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

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C09K 11/06 (2006.01)
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CPC ***H01L 51/0067*** (2013.01); ***C07D 251/24*** (2013.01); ***C07D 405/10*** (2013.01);
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(57) **ABSTRACT**

A composition comprising a first compound and a second compound is described. The composition can be a mixture of a first compound having a structure according to Formula I,
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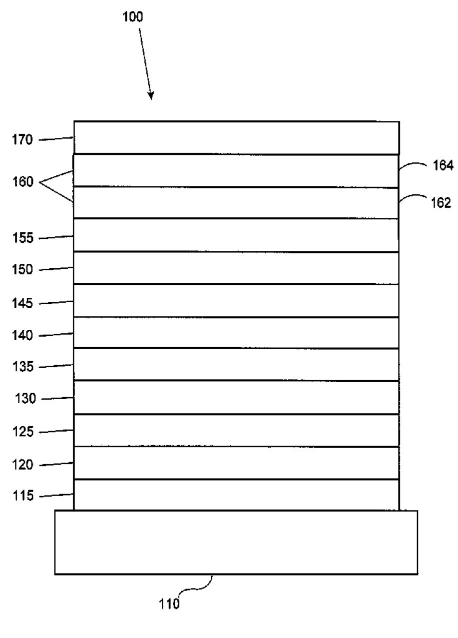
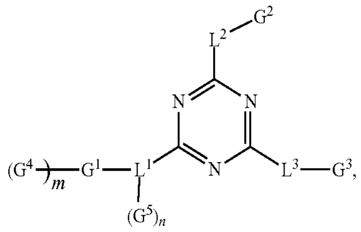
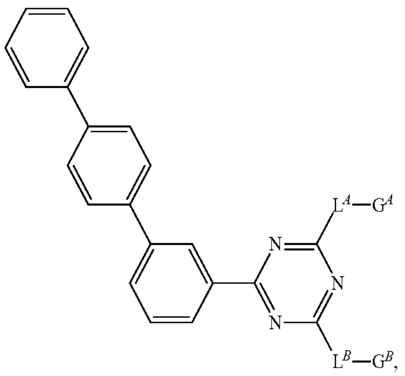




and a second compound having a structure according to Formula II,

$$Ar^1-Ar^2-Ar^3.$$

The composition can also be a mixture of a first compound having a structure according to Formula III,



and a second compound having a structure according to Formula IV,

$$G^8-\left(G^7\right)_p-G^6-Ar^4.$$

Devices, such as OLEDs, that include the compositions for Formulas I & II or Formulas III & IV, as well as, methods of making the same are also described.

20 Claims, 4 Drawing Sheets

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C09K 11/02	(2006.01)
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C07D 421/10	(2006.01)
C07D 409/04	(2006.01)
C07D 405/10	(2006.01)
H01L 51/50	(2006.01)

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

CPC ***C07D 409/04*** (2013.01); ***C07D 409/10*** (2013.01); ***C07D 421/10*** (2013.01); ***C09K 11/025*** (2013.01); ***C09K 11/06*** (2013.01); ***H01L 51/0058*** (2013.01); ***H01L 51/0073*** (2013.01); ***H01L 51/0074*** (2013.01); ***H01L 51/0085*** (2013.01); *C09K 2211/1007* (2013.01); *C09K 2211/1059* (2013.01); *C09K 2211/1092* (2013.01); *C09K 2211/1096* (2013.01); *C09K 2211/185* (2013.01); *H01L 51/5016* (2013.01); *H01L 51/5072* (2013.01)

(58) **Field of Classification Search**

CPC .. C07D 251/24; C07D 405/10; C07D 409/04; C07D 409/10; C07D 421/10; C09K 11/025; C09K 11/06; C09K 2211/1007; C09K 2211/1059; C09K 2211/1092; C09K 2211/1088

USPC 428/690, 917; 257/40, E51.029; 252/500; 544/180

See application file for complete search history.

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Notice of Reasons for Rejection dated Dec. 11, 2018 for corresponding Japanese Patent Application No. JP 2015-136658.

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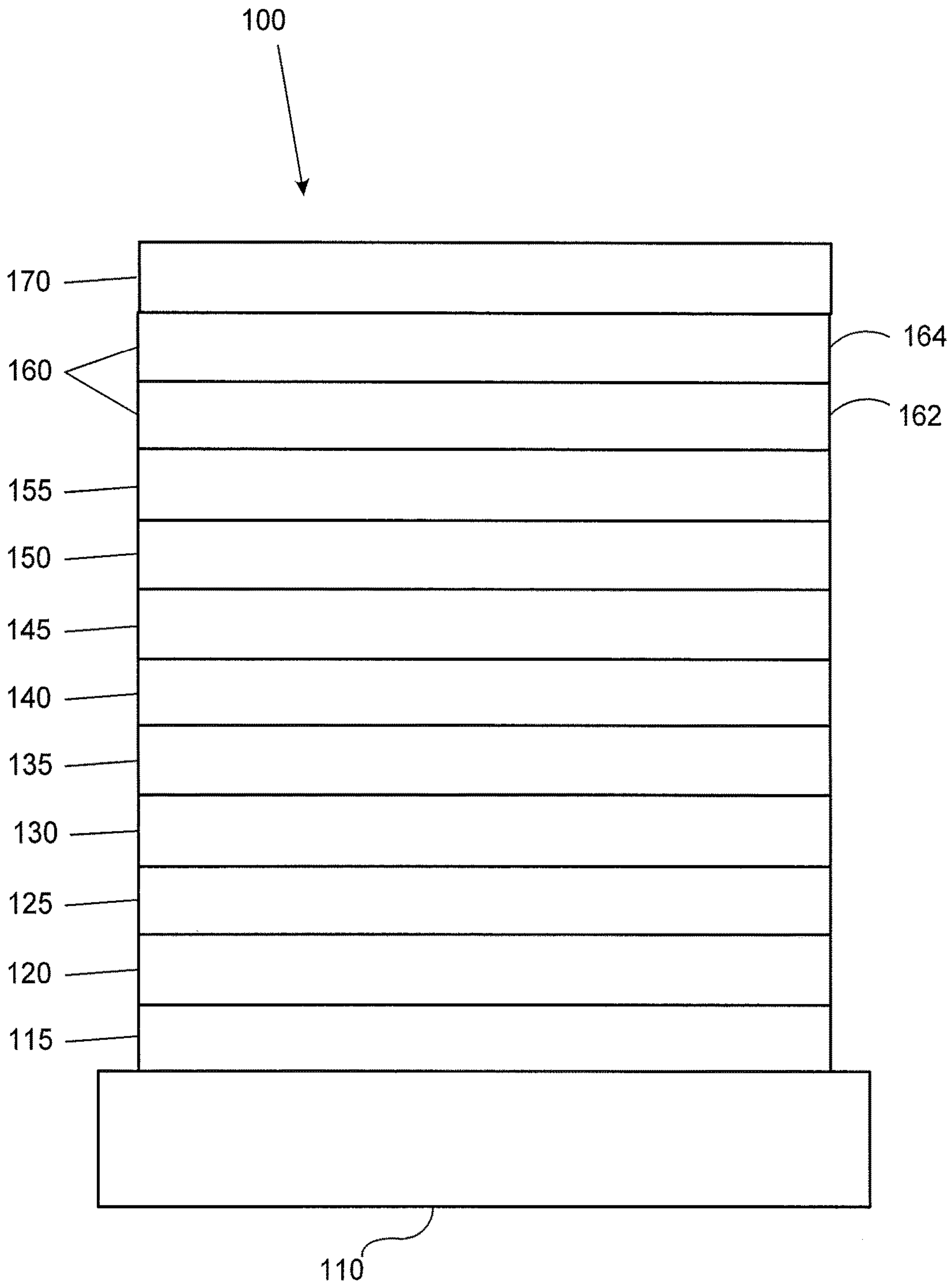


FIGURE 1

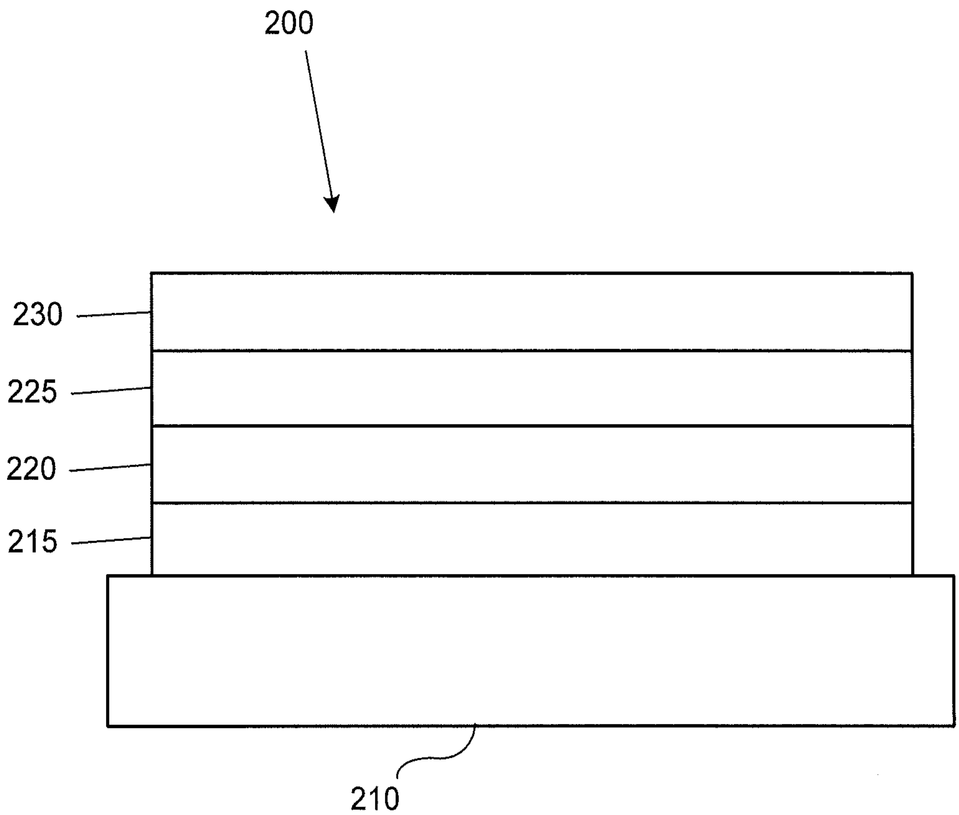
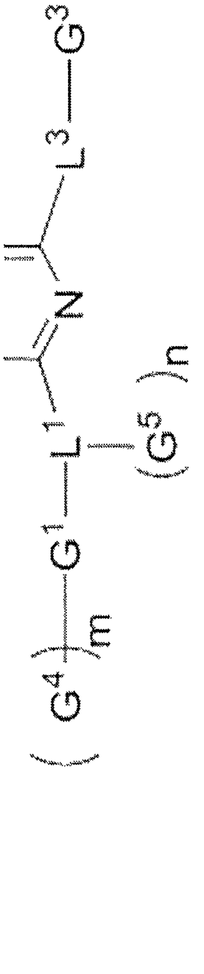


FIGURE 2

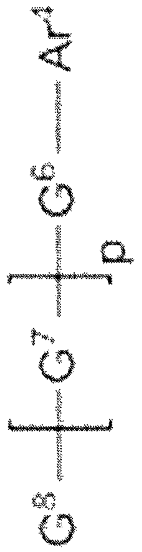
Formula II

FIGURE 4



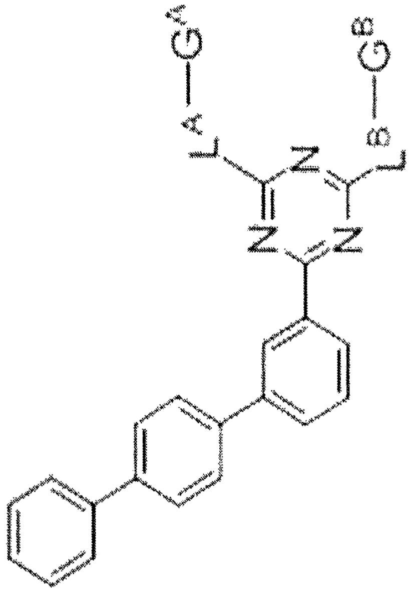
Formula I

FIGURE 3



Formula IV

FIGURE 6



Formula III

FIGURE 5

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATIONS

This application is a non-provisional of U.S. Patent Application Ser. No. 62/022,300, filed Jul. 9, 2014, U.S. Patent Application Ser. No. 62/038,925, filed Aug. 19, 2014; U.S. Patent Application Ser. No. 62/060,192, filed Oct. 6, 2014; and U.S. Patent Application Ser. No. 62/083,490, filed Nov. 24, 2014, the entire contents of which is incorporated herein by reference.

PARTIES TO A JOINT RESEARCH AGREEMENT

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

FIELD OF THE INVENTION

The present invention relates to compounds for use as hosts, blocking materials, and electron transporting materials, and devices, such as organic light emitting diodes, including the same.

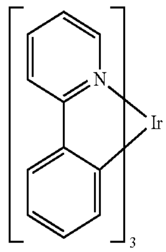
BACKGROUND

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

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

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

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



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

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

As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer.

For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

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

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

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

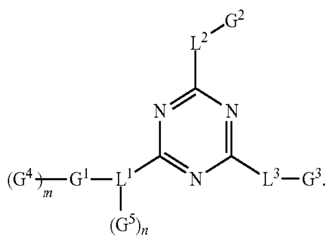
As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum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

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

SUMMARY OF THE INVENTION

According to one embodiment, a composition of materials comprising a first compound is provided. The first compound has a structure of formula:

Formula I



In Formula I:

G^1 is selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and fluorene;

L^1, L^2 and L^3 are each independently selected from the group consisting of direct bond, phenyl, biphenyl, terphenyl, pyridine, pyrimidine, and combinations thereof;

G^4 is selected from the group consisting of phenyl, biphenyl, terphenyl, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, and combinations thereof;

G^2, G^3, and G^5 are each independently selected from the group consisting of phenyl, biphenyl, terphenyl, fluorene, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, aza-fluorene, and combinations thereof;

G^2, G^3, G^4, and G^5 are each optionally further substituted with one or more unfused substituents selected from the group consisting of deuterium, alkyl, alkoxyl, cycloalkyl, cycloalkoxyl, halogen, nitro, nitrile, silyl, phenyl, biphenyl, terphenyl, pyridine, and combinations thereof;

m is an integer from 0 to 7,

n is an integer from 0 to 4;

when m or n is larger than 1, each G^4 or G^5 can be same or different;

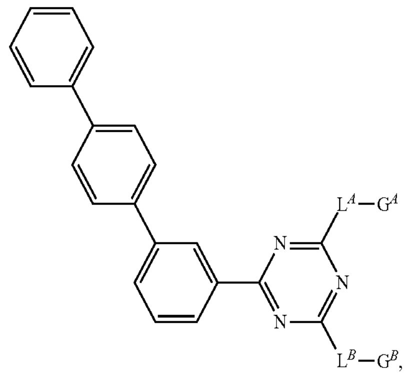
when n is 0, m is equal to or greater than 1, and each G^4 is selected from the group consisting of phenyl, and biphenyl;

when n is equal to or greater than 1, L^1 is not a direct bond; and

when m and n are both 0, L^1 is biphenyl.

According to another embodiment of the present disclosure, a composition of materials comprising a first compound having a structure of:

Formula III



is provided. In the structure of Formula III,

L^A and L^B are selected from a group consisting of direct bond, phenyl, biphenyl, pyridine, and combinations thereof;

G^A and G^B are selected from a group consisting of phenyl, biphenyl, pyridine, dibenzothiophene, dibenzofuran, dibenzoselenophene, and fluorene; and

G^A and G^B are each optionally further substituted with one or more unfused substituents selected from the group consisting of deuterium, alkyl, alkoxyl, cycloalkyl, cycloalkoxyl, halogen, nitro, nitrile, silyl, phenyl, biphenyl, terphenyl, pyridine, and combinations thereof.

According to another aspect of the present disclosure, a device that includes one or more organic light emitting devices is also provided. At least one of the one or more organic light emitting devices can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer can include a composition comprising a compound according to a structure of Formula I or Formula III, or any of the variations thereof described herein.

In yet another aspect of the present disclosure, a method for fabricating an organic light emitting device is provided. The organic light emitting device can include a first electrode, a second electrode, and a first organic layer disposed between the first electrode and the second electrode, where the first organic layer comprises a first composition comprising a mixture of a first compound and a second compound.

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 Formula I as disclosed herein.

FIG. **4** shows Formula II as disclosed herein.

FIG. **5** shows Formula III as disclosed herein.

FIG. **6** shows Formula IV as disclosed herein.

DETAILED DESCRIPTION

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

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

More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

FIG. **1** shows an organic light emitting device **100**. The figures are not necessarily drawn to scale. Device **100** may include a substrate **110**, an anode **115**, a hole injection layer **120**, a hole transport layer **125**, an electron blocking layer **130**, an emissive layer **135**, a hole blocking layer **140**, an electron transport layer **145**, an electron injection layer **150**, a protective layer **155**, a cathode **160**, and a barrier layer **170**. Cathode **160** is a compound cathode having a first conductive layer **162** and a second conductive layer **164**. Device **100** may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F_4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

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

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

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

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

Devices fabricated in accordance with embodiments of the present invention may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a mixture of a polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a "mixture", the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a non-polymeric material consists essentially of polymeric silicon and inorganic silicon.

Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of electronic component modules (or units) that can be incorporated into a variety of electronic products or intermediate components. Examples of such electronic products or intermediate components include display screens, lighting devices such as discrete light source devices or lighting panels, etc. that can be utilized by the end-user product manufacturers. Such electronic component modules can optionally include the driving electronics and/or power source(s). Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of consumer products that have one or more of the electronic component modules (or units) incorporated therein. Such consumer products would include any kind of products that include one or more light source(s) and/or one or more of some type of visual displays. Some examples of such consumer products include flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads-up displays, fully or partially transparent displays, flexible displays, laser printers, telephones, cell phones, tablets, phablets, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, 3-D displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.), but could be used outside this temperature range, for example, from −40 degree C. to +80 degree C.

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

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

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

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

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

The term "alkynyl" as used herein contemplates both straight and branched chain alkyne radicals. Preferred alkynyl groups are those containing two to fifteen carbon atoms.

Additionally, the alkynyl group may be optionally substituted.

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

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

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

The term "heteroaryl" as used herein contemplates single-ring hetero-aromatic groups that may include from one to three heteroatoms, for example, pyrrole, furan, thiophene, imidazole, oxazole, thiazole, triazole, pyrazole, pyridine, pyrazine and pyrimidine, and the like.

The term heteroaryl also includes polycyclic hetero-aromatic systems having two or more rings in which two atoms are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Additionally, the heteroaryl group may be optionally substituted.

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

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

The "aza" designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzothiophene, etc. means that one or more of the C—H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[f,h]quinoxaline and dibenzo[f,h]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein.

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

Often, the emissive layer (EML) of OLED devices exhibiting good lifetime and efficiency requires more than two components (e.g. 3 or 4 components). Fabricating such EMLs using vacuum thermal evaporation (VTE) process then requires evaporating 3 or 4 evaporation source materials in separate VTE sublimation crucibles, which is very complicated and costly compared to a standard two-component EML with a single host and an emitter, which requires only two evaporation sources.

Premixing two or more materials and evaporating them from one VTE sublimation crucible can reduce the complexity of the fabrication process. However, the co-evaporation must be stable and produce an evaporated film having a composition that remains constant through the evaporation process. Variations in the film's composition may adversely affect the device performance. In order to obtain a stable co-evaporation from a mixture of compounds under vacuum, one would assume that the materials must have the same evaporation temperature under the same condition. However, this may not be the only parameter one has to consider. When two compounds are mixed together, they may interact with each other and the evaporation property of the mixture may differ from their individual properties. On the other hand, materials with slightly different evaporation temperatures may form a stable co-evaporation mixture. Therefore, it is extremely difficult to achieve a stable co-evaporation mixture. So far, there have been very few stable co-evaporation mixture examples. "Evaporation temperature" of a material is measured in a vacuum deposition tool at a constant pressure, normally between 1×10^{-7} Torr to 1×10^{-8} Torr, at a 2 Å sec deposition rate on a surface positioned at a set distance away from the evaporation source of the material being evaporated, e.g. sublimation crucible in a VTE tool. The various measured values such as temperature, pressure, deposition rate, etc. disclosed herein are expected to have nominal variations because of the expected tolerances in the measurements that produced these quantitative values as understood by one of ordinary skill in the art.

