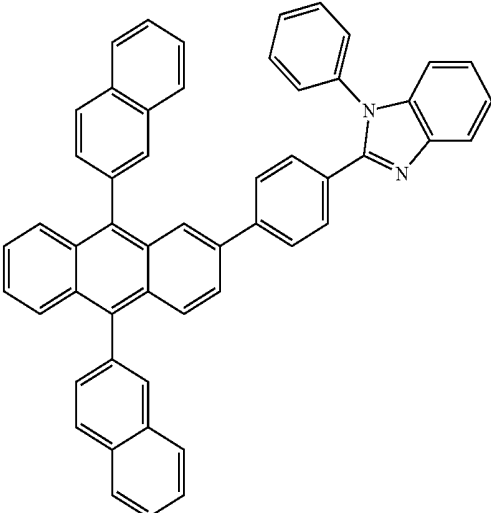
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085
Electron transporting materials		
Anthracene-benzimidazole compounds		WO2003060956

TABLE 1-continued

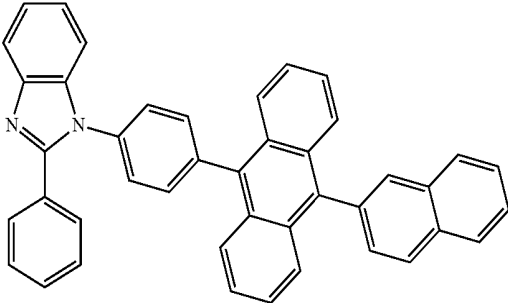
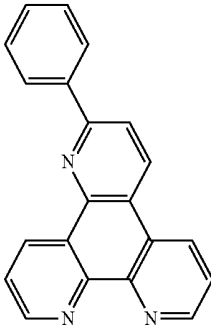
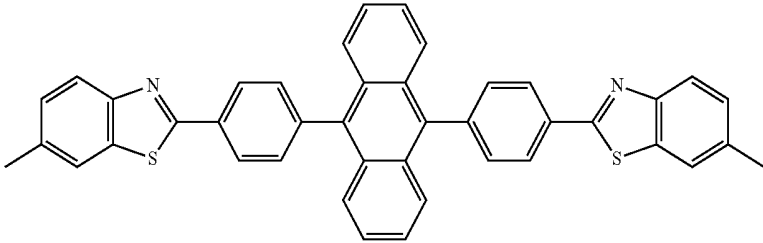
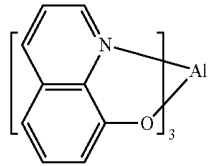
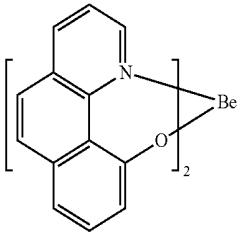
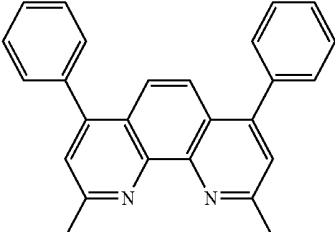
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza triphenylene derivatives		US20090179554
Anthracene-benzothiazole compounds		US20090115316
Metal 8-hydroxyquinolates (e.g., Alq ₃ , Zr _q ₄)		Appl. Phys. Lett. 89, 063504 (2006)
Metal hydroxybenoquinolates		Appl. Phys. Lett. 51, 913 (1987) US7230107
Bathocuprine compounds such as BCP, BPhen, etc		Chem. Lett. 5, 905 (1993)
		Appl. Phys. Lett. 91, 263503 (2007)

TABLE 1-continued

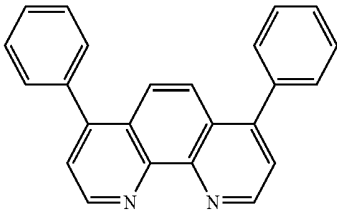
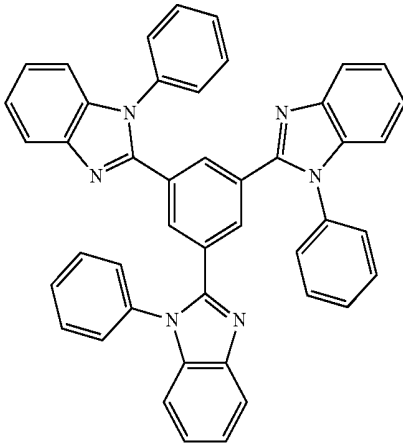
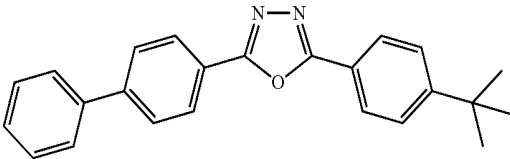
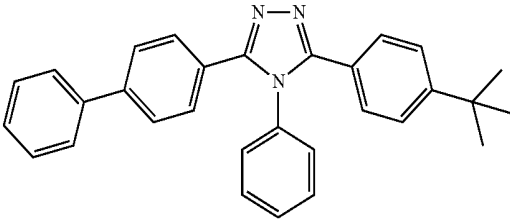
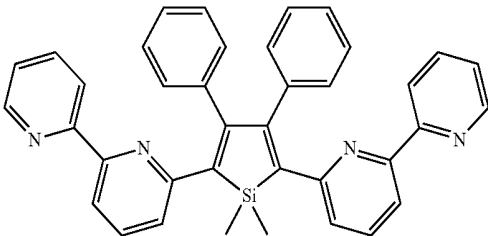
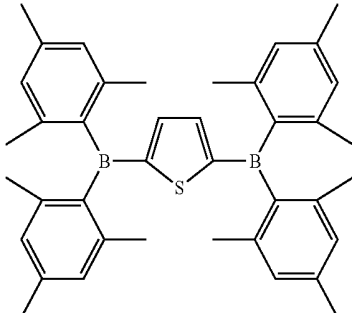
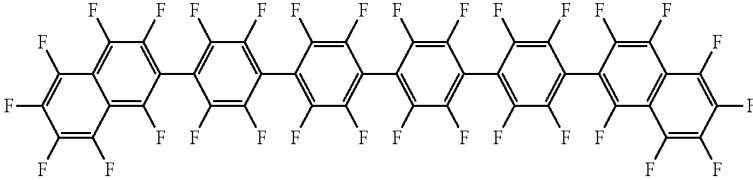
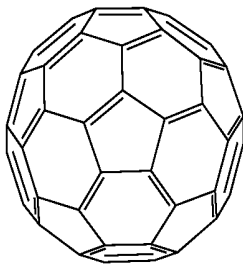
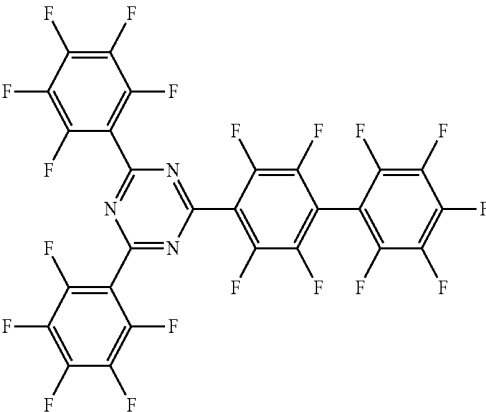
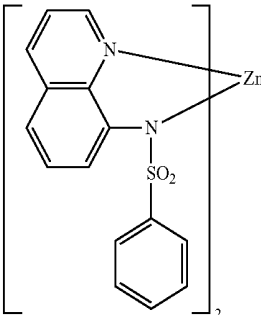
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 79, 449 (2001)
		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
Silole compounds		Jpn. J. Apply. Phys. 32, L917 (1993)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

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870
Triazine complexes		US20040036077
Zn (N ⁺ N ⁻) complexes		US6528187

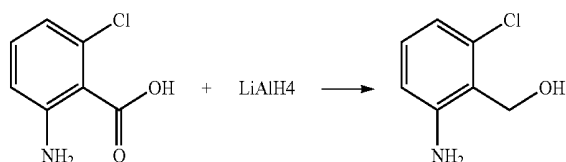
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EXPERIMENTAL

