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

(2013.01); *H01L 51/0058* (2013.01); *H01L 51/0067* (2013.01); *H01L 51/0069* (2013.01);
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(58) **Field of Classification Search**
None

See application file for complete search history.

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H01L 51/54 (2006.01)

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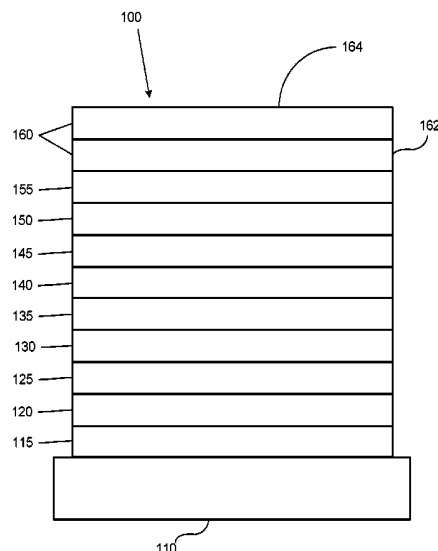
(57) **ABSTRACT**

Compounds that act as capture agents to sequester unsaturated metal complexes are provided. In particular, the compounds may be host materials, dopant materials, or dopant materials containing functional groups, such as an isocyanide or a phosphine group, which are suitable for trapping an unsaturated coordination complex. These compounds may be used in organic light emitting devices, particularly blue devices, to provide improved device lifetime.

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CPC *H01L 51/0085* (2013.01); *C09K 11/025* (2013.01); *C09K 11/06* (2013.01); *H01L 51/005* (2013.01); *H01L 51/006* (2013.01); *H01L 51/0052* (2013.01); *H01L 51/0054*

10 Claims, 7 Drawing Sheets



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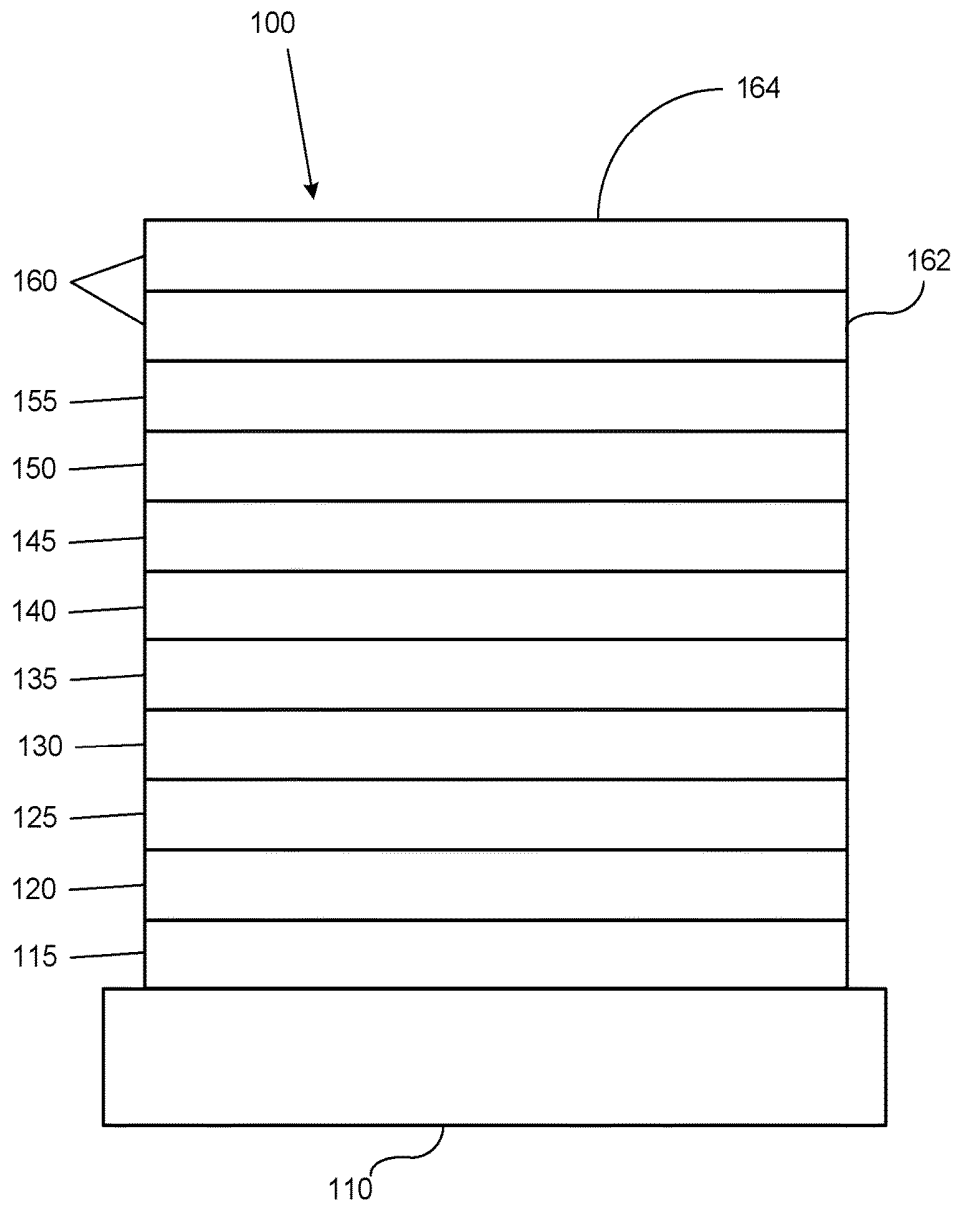


FIGURE 1

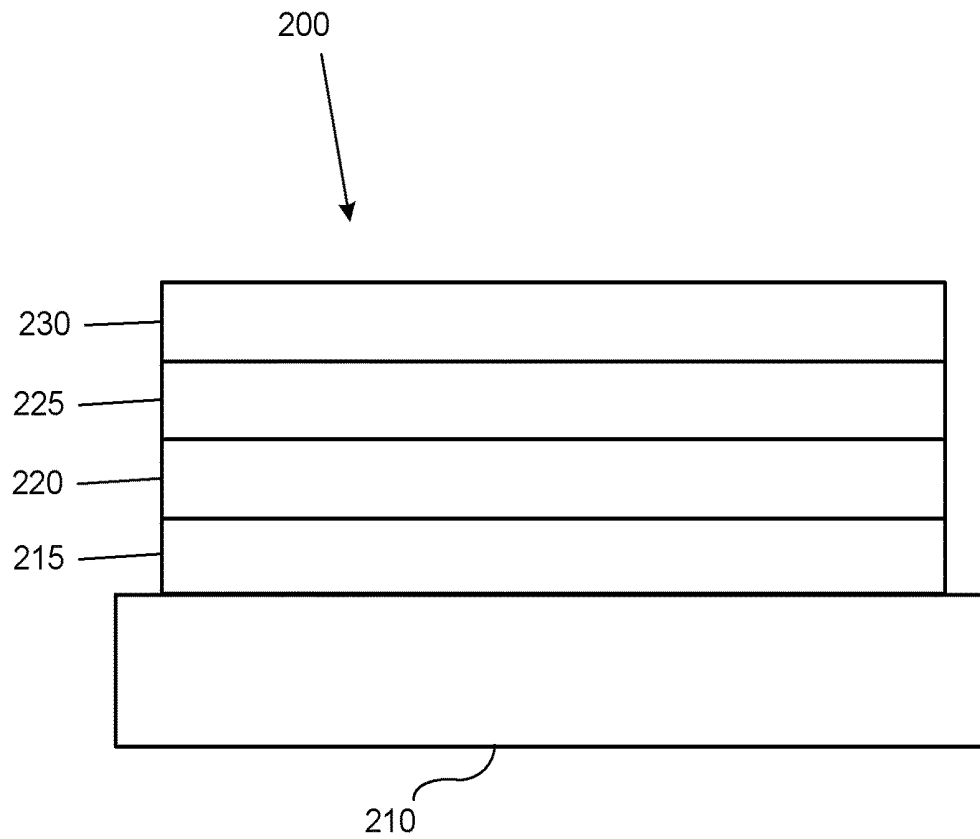


FIGURE 2

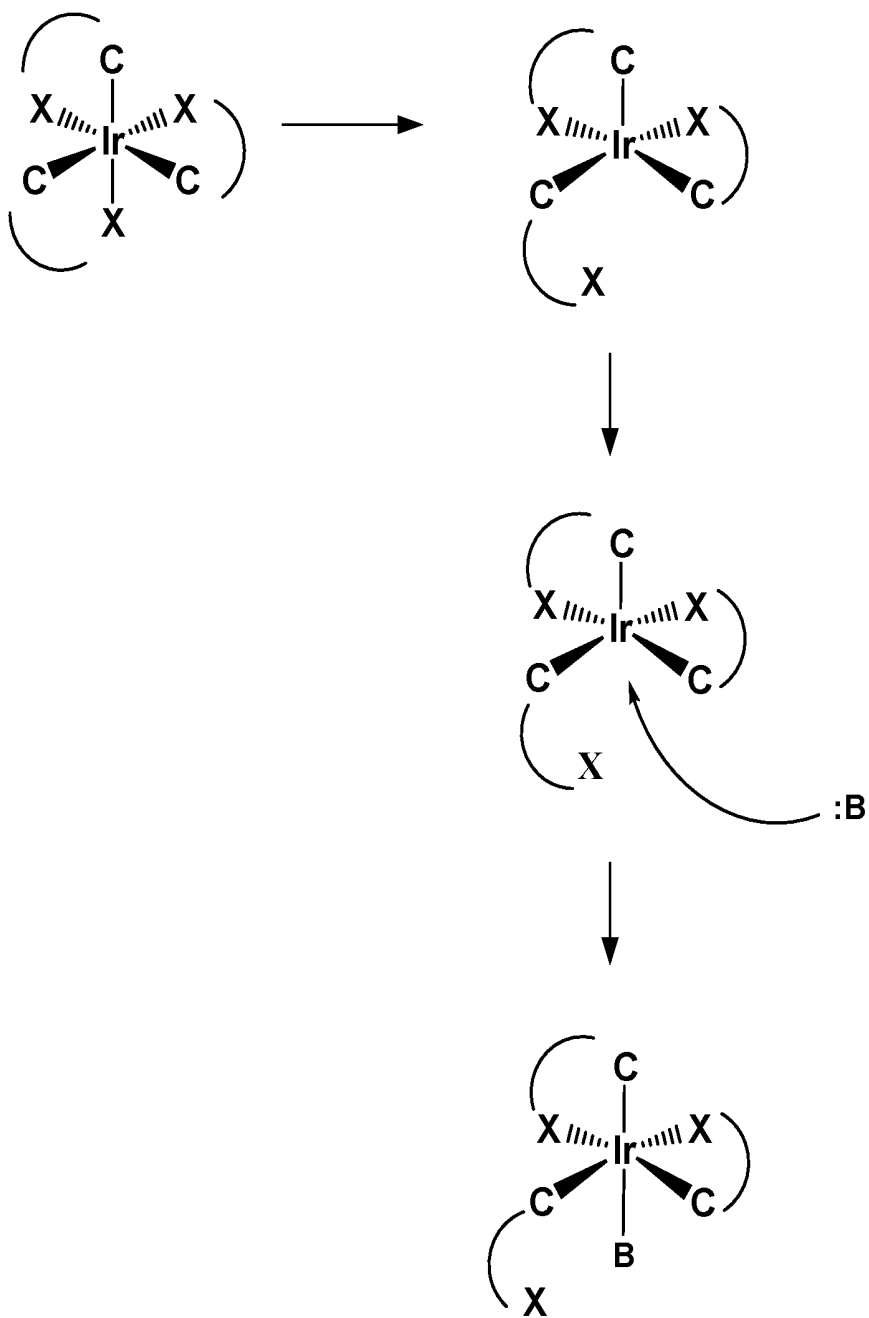
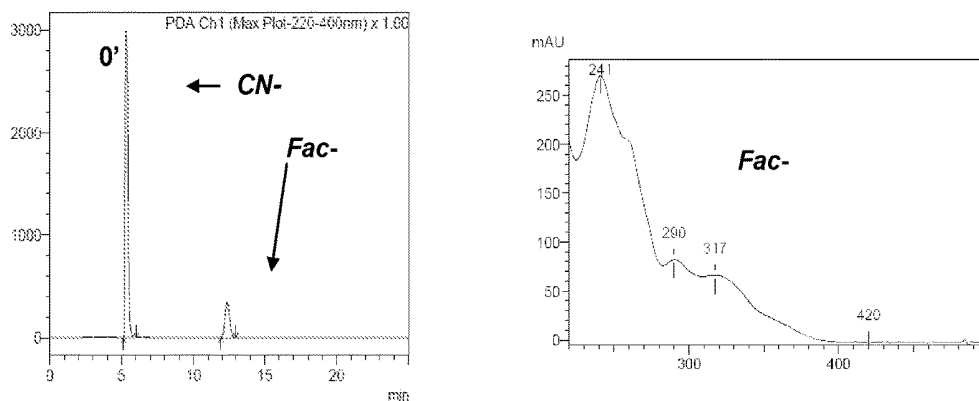


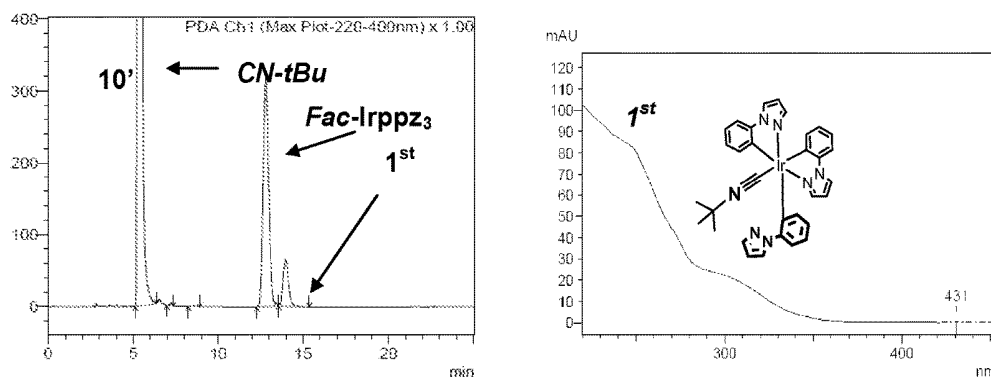
FIGURE 3

1) Results at $t = 0$ min. (left HPLC chromatogram; right Absorption spectra)



$R_t = 5.3 \text{ min CN-tBu}$; $R_t = 12.3 \text{ min Fac-Irppz}_3$ ($m/z = 623.3 [m+H]^+$)

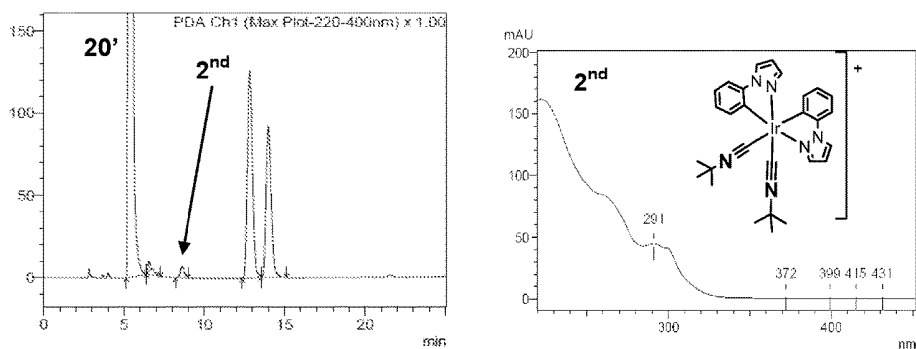
2) Results at $t = 10$ min. (left HPLC chromatogram; right Absorption spectra, inset structure of 1^{st})



$R_t = 5.3 \text{ min CN-tBu}$; $R_t = 12.3 \text{ min Fac-Irppz}_3$ ($m/z = 623.3 [m+H]^+$); $R_t = 14.0 \text{ min } 1^{st}$
 $(m/z = [1^{st}+H]^+ : 706.2; m/z [1^{st}-ppz+AcCN]^+ : 603.3)$

FIGURE 4

3) Results at $t = 20$ min. (left HPLC chromatogram; right Absorption spectra, inset structure of 2^{nd})



$Rt = 5.3$ min $CN-tBu$; $Rt = 8.7$ min 2^{nd} ($m/z = [2^{nd}]^+$: 645.3; $Rt = 12.3$ min $Fac-Irppz_3$ ($m/z = 623.3$ [$m+H$] $^+$); $Rt = 14.0$ min 1^{st} ($m/z = [1^{st}+H]^+$: 706.2; $m/z [1^{st}-ppz+AcCN]^+$: 603.3;

4) Results at $t = 60$ min

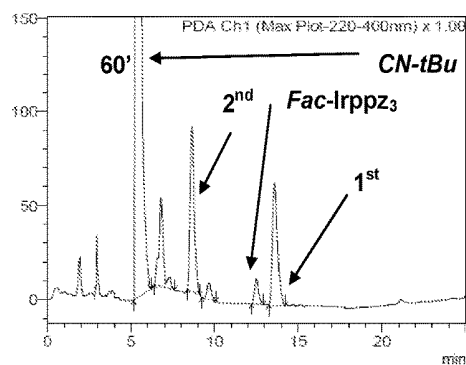
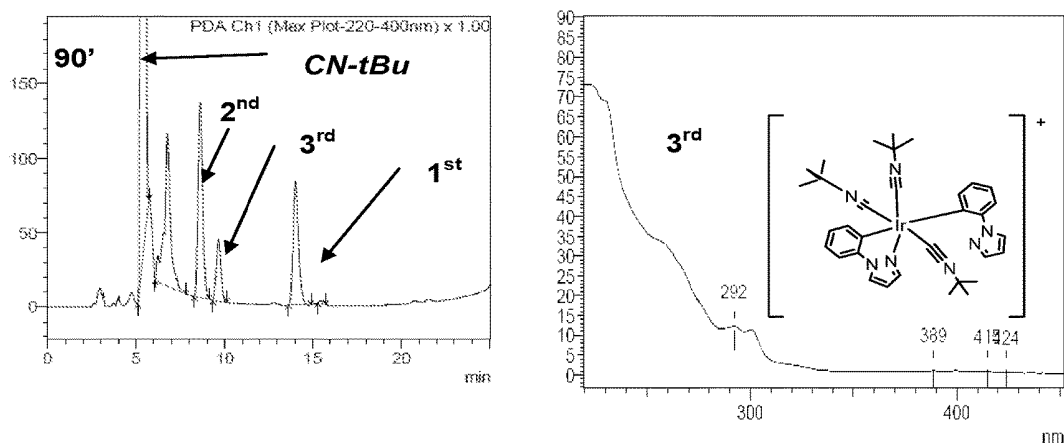


FIGURE 5

5) Results at $t = 90$ min. (left HPLC chromatogram; right Absorption spectra, inset structure of 3^{rd})



$R_t = 5.3$ min $CN-tBu$; $R_t = 8.7$ min 2^{nd} ($m/z = [2^{nd}]^+$: 645.3); $R_t = 9.6$ min 3^{rd} ($m/z = [3^{rd}]^+$: 728.4); $R_t = 12.3$ min $Fac-Irppz_3$ ($m/z = 623.3$ [$m+H$] $^+$); $R_t = 14.0$ min 1^{st} ($m/z = [1^{st}+H]^+$: 706.2; m/z [1^{st} -ppz+AcCN] $^+$: 603.3;

6) Results at $t = 120$ min.

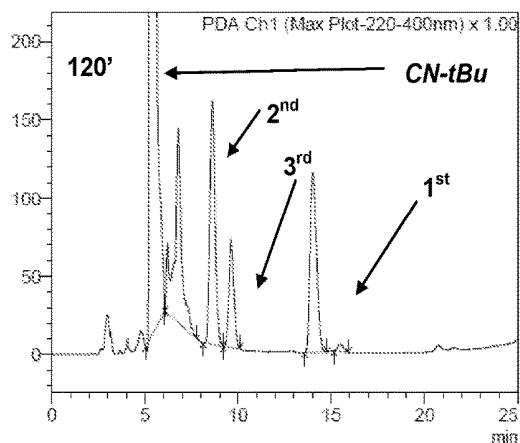
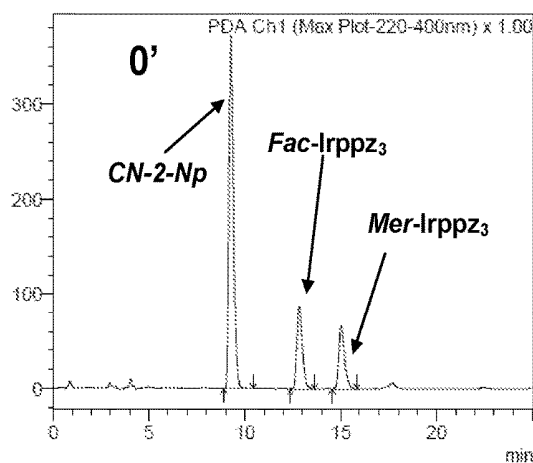


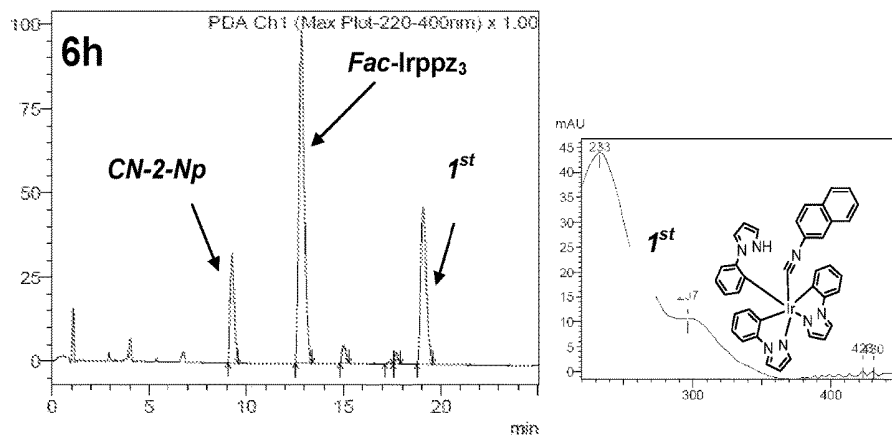
FIGURE 6

1) Results at $t = 0$ min. (HPLC chromatogram)



$R_t = 9.3$ min, CN-2-Np; $R_t = 12.9$ min, Fac-Irppz₃; $R_t = 15.1$ min, Mer-Irppz₃

2) Results at $t = 6$ hours. (left HPLC chromatogram; right Absorption spectra)



$R_t = 9.3$ min, CN-2-Np; $R_t = 12.9$ min, Fac-Irppz₃; $R_t = 15.1$ min, Mer-Irppz₃; $R_t = 19.0$ min, 1st ($m/z = [1^{st}+H]^+$: 776.2; $m/z [1^{st}-ppz+AcCN]^+$: 673.3)

FIGURE 7

1

ORGANIC ELECTROLUMINESCENT
MATERIALS AND DEVICESCROSS REFERENCE TO RELATED
APPLICATIONS

This application is a divisional application of U.S. patent application Ser. No. 13/302,436 filed on Nov. 22, 2011, which claims priority to U.S. Provisional Application No. 61/420,473, filed Dec. 7, 2010, the disclosures of which are expressly incorporated herein by reference in their entirety.

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 and organic materials for use in such devices. More specifically, the invention relates to compounds that act as capture agents to sequester unsaturated metal complexes.

BACKGROUND

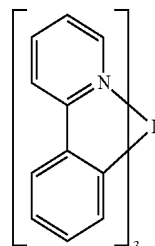
Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, 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.

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



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

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

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

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

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

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

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HOMO or LUMO energy level appears closer to the top of such a diagram than a “lower” HOMO or LUMO energy level.

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

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

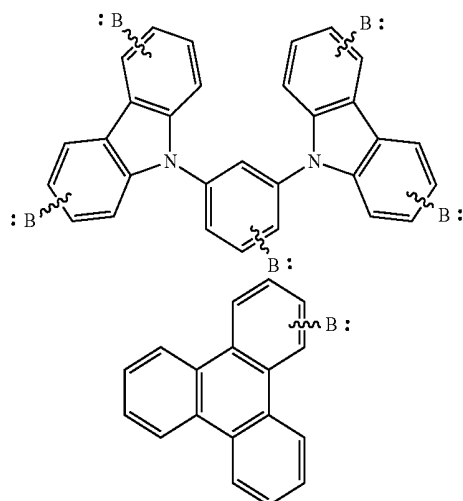
SUMMARY OF THE INVENTION

Methods for trapping a low coordinate structure, resulting from cleavage of a metal-ligand bond in the compound, and converting it back to the original coordination number are provided. The method comprising operating an organic light emitting device comprising a first organic compound containing a metal-ligand bond and a second organic compound comprising a functional group capable of trapping an unsaturated coordination complex. A metal-ligand bond in the first organic compound cleaves during operation of the device; thereby creating a coordinatively unsaturated intermediate complex. The second organic compound reacts with the coordinatively unsaturated intermediate complex.

In one aspect, the method further comprises suppressing the ability of the coordinatively unsaturated intermediate complex to trap charge and excitons.

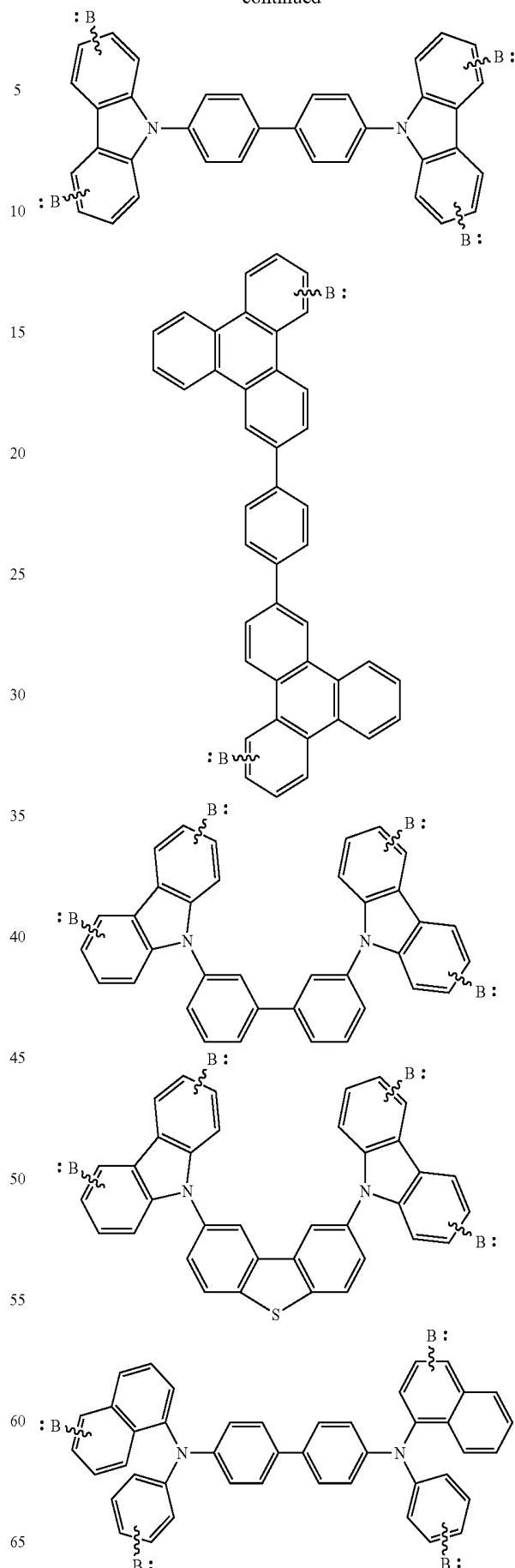
In one aspect, the functional group capable of trapping an unsaturated coordination complex is a phosphine or an isocyanide. Preferably, the phosphine has the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. Preferably, the isocyanide has the formula $\text{—N}\equiv\text{C}$.