Many factors other than temperature can contribute to the ability to achieve stable co-evaporation, such as the miscibility of the different materials and the phase transition temperatures of the different materials. The inventors found that when two materials have similar evaporation temperatures, and similar mass loss rate or similar vapor pressures, the two materials can co-evaporate consistently. "Mass loss rate" of a material is defined as the percentage of mass lost over time ("percentage/minute" or "%/min") and is determined by measuring the time it takes to lose the first 10% of the mass of a sample of the material as measured by thermal gravity analysis (TGA) under a given experimental condition at a given constant temperature for a given material after the a steady evaporation state is reached. The given constant temperature is one temperature point that is chosen so that the value of mass loss rate is between about 0.05 to 0.50%/min. A skilled person in this field should appreciate that in order to compare two parameters, the experimental condition should be consistent. The method of measuring mass loss rate and vapor pressure is well known in the art and can be found, for example, in Bull. et al. Mater. Sci. 2011, 34, 7.

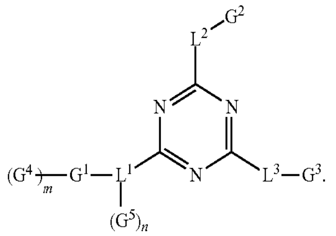
In the state of the art OLED devices, the EML may consist of three or more components. In one example, the EML can consist of two host-type compounds and an emitter combination (e.g. a hole transporting cohost (h-host), an electron transporting cohost (e-host), and a compound capable of functioning as an emitter in an OLED at room temperature). In another example, the EML can consist of one host-type compound and two emitter-type compounds (e.g., a host compound and two compounds each capable of functioning as an emitter in an OLED at room temperature). Conventionally, in order to fabricate such EMLs having three or more components using VTE process, three or more evaporation sources are required, one for each of the components. Because the concentration of the components are important for the device performance, typically, the rate of deposition of each component is measured individually during the deposition process. This makes the VTE process complicated and costly. Thus, it is desired to premix at least two of the components of such EMLs to reduce the number of VTE evaporation sources.

If any two of the three or more components of the EMLs can be premixed and form a stable mixture of co-evaporation source, then the number of evaporation sources required for EML layer fabrication would be reduced. In order for materials to be premixable into an evaporation source, they should co-evaporate and deposit uniformly without changing the ratio. The ratio of the components in the mixture should be the same as the ratio of the components in the evaporation deposited films from these premixed materials. Therefore, the concentration of the two components in the deposited film is controlled by their concentration in the premixed evaporation source.

This disclosure describes a new class of h- and e-hosts that can be premixed and stably co-evaporated from a single source.

According to one embodiment, a composition of materials comprising a first compound is disclosed. The first compound has a structure of formula:

Formula I



In Formula I:

G^1 is selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and fluorene;

L^1, L^2 and L^3 are each independently selected from the group consisting of direct bond, phenyl, biphenyl, terphenyl, pyridine, pyrimidine, and combinations thereof;

G^4 is selected from the group consisting of phenyl, biphenyl, terphenyl, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, and combinations thereof;

G^2, G^3, and G^5 are each independently selected from the group consisting of phenyl, biphenyl, terphenyl, fluorene, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, aza-fluorene, and combinations thereof;

G^2, G^3, G^4, and G^5 are each optionally further substituted with one or more unfused substituents selected from the group consisting of deuterium, alkyl, alkoxyl, cycloalkyl, cycloalkoxyl, halogen, nitro, nitrile, silyl, phenyl, biphenyl, terphenyl, pyridine, and combinations thereof;

m is an integer from 0 to 7,

n is an integer from 0 to 4;

when m or n is larger than 1, each G^4 or G^5 can be same or different;

when n is 0, m is equal to or greater than 1, and each G^4 is selected from the group consisting of phenyl, and biphenyl;

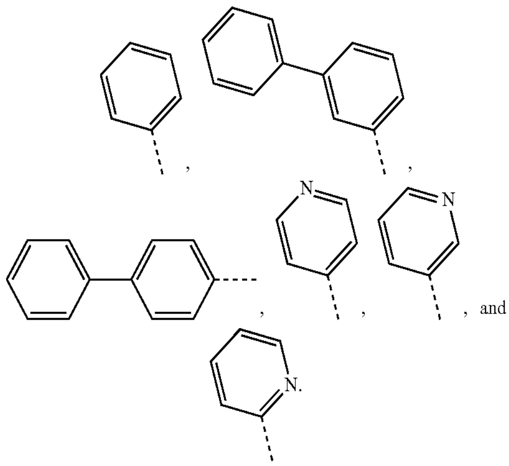
when n is equal to or greater than 1, L^1 is not a direct bond; and

when m and n are both 0, L^1 is biphenyl.

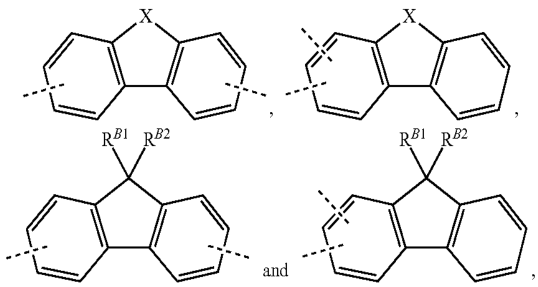
In some embodiments, one or more of L^1, L^2 and L^3 can be a direct bond, and the direct bond can be a single bond or a double bond. When L^1 is a direct bond, n=0.

In some embodiments, n is 0, while n is equal to or greater than 1 in other embodiments. In some embodiments, m and n are both 0. In some embodiments, m is equal to or greater than 1.

In some embodiments, G^4 has the structure selected from the group consisting of:



In some embodiments, G^1 has the structure selected from the group consisting of:



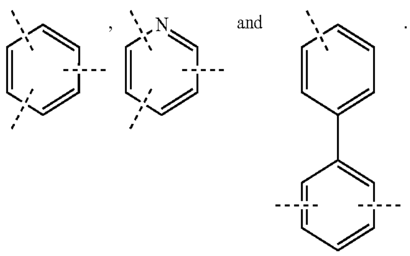
wherein:

X is selected from a group consisting of O, S and Se;

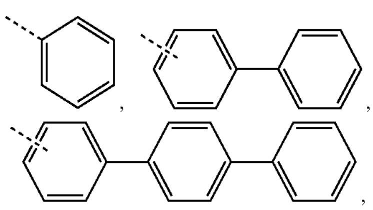
R^{B1} and R^{B2} are independently selected from a group consisting of hydrogen, deuterium, alkyl, cycloalkyl, alkoxyl, aryl, heteraryl, halogen, and combinations thereof; and

R^{B1} and R^{B2} are optionally joined to form a ring.

In some embodiments, L^1 is selected from the group consisting of:



In some embodiments, G^2, G^3 and G^5 are independently selected from the group consisting of:



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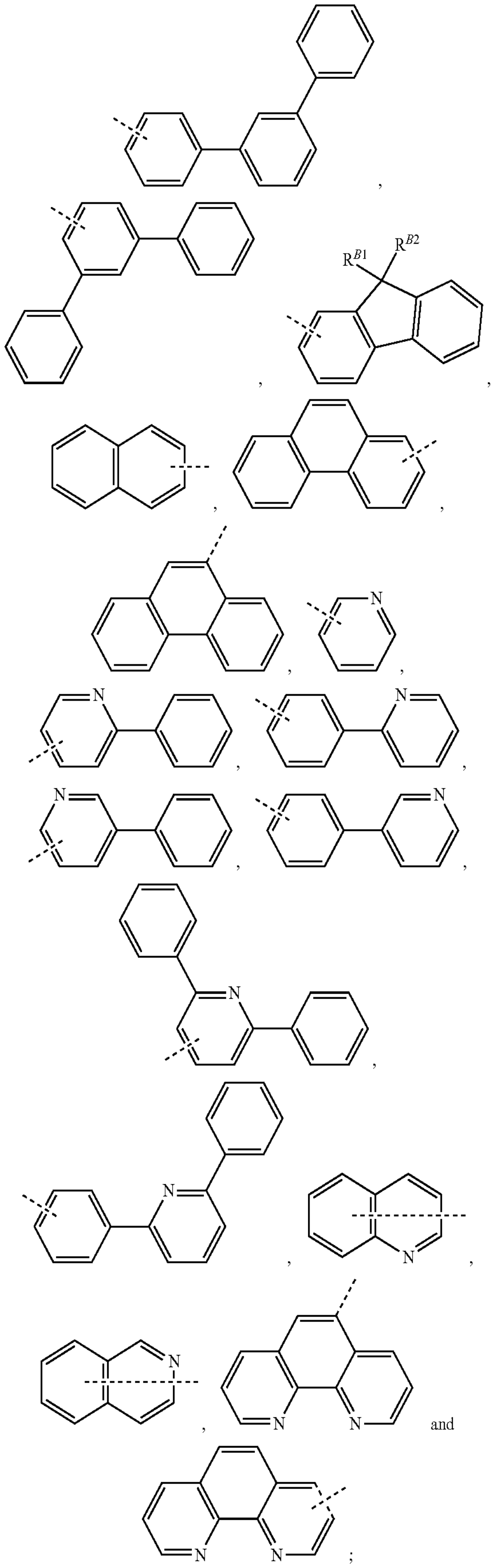


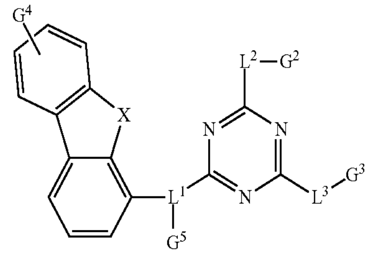
wherein

R^{B1} and R^{B2} are independently selected from a group consisting of hydrogen, deuterium, alkyl, cycloalkyl, alkoxyl, aryl, heteraryl, halogen, and combinations thereof; and

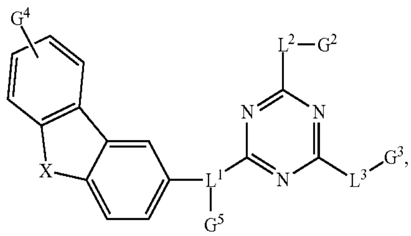
R^{B1} and R^{B2} are optionally joined to form a ring.

In some embodiments, at least one of G^2, G^3, G^4 and G^5 is substituted with at least one fluorine atom.

In some embodiments, the first compound has the formula:



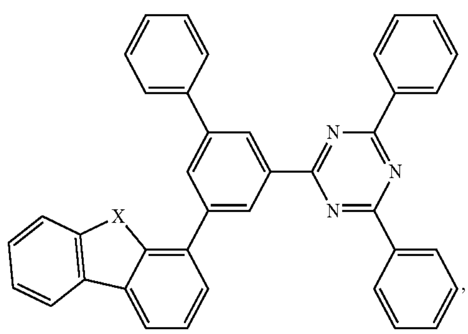
or



where X is selected from a group consisting of O, S and Se.

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

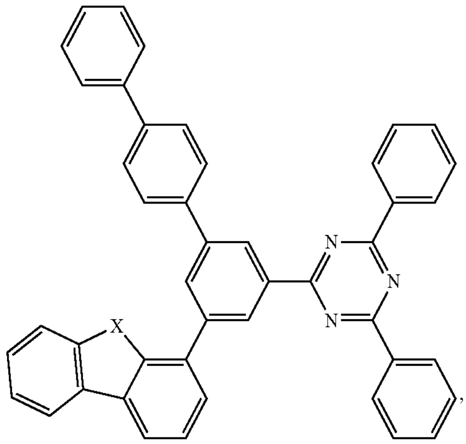
Compound A1 through A3, each represented by the formula



wherein in Compound A1: X = O,
in Compound A2: X = S,
in Compound A3: X = Se

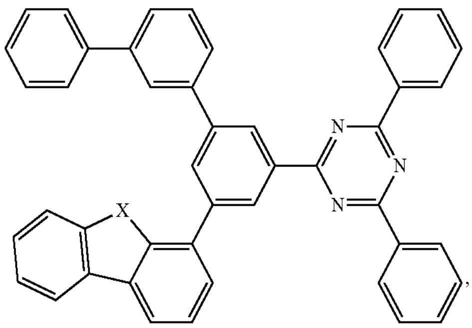
-continued

Compound A4 through A6, each represented by the formula



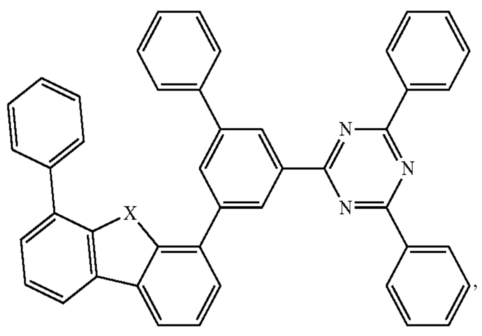
wherein in Compound A4: X = O,
in Compound A5: X = S,
in Compound A6: X = Se

Compound A7 through A9, each represented by the formula



wherein in Compound A7: X = O,
in Compound A8: X = S,
in Compound A9: X = Se

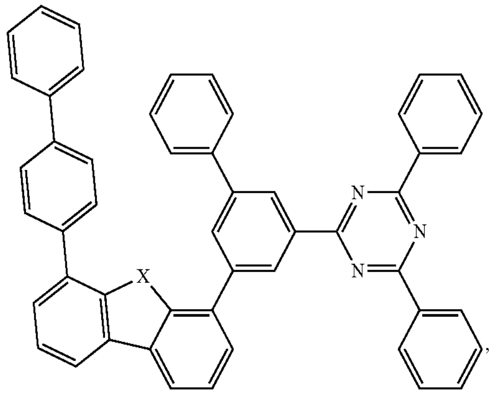
Compound A10 through A12, each represented by the formula



wherein in Compound A10: X = O,
in Compound A11: X = S,
in Compound A12: X = Se

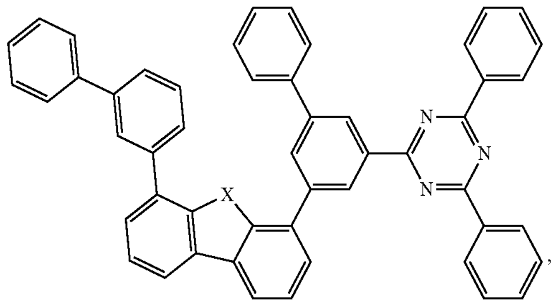
-continued

Compound A13 through A15, each represented by the formula



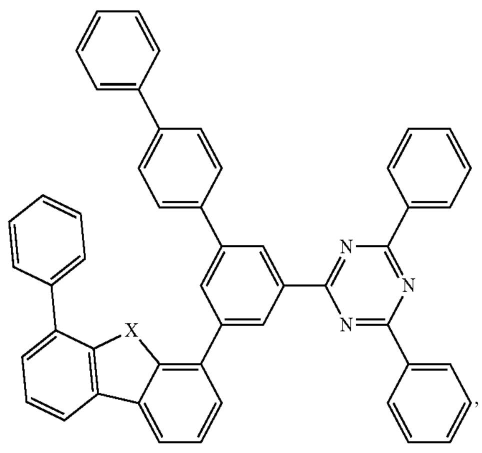
wherein in Compound A13: X = O,
in Compound A14: X = S,
in Compound A15: X = Se

Compound A16 through A18, each represented by the formula



wherein in Compound A16: X = O,
in Compound A17: X = S,
in Compound A18: X = Se

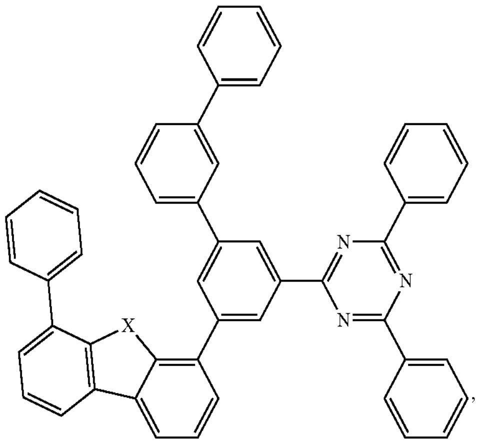
Compound A19 through A21, each represented by the formula



wherein in Compound A19: X = O,
in Compound A20: X = S,
in Compound A21: X = Se

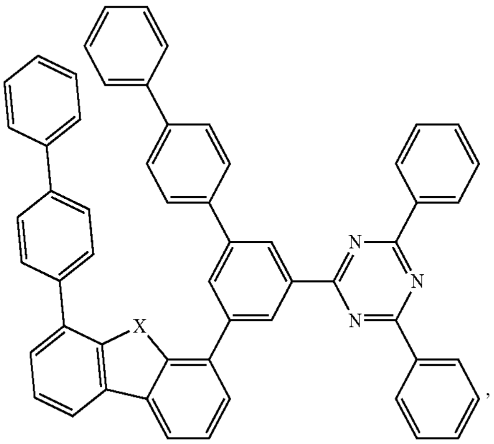
-continued

Compound A22 through A24, each represented by the formula



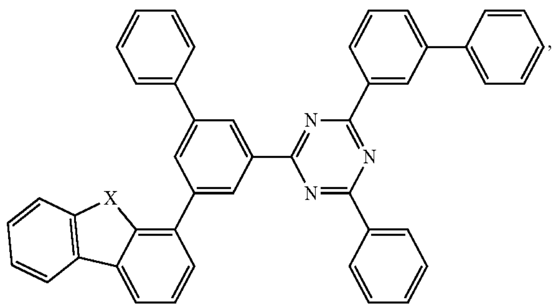
wherein in Compound A22: X = O,
in Compound A23: X = S,
in Compound A24: X = Se

Compound A25 through A27, each represented by the formula



wherein in Compound A25: X = O,
in Compound A26: X = S,
in Compound A27: X = Se

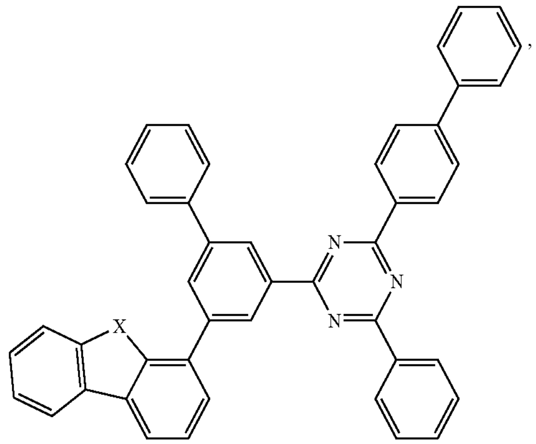
Compound A28 through A30, each represented by the formula



wherein in Compound A28: X = O,
in Compound A29: X = S,
in Compound A30: X = Se

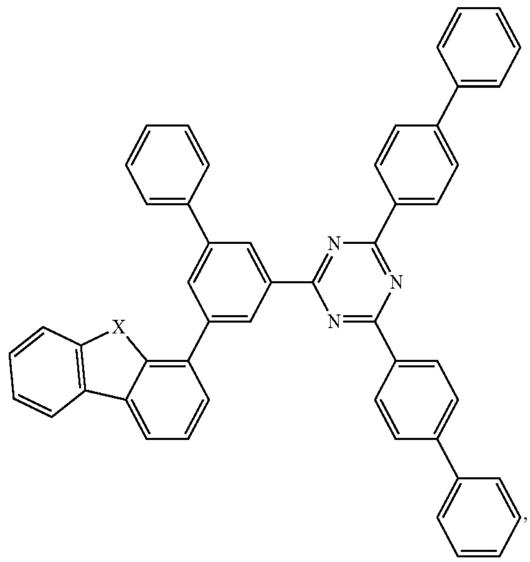
-continued

Compound A31 through A33, each represented by the formula



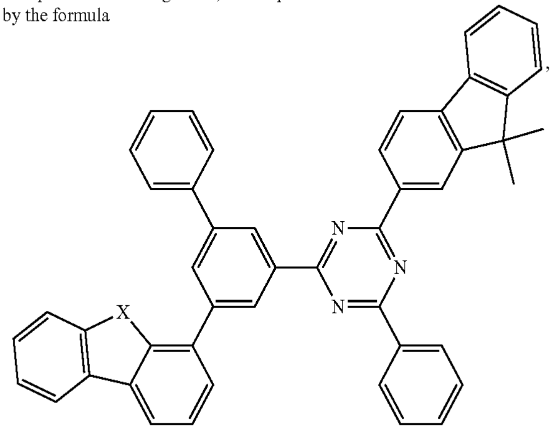
wherein in Compound A31: X = O,
in Compound A32: X = S,
in Compound A33: X = Se