Compound Examples

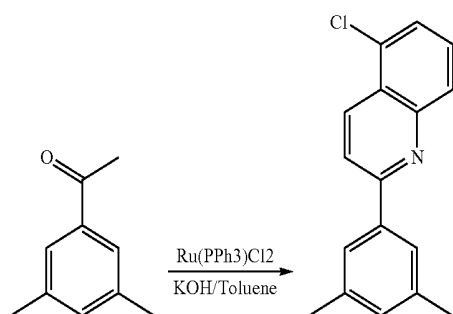
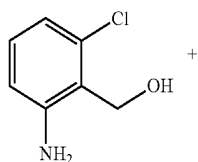
Example 1

Synthesis of Compound 1



Synthesis of (2-amino-6-chlorophenyl)methanol

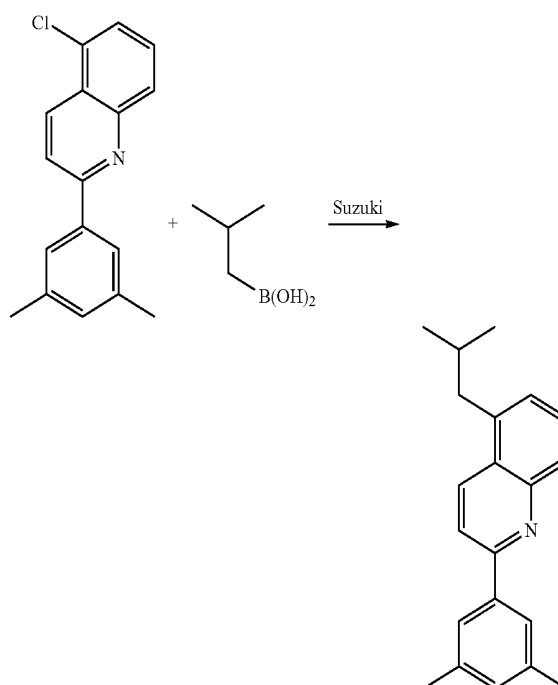
2-Amino-6-chlorobenzoic acid (25.0 g, 143 mmol) was dissolved in 120 mL of anhydrous THF in a 500 mL 2 neck round bottom flask. The solution was cooled in an ice-water bath. 215 mL of 1.0 M lithium aluminum hydride (LAH) THF solution was then added dropwise. After all of the LAH was added, the reaction mixture was allowed to warm up to room temperature and then stirred at room temperature overnight. ~10 mL of water was added to the reaction mixture followed by 7 g 15% NaOH. An additional 20 g of water was added to the reaction mixture. The organic THF phase was decanted and ~200 mL of ethyl acetate was added to the solid with stirring. Na_2SO_4 was added as a drying agent to the combined ethyl acetate organic portion and THF portion. The mixture was filtered and evaporated. ~20 g yellow solid was obtained and taken on to the next step without further purification.



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Synthesis of
5-chloro-2-(3,5-dimethylphenyl)quinoline

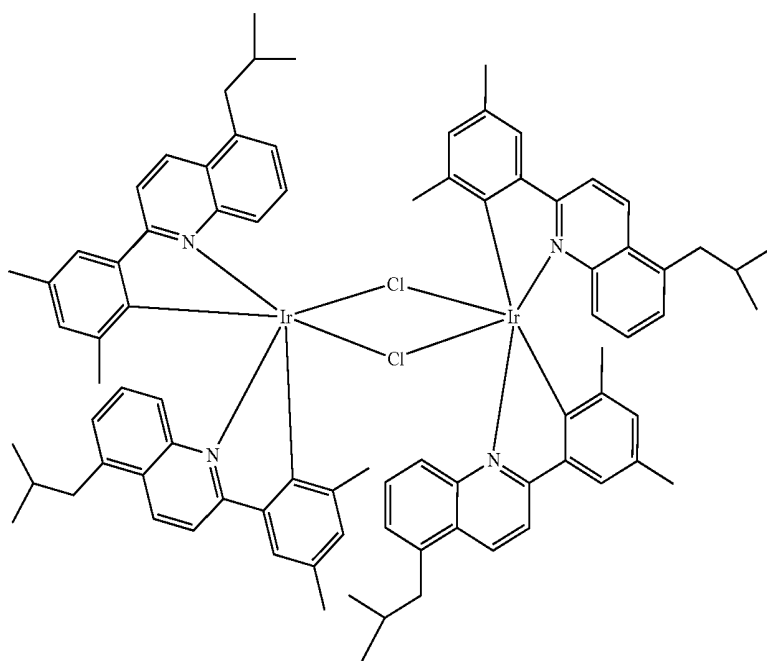
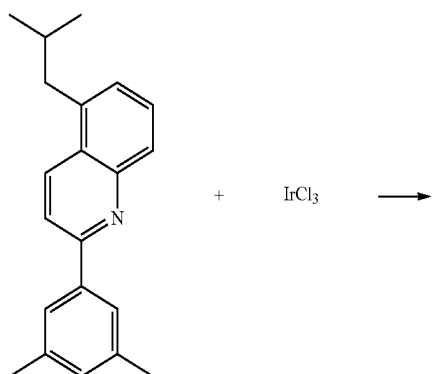
(2-Amino-6-chlorophenyl)methanol (16 g, 102 mmol), 3,5-dimethylacetophenone (22.6 g, 152 mmol), $\text{RuCl}_2(\text{PPh}_3)_3$ (0.973 g, 1.015 mmol), and KOH (10.25 g, 183 mmol) were refluxed in 270 mL of toluene for 18 h. Water was collected from the reaction using a Dean-stark trap. The reaction mixture was allowed to cool to room temperature, filtered through a silica gel plug and eluted with 5% ethyl acetate in hexanes. The product was further purified by Kugelrohr distillation to give 23.5 g of crude product, which was crystallized from 60 mL of MeOH to give 8.6 g (32% yield) of the desired product.

Synthesis of
2-(3,5-dimethylphenyl)-5-isobutylquinoline

5-Chloro-2-(3,5-dimethylphenyl)quinoline (4.3 g, 16.06 mmol), isobutylboronic acid (3.2 g, 31.4 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.538 g, 1.31 mmol), and potassium phosphate monohydrate (18.3 g, 79 mmol) were mixed in 114 mL of toluene. The system was degassed for 20 minutes. $\text{Pd}_2(\text{dba})_3$ was then added and the system was refluxed overnight. After cooling to room temperature, the reaction mixture was filtered through a Celite® plug and eluted with dichloromethane. The product was further purified by a Kugelrohr distillation and then further purified by column chromatography using 5% ethyl acetate in hexanes. This was followed by another Kugelrohr distillation to give 3.2 g (72% yield) of product.