In one aspect, the second organic compound coordinates to the metal center of the first organic compound. In another aspect, the second organic compound is a host material. Preferably, the host material is selected from the group consisting of:



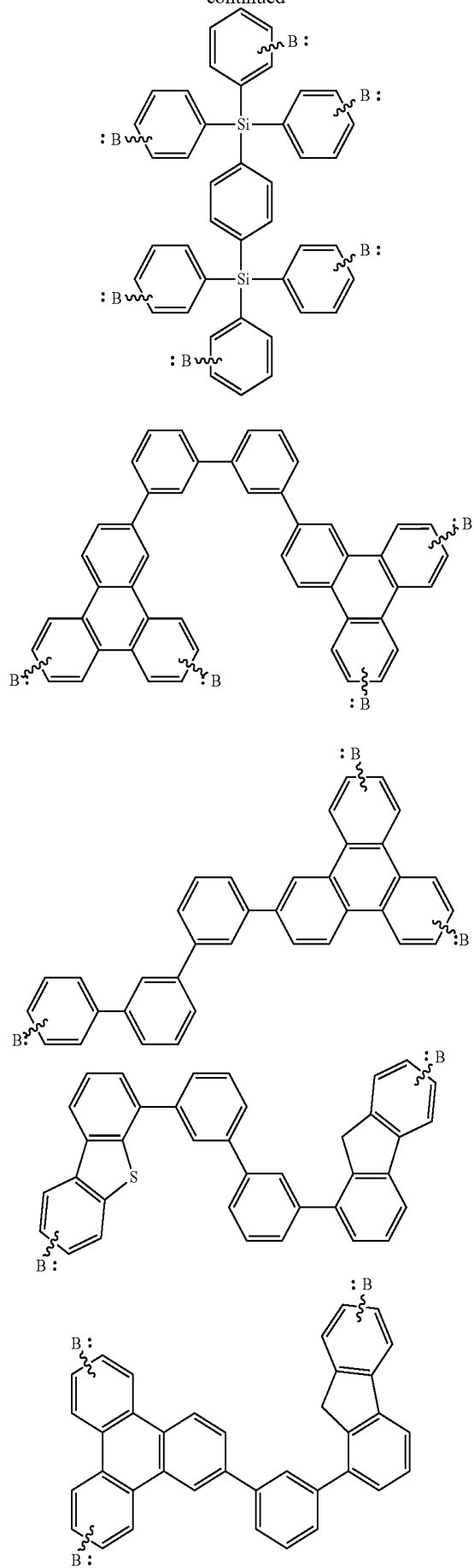
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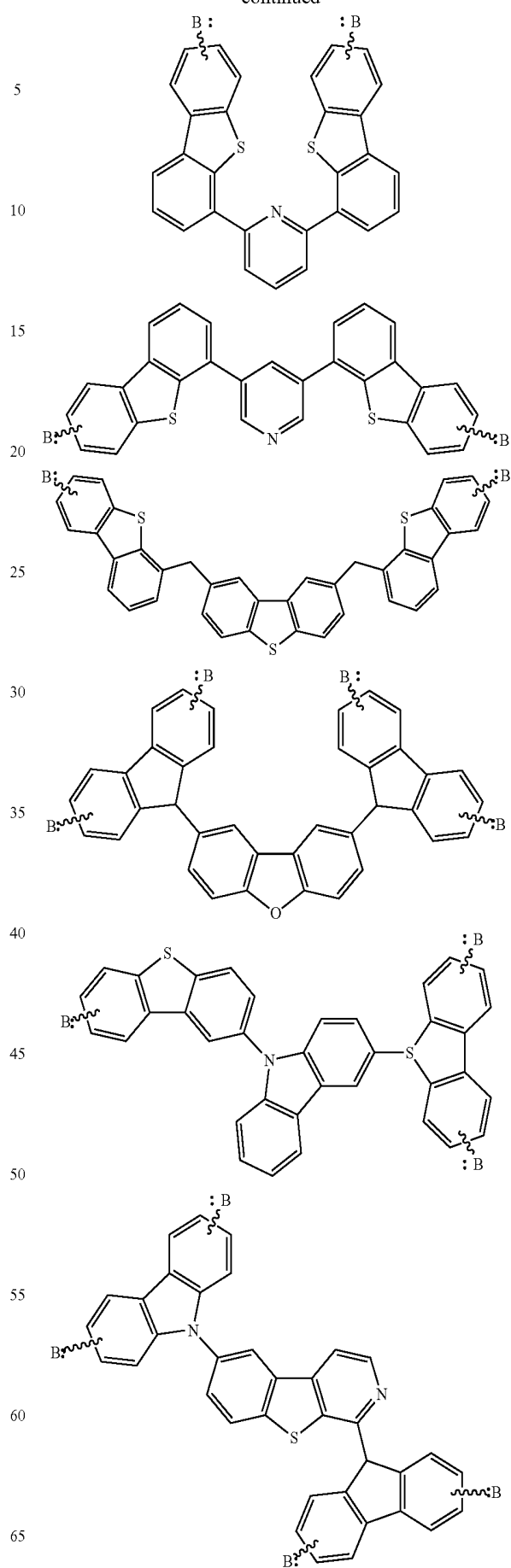


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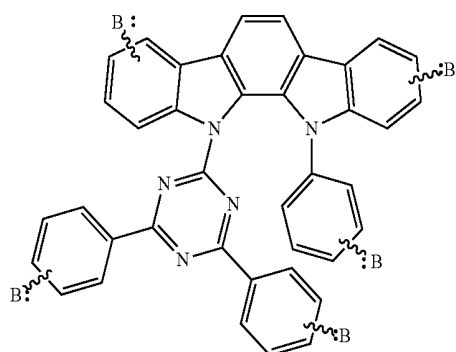
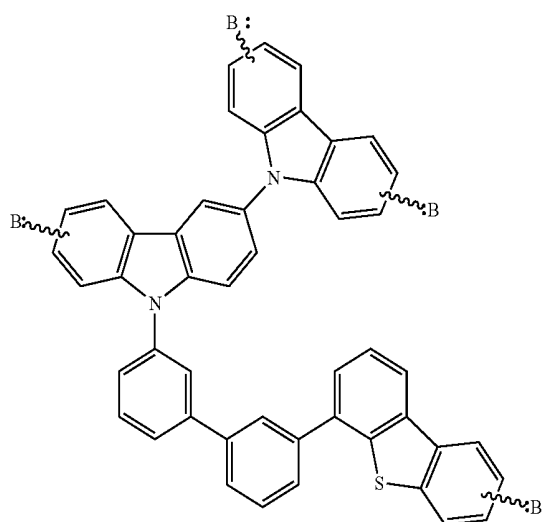
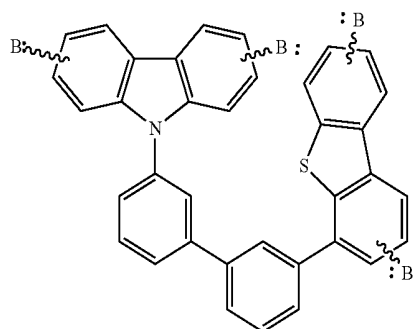
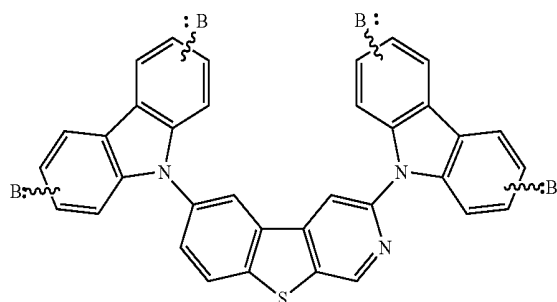
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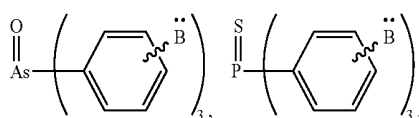
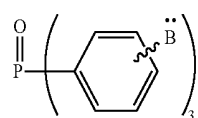
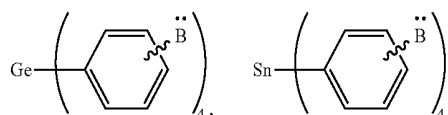
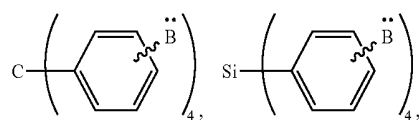
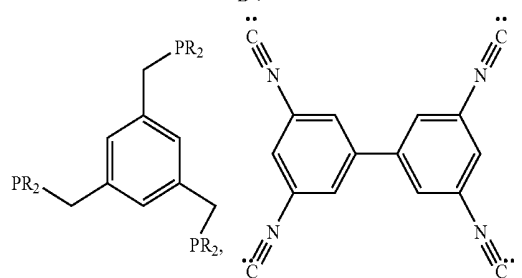
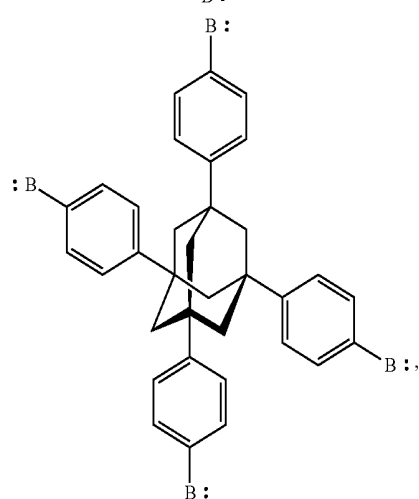
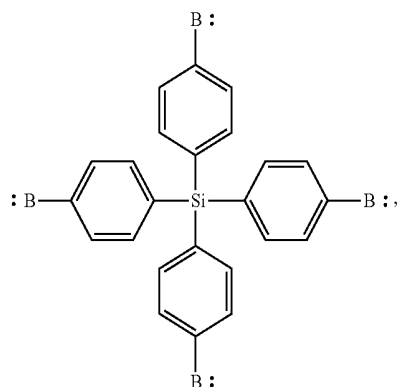
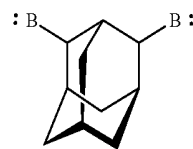
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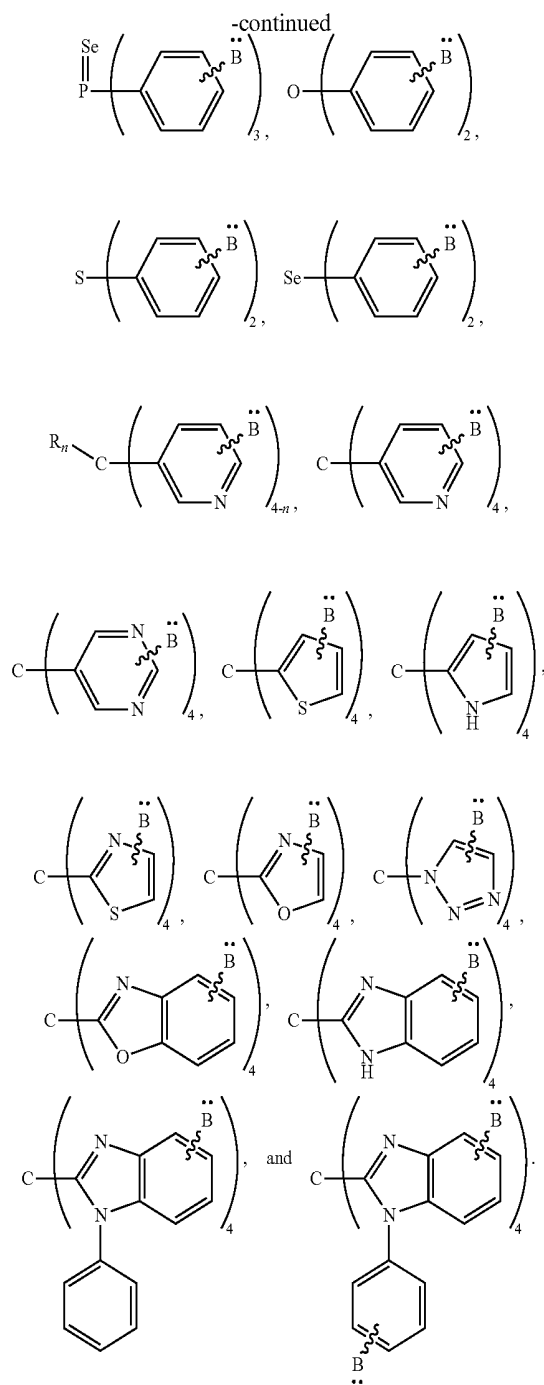
In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

In one aspect, the second organic compound is a dopant material. In another aspect, the dopant material is not capable of carrying charge. Preferably, the dopant material is selected from the group consisting of:

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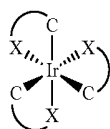
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In one aspect, :B is a phosphine having the formula —PR_2 and R is selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

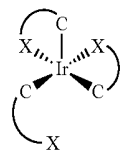
In one aspect, the dopant material is capable of carrying a charge.

In one aspect, the metal-ligand bond of the first organic compound having the formula:

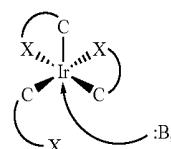


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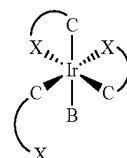
is broken, forming the coordinatively unsaturated intermediate complex having formula:



The second organic compound containing functional group :B, binds to the unsaturated intermediate complex:



forming a complex having the formula



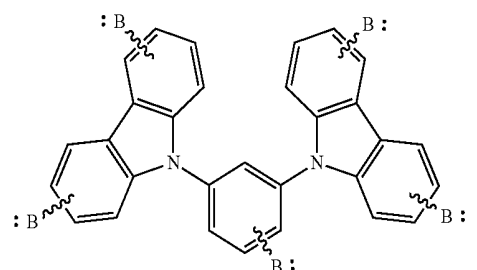
In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$. X is selected from the group consisting of N, C, O, and S. Preferably, X is N or C.

In one aspect, the first organic compound is bidentate.

In another aspect, the organic light emitting device comprises an emissive layer, and the emissive layer comprises the second organic compound.

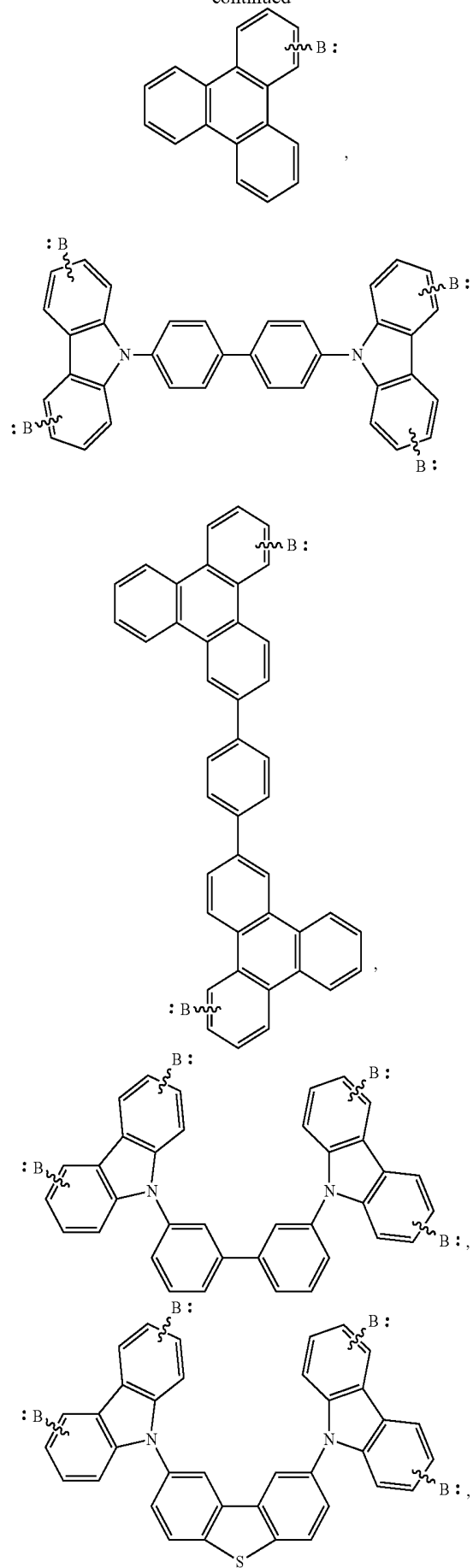
Additionally, a device comprising a trap charge compound is provided. A first device comprises an organic light emitting device, which further comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises a first organic compound containing a metal-ligand bond and a second organic compound comprising a functional group capable of trapping an unsaturated coordination complex.

In one aspect, the second organic compound coordinates to the metal center of the first organic compound. In another aspect, the second organic compound is a host material. Preferably, the host material is selected from the group consisting of:

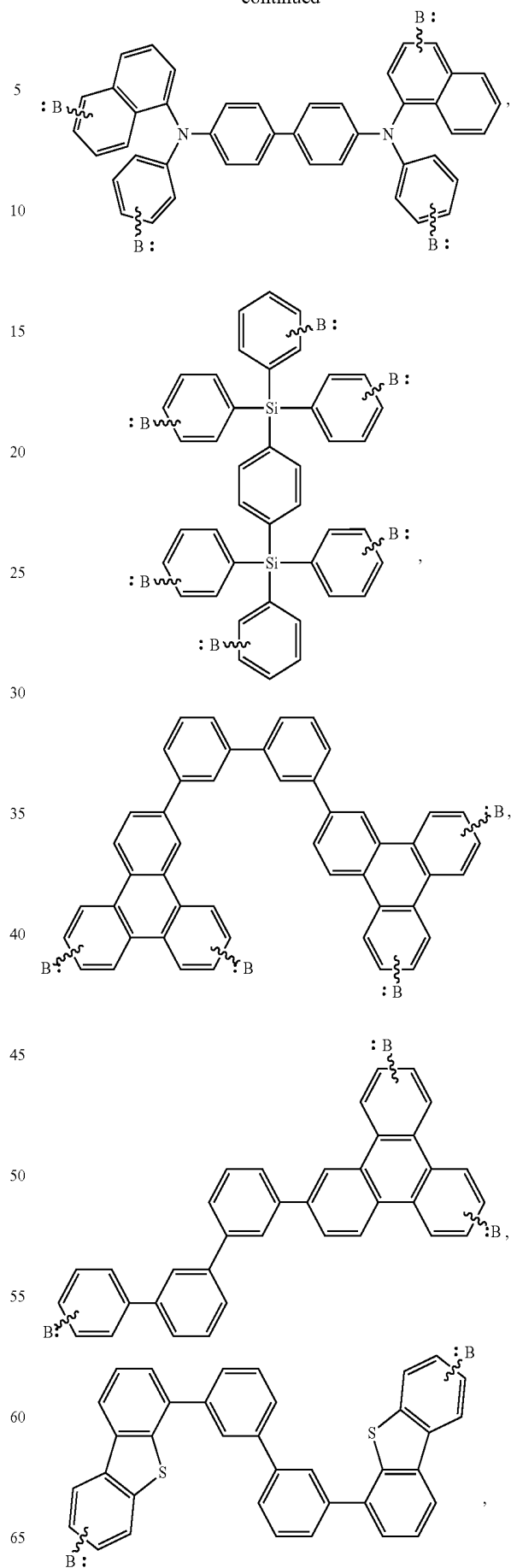


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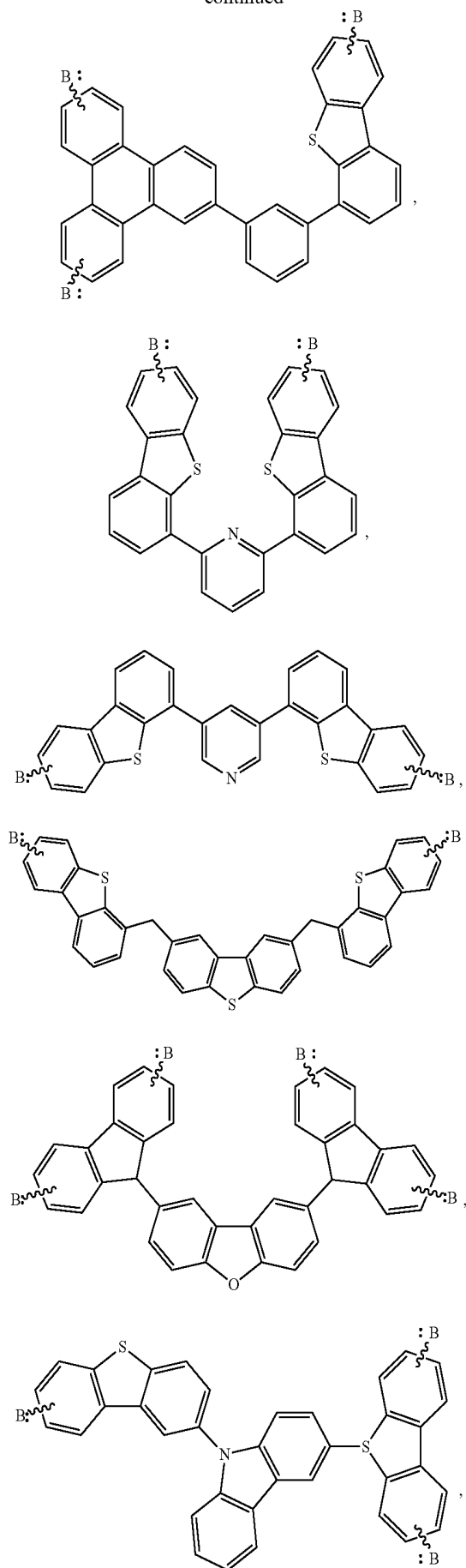
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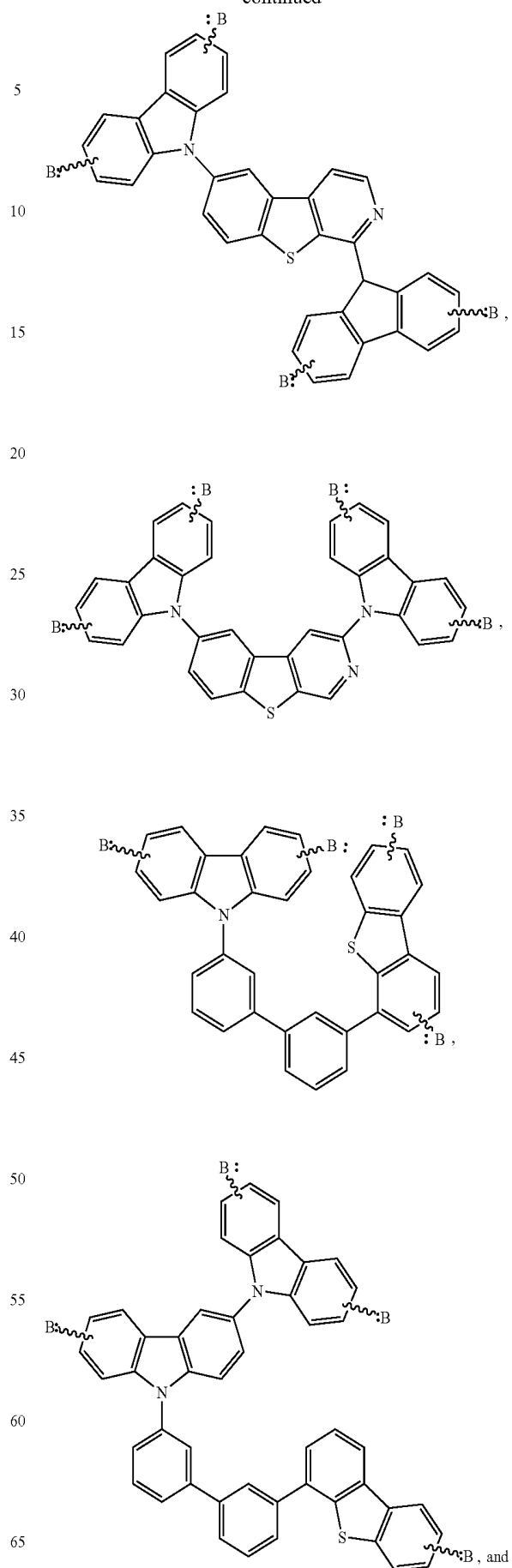
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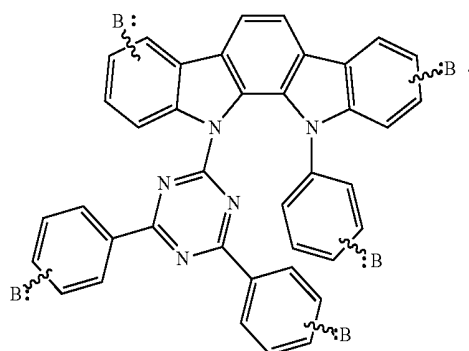
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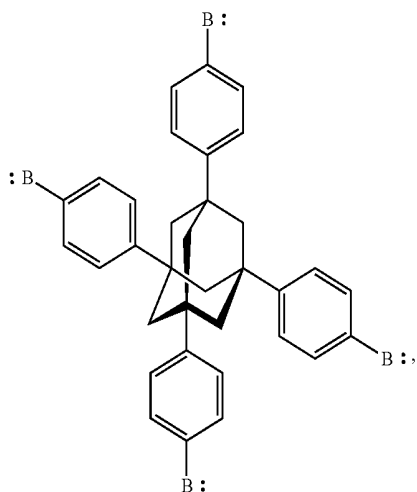
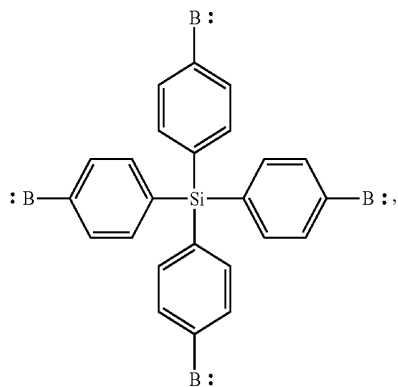
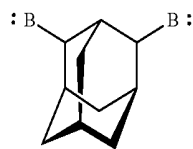
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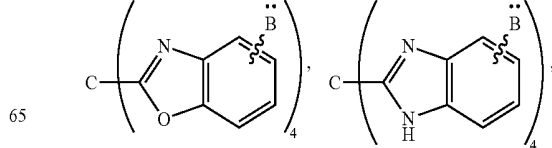
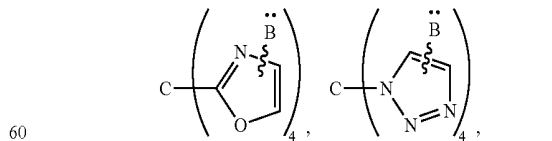
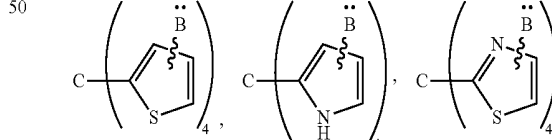
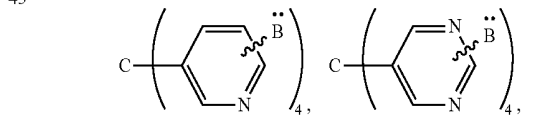
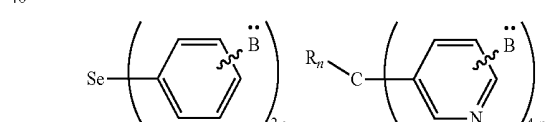
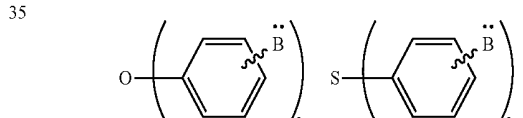
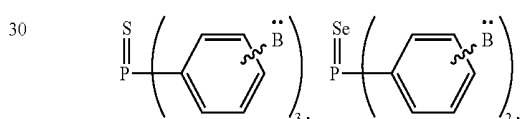
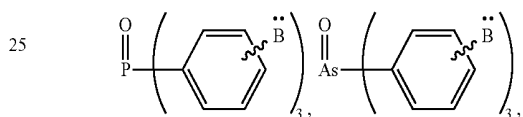
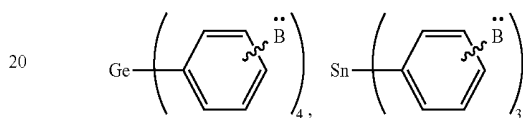
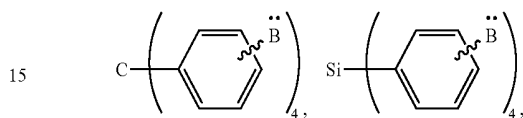
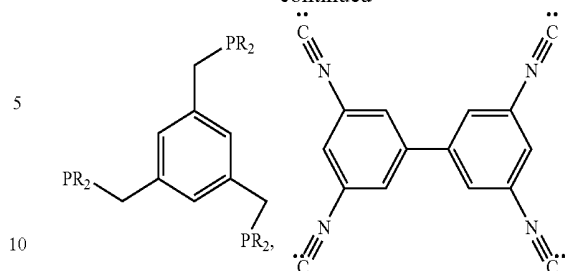
In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

In one aspect, the second organic compound is a dopant material. In another aspect, the dopant material is not capable of carrying charge. Preferably, the dopant material is selected from the group consisting of:

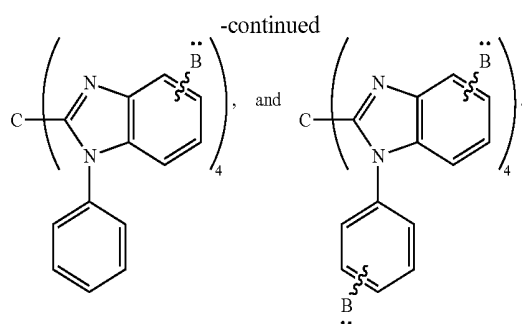


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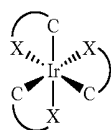


In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

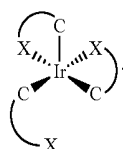
In one aspect, the dopant material is capable of carrying a charge.