Compound A34 through A36, each represented by the formula



wherein in Compound A34: X = O,
in Compound A35: X = S,
in Compound A36: X = Se

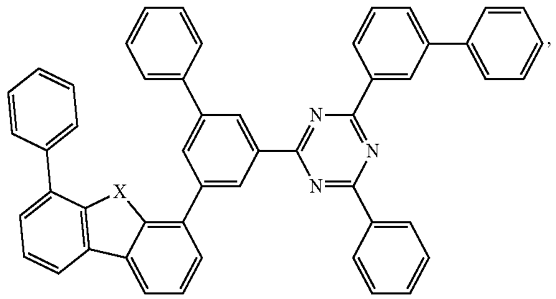
Compound A37 through A39, each represented by the formula



wherein in Compound A37: X = O,
in Compound A38: X = S,
in Compound A39: X = Se

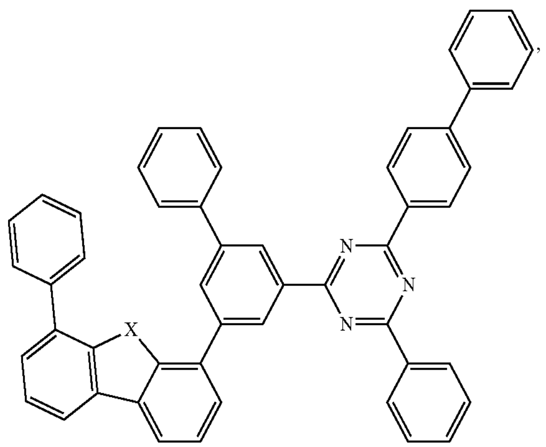
-continued

Compound A40 through A42, each represented by the formula



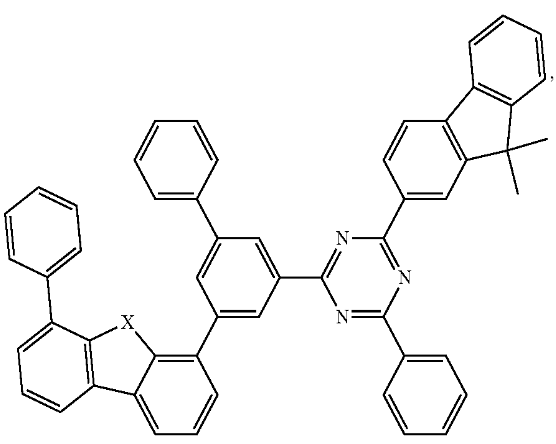
wherein in Compound A40: X = O,
in Compound A41: X = S,
in Compound A42: X = Se

Compound A43 through A45, each represented by the formula



wherein in Compound A43: X = O,
in Compound A44: X = S,
in Compound A45: X = Se

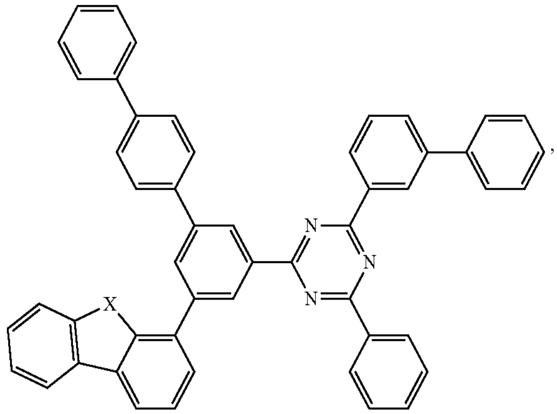
Compound A46 through A48, each represented by the formula



wherein in Compound A46: X = O,
in Compound A47: X = S,
in Compound A48: X = Se

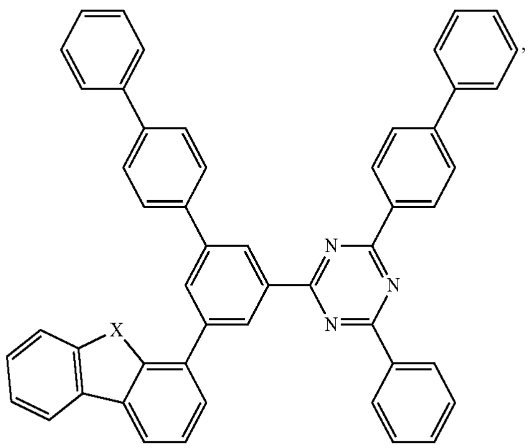
-continued

Compound A49 through A51, each represented by the formula



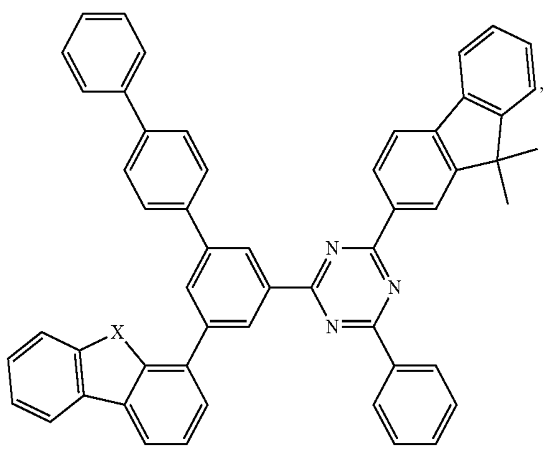
wherein in Compound A49: X = O,
in Compound A50: X = S,
in Compound A51: X = Se

Compound A52 through A54, each represented by the formula



wherein in Compound A52: X = O,
in Compound A53: X = S,
in Compound A54: X = Se

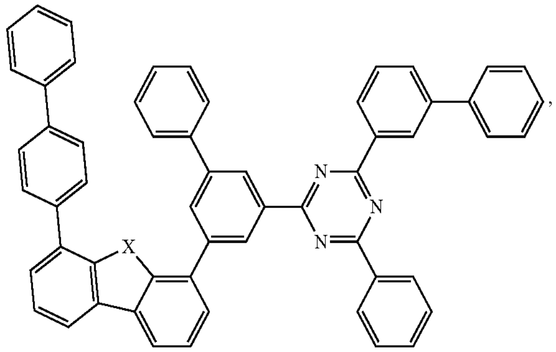
Compound A55 through A57, each represented by the formula



wherein in Compound A55: X = O,
in Compound A56: X = S,
in Compound A57: X = Se

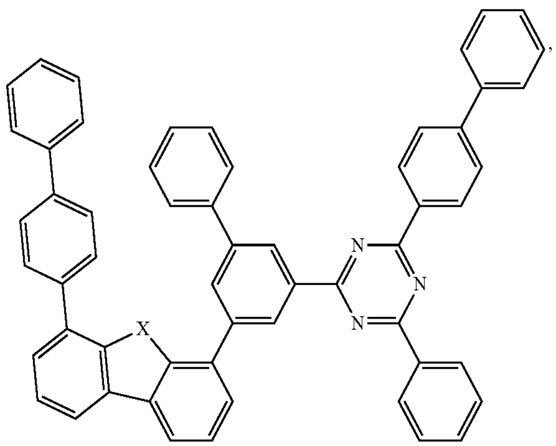
-continued

Compound A58 through A60, each represented by the formula



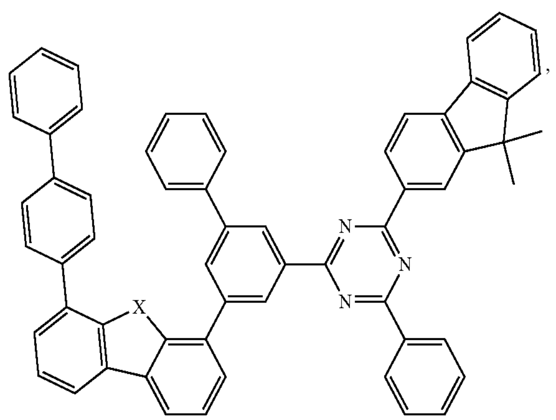
wherein in Compound A58: X = O, in Compound A59: X = S, in Compound A60: X = Se

Compound A61 through A63, each represented by the formula



wherein in Compound A61: X = O, in Compound A62: X = S, in Compound A63: X = Se

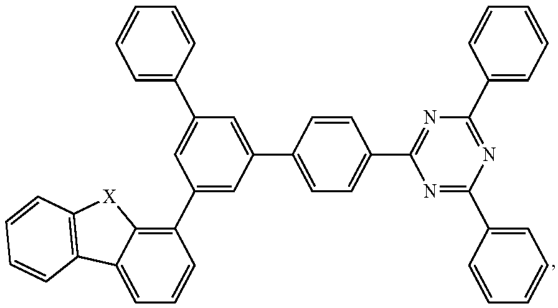
Compound A64 through A66, each represented by the formula



wherein in Compound A64: X = O, in Compound A65: X = S, in Compound A66: X = Se

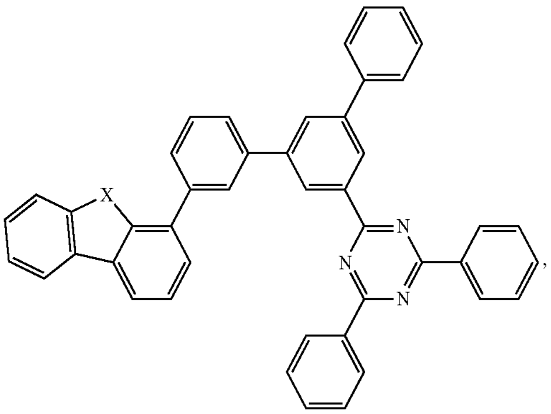
-continued

Compound A67 through A69, each represented by the formula



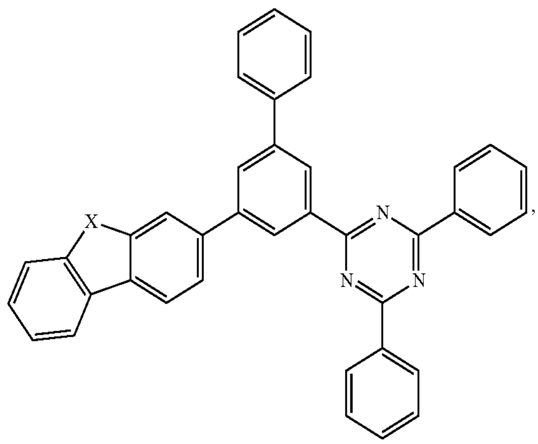
wherein in Compound A67: X = O, in Compound A68: X = S, in Compound A69: X = Se

Compound A70 through A72, each represented by the formula



wherein in Compound A70: X = O, in Compound A71: X = S, in Compound A72: X = Se

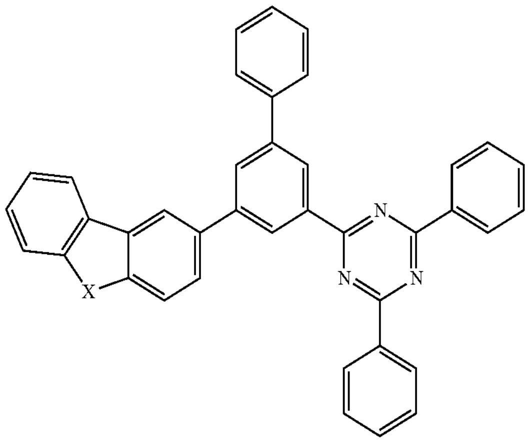
Compound A73 through A75, each represented by the formula



wherein in Compound A73: X = O, in Compound A74: X = S, in Compound A75: X = Se

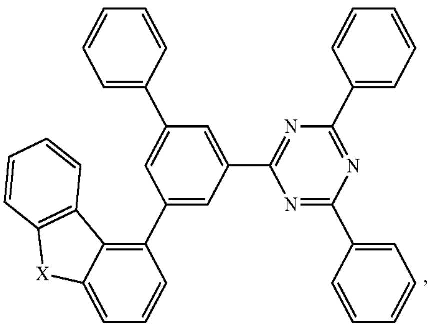
-continued

Compound A76 through A78, each represented by the formula



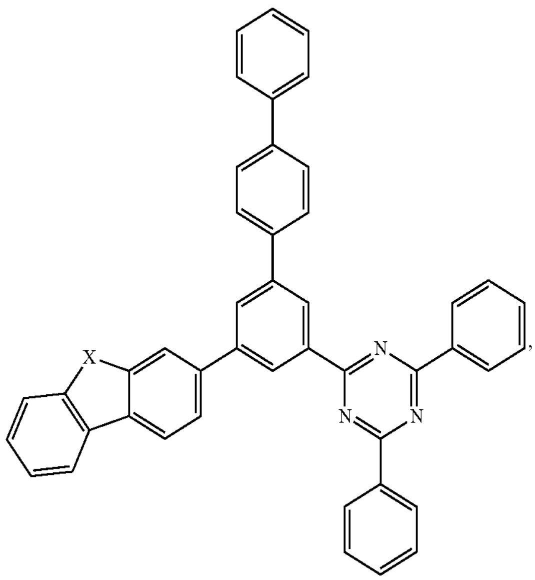
wherein in Compound A76: X = O,
in Compound A77: X = S,
in Compound A78: X = Se

Compound A79 through A81, each represented by the formula



wherein in Compound A79: X = O,
in Compound A80: X = S,
in Compound A81: X = Se

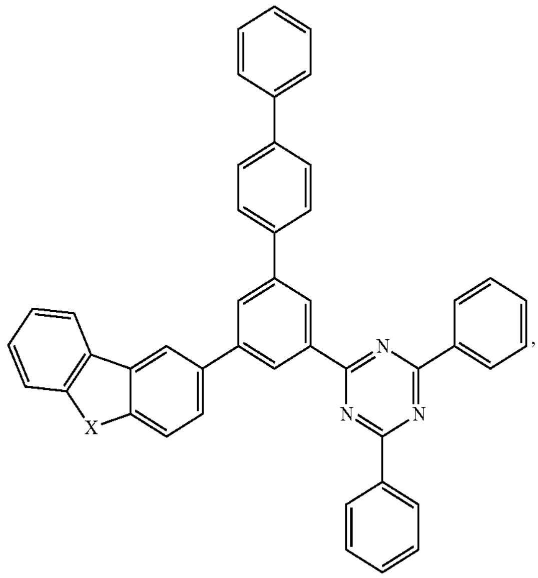
Compound A82 through A84, each represented by the formula



wherein in Compound A82: X = O,
in Compound A83: X = S,
in Compound A84: X = Se

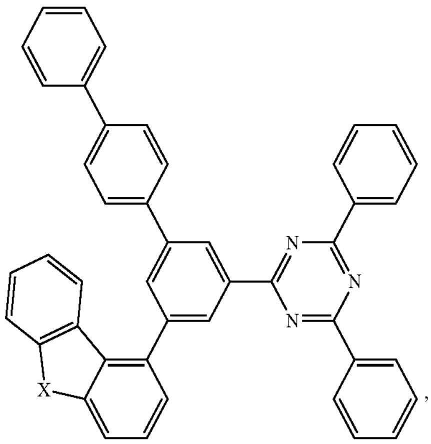
-continued

Compound A85 through A87, each represented by the formula



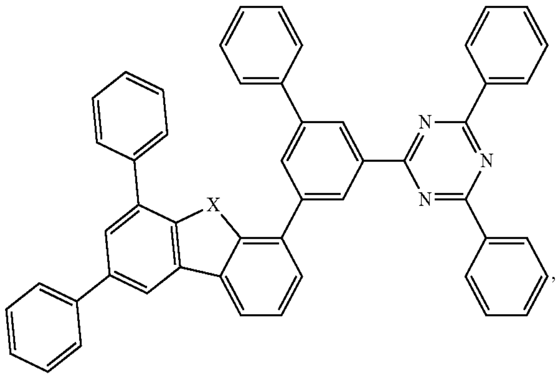
wherein in Compound A85: X = O,
in Compound A86: X = S,
in Compound A87: X = Se

Compound A88 through A90, each represented by the formula



wherein in Compound A88: X = O,
in Compound A89: X = S,
in Compound A90: X = Se

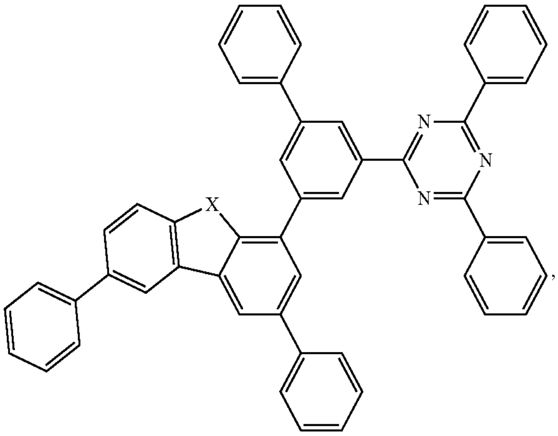
Compound A91 through A93, each represented by the formula



wherein in Compound A91: X = O,
in Compound A92: X = S,
in Compound A93: X = Se

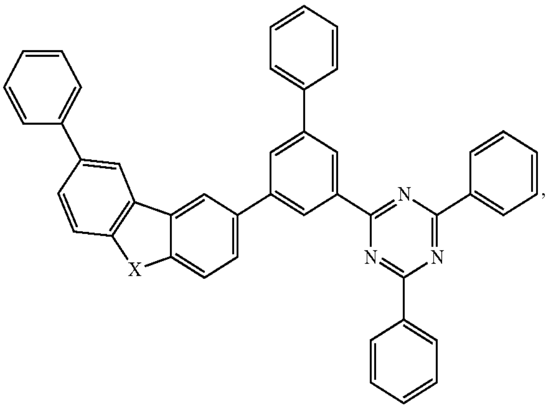
-continued

Compound A94 through A96, each represented by the formula



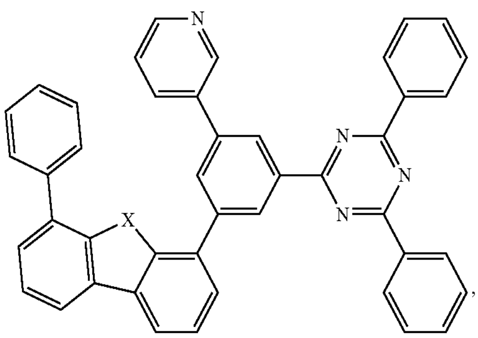
wherein in Compound A94: X = O,
in Compound A95: X = S,
in Compound A96: X = Se

Compound A97 through A99, each represented by the formula



wherein in Compound A97: X = O,
in Compound A98: X = S,
in Compound A99: X = Se

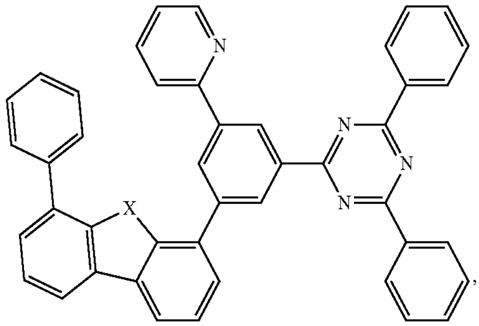
Compound A100 through A102, each represented by the formula



wherein in Compound A100: X = O,
in Compound A101: X = S,
in Compound A102: X = Se