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Synthesis of Iridium Dimer

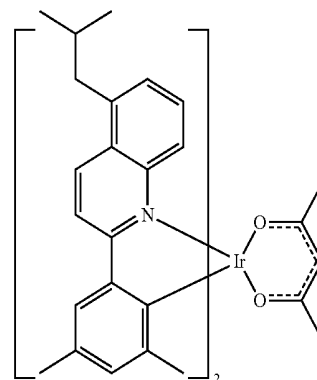
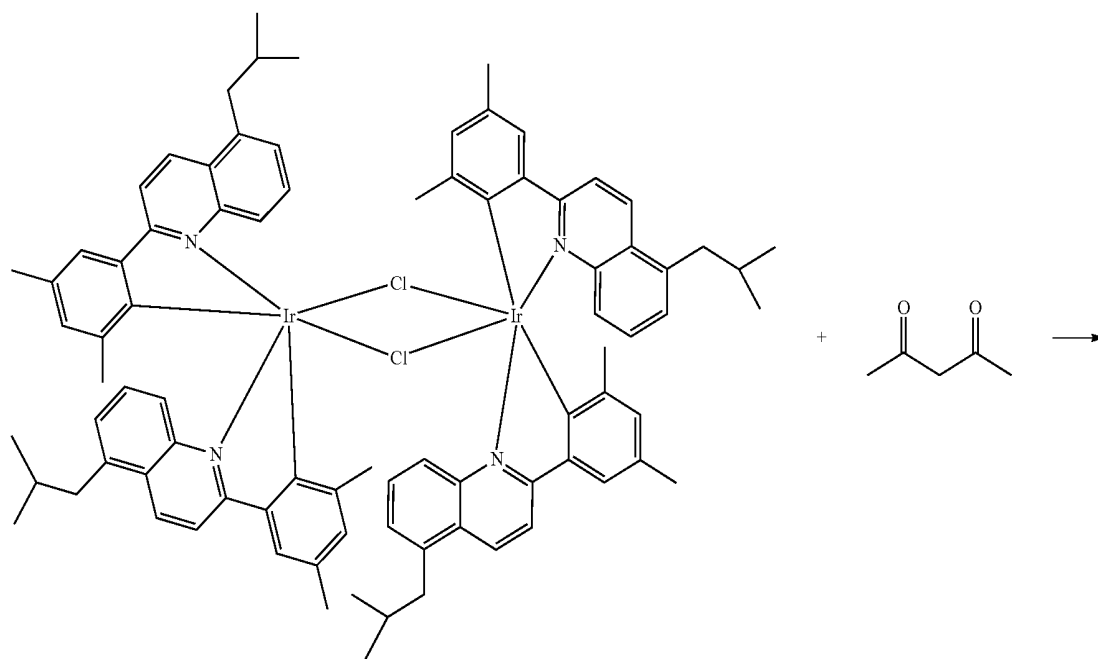
A mixture of 2-(3,5-dimethylphenyl)-5-isobutylquinoline (3.2 g, 11.06 mmol), $\text{IrCl}_3 \cdot 4\text{H}_2\text{O}$ (1.79 g, 4.83 mmol), 2-ethoxyethanol (45 mL) and water (105 mL) was refluxed

60

under nitrogen overnight. The reaction mixture was filtered and washed with MeOH (3×10 mL). ~2.9 g of dimer was obtained after vacuum drying. The dimer was used for the next step without further purification.

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Compound 1

Synthesis of Compound 1

Dimer (2.9 g, 1.80 mmol), pentane-2,4-dione (1.80 g, 18.02 mmol), K_2CO_3 (2.49 g, 18.02 mmol) and 2-ethoxyethanol (22 mL) were stirred at room temperature for 24 h. The 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 (TEA) in hexanes and eluted with methylene chloride. 2-Propanol was added to the filtrate. The filtrate was concentrated, but not to dryness. 1.6 g of product was obtained after filtration. The solid was sublimed twice under high vacuum at 240° C. to give 1.0 g (64%) of Compound 1.

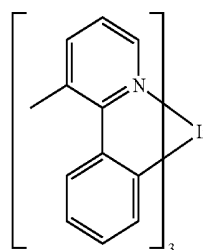
The stack of the device examples consisted of sequentially, from the 1200 Å ITO surface, 100 Å of Compound A as the hole injection layer (HIL), 400 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (α -NPD) as the hole transporting layer (HTL), 300 Å of the 7 wt % invention compound doped into BALq host as the emissive layer (EML), 550 Å of Alq_3 (tris-8-hydroxyquinoline aluminum) as the ETL.

Comparative Examples were fabricated similarly to the Device Examples except that Compound B, C or D was used as the emitter in the EML.

As used herein, the following compounds have the following structures:

Device Examples

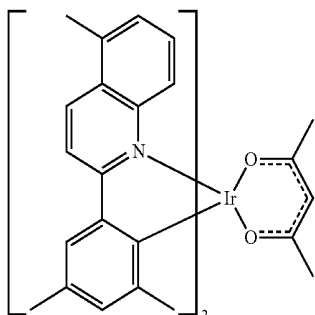
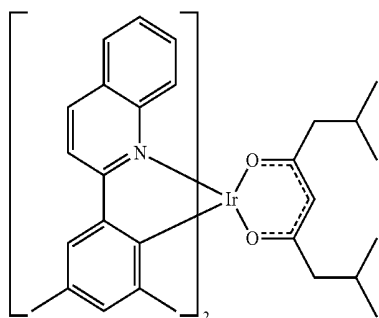
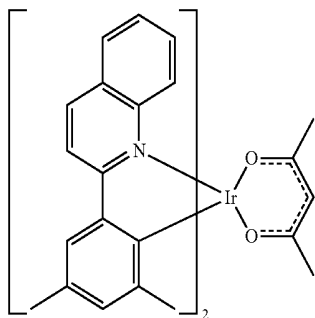
All example devices were fabricated by high vacuum (<10⁻⁷ Torr) thermal evaporation. The anode electrode is 1200 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1000 Å of Al. All devices are encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H₂O and O₂) immediately after fabrication, and a moisture getter was incorporated inside the package.



Compound A

99

-continued



Particular emissive dopants for the emissive layer of an OLED are provided. These compounds may lead to devices having particularly good properties.

The device structures and device data are summarized in Table 2.

100

Compound B

As seen from the Table 2, the EQE of Compound 1 at 1000 nits is up to 10% higher than Compounds B, C, and D.

Additionally, the EL spectral full width at half maximum (FWHM) of Compound 1 (58 nm) is also narrower than Compound B (62 nm) and Compound D (64 nm), which is a

desirable device property. The FWHM of Compound 1 is the same as the FWHM of Compound C (58 nm). The color saturation (CIE) of Compound 1 and Compound B are also

Compound C

the same. These results indicate that Compound 1 is a more efficient red emitter than Compounds B, C and D with a desirable narrower FWHM.

Compound 1 also has almost a double lifetime at room temperature compared to Compound D. The only difference between these two compounds is that Compound 1 has a bulkier group at 5-position. This clearly indicates that a bulkier group than methyl in the 5-position of 2-phenylquinoline may indeed provide a significant improvement in overall device performance.

Compound D

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.

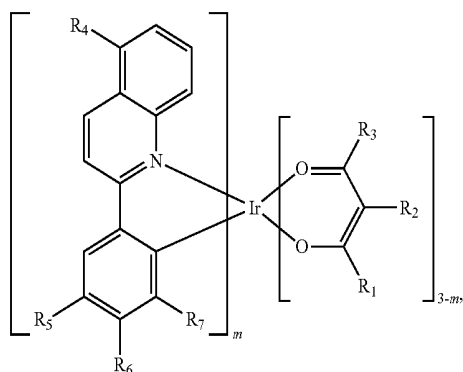
TABLE 2

Emitter	At 1,000 nits									At 40 mA/cm ²		
	1931 CIE		λ_{max}	FWHM	V	LE	EQE	PE	cd/A per	L ₀	LT _{80%} [h]	
	x	y	[nm]	[nm]	[V]	[cd/A]	[%]	[lm/W]	EQE		RT	70° C.
Compound 1 (Device Example)	0.666	0.331	622	58	7.8	22.2	20.5	9.0	1.08	6,852	600	66
Compound B (Comparative Example)	0.667	0.331	622	62	8.1	19.9	18.8	7.7	1.06	6,447	878	70
Compound C (Comparative Example)	0.662	0.335	620	58	7.4	21.9	18.9	9.3	1.16	6,927	565	73
Compound D (Comparative Example)	0.664	0.334	620	64	8.1	21.1	19.4	8.1	1.09	6,666	321	44

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The invention claimed is:

1. A compound having the formula:



Formula III

wherein each of R₁, R₂, R₃, R₅, R₆ and R₇ is independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl;

wherein R₄ is selected from the group consisting of isopropyl, isobutyl, and t-butyl; and

wherein m=2.

2. The compound of claim 1, wherein each of R₁ and R₃ are a branched alkyl with branching at a position further than the α position to the carbonyl group.

3. The compound of claim 1, wherein each of R₅, R₆ and R₇ are independently selected from methyl and hydrogen, and at least one of R₅, R₆ and R₇ is methyl.

