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

(71) Applicant: **Universal Display Corporation**, Ewing, NJ (US)

(72) Inventors: **Chuanjun Xia**, Lawrenceville, NJ (US); **Raymond C. Kwong**, Plainsboro, NJ (US); **Suman Layek**, Lawrenceville, NJ (US)

(73) Assignee: **UNIVERSAL DISPLAY CORPORATION**, Ewing, NJ (US)

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(51) **Int. Cl.**

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C09K 11/06	(2006.01)
H01L 51/00	(2006.01)
C07F 15/00	(2006.01)
H05B 33/10	(2006.01)
H01L 51/50	(2006.01)

(52) **U.S. Cl.**

CPC ***H01L 51/0085*** (2013.01); ***C07F 15/0033*** (2013.01); ***C09K 11/06*** (2013.01); ***H05B 33/10*** (2013.01); *C09K 2211/1007* (2013.01); *C09K 2211/1011* (2013.01); *C09K 2211/1029* (2013.01); *C09K 2211/1088* (2013.01); *C09K 2211/1092* (2013.01); *C09K 2211/185* (2013.01); *H01L 51/5016* (2013.01)

(58) **Field of Classification Search**

None

See application file for complete search history.

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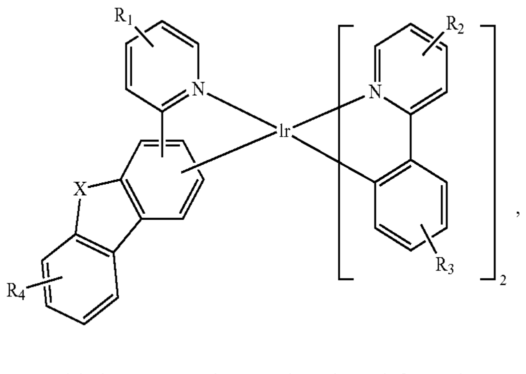
Primary Examiner — Marie R. Yamnitzky

(74) *Attorney, Agent, or Firm* — Duane Morris LLP

(57) **ABSTRACT**

Novel heteroleptic iridium complexes having the structure of Formula I,



are provided. In Formula I, X is selected from the group consisting of NR, BR, and Se; R is selected from hydrogen and alkyl, and each R_1, R_2, R_3, and R_4 is independently selected from hydrogen, alkyl, and aryl. The compounds may be used in organic light emitting devices, particularly as emitting dopants, to provide devices having improved efficiency, lifetime, and manufacturing.

19 Claims, 3 Drawing Sheets

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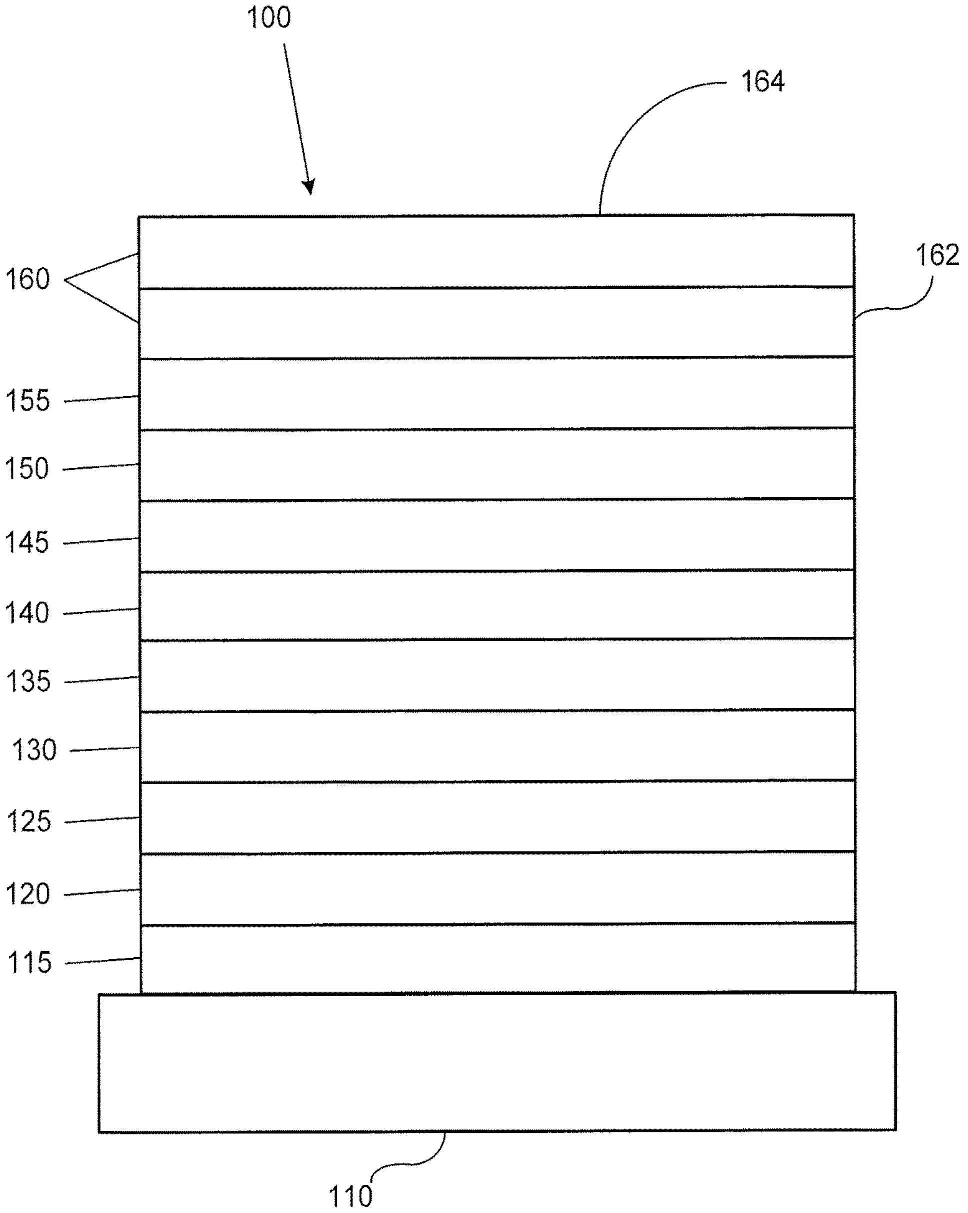


FIGURE 1

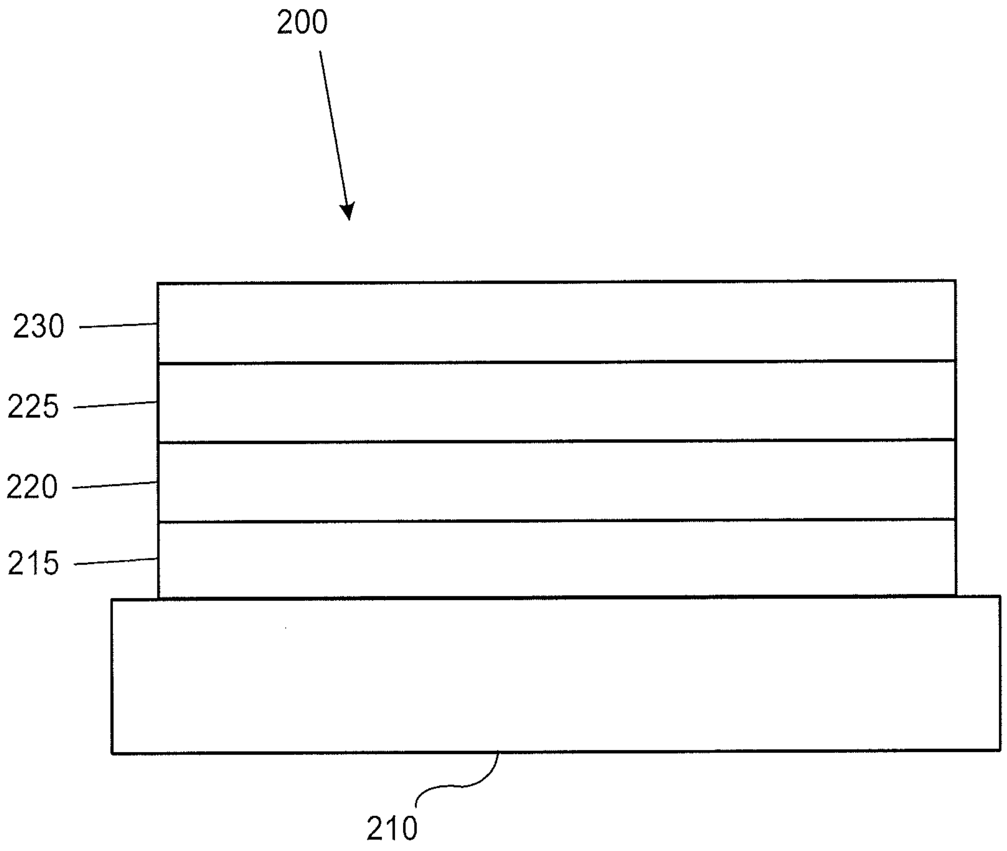


FIGURE 2

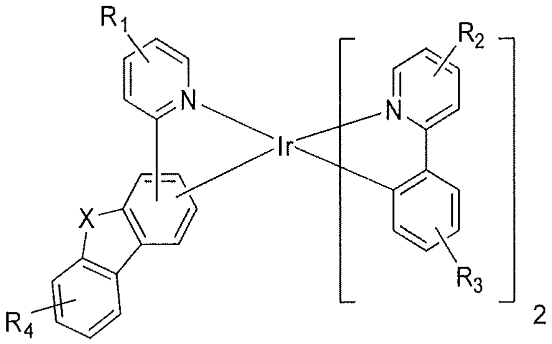


FIGURE 3

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

This application is a continuation of U.S. application Ser. No. 12/727,615, filed Mar. 19, 2010, which claims priority to U.S. Provisional Application No. 61/162,476, filed Mar. 23, 2009, the disclosures of which are herein expressly incorporated 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 novel organic complexes that may be advantageously used in organic light emitting devices. More particularly, the present invention relates to novel heteroleptic iridium complexes containing a pyridyl dibenzo-substituted ligand and devices containing these compounds.

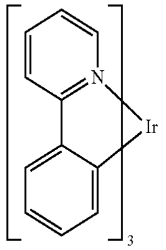
BACKGROUND

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

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

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

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



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

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

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

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

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

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

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

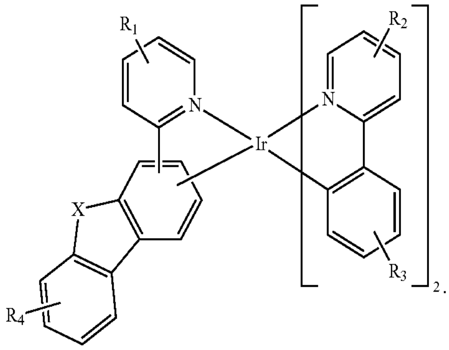
As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum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

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

SUMMARY OF THE INVENTION

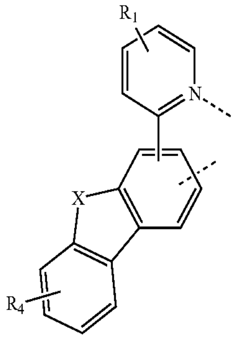
Novel phosphorescent emissive compounds are provided. The compounds comprise heteroleptic iridium complexes having the formula:

FORMULA I



The compound comprises a ligand having the structure

FORMULA II



X is selected from the group consisting of NR, O, S, BR, and Se. R is selected from hydrogen and alkyl. Preferably, R has 4 or fewer carbon atoms. R_1, R_2, R_3, and R_4 may represent mono, di, tri, or tetra substitutions. Each of R_1, R_2, R_3, and R_4 are independently selected from the group consisting of hydrogen, alkyl, and aryl. Preferably, alkyls in the R_1, R_2, R_3 and/or R_4 positions of Formula I have four or fewer carbon atoms (e.g., methyl, ethyl, propyl, butyl, and isobutyl). Preferably, R_1 and R_4 are independently hydrogen or alkyl having four or fewer carbon atoms; more preferably, R_1 and R_4 are independently hydrogen or methyl. Preferably, R_2 and R_3 are independently hydrogen or alkyl having four or fewer carbon atoms; more preferably, R_2 and R_3 are independently hydrogen or methyl; most preferably, R_2 and R_3 are hydrogen.

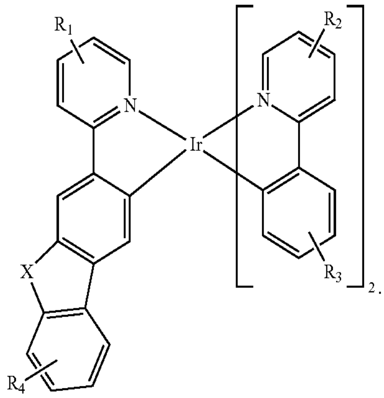
Preferably, R_1 and R_4 are independently hydrogen, alkyl having four or fewer carbon atoms or aryl with 6 or fewer atoms in the ring; more preferably, R_1 and R_4 are independently hydrogen, methyl or phenyl. Preferably, R_2 and R_3 are independently hydrogen, alkyl having four or fewer carbon atoms or aryl with 6 or fewer atoms in the ring; more preferably, R_2 and R_3 are independently hydrogen, methyl or phenyl; most preferably, R_2 and R_3 are hydrogen.

In one aspect, compounds are provided wherein R_1, R_2, R_3, and R_4 are independently selected from the group consisting of hydrogen and alkyl having four or fewer carbon atoms. In another aspect, compounds are provided wherein R_1, R_2, R_3, and R_4 are independently selected from the group consisting of hydrogen and methyl. In yet another aspect, compounds are provided wherein R_1, R_2, R_3, and R_4 are hydrogen.

In another aspect, compounds are provided wherein R_1, R_2, R_3, and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms and aryl with 6 or fewer atoms in the ring. In another aspect, compounds are provided wherein R_1, R_2, R_3, and R_4 are independently selected from the group consisting of hydrogen, methyl and phenyl. In yet another aspect, compounds are provided wherein R_1, R_2, R_3, and R_4 are hydrogen.

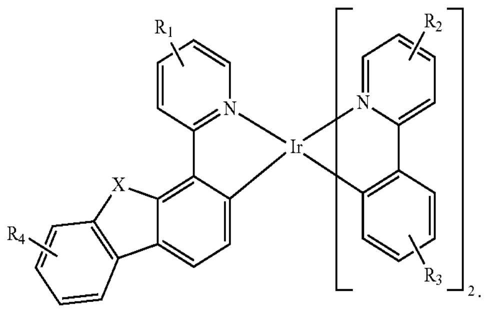
Particular heteroleptic iridium complexes are also provided. In one aspect, heteroleptic iridium complexes are provided having the formula:

FORMULA III



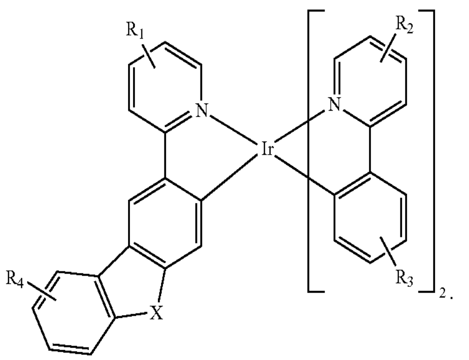
In another aspect, heteroleptic iridium complexes are provided having the formula:

FORMULA IV



In yet another aspect, heteroleptic iridium complexes are provided having the formula:

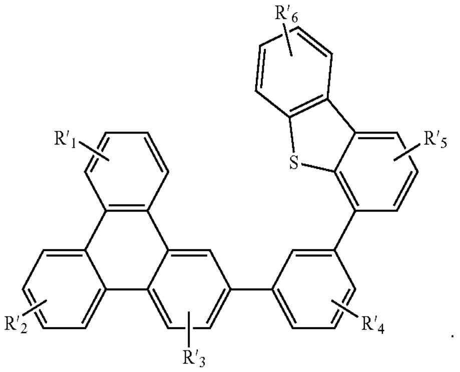
FORMULA V



Specific examples of heteroleptic iridium complex are provided including Compounds 1-36. In particular, heteroleptic compounds are provided wherein X is O (i.e., pyridyl dibenzofuran), for example, Compounds 1-12. Additionally, heteroleptic compounds are provided wherein X is S (i.e., pyridyl dibenzothiophene), for example, Compounds 13-24. Moreover, heteroleptic compounds are provided wherein X is NR (i.e., pyridyl carbazole), for example, Compounds 25-36.

Additional specific examples of heteroleptic iridium complexes are provided, including Compounds 37-108. In particular, heteroleptic compounds are provided wherein X is O, for example, Compounds 37-60. Further, heteroleptic compounds are provided wherein X is S, for example, Compounds 61-84. Moreover, heteroleptic compounds are provided wherein X is NR, for example, Compounds 85-108.

Additionally, an organic light emitting device is also provided. The device has an anode, a cathode, and an organic layer disposed between the anode and the cathode, where the organic layer comprises a compound having FORMULA I. In particular, the organic layer of the device may comprise a compound selected from Compounds 1-36. The organic layer may further comprise a host. Preferably, the host contains a triphenylene moiety and a dibenzothiophene moiety. More preferably, the host has the formula:



R'_1, R'_2, R'_3, R'_4, R'_5, and R'_6 may represent mono, di, tri, or tetra substitutions. R'_1, R'_2, R'_3, R'_4, R'_5, and R'_6 are independently selected from the group consisting of hydrogen, alkyl, and aryl.

The organic layer of the device may comprise a compound selected from the group consisting of Compounds 1-108. In particular, the organic layer of the device may also comprise a compound selected from Compounds 37-108.

A consumer product comprising a device is also provided. The device contains an anode, a cathode, and an organic layer disposed between the anode and the cathode, where the organic layer further comprises a compound having FORMULA I.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. **1** shows an organic light emitting device.

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

FIG. **3** shows a heteroleptic iridium complex.

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 outcoupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen Or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as inkjet and OVJD. Other methods may also be used, The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing, Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processibility than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

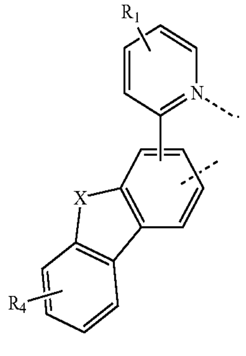
Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent 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.

Novel compounds are provided, the compounds comprising a heteroleptic iridium complex (illustrated in FIG. 3). In particular, the complex has two phenylpyridine ligands and one ligand having the structure

FORMULA II



The ligand having the structure FORMULA II consists of a pyridine joined to a dibenzofuran, dibenzothiophene, carbazole, dibenzoborole, or dibenzoselenophene (herein also referred to as “pyridyl dibenzo-substituted”). These compounds may be advantageously used in organic light emitting devices as an emitting dopant in an emissive layer.

Iridium complexes containing two or three pyridyl dibenzofuran, dibenzothiophene, carbazole, and fluorene ligands have been reported. By replacing the phenyl group in tris(2-phenylpyridine)iridium with dibenzofuran, dibenzothiophene, carbazole, and fluorene groups, the HOMO-LUMO energy levels, photophysical properties, and electronic properties of the resulting complex can be significantly affected. A variety of emission colors, ranging from green to red, have been achieved by using complexes with different combinations of pyridyl dibenzo-substituted ligands (i.e., bis and tris complexes). However, the existing complexes may have practical limitations. For example, iridium complexes having two or three of these types of ligands (e.g., pyridyl dibenzofuran, dibenzothiophene, or carbazole) have high molecular weights, which often results in a high sublimation temperature. In some instances, these complexes can become non-sublimable due to the increased molecular weight. For example, tris(2-(dibenzo[b,d]furan-4-yl)pyridine)Iridium(III) decomposed during sublimation attempts. Additionally, known compounds comprising a pyridyl fluorene ligand may have reduced stability. Fluorene groups (e.g., C=O and CRR') disrupt conjugation within the ligand structure resulting in a diminished ability to stabilize electrons. Therefore, compounds with the beneficial properties of pyridyl dibenzo-substituted ligands (e.g., dibenzofuran, dibenzothiophene, carbazole, dibenzoborole, and dibenzoselenophene) and a relatively low sublimation temperature are desirable.

Additionally, iridium complexes having two or three of the ligands having FORMULA II have high molecular weights and stronger intermolecular interactions, which often results in a high sublimation temperature. In some instances, these complexes can become non-sublimable due to the increased molecular weight and strong intermolecular interactions.

Novel heteroleptic iridium complexes are provided herein. The complexes contain pyridyl dibenzo-substituted ligands having the structure FORMULA II. In particular, the novel heteroleptic complexes include a single pyridyl dibenzo-substituted ligand wherein the ligand contains O, S, N, Se, or B (i.e. the ligand is pyridyl dibenzofuran, pyridyl dibenzothiophene, pyridyl carbazole, pyridyl dibenzoselenophene, or pyridyl dibenzoborole) and two phenylpyridine ligands. As a result of the particular combination of ligands in the heteroleptic compounds disclosed herein, these compounds can provide both improved photochemical and electrical properties as well as improved device manufacturing. In particular, by containing only one of the dibenzo-substituted pyridine ligands having FORMULA II, the complexes provided herein will likely have lower sublimation temperatures (correlated with reduced molecular weight and/or weaker intermolecular interactions). Additionally, these compounds maintain all of the benefits associated with the pyridyl dibenzo-substituted ligand, such as improved stability, efficiency, and narrow line width. Therefore, these compounds may be used to provide improved organic light emitting devices and improved commercial products comprising such devices. In particular, these compounds may be particularly useful in red and green phosphorescent organic light emitting devices (PHOLEDs).

As mentioned previously, bis or tris iridium complexes containing ligands having FORMULA II may be limited in practical use due to the high sublimation temperature of the complex. The invention compounds, however, have a lower sublimation temperature which can improve device manufacturing. Table 1 provides the sublimation temperature for several compounds provided herein and the corresponding bis or tris complex. For example, Compound 1 has a sublimation temperature of 243° C. while the corresponding tris complex fails to sublime. Additionally, other tris complexes comprising three pyridyl dibenzo-substituted ligands (i.e., tris complex comprising pyridyl dibenzothiophene) fail to sublime. Therefore, the compounds provided herein may allow for improved device manufacturing as compared to previously reported bis and tris compounds.

TABLE 1

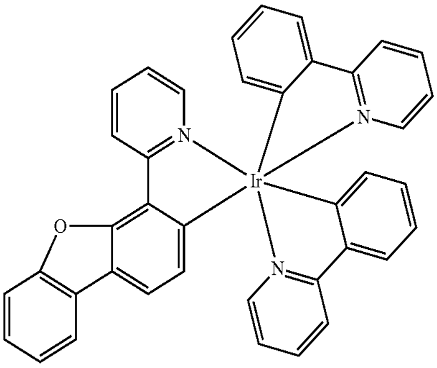
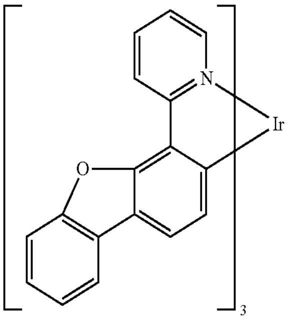
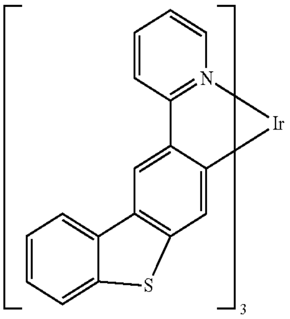
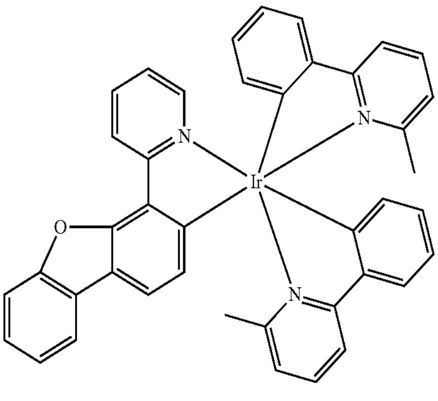
Compounds	Sublimation temperature (° C.)
 Compound 1	243
	Fail to sublime
	Fail to sublime
 Compound 4	218

TABLE 1-continued

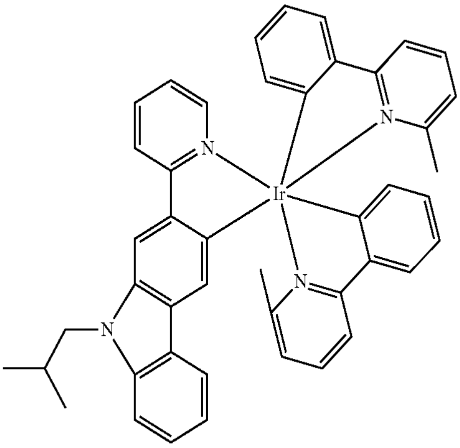
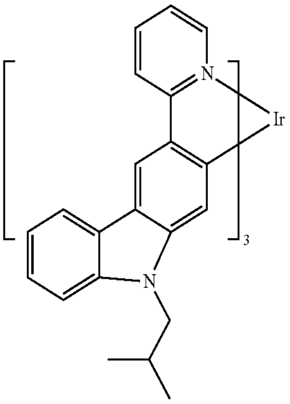
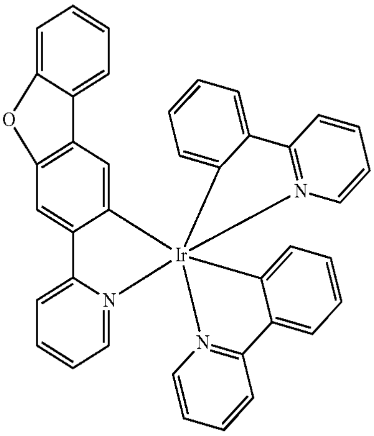
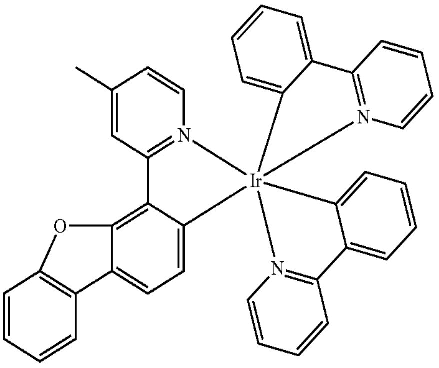
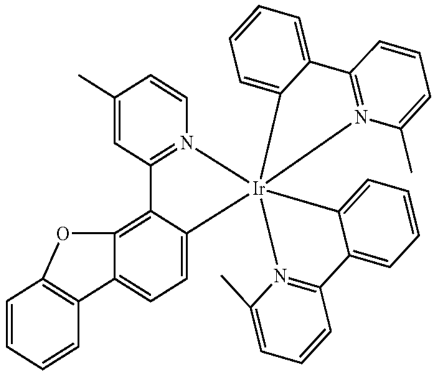
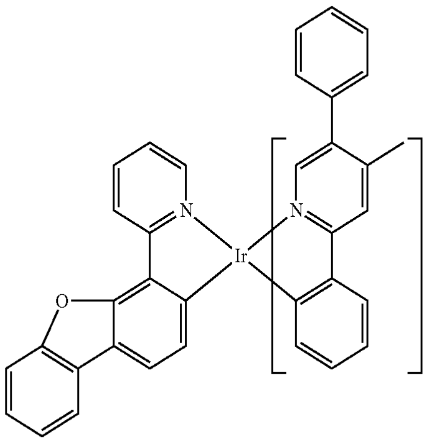
Compounds	Sublimation temperature (° C.)
 Compound 29	230
	290
 Compound 2	232

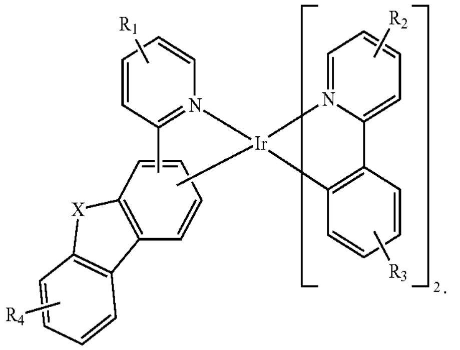
TABLE 1-continued

Compounds	Sublimation temperature (° C.)
 Compound 7	256
 Compound 10	240
 Compound 37	224

Generally, the dibenzo-substituted pyridine ligand would be expected to have lower triplet energy than the phenylpyridine ligand, and consequently the dibenzo-substituted pyridine ligand would be expected to control the emission properties of the compound. Therefore, modifications to the dibenzo-substituted pyridine ligand may be used to tune the emission properties of the compound. The compounds disclosed herein contain a dibenzo-substituted pyridine ligand containing a heteroatom (e.g., O, S, or NR) and optionally further substituted by chemical groups at the R_1 and R_4 positions. Thus, the emission properties of the compounds may be tuned by selection of a particular heteroatom and/or varying the substituents present on the dibenzo-substituted pyridine ligand.

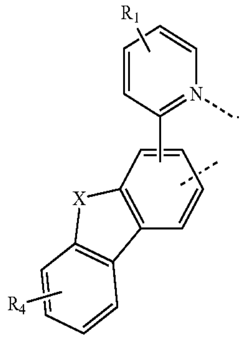
The compounds described herein comprise heteroleptic iridium complexes having the formula:

FORMULA I



Features of the compounds having FORMULA I include comprising one ligand having the structure

FORMULA II



and two phenylpyridine ligands that may have further substitution, wherein all ligands are coordinated to Ir.

X is selected from the group consisting of NR, O, S, BR, and Se. R is selected from hydrogen and alkyl. R_1, R_2, R_3 and R_4 may represent mono, di, tri, or tetra substitutions; and each of R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms, and aryl.

In another aspect, R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms, and aryl with 6 or fewer atoms in the ring.

The term "aryl" as used herein refers to an aryl, comprising either carbon atoms or heteroatoms, that is not fused to the phenyl ring of the phenylpyridine ligand (i.e., aryl is a non-fused aryl). The term "aryl" as used herein contemplates single-ring groups and polycyclic ring systems. The polycyclic rings may have two or more rings in which two carbons are common by two adjoining rings (the rings are "fused") wherein at least one of the rings is aromatic, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles and/or heteroaryls. Additionally, the aryl group may be optionally substituted with one or more substituents selected from halo, CN, CO_2R, C(O)R, NR_2, cyclic-amino, NO_2, and OR. "Aryl" also encompasses a heteroaryl, such as single-ring hetero-aromatic groups that may include from one to three heteroatoms, for example, pyrrole, furan, thiophene, imidazole, oxazole, thiazole, triazole, pyrazole, pyridine, pyrazine and pyrimidine, and the like. This includes polycyclic hetero-aromatic systems having two or more rings in which two atoms are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles and/or heteroaryls. Additionally, the heteroaryl group may be optionally substituted with one or more substituents selected from halo, CN, CO_2R, C(O)R, NR_2, cyclic-amino, NO_2, and OR. For example, R_1, R_2, R_3 and/or R_4 may be an aryl, including an heteroaryl, that is not used to the phenyl ring of the phenylpyridine.

The term "alkyl" as used herein contemplates both straight and branched chain alkyl radicals. Examples include methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tert-butyl, and the like. Additionally, the alkyl group may be optionally substituted with one or more substituents selected from halo, CN, CO_2R, C(O)R, NR_2, cyclic-amino, NO_2, and OR, wherein each R is independently selected from H, alkyl, alkenyl, alkynyl, aralkyl, aryl and heteroaryl. Preferably, in order to make the compounds sublimable and/or to reduce sublimation temperature, alkyls in the R_1, R_2, R_3 and/or R_4 positions of Formula I have four or fewer carbon atoms (e.g., methyl, ethyl, propyl, butyl, and isobutyl).

In general, the compounds provided herein have relatively low sublimation temperatures compared to previously reported compounds. Thus, these novel compounds provide improved device fabrication among other beneficial properties. Moreover, it is believed that heteroleptic compounds having FORMULA I wherein R_1, R_2, R_3 and R_4 are selected from smaller substituents may be particularly beneficial. A smaller substituents includes, for example, hydrogen or alkyl. In particular, it is believed that compounds wherein the substituents R_1, R_2, R_3 and/or R_4 are selected from smaller substituents may have even lower sublimation temperatures thereby further improving manufacturing while maintaining the desirable properties (e.g., improved stability and lifetimes) provided by the ligand having the structure FORMULA II.

Generally, the compounds provided having FORMULA I have substituents such that R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, alkyl, and aryl. Preferably, any alkyl has four or fewer carbon atoms. To minimize molecular weight and thereby lower the sublimation temperature, compounds having smaller substituents on the ligand having the structure FORMULA II are preferred. Preferably, R_1 and R_4 are independently selected from the group consisting of hydrogen and alkyl having four or fewer carbon atoms; more preferably, R_1 and R_4 are independently selected from the group consisting of hydrogen and methyl.

For similar reasons, compounds are preferred having smaller substituents present on the phenylpyridine ligand. Additionally, the phenylpyridine ligand is believed to contribute less to the emission of the complex. Moreover, the complex contains two of the phenylpyridine ligand, thus substituents present on the phenylpyridine ligand contribute more to the overall molecular weight of the complex. For at least these reasons, preferably R_2 and R_3 are independently selected from hydrogen and alkyl having four or fewer carbon atoms; more preferably, R_2 and R_3 are independently selected from hydrogen and methyl; most preferably, R_2 and R_3 are hydrogen.

Compounds having alkyl and aryl substitutions that can decrease intermolecular interactions are also preferred.

In another aspect, preferably R_2 and R_3 are independently selected from hydrogen, alkyl having four or fewer carbon atoms and aryl with 6 or fewer atoms in the ring; more preferably, R_2 and R_3 are independently selected from hydrogen, methyl and phenyl; most preferably, R_2 and R_3 are hydrogen.

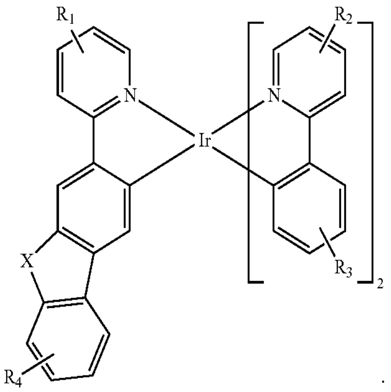
Compounds are preferred wherein the overall molecular weight of the complex is low to reduce the sublimation temperature and improve device manufacturing. Toward this end, compounds wherein all substituents are relatively small are preferred. In one aspect, preferably R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen and alkyl having four or fewer carbon atoms; more preferably, R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen and methyl; most preferably, R_1, R_2, R_3 and R_4 are hydrogen.

In another aspect, preferably R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms and aryl with 6 or fewer atoms in the ring; more preferably, R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, methyl and phenyl; most preferably, R_1, R_2, R_3 and R_4 are hydrogen.

As discussed above, X can also be BR. Preferably, R has 4 or fewer carbon atoms. For similar reasons as those previously discussed, smaller alkyl groups (i.e., alkyls having 4 or fewer carbon atoms) on the carbazole portion of the substituted ligand will likely lower the sublimation temperature of the complex and thus improve device manufacturing.