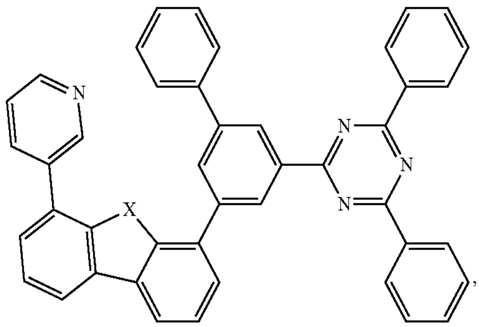
-continued

Compound A103 through A105, each represented by the formula



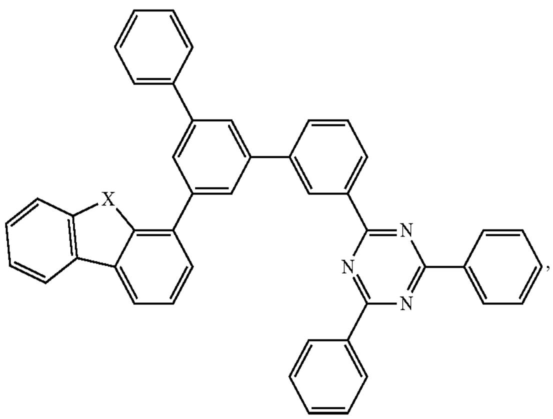
wherein in Compound A103: X = O,
in Compound A104: X = S,
in Compound A105: X = Se

Compound A106 through A108, each represented by the formula



wherein in Compound A106: X = O,
in Compound A107: X = S,
in Compound A108: X = Se

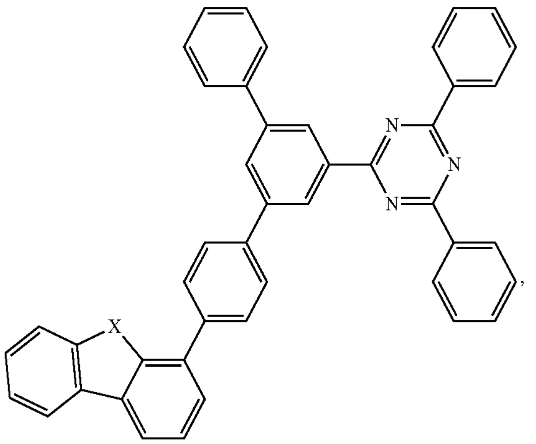
Compound A109 through A111, each represented by the formula



wherein in Compound A109: X = O,
in Compound A110: X = S,
in Compound A111: X = Se

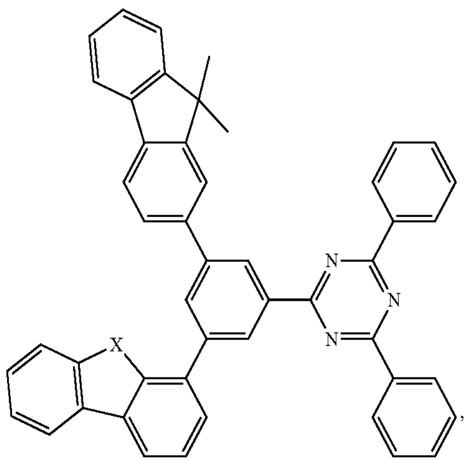
-continued

Compound A112 through A114, each represented by the formula



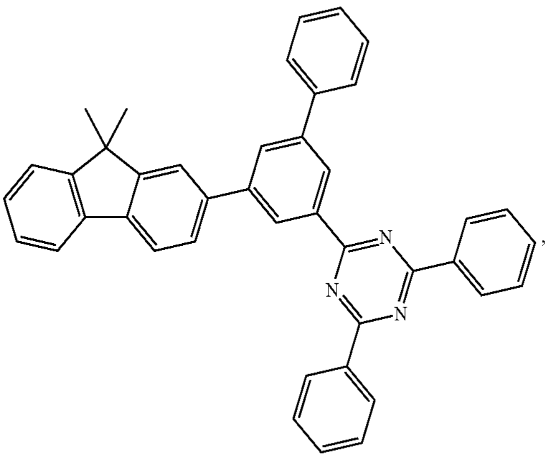
wherein in Compound A112: X = O,
in Compound A113: X = S,
in Compound A114: X = Se

Compound A115 through A117, each represented by the formula



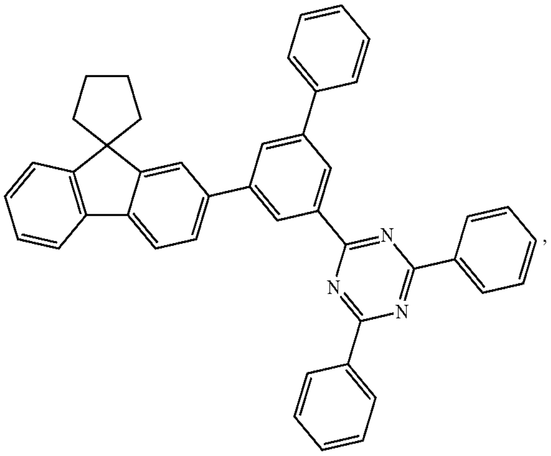
wherein in Compound A115: X = O,
in Compound A116: X = S,
in Compound A117: X = Se

Compound B1

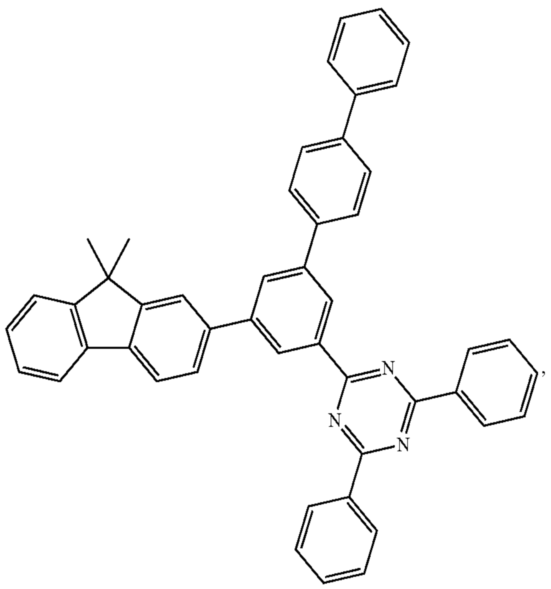


-continued

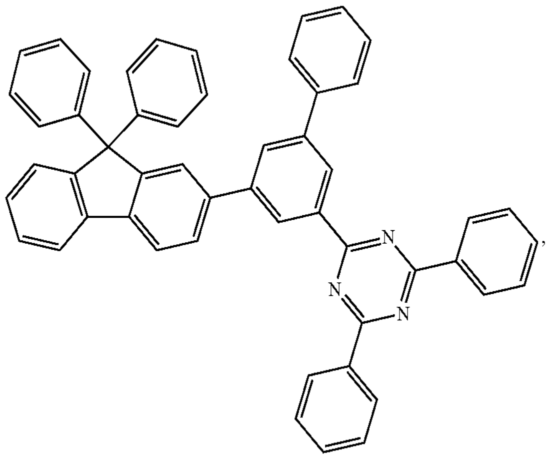
Compound B2



Compound B3

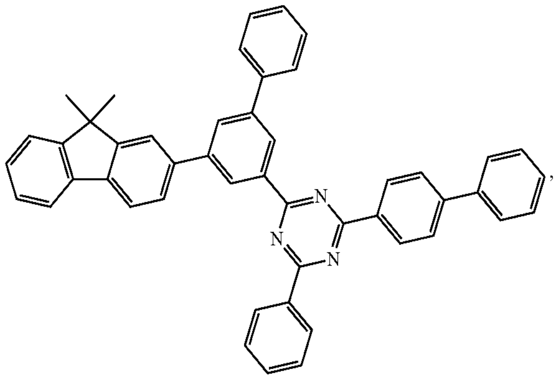


Compound B4

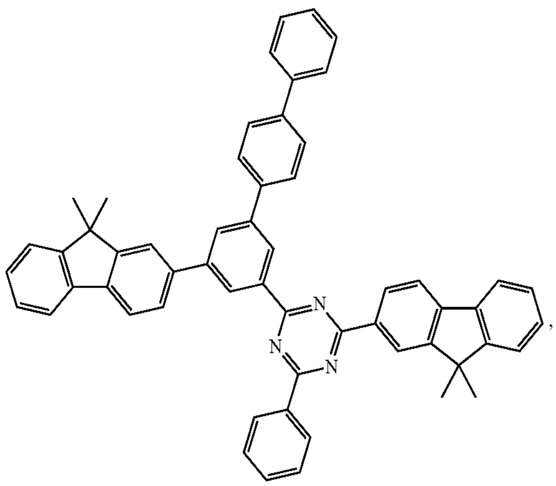


-continued

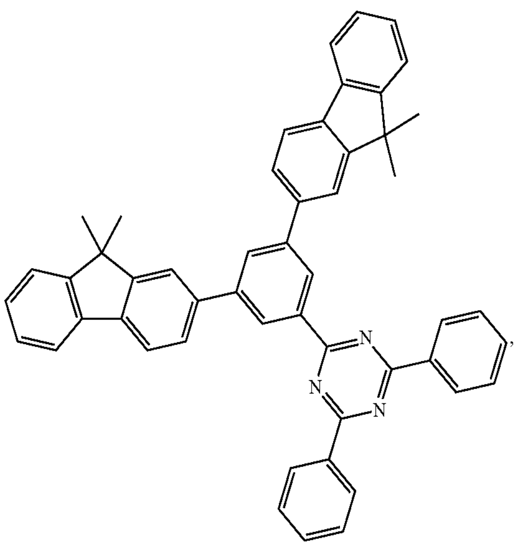
Compound B5



Compound B6



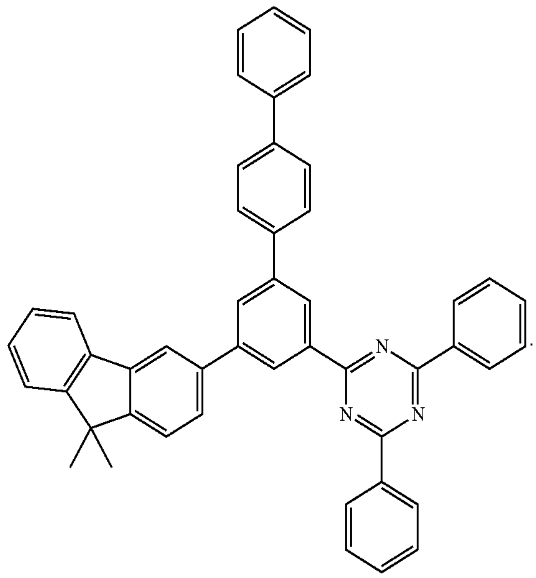
Compound B7



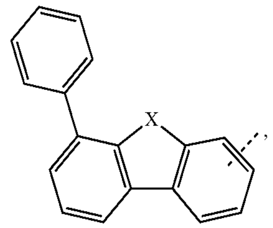
and

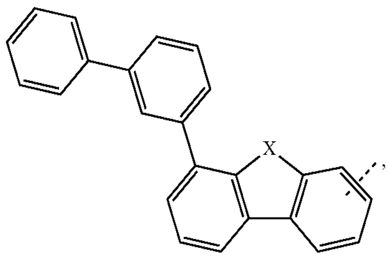
-continued

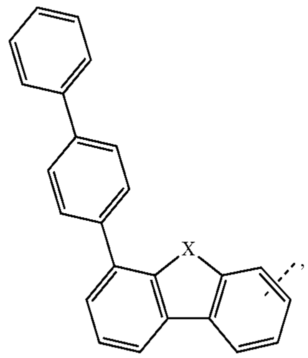
Compound B8

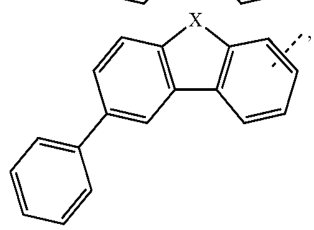


In some embodiments, n is 0, m is 1, and G^4-G^1 has a structure selected from the group consisting of:









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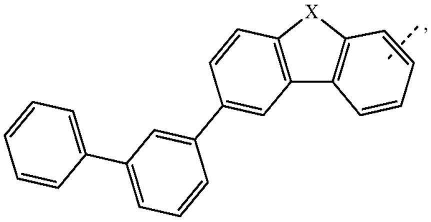
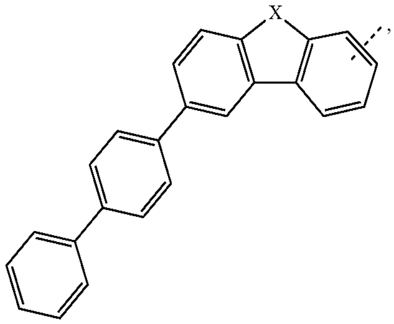
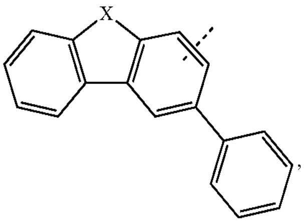
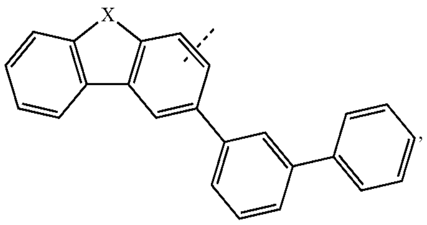
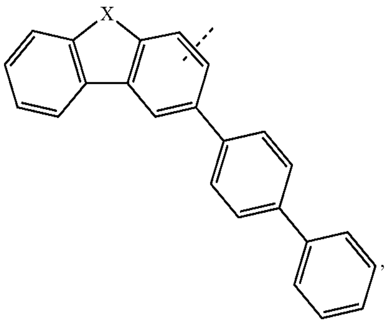
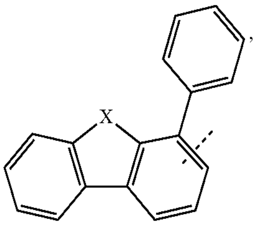


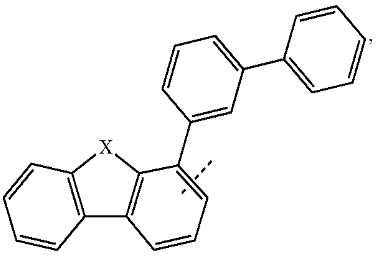






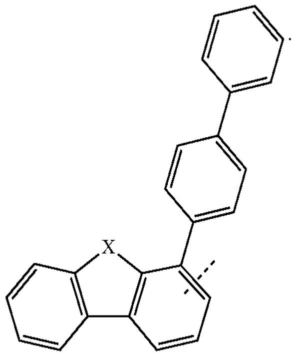






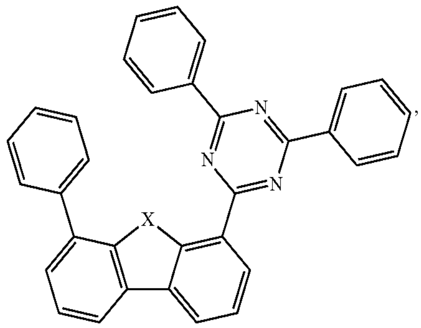
and

-continued



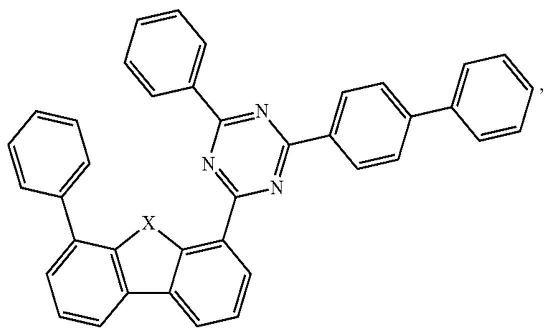
In some embodiments, the first compound is selected from the group consisting of:

Compound C1 through C3, each represented by the formula



wherein in Compound C1: X = O,
in Compound C2: X = S,
in Compound C3: X = Se

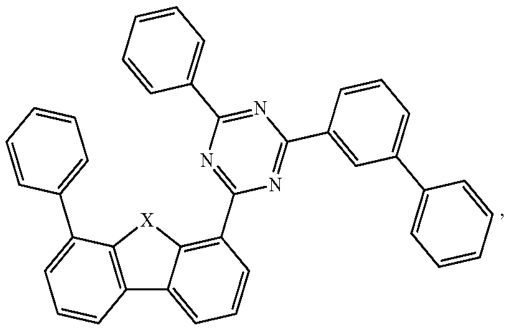
Compound C4 through C6, each represented by the formula



wherein in Compound C4: X = O,
in Compound C5: X = S,
in Compound C6: X = Se

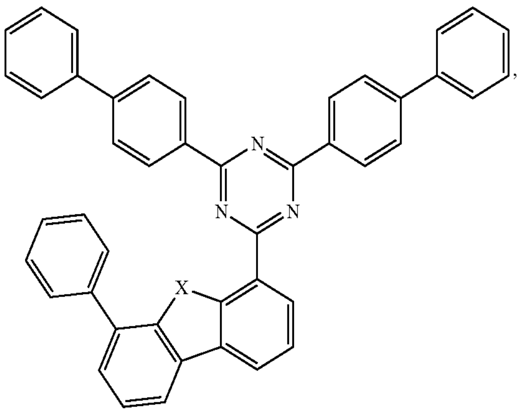
-continued

Compound C7 through C9, each represented by the formula



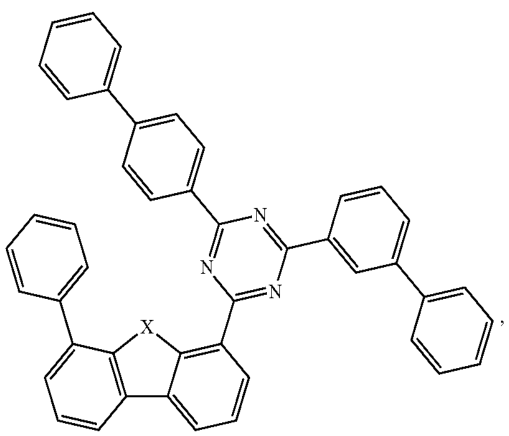
wherein in Compound C7: X = O,
in Compound C8: X = S,
in Compound C9: X = Se

Compound C10 through C12, each represented by the formula



wherein in Compound C10: X = O,
in Compound C11: X = S,
in Compound C12: X = Se

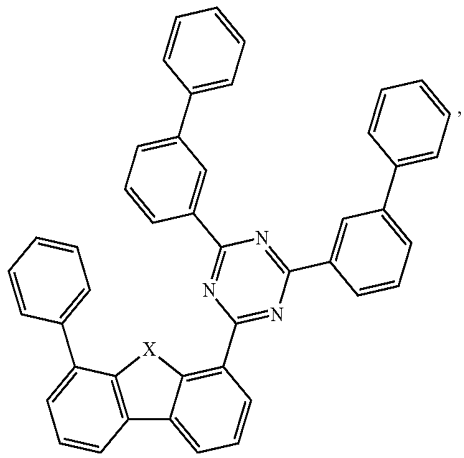
Compound C13 through C16, each represented by the formula



wherein in Compound C13: X = O,
in Compound C14: X = S,
in Compound C15: X = Se

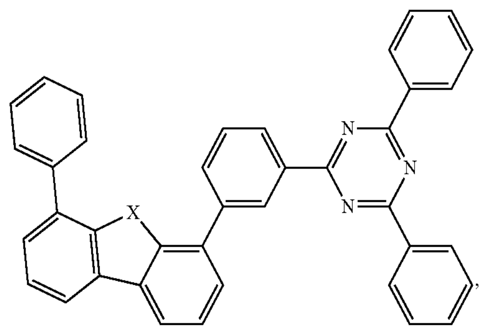
-continued

Compound C16 through C18, each represented by the formula



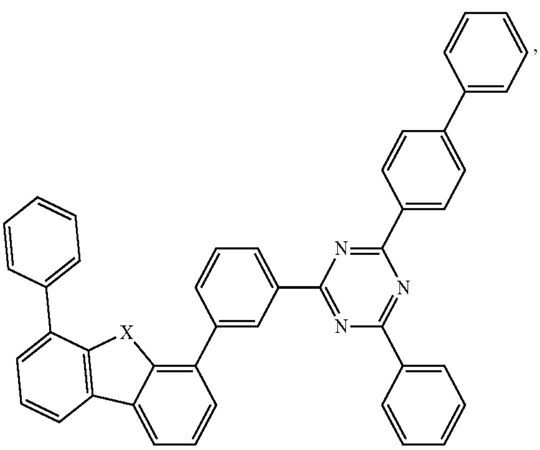
wherein in Compound C16: X = O,
in Compound C17: X = S,
in Compound C18: X = Se