4. The compound of claim 1, wherein each of R₅ and R₇ are methyl, and R₆ is hydrogen.

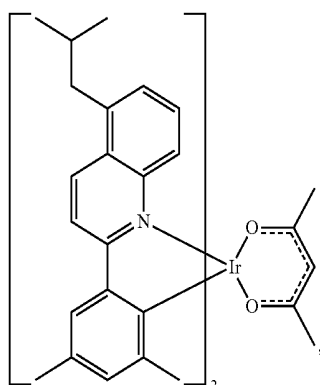
5. The compound of claim 1, wherein each of R₅ and R₆ are methyl, and R₇ is hydrogen.

6. The compound of claim 1, wherein each of R₅, R₆ and R₇ are methyl.

7. The compound of claim 1, wherein R₄ is isobutyl.

8. The compound of claim 1, wherein R₄ is isopropyl.

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

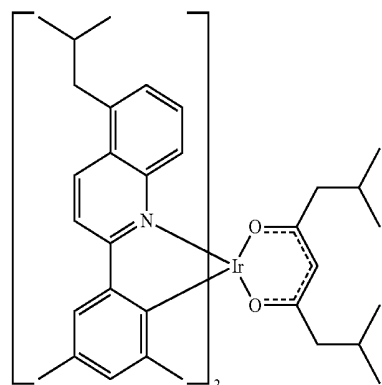


Compound 1

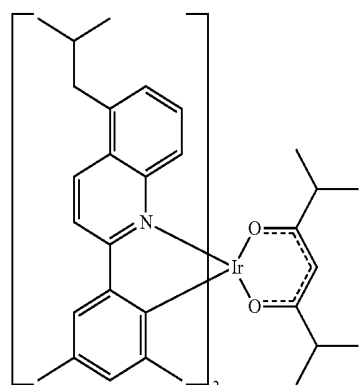
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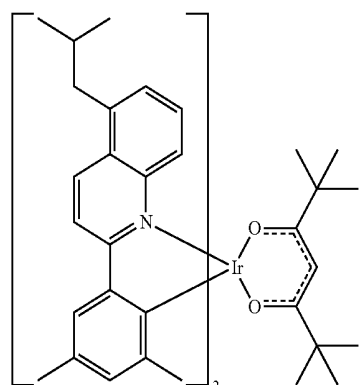
Compound 2



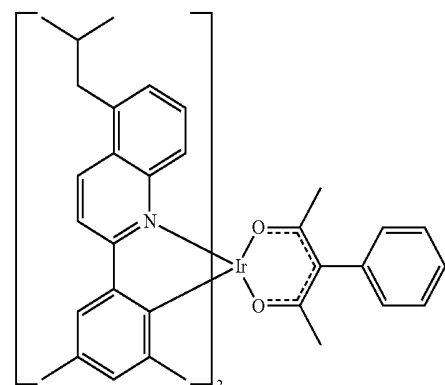
Compound 3



Compound 4

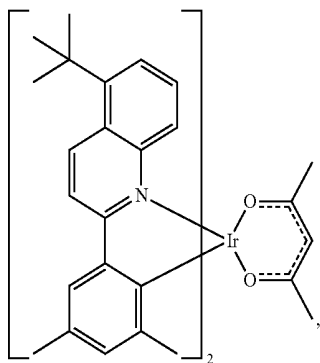


Compound 5



103

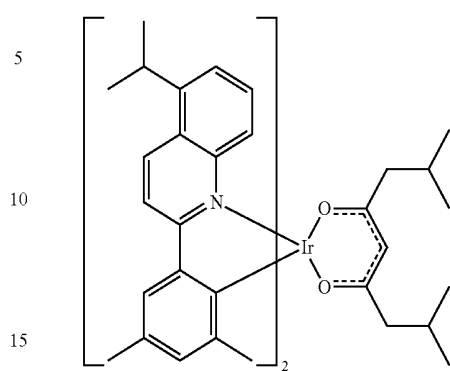
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Compound 15

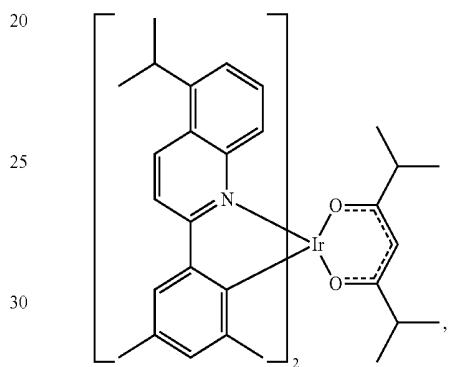
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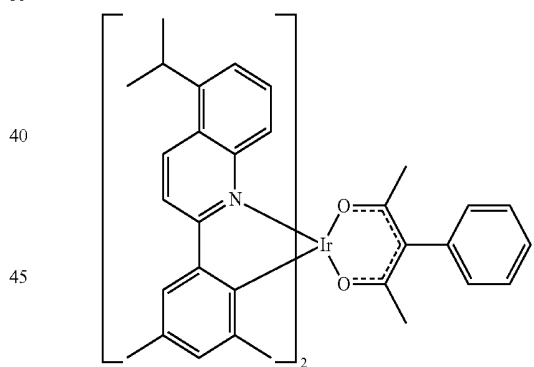
Compound 19

Compound 16



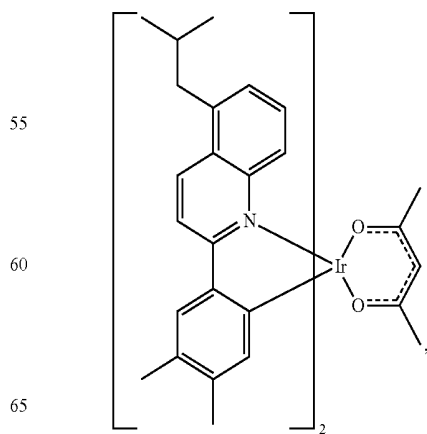
Compound 20

Compound 17



Compound 21

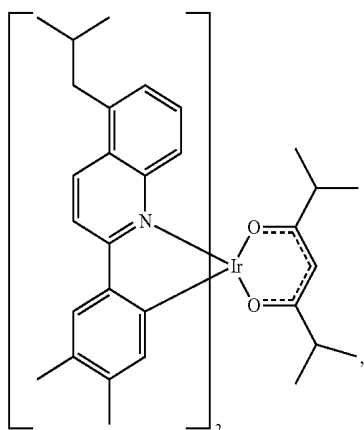
Compound 18



Compound 33

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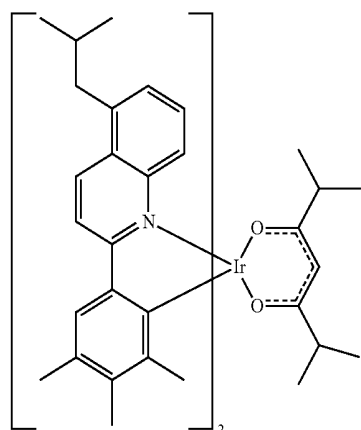
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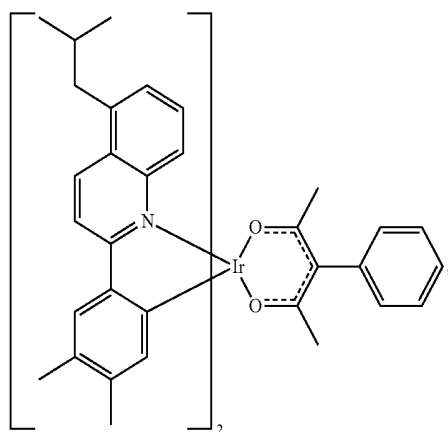
Compound 35