In one aspect, the functional group capable of trapping an unsaturated coordination complex is a phosphine or an isocyanide. Preferably, the phosphine has the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. Preferably, the isocyanide has the formula $\text{—N}\equiv\text{C}$.

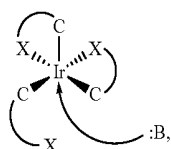
In one aspect, the metal-ligand bond of the first organic compound having the formula:



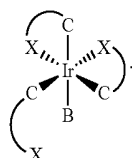
is broken, forming the coordinatively unsaturated intermediate complex having formula:



The second organic compound containing functional group :B, binds to the unsaturated intermediate complex:



forming a complex having the formula

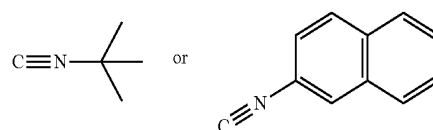


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In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$. X is selected from the group consisting of N, C, O, and S. Preferably, X is N or C.

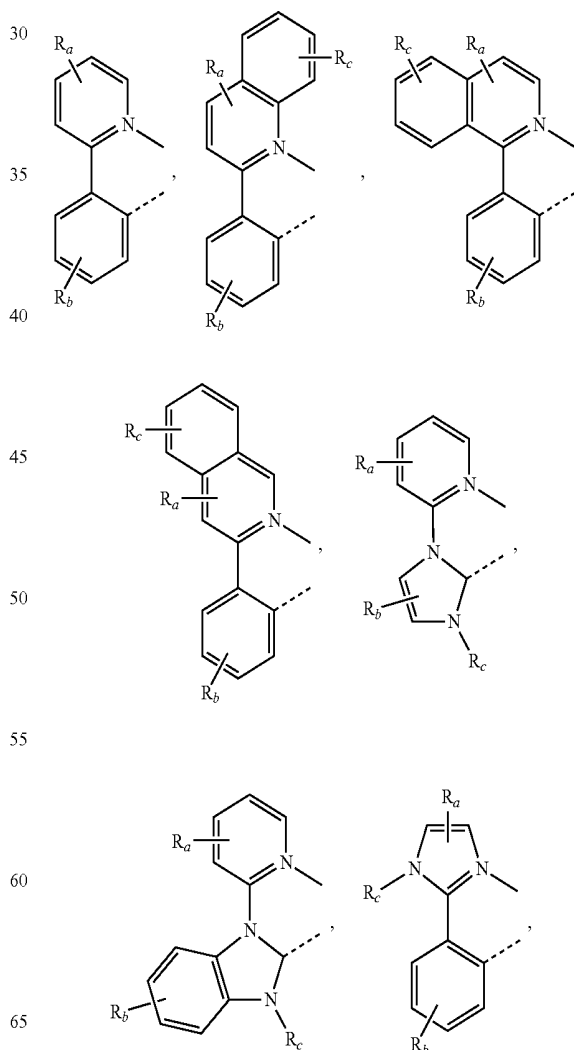
In one aspect, the first organic compound is bidentate.

In another aspect, the organic light emitting device comprises an emissive layer, and the emissive layer comprises the second organic compound. Preferably, the second compound is



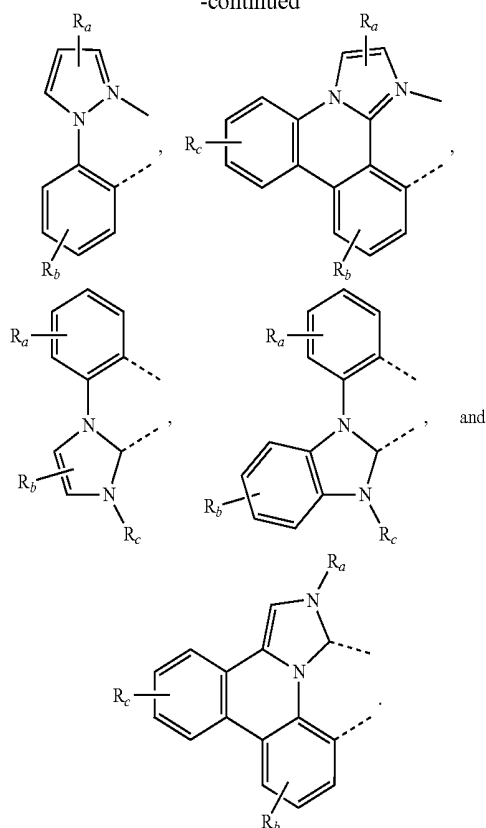
In one aspect, the organic light emitting device is a blue phosphorescent OLED.

In another aspect, the first organic compound is a transition metal complex having at least one ligand selected from the group consisting of:



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Each of R_a , R_b and R_c may represent mono, di, tri, or tetra substituents. Each of R_a , R_b and R_c substituent are independently selected from a group consisting of hydrogen, deuterium, heteroalkyl, aryl, or heteroaryl. Two adjacent substituents may form into a ring.

Additionally, a first device comprising a compound containing a cleaved metal-ligand bond is provided. A first device comprises an organic light emitting device, which further comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises a first compound containing a cleaved metal-ligand bond and a second compound comprising a functional group capable of trapping an unsaturated coordination complex.

Moreover, devices comprising an isonitrile-substituted host material are also provided. In particular, a first device comprises an organic light emitting device, which further comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises an isonitrile-substituted host material. Preferably, the organic layer is an emissive layer.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 shows an organic light emitting device.

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

FIG. 3 shows a trap capture compound binding to an unsaturated intermediate complex.

FIG. 4 shows HPLC chromatograms at 0 minute and 10 minute time points during a photolysis experiment.

FIG. 5 shows HPLC chromatograms at 20 minute and 60 minute time points during a photolysis experiment.

FIG. 6 shows HPLC chromatograms at 90 minute and 120 minute time points during a photolysis experiment.

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FIG. 7 shows HPLC chromatograms at 0 minute and 6 house points during a photolysis experiment.

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. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution 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 consumer 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.

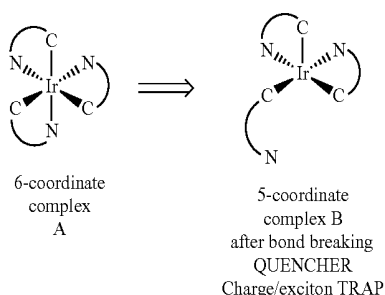
One possible reason for the short working lifetime of blue phosphorescent OLEDs is cleavage of a metal-ligand bond during operation of the device in the complex used as a luminescent dopant. The resulting coordinatively unsaturated intermediate complex is expected to have lower triplet and higher ground energy than the parent species and can thus serve as an exciton and/or charge trap for the remaining luminescent dopants. The presence of these traps may further degrade the luminescent output of the OLED. Compounds that can react with the unsaturated complex by

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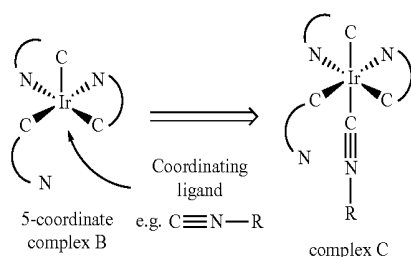
coordinating to the metal center and suppress its ability to trap energy/charge, thereby extending the operating lifetime of a blue phosphorescent OLED, are provided herein. The compound, a trap capture agent, can be added to the emissive layer of an OLED either as a host or a dopant.

Incorporation of these trap capture compounds may provide several benefits. The addition of the trap capture compound to an unsaturated intermediate complex may lower the energy for holes, such that the complex will not trap holes. Furthermore, addition of the trap capture compound to an unsaturated intermediate complex may also prevent the complex from trapping excitons, resulting in blue shift emission of the complex.

Several experiments have been performed using the model compound fac-Ir(ppz)₃ in order to verify the formation and capture of an unsaturated five-coordinate complex caused by photolytic metal-ligand bond breaking. The six coordinate complex (A) has a high triplet energy that causes it to undergo bond breaking before it can relax to the ground state. Complex B is a 16 electron complex that is expected to have lower triplet energy than A and therefore, act as non-emissive charge exciton trap reducing the efficiency of the OLED.



It has been demonstrated that a molecule bearing an isocyanide group can intercept the intermediate complex B and bind strongly to iridium complex to form complex C.



This reaction enables complex C to regain an octahedral saturated coordination sphere. Moreover, the inductive electron-withdrawing effect of the strong field isocyanide ligand leads to a blue-shift in the absorption spectrum and raises the triplet energy of C compared to A.

The trap charge compounds provided herein may include host materials suitable for blue dopant phosphors and dopant materials, which are endowed with proper functional group able to trap an unsaturated coordination complex, for example, an isocyanide or a phosphine group. For example, cyclometallated blue phosphorescent materials with a C⁺N cyclometallated ligand or a C⁺C metal-carbene system endowed with proper functional groups to trap an unsaturated complex are suitable for use as a trap charge compound.

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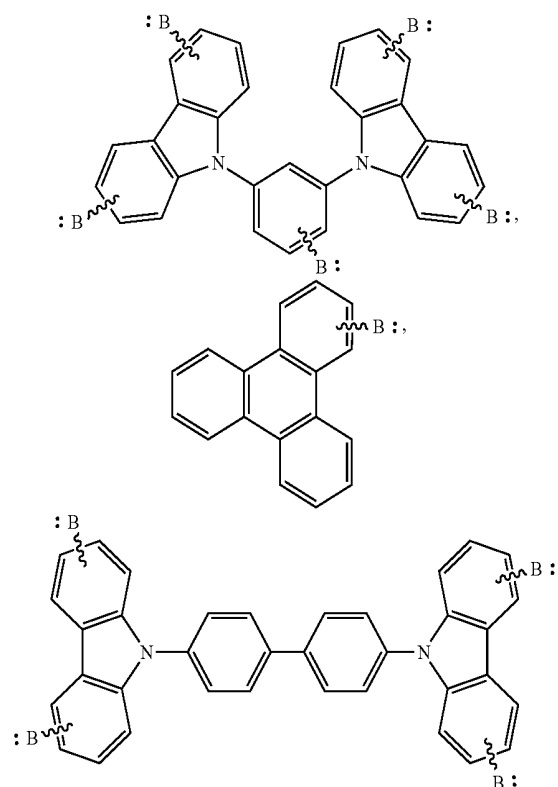
Methods for trapping a low coordinate structure, resulting from cleavage of a metal-ligand bond in the compound, and converting it back to the original coordination number are provided. Generally, the methods consist of operating an organic light emitting device comprising a first organic compound containing a metal-ligand bond and a second organic compound comprising a functional group capable of binding to the metal of an unsaturated coordination complex. A metal-ligand bond in the first organic compound cleaves during operation of the device, thereby creating a coordinatively unsaturated intermediate complex. The second organic compound reacts with the coordinatively unsaturated intermediate complex, which can suppress the ability of the coordinatively unsaturated intermediate complex to trap charge and excitons.

The methods provided herein comprise operating an organic light emitting device comprising a first organic compound containing a metal-ligand bond and a second organic compound comprising a functional group capable of trapping an unsaturated coordination complex; cleaving the metal-ligand bond in the first organic compound, thereby creating a coordinatively unsaturated intermediate complex; and reacting the second organic compound with the coordinatively unsaturated intermediate complex.

In one aspect, the method further comprises suppressing the ability of the coordinatively unsaturated intermediate complex to trap charge and excitons.

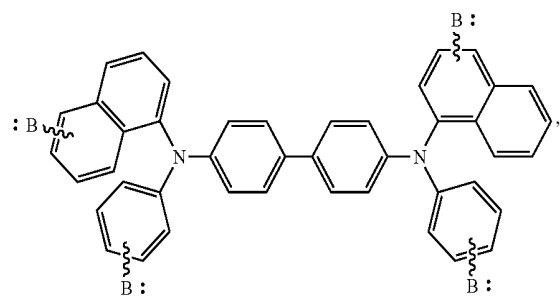
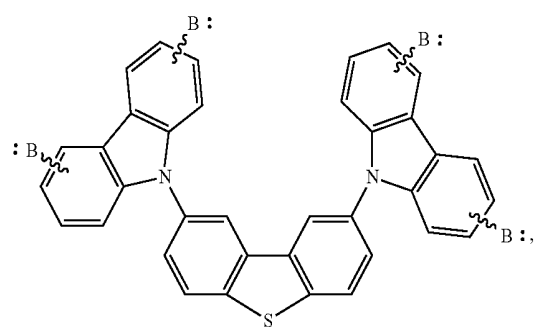
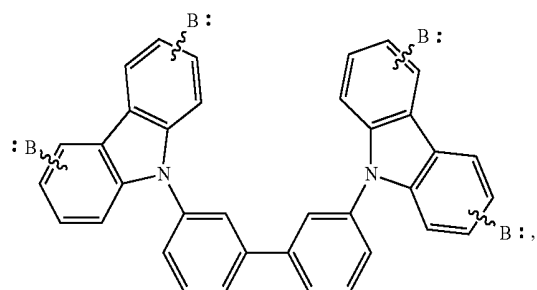
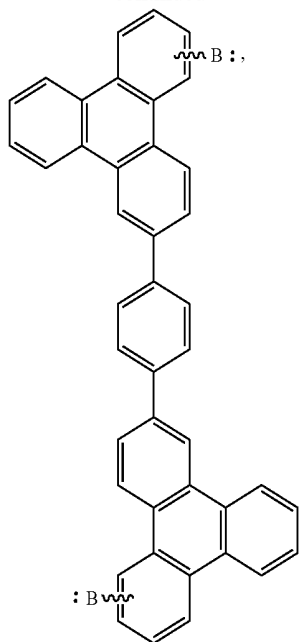
In one aspect, the functional group capable of trapping an unsaturated coordination complex is a phosphine or an isocyanide. Preferably, the phosphine has the formula —PR₂ and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. Preferably, the isocyanide has the formula —N≡C.

In one aspect, the second organic compound coordinates to the metal center of the first organic compound. In another aspect, the second organic compound is a host material. Preferably, the host material is selected from the group consisting of:

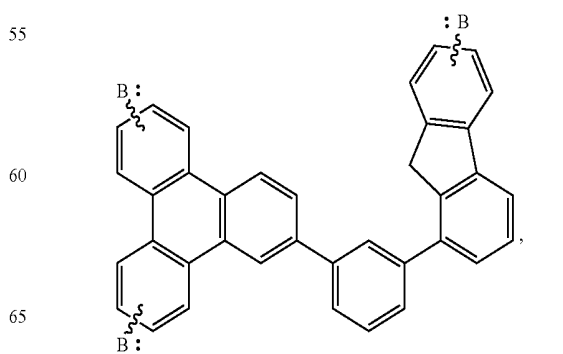
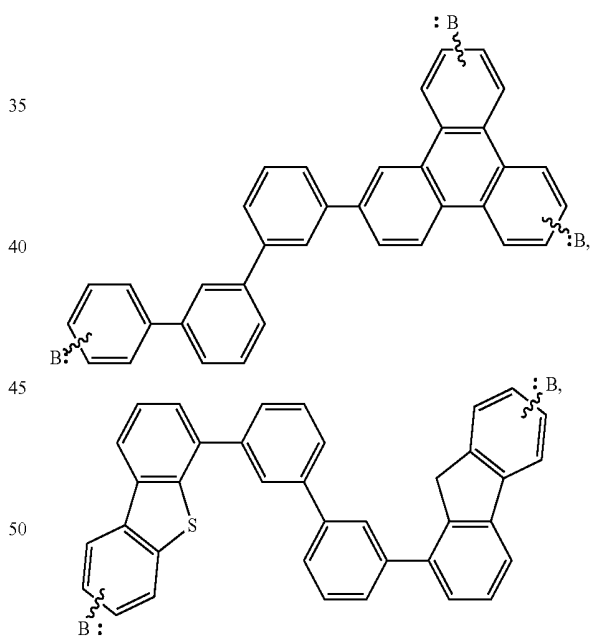
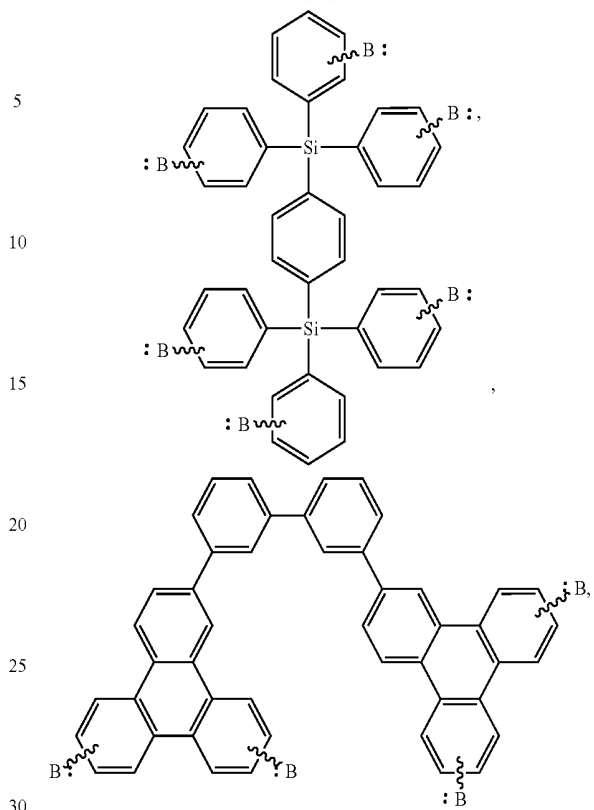


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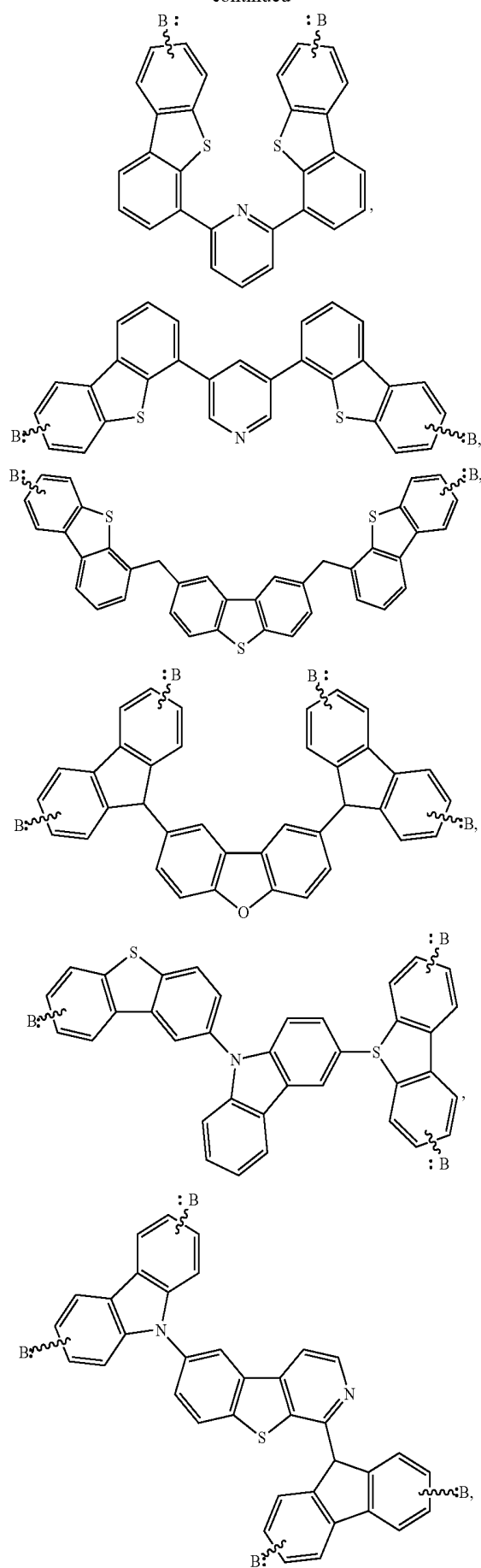
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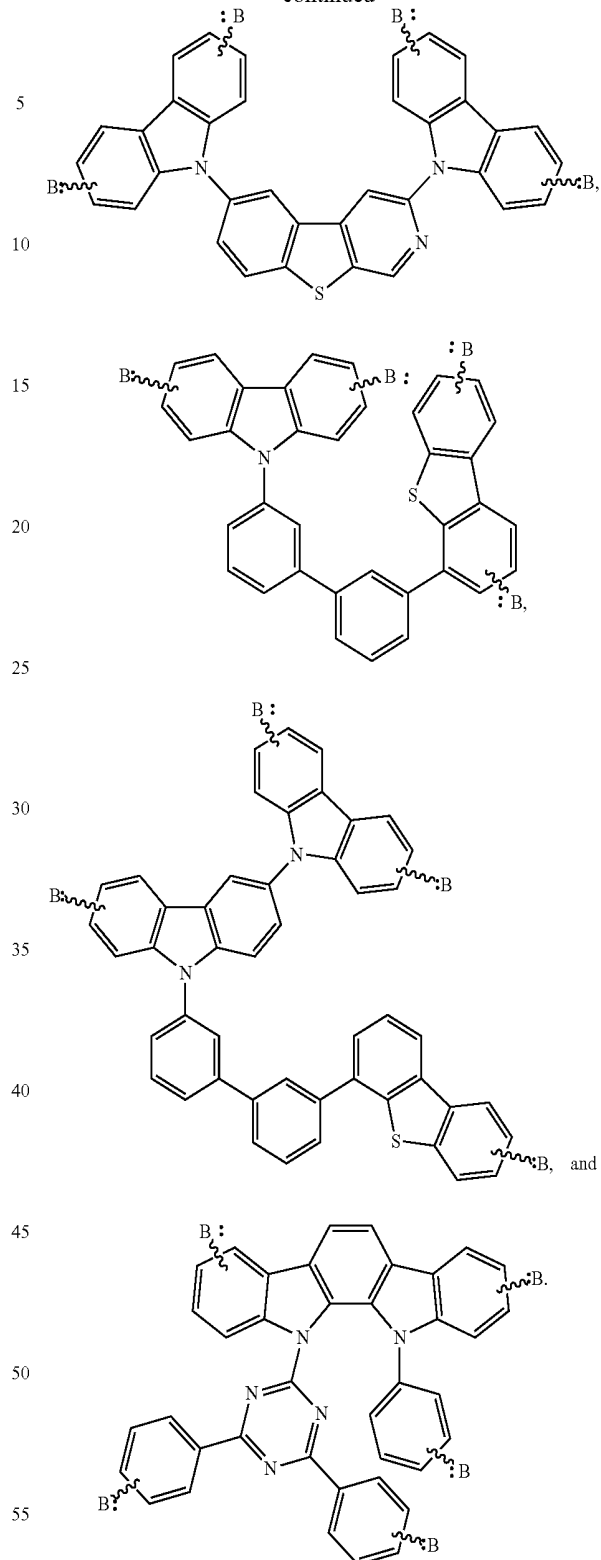
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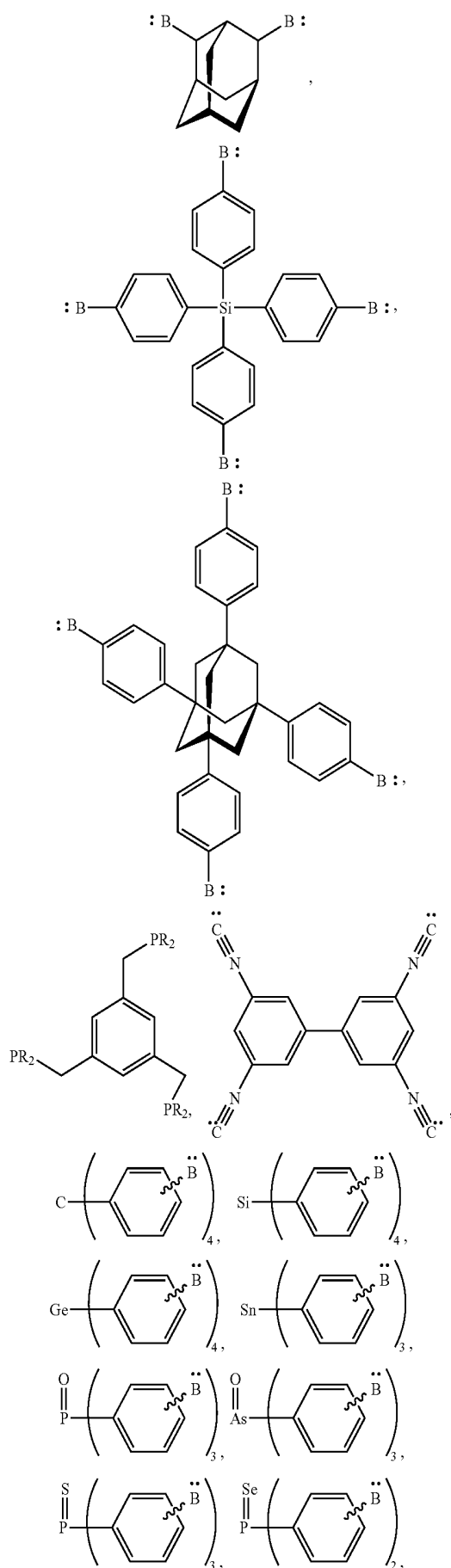
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In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

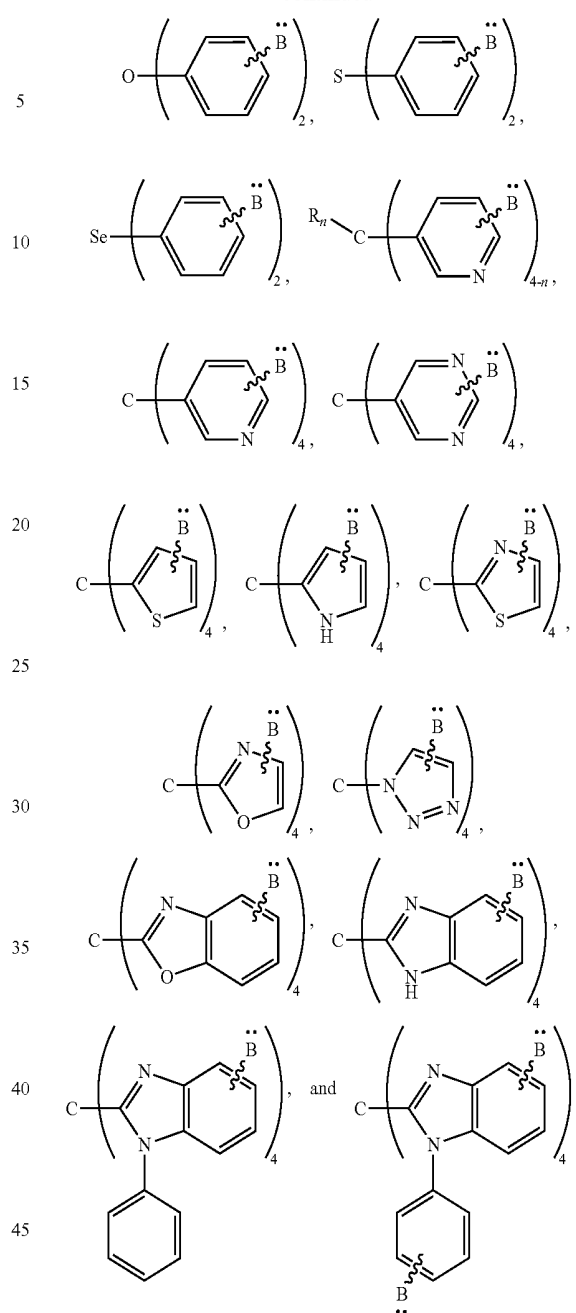
In one aspect, the second organic compound is a dopant material. In another aspect, the dopant material is not capable of carrying charge. Preferably, the dopant material is selected from the group consisting of:

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50 In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

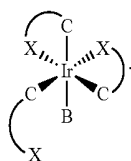
55 In one aspect, the dopant material is capable of carrying a charge.