Compound C19 through C21, each represented by the formula



wherein in Compound C19: X = O,
in Compound C20: X = S
in Compound C21: X = Se

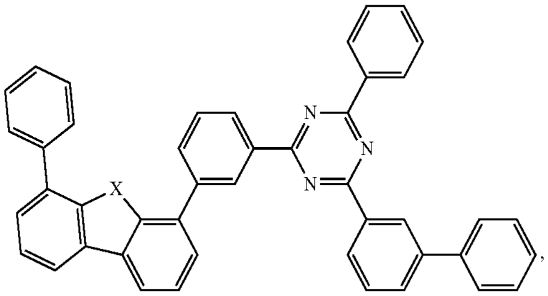
Compound C22 through C24, each represented by the formula



wherein in Compound C22: X = O,
in Compound C23: X = S
in Compound C24: X = Se

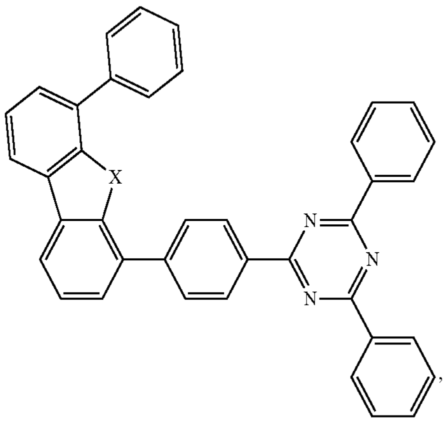
-continued

Compound C25 through C27, each represented by the formula



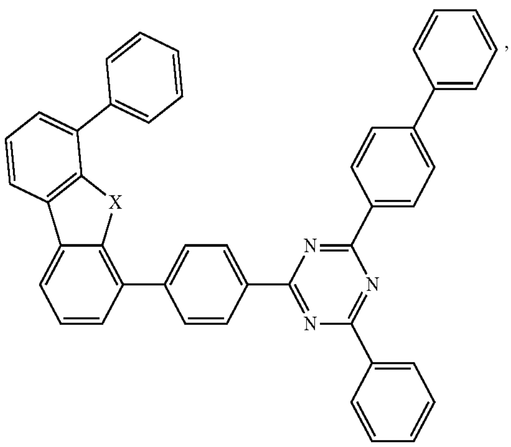
wherein in Compound C25: X = O,
in Compound C26: X = S
in Compound C27: X = Se

Compound C28 through C30, each represented by the formula



wherein in Compound C28: X = O,
in Compound C29: X = S
in Compound C30: X = Se

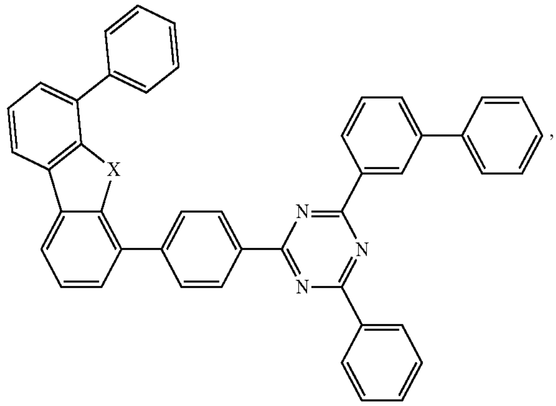
Compound C31 through C33, each represented by the formula



wherein in Compound C31: X = O,
in Compound C32: X = S
in Compound C33: X = Se

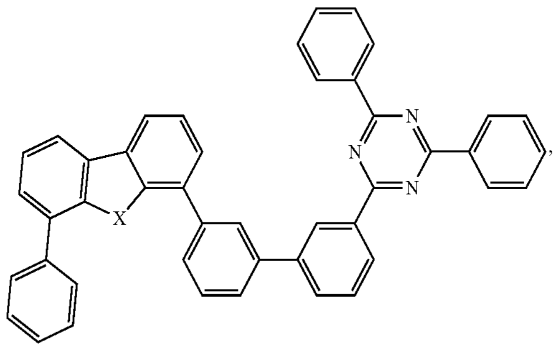
-continued

Compound C34 through C36, each represented by the formula



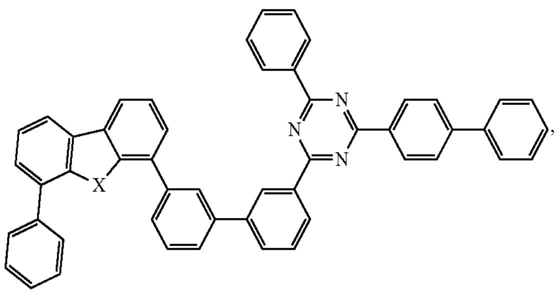
wherein in Compound C34: X = O,
in Compound C35: X = S
in Compound C36: X = Se

Compound C37 through C39, each represented by the formula



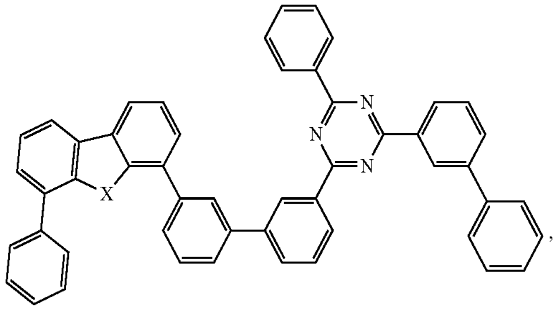
wherein in Compound C37: X = O,
in Compound C38: X = S
in Compound C39: X = Se

Compound C40 through C42, each represented by the formula



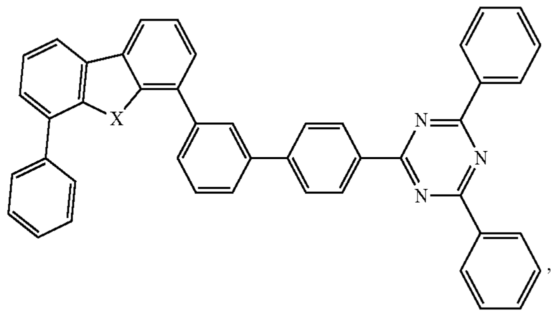
wherein in Compound C40: X = O,
in Compound C41: X = S
in Compound C42: X = Se

Compound C43 through C45, each represented by the formula



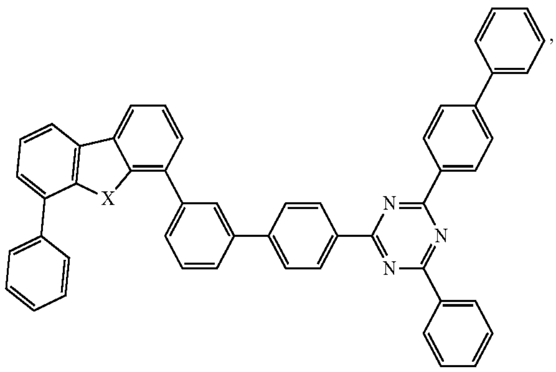
wherein in Compound C43: X = O,
in Compound C44: X = S
in Compound C45: X = Se

Compound C46 through C48, each represented by the formula



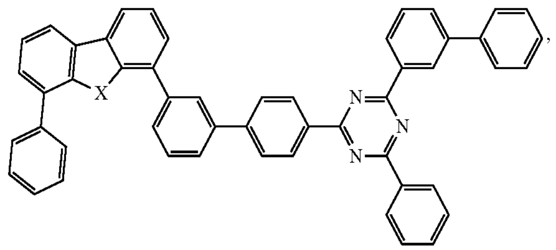
wherein in Compound C46: X = O,
in Compound C47: X = S
in Compound C48: X = Se

Compound C49 through C51, each represented by the formula



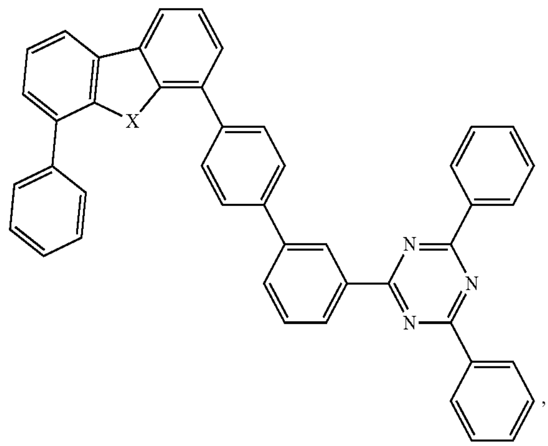
wherein in Compound C49: X = O,
in Compound C50: X = S
in Compound C51: X = Se

Compound C52 through C54, each represented by the formula



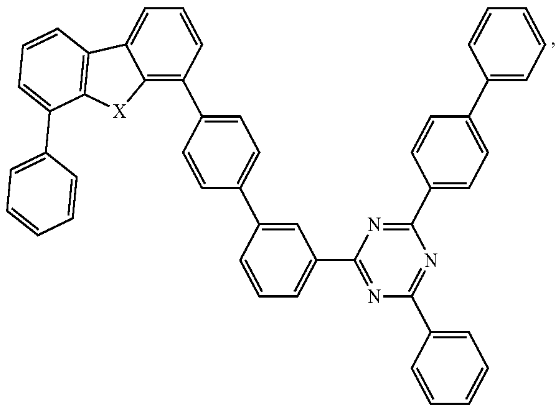
wherein in Compound C52: X = O,
in Compound C53: X = S
in Compound C54: X = Se

Compound C55 through C57, each represented by the formula



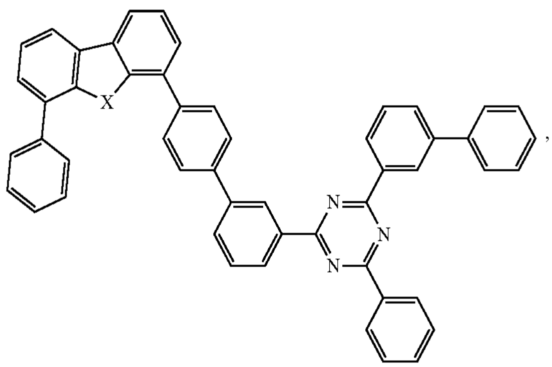
wherein in Compound C55: X = O,
in Compound C56: X = S
in Compound C57: X = Se

Compound C58 through C60, each represented by the formula



wherein in Compound C58: X = O,
in Compound C59: X = S
in Compound C60: X = Se

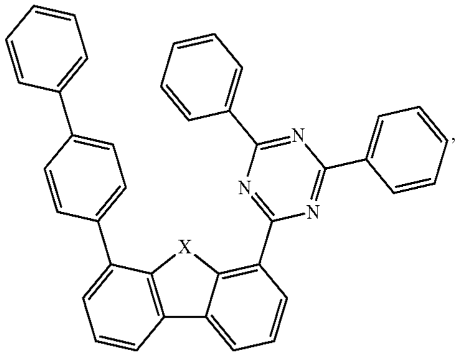
Compound C61 through C63, each represented by the formula



wherein in Compound C61: X = O,
in Compound C62: X = S
in Compound C63: X = Se

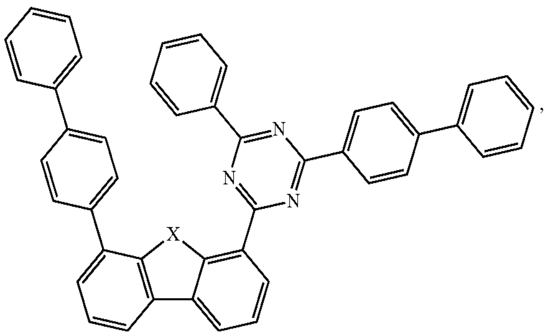
-continued

Compound C64 through C66, each represented by the formula



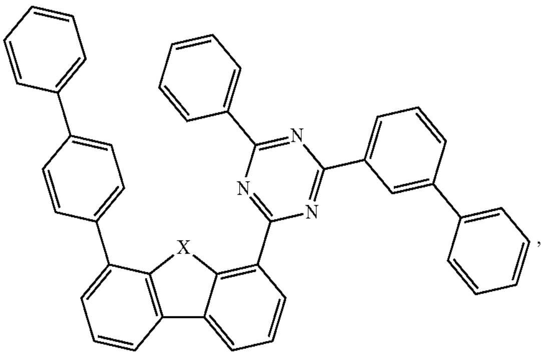
wherein in Compound C64: X = O,
in Compound C65: X = S,
in Compound C66: X = Se

Compound C67 through C69, each represented by the formula



wherein in Compound C67: X = O,
in Compound C68: X = S,
in Compound C69: X = Se

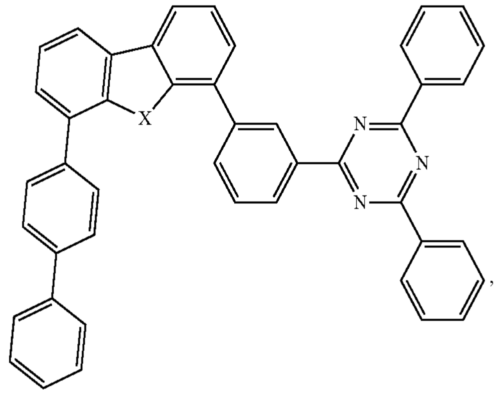
Compound C70 through C72, each represented by the formula



wherein in Compound C70: X = O,
in Compound C71: X = S,
in Compound C72: X = Se

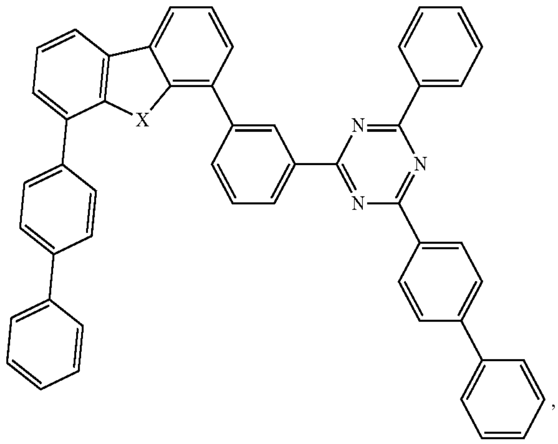
-continued

Compound C73 through C75, each represented by the formula



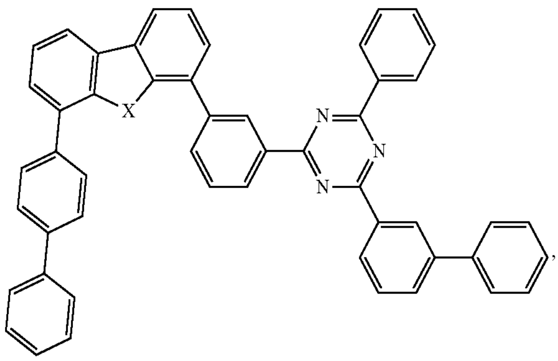
wherein in Compound C73: X = O,
in Compound C74: X = S
in Compound C75: X = Se

Compound C76 through C78, each represented by the formula



wherein in Compound C76: X = O,
in Compound C77: X = S
in Compound C78: X = Se

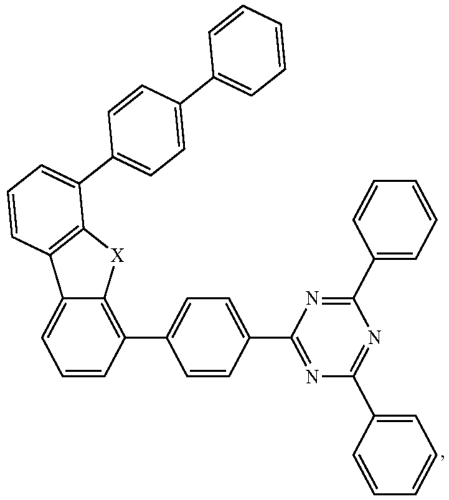
Compound C79 through C81, each represented by the formula



wherein in Compound C79: X = O,
in Compound C80: X = S
in Compound C81: X = Se

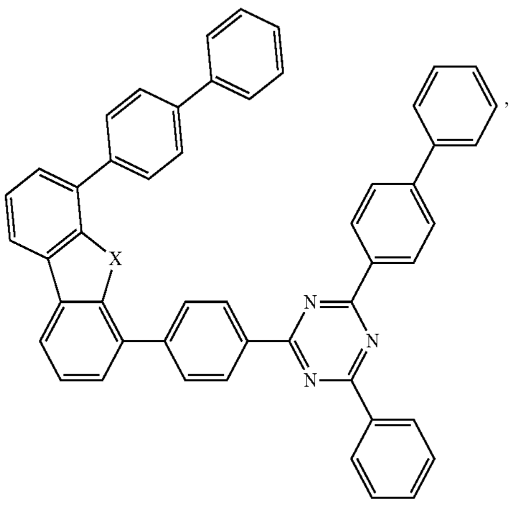
-continued

Compound C82 through C84, each represented by the formula



wherein in Compound C82: X = O,
in Compound C83: X = S
in Compound C84: X = Se

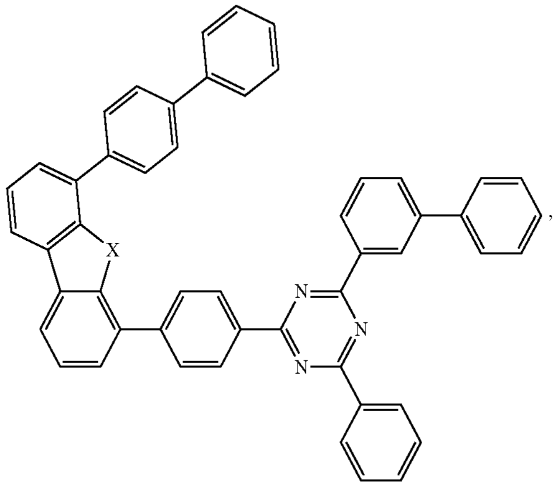
Compound C85 through C87, each represented by the formula



wherein in Compound C85: X = O,
in Compound C86: X = S
in Compound C87: X = Se

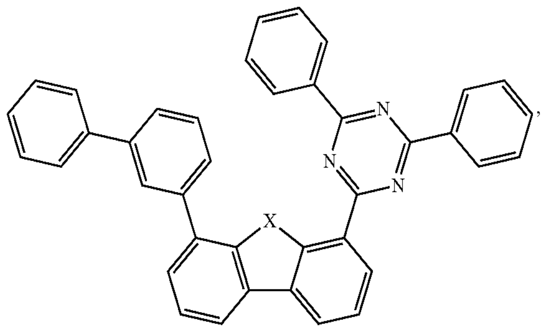
-continued

Compound C88 through C90, each represented by the formula



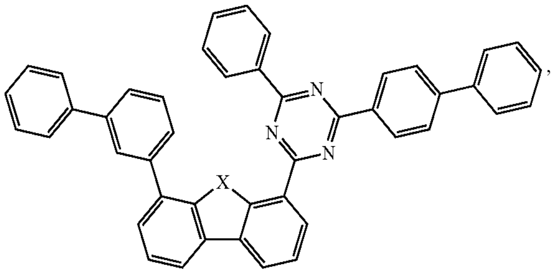
wherein in Compound C88: X = O,
in Compound C89: X = S
in Compound C90: X = Se