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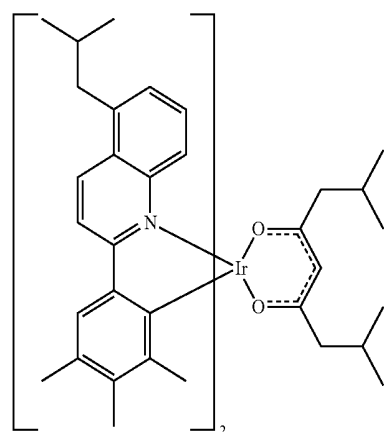
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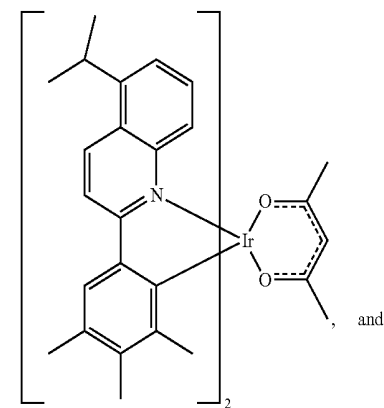
Compound 42



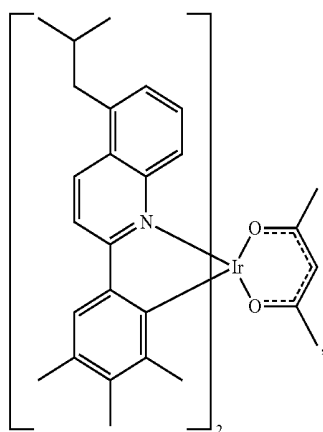
Compound 37



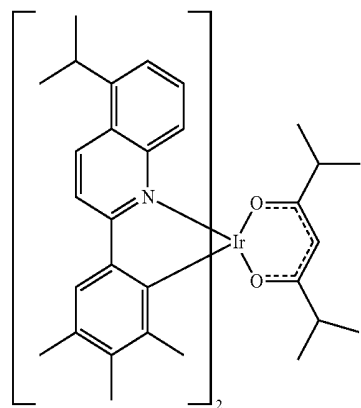
Compound 43



Compound 45



Compound 41

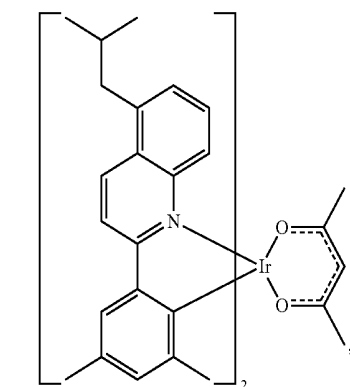


Compound 46

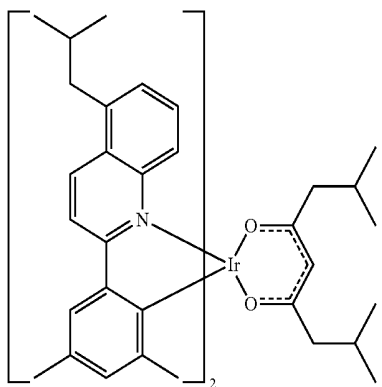
107

10. The compound of claim 1, wherein each of R_1 , R_2 , R_3 , R_5 , R_6 and R_7 is independently selected from the group consisting of hydrogen, deuterium, and alkyl.

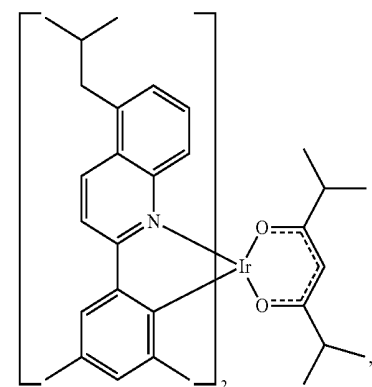
11. The composition of claim 1, wherein the compound is selected from the group consisting of:



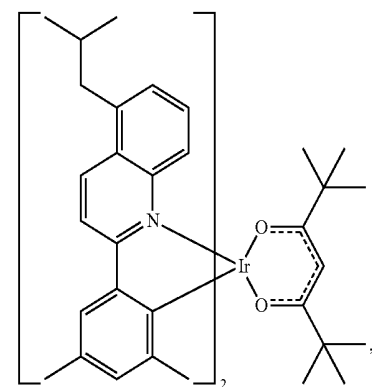
Compound 1



Compound 2



Compound 3

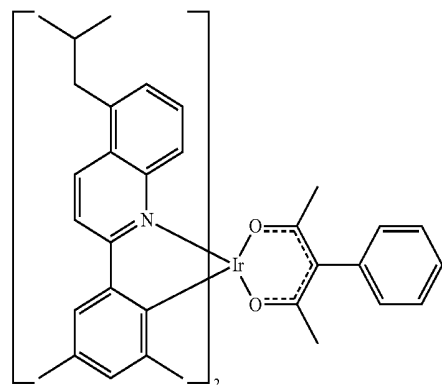


Compound 4

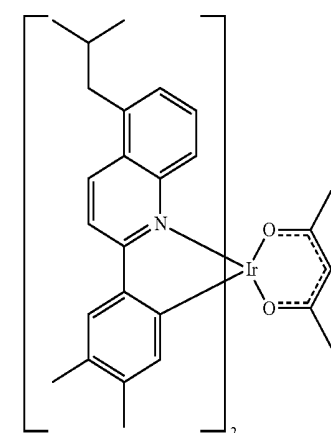
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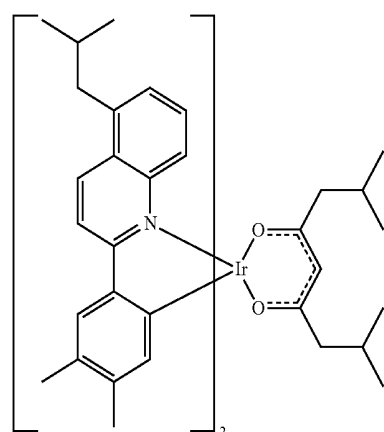
Compound 5



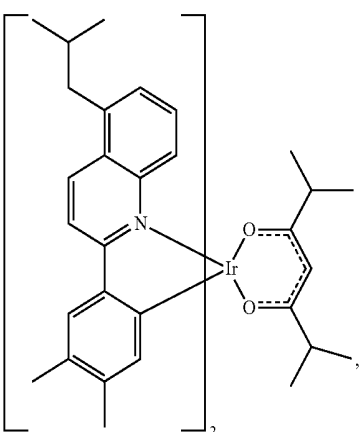
Compound 33



Compound 34

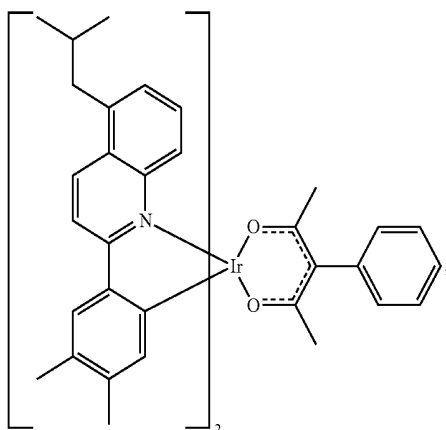


Compound 35



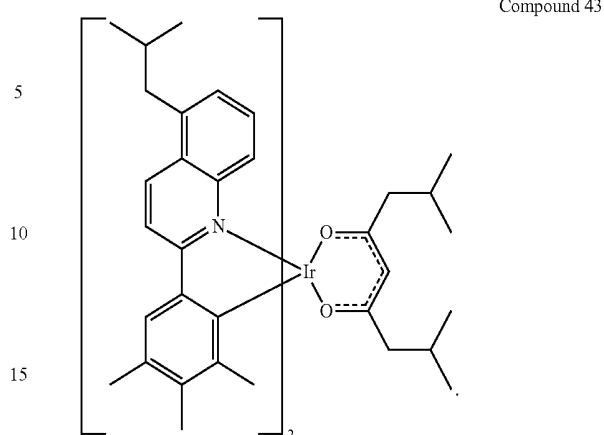
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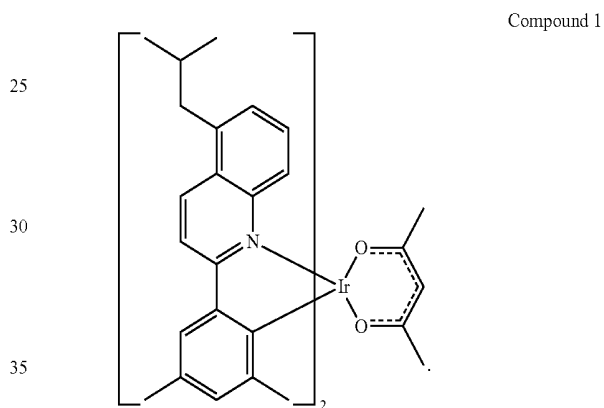
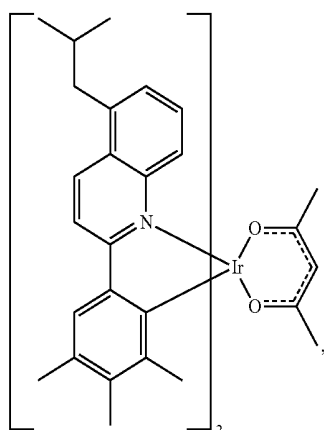