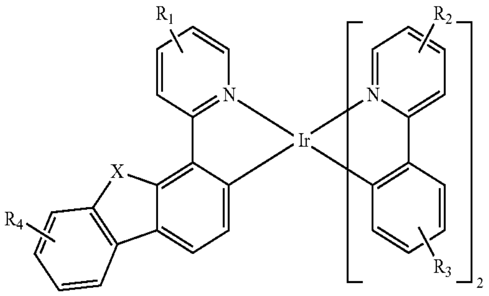
Particular heteroleptic iridium complexes are also provided. In one aspect, heteroleptic iridium complexes are provided having the formula:

FORMULA III



In another aspect, heteroleptic iridium complexes are provided having the formula:

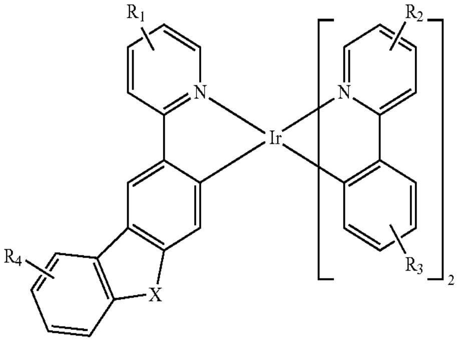
FORMULA IV



.

In yet another aspect, heteroleptic iridium complexes are provided having the formula:

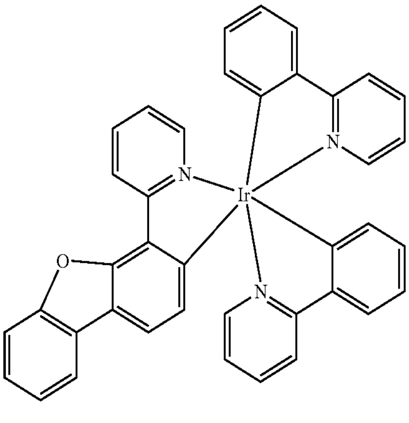
FORMULA V



.

Specific examples of heteroleptic iridium complexes are provided, and include compounds selected from the group consisting of:

Compound 1



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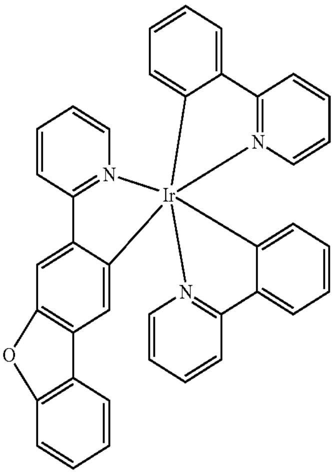
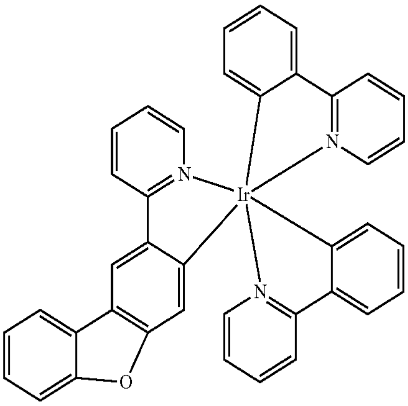
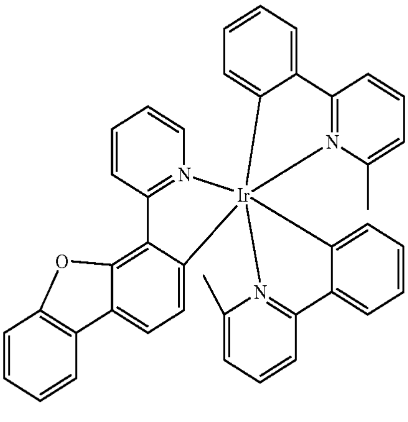
Compound 2



Compound 3



Compound 4



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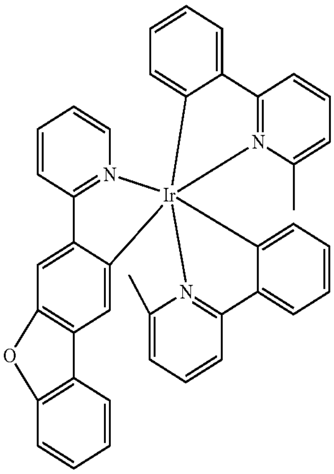
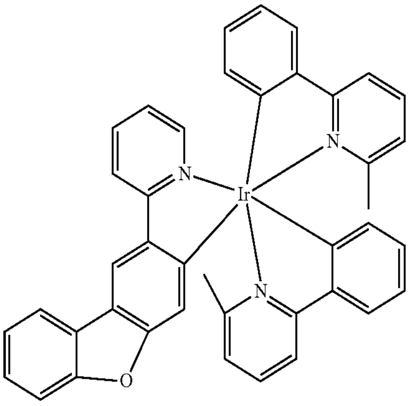
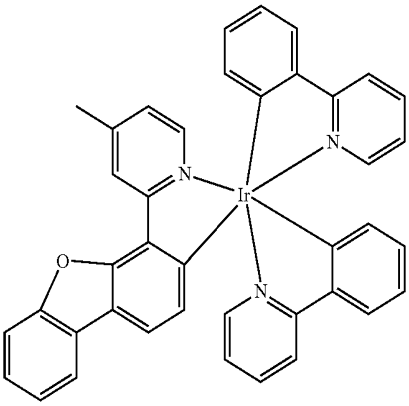
Compound 5



Compound 6



Compound 7



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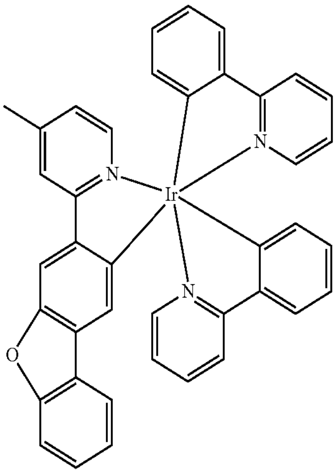
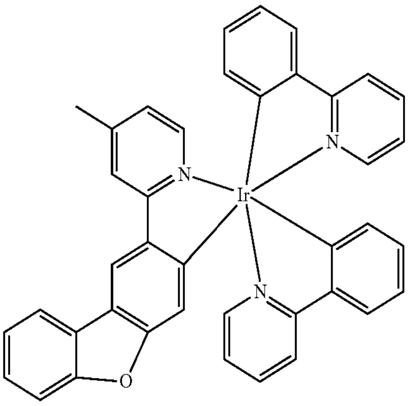
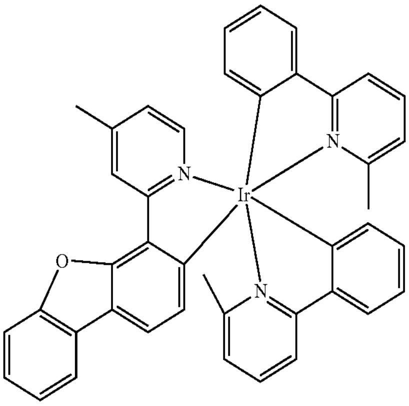
Compound 8



Compound 9



Compound 10



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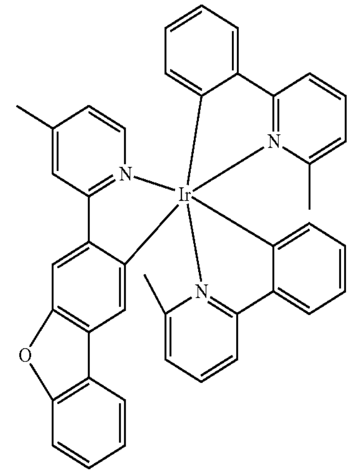
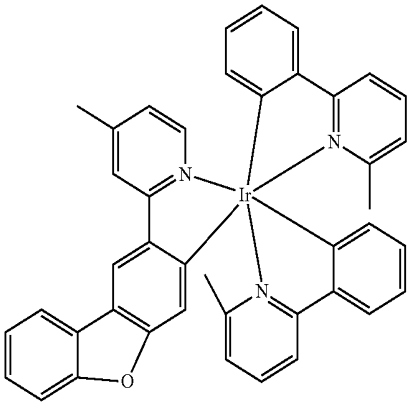
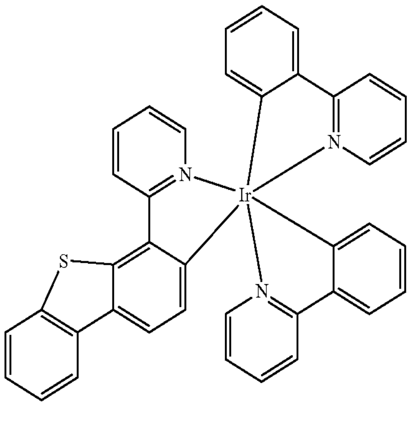
Compound 11



Compound 12



Compound 13



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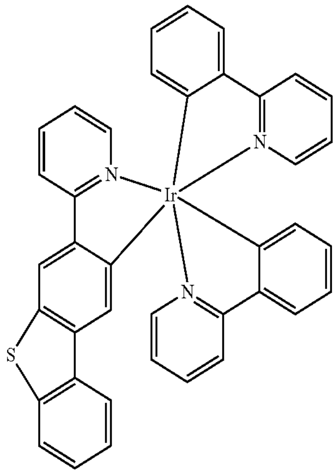
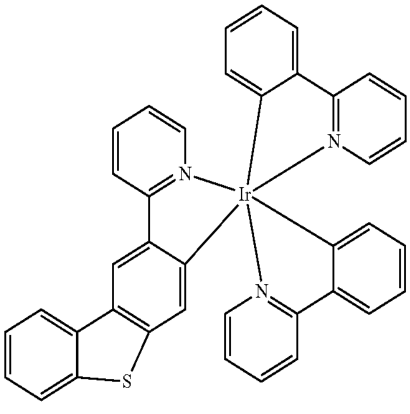
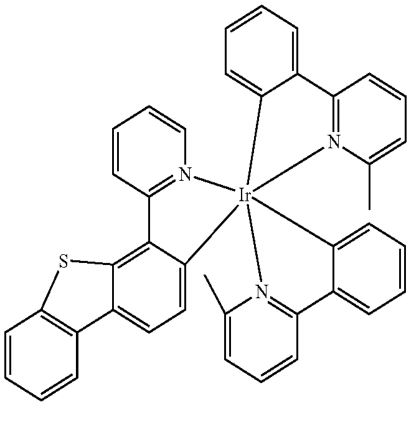
Compound 14



Compound 15



Compound 16



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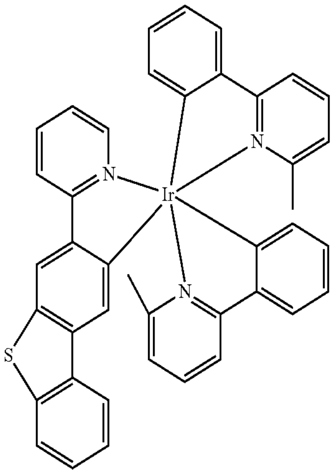
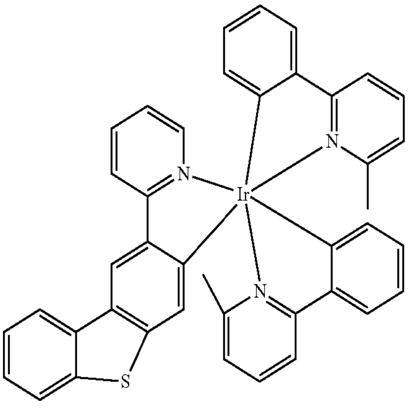
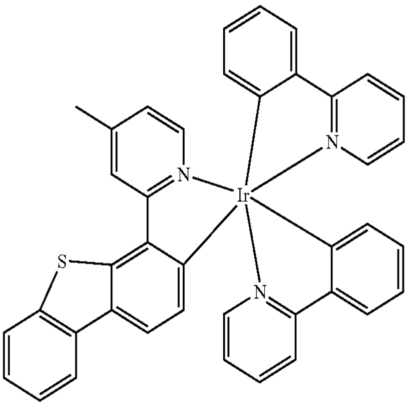
Compound 17



Compound 18



Compound 19



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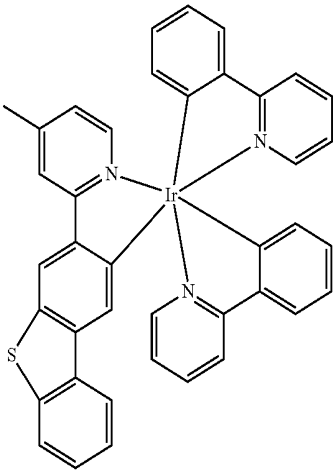
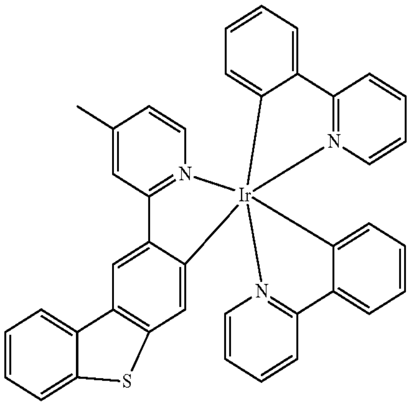
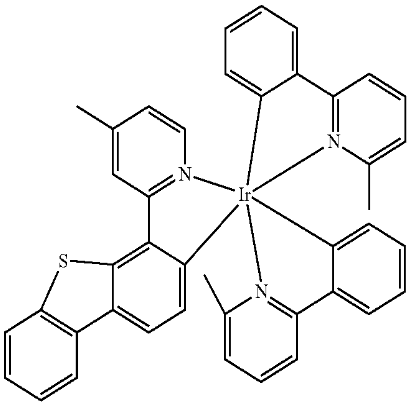
Compound 20



Compound 21



Compound 22



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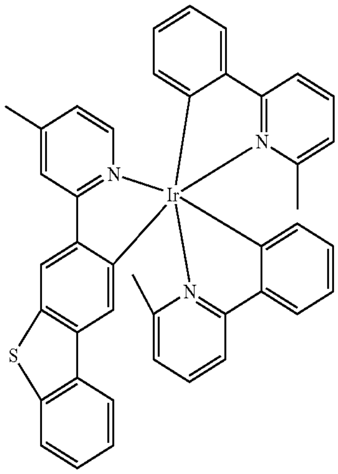
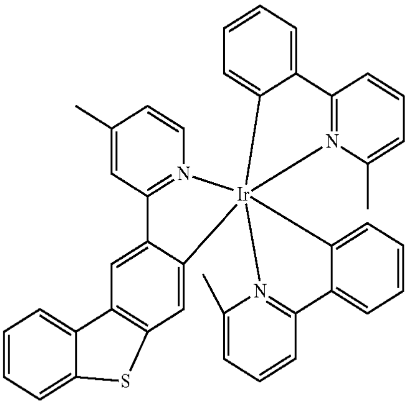
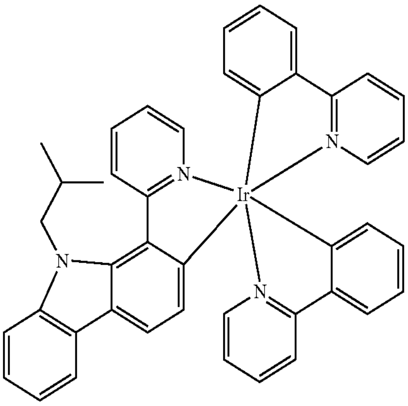
Compound 23



Compound 24



Compound 25



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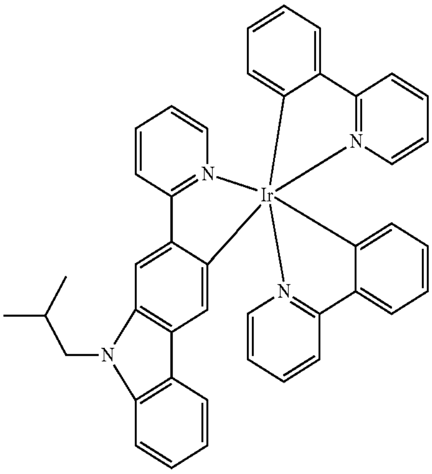
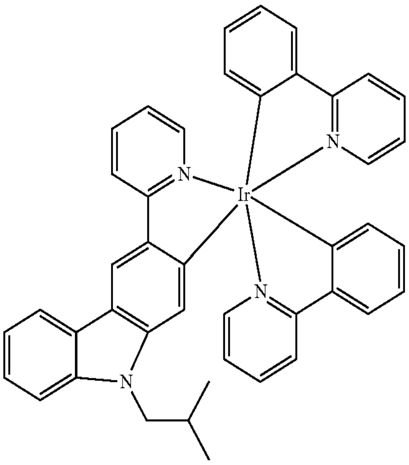
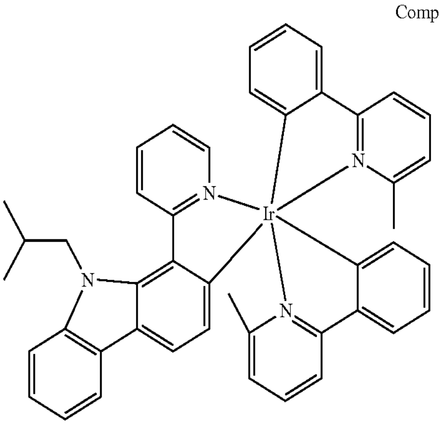
Compound 26



Compound 27



Compound 28



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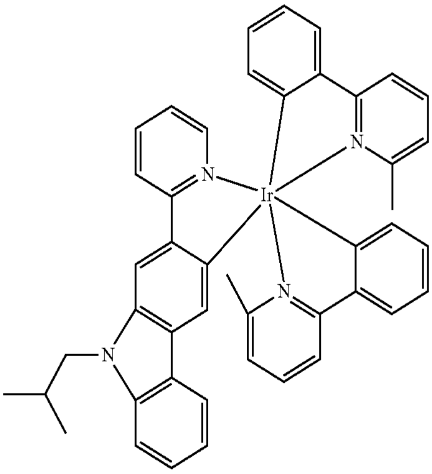
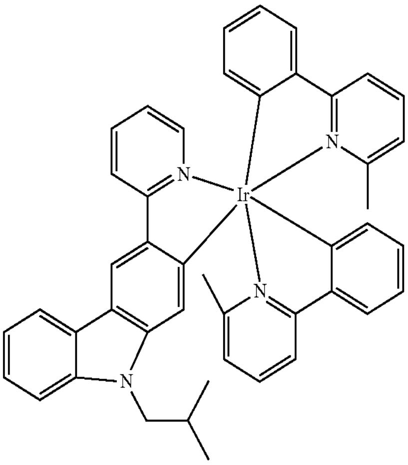
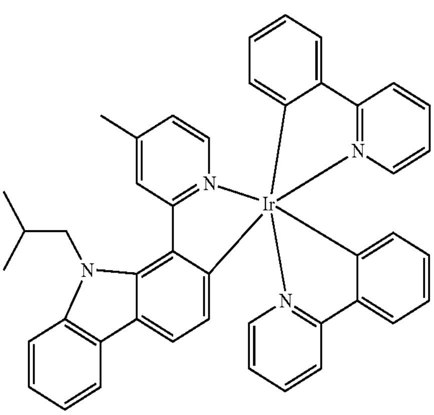
Compound 29



Compound 30



Compound 31



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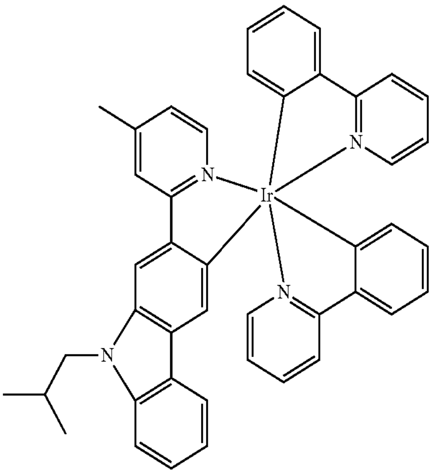
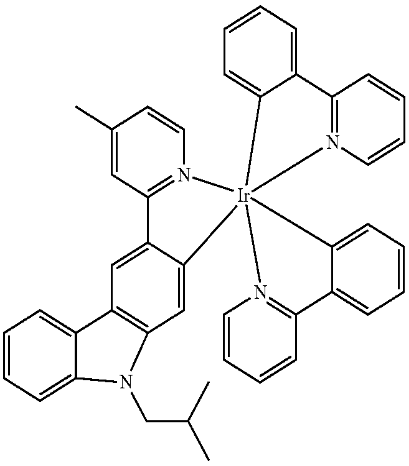
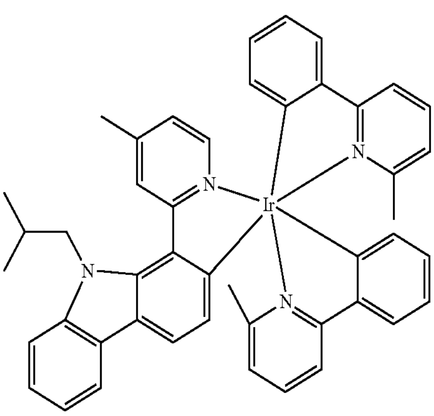
Compound 32



Compound 33



Compound 34



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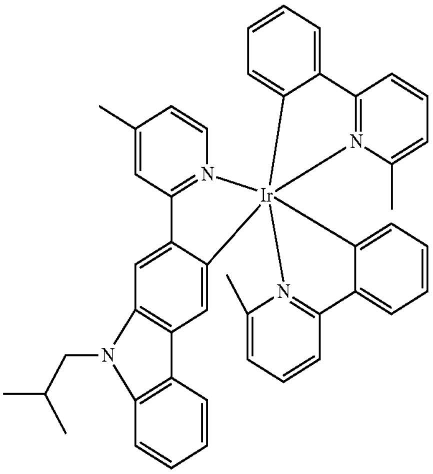
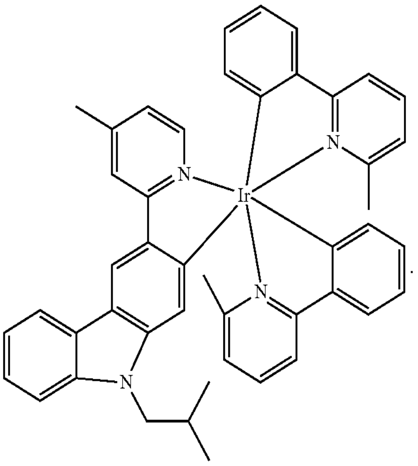
Compound 35

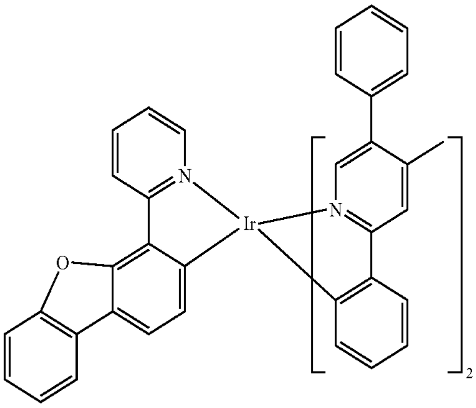


Compound 36



Additional specific examples of heteroleptic iridium complexes are provided, and include compounds selected from the group consisting of:

Compound 37



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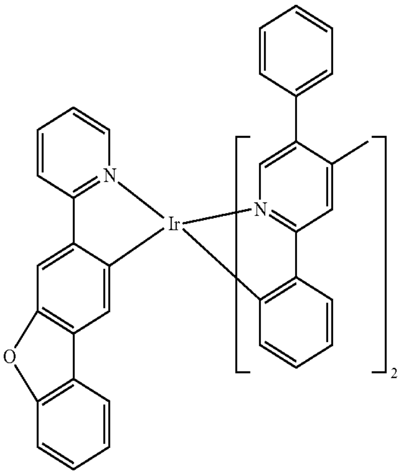
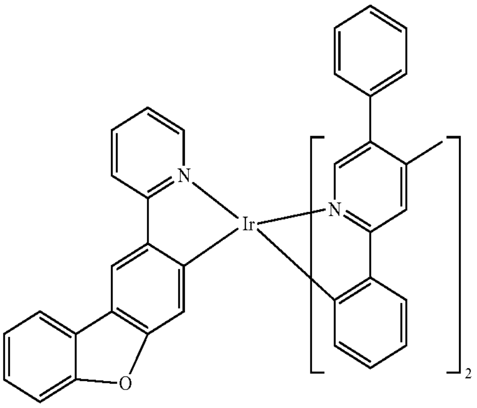
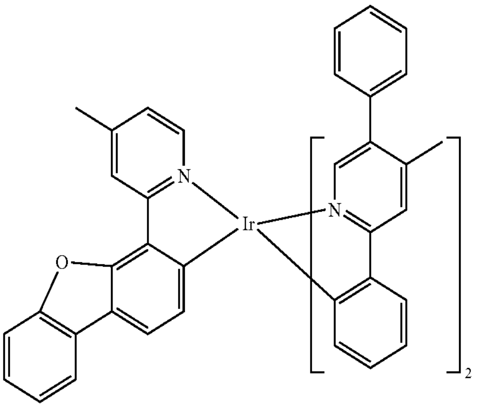
Compound 38



Compound 39



Compound 40



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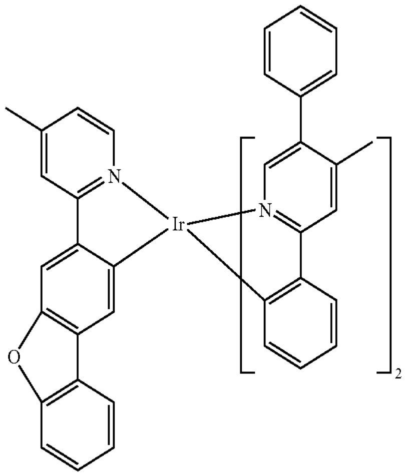
Compound 41



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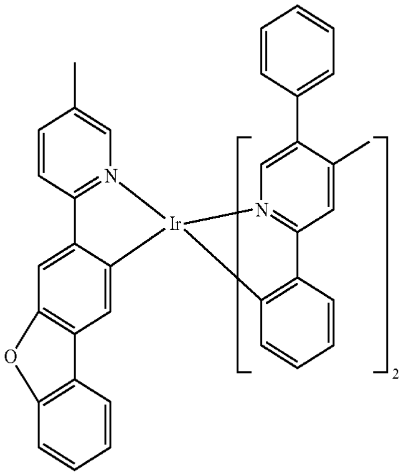
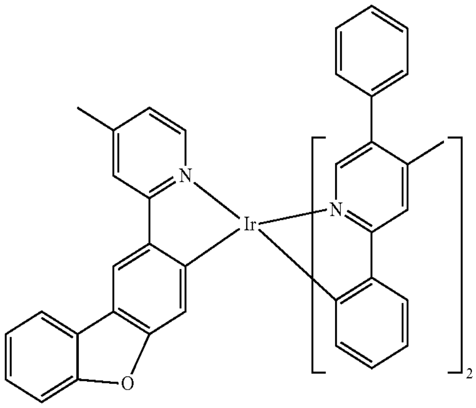
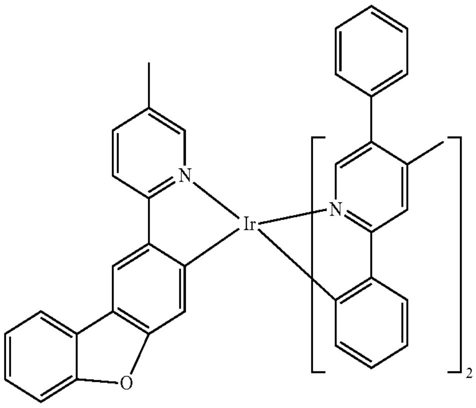
Compound 44



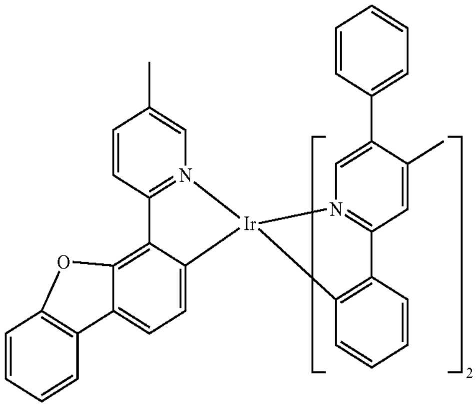
Compound 42



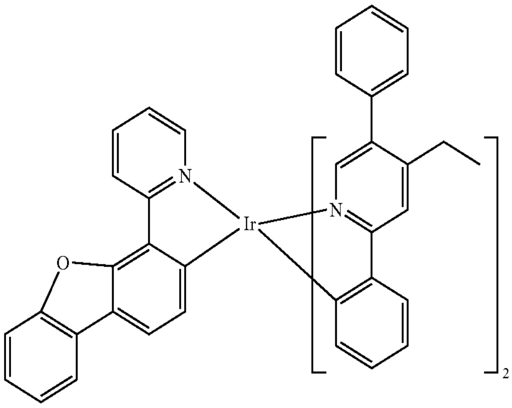
Compound 45



Compound 43



Compound 46



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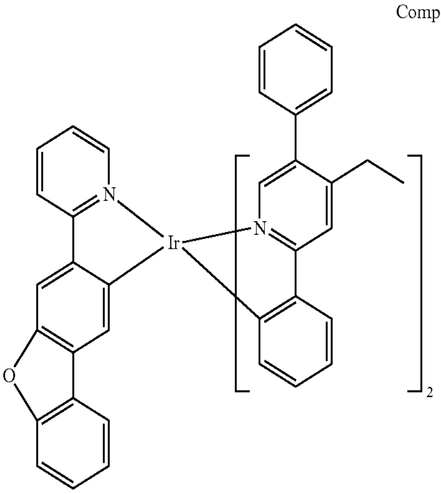
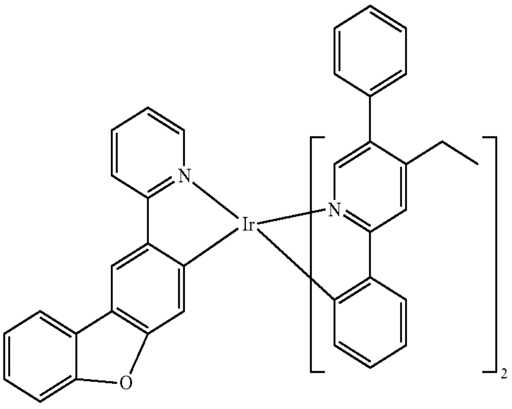
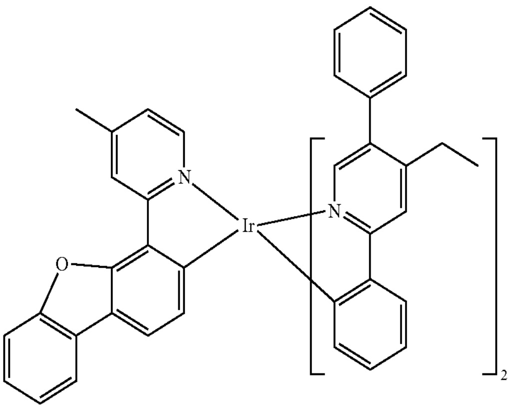
Compound 47



Compound 48



Compound 49



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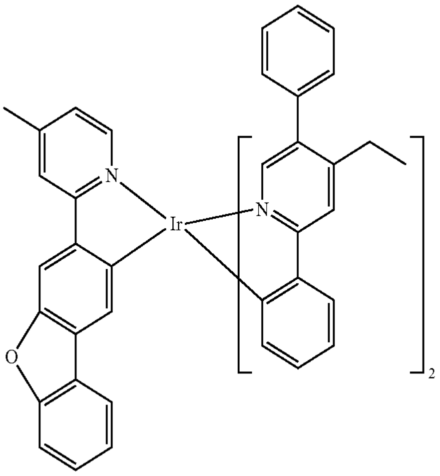
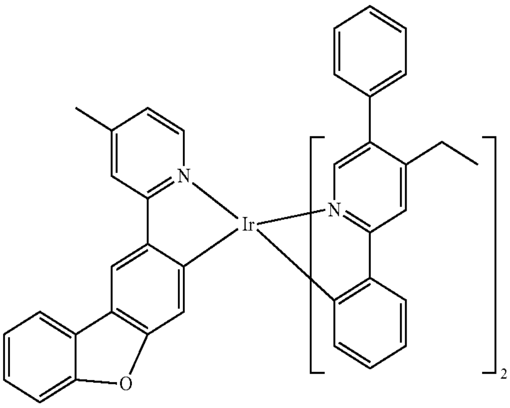
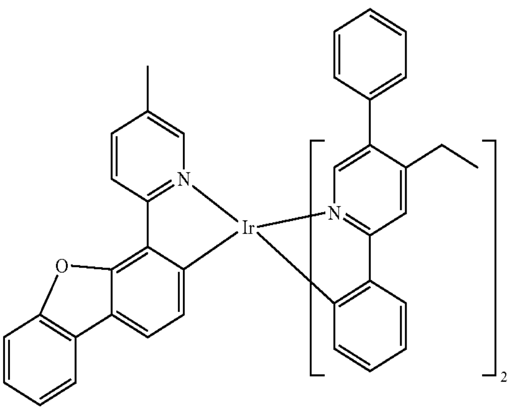
Compound 50



Compound 51



Compound 52



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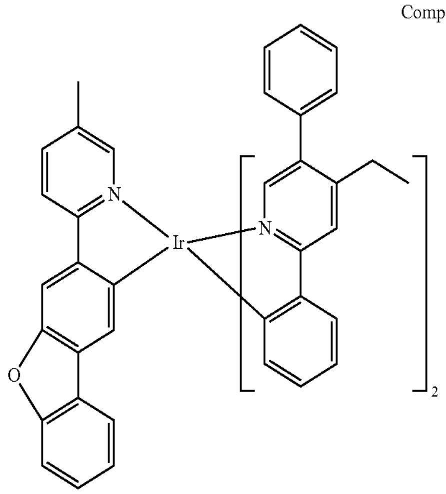
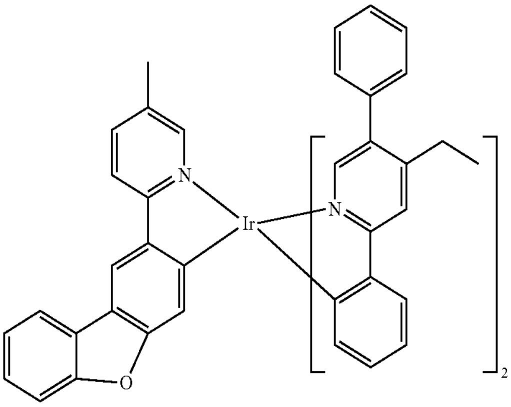
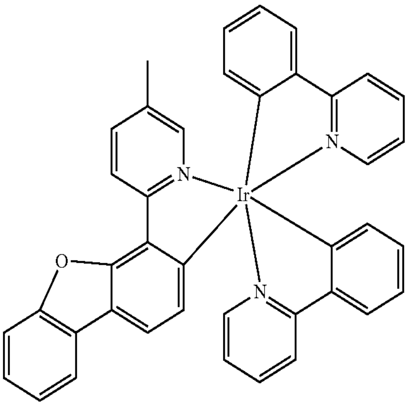
Compound 53