Compound C91 through C93, each represented by the formula



wherein in Compound C91: X = O,
in Compound C92: X = S,
in Compound C93: X = Se

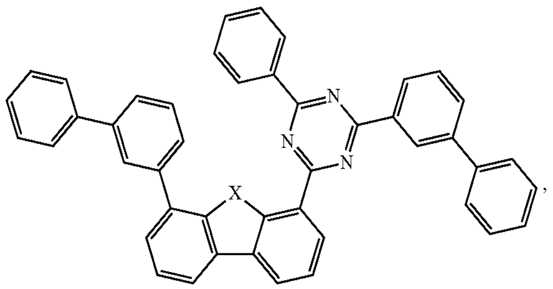
Compound C94 through C96, each represented by the formula



wherein in Compound C94: X = O,
in Compound C95: X = S,
in Compound C96: X = Se

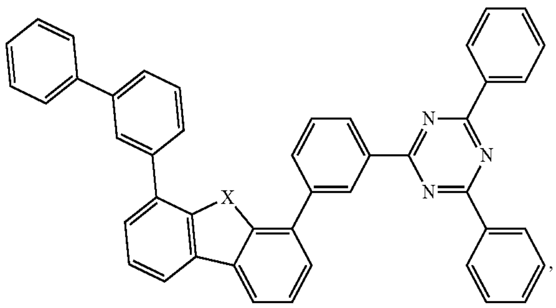
-continued

Compound C97 through C99, each represented by the formula



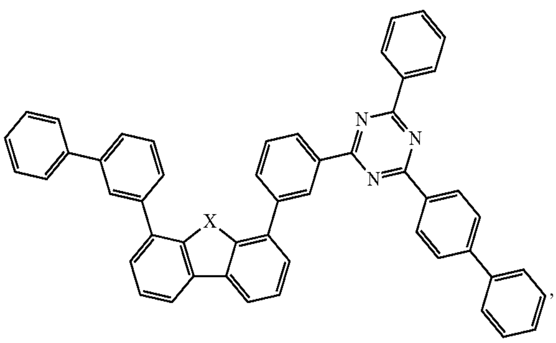
wherein in Compound C97: X = O,
in Compound C98: X = S,
in Compound C99: X = Se

Compound C100 through C102, each represented by the formula



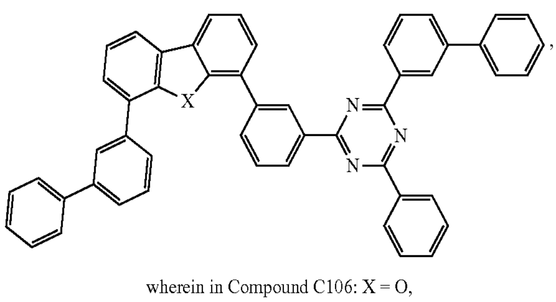
wherein in Compound C100: X = O,
in Compound C101: X = S
in Compound C1021: X = Se

Compound C103 through C105, each represented by the formula



wherein in Compound C103: X = O,
in Compound C104: X = S,
in Compound C105: X = Se

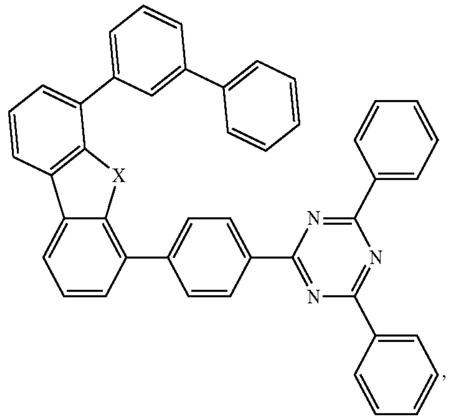
Compound C106 through C108, each represented by the formula



wherein in Compound C106: X = O,
in Compound C107: X = S,
in Compound C108: X = Se

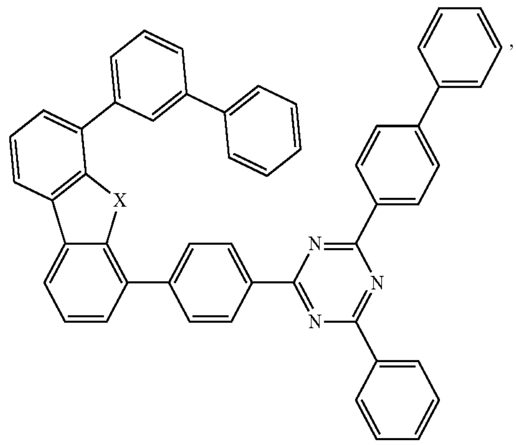
-continued

Compound C109 through C111, each represented by the formula



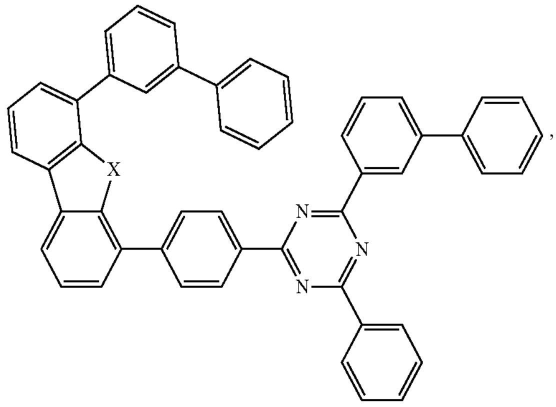
wherein in Compound C109: X = O,
in Compound C110: X = S
in Compound C111: X = Se

Compound C112 through C114, each represented by the formula



wherein in Compound C112: X = O,
in Compound C113: X = S
in Compound C114: X = Se

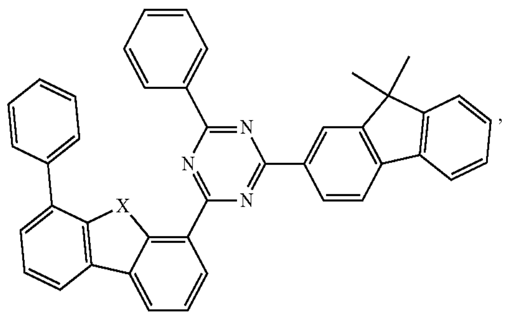
Compound C115 through C117, each represented by the formula



wherein in Compound C115 X = O,
in Compound C116: X = S
in Compound C117: X = Se

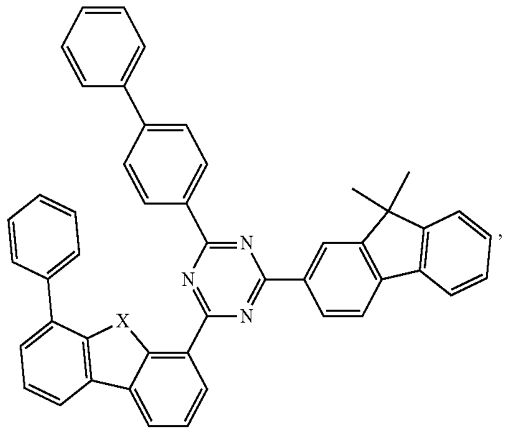
-continued

Compound C118 through C120, each represented by the formula



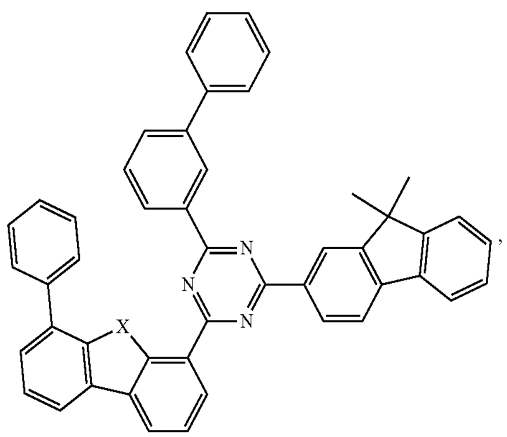
wherein in Compound C118: X = O,
in Compound C119: X = S
in Compound C120: X = Se

Compound C121 through C123, each represented by the formula



wherein in Compound C121: X = O,
in Compound C122: X = S
in Compound C123: X = Se

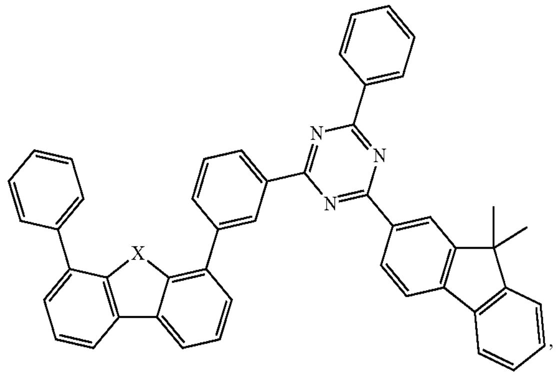
Compound C124 through C126, each represented by the formula



wherein in Compound C124: X = O,
in Compound C125: X = S
in Compound C126: X = Se

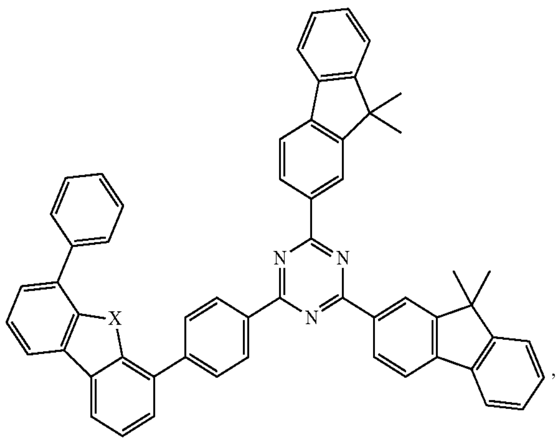
-continued

Compound C127 through C129, each represented by the formula



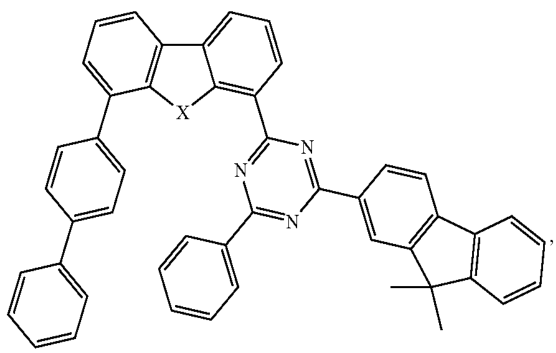
wherein in Compound C127: X = O,
in Compound C128: X = S,
in Compound C129: X = Se

Compound C130 through C132, each represented by the formula



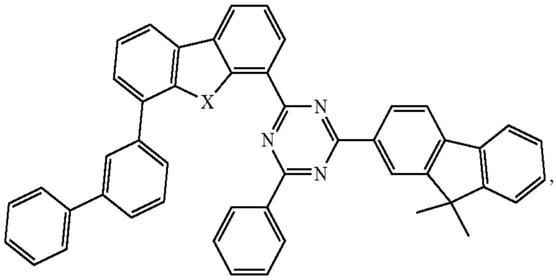
wherein in Compound C130: X = O,
in Compound C131: X = S,
in Compound C132: X = Se

Compound C133 through C135, each represented by the formula



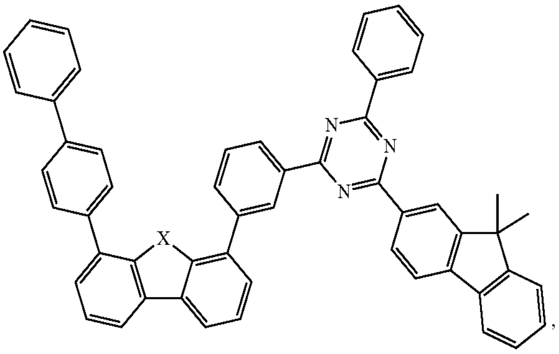
wherein in Compound C133: X = O,
in Compound C134: X = S,
in Compound C135: X = Se

Compound C136 through C138, each represented by the formula



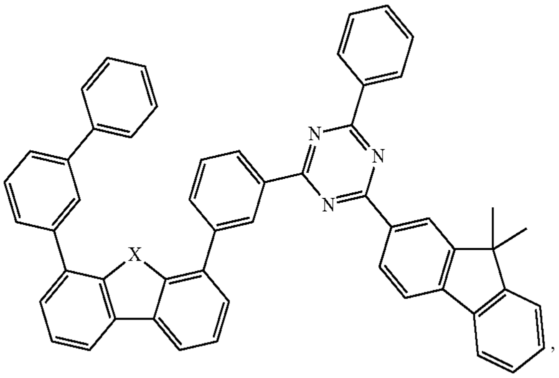
wherein in Compound C133: X = O,
in Compound C134: X = S,
in Compound C135: X = Se

Compound C139 through C141, each represented by the formula



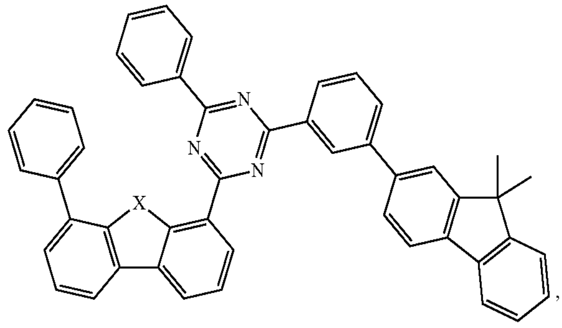
wherein in Compound C139: X = O,
in Compound C140: X = S,
in Compound C141: X = Se

Compound C142 through C144, each represented by the formula



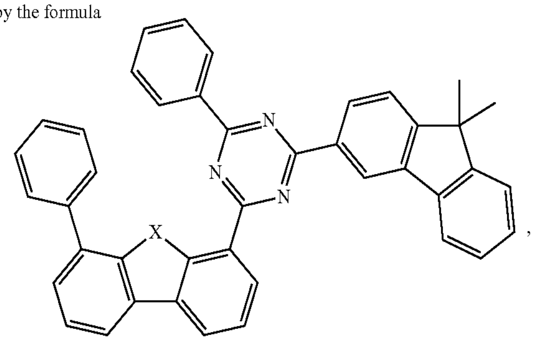
wherein in Compound C142: X = O,
in Compound C143: X = S,
in Compound C144: X = Se

Compound C145 through C147, each represented by the formula



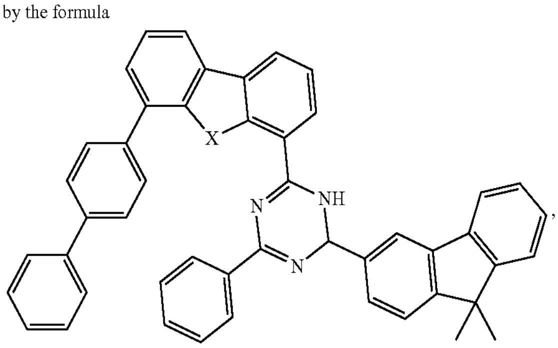
wherein in Compound C145: X = O,
in Compound C146: X = S,
in Compound C147: X = Se

Compound C148 through C150, each represented by the formula



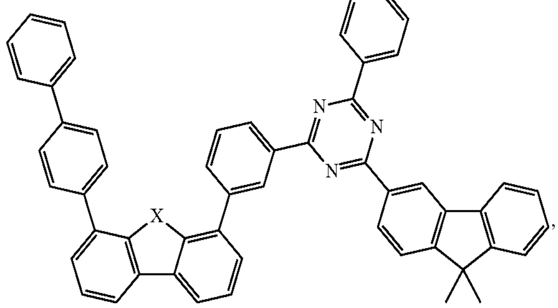
wherein in Compound C148: X = O,
in Compound C149: X = S,
in Compound C150: X = Se

Compound C151 through C153, each represented by the formula



wherein in Compound C151: X = O,
in Compound C152: X = S,
in Compound C153: X = Se

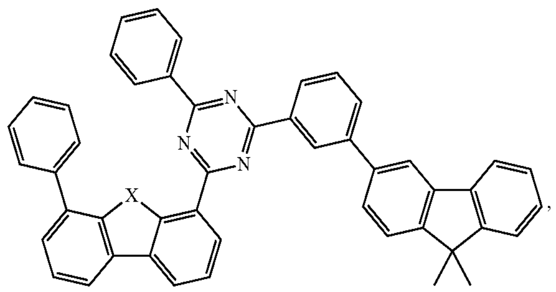
Compound C154 through C156, each represented by the formula



wherein in Compound C154: X = O,
in Compound C155: X = S,
in Compound C156: X = Se

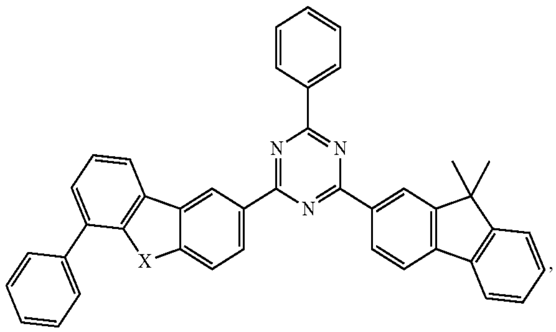
-continued

Compound C157 through C159, each represented by the formula



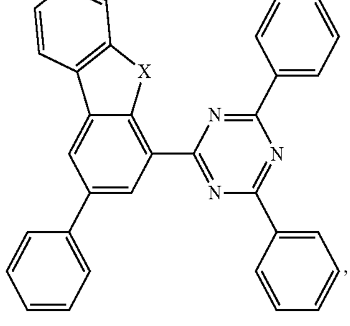
wherein in Compound C157: X = O,
in Compound C158: X = S,
in Compound C159: X = Se

Compound C160 through C162, each represented by the formula



wherein in Compound C160: X = O,
in Compound C161: X = S,
in Compound C162: X = Se

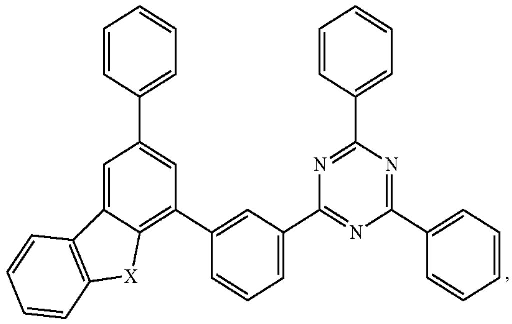
Compound C163 through C165, each represented by the formula



wherein in Compound C163: X = O,
in Compound C164: X = S,
in Compound C165: X = Se

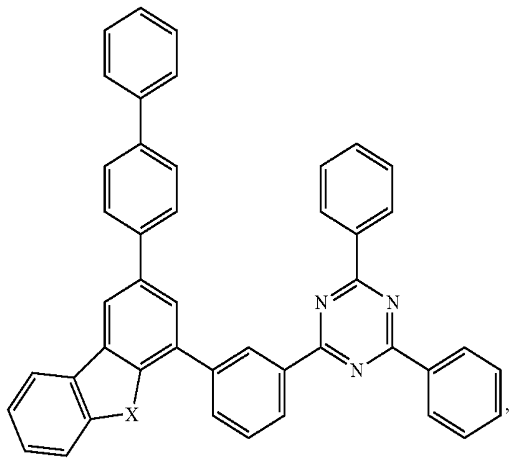
-continued

Compound C166 through C168, each represented by the formula



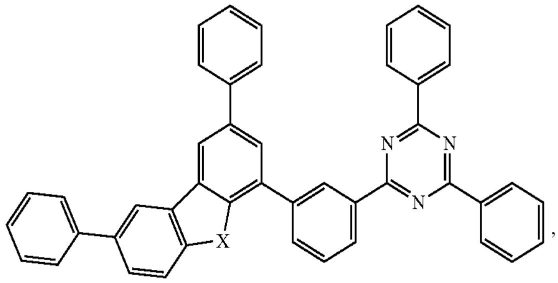
wherein in Compound C166: X = O,
in Compound C167: X = S,
in Compound C168: X = Se