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12. The composition of claim 1, wherein the compound is



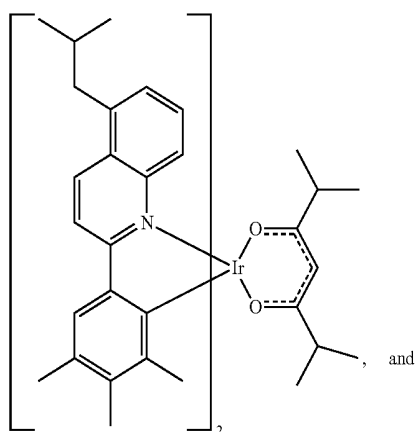
13. The compound of claim 1, wherein R_4 is t-butyl.

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

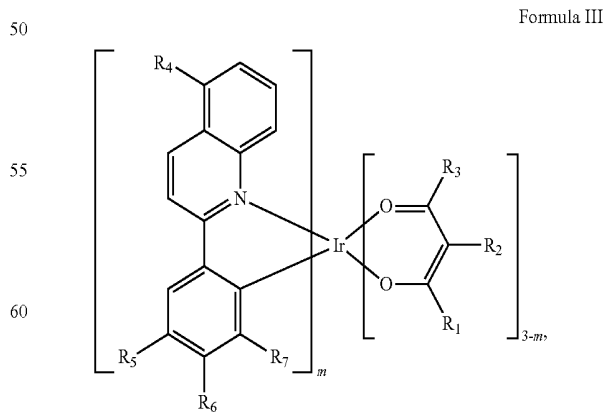
an anode;

a cathode; and

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



Compound 42



wherein each of R_1 , R_2 , R_3 , R_5 , R_6 and R_7 is independently selected from the group consisting of hydrogen, deute-

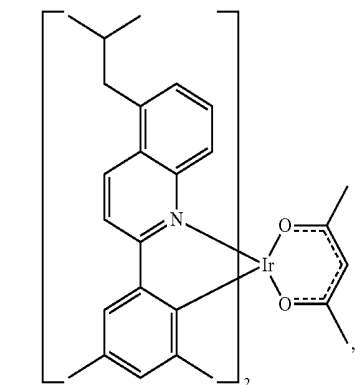
111

rium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl;

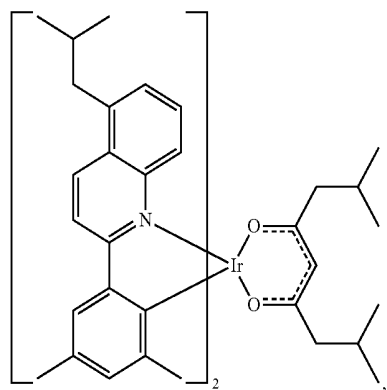
wherein R_4 is selected from the group consisting of isopropyl, t-butyl, and isobutyl; and

wherein $m=2$.

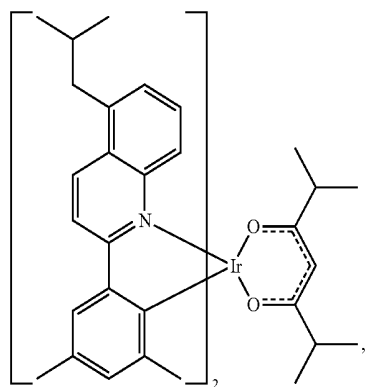
15. The first device of claim **14**, wherein the compound is selected from the group consisting of:



Compound 1



Compound 2

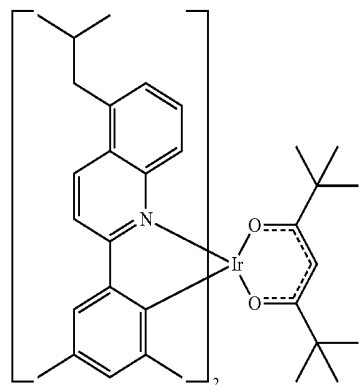


Compound 3

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Compound 4

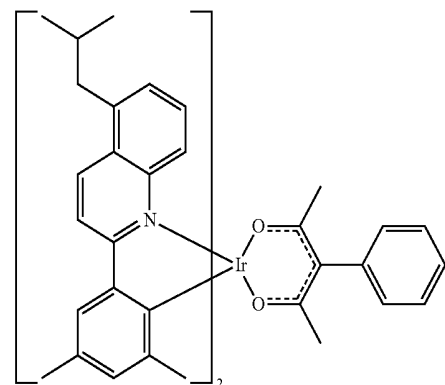


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Compound 5

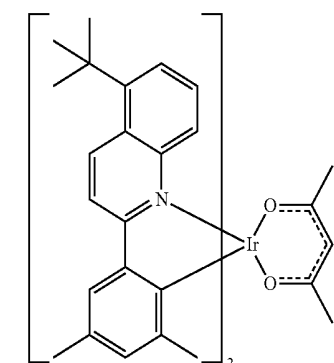


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Compound 15

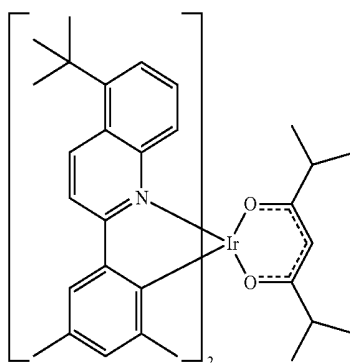


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Compound 16



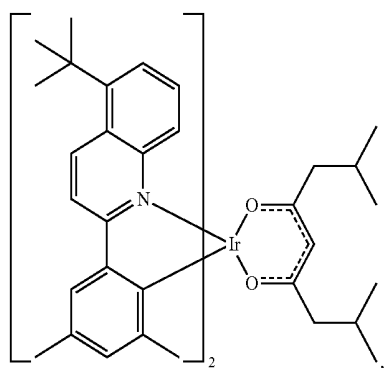
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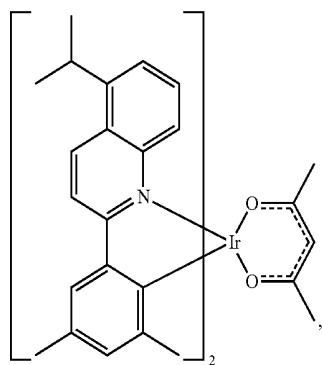
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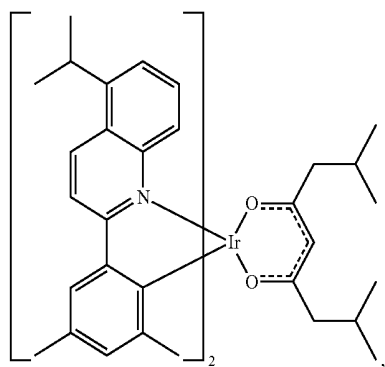
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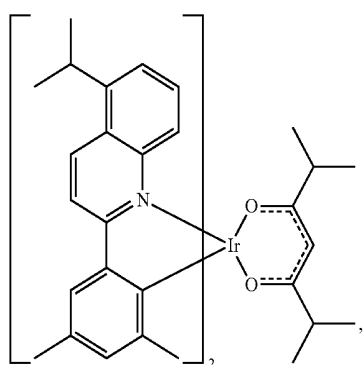
Compound 17