Compound 54



Compound 55



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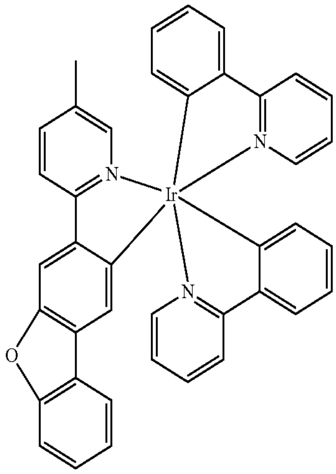
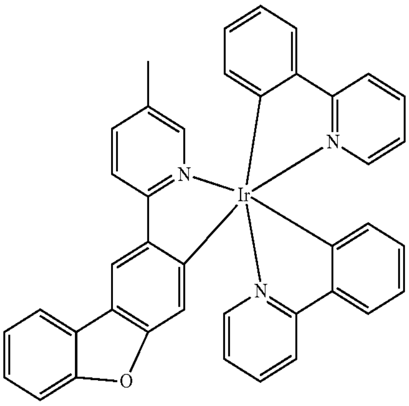
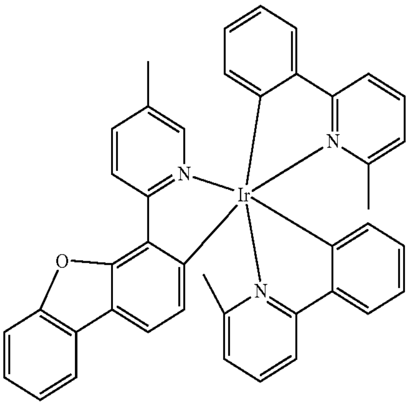
Compound 56



Compound 57



Compound 58



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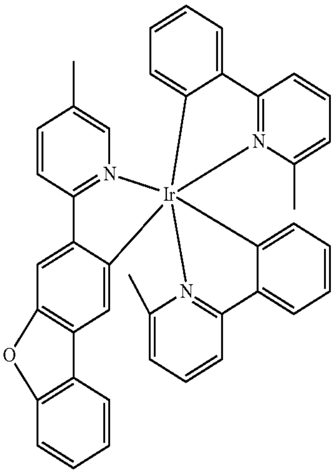
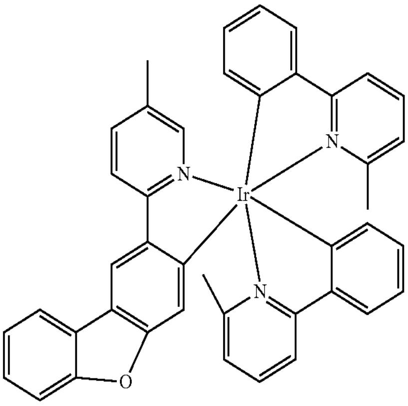
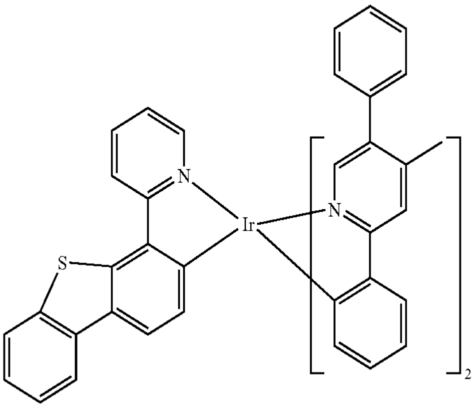
Compound 59



Compound 60



Compound 61



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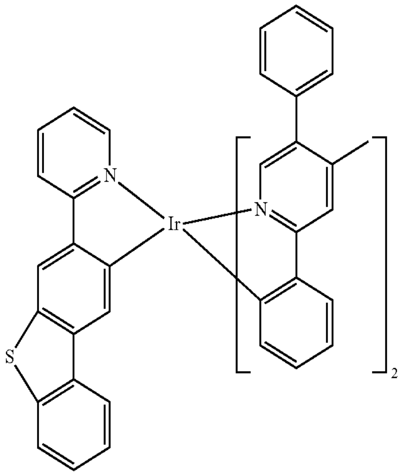
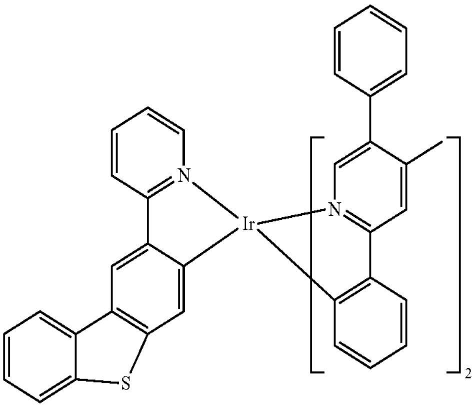
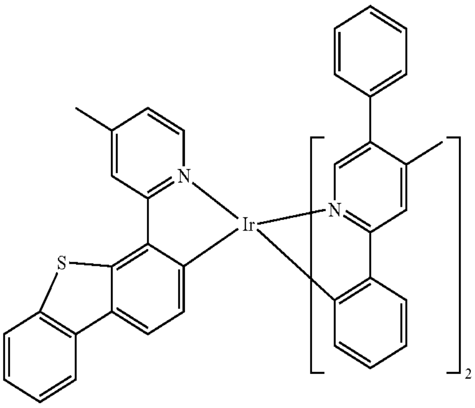
Compound 62



Compound 63



Compound 64



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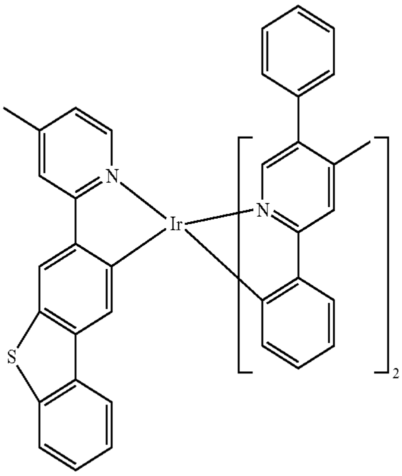
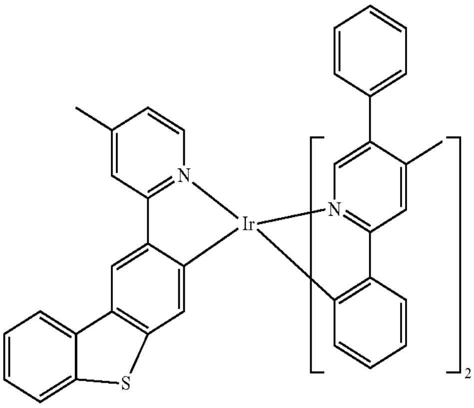
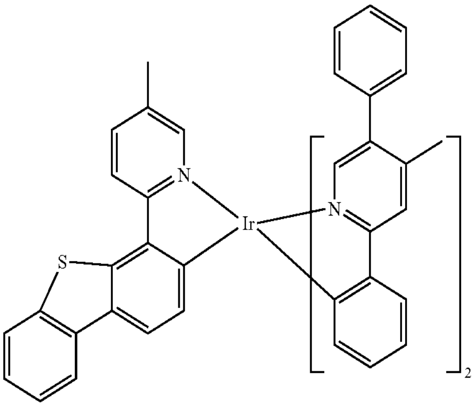
Compound 65



Compound 66



Compound 67



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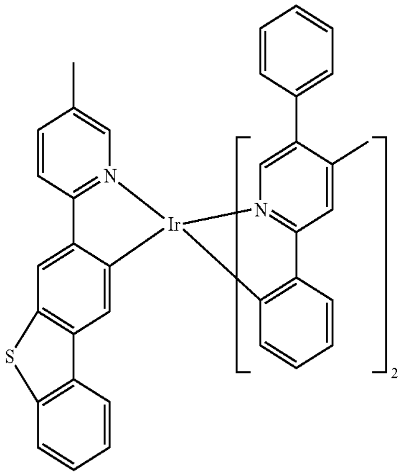
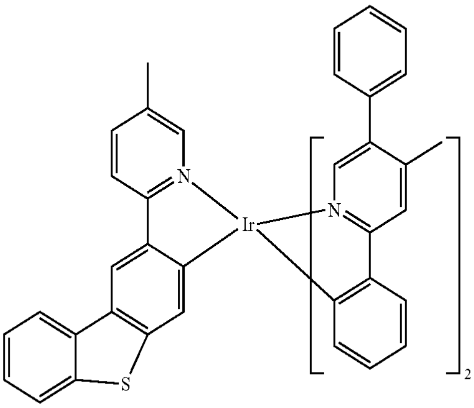
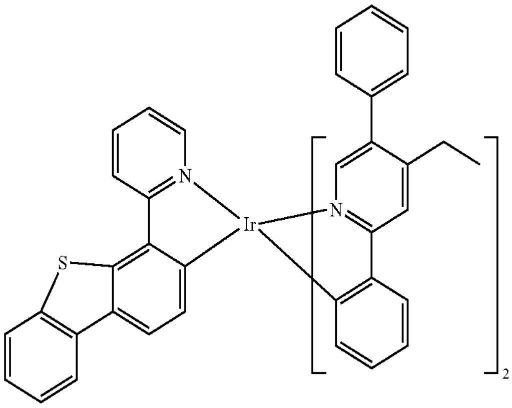
Compound 68



Compound 69



Compound 70



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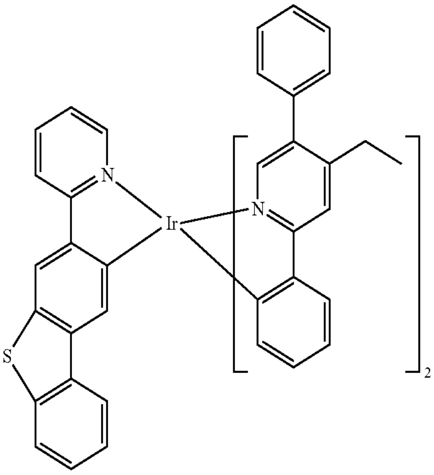
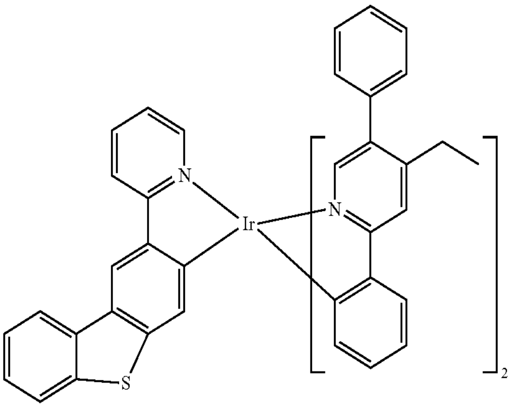
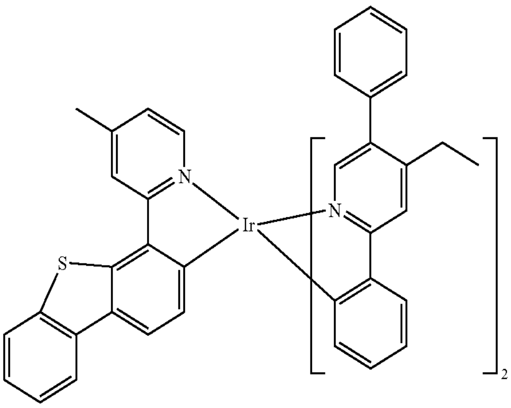
Compound 71



Compound 72



Compound 73



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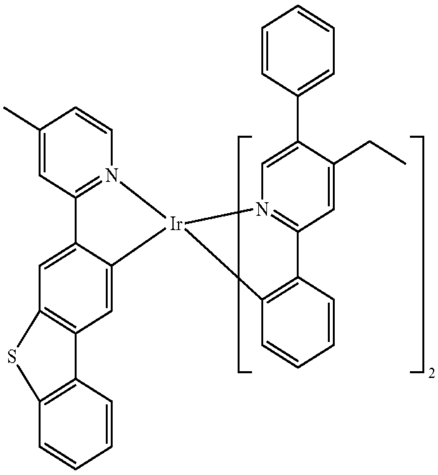
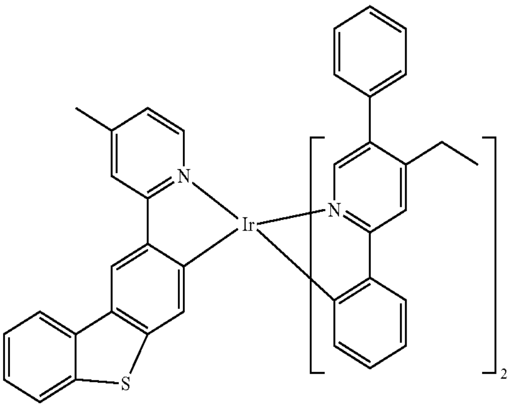
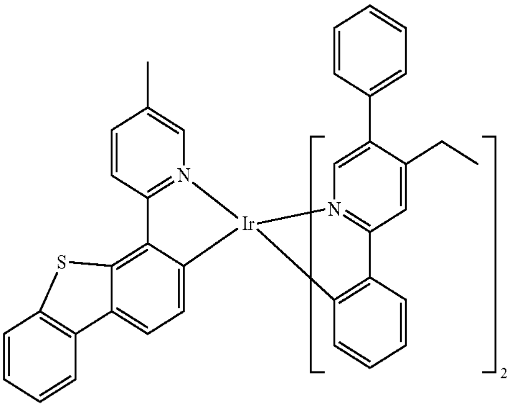
Compound 74



Compound 75



Compound 76



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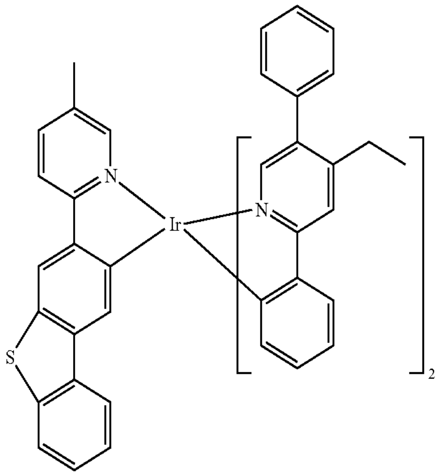
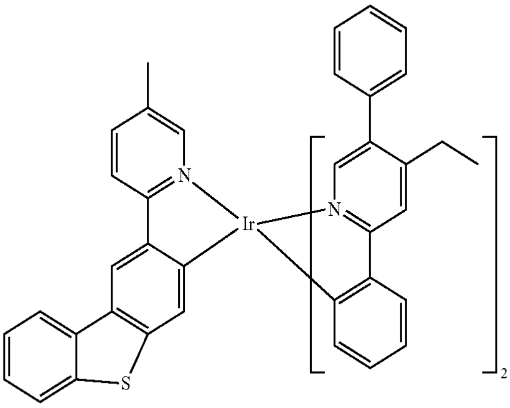
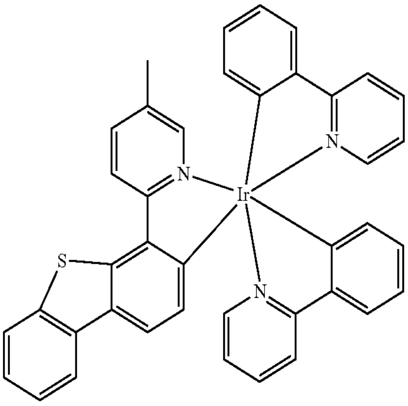
Compound 77



Compound 78



Compound 79



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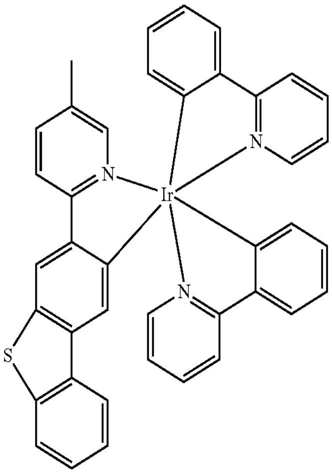
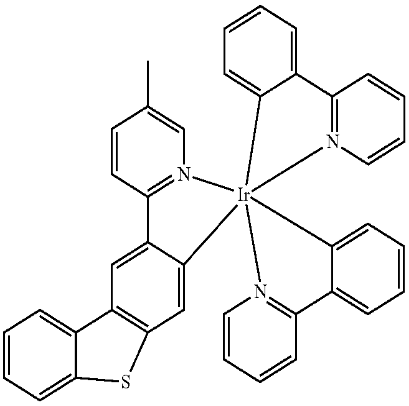
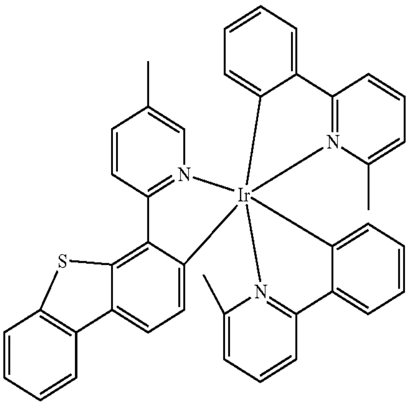
Compound 80



Compound 81



Compound 82



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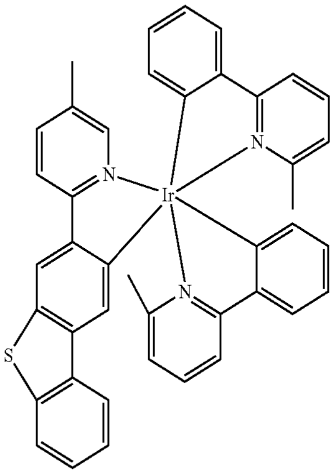
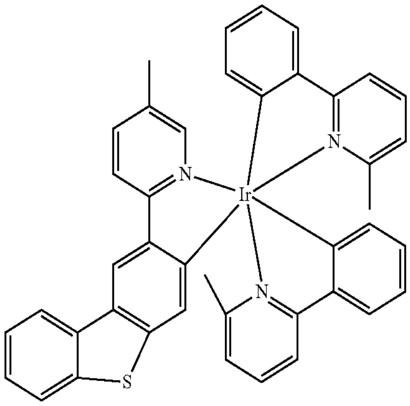
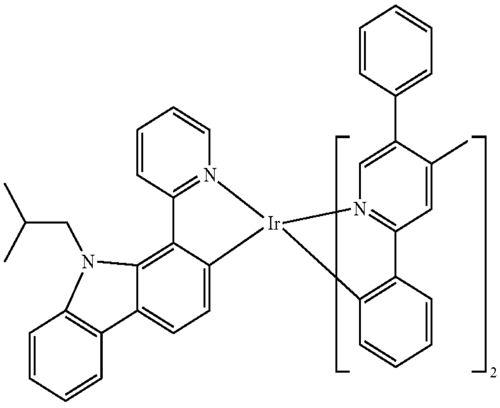
Compound 83



Compound 84



Compound 85



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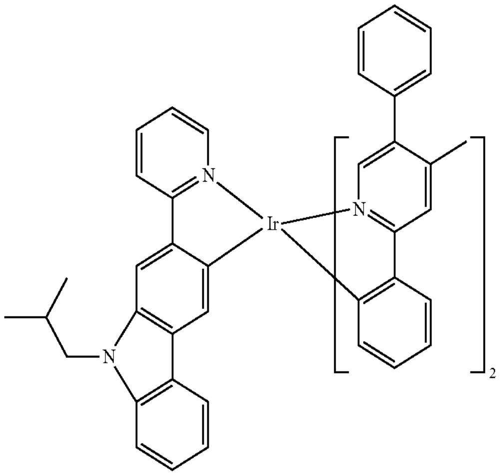
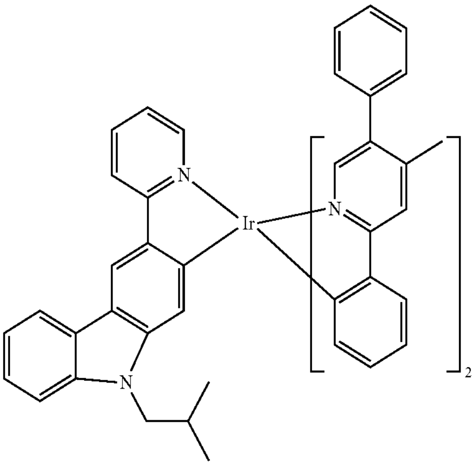
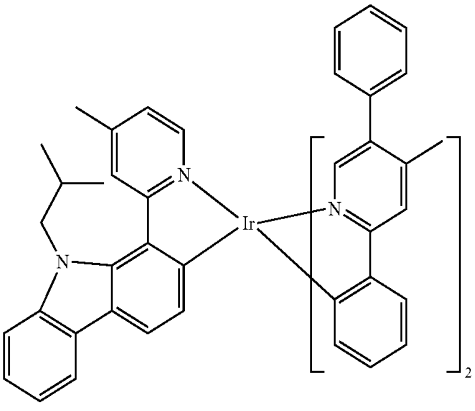
Compound 86



Compound 87



Compound 88



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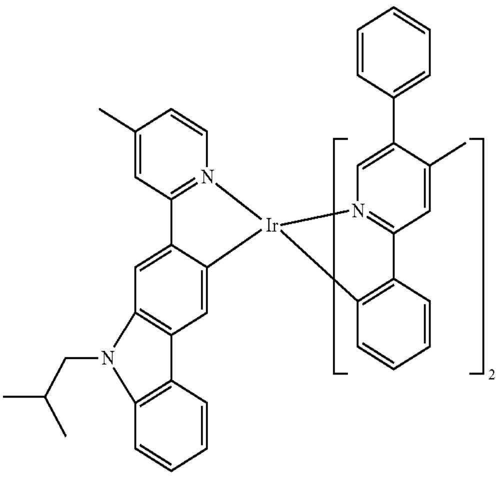
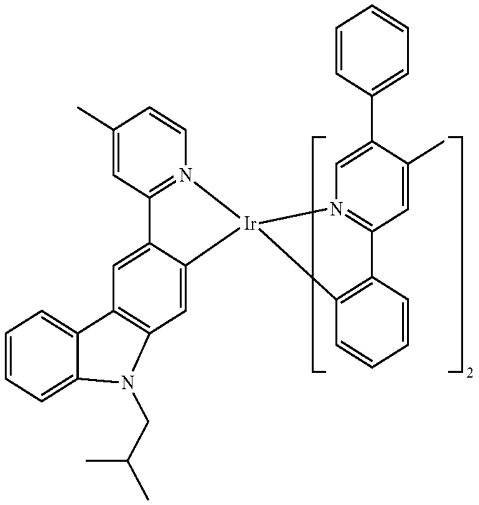
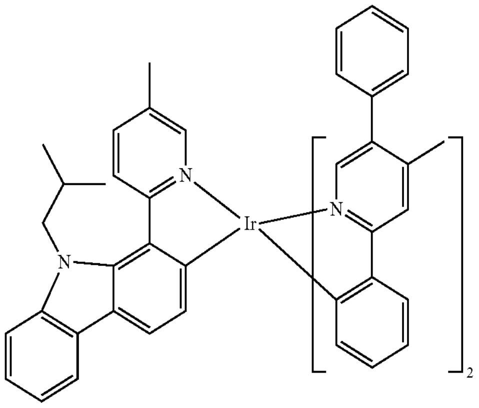
Compound 89



Compound 90



Compound 91



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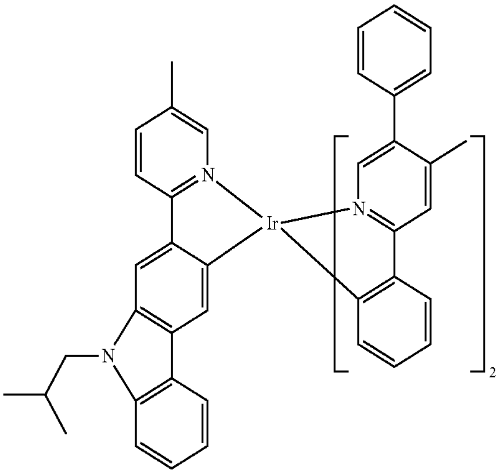
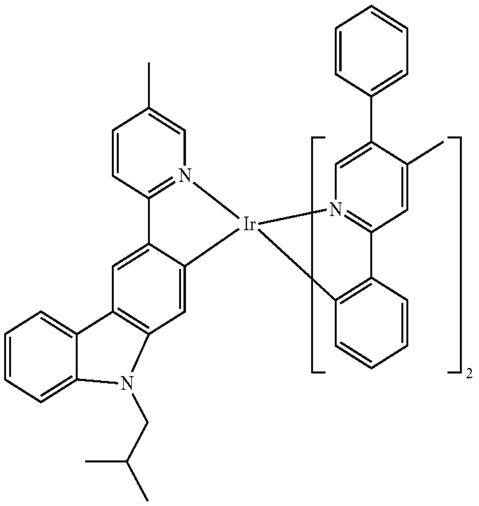
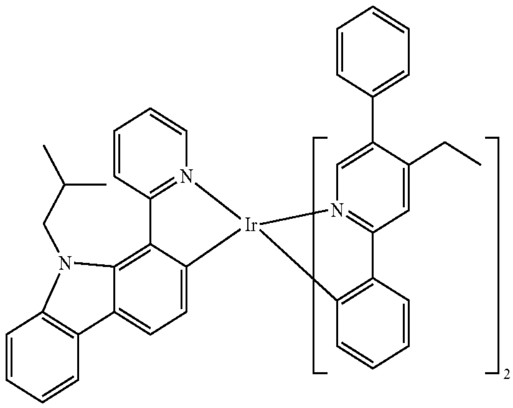
Compound 92



Compound 93



Compound 94



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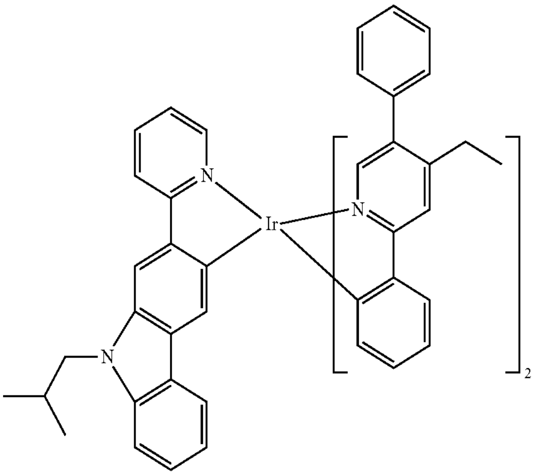
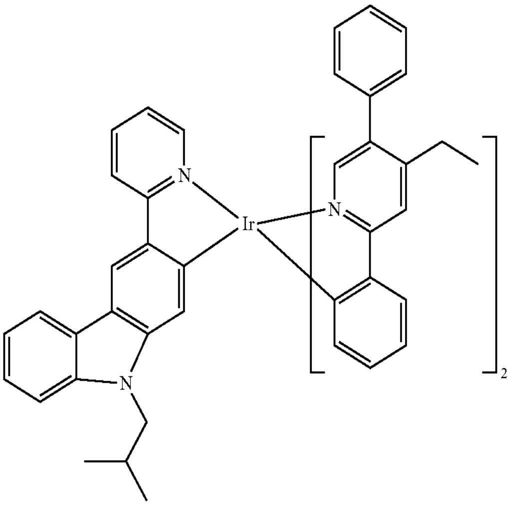
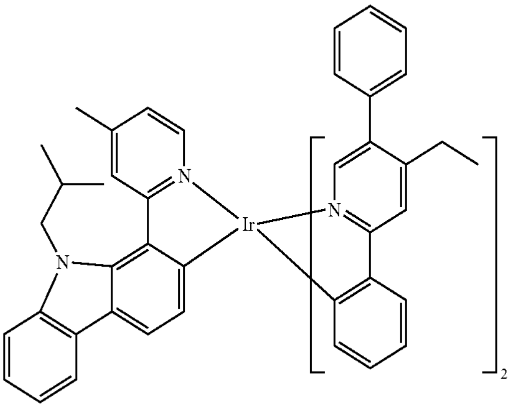
Compound 95



Compound 96



Compound 97



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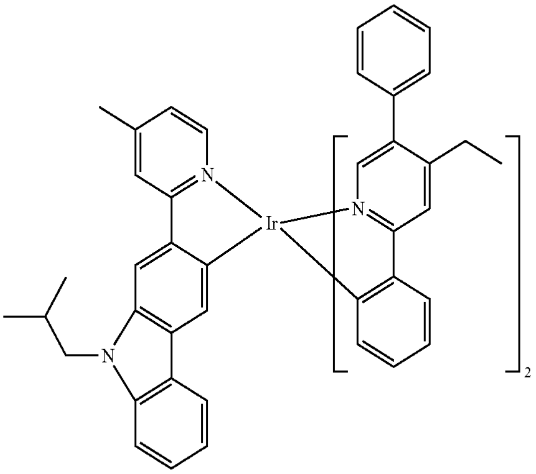
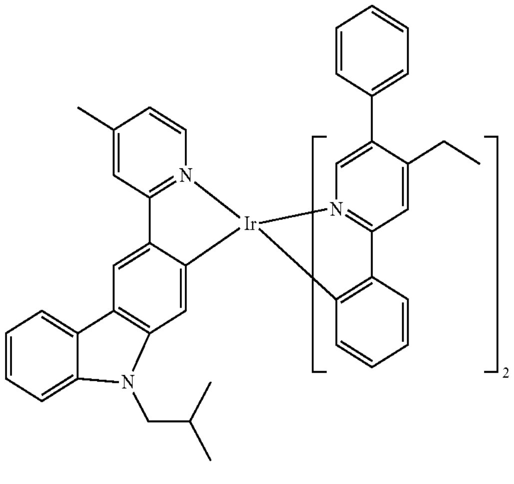
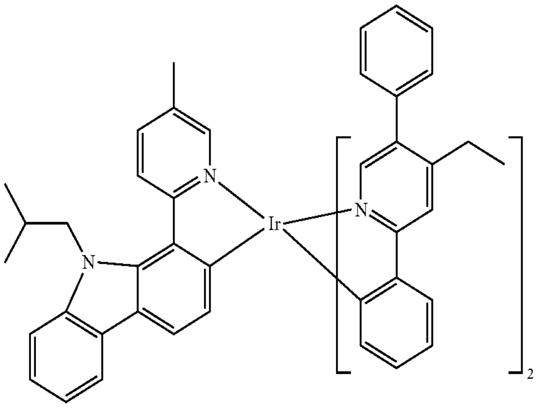
Compound 98



Compound 99



Compound 100



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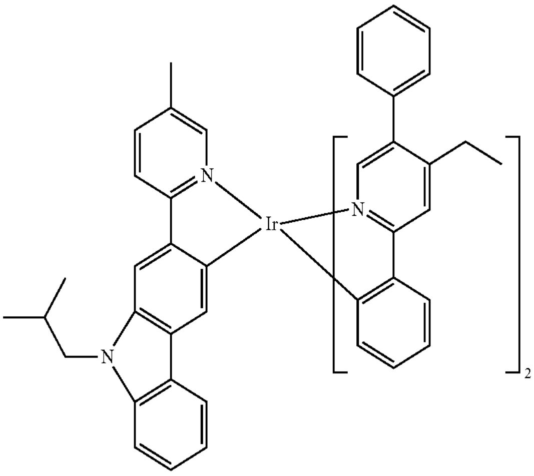
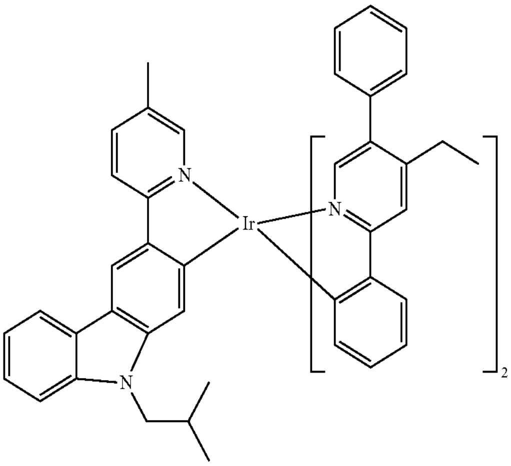
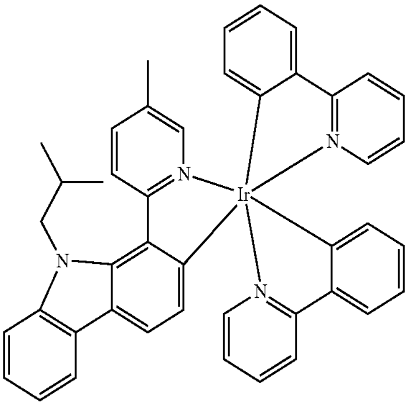
Compound 101



Compound 102

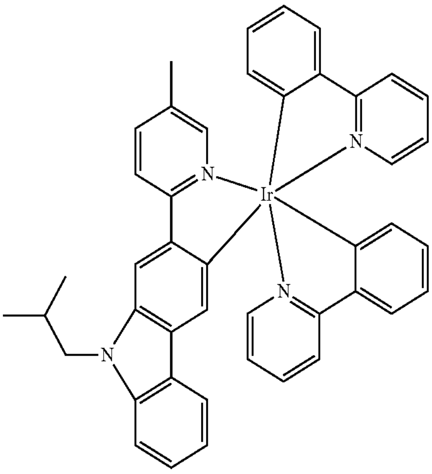


Compound 103

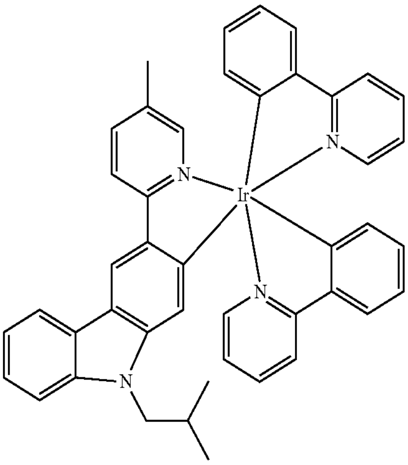


-continued

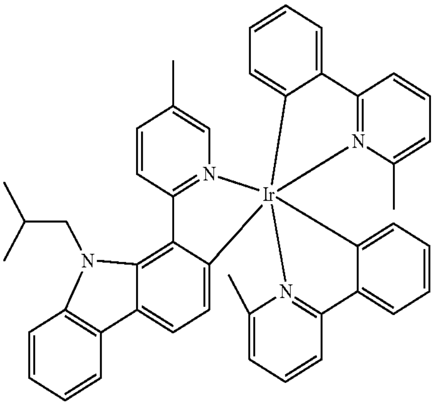
Compound 104



Compound 105



Compound 106



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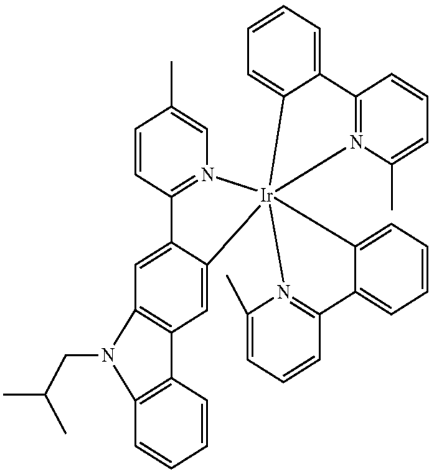
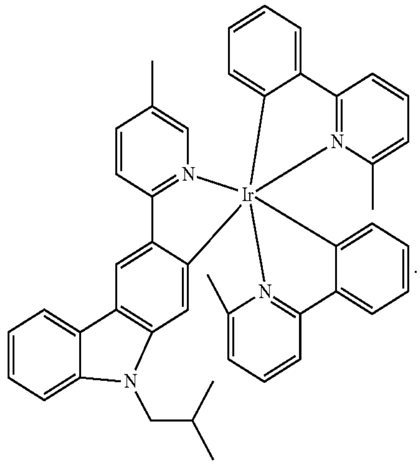
Compound 107



Compound 108



The heteroleptic iridium compound may be selected from the group consisting of Compound 1-Compound 108.