In one aspect, the metal-ligand bond of the first organic compound having the formula:

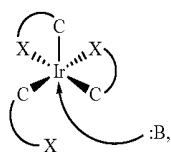


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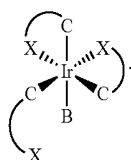
Is broken, forming the coordinatively unsaturated intermediate complex having formula:



The second organic compound containing functional group :B binds to the unsaturated intermediate complex:



forming a complex having the formula



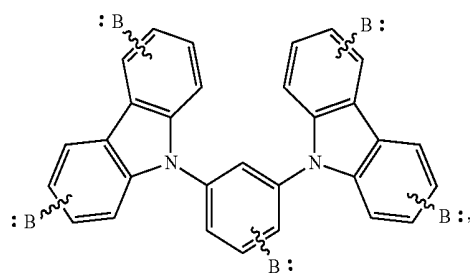
in one aspect, :B is a phosphine having the formula —PR, and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula —N≡C, X is selected from the group consisting of N, C, O, and S. Preferably, X is N or C. Additionally, we believe that this is the first report of trapping the intermediate complex along the transition pathway from meridional to facial.

Most phosphorescent materials used in OLEDs are bidentate. Therefore, in one aspect, the first organic compound is bidentate.

In another aspect, the organic light emitting device comprises an emissive layer, and the emissive layer comprises the second organic compound.

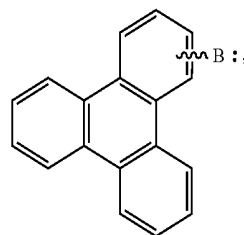
Additionally, a device comprising a trap charge compound is provided. A first device comprises an organic light emitting device, which further comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises a first organic compound containing a metal-ligand bond and a second compound comprising a functional group capable of trapping an unsaturated coordination complex.

In one aspect, the second organic compound coordinates to the metal center of the first organic compound. In another aspect, the second organic compound is a host material. Preferably, the host material is selected from the group consisting of:



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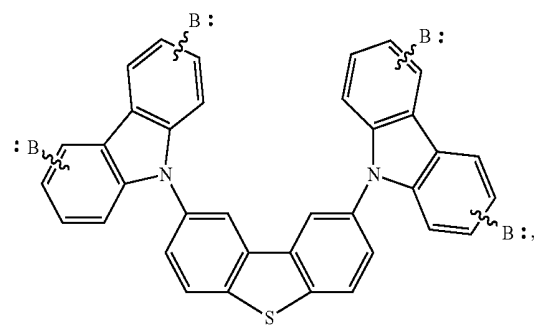
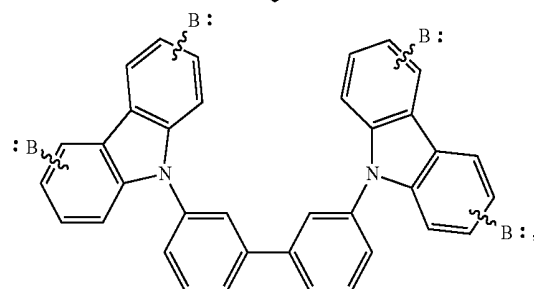
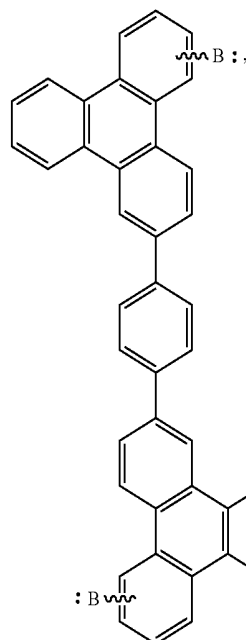
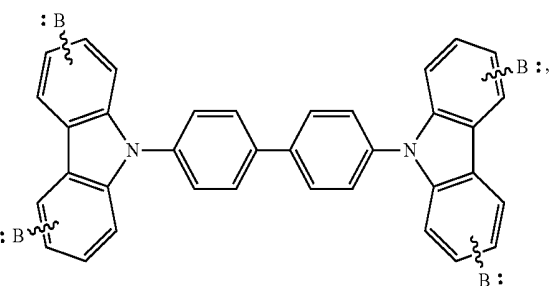
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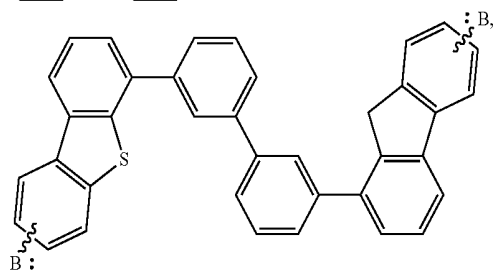
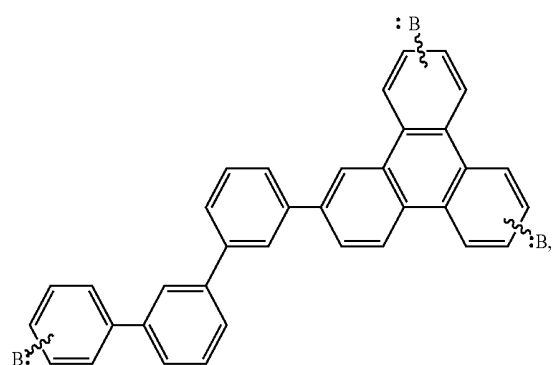
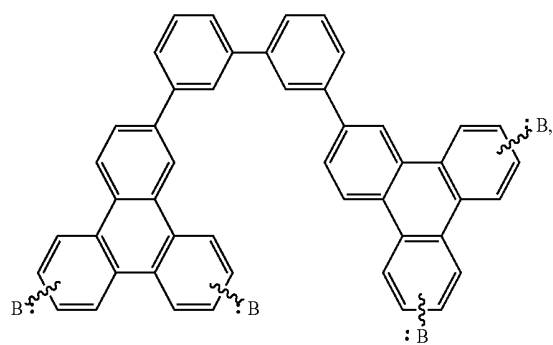
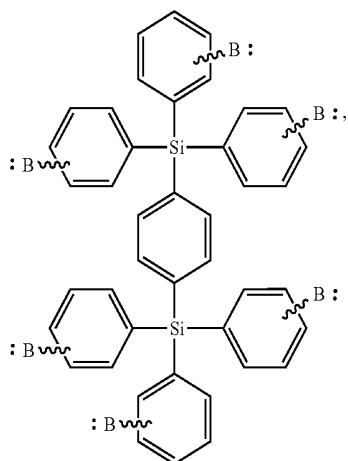
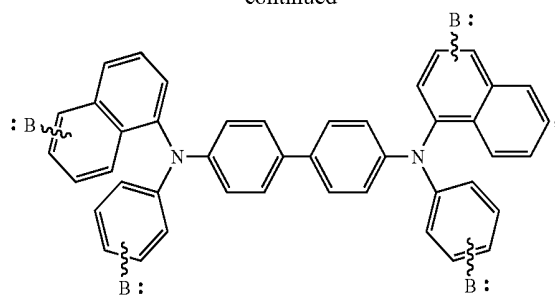
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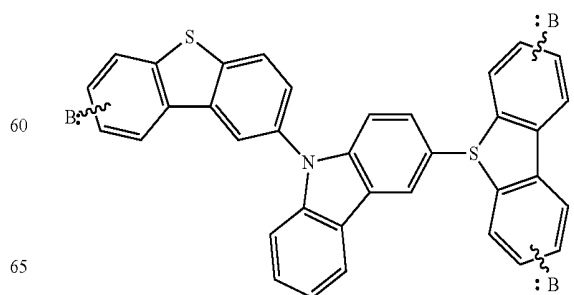
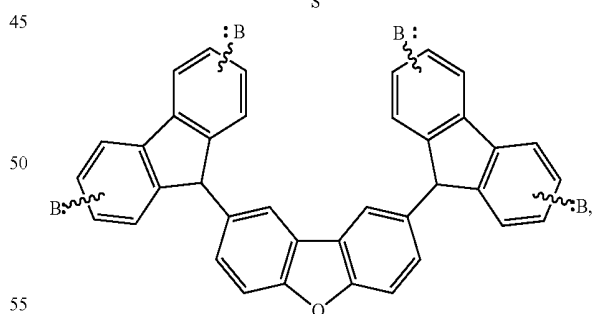
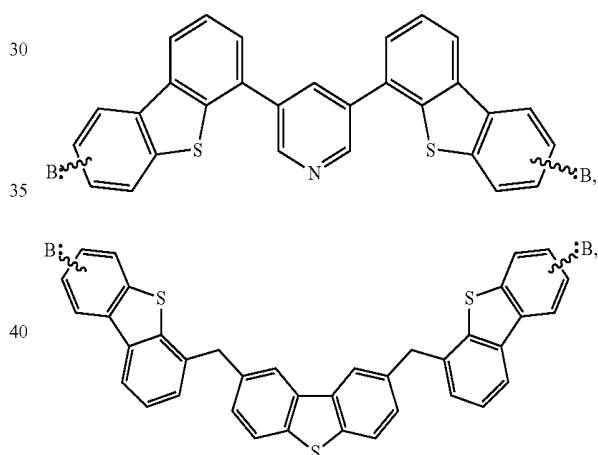
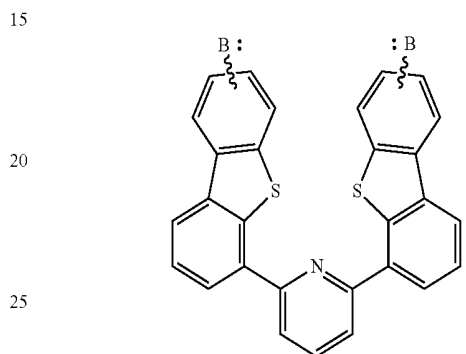
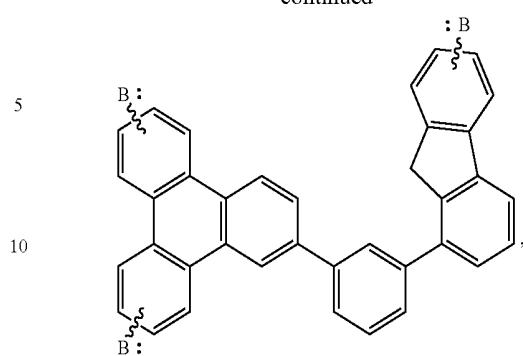


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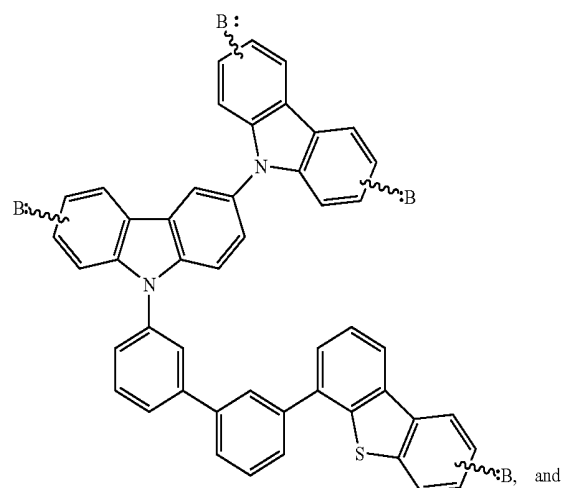
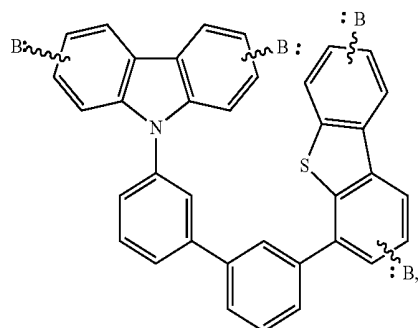
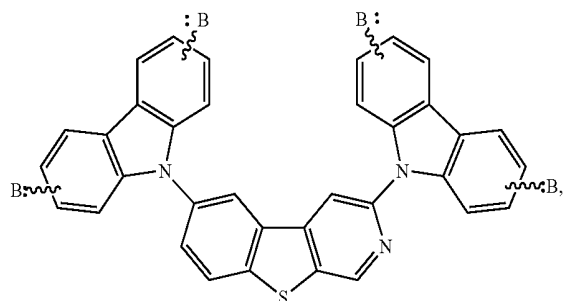
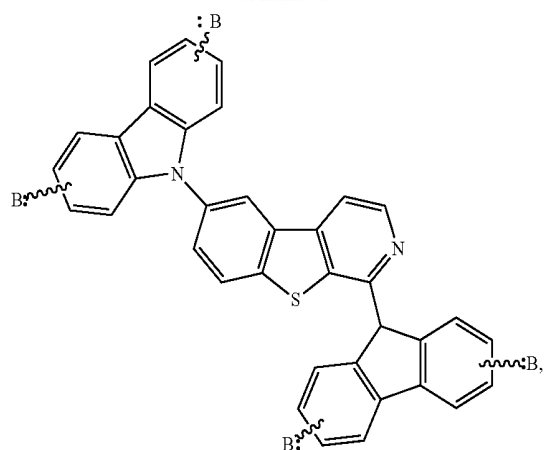
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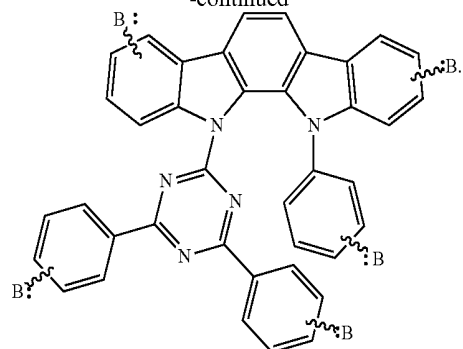
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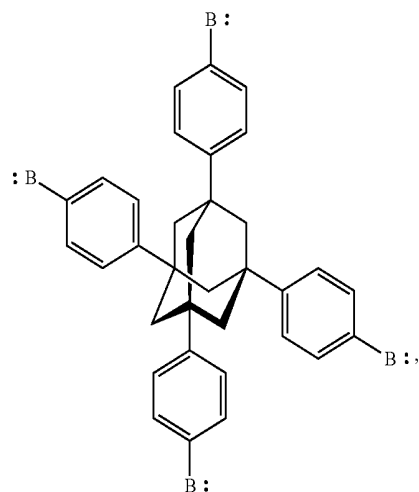
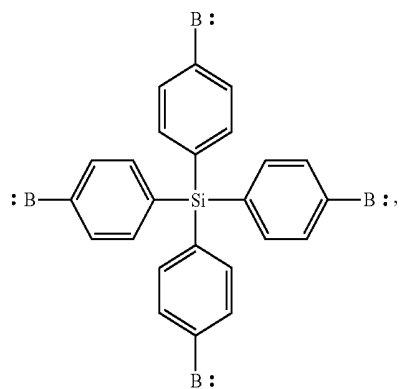
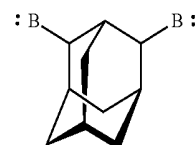
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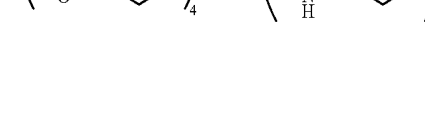
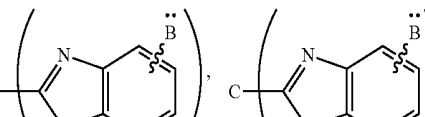
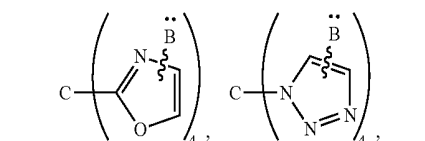
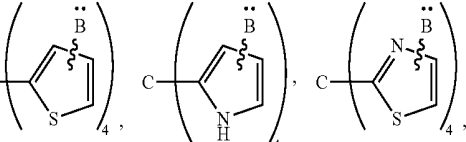
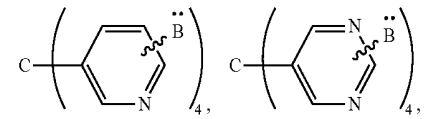
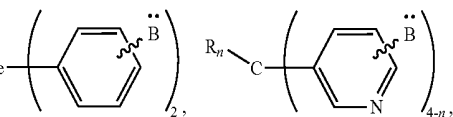
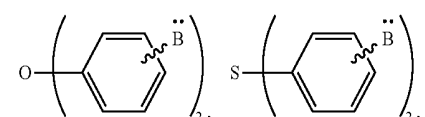
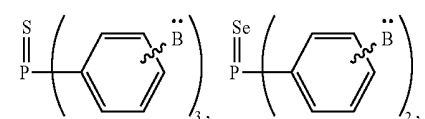
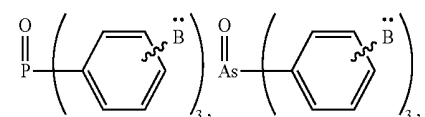
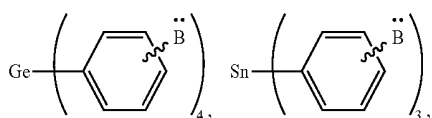
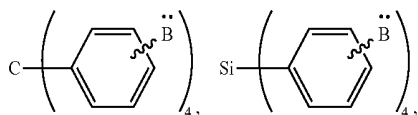
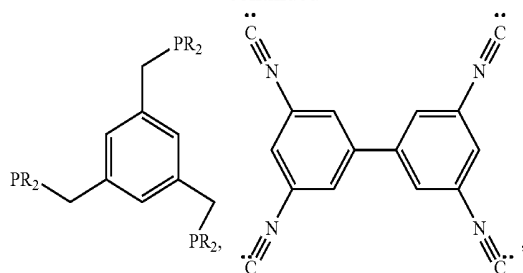
In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

In one aspect, the second organic compound is a dopant material. In another aspect, the dopant material is not capable of carrying charge. Preferably, the dopant material is selected from the group consisting of:



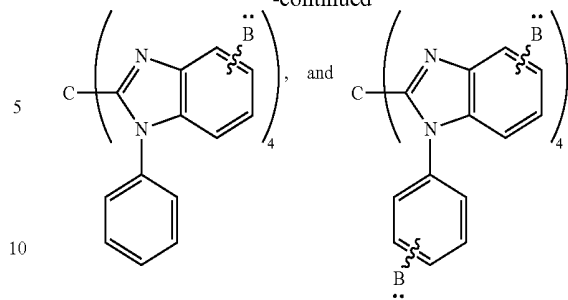
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In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$.

In one aspect, the dopant material is capable of carrying a charge.

In one aspect, the functional group capable of trapping an unsaturated coordination complex is a phosphine or an isocyanide. Preferably, the phosphine has the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. Preferably, the isocyanide has the formula $\text{—N}\equiv\text{C}$.

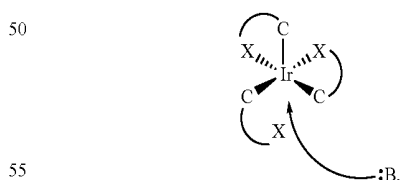
In one aspect, the metal-ligand bond of the first organic compound having the formula:



is broken, forming the coordinatively unsaturated intermediate complex having formula:



The second organic compound containing functional group :B binds to the unsaturated intermediate complex:



forming a complex having the formula

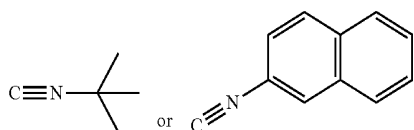


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In one aspect, :B is a phosphine having the formula —PR_2 and R selected from the group consisting of hydrogen, methyl, ethyl, propyl, butyl, alkyl, and phenyl. In another aspect, :B is an isocyanide having the formula $\text{—N}\equiv\text{C}$. X is selected from the group consisting of N, C, O, and S. Preferably, X is N or C.

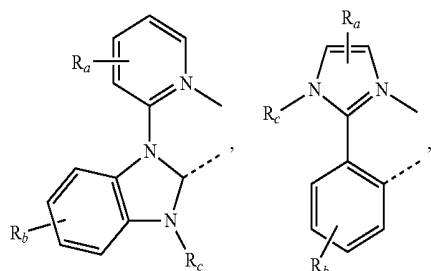
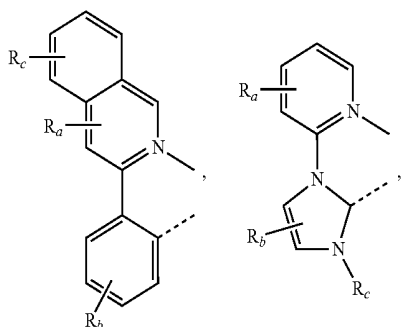
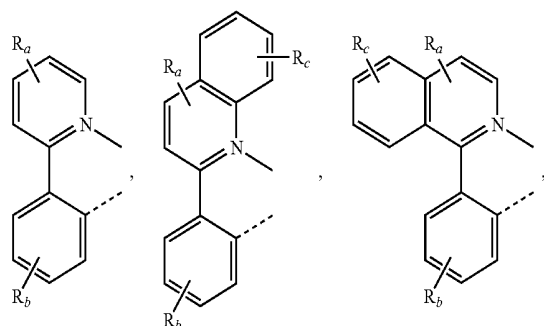
In one aspect, the first organic compound is bidentate.

In another aspect, the organic light emitting device comprises an emissive layer, and the emissive layer comprises the second organic compound. Preferably, the second compound is



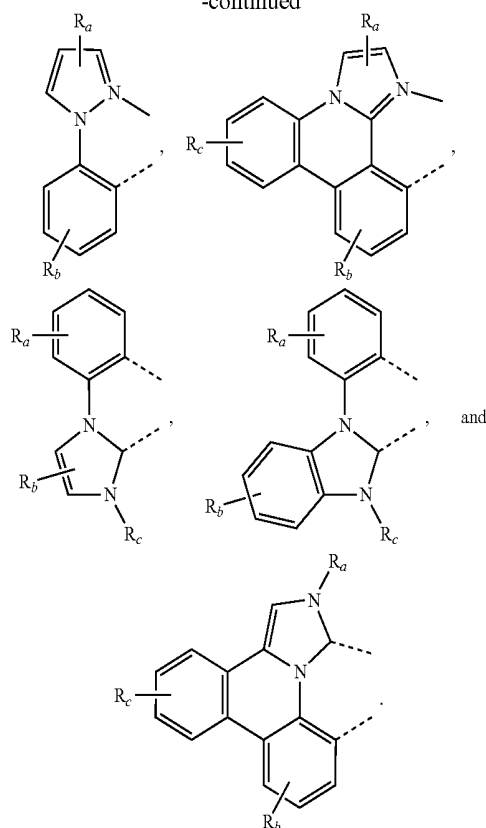
In one aspect, the organic light emitting device is a blue phosphorescent OLED.

In another aspect, the first organic compound is a transition metal complex having at least one ligand selected from the group consisting of:



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Each of R_a , R_b and R_c may represent mono, di, tri, or tetra substituents. Each of R_a , R_b and R_c substituent are independently selected from a group consisting of hydrogen, deuterium, heteroalkyl, aryl, or heteroaryl. Two adjacent substituents may form into a ring.

Additionally, a first device comprising a compound containing a cleaved metal-ligand bond is provided. A first device comprises an organic light emitting device, which further comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises a first organic compound containing a cleaved metal-ligand bond and a second compound comprising a functional group capable of trapping an unsaturated coordination complex.

Moreover, devices comprising an isonitrile-substituted host material are also provided. In particular, a first device comprises an organic light emitting device, which further comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises an isonitrile-substituted host material. Preferably, the organic layer is an emissive layer.

55 Combination with other Materials

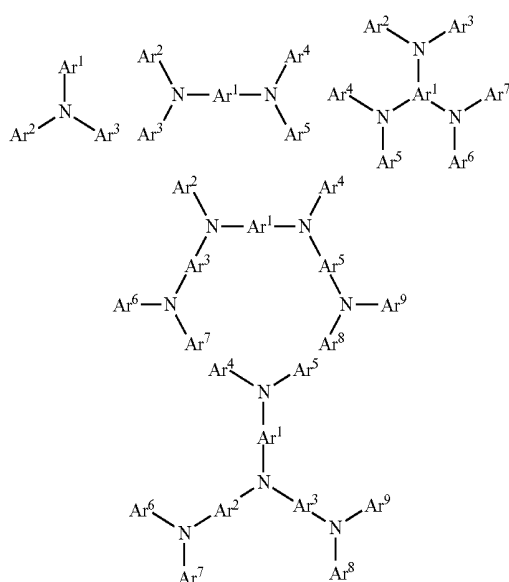
The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

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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 not limit to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as MoO_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 HIL, or HTL include, but not limit to the following general structures:

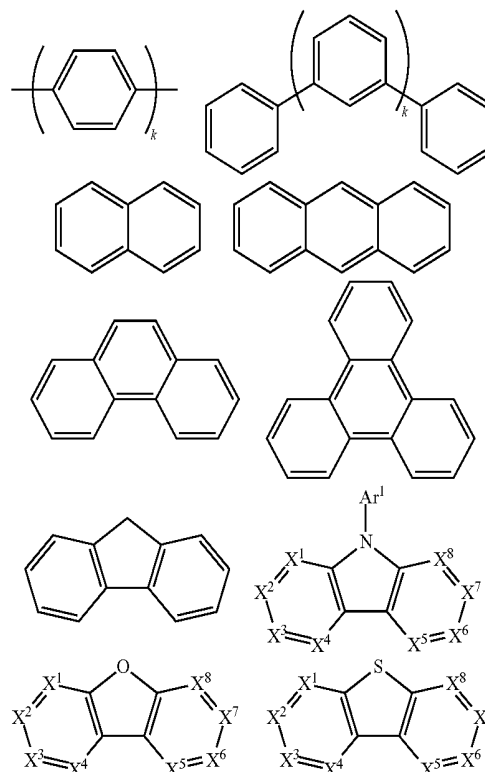


Each of Ar^1 to Ar^9 is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenylene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothio-
 phene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolidopyridine, 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, xan-
 thene, acridine, phenazine, phenothiazine, phenoxazine, benzofuro-
 pyridine, furodipyr-
 idine, benzothienopyridine, thienodipyr-
 idine, benzoselenophenopyridine, and seleno-
 phenodipyr-
 idine; and group consisting of 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron

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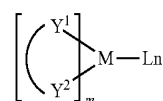
atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

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 are used in HIL or HTL include, but not limit 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 cabene 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.

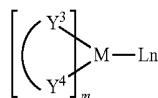
Host:

The light emitting layer of the organic EL device in embodiments of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant

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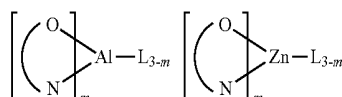
material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant.