Compound 18



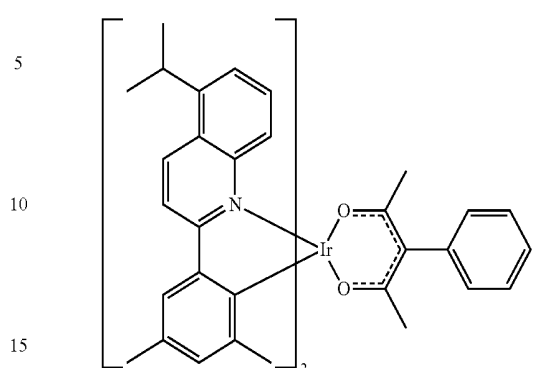
Compound 19



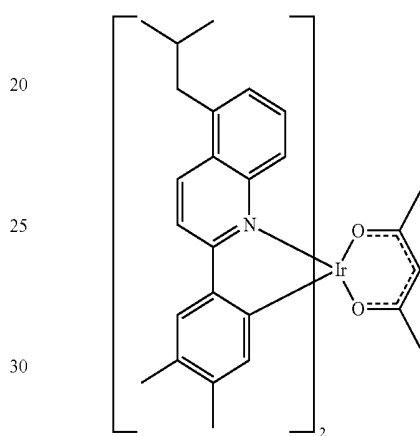
Compound 20

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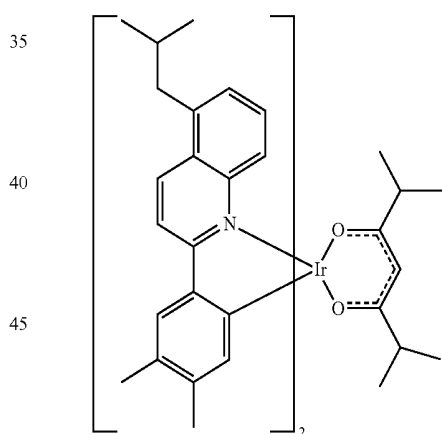
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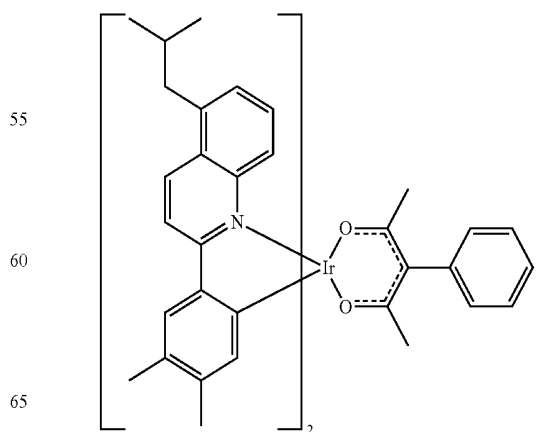
Compound 21



Compound 33



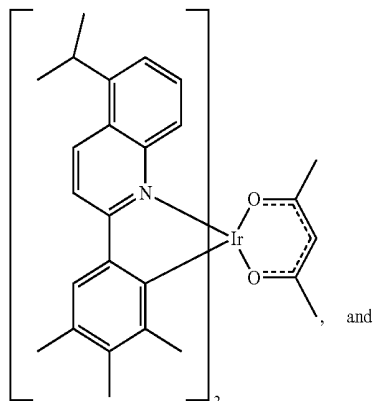
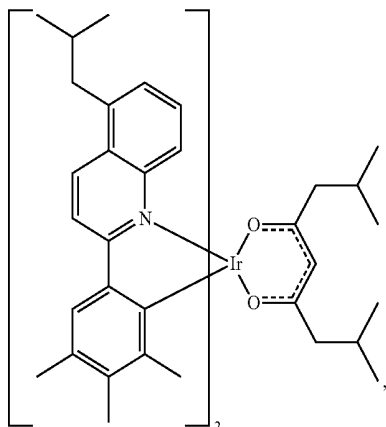
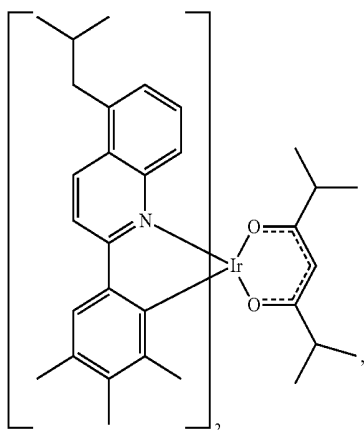
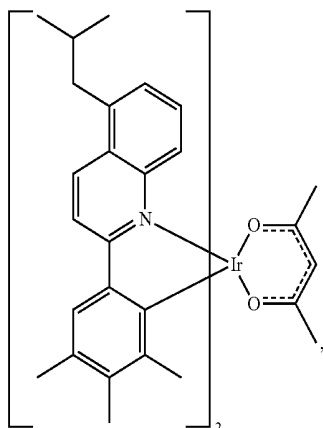
Compound 35



Compound 37

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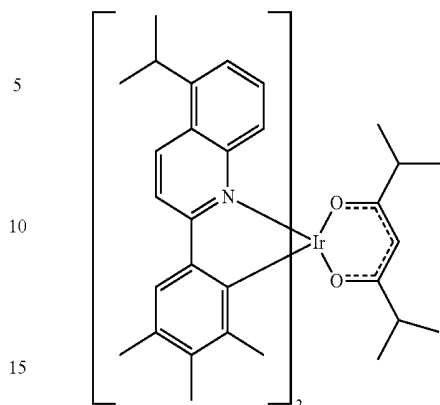
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Compound 41



Compound 46

Compound 42

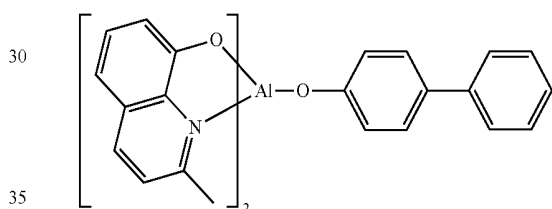
16. The first device of claim 14, wherein the organic layer is an emissive layer and the compound is an emissive dopant.

17. The first device of claim 16, 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 18, wherein the host is:

Compound 43

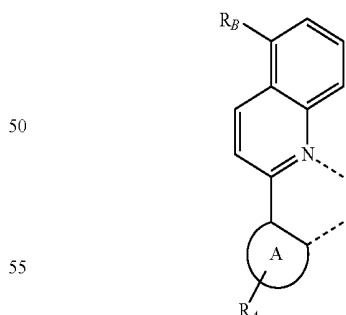


20. The first device of claim 14, wherein the first device is a consumer product.

21. The first device of claim 14, wherein the first device is an organic light emitting device.

22. A compound comprising a ligand L having the formula:

Compound 45



Formula I

wherein A is a 5-membered or 6-membered carbocyclic or heterocyclic ring;

wherein R_A may represent mono, di, tri, or tetra substitutions;

wherein each of R_A is independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl;

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wherein R_B is selected from the group consisting of amino and silyl;

wherein, when R_B is silyl, a Si atom of the silyl is bonded directly to the quinoline ring of Formula I;

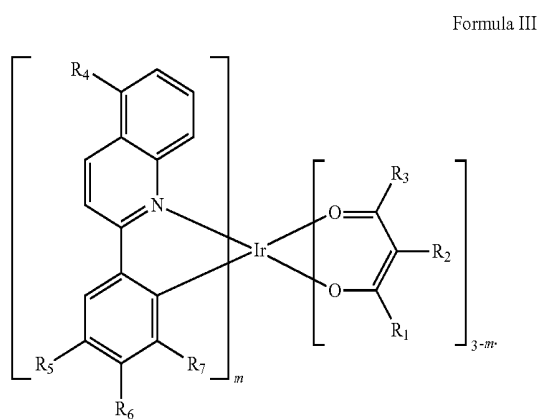
wherein, when R_B is amino, a N atom of the amino is bonded directly to the quinoline ring of Formula I; and

wherein the ligand L is coordinated to a metal M having an atomic number greater than 40.