Compounds having FORMULA I in which X is selected from O, S and NR may be particularly advantageous. Without being bound by theory, it is thought that the aromaticity of the ligands comprising a dibenzofuran, dibenzothiophene or carbazole moiety (i.e., X is O, S, or NR) provides electron delocalization which may result in improved compound stability and improved devices. Moreover, it is believed that compounds wherein X is O may be more preferable than compounds wherein X is S or NR. In many cases, dibenzofuran containing compounds and devices comprising such compounds demonstrate especially desirable properties.

In one aspect, compounds are provided wherein X is O. Exemplary compounds where X is O include, but are not limited to, Compounds 1-12. Compounds wherein X is O may be especially preferred at least because these compounds may generate devices having desirable properties. For example, these compounds may provide devices having improved efficiency and a long lifetime. Additionally, the reduced sublimation temperature of these compounds can also result in improved manufacturing of such desirable devices.

Additional exemplary compounds where X is O are provided and include, without limitation, Compounds 37-60. Compounds 1-12 and 37-60 may provide devices having improved efficiency, lifetime, and manufacturing.

In another aspect, compounds are provided wherein X is S. Exemplary compounds where X is S include, but are not limited to, Compounds 13-24. These compounds, containing a pyridyl dibenzofuran ligand, may also be used in devices demonstrating good properties. For example, compounds wherein X is S may provide devices having improved stability and manufacturing.

Additional exemplary compounds where X is S are provided and include, without limitation, Compounds 61-84. Compounds 13-24 and 61-84 may provide devices having improved stability and manufacturing.

In yet another aspect, compounds are provided wherein X is NR. Exemplary compounds wherein X is NR include, but are not limited to, Compounds 25-36. These compounds containing a pyridyl carbazole ligand may also be used to provide devices having good properties, such as improved efficiency.

Additional exemplary compounds where X is NR are provided and include, without limitation, Compounds 85-108. Compounds 26-36 and 85-108 may provide devices having improved efficiency.

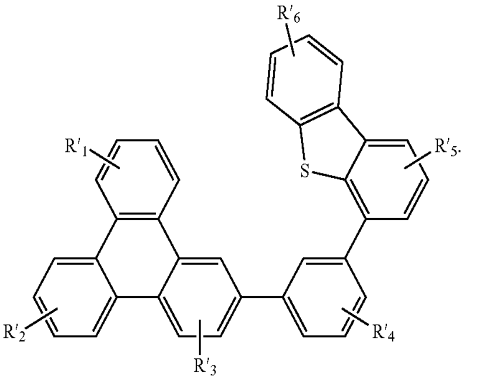
Additionally, an organic light emitting device is also provided. The device comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode, wherein the organic layer comprises a compound having FORMULA I. X is selected from the group consisting of NR, O, S, BR, and Se. R is selected from hydrogen and alkyl. Preferably, R has 4 or fewer carbon atoms. R_1, R_2, R_3 and R_4 may represent mono, di, tri, or tetra substitutions. Each of R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms, and aryl. Preferably, R_2 and R_3 are independently selected from the group consisting of hydrogen and alkyl having four or fewer carbon atoms. Selections for the heteroatoms and substituents described as preferred for the compound of FORMULA I are also preferred for use in a device that includes a compound having FORMULA I. These selections include those described for X, R, R_1, R_2 and R_3 and R_4.

In another aspect, each of R_1, R_2, R_3 and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms, and aryl with 6 or fewer atoms in the ring. Preferably, R_2 and R_3 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms and aryl with 6 or fewer atoms in the ring.

In particular, devices are provided wherein the compound is selected from the group consisting of Compounds 1-36.

In addition, devices are provided which contain a compound selected from the group consisting of Compounds 37-108. Moreover, the devices provided may contain a compound selected from the group consisting of Compounds 1-108.

In one aspect, the organic layer is an emissive layer and the compound having FORMULA I is an emitting dopant. The organic layer may further comprise a host. Preferably, the host comprises a triphenylene moiety and a dibenzothiophene moiety. More preferably, the host has the formula:



R'_1, R'_2, R'_3, R'_4, R'_5, and R'_6 may represent mono, di, tri, or tetra substitutions. Each of R'_1, R'_2, R'_3, R'_4, R'_5, and R'_6 are independently selected from the group consisting of hydrogen, alkyl, and aryl.

As discussed above, the heteroleptic compounds provided herein may be advantageously used in organic light emitting devices to provide devices having desirable properties such as improved lifetime, stability and manufacturing.

A consumer product comprising a device is also provided. The device further comprises an anode, a cathode, and an organic layer. The organic layer further comprises a heteroleptic iridium complex having FORMULA I.

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.

In addition to and/or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 2 below. Table 2 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 2

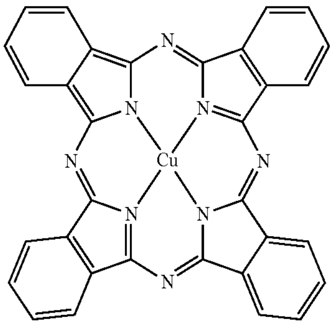
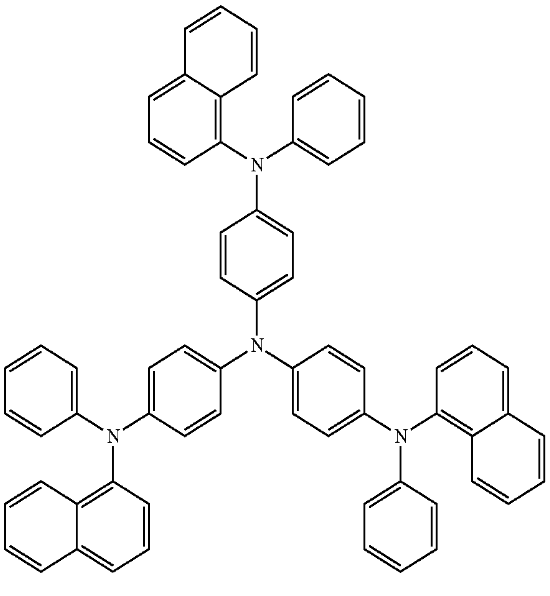
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Hole injection materials		
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)

TABLE 2-continued

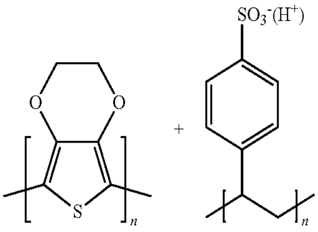
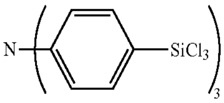
MATERIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
CF_x Fluorohydrocarbon polymer	$-\!\!\left[CH_xF_y \right]_n\!\!-$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and sliane SAMs		US20030162053

TABLE 2-continued

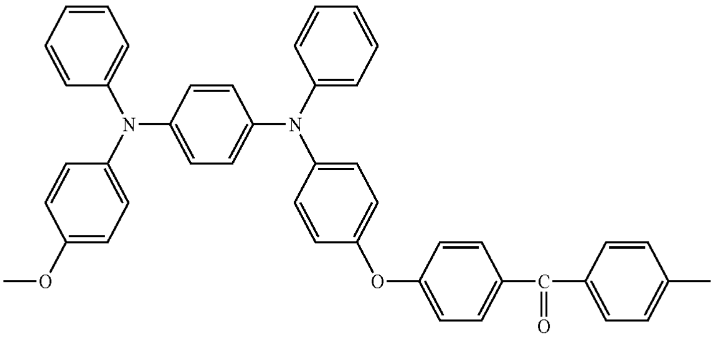
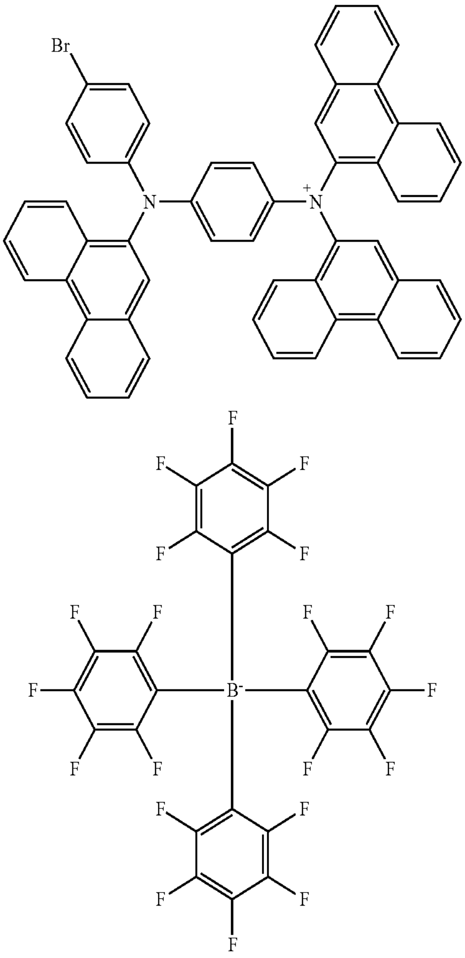
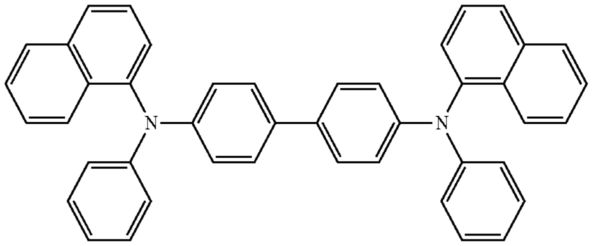
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine or polythiophene polymers with conductivity dopants	 and 	EA01725079A1
Arylamines complexed with metal oxides such as molybdenum and tungsten oxides	 + MoO_x	SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 2-continued

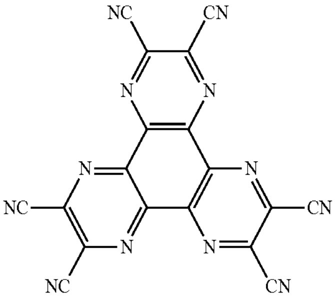
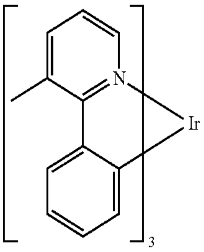
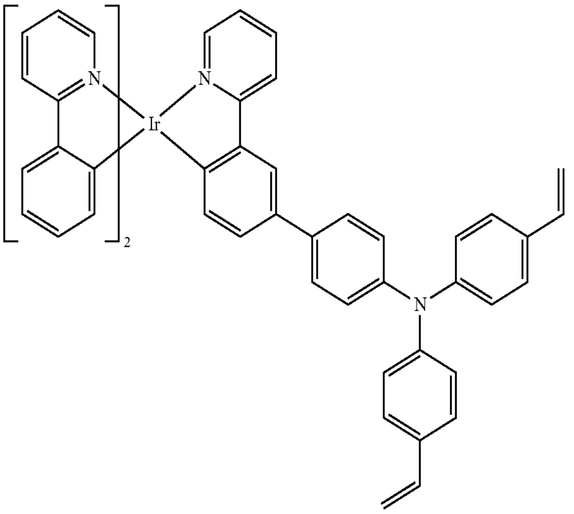
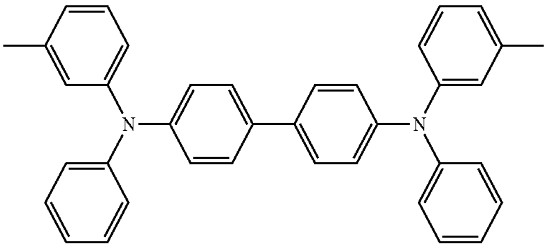
MATERIAL	EXAMPLES OF MATERIAL	PUBLI- CATIONS
p-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Hole transporting materials		
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)

TABLE 2-continued

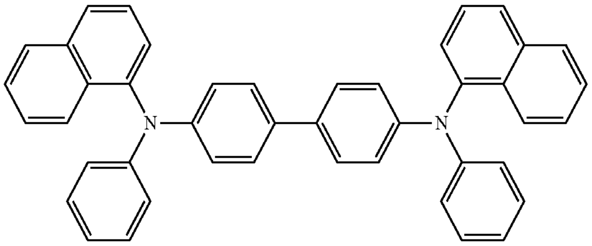
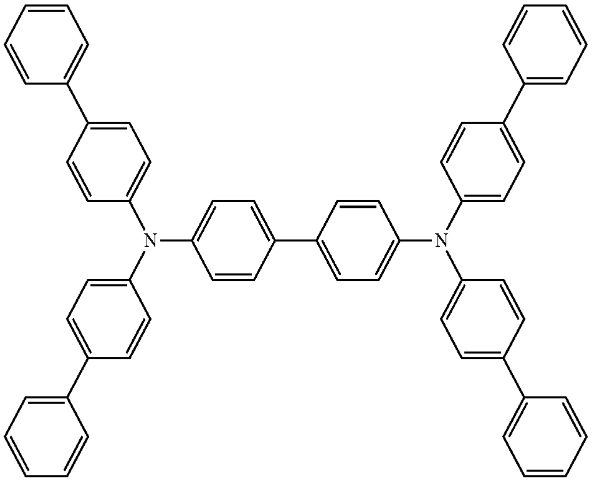
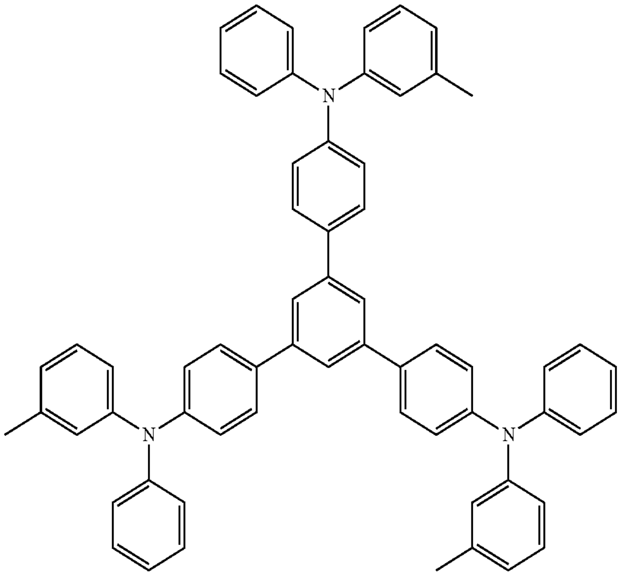
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 5,061,569
		EP650955
		J. Mater. Chem. 3, 319 (1993)

TABLE 2-continued

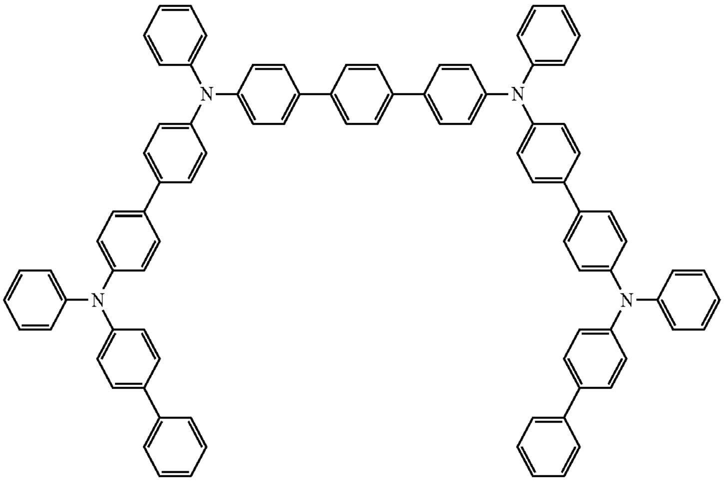
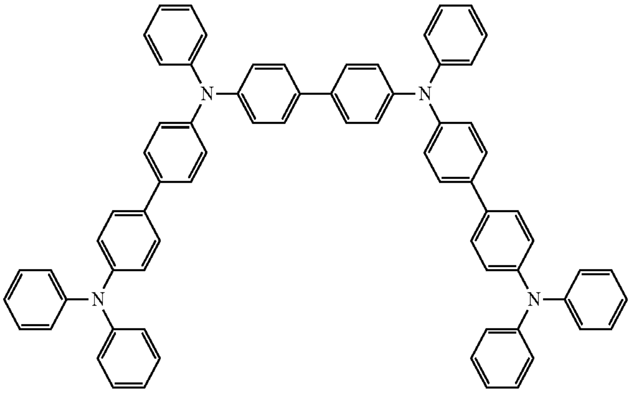
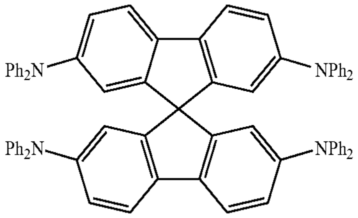
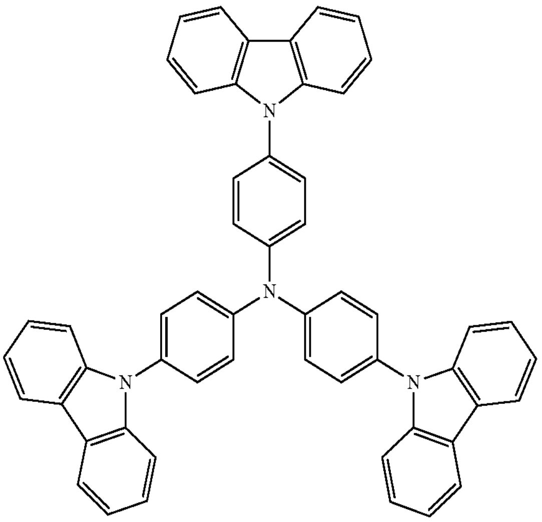
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572

TABLE 2-continued

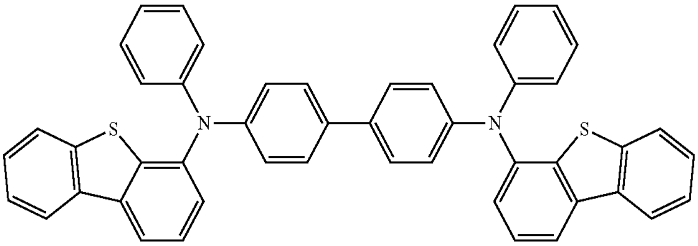
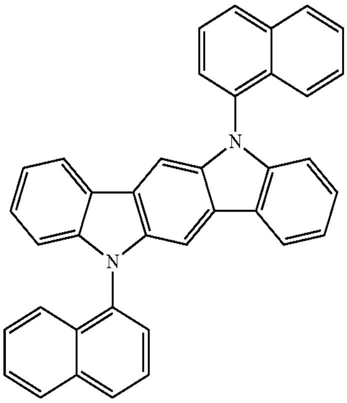
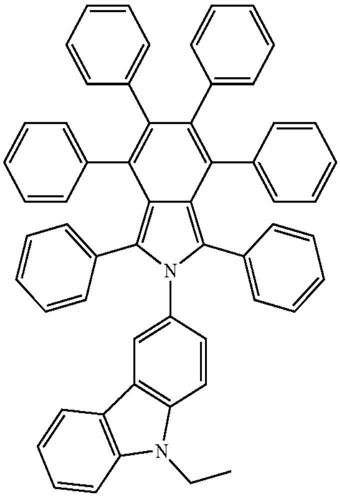
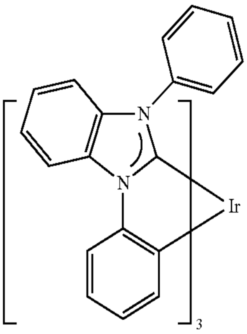
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221

TABLE 2-continued

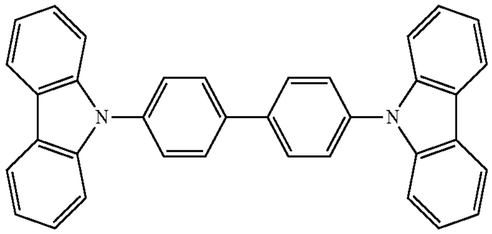
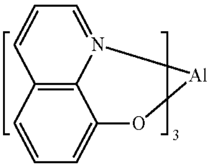
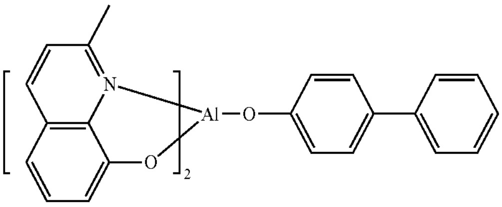
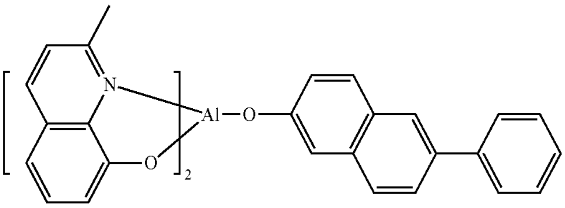
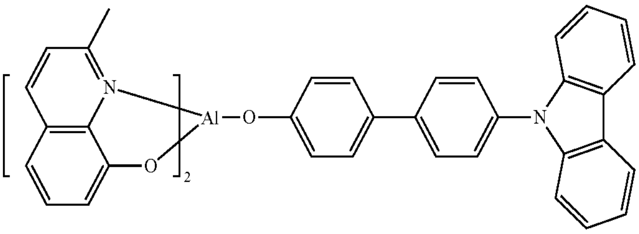
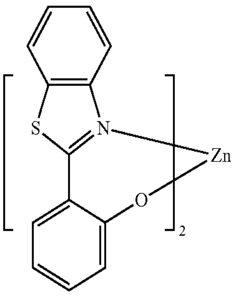
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phosphorescent OLED host materials Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxy-benzothiazole compounds		Appl.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

TABLE 2-continued

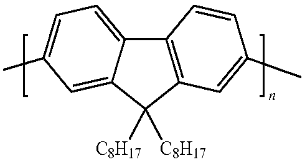
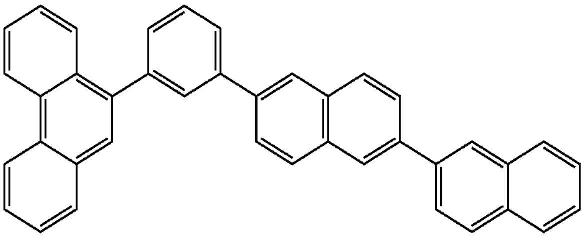
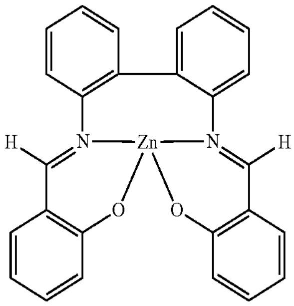
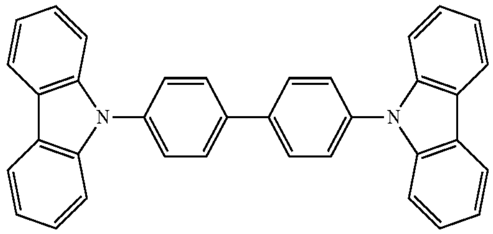
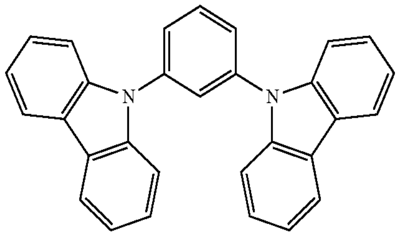
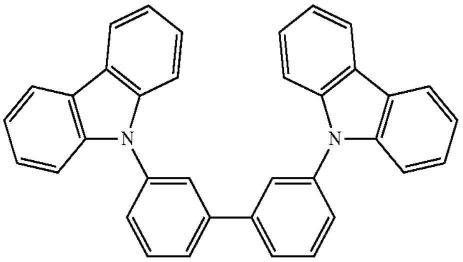
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2009062578
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234

TABLE 2-continued

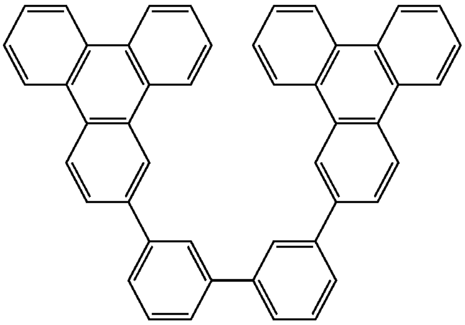
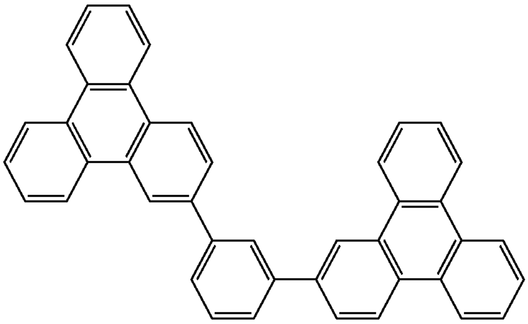
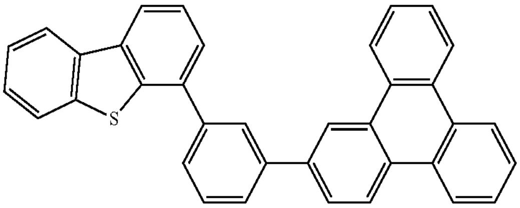
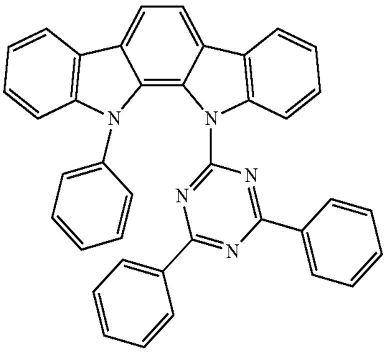
MATERIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
Aryltriphenylene compounds		US20060280965
		US20060280965
		WO2009021126
Donor acceptor type molecules		WO2008056746

TABLE 2-continued

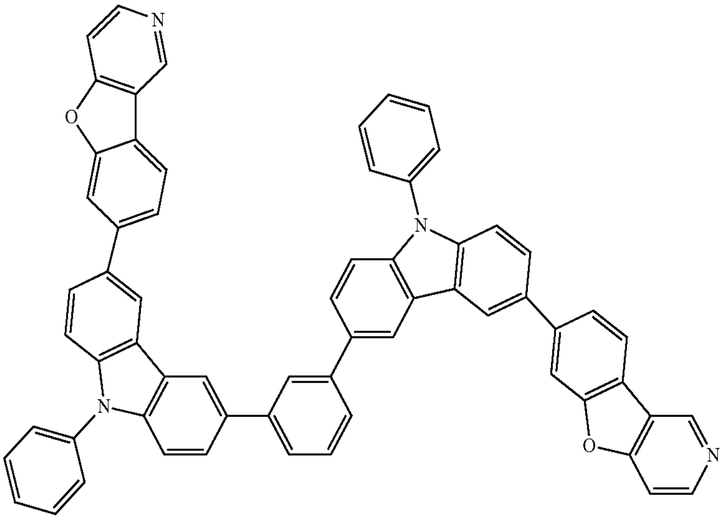
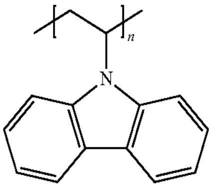
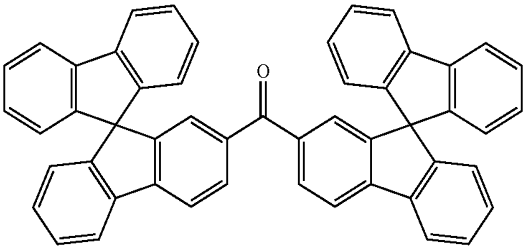
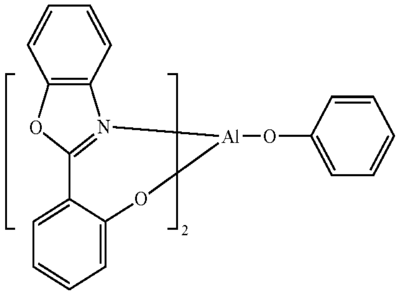
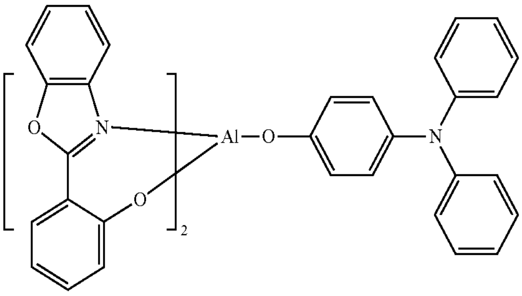
MATERIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
Aza-carbazole/ DBT/DBF		JP2008074939
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207
Metal phenoxybenzooxazole compounds		WO2005089025
		WO2006132173

TABLE 2-continued

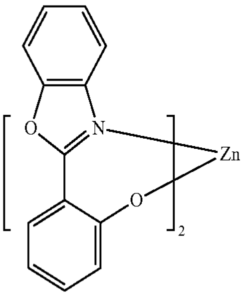
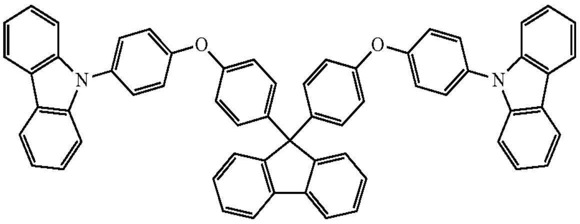
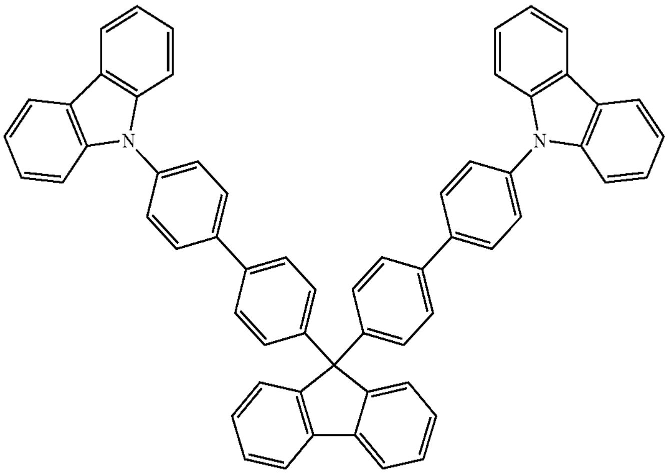
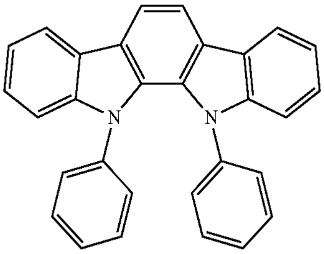
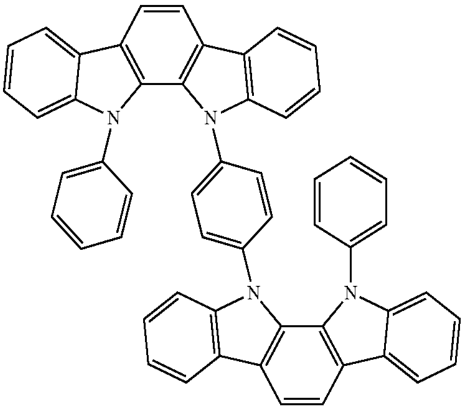
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297
Indolocabazoles		WO2007063796
		WO2007063754

TABLE 2-continued

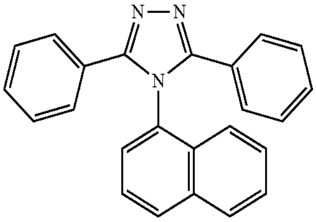
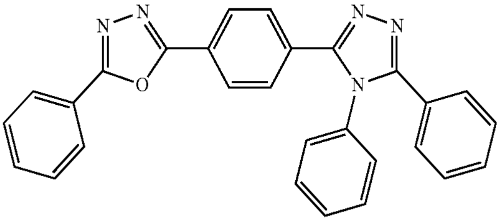
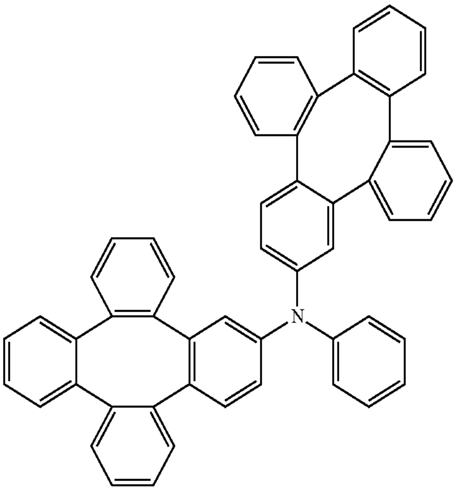
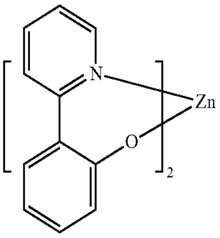
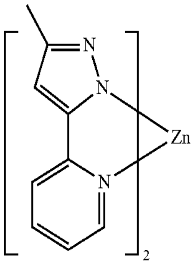
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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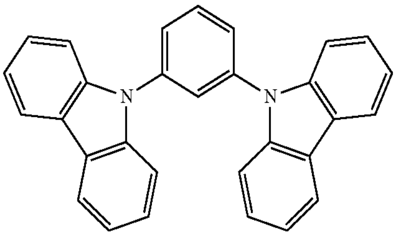
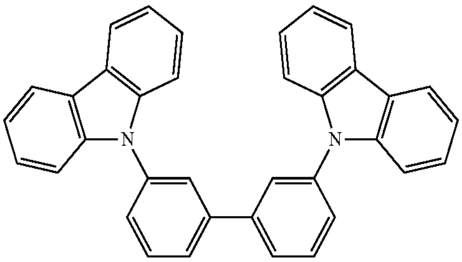
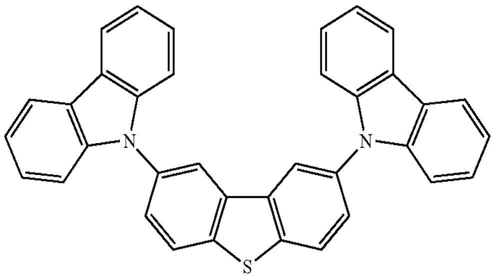
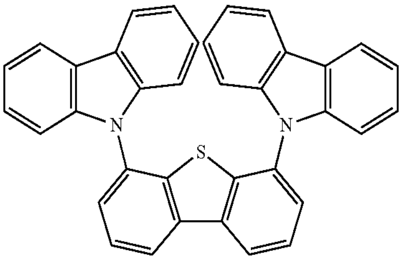
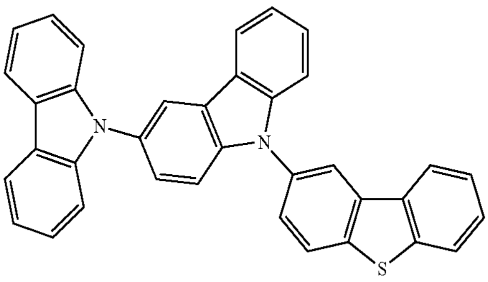
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/ Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162
		WO2009086028