Examples of metal complexes used as host 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.

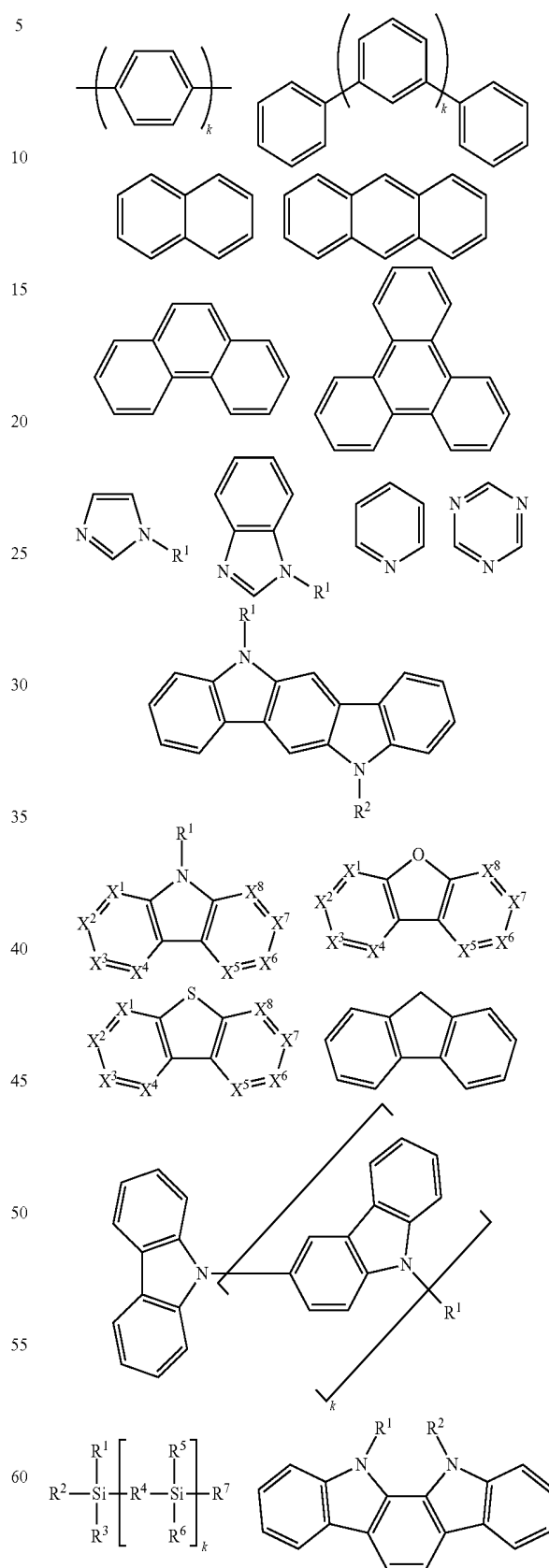
In another aspect, M is selected from Ir and Pt.

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

Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyddine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoxaline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropydine, 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, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl.

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



R¹ to R⁷ is independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl,

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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.

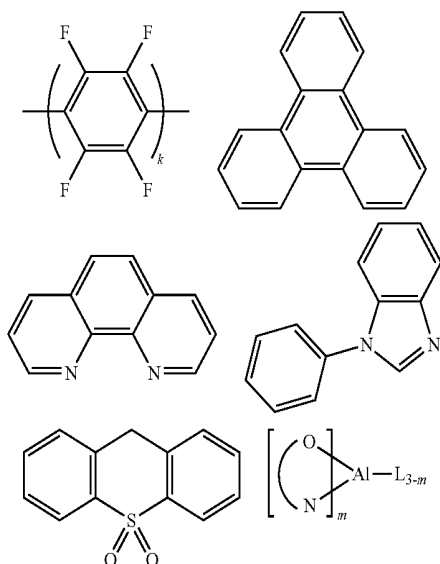
X¹ to X⁸ is selected from CH or N.

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

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

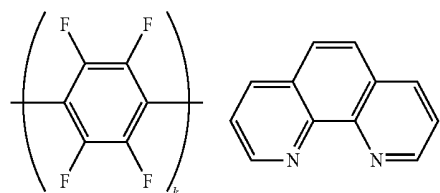


k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

ETL:

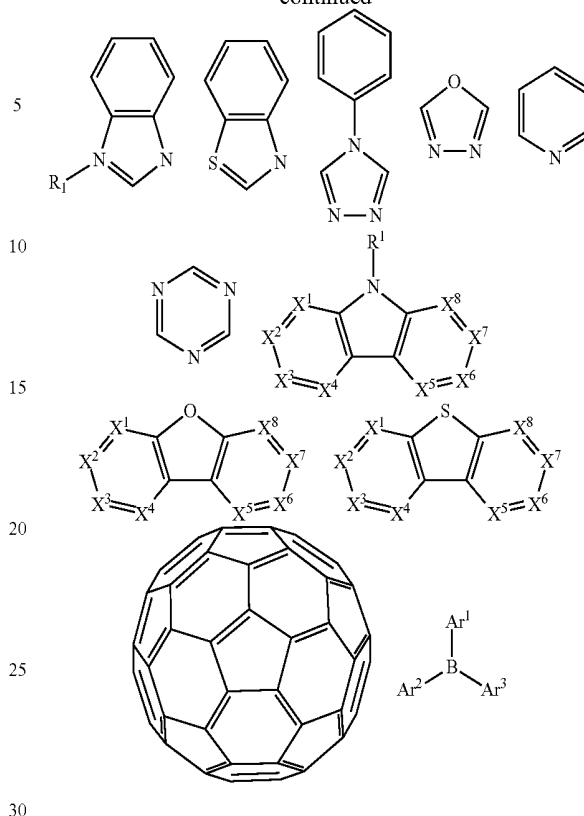
Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may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

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



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-continued



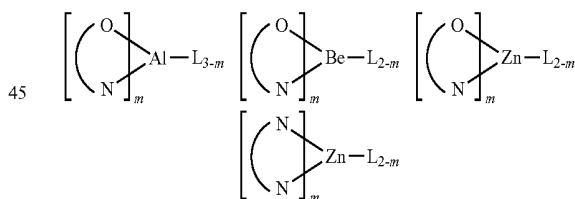
R¹ is selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

Ar¹ to Ar³ has the similar definition as Ar's mentioned above.

k is an integer from 0 to 20.

X¹ to X⁸ is selected from CH or N.

In another aspect, the metal complexes used in ETL contains, but not limit 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 transporting 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

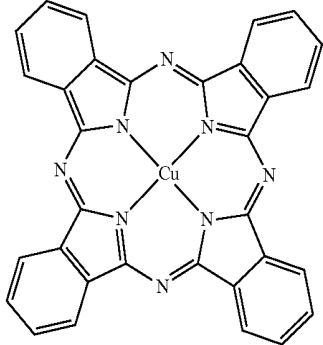
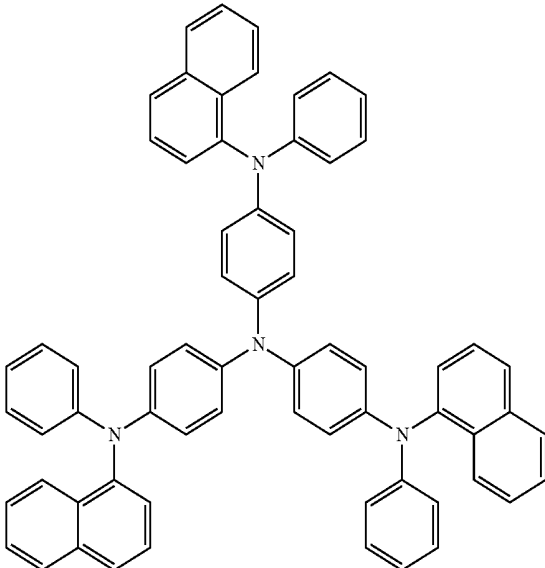
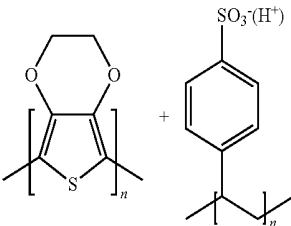
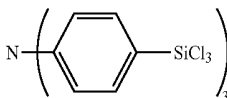
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Phthalocyanine and porphyrin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF _x Fluorohydrocarbon polymer	$\text{---}[\text{CH}_x\text{F}_y]_n\text{---}$	Appl. Phys. Lett. 78, 673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

TABLE 1-continued

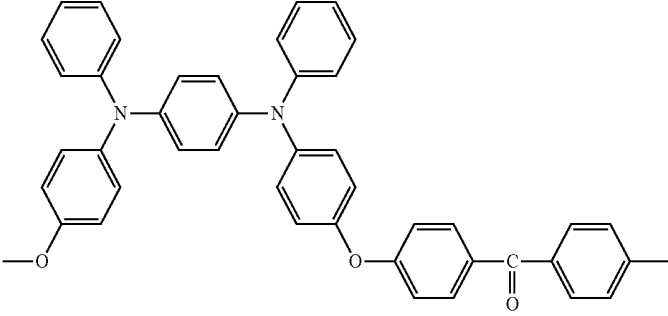
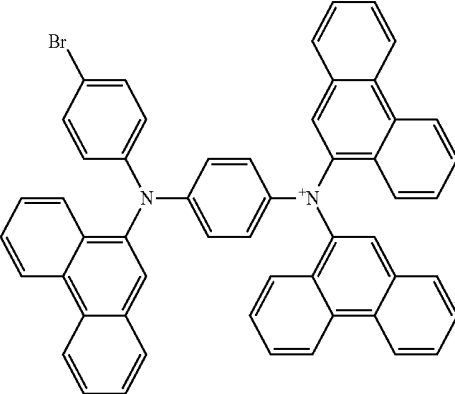
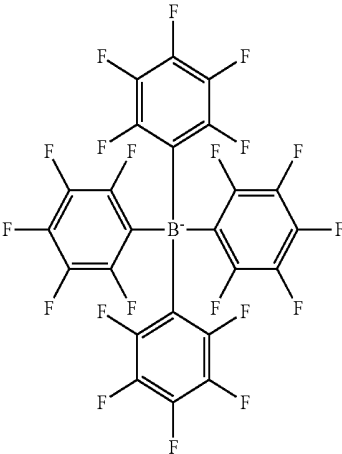
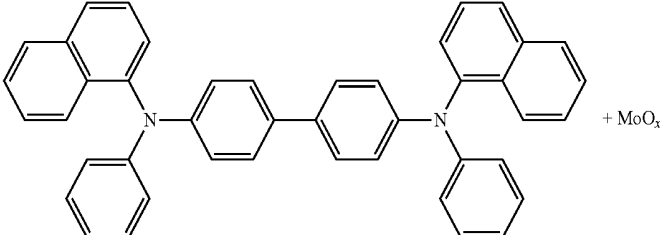
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine or polythiophene polymers with conductivity dopants		EA01725079A1
		
		
Arylamines complexed with metal oxides such as molybdenum and tungsten oxides		SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 1-continued

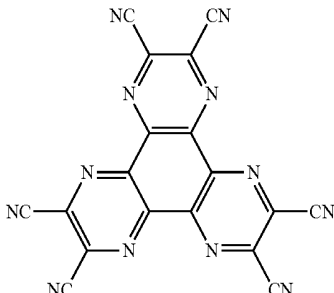
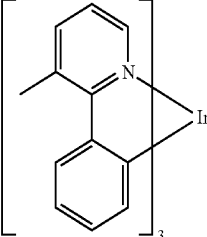
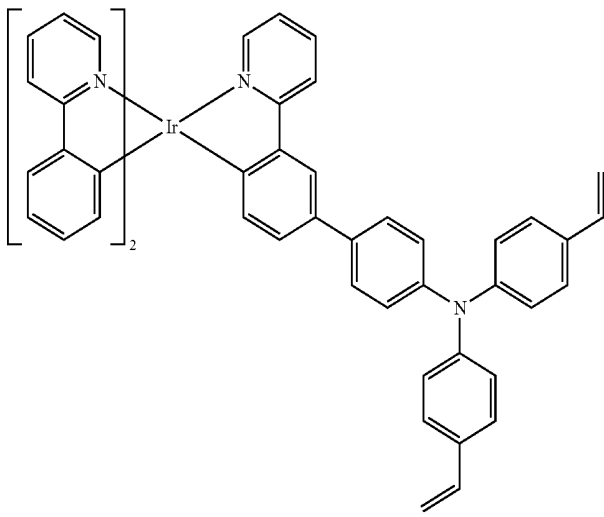
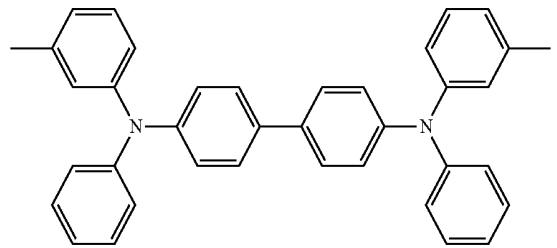
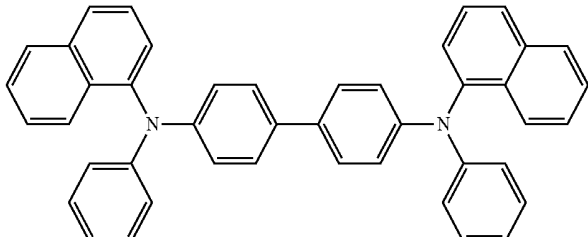
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
p-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Hole transporting materials		
Triarylamines (e.g., TPD, α -NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5,061,569

TABLE 1-continued

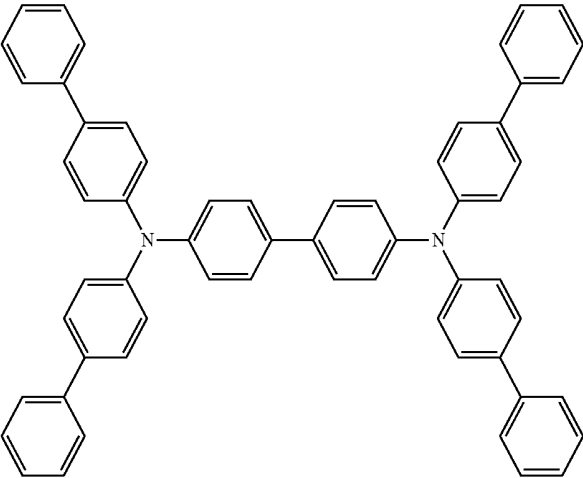
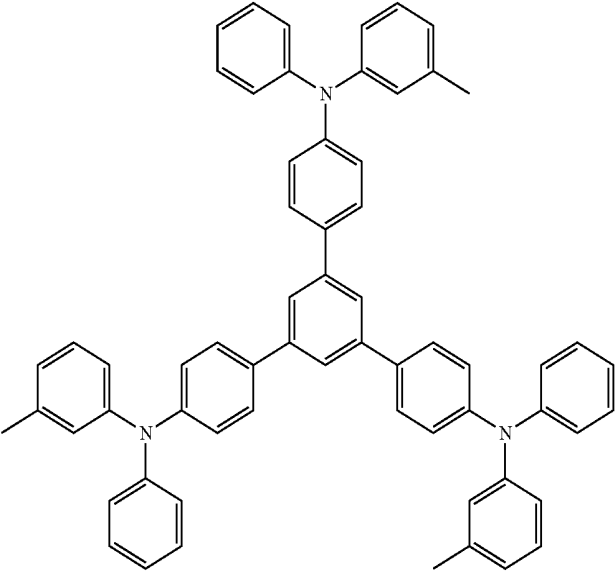
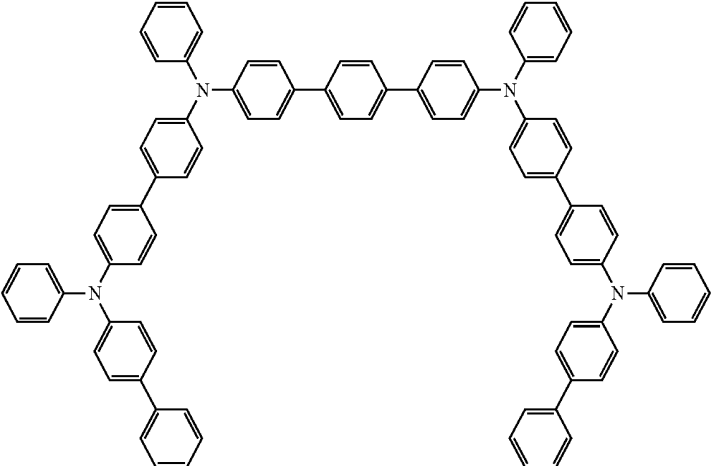
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		EP650955
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE 1-continued

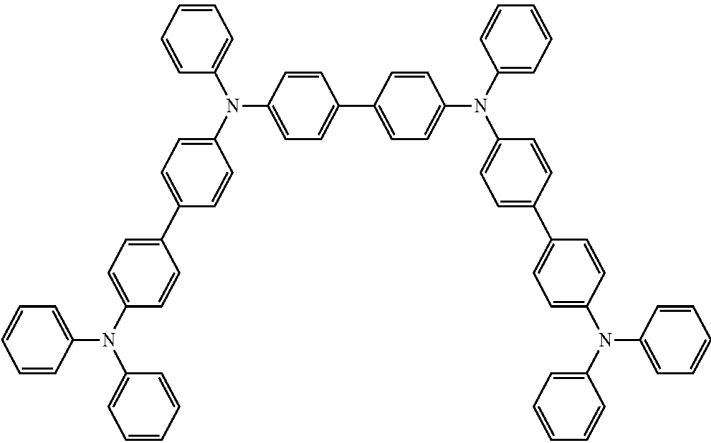
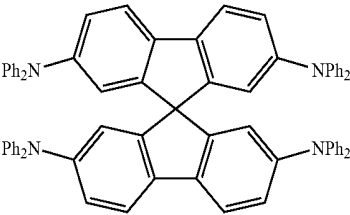
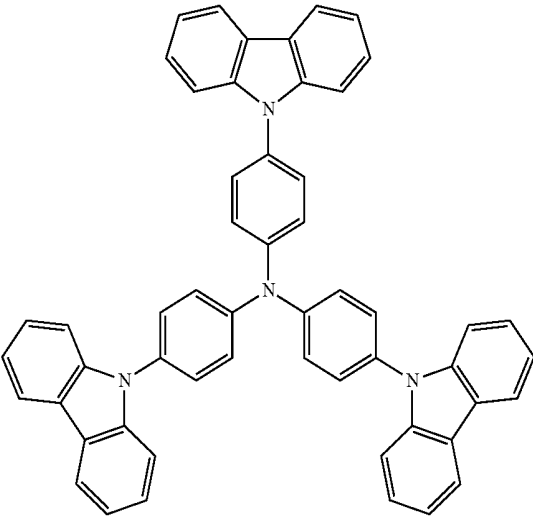
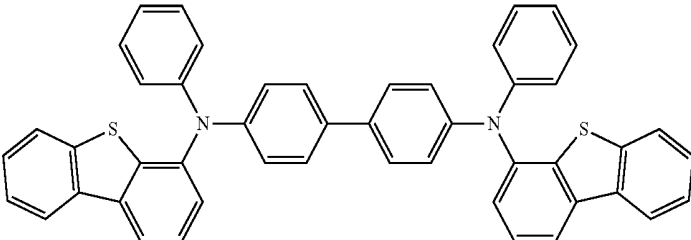
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
Triarylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190

TABLE 1-continued

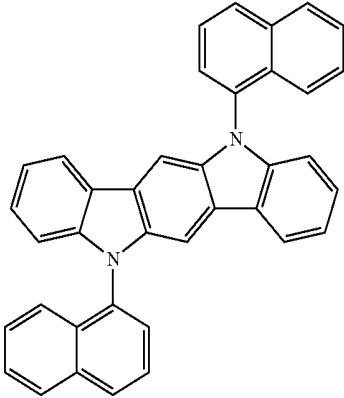
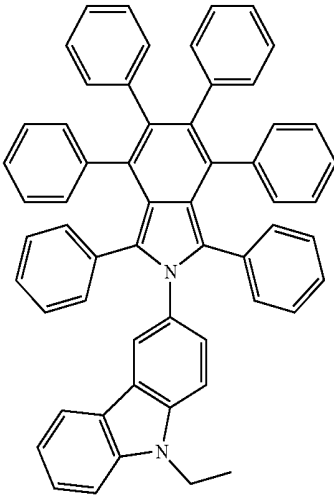
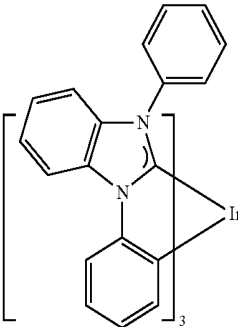
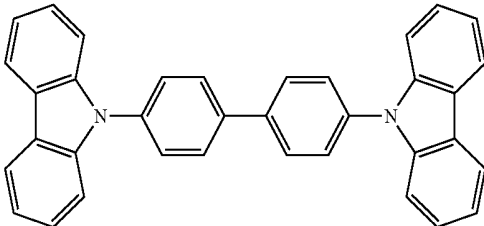
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials		
Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

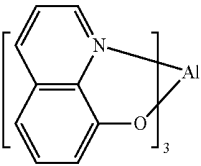
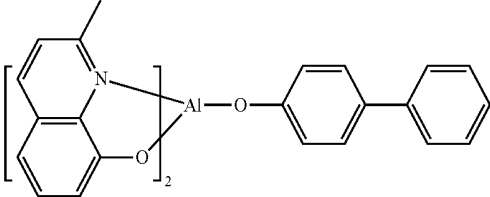
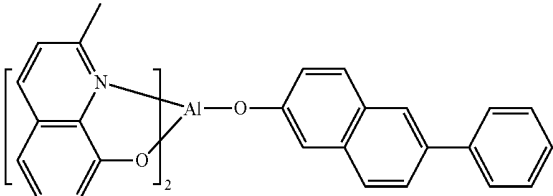
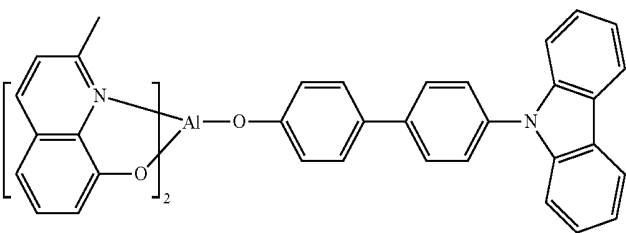
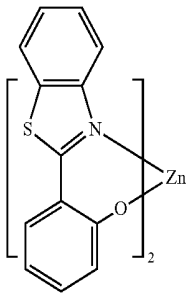
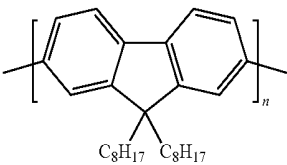
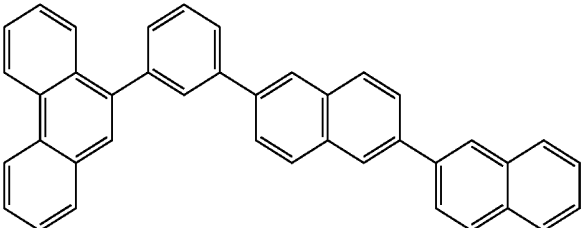
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal 8-hydroxyquinolates (e.g., Alq ₃ , BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron.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

TABLE 1-continued

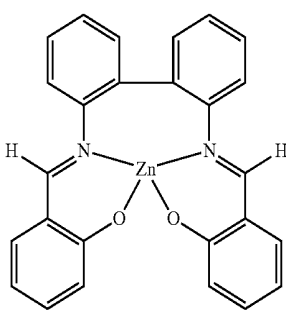
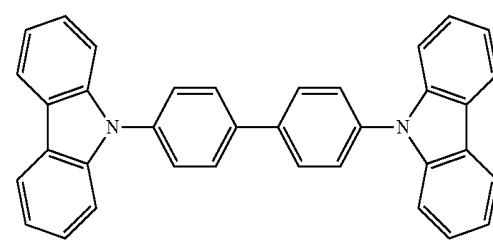
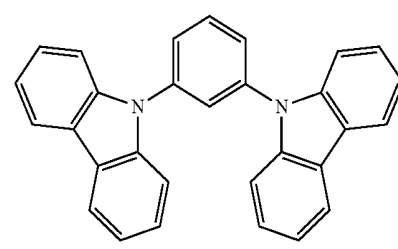
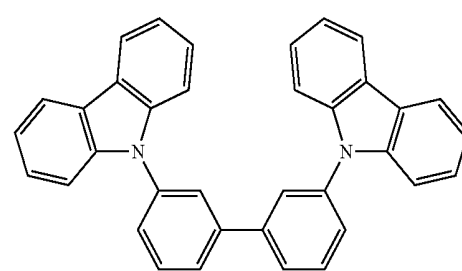
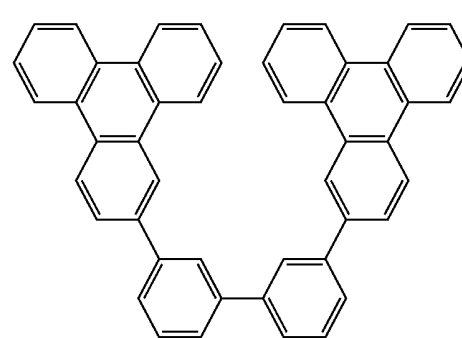
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Zinc complexes		WO2009062578
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE 1-continued

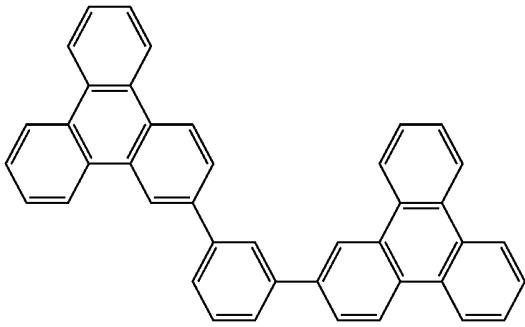
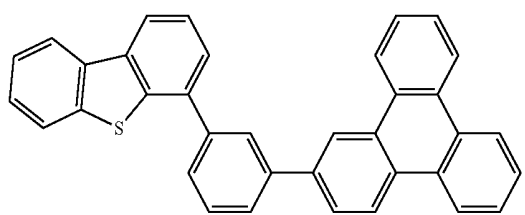
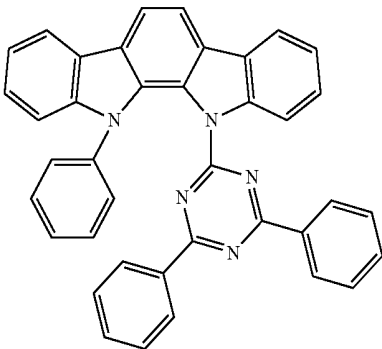
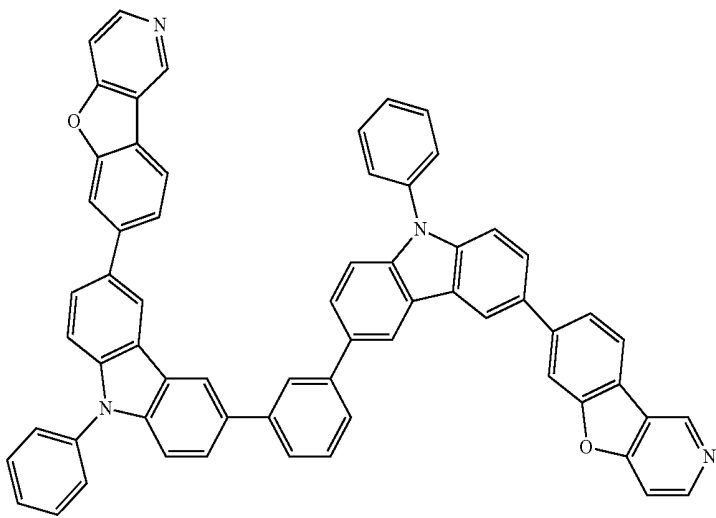
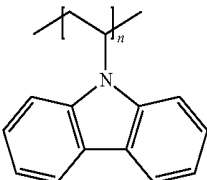
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060280965
		WO2009021126
Donor acceptor type molecules		WO2008056746
Aza-carbazole/DBT/DBF		JP2008074939
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)