23. The compound of claim 22, wherein R_B is amino.

24. The compound of claim 22, wherein R_B is silyl.

25. The compound of claim 22, wherein the compound has a structure according to Formula III:



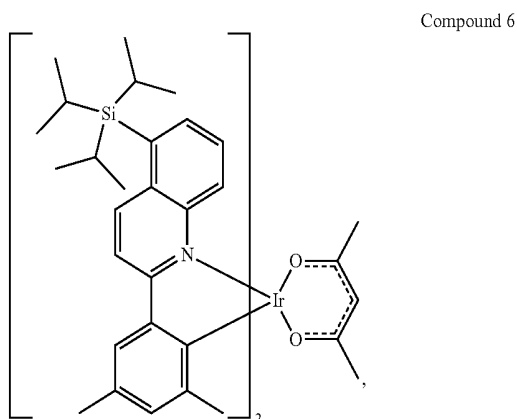
wherein each of R_1 , R_2 , R_3 , R_5 , R_6 and R_7 is independently selected from the group consisting of hydrogen, deuterium, alkyl, silyl, alkoxy, amino, alkenyl, alkynyl, arylkyl, aryl and heteroaryl;

wherein R_4 is selected from the group consisting of amino and silyl;

wherein, when R_4 is silyl, a Si atom of the silyl is bonded directly to the quinoline ring of Formula III; and

wherein, when R_4 is amino, a N atom of the amino is bonded directly to the quinoline ring of Formula III.

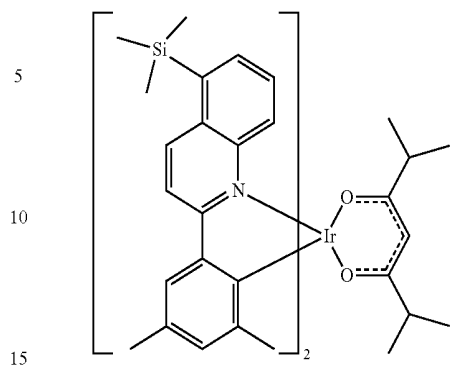
26. The compound of claim 22, wherein the compound is selected from the group consisting of:



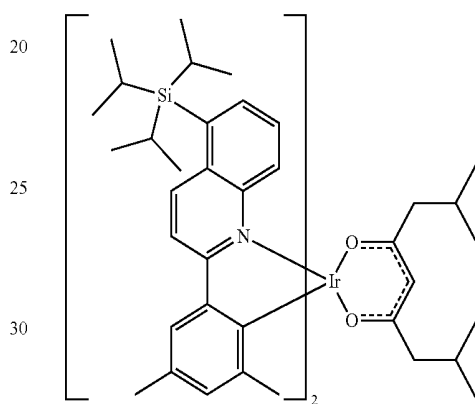
118

-continued

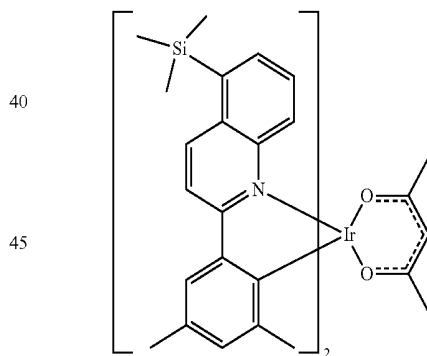
Compound 7



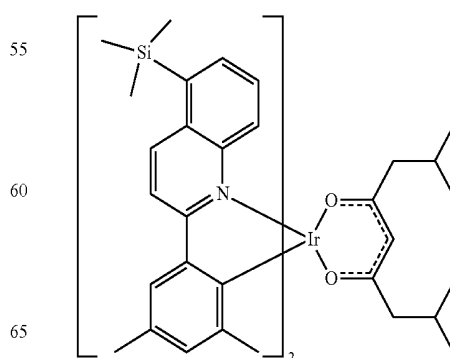
Compound 8



Compound 9

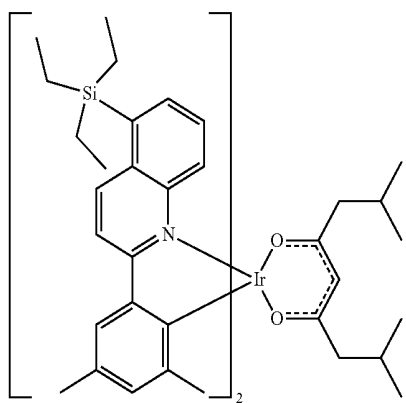
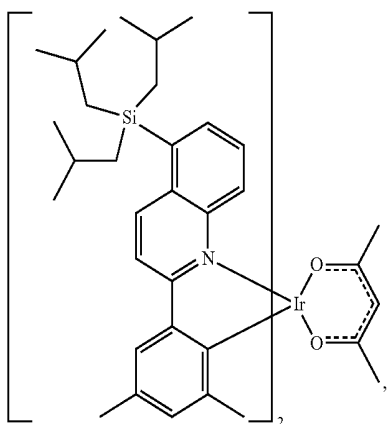
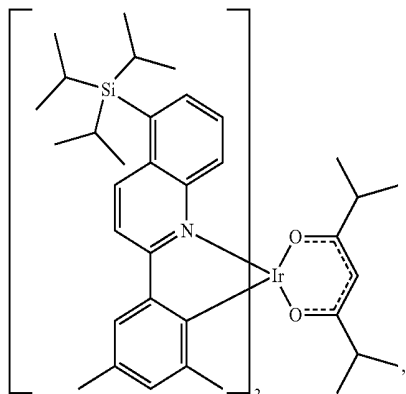


Compound 10



119

-continued



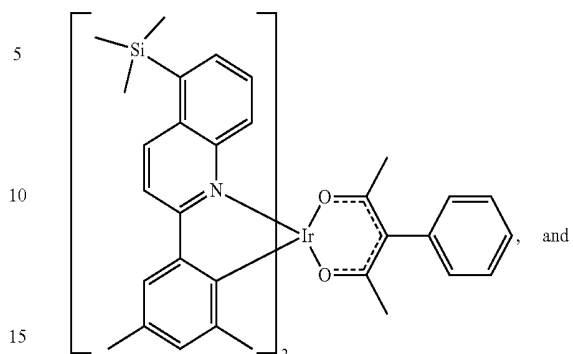
Compound 11

Compound 12

Compound 13

120

-continued



Compound 14

20

25

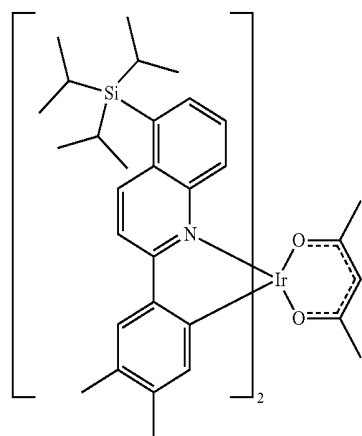
30

35

40

45

Compound 38



* * * * *

专利名称(译)	用于发光二极管的5-取代的2-苯基喹啉配合物材料		
公开(公告)号	US9130177	公开(公告)日	2015-09-08
申请号	US13/006016	申请日	2011-01-13
[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 ADAMOVICH VADIM		
发明人	MA, BIN DEANGELIS, ALAN XIA, CHUANJUN ADAMOVICH, VADIM		
IPC分类号	H01L51/54 C09K11/06 H01L51/00 C07F15/00 H01L51/50		
CPC分类号	H01L51/0085 C07F15/0033 C09K11/06 C09K2211/1029 C09K2211/185 H01L51/5016 C07C49/92 C07F15/00 C07F19/00 H01L51/50 H05B33/14		
其他公开文献	US20120181511A1		
外部链接	Espacenet USPTO		

摘要(译)

提供的化合物包含具有5-取代的2-苯基喹啉的配体。特别地，2-苯基喹啉可以在5-位被大体积烷基取代。这些化合物可用于有机发光器件中，特别是用作这种器件的发光层中的红色发光体，以提供具有改进性能的器件。