TABLE 2-continued

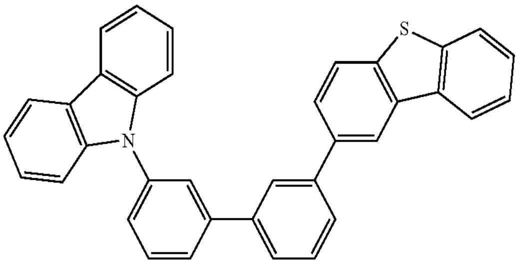
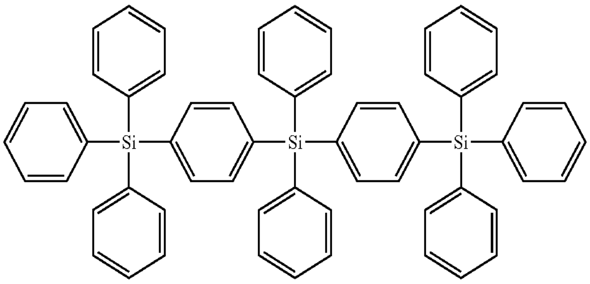
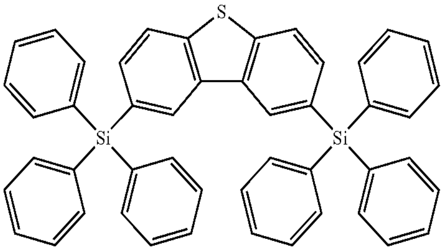
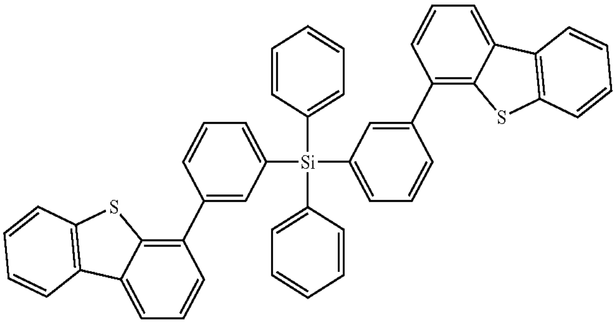
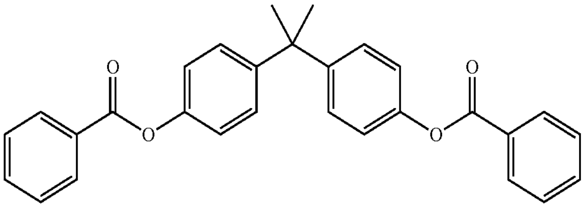
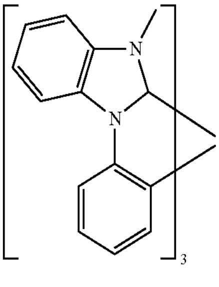
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090030202, US20090017330
Silicon aryl compounds		US20050238919
		WO2009003898
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114

TABLE 2-continued

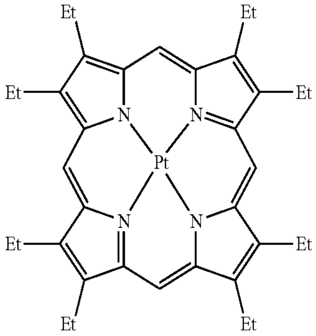
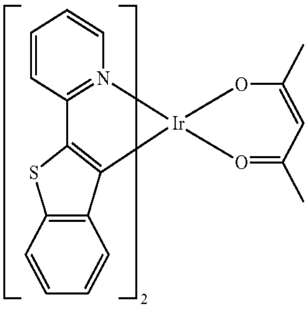
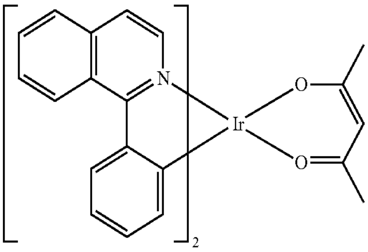
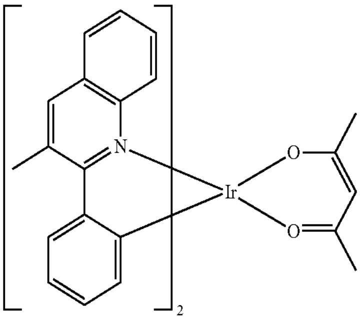
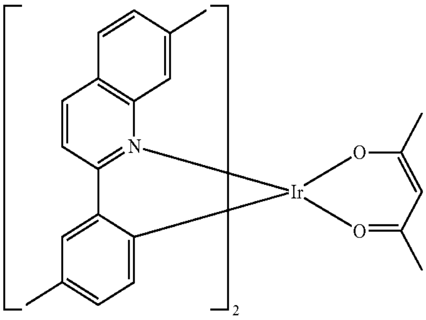
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phosphorescent dopants Red dopants		
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium (III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US2006835469
		US2006835469
		US20060202194

TABLE 2-continued

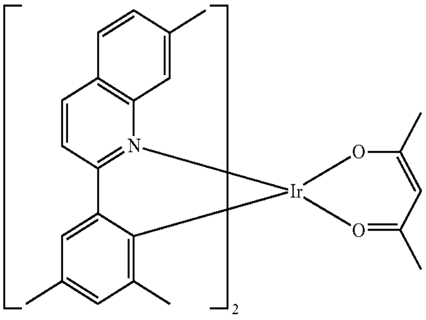
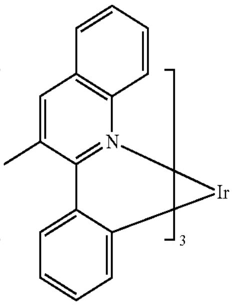
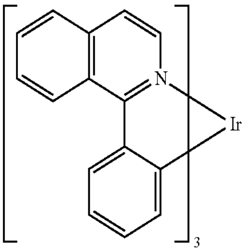
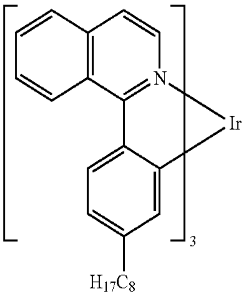
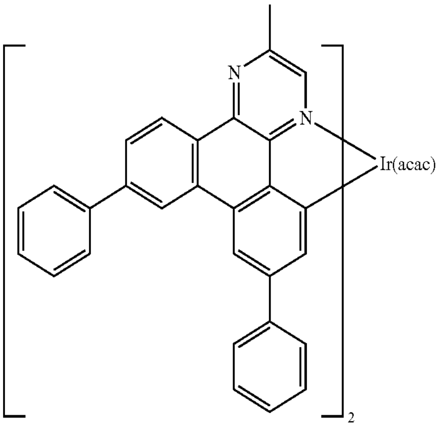
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060202194
		US20070087321
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991

TABLE 2-continued

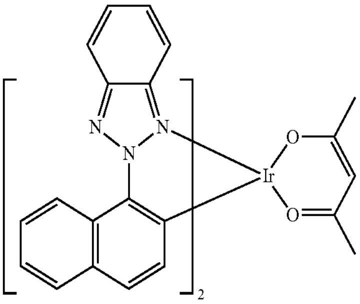
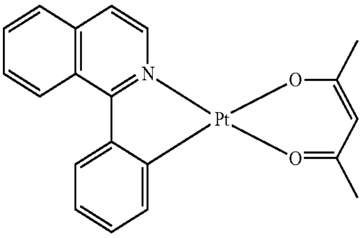
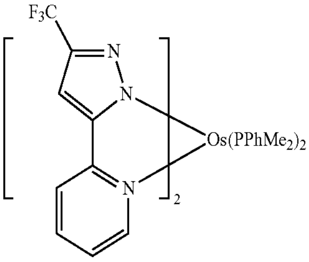
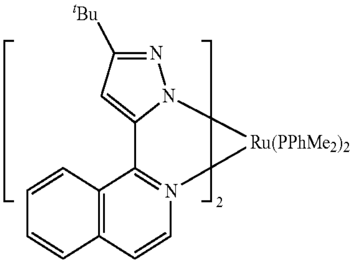
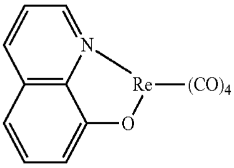
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2008101842
Platinum (II) organometallic complexes		WO2003040257
Osminum (III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium (II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673

TABLE 2-continued

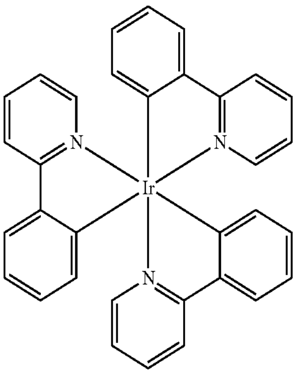
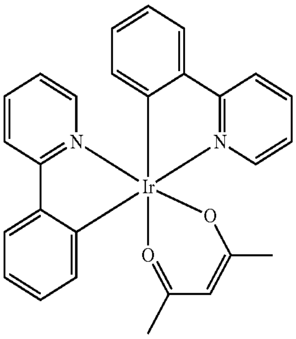
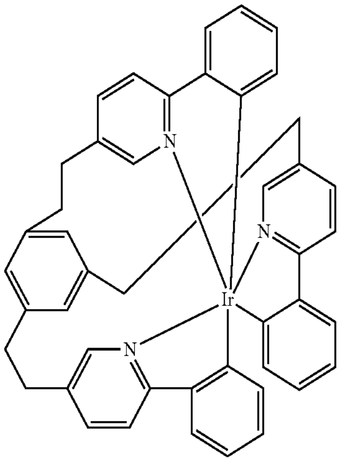
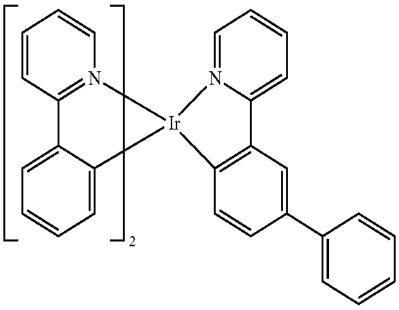
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Green dopants		
Iridium (III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656
		U.S. Pat. No. 7,332,232
		US20090108737

TABLE 2-continued

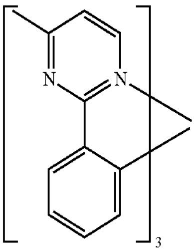
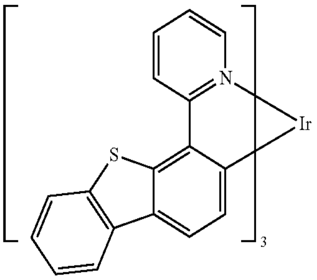
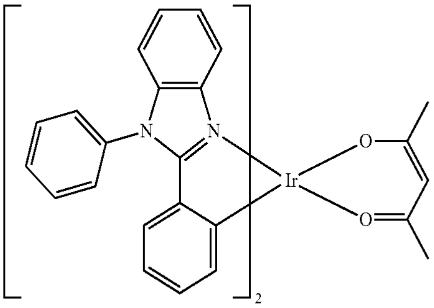
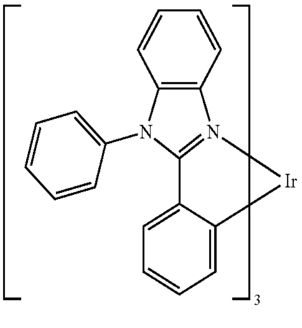
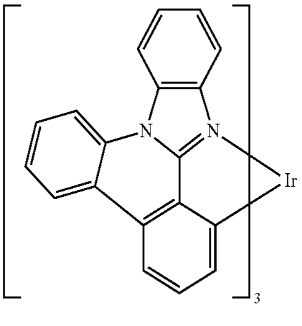
MATERIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		US20090039776
		U.S. Pat. No. 6,921,915
		U.S. Pat. No. 6,687,266
		Chem. Mater. 16, 2480 (2004)
		US20070190359

TABLE 2-continued

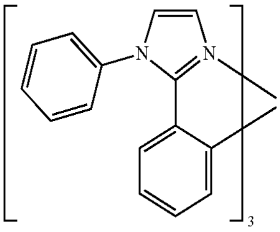
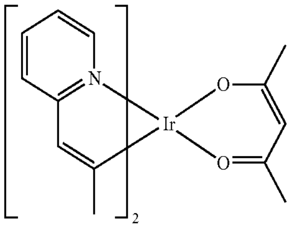
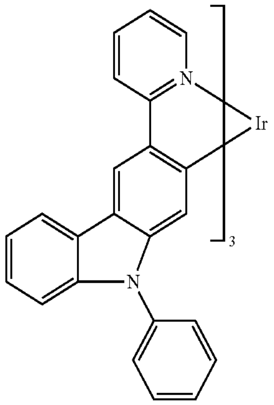
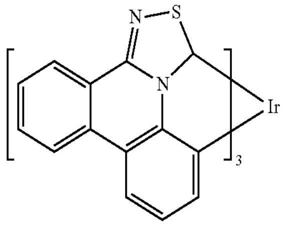
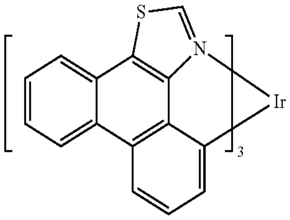
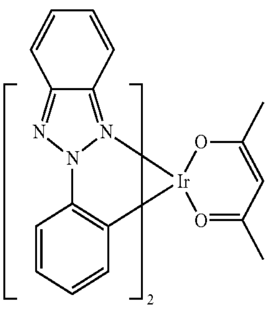
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US 20060008670 JP2007123392
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846
		US20080015355

TABLE 2-continued

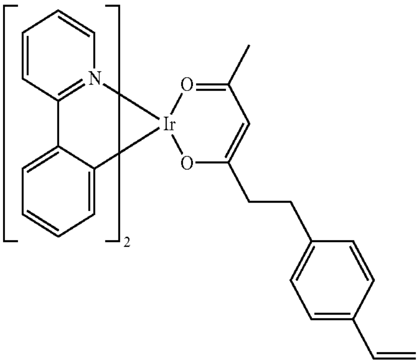
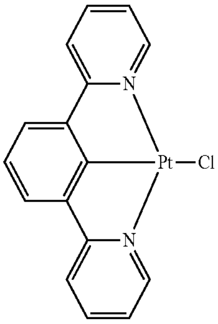
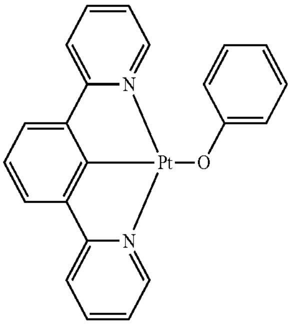
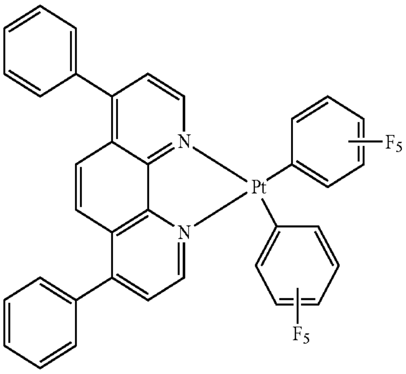
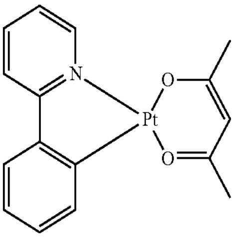
MATERIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt (II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl, Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645

TABLE 2-continued

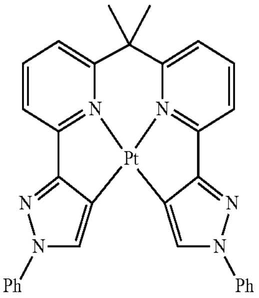
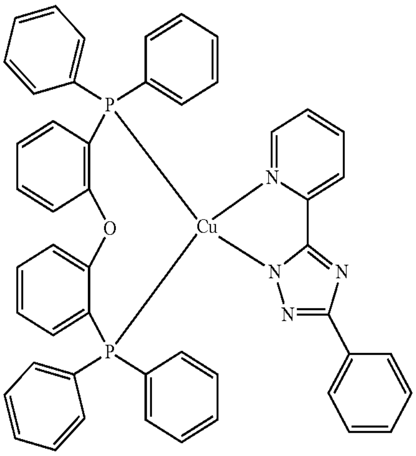
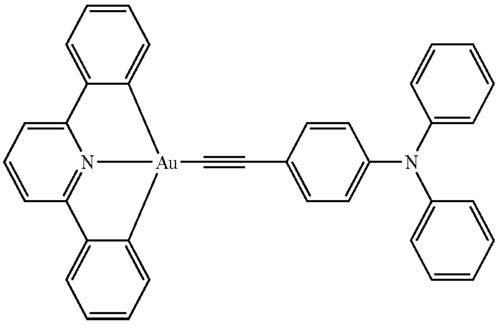
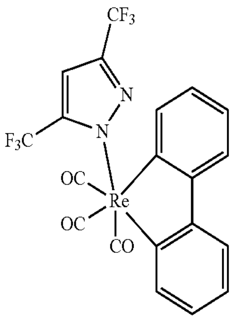
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060263635
Cu complexes		WO2009000673
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium (III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE 2-continued

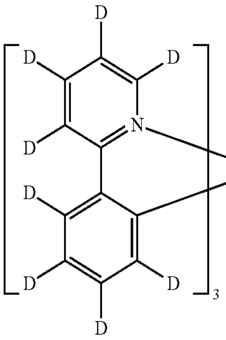
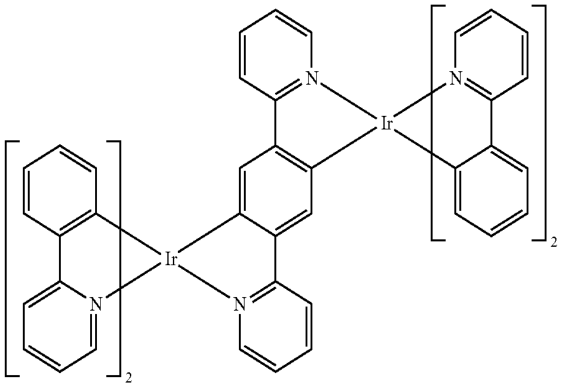
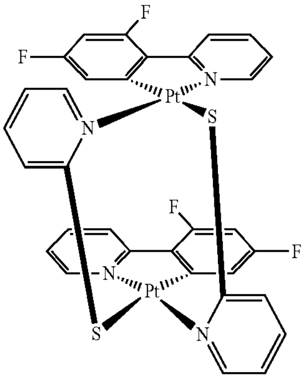
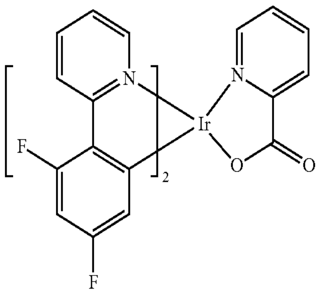
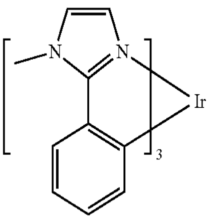
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928
Blue dopants		
Iridium (III) organometallic complexes		WO2002002714
		WO2006009024

TABLE 2-continued

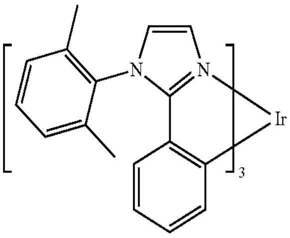
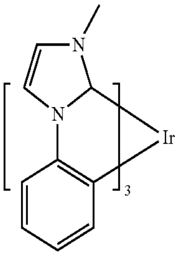
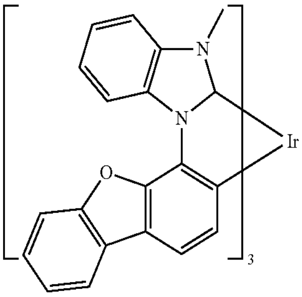
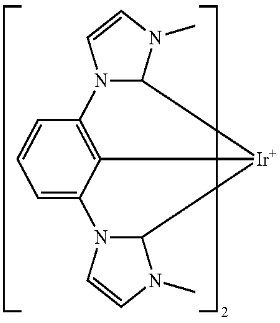
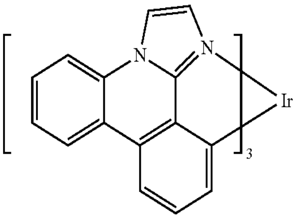
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060251923
		U.S. Pat. No. 7,393,599, WO20060564I8, US20050260441, WO2005019373
		U.S. Pat. No. 7,534,505
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033

TABLE 2-continued

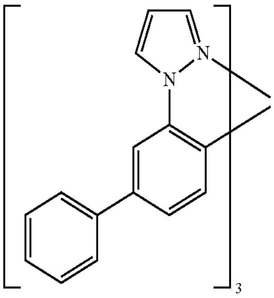
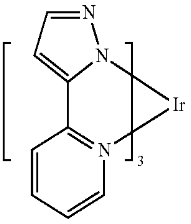
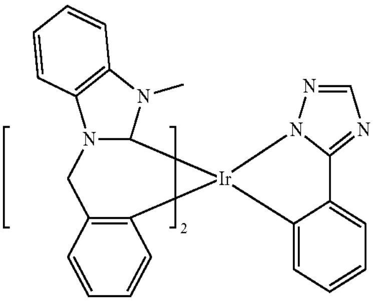
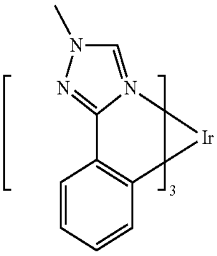
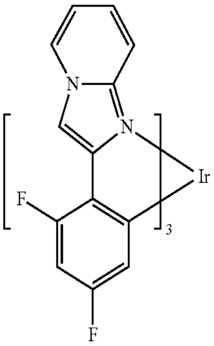
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,338,722
		US20020134984
		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)

TABLE 2-continued

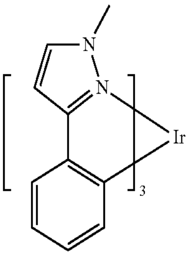
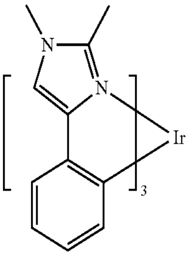
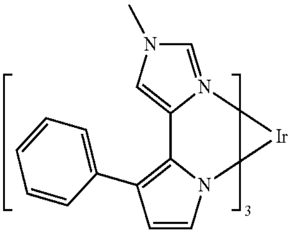
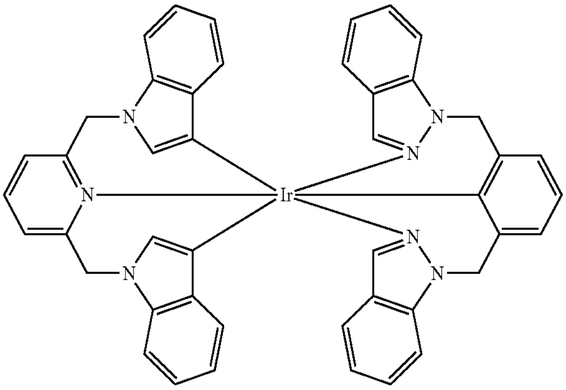
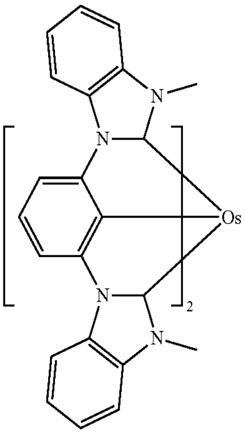
MATERIAL	EXAMPLES OF MATERIAL	PUBLI-CATIONS
		WO2005123873
		WO2005123873
		WO2007004380
		WO2006082742
Osmium (II) complexes		U.S. Pat. No. 7,279,704

TABLE 2-continued

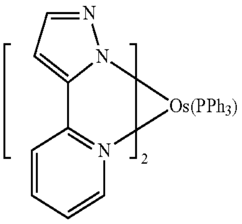
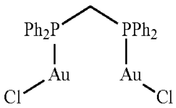
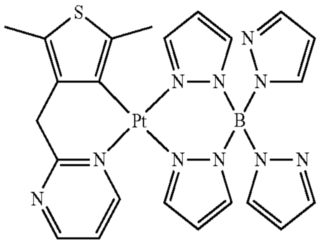
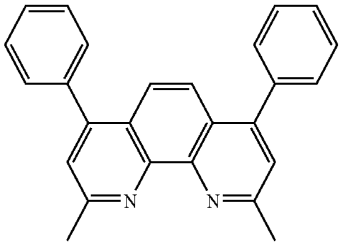
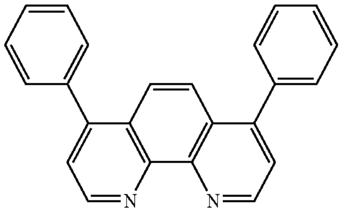
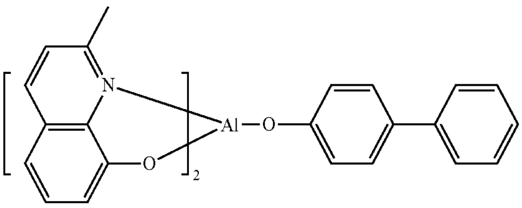
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum (II) complexes		WO2006098120, WO2006103874
Exciton/hole blocking layer materials		
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)

TABLE 2-continued

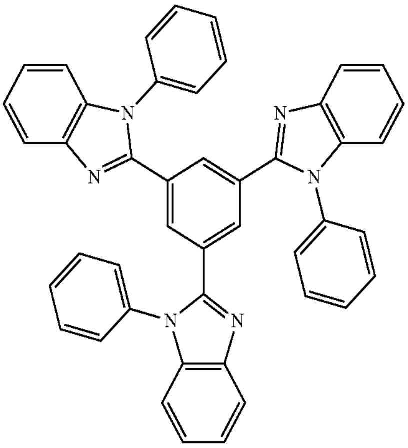
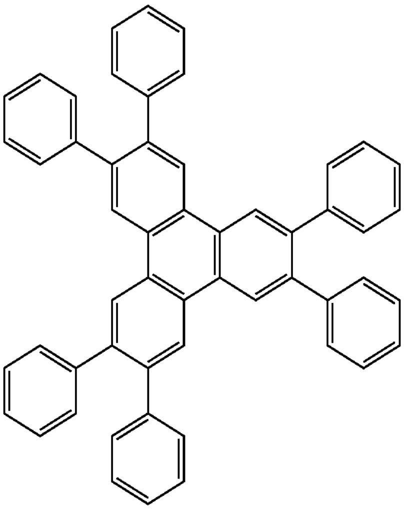
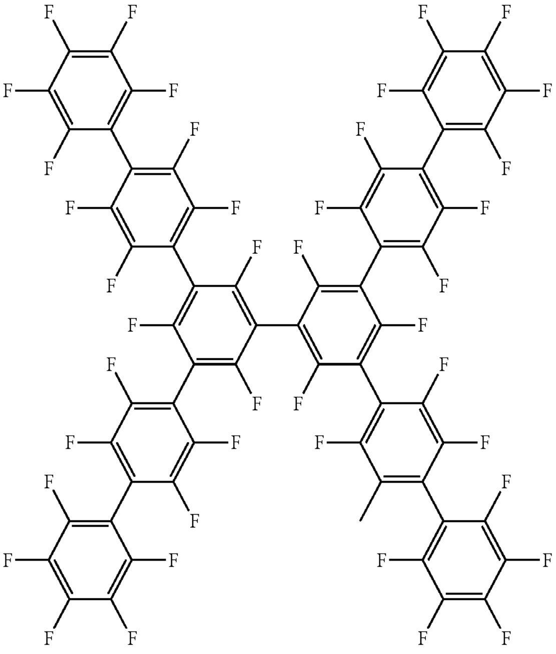
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)

TABLE 2-continued

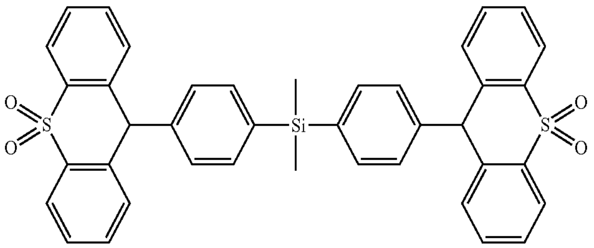
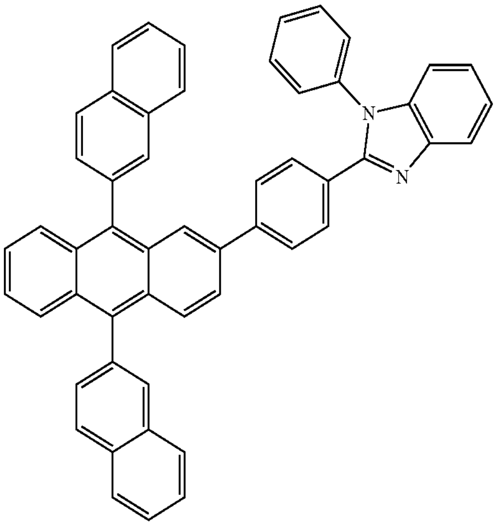
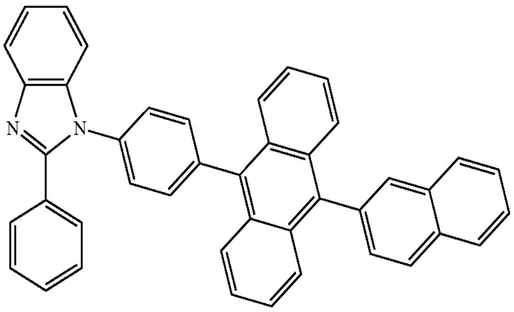
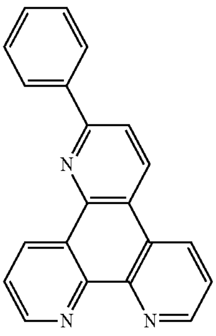
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085
Electron transporting materials		
Anthracene-benzoimidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives		US20090115316

TABLE 2-continued

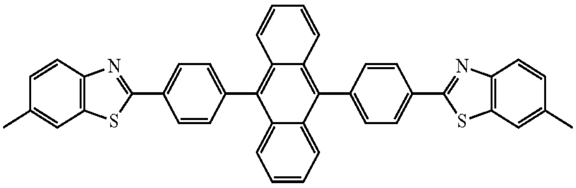
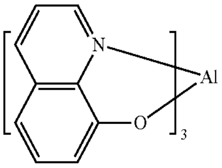
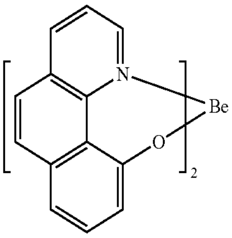
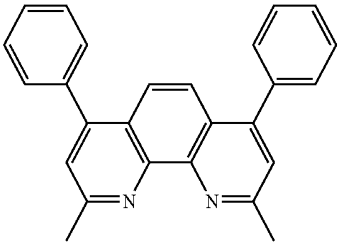
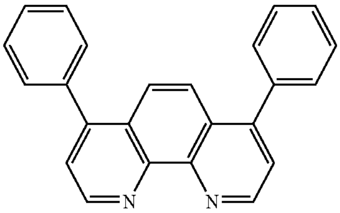
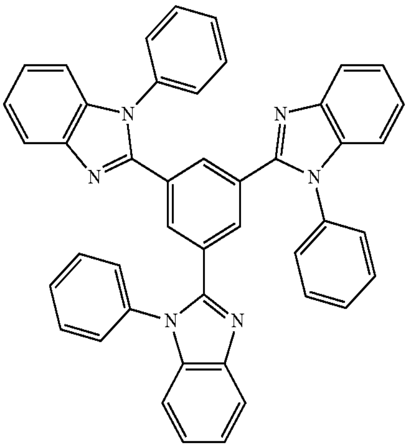
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 313 (1987) U.S. Pat. No. 7,230,107
Metal hydroxybenoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
		Appl. Phys. Lett. 79, 449 (2001)
5-member ring electron deficient heterocycles (e.g.,triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)

TABLE 2-continued

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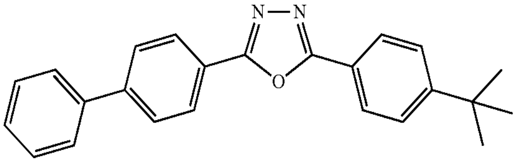
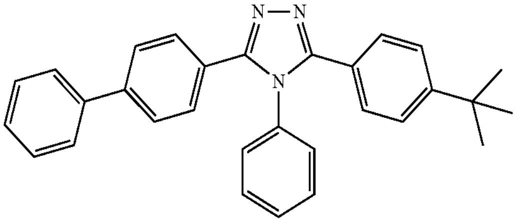
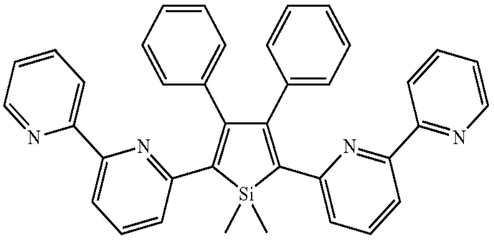
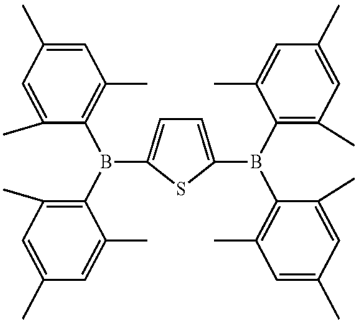
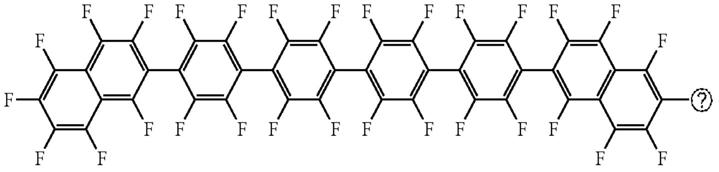
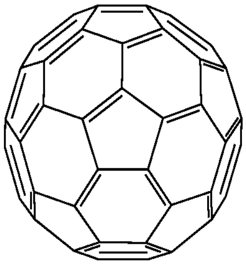
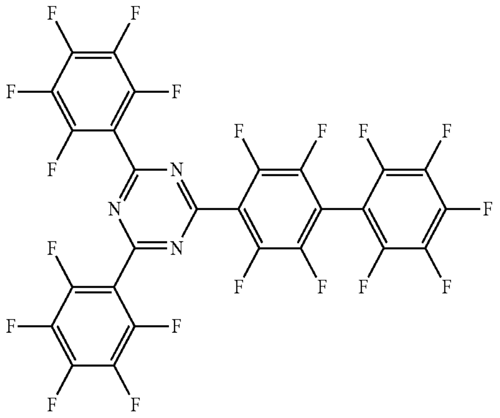
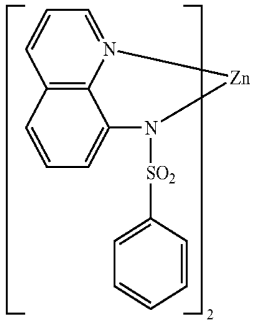
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870

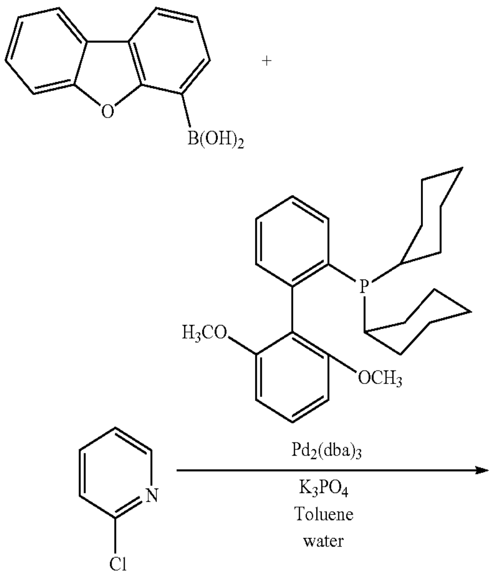
TABLE 2-continued

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

EXPERIMENTAL

Compound Examples

Example 1. Synthesis of Compound 1



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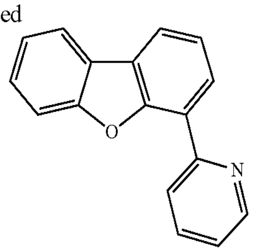
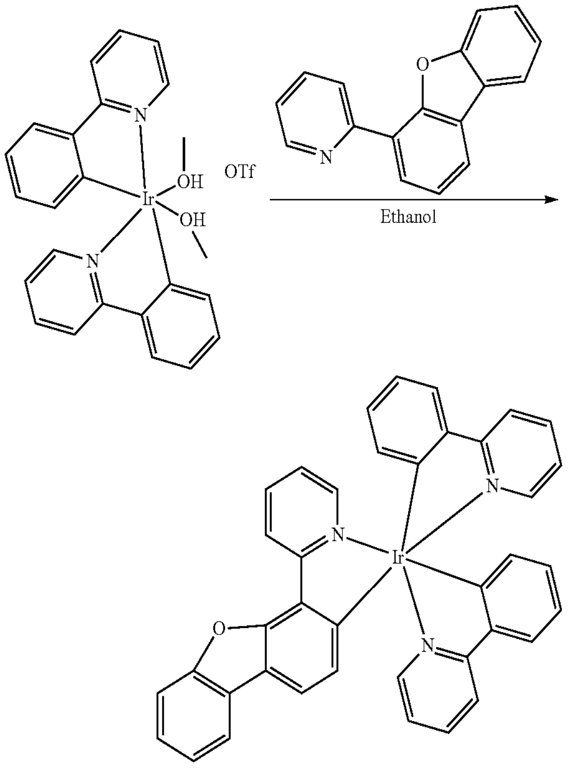


Synthesis of 2-(dibenzo[b,d]furan-4-yl)pyridine

4-dibenzofuranboronic acid (5.0 g, 23.6 mmol), 2-chloropyridine (2.2 g, 20 mmol), dicyclohexyl(2',6'-dimethoxybiphenyl-2-yl)phosphine (S-Phos) (0.36 g, 0.8 mmol), and potassium phosphate (11.4 g, 50 mmol) were mixed in 100 mL of toluene and 10 mL of water. Nitrogen is bubbled directly into the mixture for 30 minutes. Next, Pd$_2$(dba)$_3$ was added (0.18 g, 0.2 mmol) and the mixture was heated to reflux under nitrogen for 8 h. The mixture was cooled and the organic layer was separated. The organic layers are washed with brine, dried over magnesium sulfate, filtered, and evaporated to a residue. The residue was purified by column chromatography eluting with dichloromethane. 4.5 g of desired product was obtained after purification.