TABLE 1-continued

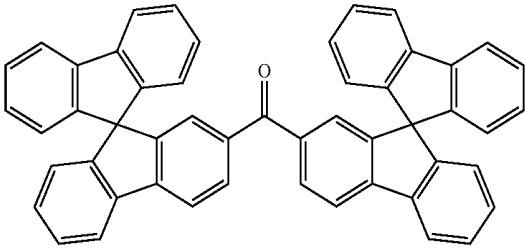
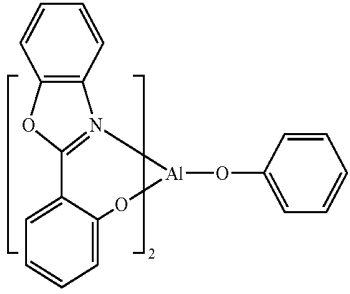
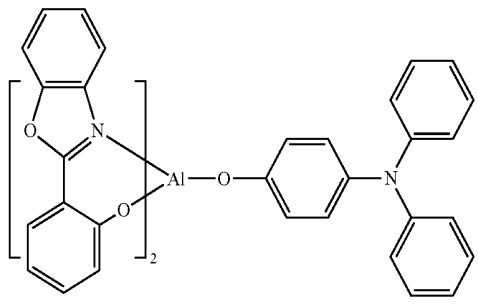
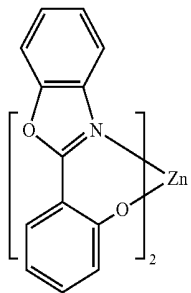
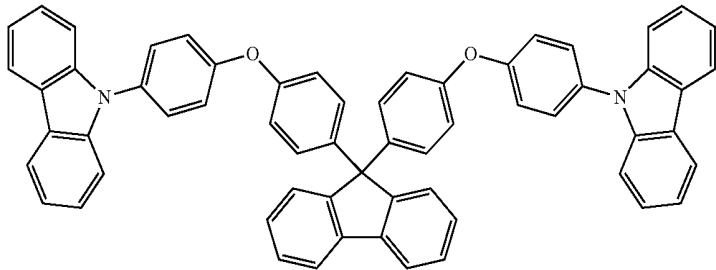
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Spirofluorene compounds		WO2004093207
Metal phenoxybenzoxazole compounds		WO2005089025
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297

TABLE 1-continued

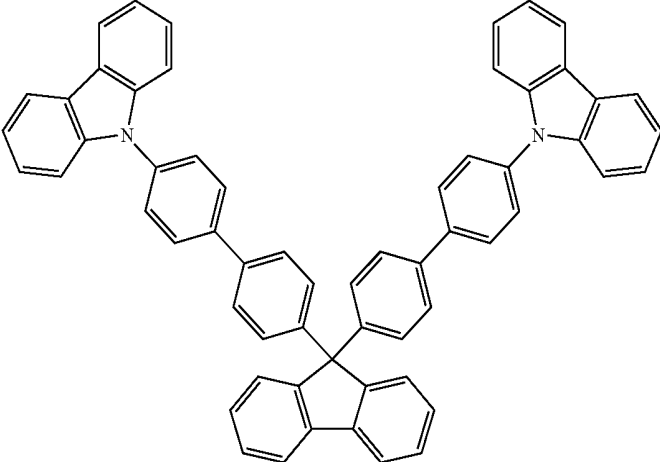
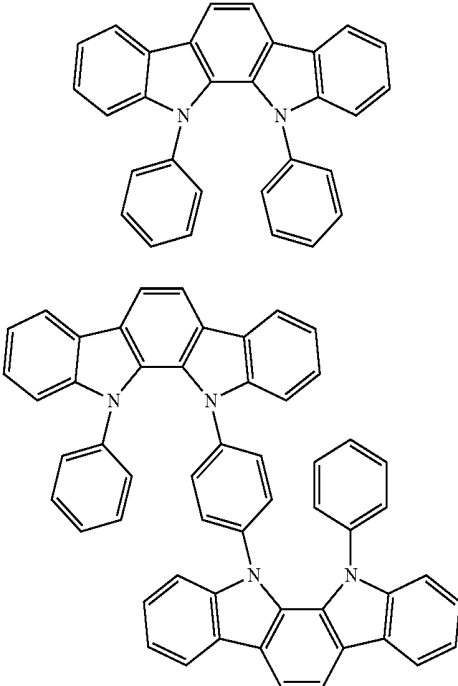
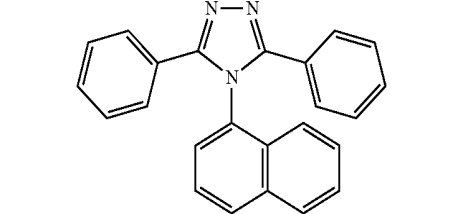
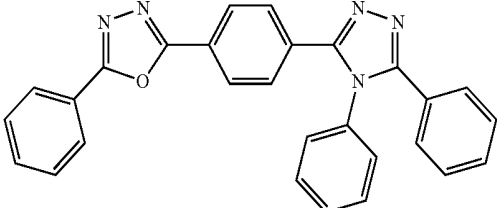
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocabazoles		JP2007254297
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)	 	WO2007063796 WO2007063754 J. Appl. Phys. 90, 5048 (2001)
		WO2004107822

TABLE 1-continued

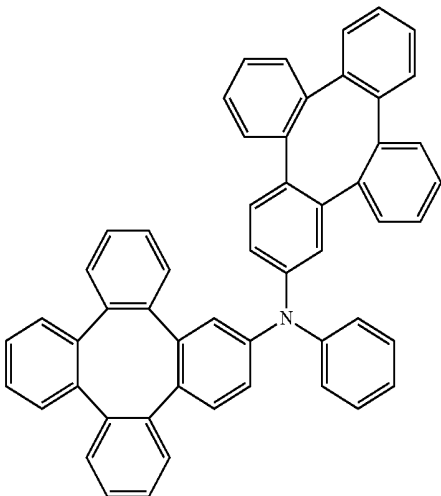
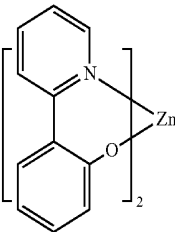
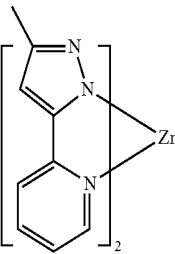
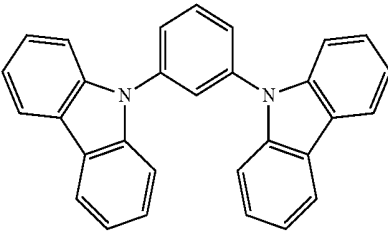
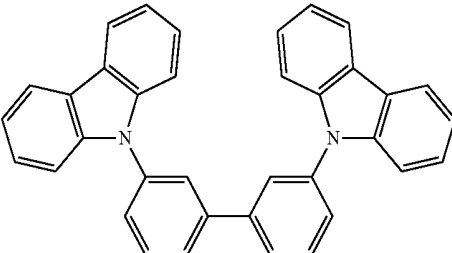
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N N ligands)		US20040137268, US20040137267
Blue hosts		
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359

TABLE 1-continued

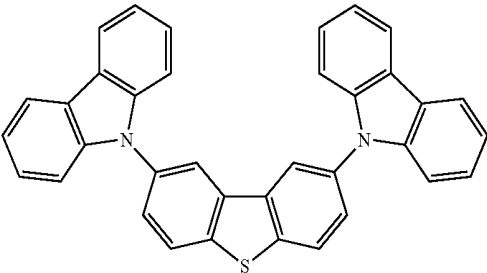
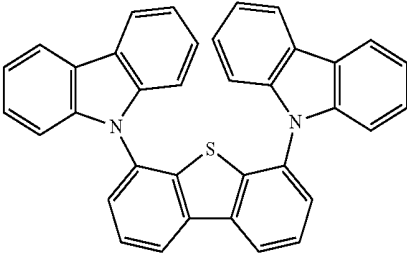
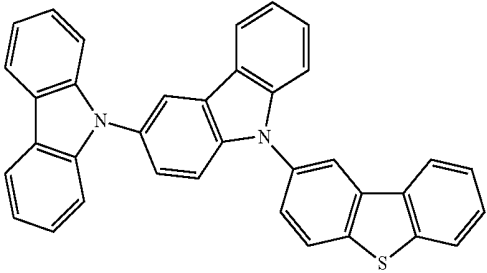
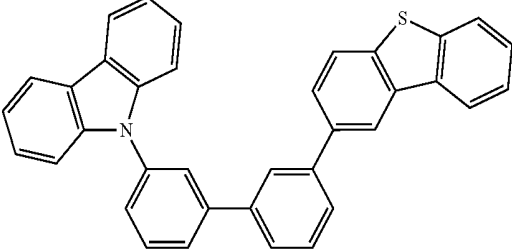
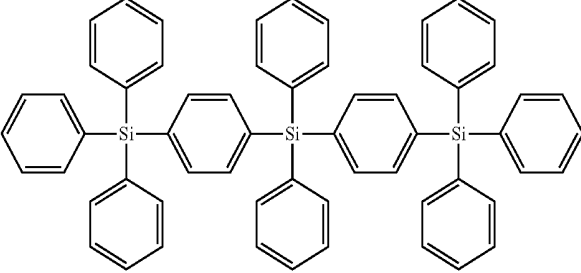
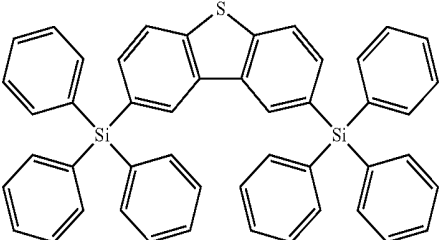
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Dibenzothiophene/Dibenzo- furan-carbazole compounds		WO2006114966, US20090167162
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		US20090030202, US20090017330
Silicon aryl compounds		US20050238919
		WO2009003898

TABLE 1-continued

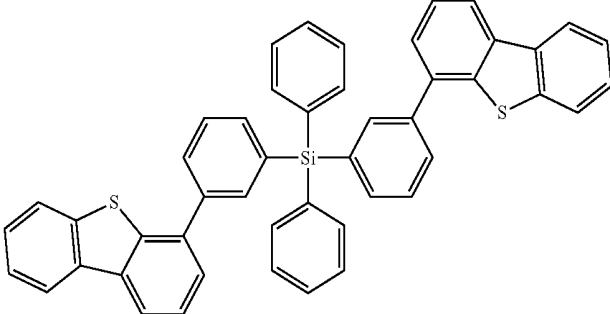
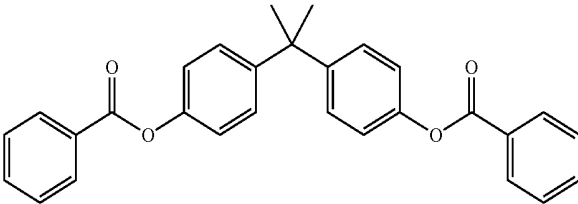
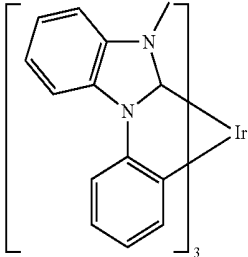
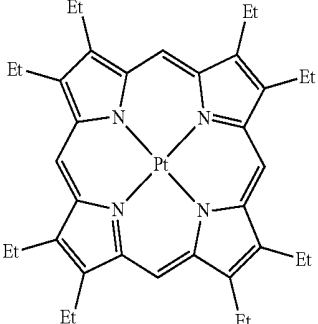
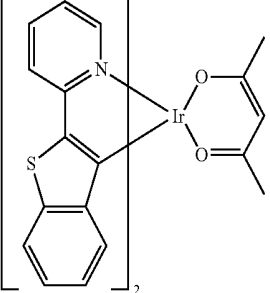
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Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114
	Phosphorescent dopants Red dopants	
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

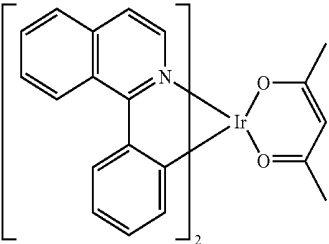
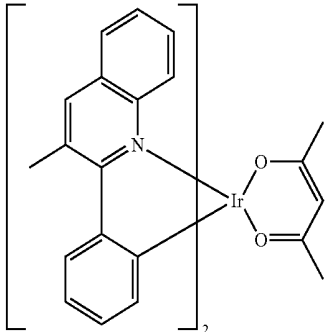
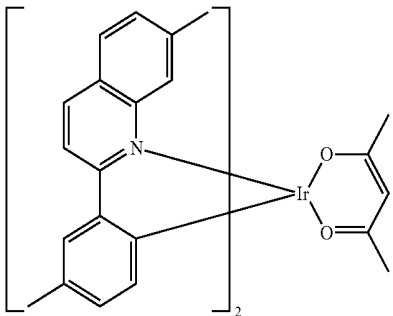
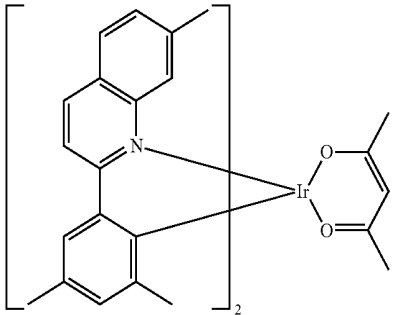
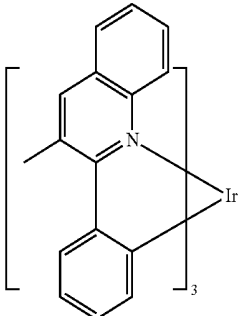
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		US20060202194
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		US20070087321

TABLE 1-continued

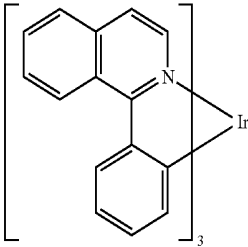
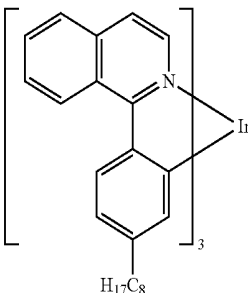
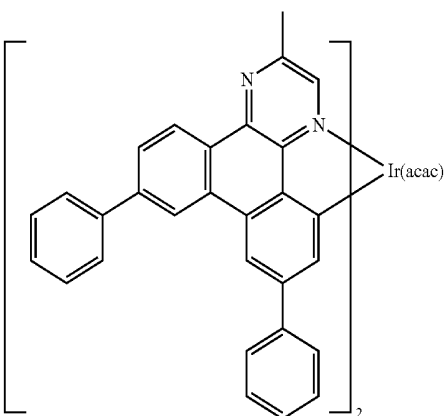
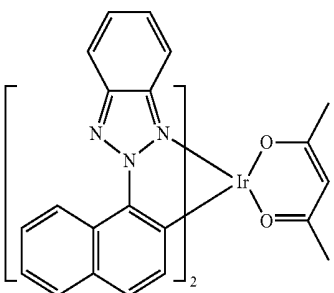
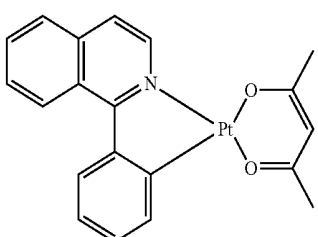
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		WO2009100991
		WO2008101842
Platinum(II) organometallic complexes		WO2003040257

TABLE 1-continued

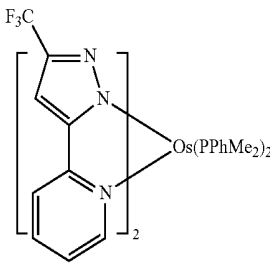
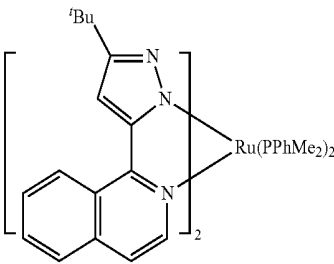
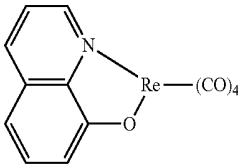
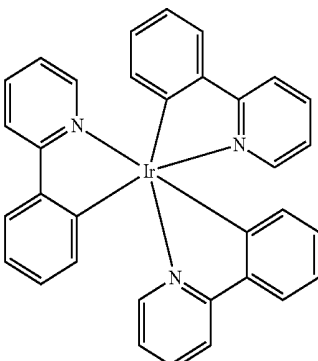
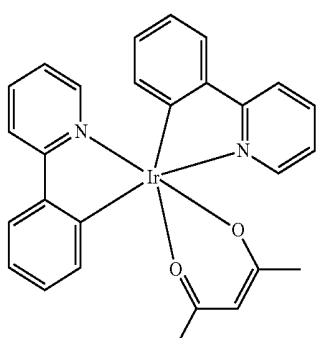
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Osmium(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
Green dopants		
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40,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

TABLE 1-continued

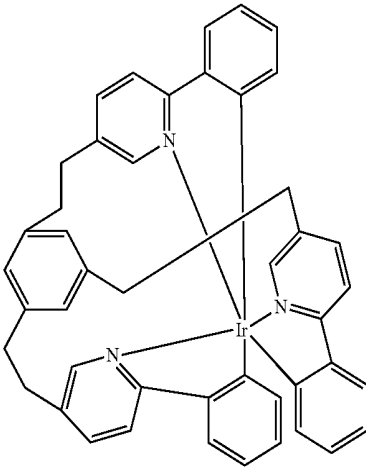
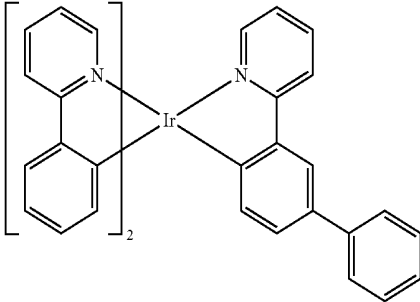
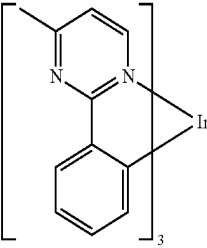
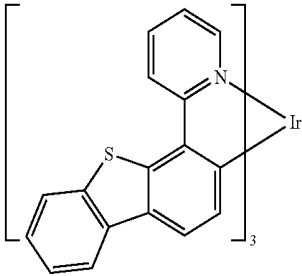
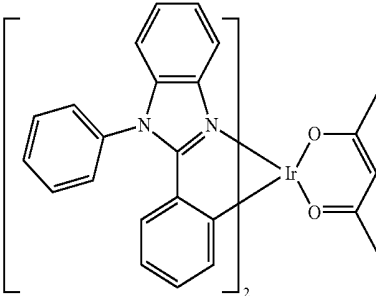
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		U.S. Pat. No. 6,921,915
		U.S. Pat. No. 6,687,266

TABLE 1-continued

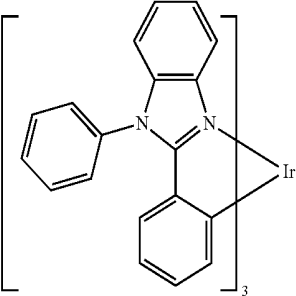
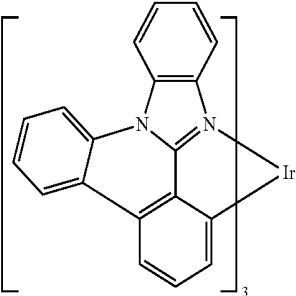
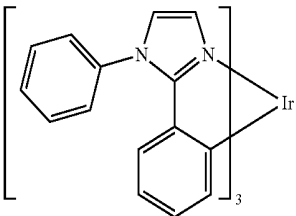
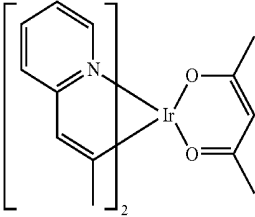
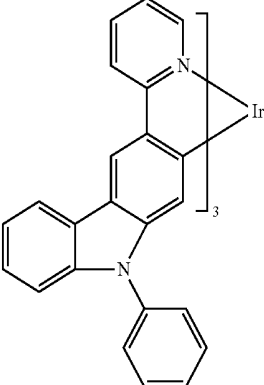
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		US20070190359
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		Angew. Chem. Int. Ed. 2006, 45, 7800

TABLE 1-continued

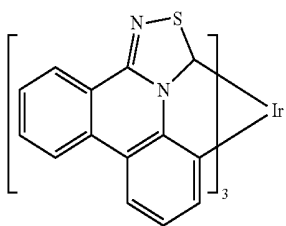
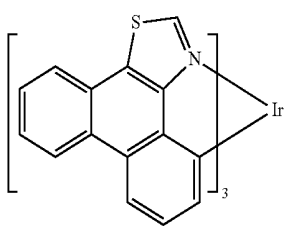
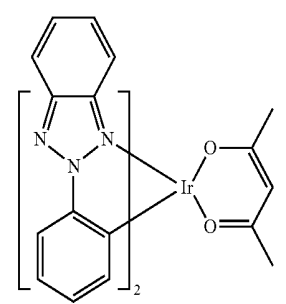
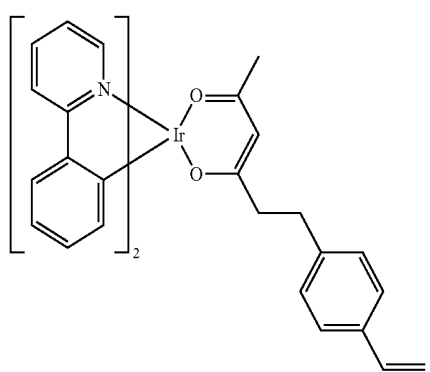
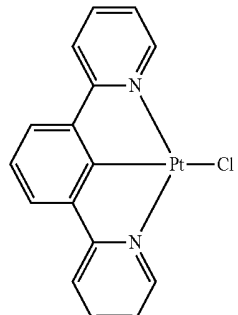
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2009050290
		US20090165846
		US20080015355
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentate ligands		Appl. Phys. Lett. 86, 153505 (2005)

TABLE 1-continued

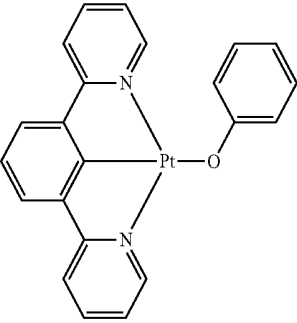
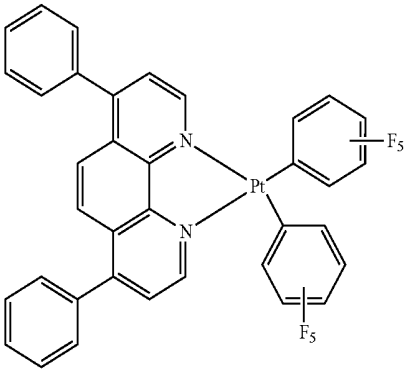
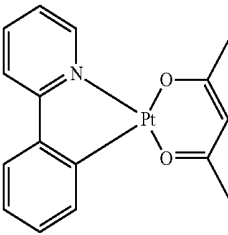
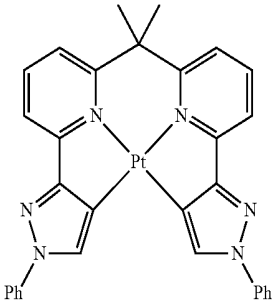
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		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635

TABLE 1-continued

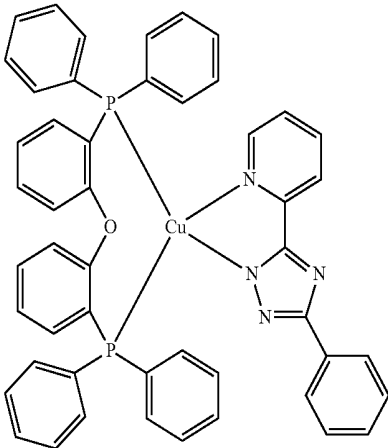
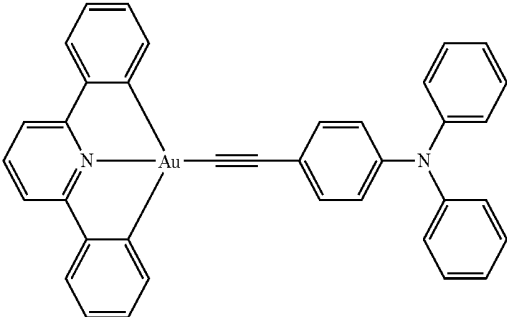
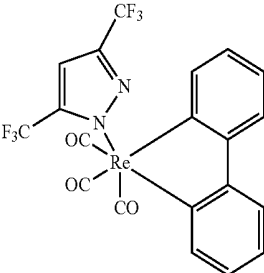
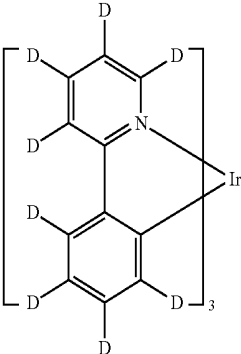
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Cu complexes		WO2009000673
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)
Deuterated organometallic complexes		US20030138657

TABLE 1-continued

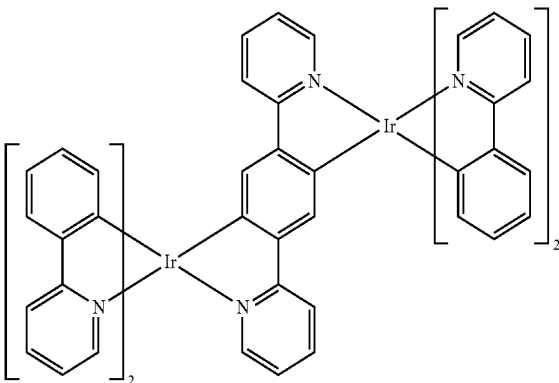
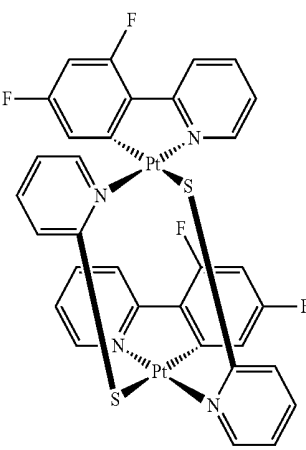
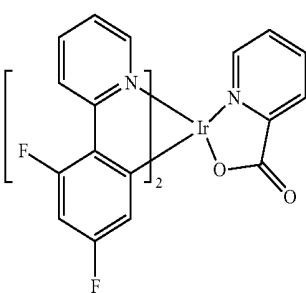
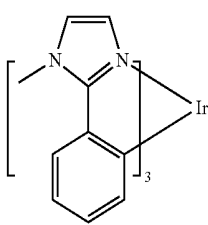
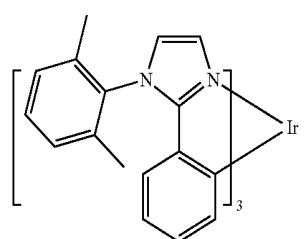
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organometallic complexes with two or more metal centers		US20030152802
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	Blue dopants	
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923