Compound C169 through C171, each represented by the formula



wherein in Compound C169: X = O,
in Compound C170: X = S,
in Compound C171: X = Se

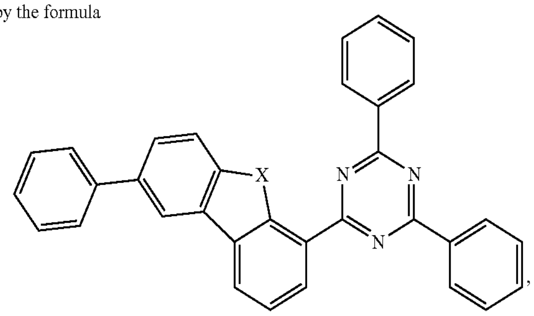
Compound C172 through C174, each represented by the formula



wherein in Compound C172: X = O,
in Compound C173: X = S,
in Compound C174: X = Se

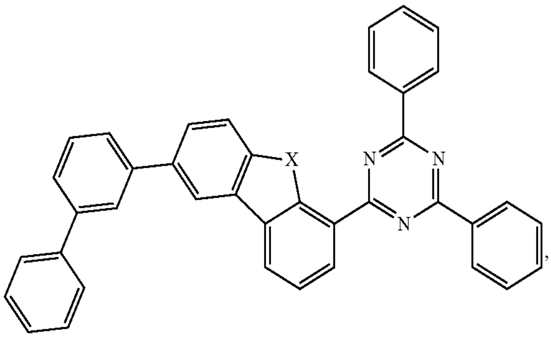
-continued

Compound C175 through C177, each represented by the formula



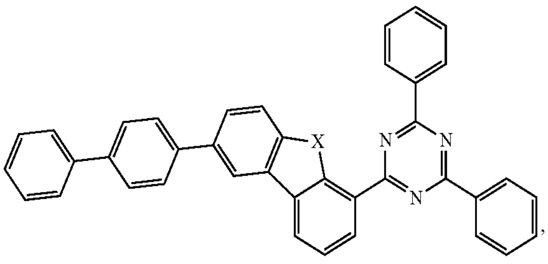
wherein in Compound C175: X = O,
in Compound C176: X = S,
in Compound C177: X = Se

Compound C178 through C180, each represented by the formula



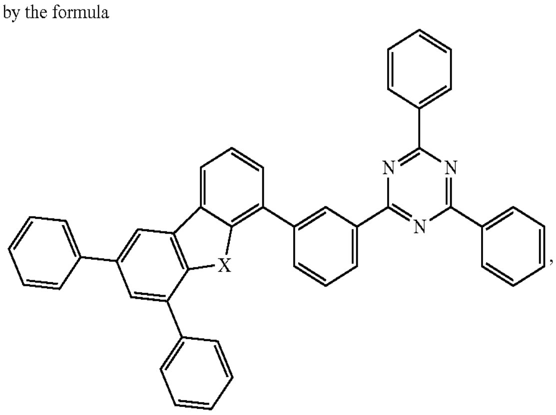
wherein in Compound C178: X = O,
in Compound C179: X = S,
in Compound C180: X = Se

Compound C181 through C183, each represented by the formula



wherein in Compound C181: X = O,
in Compound C182: X = S,
in Compound C183: X = Se

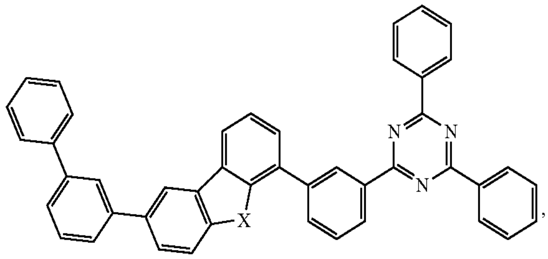
Compound C184 through C186, each represented by the formula



wherein in Compound C184: X = O,
in Compound C185: X = S,
in Compound C186: X = Se

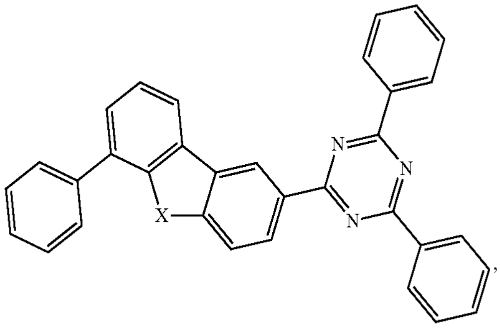
-continued

Compound C187 through C189, each represented by the formula



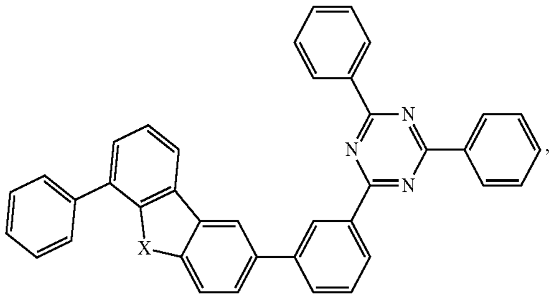
wherein in Compound C187: X = O,
in Compound C188: X = S,
in Compound C189: X = Se

Compound C190 through C192, each represented by the formula



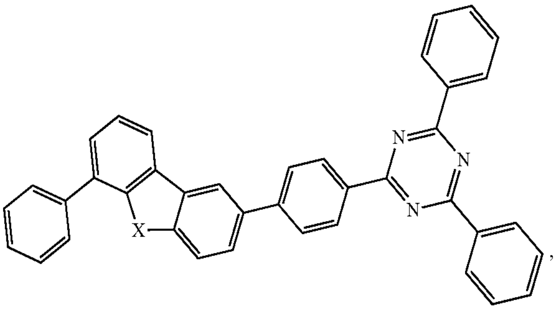
wherein in Compound C190: X = O,
in Compound C191: X = S,
in Compound C192: X = Se

Compound C193 through C195, each represented by the formula



wherein in Compound C193: X = O,
in Compound C194: X = S,
in Compound C195: X = Se

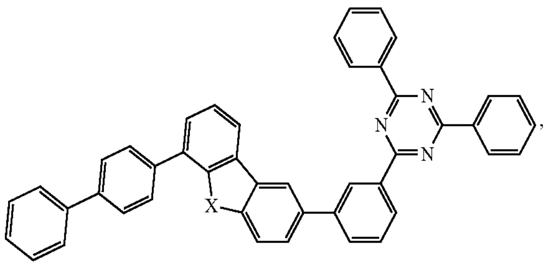
Compound C196 through C198, each represented by the formula



wherein in Compound C196: X = O,
in Compound C197: X = S,
in Compound C198: X = Se

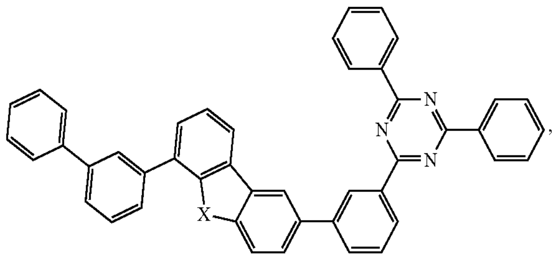
-continued

Compound C199 through C201, each represented by the formula



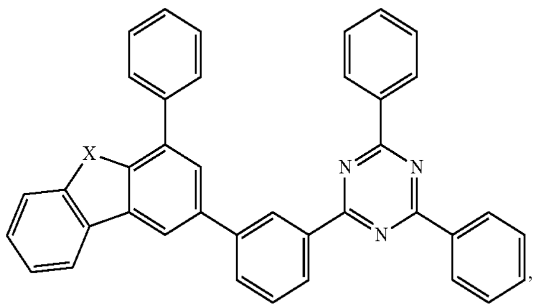
wherein in Compound C199: X = O,
in Compound C200: X = S,
in Compound C201: X = Se

Compound C202 through C204, each represented by the formula



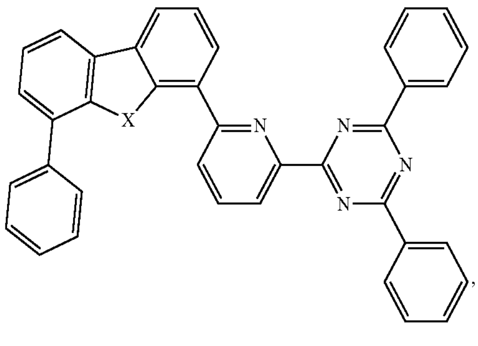
wherein in Compound C202: X = O,
in Compound C203: X = S,
in Compound C204: X = Se

Compound C205 through C207, each represented by the formula



wherein in Compound C205: X = O,
in Compound C206: X = S,
in Compound C207: X = Se

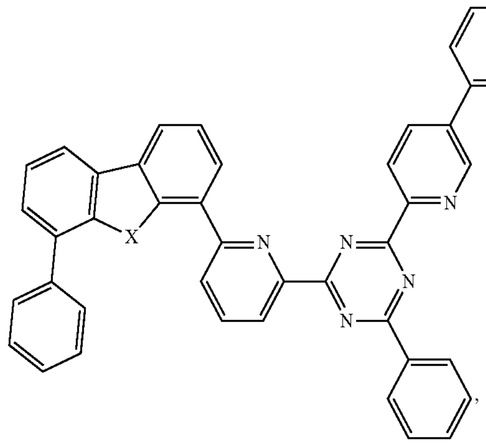
Compound C208 through C210, each represented by the formula



wherein in Compound C208: X = O,
in Compound C209: X = S
in Compound C210: X = Se

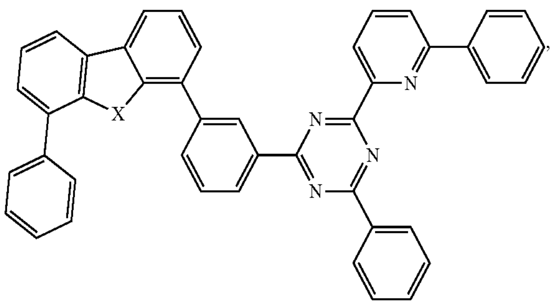
-continued

Compound C211 through C13, each represented by the formula



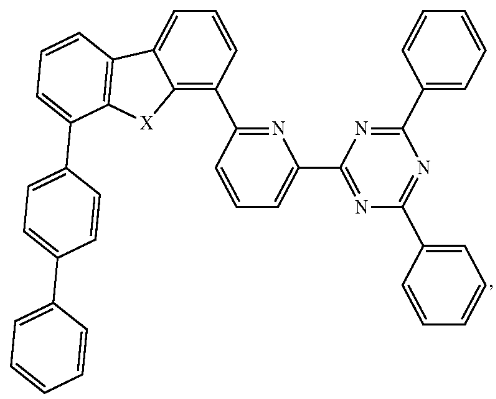
wherein in Compound C211: X = O,
in Compound C212: X = S
in Compound C213: X = Se

Compound C214 through C216, each represented by the formula



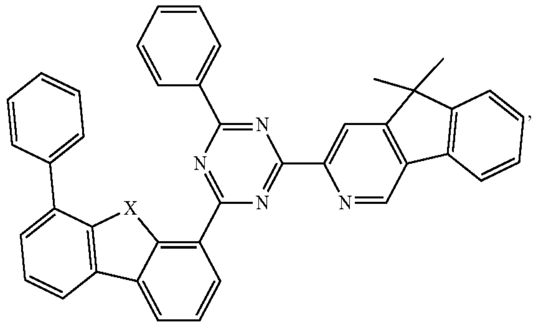
wherein in Compound C214: X = O,
in Compound C215: X = S
in Compound C216: X = Se

Compound C217 through C219, each represented by the formula



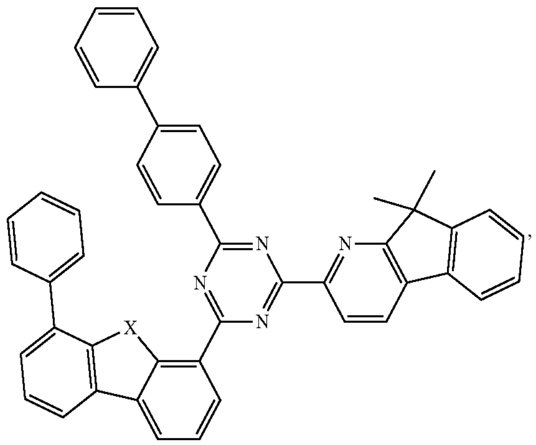
wherein in Compound C217: X = O,
in Compound C218: X = S
in Compound C219: X = Se

Compound C220 through C222, each represented by the formula



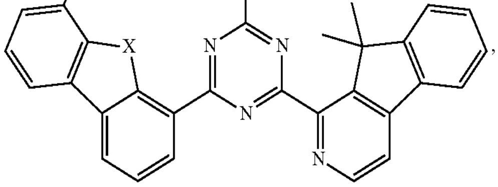
wherein in Compound C222: X = O,
in Compound C223: X = S
in Compound C224: X = Se

Compound C223 through C225, each represented by the formula



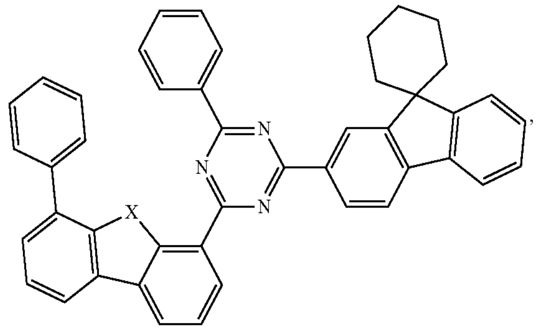
wherein in Compound C222: X = O,
in Compound C223: X = S
in Compound C224: X = Se

Compound C226 through C228, each represented by the formula



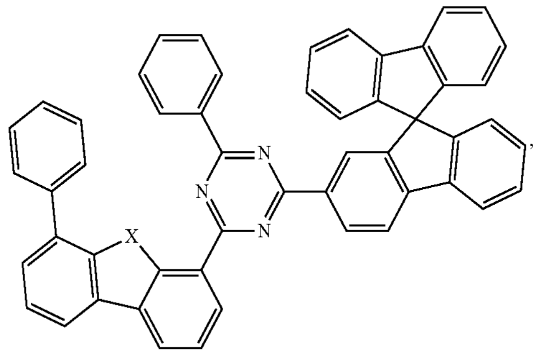
wherein in Compound C226: X = O,
in Compound C227: X = S
in Compound C228: X = Se

Compound C229 through C231, each represented by the formula



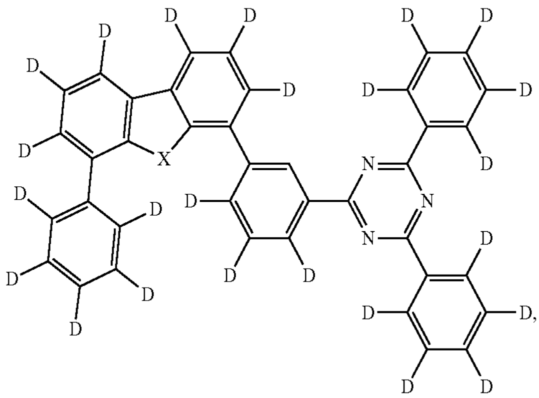
wherein in Compound C229: X = O,
in Compound C230: X = S
in Compound C231: X = Se

Compound C232 through C234, each represented by the formula



wherein in Compound C232: X = O,
in Compound C233: X = S
in Compound C234: X = Se

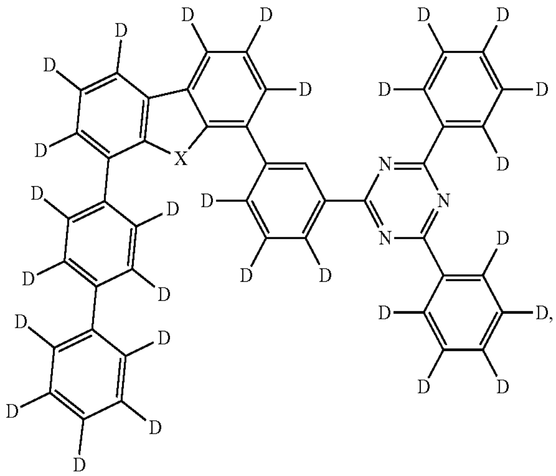
Compound C235 through C237, each represented by the formula



wherein in Compound C235: X = O,
in Compound C236 X = S,
in Compound C237: X = Se

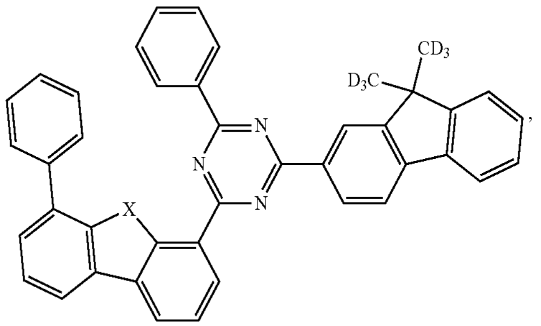
-continued

Compound C234 through C240, each represented by the formula



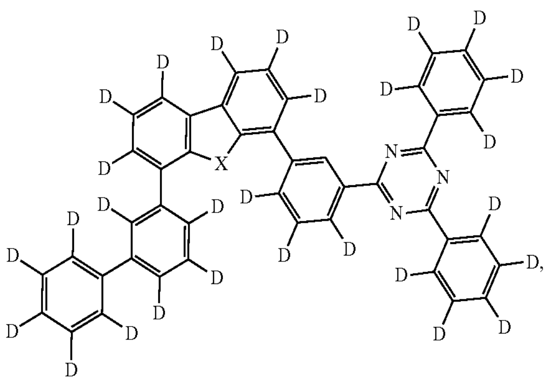
wherein in Compound C235: X = O,
in Compound C236 X = S,
in Compound C237: X = Se

Compound C241 through C243, each represented by the formula



wherein in Compound C241: X = O,
in Compound C242 X = S,
in Compound C243: X = Se

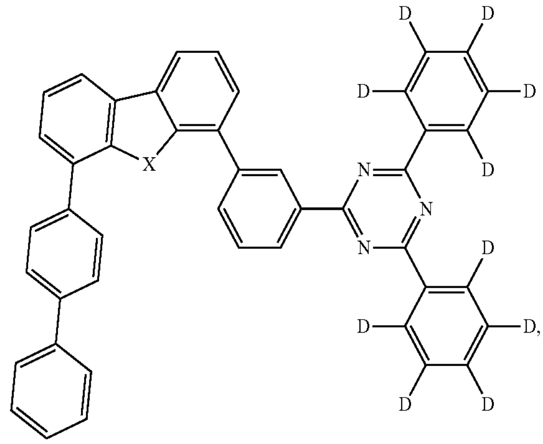
Compound C244 through C246, each represented by the formula



wherein in Compound C244: X = O,
in Compound C245 X = S,
in Compound C246: X = Se

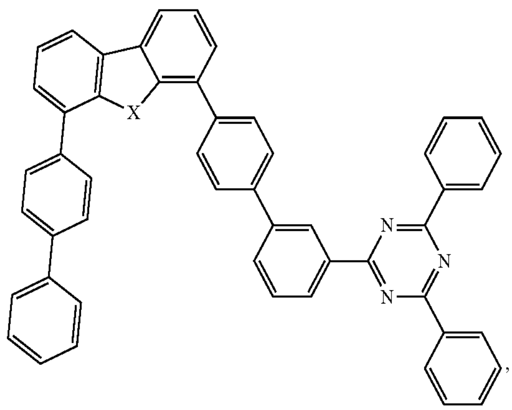
-continued

Compound C247 through C249, each represented by the formula



wherein in Compound C247: X = O,
in Compound C248 X = S,
in Compound C249: X = Se

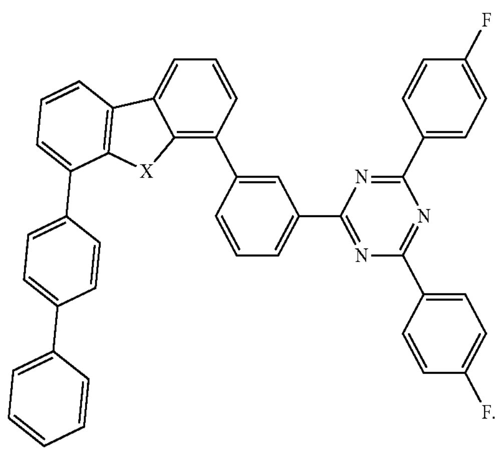
Compound C250 through C252, each represented by the formula



and

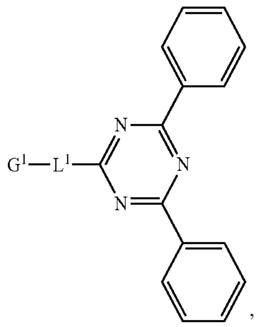
wherein in Compound C250: X = O,
in Compound C251 X = S,
in Compound C252: X = Se

Compound C253 through C255, each represented by the formula



wherein in Compound C253: X = O,
in Compound C254: X = S,
in Compound C255: X = Se

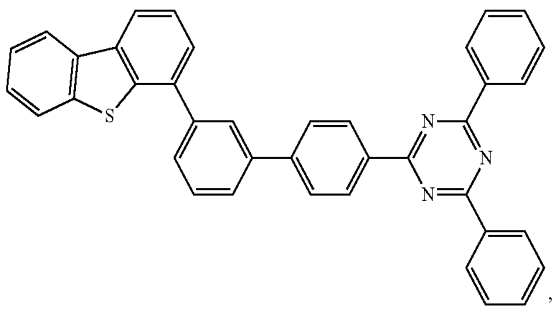
In some embodiments, the first compound has a formula:



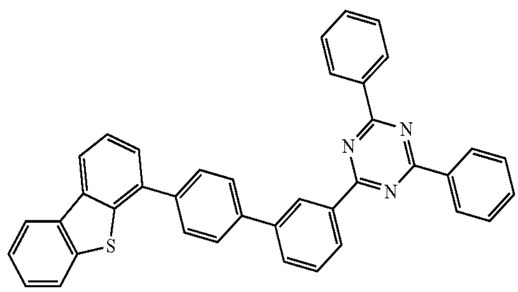
where L^1 is biphenyl.