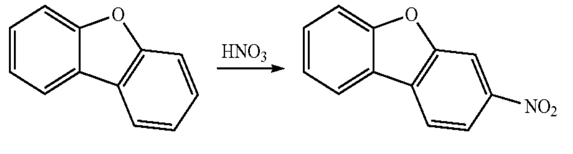


Compound 1

Synthesis of Compound 1

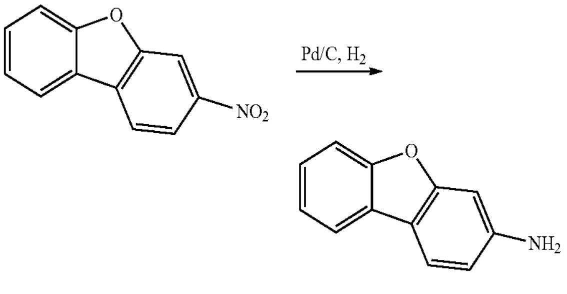
The iridium triflate precursor (0.97 g, 1.4 mmol) and 2-(dibenzo[b,d]furan-4-yl)pyridine (1.0 g, 4.08 mmol) were mixed in 50 mL of ethanol. The mixture was heated at reflux for 24 h under nitrogen. Precipitate formed during reflux. The reaction mixture was filtered through a celite bed. The product was washed with methanol and hexanes. The solid was dissolved in dichloromethane and purified by column using 1:1 of dichloromethane and hexanes. 0.9 g of pure product was obtained after the column purification. (HPLC purity: 99.9%)

Example 2. Synthesis of Compound 2



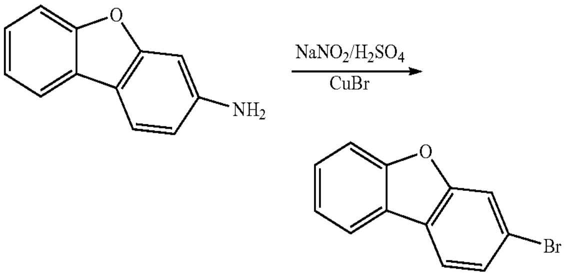
Synthesis of 3-nitrodibenzofuran

To 80 mL trifluroacetic acid in a 250 mL round bottom flask was added dibenzofuran (7.06 g, 42 mmol) and stirred vigorously to dissolve the content at room temperature. The solution was then cooled on ice and 1.2 equivalent 70% HNO_3 (4.54 g, 50.40 mmol) in 20 mL trifluroacetic acid was poured into the stirred solution slowly. After stirring for 30 minutes contents from the flask was poured into 150 mL ice-water and stirred for another 15 minutes. Off white color precipitate was then filtered out and finally washed with 2M NaOH and water. Moist material was then recrystallized from 1.5 L boiling ethanol in the form of light yellow color crystal. 7.2 g of product was isolated.



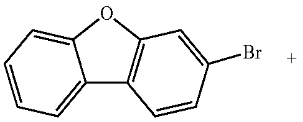
Synthesis of 3-aminodibenzofuran

3-nitrodibenzofuran (6.2 g, 29.08 mmol) was dissolved in 360 mL ethyl acetate and was degassed 5 minutes by passing nitrogen gas through the solution. 500 mg of Pd/C was added to the solution and the content was hydrogenated at 60 psi pressure. Reaction was let go until pressure in hydrogenation apparatus stabilizes at 60 psi for 15 minutes. Reaction content was then filtered through a small celite pad and off white color product was obtained. (5.3 g, 28.9 mmol)



Synthesis of 3-bromodibenzofuran

$NaNO_2$ (2.21 g, 32.05 mmol) was dissolved in 20 mL conc. H_2SO_4 in conical flask kept at 0° C. Solution of 2-aminodibenzofuran (5.3 g, 28.9 mmol) in minimum volume of glacial acetic acid was then slowly added to the flask so that temperature never raised above 5-8° C. and the mixture was stirred at 0° C. for another 1.5 h. 100 mL ether was added to the stirred mixture and precipitate of corresponding diazo salt immediately settled down. Brown color diazo salt was immediately filtered out and transferred to a flask containing CuBr (6.25 g, 43.5 mmol) in 150 mL 48% HBr. The flask was then placed in a water bath maintained at 64° C. and stirred for 2 h. After cooling down to room temperature, the dark color reaction content was filtered out and the precipitate was washed with water twice. Isolated solid was then flashed over Silica gel column with 5-10% DCM/Hexane to give 4.79 g final compound.



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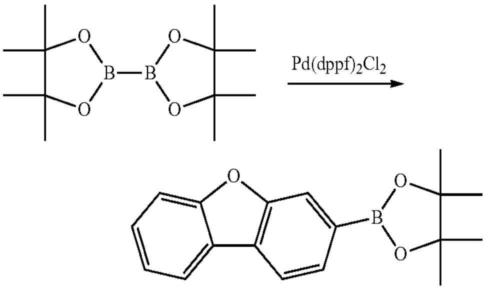
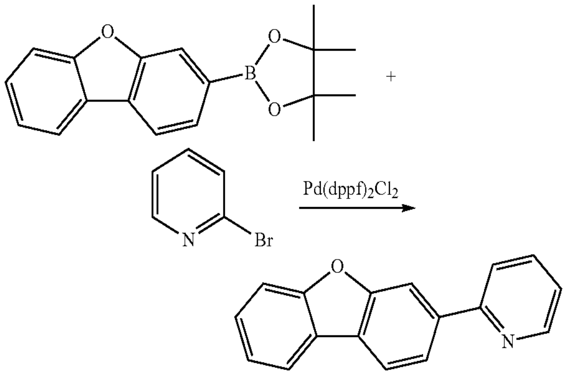


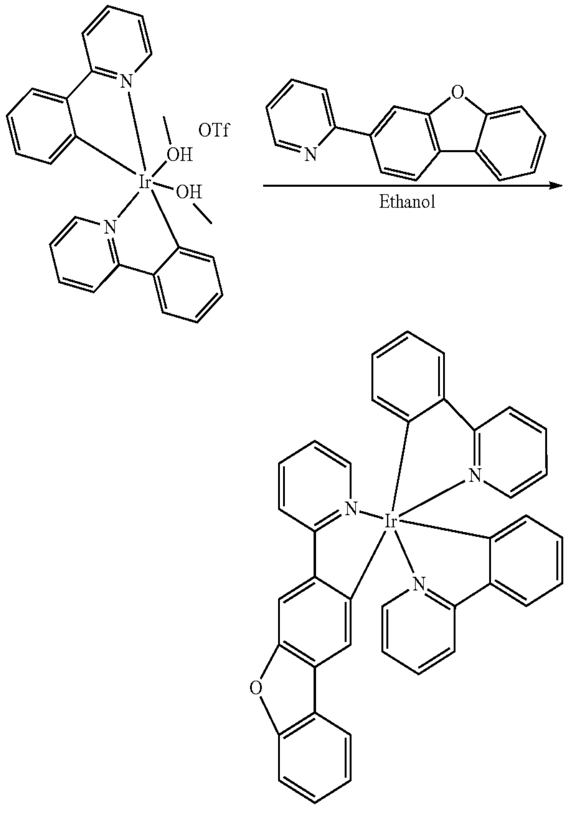
Synthesis of 2-(dibenzo[b,d]furan-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

3-bromodibenzofuran (4.79 g, 19.39 mmol), bispinacolatodiboron (6.4 g, 25.2 mmol), KOAc (7.61 g, 77.54 mmol) was added to 100 mL of dioxane in a r.b. flask. Content was degassed for 30 minutes under bubbling nitrogen gas and Pd(dppf)$_2$Cl$_2$ (158 mg, 0.019 mmol) was added to the reaction mixture. After degassing for another 10 minutes, the reaction mixture was heated to 80° C. and stirred overnight. Reaction flask was then cooled to room temperature and filtered through a pad of celite. Deep brown color solution was then partitioned in between brine and ethyl acetate. Organic layer was collected, dried over anhydrous Na$_2$SO$_4$ and excess solvent was evaporated under vacuum. Brown colored solid was then dry loaded in silica gel column and quickly flashed with 5% ethylacetate/hexane/0.005% triethylamine to give 5.08 g final product.



Synthesis of 2-(dibenzofuran-3-yl)pyridine

Dibenzofuran boronate ester (5.85 g, 20 mmol), 2-bromopyridine (2.93 mL, 30 mmol), 30 mL 2 M Na$_2$CO$_3$ (60 mmol) was slurried in 200 mL toluene/ethanol (1:1) in a 500 mL 3-neck round bottom flask and degassed for 30 minutes under bubbling nitrogen gas. Pd(dppf)$_2$Cl$_2$ (160 mg, 0.2 mmol) was added to the slurry and degassing continued for another 10 minutes. The reaction contents were then refluxed overnight. Reaction content was cooled to room temperature and filtered thru a small celite pad. Brown color biphasic solution was then partitioned between brine and ethylacetate. Organic layer was dried over anhydrous Na$_2$SO$_4$ and excess solvent was removed under vacuum. Residue from previous step was dry loaded in silica gel column and eluted with 5-8% ethylacetate/hexane to give 4.3 g final product.

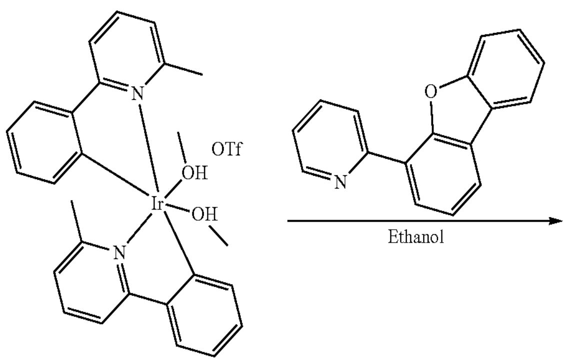


Compound 2

Synthesis of Compound 2

The iridium triflate precursor (2.8 g, 3.9 mmol), 2-(dibenzofuran-3-yl)pyridine (4 g, 16.3 mmol) were refluxed in 100 mL ethanol overnight. Bright yellow precipitate was filtered out, dried and dry loaded in a silica gel column. 210 mg final compound was isolated after elution with 3:2 DCM/hexane.

Example 3. Synthesis of Compound 4



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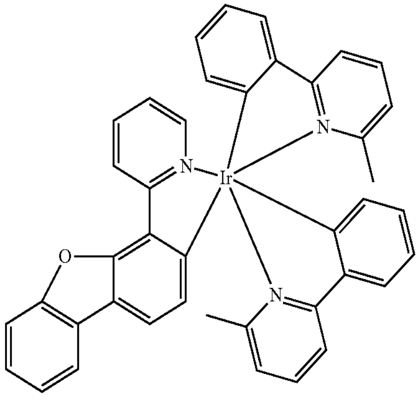
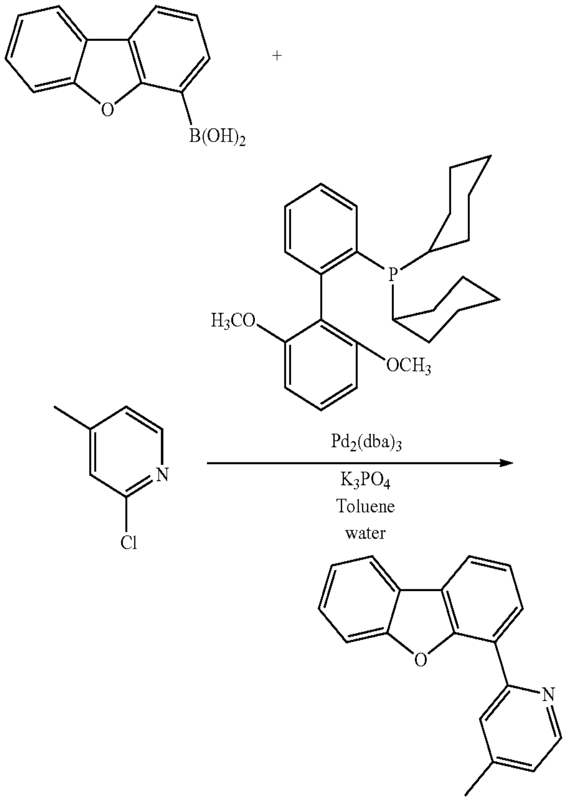


Compound 4

Synthesis of Compound 4

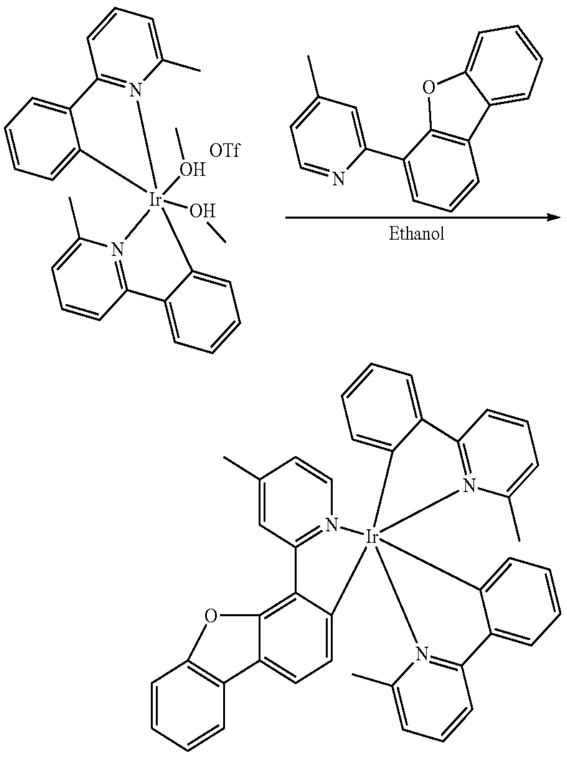
The iridium triflate precursor (1.6 g, 2.2 mmol) and 2-(dibenzo[b,d]furan-4-yl)pyridine (1.6 g, 6.5 mmol) were mixed in 50 mL of ethanol. The mixture was heated at reflux for 24 h under nitrogen. Precipitate formed during reflux. The reaction mixture was filtered through a celite bed. The product was washed with methanol and hexanes. The solid was dissolved in dichloromethane and purified by column using 1:1 of dichloromethane and hexanes. 1.4 g of pure product was obtained after the column purification.

Example 4. Synthesis of Compound 10



Synthesis of 4-methyl-2-(dibenzo[b,d]furan-4-yl) pyridine

4-dibenzofuranboronic acid (5.0 g, 23.6 mmol), 2-chloro-4-methylpyridine (2.6 g, 20 mmol), dicyclohexyl(2',6'-dimethoxybiphenyl-2-yl)phosphine (S-Phos) (0.36 g, 0.8 mmol), and potassium phosphate (11.4 g, 50 mmol) were mixed in 100 mL of toluene and 10 mL of water. Nitrogen is bubbled directly into the mixture for 30 minutes. Next, $Pd_2(dba)_3$ was added (0.18 g, 0.2 mmol) and the mixture was heated to reflux under nitrogen for 8 h. The mixture was cooled and the organic layer was separated. The organic layers are washed with brine, dried over magnesium sulfate, filtered, and evaporated to a residue. The residue was purified by column chromatography eluting with dichloromethane. 4.7 g of desired product was obtained after purification.

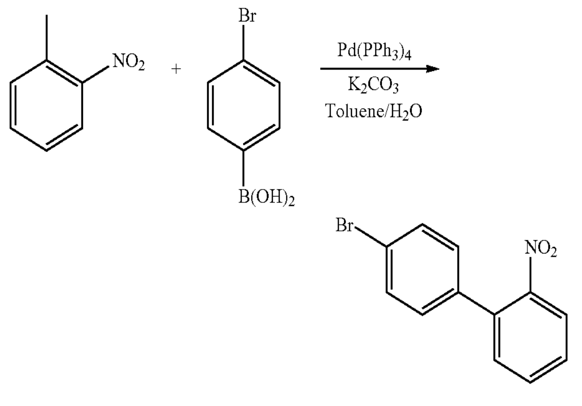


Compound 10

Synthesis of Compound 10

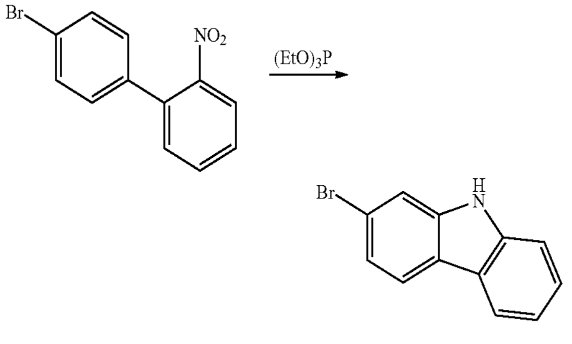
The iridium triflate precursor (2.0 g, 2.7 mmol) and 4-methyl-2-(dibenzo[b,d]furan-4-yl)pyridine (2.1 g, 8.1 mmol) were mixed in 60 mL of ethanol. The mixture was heated at reflux for 24 h under nitrogen. Precipitate formed during reflux. The reaction mixture was filtered through a celite bed. The product was washed with methanol and hexanes. The solid was dissolved in dichloromethane and purified by column using 1:1 of dichloromethane and hexanes. 1.6 g of pure product was obtained after the column purification.

Example 5. Synthesis of Compound 29



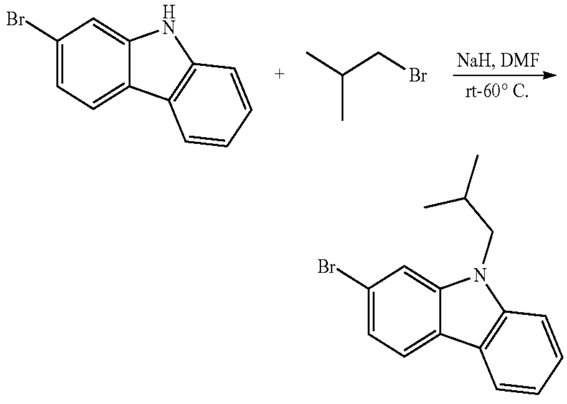
Synthesis of 4'-bromo-2-nitrobiphenyl

o-iodonitrobenzene (9.42 g, 37.84 mmol), 4-bromobenzeneboronic acid (7.6 g, 37.84 mmol), potassium carbonate (21 g, 151.36 mmol) was added to 190 mL DME/water (3:2) solution and degassed for 30 minutes. $Pd(PPh_3)_4$ (437 mg, 0.38 mmol) was added to the slurry under nitrogen and the slurry was degassed for another 5 minutes. The reaction was refluxed under nitrogen for 6 h. Content of the flask was filtered through a pad of celite and partitioned in ethyl acetate and brine. Organic phase was dried over anhydrous Na_2SO_4 and evaporated under vacuum. Crude yellow oil was flashed over silica gel using 5% ethylacetate/hexane. Final compound was isolated as colorless oil (9.8 g, 35.4 mmol).



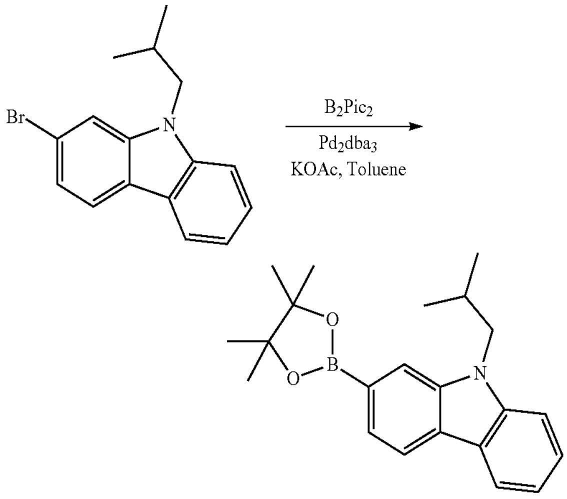
Synthesis of 2-bromo-9H-carbazole

4'-bromo-2-nitrobiphenyl (9.8 g, 35.4 mmol) was refluxed with 30 mL triethylphosphite overnight. After cooling down the solution to room temperature, 40 mL 6(N) HCl was added to it slowly and heated to 80° C. for 3 h. Acidic solution was halfway neutralized with conc. NaOH, rest of the acidic solution was neutralized with solid Na_2CO_3. Cloudy solution was extracted three times with ethylacetate (500 mL). Combined organic layer was evaporated under vacuum and crude was flashed on silica gel (15% to 30% ethylacetate/hexane). 4.1 g final compound was isolated as off white solid.



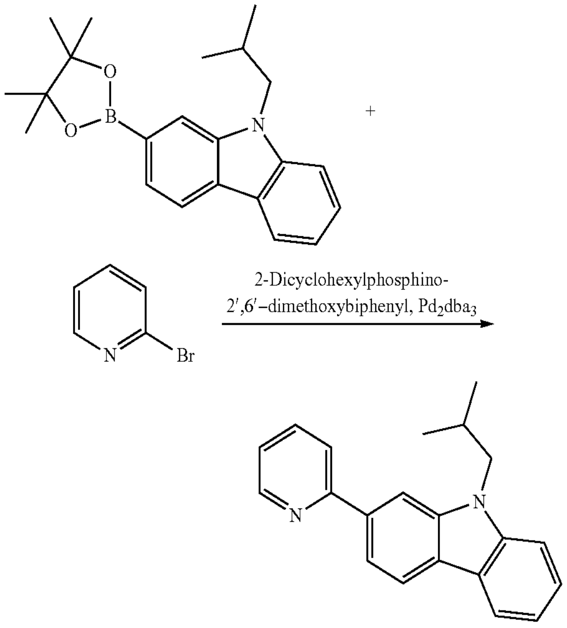
Synthesis of 2-bromo-9-isobutyl-9H-carbazole

2-bromo-9H-carbazole (4.1 g, 16.74 mmol) was dissolved in DMF. To the stirred solution was slowly added NaH (1.8 g, 75.5 mmol) in 3 portions. Isobutylbromide (4.8 mL, 43.2 mmol) was added to the stirred slurry and after waiting for 20 minute, warmed up to 60° C. for 4 h. Reaction mixture was cooled to room temperature and carefully quenched with drop wise addition of saturated NH_4Cl solution. Content was then partitioned in brine and ethylacetate. Organic layer was dried over anhydrous Na_2SO_4 and evaporated under vacuum. The crude product was flashed over silica gel with 10% ethylacetate/hexane. Final product (4.45 g, 14.8 mmol) was isolated as white solid.



Synthesis of 9-isobutyl-2-pinacolboron-9H-carbazole

2-bromo-9-isobutyl-9H-carbazole (4.45 g, 14.78 mmol), bisboronpinacolate (4.7 g, 18.5 mmol), potassium acetate (5.8 g, 59.1 mmol) were taken in 75 mL anhydrous toluene and degassed for 30 minutes. Pd_2dba_3 (362 mg, 0.443 mmol) was added to the slurry under nitrogen and the slurry was degassed for another 5 minutes. After overnight reflux, content of the reaction was cooled down and filtered through a celite pad. Toluene solution was partitioned in water and ethylacetate. Organic layer was dried over anhydrous Na_2SO_4 and solvent was evaporated under vacuum. Solid crude was flashed in silica gel using 10% ethylacetate/hexane. Isolated solid was subjected to Kugelrohr distillation at 133° C. to remove traces of bisboronpinacolate. Final product (4.77 g, 13.7 mmol) was isolated as off white solid.



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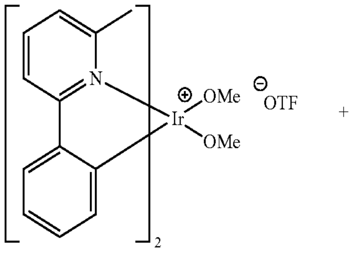
Synthesis of 9-isobutyl-2-(pyridine-2-yl)-9H-carbazole

9-isobutyl-2-pinacolboron-9H-carbazole (1.45 g, 4 mmol), 2-bromopyridine (760 mg, 4.8 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (67 mg, 0.16 mmol), $K_3PO_4.H_2O$ (3.68 g, 16 mmol) were added to 40 mL mixture of 9:1 toluene and water. Contents were degassed for 30 minutes before addition of Pd_2dba_3 (37 mg, 0.04 mmol) and degassed for another 5 minutes. After overnight reflux, reaction content was cooled to room temperature and filtered through a pad of celite. Filtrate was partitioned in water and ethylacetate. Organic layer was isolated, dried over anhydrous Na_2SO_4 and evaporated under vacuum. Crude was then flashed over silica gel using 10%-30% ethylacetate/hexane to remove the protodeborylation product. Final compound (620 mg, 2.1 mmol) was isolated as white solid.



Intermediate-1

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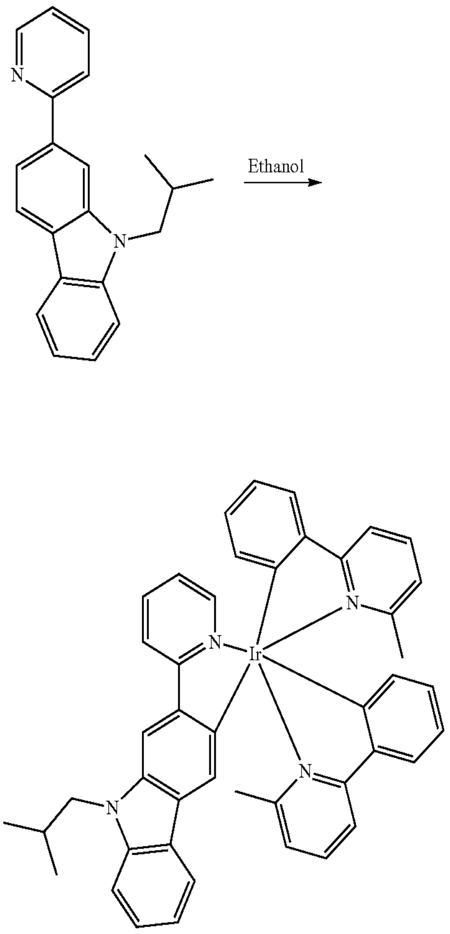
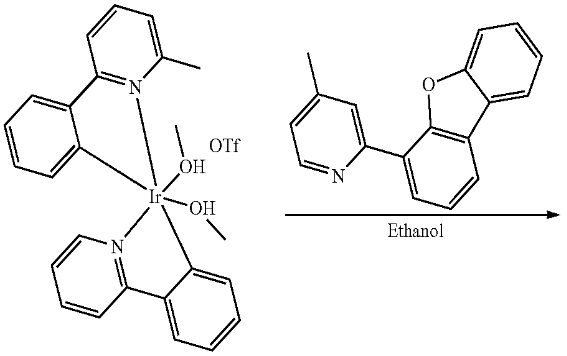


Compound 29

Synthesis of Compound 29

Carbazole ligand (620 mg, 2.1 mmol) from previous step was dissolved in ethanol and Intermediate-1 was added to it under nitrogen. Solution was then refluxed overnight. Deep orange color precipitate was filtered out and flashed over silica gel with 50% DCM/hexane. Isolated product was then sublimed to give 310 mg 99.7% pure product.

Example 6. Synthesis of Compound 7



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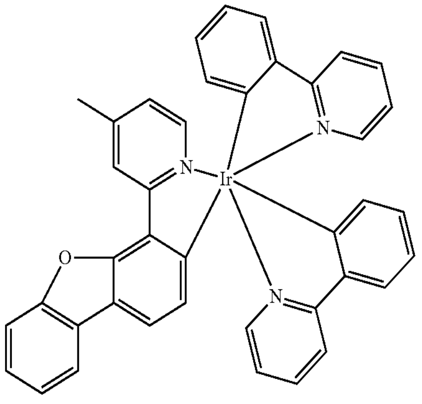
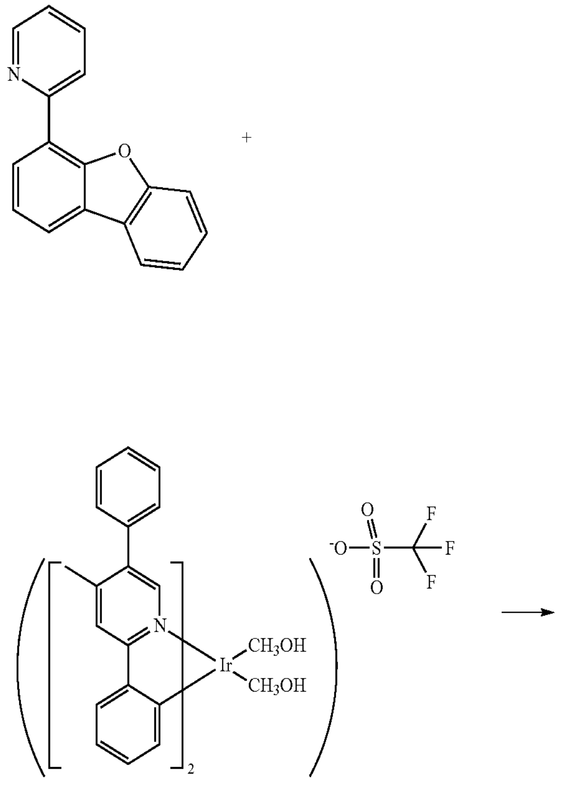


Compound 7

Synthesis of Compound 7

The iridium triflate precursor (2.0 g, 2.7 mmol) and 4-methyl-2-(dibenzo[b,d]furan-4-yl)pyridine (2.1 g, 8.1 mmol) were mixed in 60 mL of ethanol. The mixture was heated at reflux for 24 h under nitrogen. Precipitate formed during reflux. The reaction mixture was filtered through a celite bed. The product was washed with methanol and hexanes. The solid was dissolved in dichloromethane and purified by column using 1:1 of dichloromethane and hexanes. 1.0 g of pure product was obtained after the column purification.

Example 7. Synthesis of Compound 37



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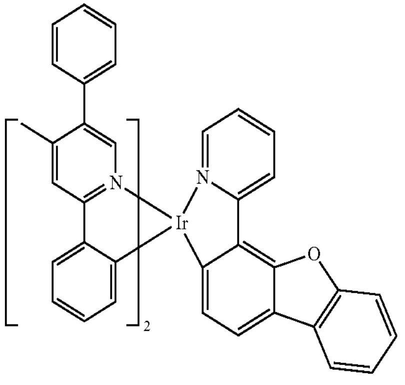


Compound 37

Synthesis of Compound 37

2-(dibenzo[b,d]furan-4-yl)pyridine (5.0 g, 20.39 mmol) and the iridium triflate (5.0 g, 5.59 mmol) were placed in a 250 mL round bottom flask with 100 mL of a 1:1 solution of ethanol and methanol. The reaction mixture was refluxed for 24 h. A bright yellow precipitate was obtained. The reaction was cooled to room temperature and diluted with ethanol. Celite was added to and the reaction mixture was filtered through a silica gel plug. The plug was washed with ethanol (2×50 mL) followed by hexanes (2×50 mL). The product which remained on the silica gel plug was eluted with dichloromethane into a clean receiving flask. The dichloromethane was removed under vacuum and the product was recrystallized from a combination of dichloromethane and isopropanol. The yellow solid was filtered, washed with methanol followed by hexanes to give bright yellow crystalline product. The product was further purified by recrystallization from toluene followed by recrystallization from acetonotrile to give 1.94 g (37.5% yield) of product with purity 99.5% by HPLC.

Device Examples

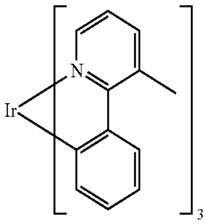
All example devices were fabricated by high vacuum ($<10^{-7}$ Torr) thermal evaporation. The anode electrode is 800 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1000 Å of Al. All devices are encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H_2O and O_2) immediately after fabrication, and a moisture getter was incorporated inside the package.

Particular devices are provided wherein an invention compound, Compound 1, 2, 4, 7, 10 or 29, is the emitting dopant and H1 is the host. The organic stack of Device Examples 1-11 consisted of, sequentially from the ITO surface, 100 Å of E1 as the hole injecting layer (HIL), 300 Å of 4,4'-bis-[N-(1-naphthyl)-N-phenylamino]biphenyl (α-NPD) as the hole transport layer (HTL), 300 Å of H1 doped with 7% or 10% of the invention compound, an Ir phosphorescent compound, as the emissive layer (EML), 50 Å of H1 as the blocking layer (BL) and 400 Å of Alq_3 (tris-8-hydroxyquinoline aluminum) as the ETL1.

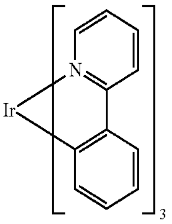
Comparative Examples 1 and 2 were fabricated similarly to the Device Examples, except that E1 and E2. respectively, were used as the emitting dopant.