TABLE 1-continued

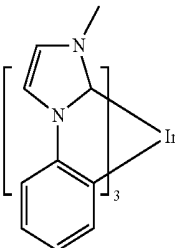
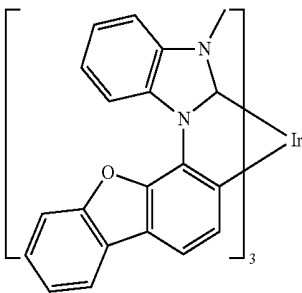
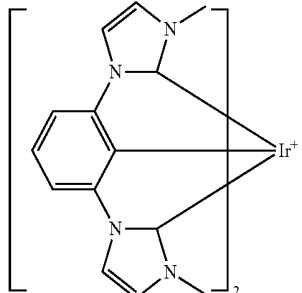
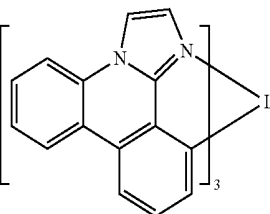
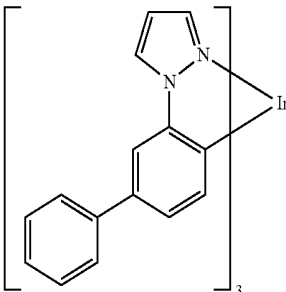
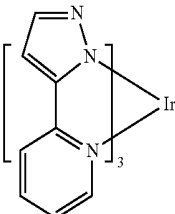
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		U.S. Pat. No. 7,534,505
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033
		U.S. Pat. No. 7,338,722
		US20020134984

TABLE 1-continued

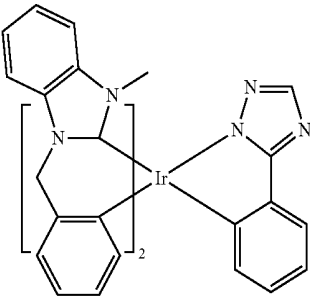
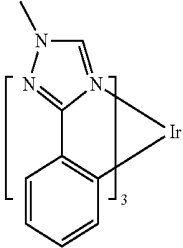
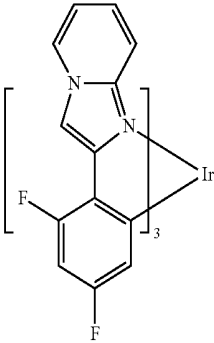
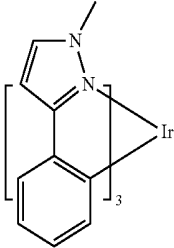
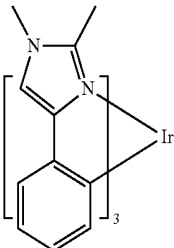
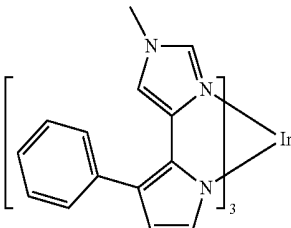
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		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873
		WO2007004380

TABLE 1-continued

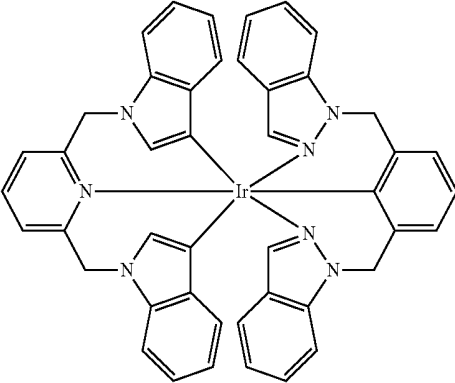
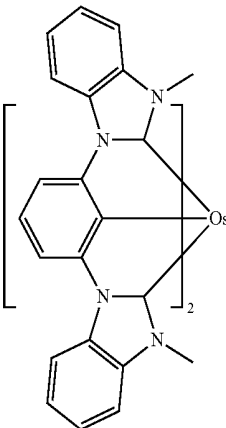
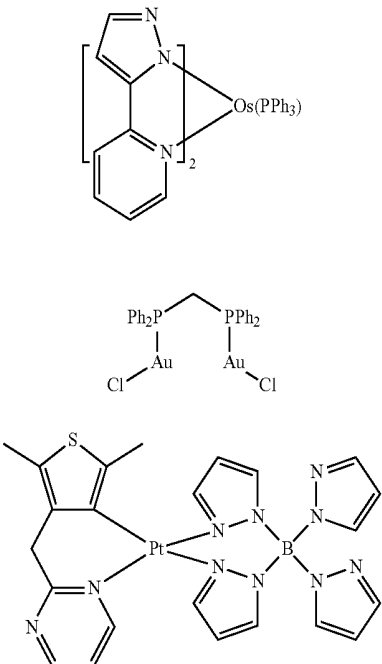
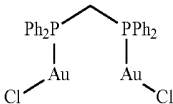
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Osmium(II) complexes		WO2006082742
Gold complexes		U.S. Pat. No. 7,279,704
Platinum(II) complexes		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 136 (1999)

TABLE 1-continued

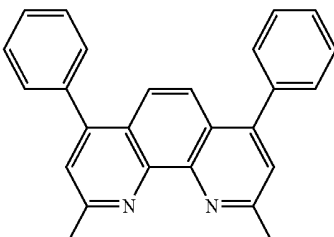
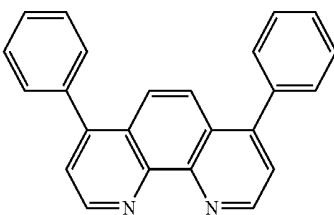
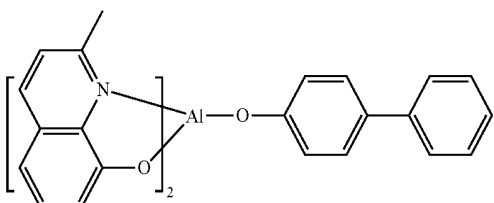
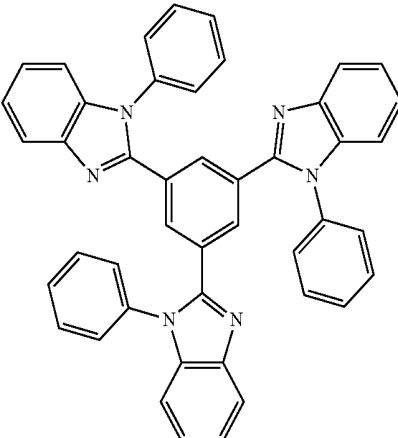
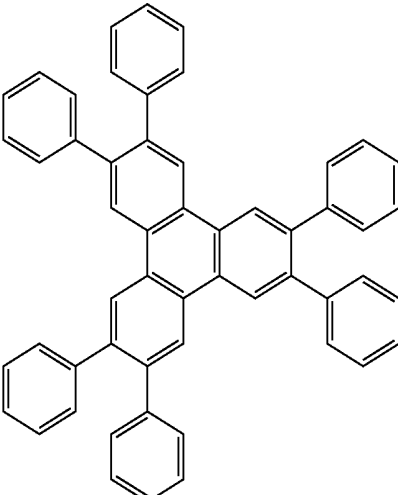
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)	 	Appl. Phys. Lett. 75, 4 (1999) Appl. Phys. Lett. 79 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993

TABLE 1-continued

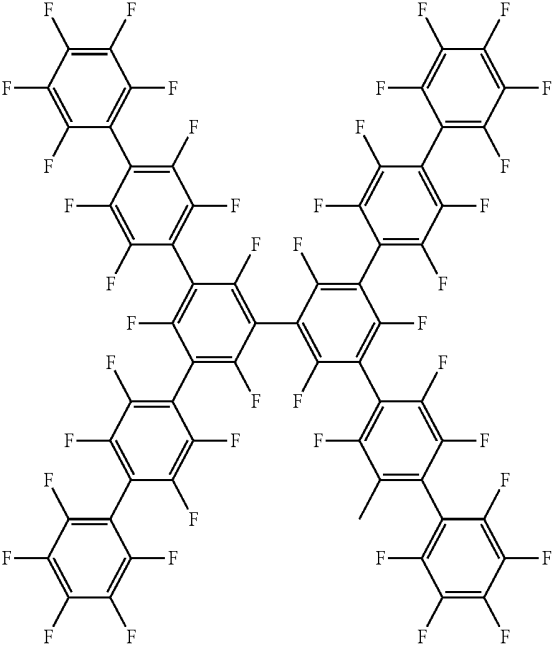
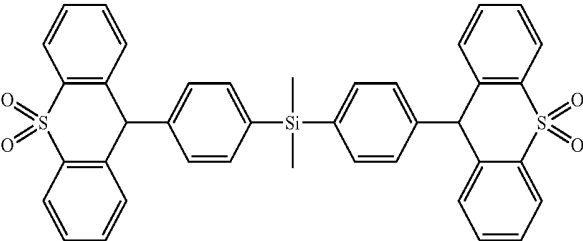
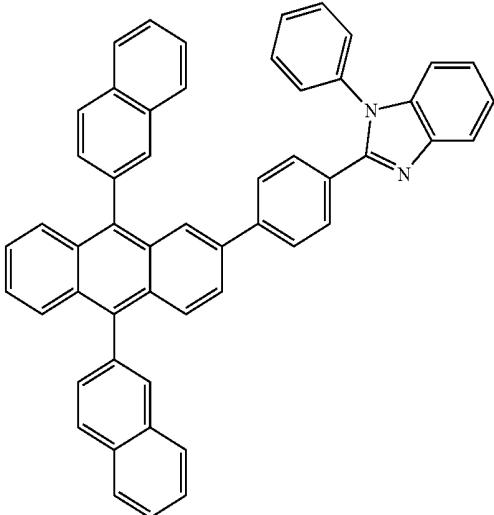
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085
Electron transporting materials		
Anthracene-benzimidazole compounds		WO2003060956

TABLE 1-continued

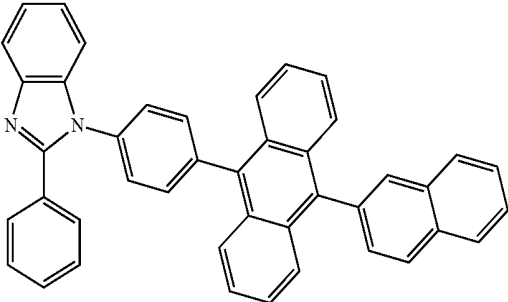
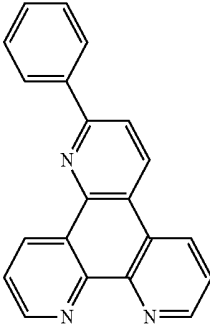
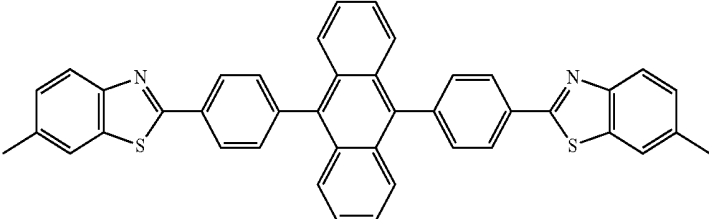
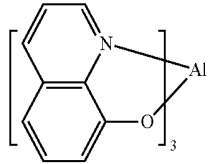
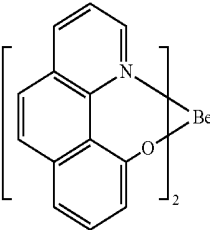
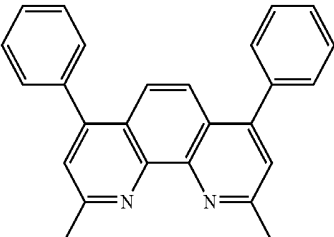
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza triphenylene derivatives		US20090179554
Anthracene-benzothiazole compounds		US20090115316
Metal 8-hydroxyquinolates (e.g., Alq ₃ , Zrq ₄)		Appl. Phys. Lett. 89, 063504 (2006)
Metal hydroxybenzoquinolates		Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7,230,107
Metal hydroxybenzoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)

TABLE 1-continued

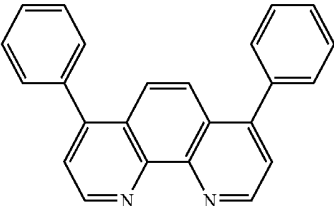
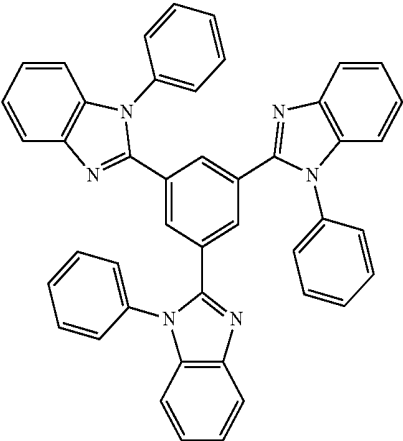
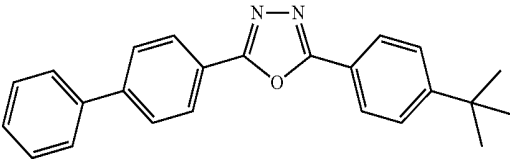
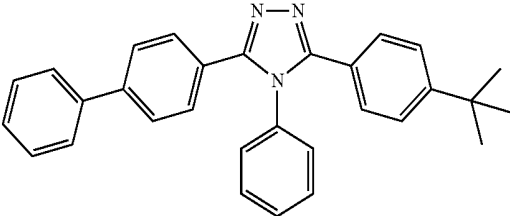
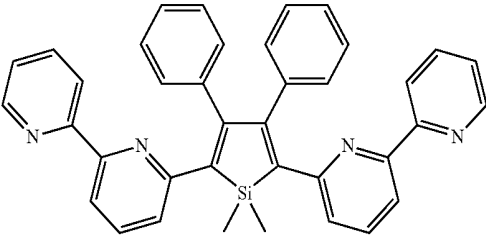
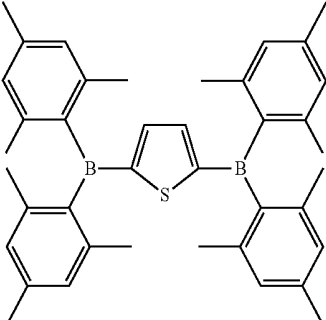
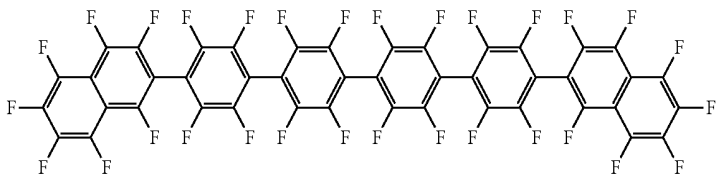
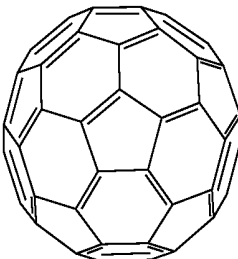
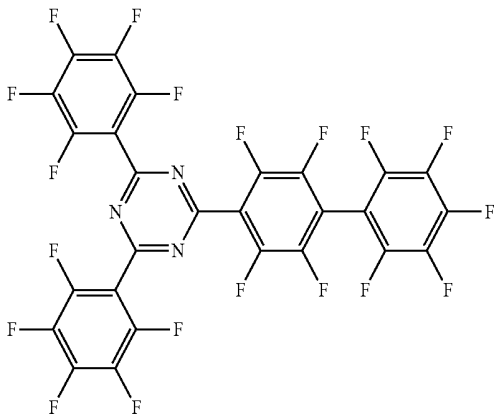
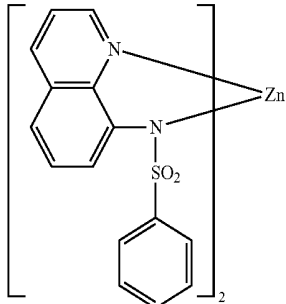
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 79, 449 (2001)
		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
Silole compounds		Jpn. J. Apply. Phys. 32, L917 (1993)
		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., C ₆₀)		US20090101870
Triazine complexes		US20040036077
Zn (N ⁺ N) complexes		U.S. Pat. No. 6,528,187

EXPERIMENTAL

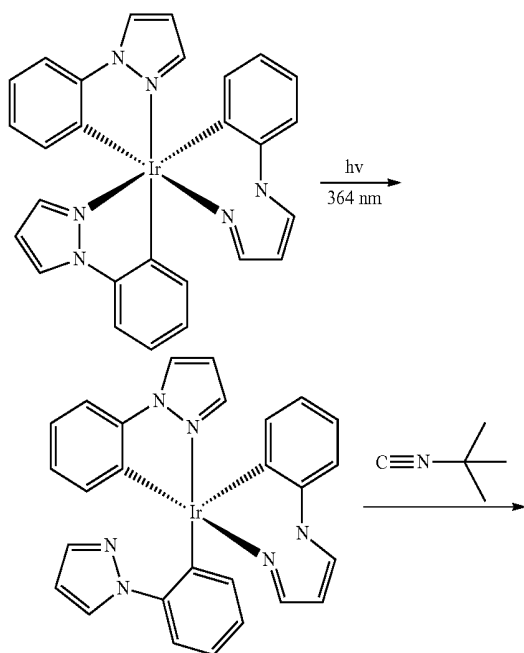
General Methods:

HPLC-MS. HPLC analysis was performed on a Shimadzu Prominence-LCMS 2020 equipped with a column oven (T=40° C.), a PDA photodetector (200-800 nm) and an MS spectrometer (LCNIS 2020; m/z range: 0-2000; ionization modes: ESI/APCI). The ESI/APCI conditions were: nitro-
 65 gas pressure 100 psi; nitrogen gas flow rate 1.5 L/minute; auxiliary nitrogen gas flow rates 15 L/minute; interface

voltage -3.5 kV; interface current 0.1 uA; corona needle voltage -3.5 kV; corona needle current 0.1 uA; dissolution line (DL) voltage 0V; DL temperature 250° C.; heat block temperature 400° C.; Q-array RF voltage 14.6 V; detector voltage 0.95 V; IG vacuum 7×10⁻⁴ Pa. HPLC was performed with the following protocol on a Inertsil C18, column 5 μm;
 60 4.6×250 mm; flow rate: 0.6 mL/min; Gradient acetonitrile-H₂O: 0-5 minutes, 80%; 20 minutes, 90%; 23 minutes, 80%; 25 minutes end of the program.

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Photolysis Experiments No. 1:

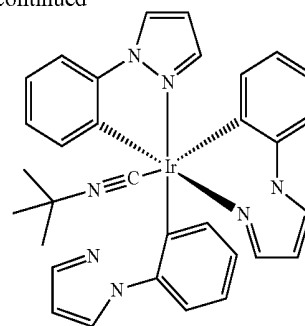


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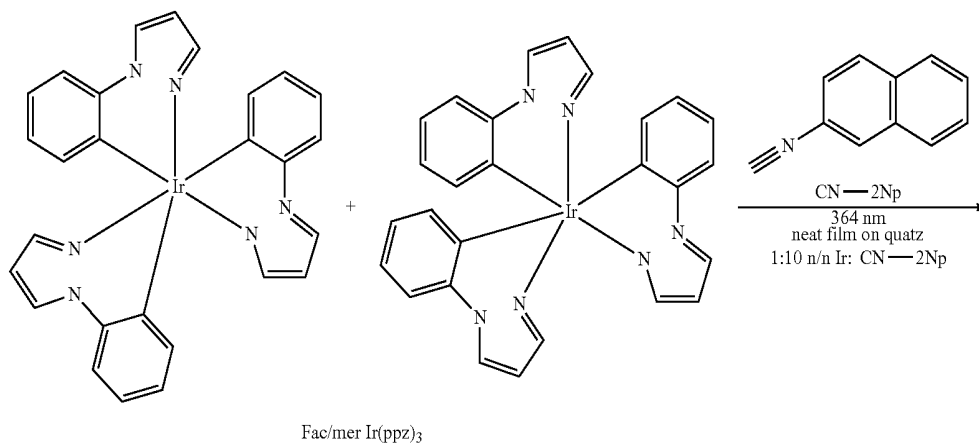
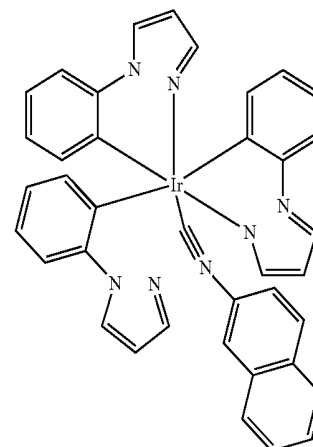
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- 15 A stirred nitrogen degassed solution of fac-Ir(ppz)₃, 1 mg/mL, in tert-butylisocyanide (CN-tBu) is photolyzed in a photo reactor equipped with 364 nm lamps (FIGS. 4-6). A reference sample is taken before photolysis starts. Photolysis is carried on for 120 minutes. 50 μL aliquot of the solution is taken for analysis after 10 minutes, 20 minutes, 60 minutes, 90 minutes and 120 minutes of irradiation. The sample aliquot is diluted in 1 mL of acetonitrile (AcCN) and analyzed by HPLC-MS in the condition previously indicated.
- 25

Photolysis Experiments No. 2 Neat Film:

Fac/mer Ir(ppz)₃

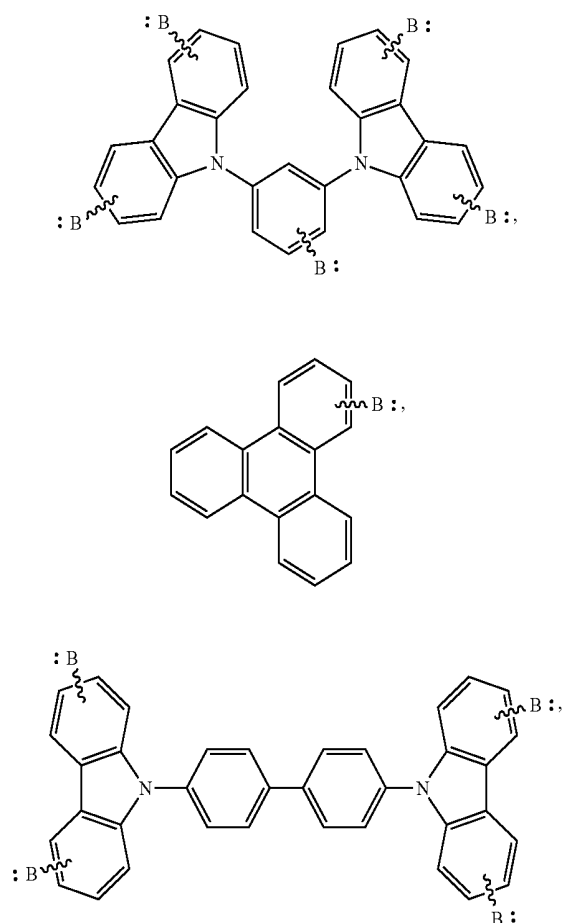
111

A mixture of 10 mg (1 equiv) of fac/mer-Ir(ppz)₃ (56/46 molar ratio) and 24.6 mg of CN-2-Np (10 equiv) dissolved in 1.5 mL of CH₂Cl₂ is spin coated on a quartz substrate at 2000 rpm for 40 seconds (nominal film thickness 200-300 Å). The film is irradiated under nitrogen or under vacuum in a photo reactor equipped with 364 nm lamps (FIG. 7). A reference sample film is not irradiated. Photolysis is carried on for 6 hours. The film is dissolved in 1 mL of acetonitrile (ACN) and analyzed by HPLC-MS in the condition previously indicated.

It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

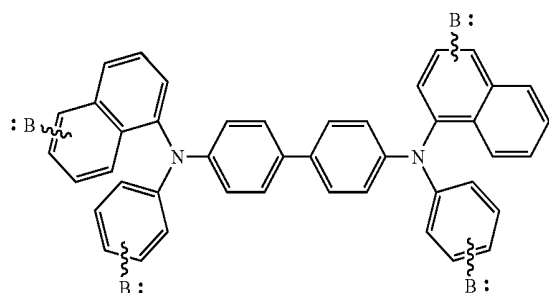
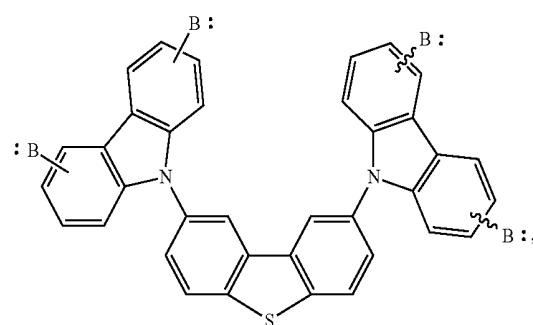
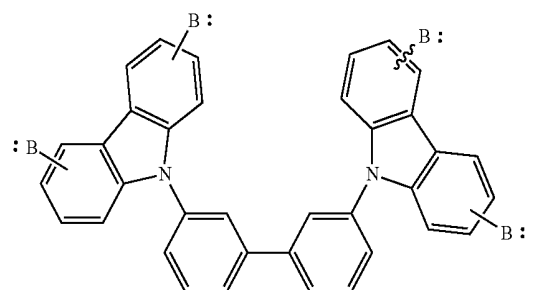
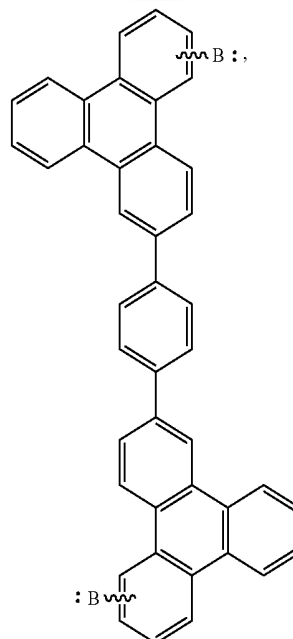
We claim:

1. An organic light emitting device, comprising: an anode; a cathode; and an organic layer disposed between the anode and the cathode, the organic layer comprising a first organic compound containing a metal-ligand bond and a second organic compound, wherein the second organic compound is a host selected from the group consisting of