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

E1



E2



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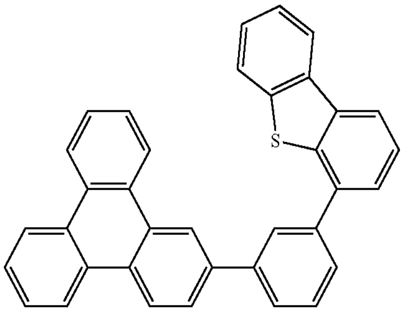
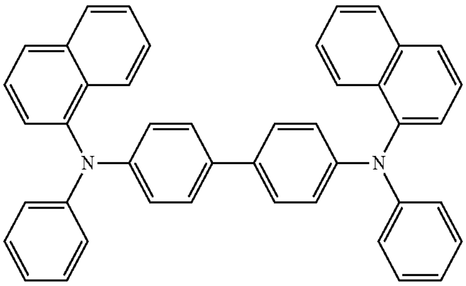
H1



NPD



The device structures and device data are summarized below in Table 3 and Table 4. Table 3 shows the device structure, and Table 4 shows the corresponding measured results for the devices. Ex. is an abbreviation of Example.

TABLE 3

Example	HIL	HTL	Host	A %	BL	ETL
Example 1	E1 100 Å	NPD 300 Å	H1	Compound 1 7%	H1 50 Å	Alq 400 Å
Example 2	E1 100 Å	NPD 300 Å	H1	Compound 1 10%	H1 50 Å	Alq 400 Å
Example 3	E1 100 Å	NPD 300 Å	H1	Compound 2 7%	H1 50 Å	Alq 400 Å
Example 4	E1 100 Å	NPD 300 Å	H1	Compound 2 10%	H1 50 Å	Alq 400 Å
Example 5	E1 100 Å	NPD 300 Å	H1	Compound 4 7%	H1 50 Å	Alq 400 Å
Example 6	E1 100 Å	NPD 300 Å	H1	Compound 4 10%	H1 50 Å	Alq 400 Å
Example 7	E1 100 Å	NPD 300 Å	H1	Compound 7 7%	H1 50 Å	Alq 400 Å
Example 8	E1 100 Å	NPD 300 Å	H1	Compound 7 10%	H1 50 Å	Alq 400 Å
Example 9	E1 100 Å	NPD 300 Å	H1	Compound 10 7%	H1 50 Å	Alq 400 Å
Example 10	E1 100 Å	NPD 300 Å	H1	Compound 10 10%	H1 50 Å	Alq 400 Å
Example 11	E1 100 Å	NPD 300 Å	H1	Compound 29 10%	H1 50 Å	Alq 400 Å
Comparative Example 1	E1 100 Å	NPD 300 Å	H1	Compound E1 7%	H1 50 Å	Alq 400 Å
Comparative Example 2	E1 100 Å	NPD 300 Å	H1	Compound E2 7%	H1 50 Å	Alq 400 Å

TABLE 4

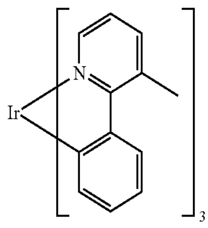
				At 1000 nits				At 40 mA/cm^2	
	λ max,	CIE		V	LE	EQE	PE	Lo,	
Example	nm	X	Y	(V)	(cd/A)	(%)	(lm/W)	nits	RT$_{80\%}$, h
Ex. 1	532	0.354	0.616	6.1	60.1	15.9	31	17,382	180
Ex. 2	530	0.367	0.607	6.5	43.2	11.5	21	13,559	170
Ex. 3	527	0.355	0.612	6.2	51.7	13.9	26.1	14,565	210
Ex. 4	528	0.361	0.609	6	44.4	11.9	23.3	13,618	360
Ex. 5	528	0.348	0.620	5.7	68.7	18.1	37.7	19,338	98
Ex. 6	528	0.356	0.616	5.2	70.1	18.5	42.4	21,199	96
Ex. 7	522	0.326	0.630	5.6	68.2	18.4	38.6	18,431	120
Ex. 8	524	0.336	0.623	5.2	58.2	15.7	35.0	17,606	200
Ex. 9	522	0.320	0.634	5.4	70.7	19	41.4	19,996	75
Ex. 10	522	0.327	0.631	5	71.1	19.1	44.9	21,703	58
Ex. 11	576	0.538	0.459	5.6	50.6	19	28.1	14,228	800
Comparative Ex. 1	527	0.344	0.614	6.4	56.7	15.6	27.6	15,436	155
Comparative Ex. 2	519	0.321	0.621	6	45.1	12.6	23.6	13,835	196

From Device Examples 1-11, it can be seen that the invention compounds as emitting dopants in green phosphorescent devices provide high device efficiency and longer lifetime. In particular, the lifetime, RT$_{80\%}$ (defined as the time for the initial luminance, L_0, to decay to 80% of its value, at a constant current density of 40 mA/cm^2 at room temperature) of devices containing Compounds 1, 2, 7 and 29 are notably higher than that measured for Comparative Example 2 which used the industry standard emitting dopant Ir(ppy)$_3$. Additionally, Compound 1 in Device Example 1 achieved high device efficiency (i.e., LE of 60 cd/A at 1000 cd/m^2), indicating that the inventive compounds comprising a single substituted pyridyl ligand (e.g., pyridyl dibenzofuran) have a high enough triplet energy for efficient green electrophosphorescence.

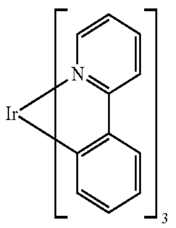
Additional device structures and device data are summarized below. The device structures and device data are summarized below in Table 5 and Table 6. Table 5 shows the device structure, and Table 6 shows the corresponding measured results for the devices. Ex. is an abbreviation of Example.

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

E1



E2



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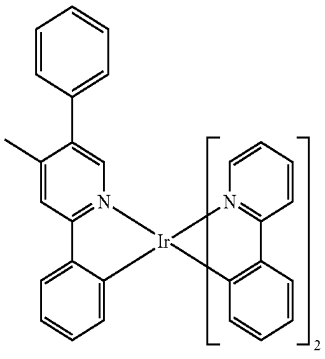
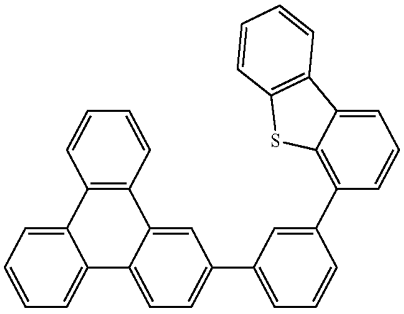
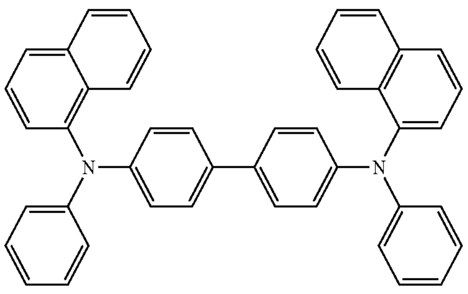
E3



H1



NPD



H2 is a compound available as NS60 from Nippon Steel Company (NSCC) of Tokyo, Japan.

TABLE 5

Example	HIL	HTL	Host	A %	BL	ETL
Example 12	E1 100 Å	NPD 300 Å	H2	Compound 1 10%	H2 100 Å	Alq 400 Å
Example 13	E1 100 Å	NPD 300 Å	H2	Compound 2 7%	H2 100 Å	Alq 400 Å
Example 14	E1 100 Å	NPD 300 Å	H2	Compound 2 10%	H2 100 Å	Alq 400 Å
Example 15	E1 100 Å	NPD 300 Å	H2	Compound 4 10%	H2 100 Å	Alq 400 Å
Example 16	E1 100 Å	NPD 300 Å	H2	Compound 7 10%	H2 100 Å	Alq 400 Å
Example 17	E1 100 Å	NPD 300 Å	H2	Compound 10 10%	H2 100 Å	Alq 400 Å
Example 18	E1 100 Å	NPD 300 Å	H2	Compound 29 10%	H2 100 Å	Alq 400 Å
Example 19	E3 100 Å	NPD 300 Å	H1	Compound 37 7%	H1 100 Å	Alq 400 Å
Example 20	E3 100 Å	NPD 300 Å	H1	Compound 37 10%	H1 100 Å	Alq 400 Å
Example 21	E3 100 Å	NPD 300 Å	H2	Compound 37 10%	H2 100 Å	Alq 400 Å

TABLE 6

				At 1000 nits				At 40 mA/cm^2	
		CIE		V	LE	EQE	PE	Lo,	
Example	λ max, nm	X	Y	(V)	(cd/A)	(%)	(lm/W)	nits	RT$_{80\%}$, h
Ex. 12	530	0.361	0.612	4.1	78.6	20.9	60.0	24,069	220
Ex. 13	526	0.354	0.615	4.7	48.9	13.1	33.0	14,002	210
Ex. 14	527	0.349	0.620	4.9	49.8	13.3	31.6	14,510	190
Ex. 15	528	0.363	0.612	5.1	67.8	18	42.1	21,146	116
Ex. 16	522	0.334	0.626	4.8	65.9	17.8	43.1	20,136	170
Ex. 17	522	0.333	0.627	5.7	62.1	16.7	34.0	18,581	98
Ex. 18	576	0.542	0.455	6.4	36.2	13.9	17.9	10,835	740
Ex. 19	532	0.386	0.593	5.6	67.8	18.5	37.9	21,426	98
Ex. 20	532	0.386	0.593	5.7	67.7	18.5	37.5	21,050	103
Ex. 21	532	0.380	0.598	6.5	54.8	14.8	26.7	16,798	315

From Device Examples 12-21, it can be seen that the invention compounds as emitting dopants in green phosphorescent devices provide devices with high efficiency and long lifetimes. In particular, the lifetime, RT$_{80\%}$ (defined as the time for the initial luminance, L_0, to decay to 80% of its value, at a constant current density of 40 mA/cm^2 at room temperature) of devices containing Compounds 29 and 37 are notably higher than those measured for the Comparative Examples. In particular, Compound 29 in Device Example 18 and Compound 37 in Device Example 21 measured 740 h and 315 h, respectively. Devices with Compound 1 in H2, as shown in Example 12, had exceptionally high efficiency, 78.6 cd/A and long lifetime. It is unexpected that Compound 1 worked extremely well in H2. Additionally, Compounds 1, 4, 7, 29, and 37 in Device Examples 12, 15, 17, 19, and 20, respectively, achieved high device efficiency (i.e., LE of greater than 60 cd/A at 1000 cd/m^2), indicating that the inventive compounds comprising a single substituted pyridyl ligand (e.g., pyridyl dibenzofuran) have a high enough triplet energy for efficient green electrophosphorescence.

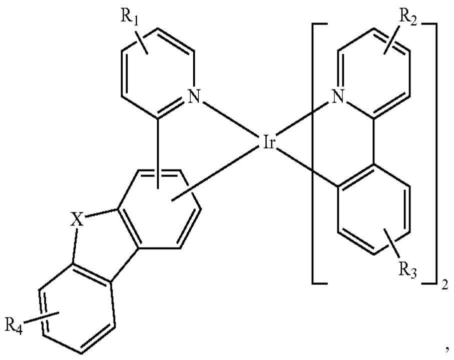
The above data suggests that the heteroleptic iridium complexes provided herein can be excellent emitting dopants for phosphorescent OLEDs, providing devices having improved efficiency and longer lifetime that may also have improved manufacturing.

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 includes 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.

The invention claimed is:

1. A heteroleptic compound having the formula:

FORMULA I



,

wherein X is NR;

wherein R is isobutyl;

wherein R_1, R_2, R_3, and R_4 may represent mono, di, tri, or tetra substitutions; and

wherein each of R_1, R_2, R_3, and R_4 is independently selected from the group consisting of hydrogen, alkyl, and aryl.

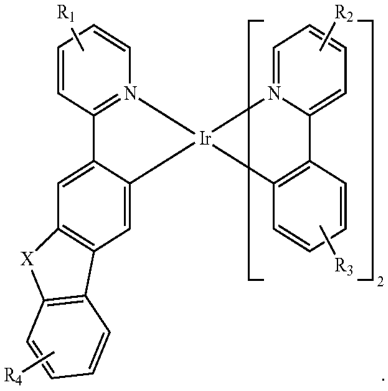
2. The heteroleptic compound of claim **1**, wherein R_1 and R_4 are independently selected from the group consisting of hydrogen and alkyl having four or fewer carbon atoms.

3. The heteroleptic compound of claim **1**, wherein R_2 and R_3 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms and aryl comprising an aryl ring with 5 or 6 atoms in the aryl ring.

4. The heteroleptic compound of claim **1**, wherein R_1, R_2, R_3, and R_4 are independently selected from the group consisting of hydrogen, alkyl having four or fewer carbon atoms and aryl comprising an aryl ring with 5 or 6 atoms in the aryl ring.

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

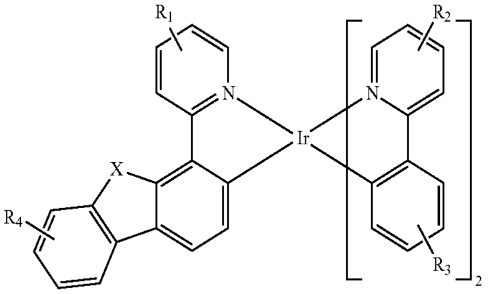
FORMULA III



.

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

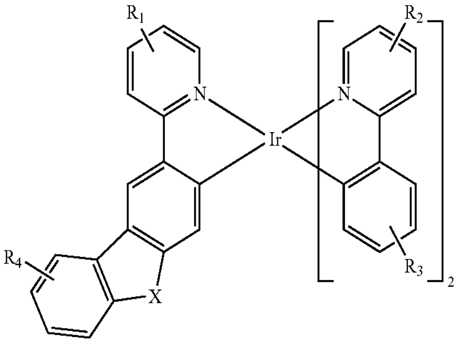
FORMULA IV



.

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

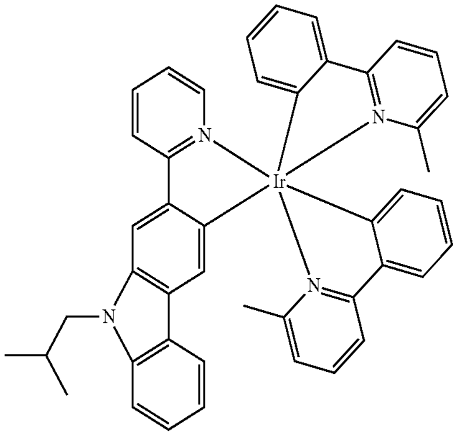
FORMULA V



.

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

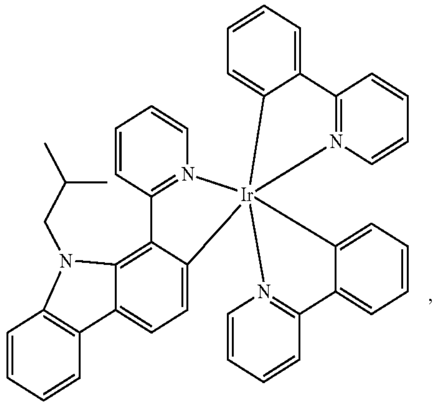
Compound 29



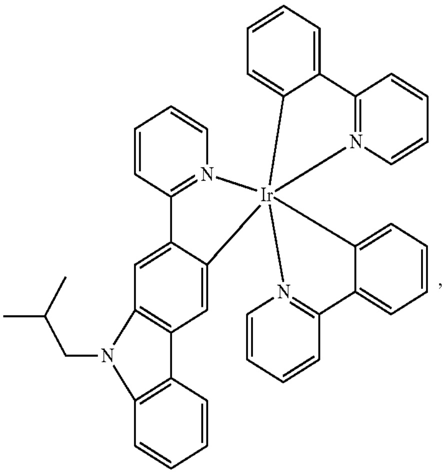
.

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

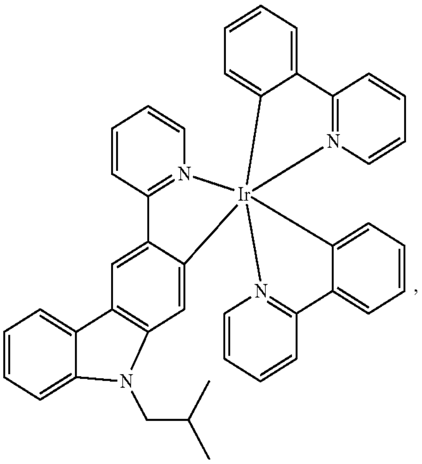
Compound 25



Compound 26



Compound 27



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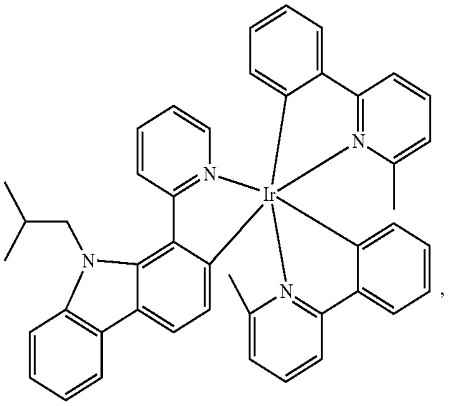
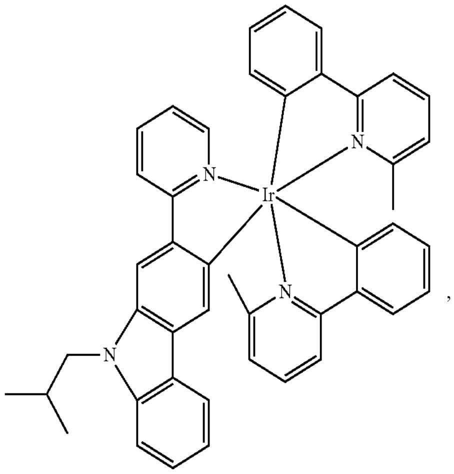
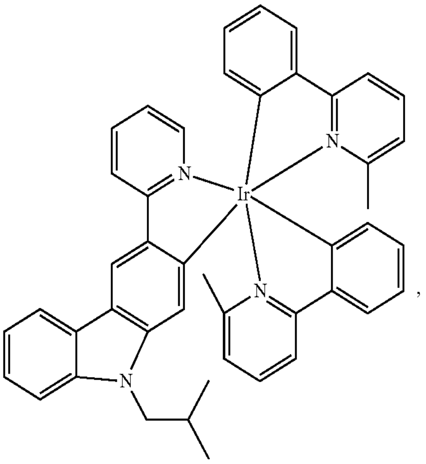
Compound 28



Compound 29



Compound 30



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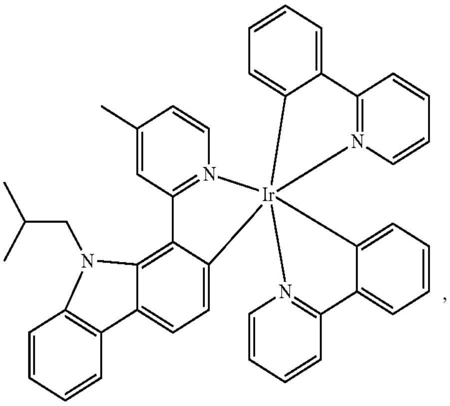
Compound 31



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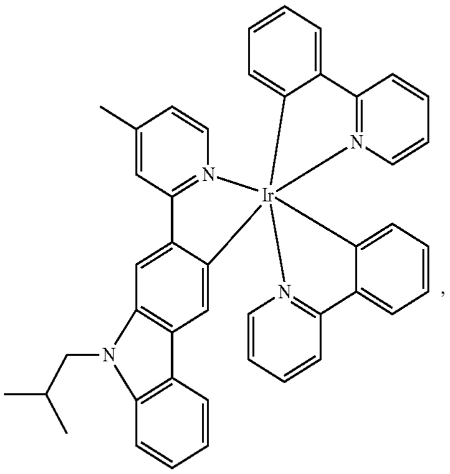
Compound 32



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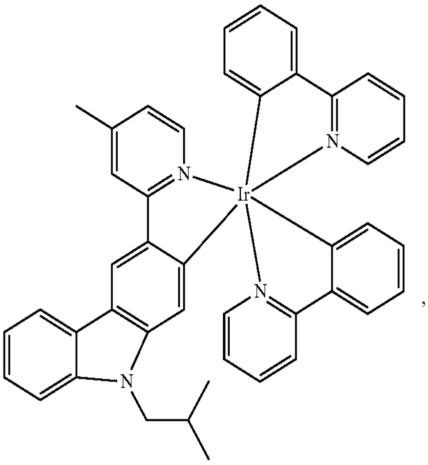
Compound 33



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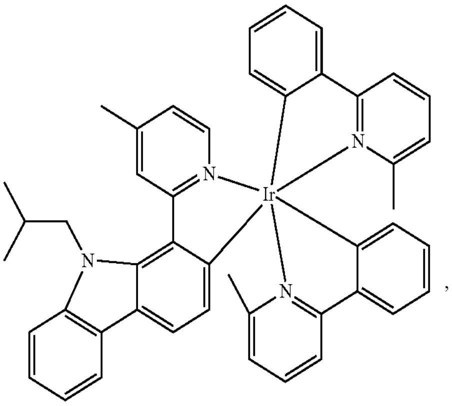
Compound 34



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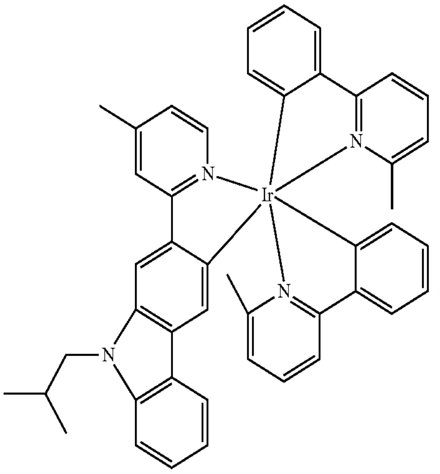
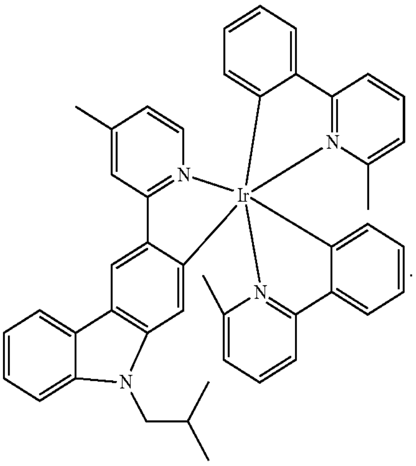
Compound 35



, and

Compound 36



.

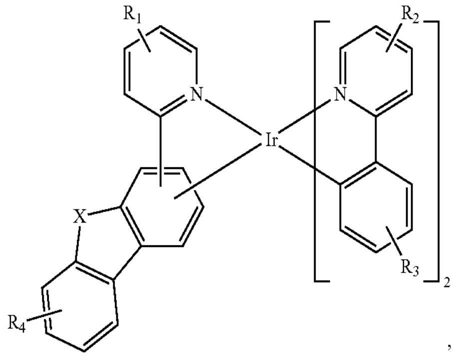
10. A first device comprising an organic light emitting device, comprising:

an anode;

a cathode; and

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

FORMULA I



,

wherein X is NR;

wherein R is isobutyl;

wherein R_1, R_2, R_3 and R_4 may represent mono, di, tri, or tetra substitutions;

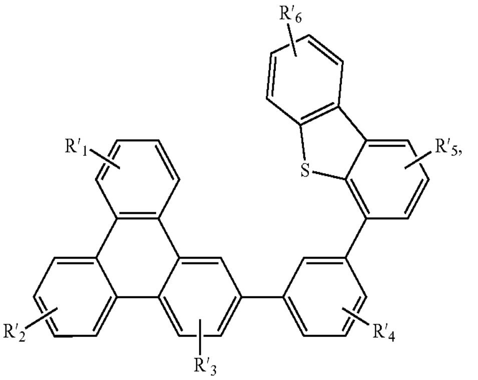
wherein each of R_1, R_2, R_3 and R_4 is independently selected from the group consisting of hydrogen, alkyl, and aryl.

11. The device of claim **10**, wherein the organic layer is an emissive layer and the heteroleptic compound is an emitting dopant.

12. The device of claim **10**, wherein the organic layer further comprises a host.

13. The device of claim **12**, wherein the host comprises a triphenylene moiety and a dibenzothiophene moiety.

14. The device of claim **12**, wherein the host has the formula:



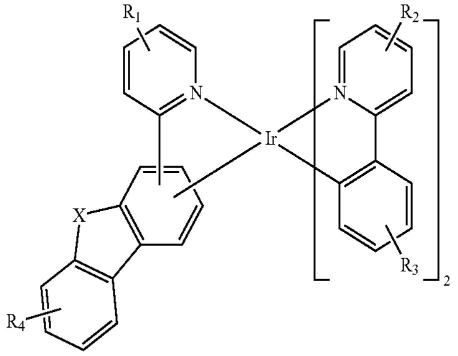
wherein R'_1, R'_2, R'_4, and R'_6 may represent mono, di, tri, or tetra substitutions;

wherein R'_3 and R'_5 may represent mono, di, or tri substitutions; and

wherein each of R'_1, R'_2, R'_3, R'_4, R'_5, and R'_6 is independently selected from the group consisting of hydrogen, alkyl, and aryl.

15. A heteroleptic compound having the formula:

FORMULA I



,

wherein X is selected from the group consisting of BR and Se;

wherein R is selected from hydrogen and alkyl;

wherein R_1, R_2, R_3, and R_4 may represent mono, di, tri, or tetra substitutions; and

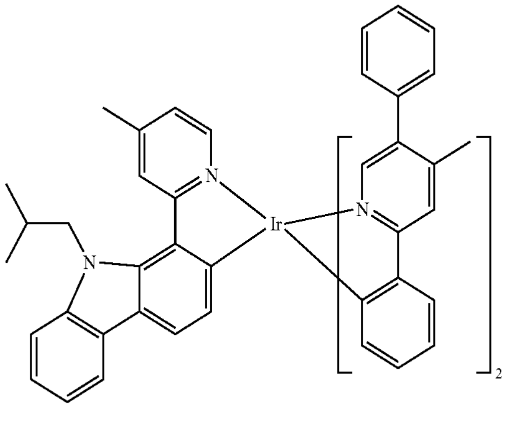
wherein each of R_1, R_2, R_3, and R_4 is independently selected from the group consisting of hydrogen, alkyl, and aryl.

16. The heteroleptic compound of claim **15**, wherein X is Se.

17. The heteroleptic compound of claim **15**, wherein X is BR.

18. The heteroleptic compound of claim **1** wherein the compound is selected from the group consisting of:

Compound 85



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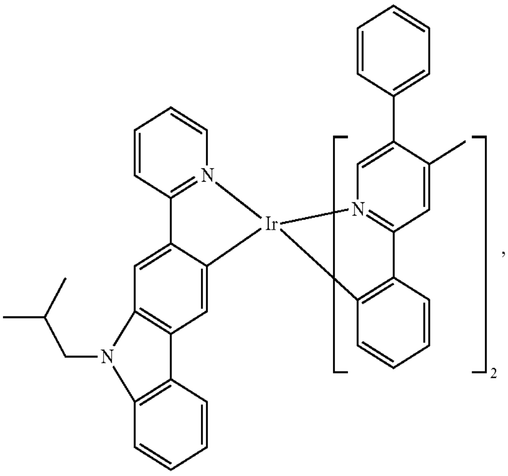
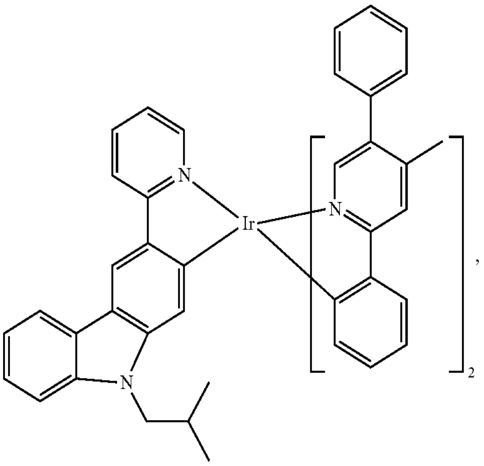
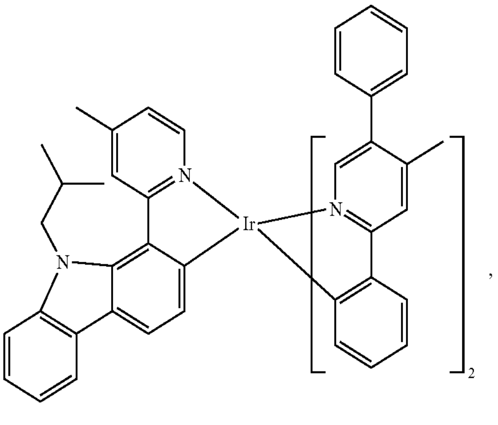
Compound 86



Compound 87



Compound 88



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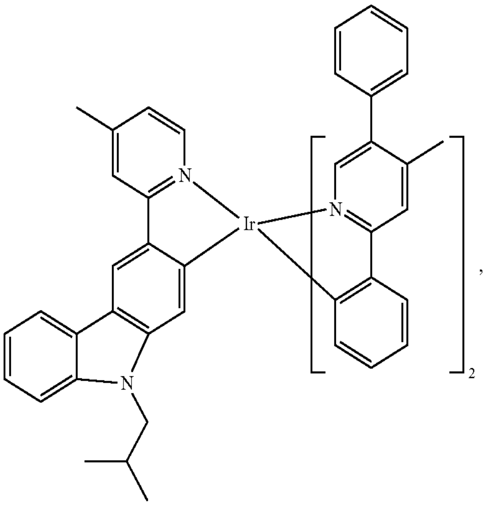
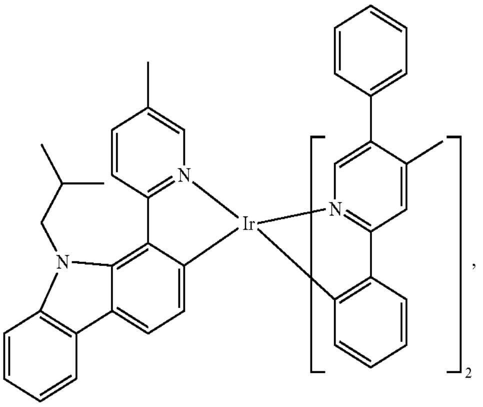
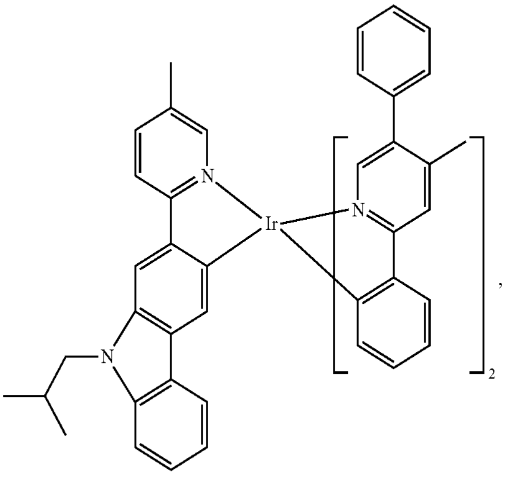
Compound 90



Compound 91

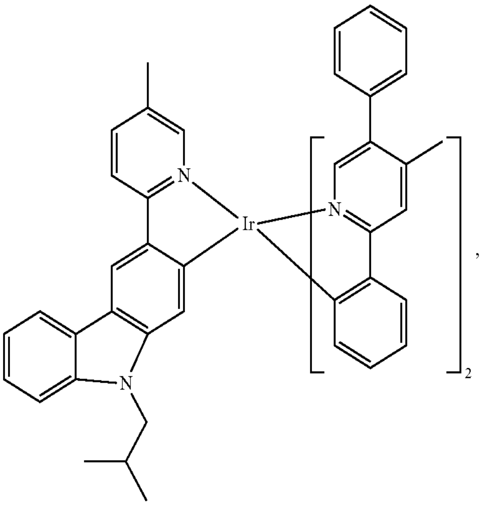


Compound 92

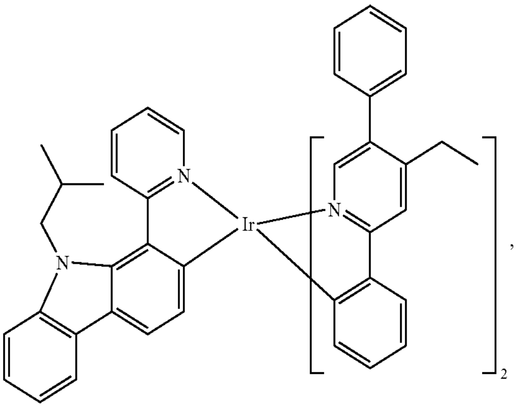


-continued

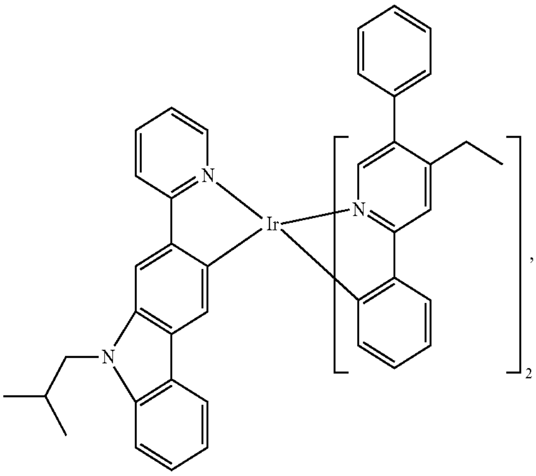
Compound 93



Compound 94



Compound 95



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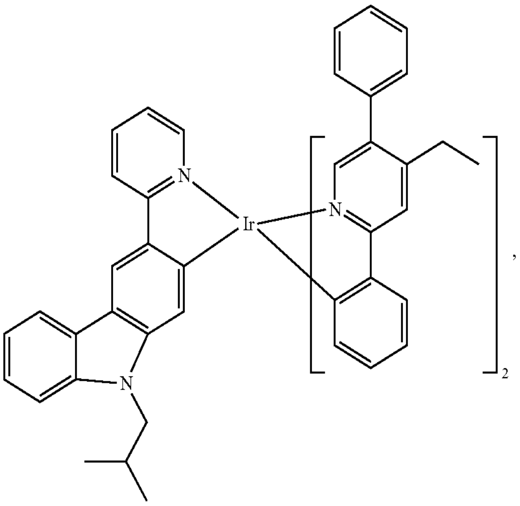
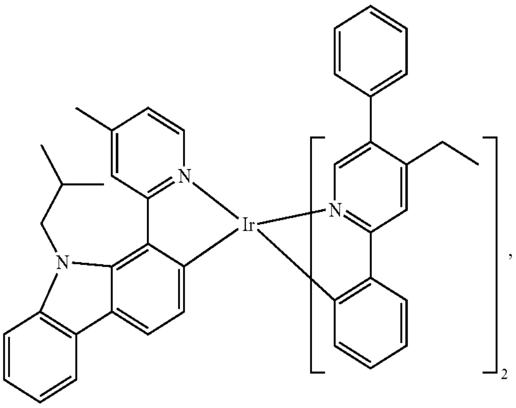
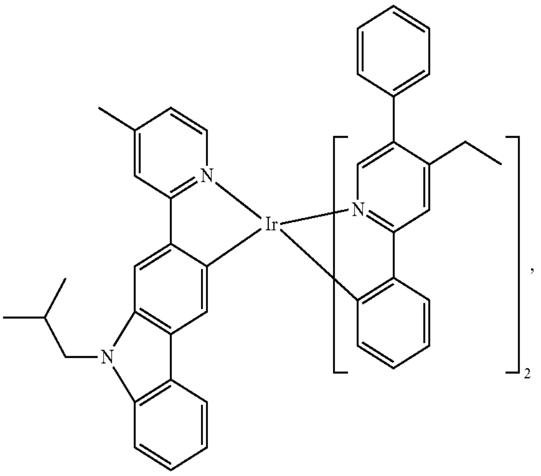
Compound 96