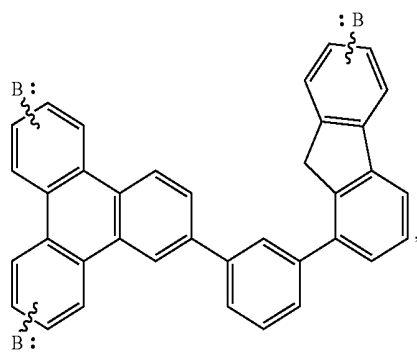
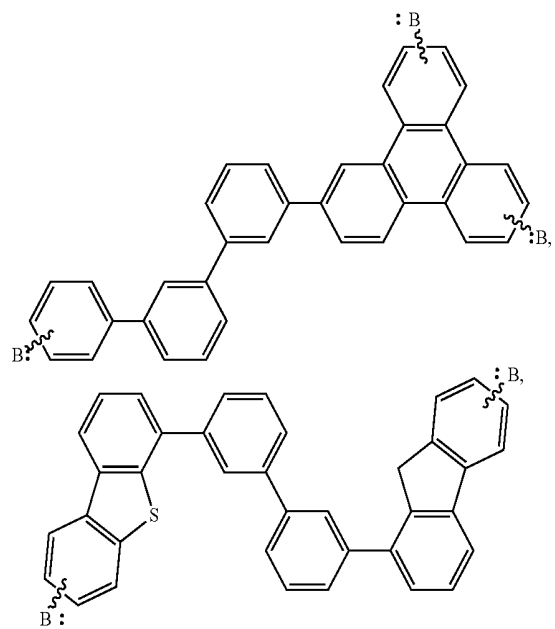
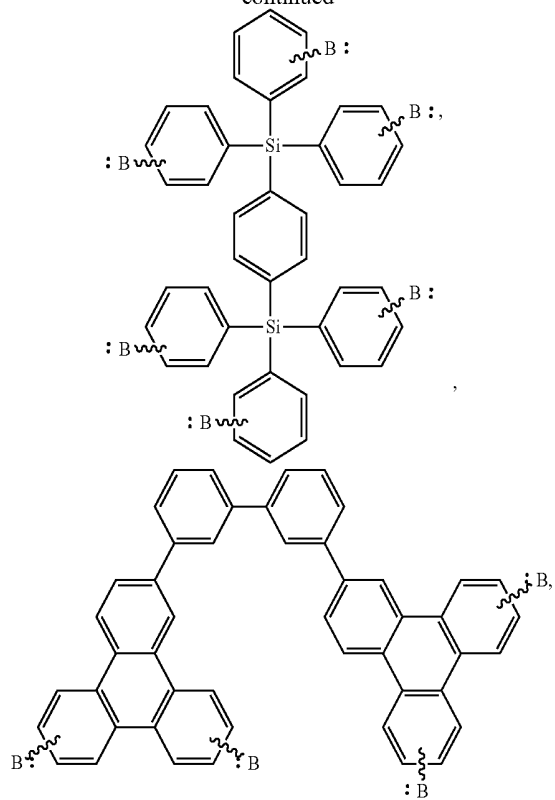
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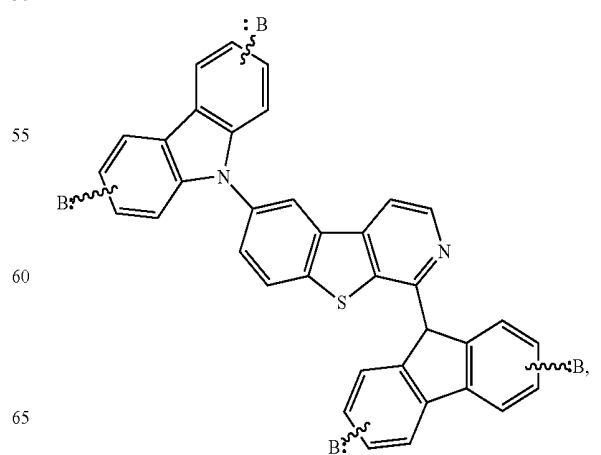
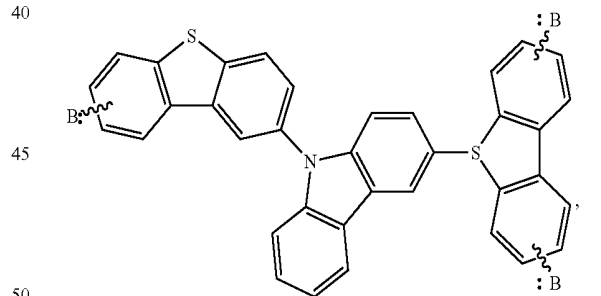
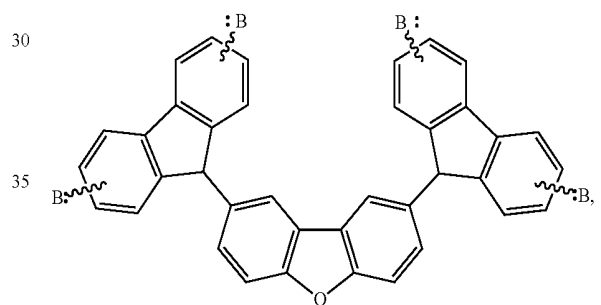
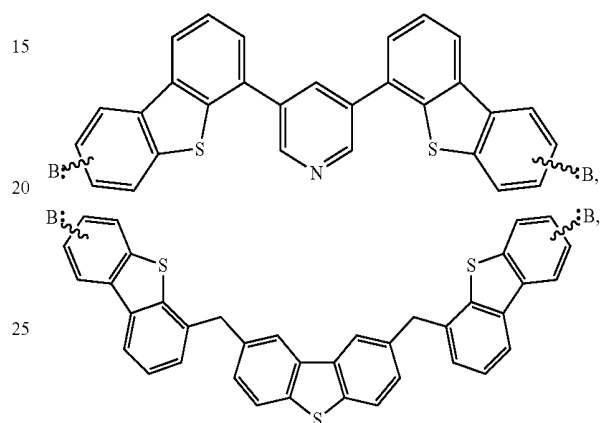
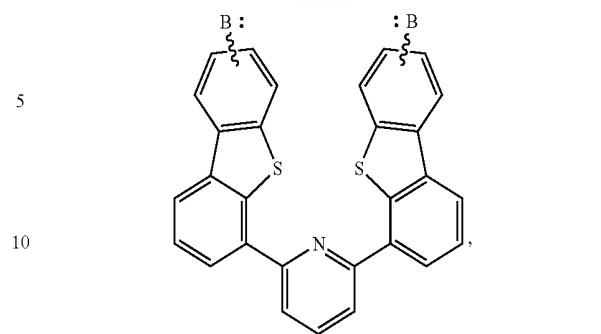


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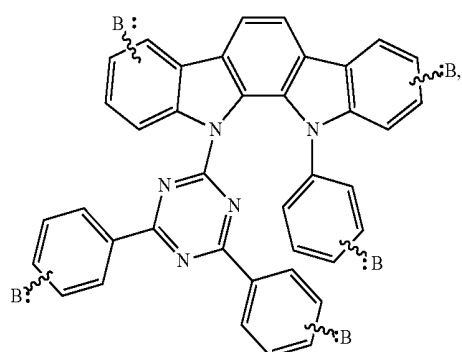
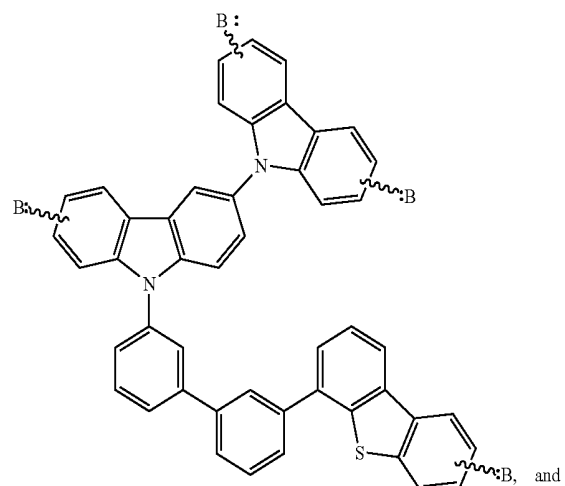
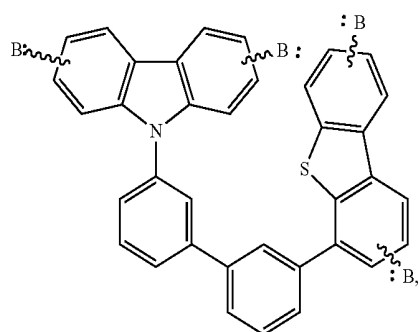
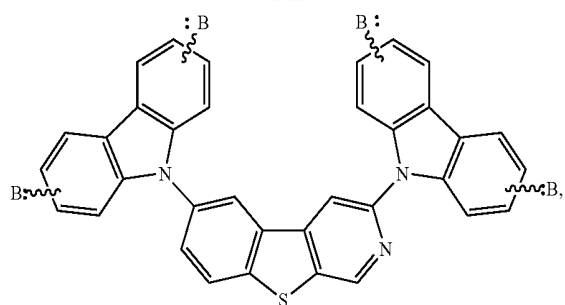
**114**

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115

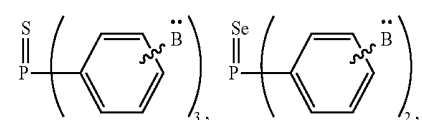
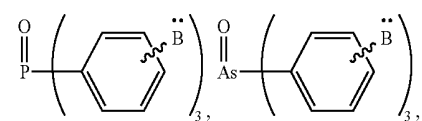
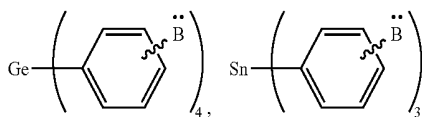
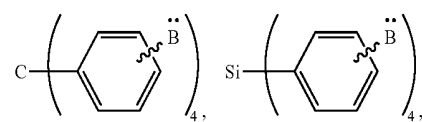
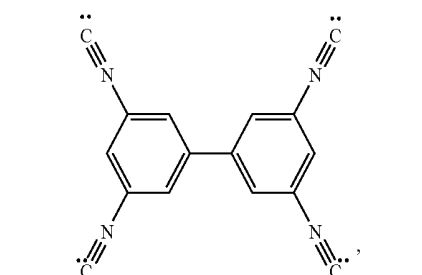
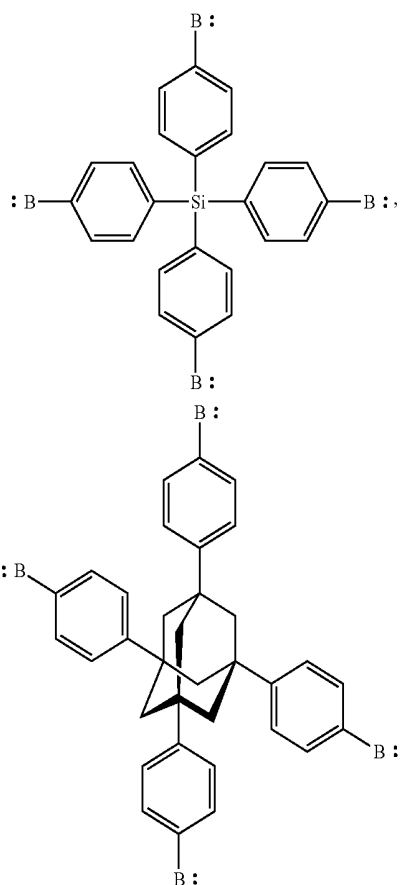
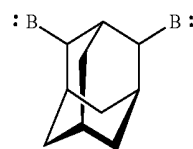
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wherein :B and B: represent an isocyanide having the formula $\text{—N}\equiv\text{C}$.

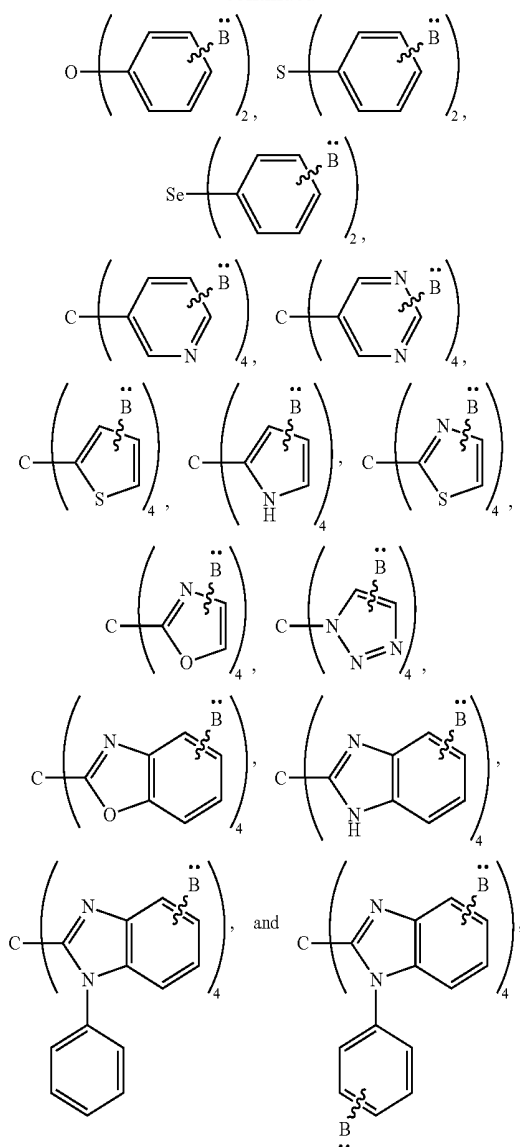
2. An organic light emitting device comprising: an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer comprises a first organic compound containing a metal-ligand bond and a second organic compound, and the second organic compound is selected from the group consisting of

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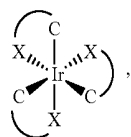
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-continued



wherein :B and B: and $\ddot{B}$ and $\ddot{B}$ represent an isocyanide having the formula $—N\equiv C$.

3. The device of claim 1, wherein the first organic compound is of the formula:



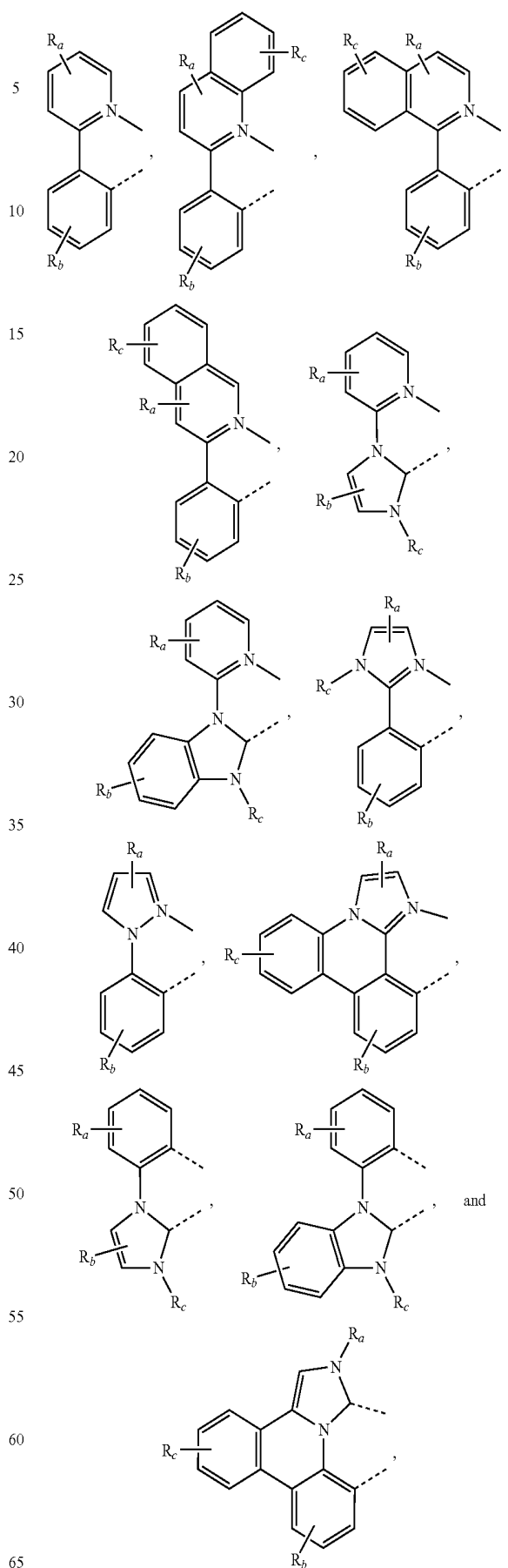
wherein X is selected from the group consisting of N, C, O, and S.

4. The device of claim 3, wherein X is N or C.

5. The device of claim 1, wherein the organic layer is an emissive layer of the organic light emitting device, and the first organic compound is a blue phosphorescent compound.

6. The device of claim 1, wherein the first organic compound is a transition metal complex having at least one ligand selected from the group consisting of:

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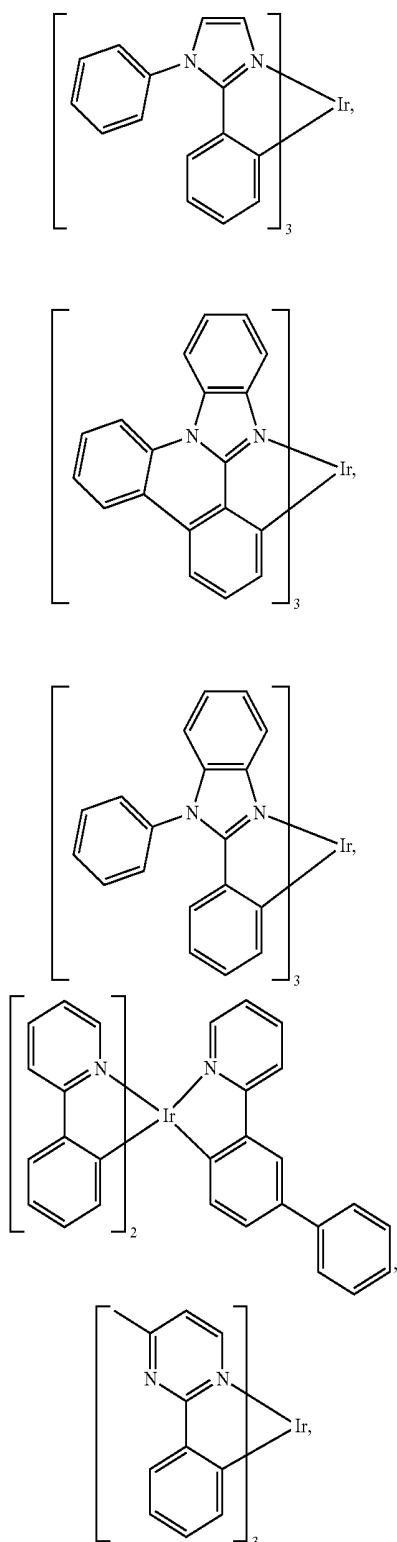
119

wherein R_a , R_b and R_c represent mono, di, tri, or tetra substituents;

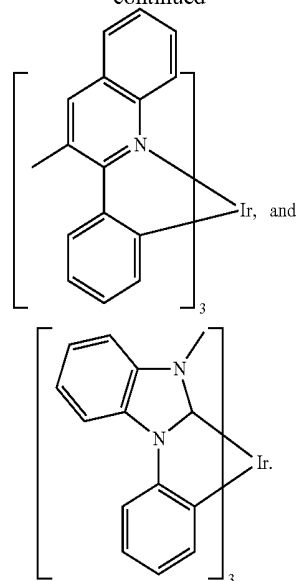
each of R_a , R_b and R_c are independently selected from the group consisting of hydrogen, deuterium, alkyl, heteroalkyl, aryl, and heteroaryl; and

two adjacent R_a , R_b , and R_c can form into a ring.

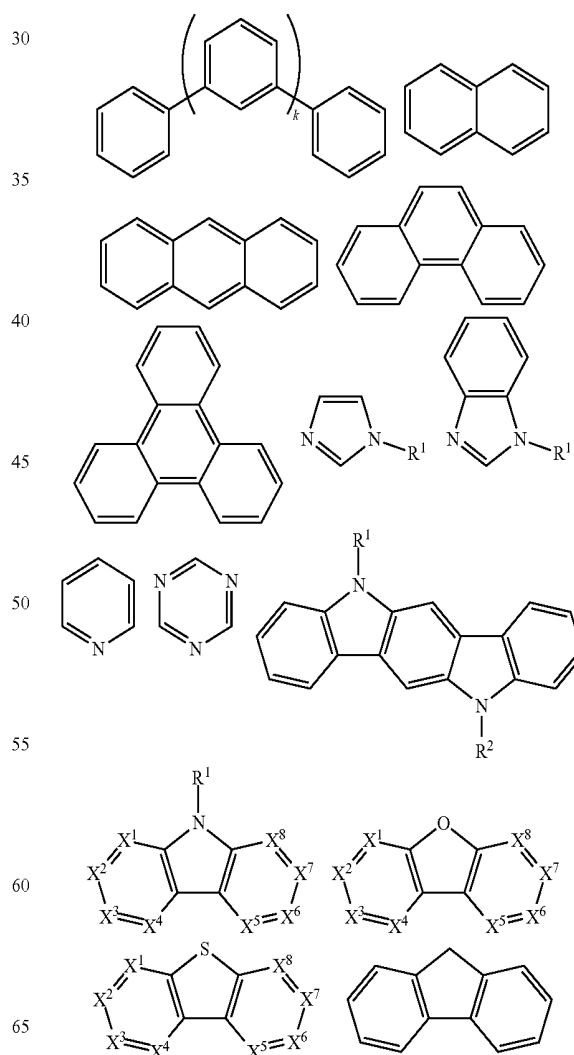
7. The device of claim 1, wherein the organic layer further comprises a compound selected from the group consisting of

**120**

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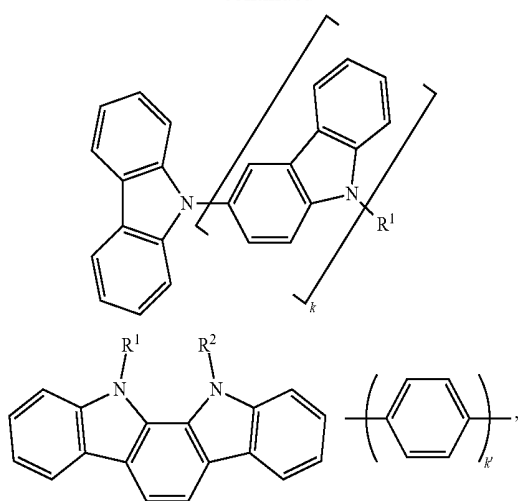


8. The device of claim 1, wherein the organic layer further comprises a host that includes at least one of the following groups selected from the group consisting of



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-continued



wherein

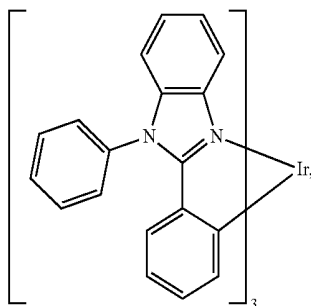
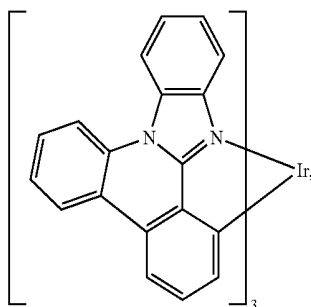
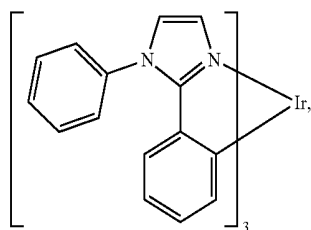
R^1 and R^2 are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl;

k is an integer from 0 to 20;

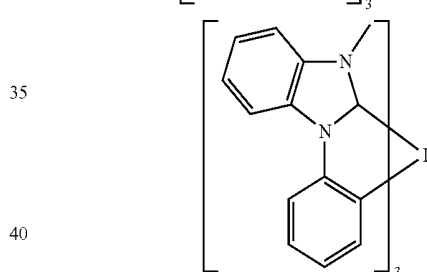
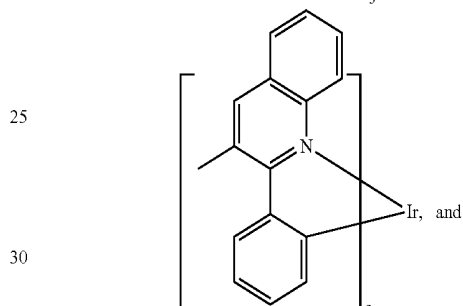
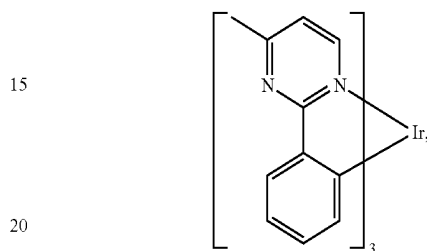
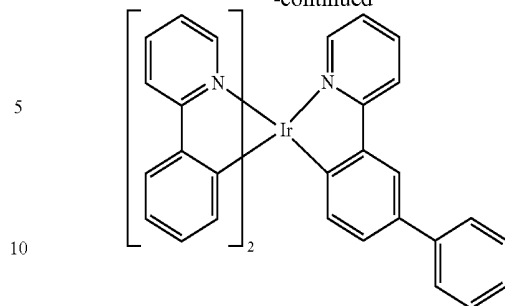
k' is an integer from 1 to 20; and

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

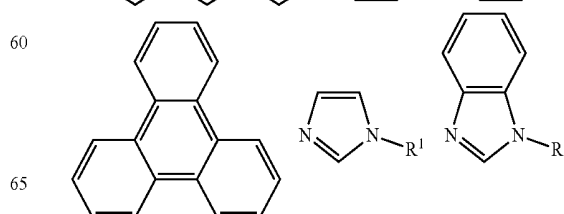
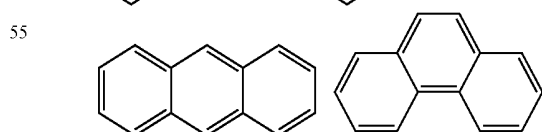
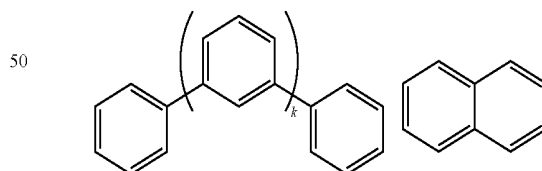
9. The device of claim 2, wherein the organic layer further comprises a compound selected from the group consisting of

**122**

-continued

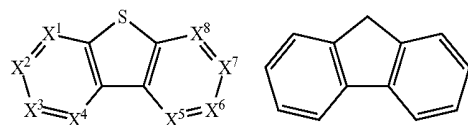
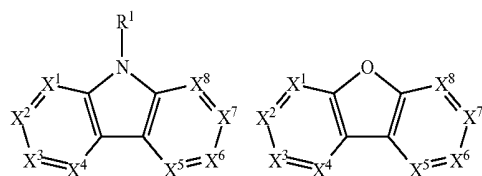
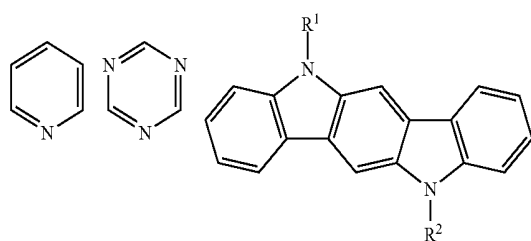


10. The device of claim 2, wherein the organic layer further comprises a host that includes at least one of the following groups selected from the group consisting of

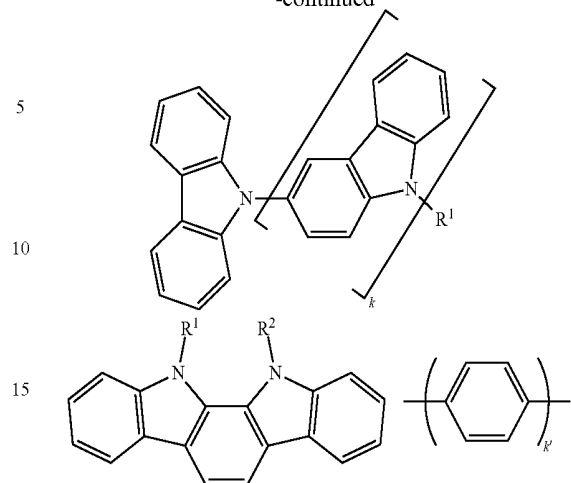


123

-continued

**124**

-continued



wherein

R^1 and R^2 are independently selected from the group consisting of hydrogen, alkyl, alkoxy, amino, alkenyl, alkynyl, arylalkyl, heteroalkyl, aryl and heteroaryl;

k is an integer from 0 to 20;

k' is an integer from 1 to 20; and

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

* * * * *

专利名称(译)	有机电致发光材料和器件		
公开(公告)号	US10147892	公开(公告)日	2018-12-04
申请号	US15/008654	申请日	2016-01-28
[标]申请(专利权)人(译)	南加利福尼亚大学		
申请(专利权)人(译)	南加州大学		
当前申请(专利权)人(译)	南加州大学		
[标]发明人	THOMPSON MARK E BOSSI ALBERTO DJUROVICH PETER		
发明人	THOMPSON, MARK E. BOSSI, ALBERTO DJUROVICH, PETER		
IPC分类号	H01L51/54 H01L51/50 C09K11/06 H01L51/00 C09K11/02		
CPC分类号	H01L51/0085 C09K11/06 H01L51/005 H01L51/006 H01L51/0052 H01L51/0054 H01L51/0058 H01L51/0067 H01L51/0069 H01L51/0072 H01L51/0073 H01L51/0074 H01L51/0077 H01L51/0094 H01L51/5016 H01L51/5024 C09K11/025 H01L51/5028 C09K2211/1007 C09K2211/1011 C09K2211/1044 C09K2211/185		
代理机构(译)	DUANE MORRIS LLP		
优先权	61/420473 2010-12-07 US		
其他公开文献	US20160141524A1		
外部链接	Espacenet		

摘要(译)

提供了作为捕获剂以整合不饱和金属配合物的化合物。特别地，化合物可以是主体材料，掺杂剂材料或含有官能团的掺杂剂材料，例如异氰化物或膦基团，其适合于捕获不饱和配位络合物。这些化合物可用于有机发光器件，特别是蓝色器件，以提供改善的器件寿命。