Compound 97



Compound 98



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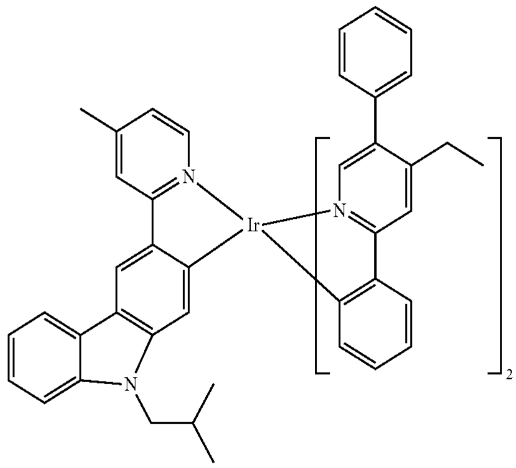
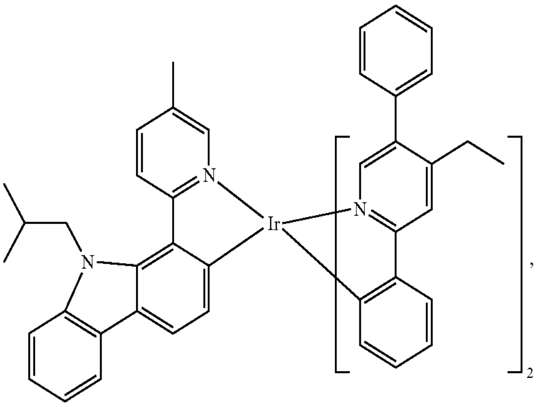
Compound 99



Compound 100



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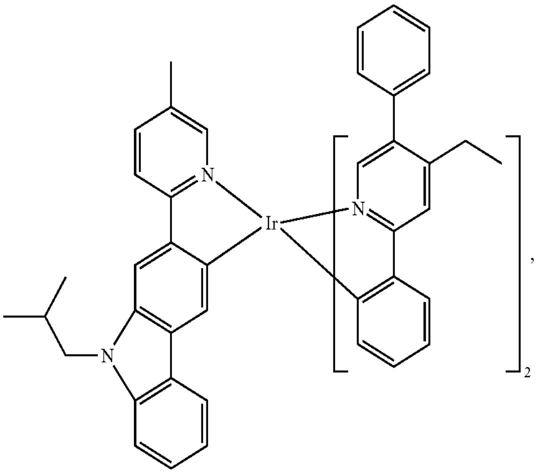

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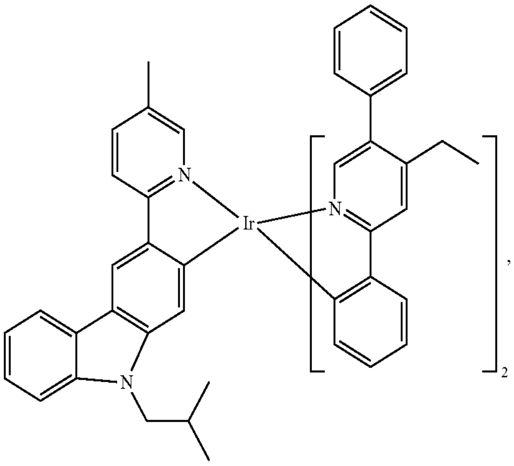
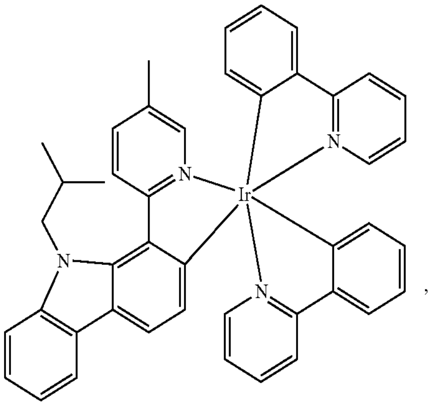
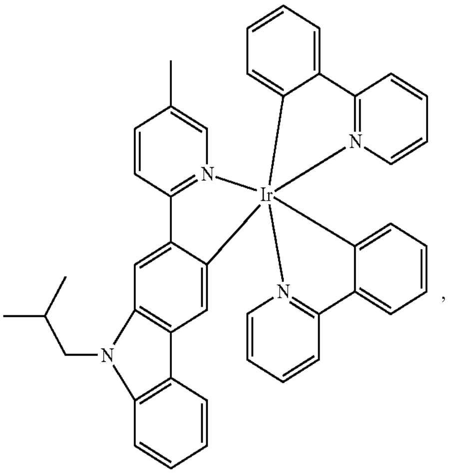
Compound 102



Compound 103



Compound 104



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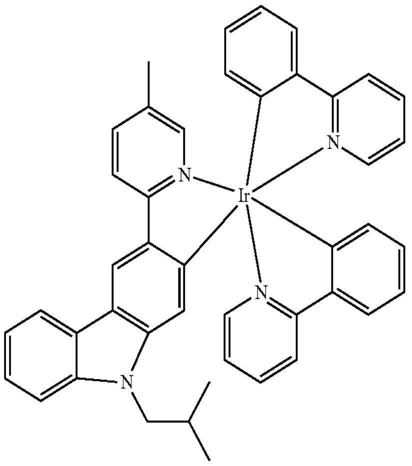
Compound 105



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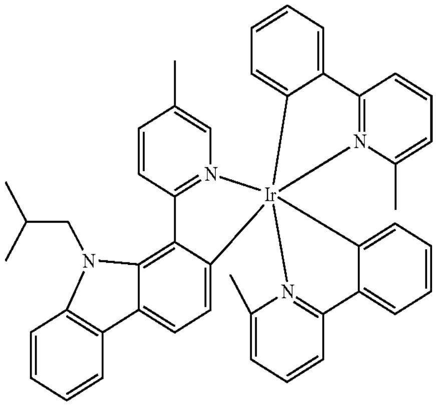

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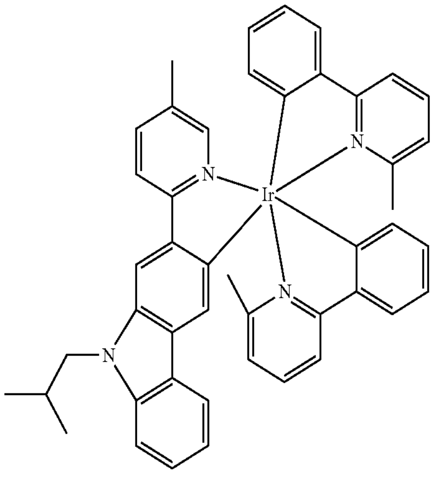
Compound 107



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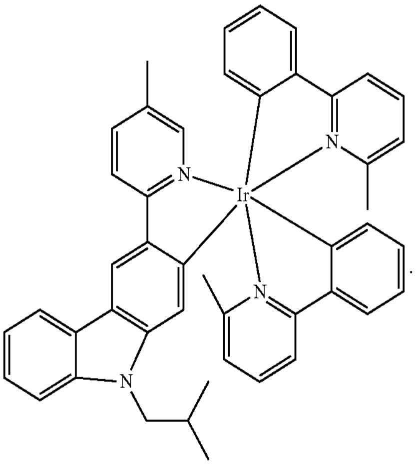
Compound 108



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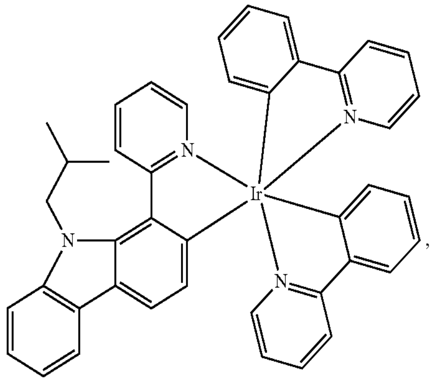
19. The heteroleptic compound of claim **1**, wherein the compound is selected from the group consisting of:

Compound 25



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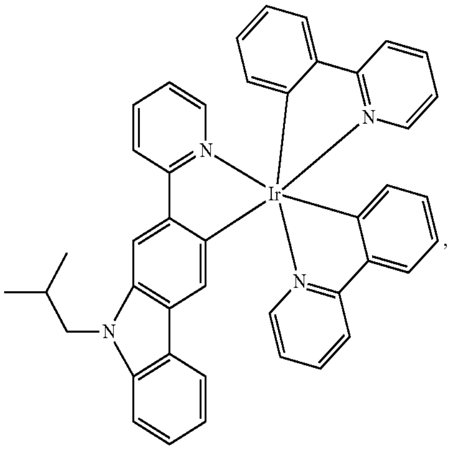
Compound 26



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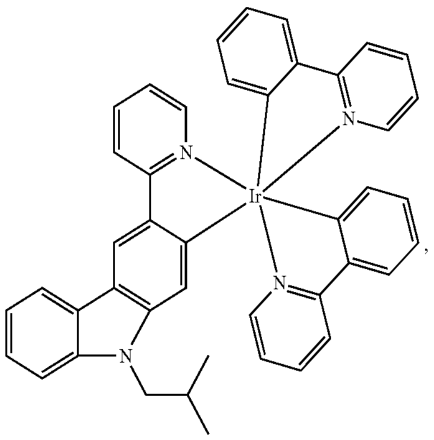
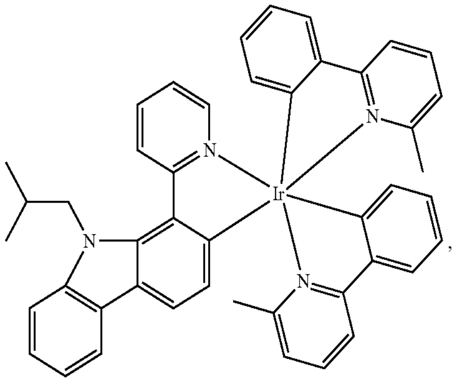
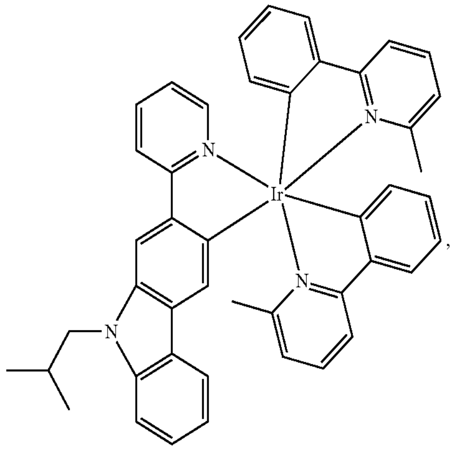
Compound 27



Compound 28



Compound 29



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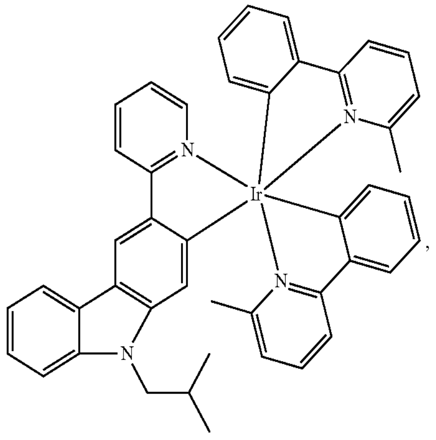
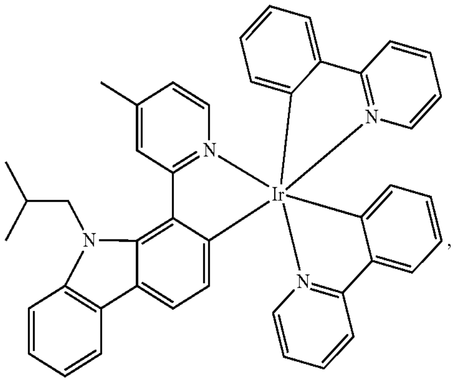
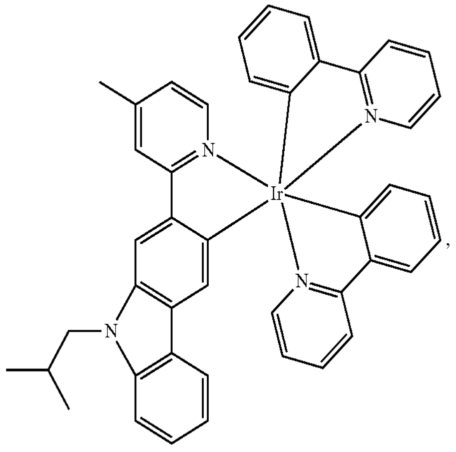
Compound 30



Compound 31



Compound 32



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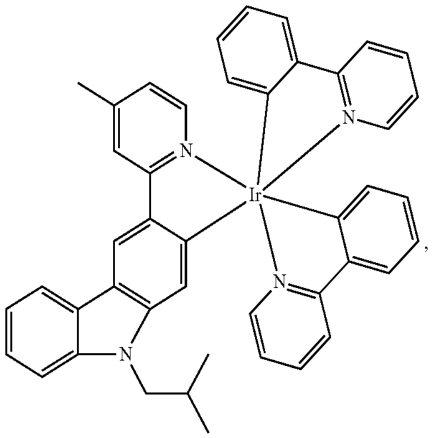
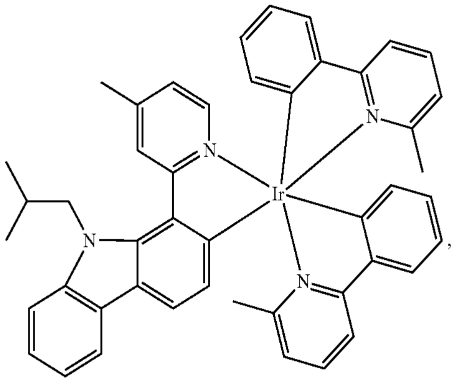
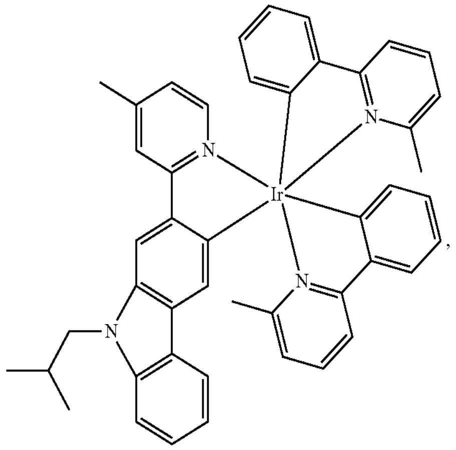
Compound 33



Compound 34



Compound 35



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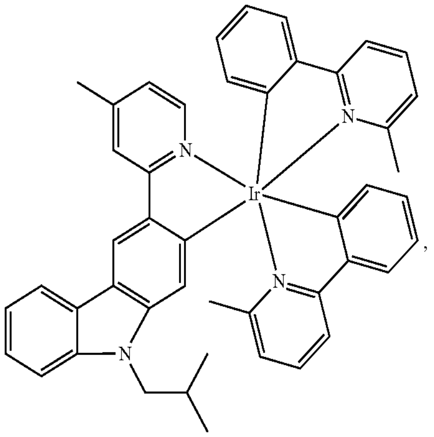
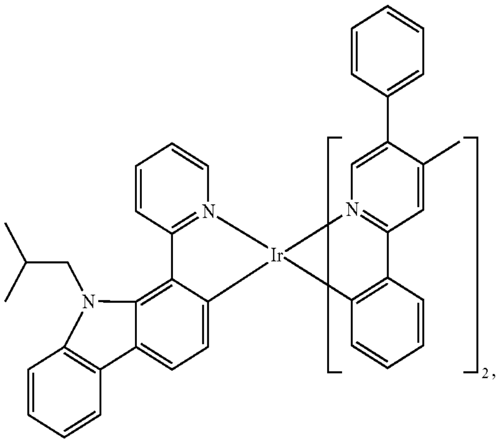
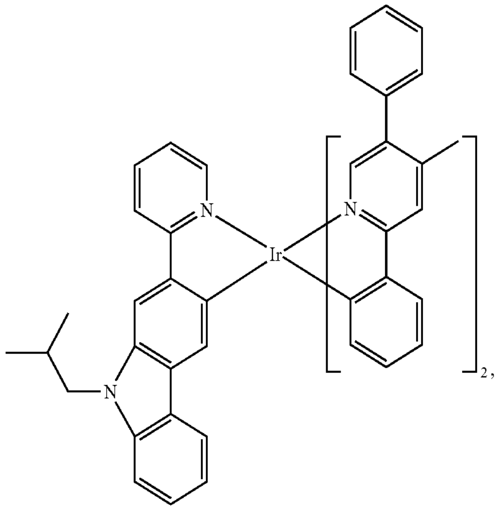
Compound 36



Compound 85



Compound 86



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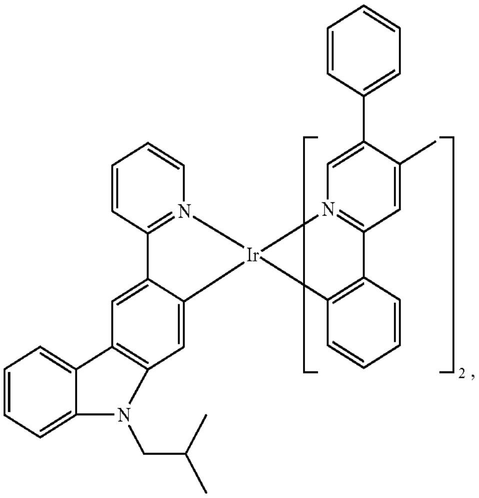
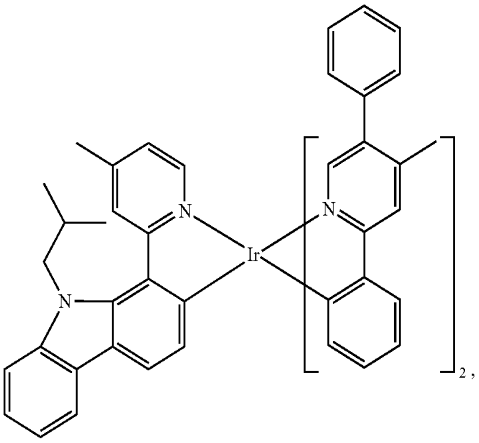
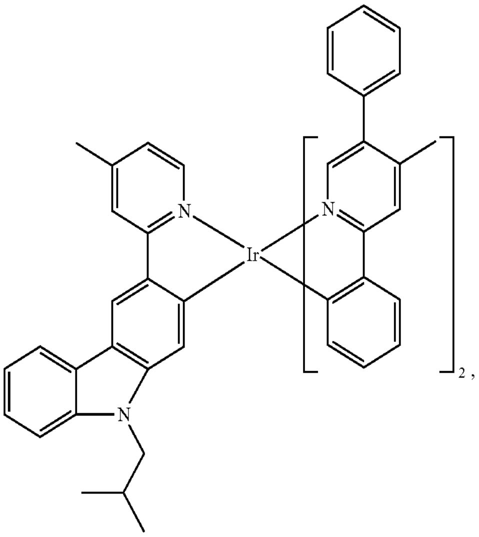
Compound 87



Compound 88



Compound 90



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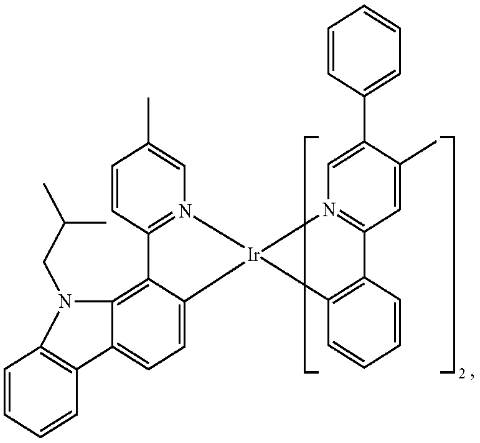
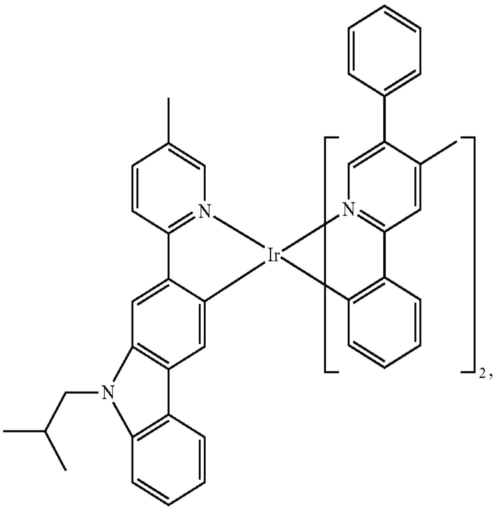
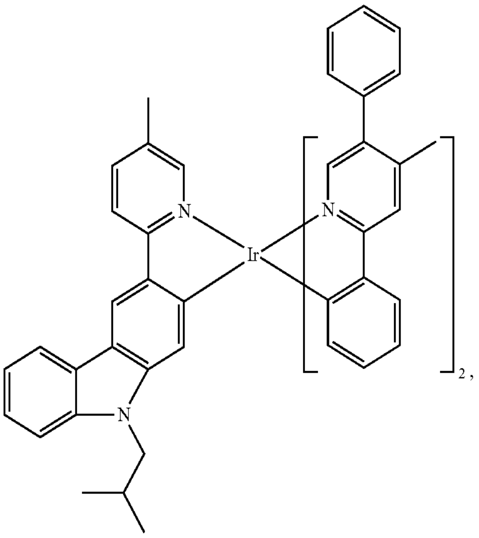


Compound 92



Compound 93



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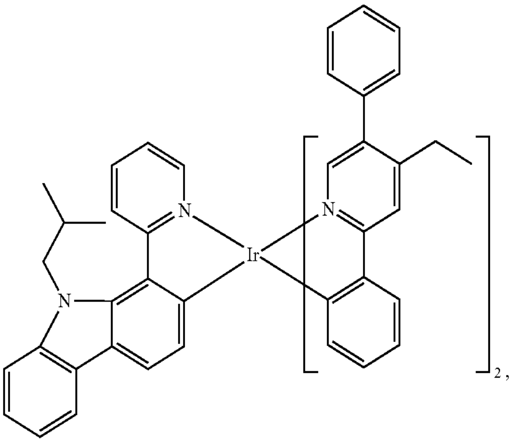
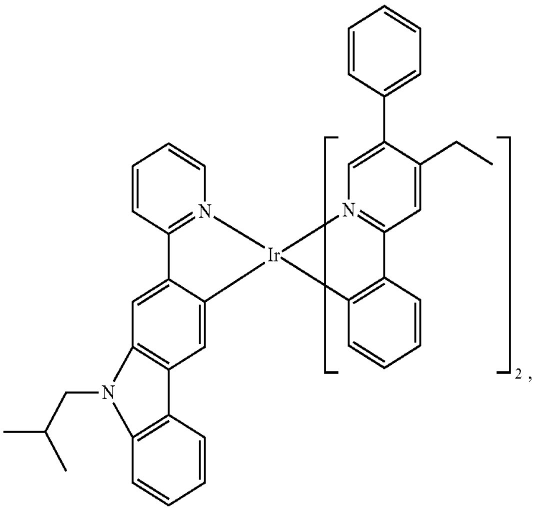
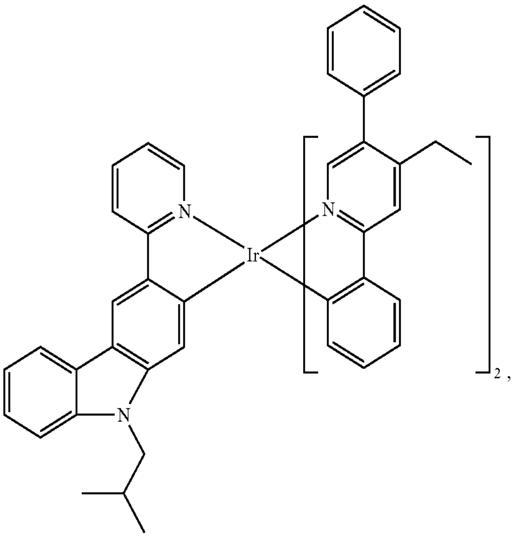
Compound 95



Compound 95



Compound 96



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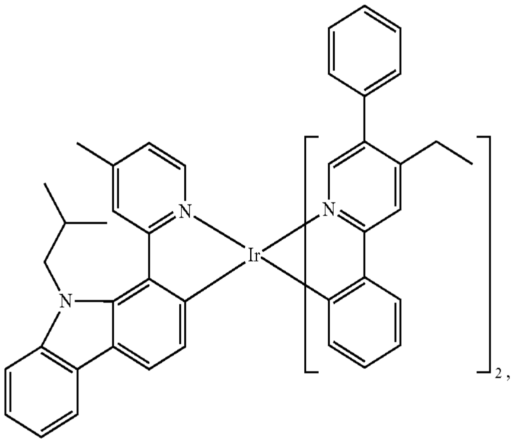
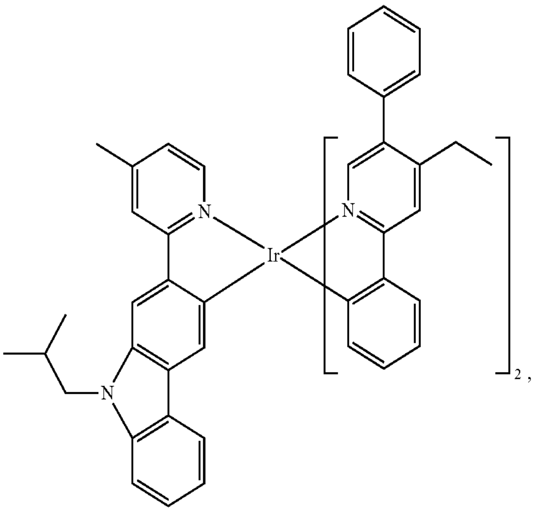
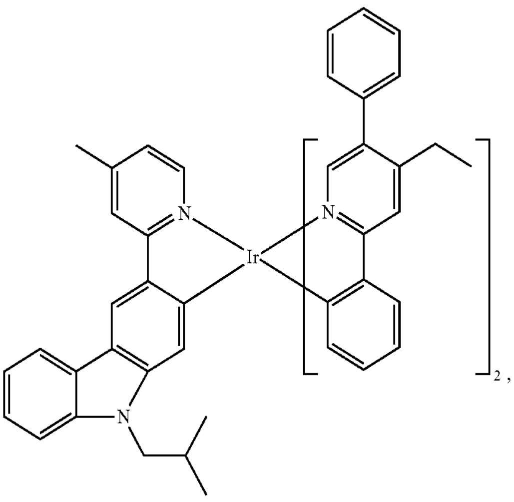
Compound 97



Compound 98



Compound 99



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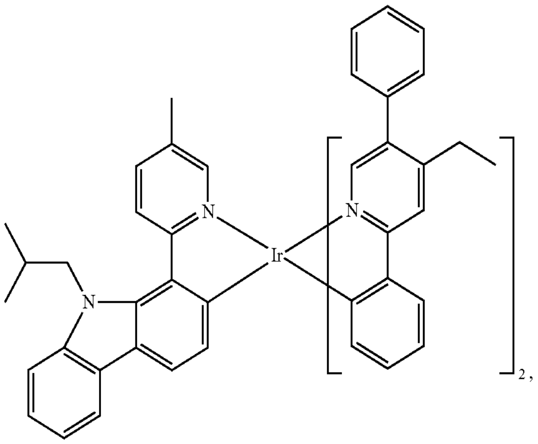
Compound 100



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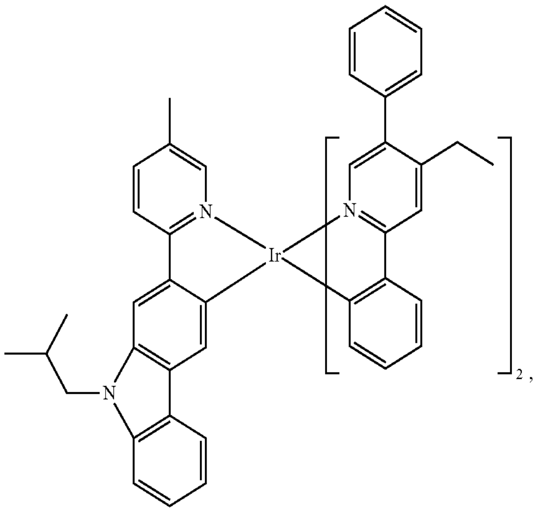
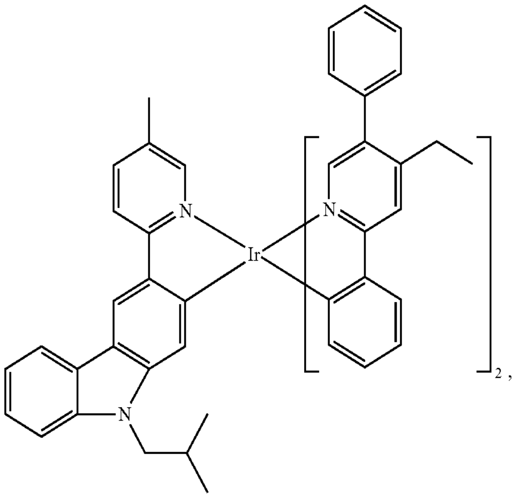


Compound 102



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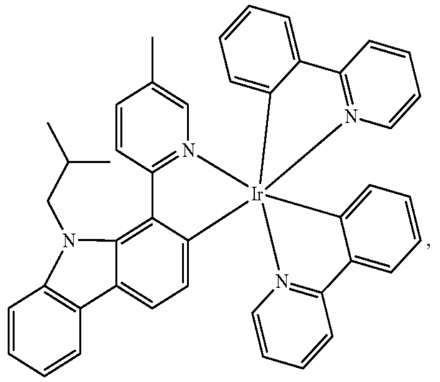
Compound 103



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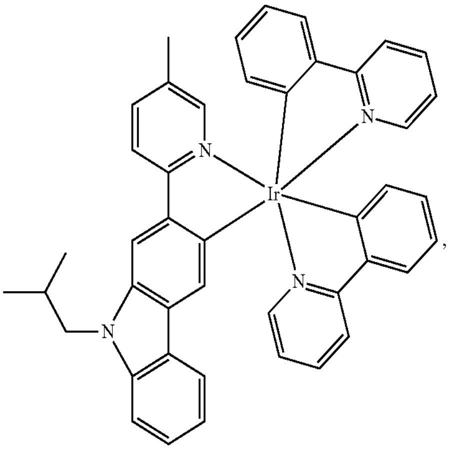

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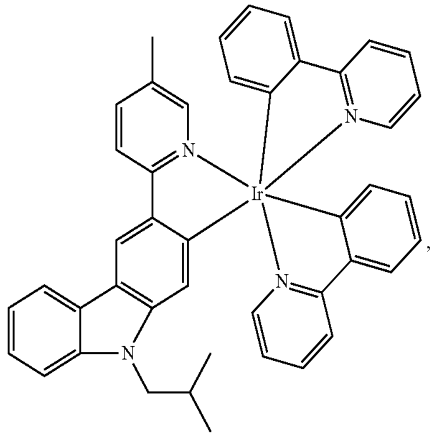

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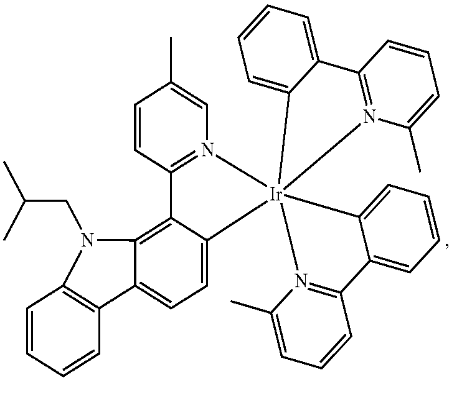

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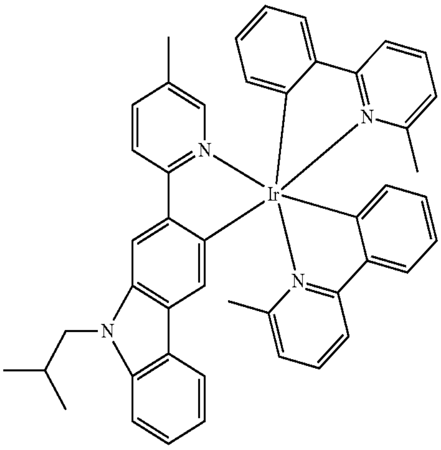
Compound 107



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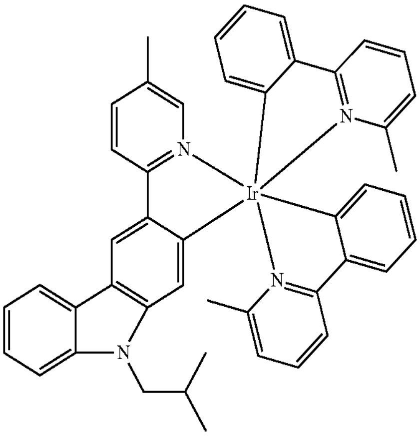
Compound 108



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专利名称(译)	有机电致发光材料和器件		
公开(公告)号	US10056566	公开(公告)日	2018-08-21
申请号	US14/225591	申请日	2014-03-26
[标]申请(专利权)人(译)	环球展览公司		
申请(专利权)人(译)	通用显示器公司		
当前申请(专利权)人(译)	通用显示器公司		
[标]发明人	XIA CHUANJUN KWONG RAYMOND C LAYEK SUMAN		
发明人	XIA, CHUANJUN KWONG, RAYMOND C. LAYEK, SUMAN		
IPC分类号	H01L51/54 C09K11/06 H01L51/00 C07F15/00 H05B33/10 H01L51/50		
CPC分类号	H01L51/0085 C07F15/0033 C09K11/06 H05B33/10 C09K2211/1007 H01L51/5016 C09K2211/1029 C09K2211/1088 C09K2211/1092 C09K2211/185 C09K2211/1011 H01L51/5012 H01L51/5024		
代理机构(译)	DUANE MORRIS LLP		
优先权	61/162476 2009-03-23 US		
其他公开文献	US20140203268A1		
外部链接	Espacenet		

摘要(译)

具有式I结构的新型杂配铱配合物， 提供。在式I中，X选自NR，BR和Se; R选自氢和烷基，并且每个R 1 ，R 2 ，R 3 和R 4 R 1独立地选自氢，烷基和芳基。该化合物可用于有机发光器件中，特别是用作发光掺杂剂，以提供具有改进的效率，寿命和制造的器件。