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

Compound D1

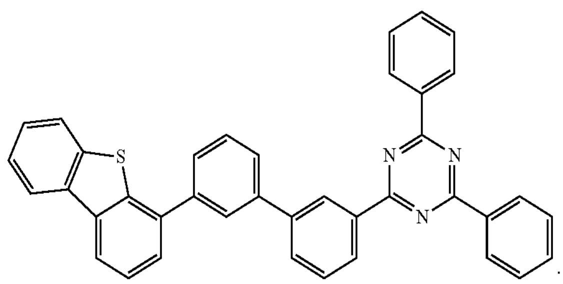


Compound D2



, and

Compound D3



In some embodiments, the composition comprises a second compound having a structure of formula II:

Formula II

$$Ar^1—Ar^2—Ar^3.$$

In the structure of Formula II:

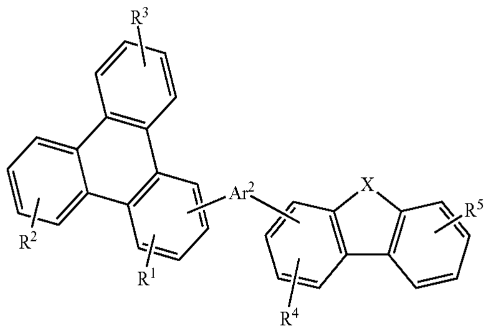
Ar^1 is selected from the group consisting of triphenylene, and aza-triphenylene;

Ar^2 is selected from the group consisting of a direct bond, phenyl, biphenyl, terphenyl, naphthalene, pyridine, dibenzofuran, dibenzothiophene, dibenzoselenophene, aza-dibenzofuran, aza-dibenzothiophene, aza-dibenzoselenophene, and combinations thereof;

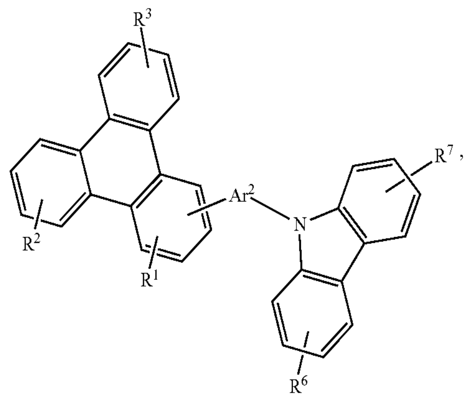
Ar^3 is selected from the group consisting of benzene, biphenyl, terphenyl, naphthalene, pyridine, dibenzofuran, dibenzothiophene, dibenzoselenophene, aza-dibenzofuran, aza-dibenzothiophene, aza-dibenzoselenophene, carbazole, aza-carbazole, and combinations thereof; and

Ar^1, Ar^2 and Ar^3 are each, independently, optionally further substituted with one or more substitutions selected from the group consisting of deuterium, halogen, alkyl, aryl, heteroaryl, and combinations thereof.

In some embodiments, the second compound is selected from the group consisting of



and



where:

X is selected from the group consisting of O, S and Se;

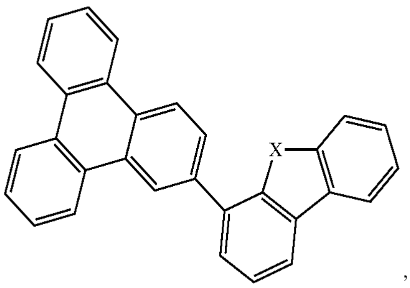
R^1 and R^4 each independently represents mono, di, or tri, substitution, or no substitution;

R^2, R^3, R^5, and R^6 each independently represents mono, di, tri, or tetra substitution, or no substitution; and

R^1 to R^6 are each independently selected from the group consisting of hydrogen, deuterium, benzene, biphenyl, terphenyl, naphthalene, fluorene, triphenylene, phenanthrene, dibenzofuran, dibenzothiophene, carbazole and combinations thereof.

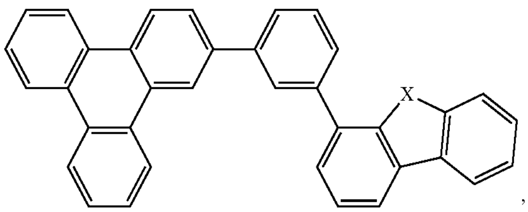
In some embodiments, the second compound is selected from the group consisting of

Compound E1 through E3, each represented by the formula



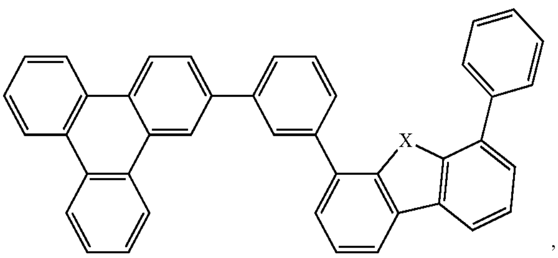
wherin in Compound E1: X = O,
in Compound E2: X = S,
in Compound E3: X = Se

Compound E4 through E6, each represented by the formula



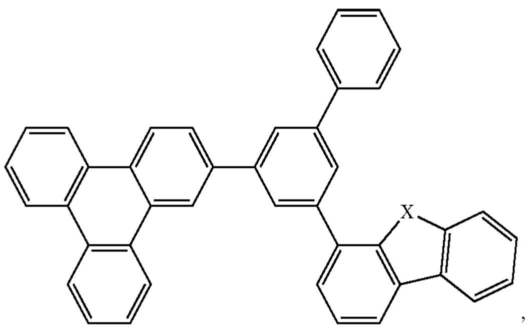
wherin in Compound E4: X = O,
in Compound E5: X = S,
in Compound E6: X = Se

Compound E7 through E9, each represented by the formula



wherin in Compound E7: X = O,
in Compound E8: X = S,
in Compound E9: X = Se

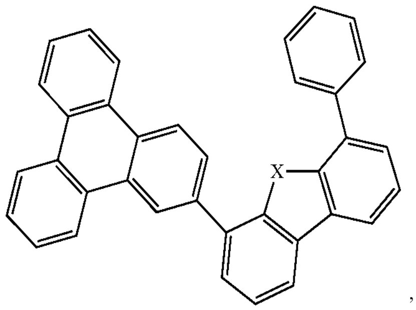
Compound E10 through E12, each represented by the formula



wherin in Compound E10: X = O,
in Compound E11: X = S,
in Compound E12: X = Se

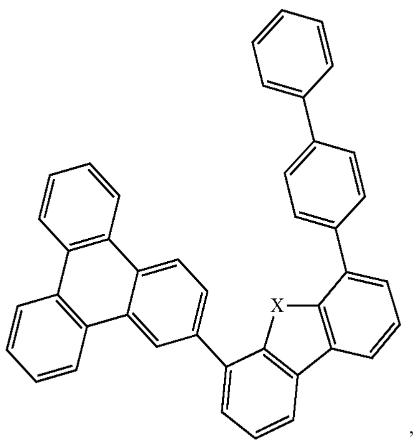
-continued

Compound E13 through E15, each represented by the formula



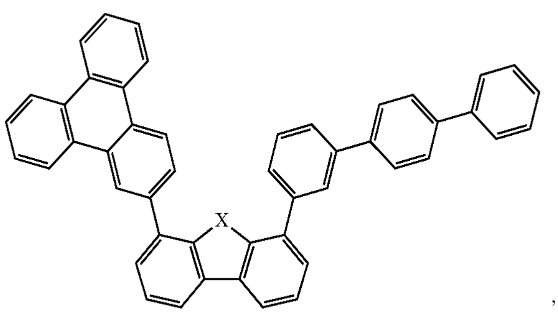
wherin in Compound E13: X = O,
in Compound E14: X = S,
in Compound E15: X = Se

Compound E16 through E18, each represented by the formula



wherin in Compound E16: X = O,
in Compound E17: X = S,
in Compound E18: X = Se

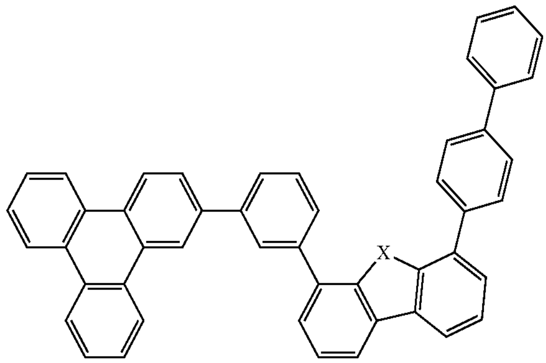
Compound E19 through E21, each represented by the formula



wherin in Compound E19: X = O,
in Compound E20: X = S,
in Compound E21: X = Se

-continued

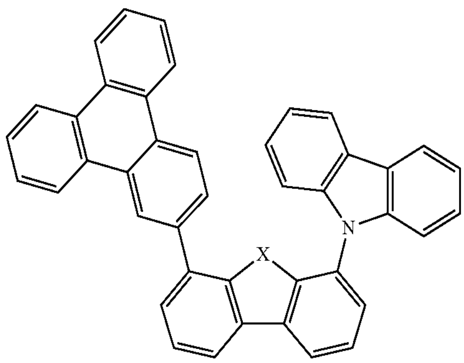
Compound E22 through E24, each represented by the formula



,

wherin in Compound E22: X = O,
in Compound E23: X = S,
in Compound E24: X = Se

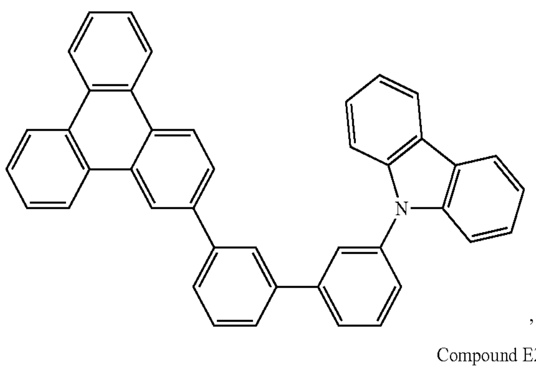
Compound E25 through E27, each represented by the formula



,

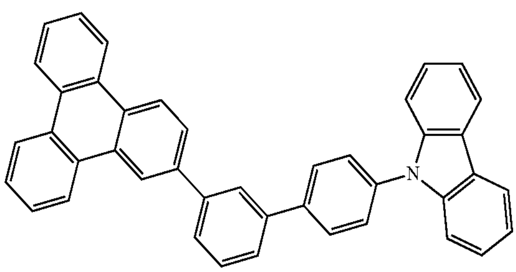
wherin in Compound E25: X = O,
in Compound E26: X = S,
in Compound E27: X = Se

Compound E28



,

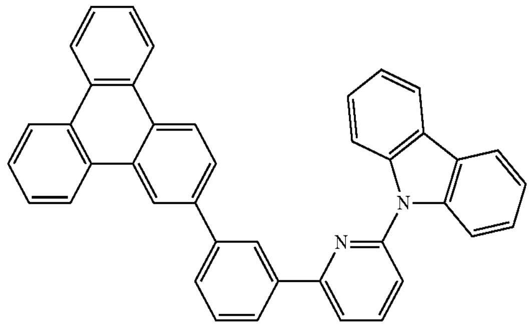
Compound E29



, and

-continued

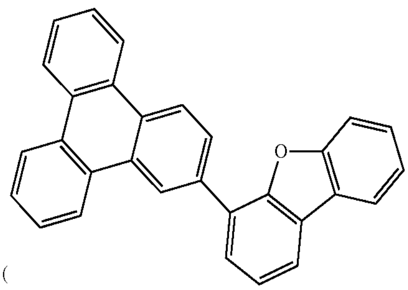
Compound E30



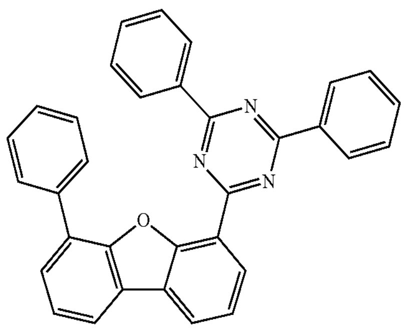
.

In some embodiments, the mixture of the first compound and the second compound is selected from the group consisting of:

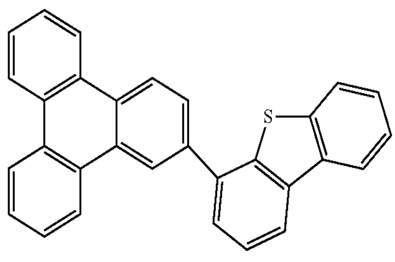
Compound E1

( ,

Compound C1

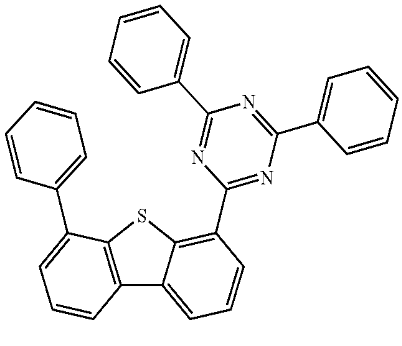
);

Compound E2

( ,

-continued

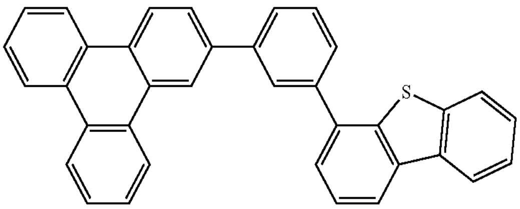
Compound C2



);

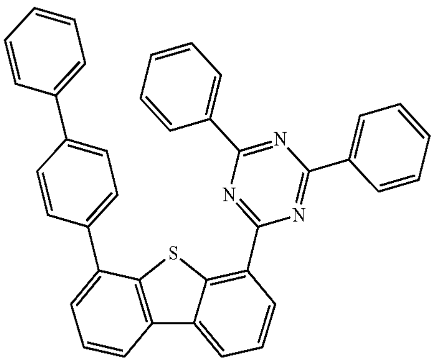
Compound E5

(



,

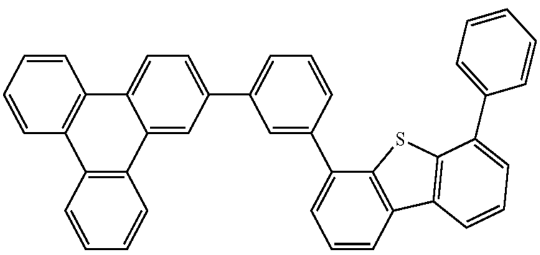
Compound C65



);

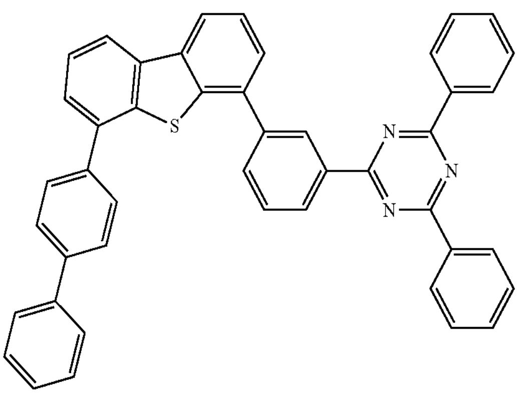
Compound E8

(



,

Compound C74

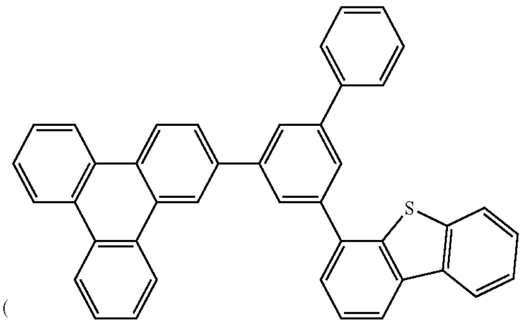


);

-continued

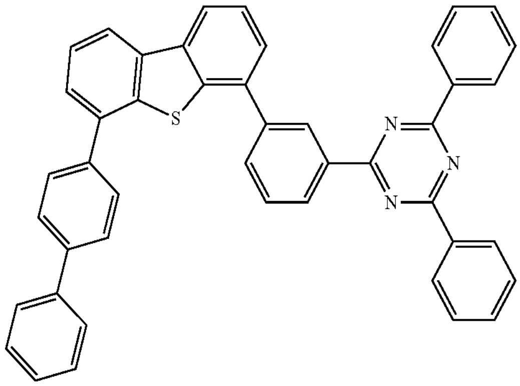
Compound E11

(



,

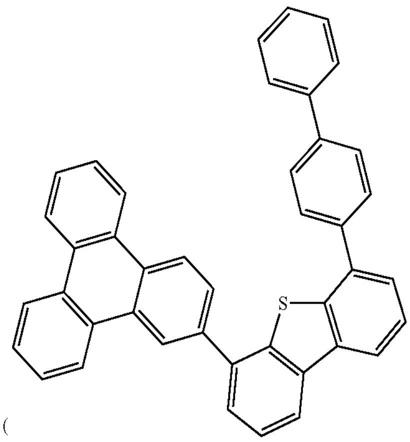
Compound C74



);

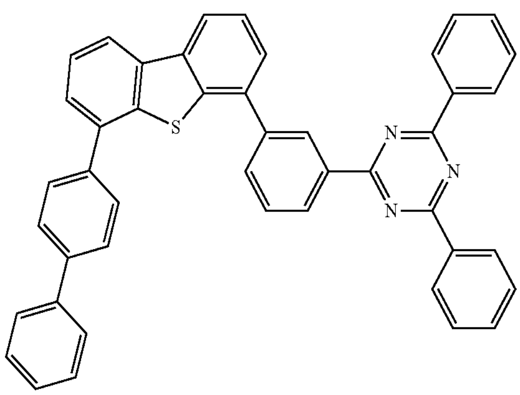
Compound E17

(



,

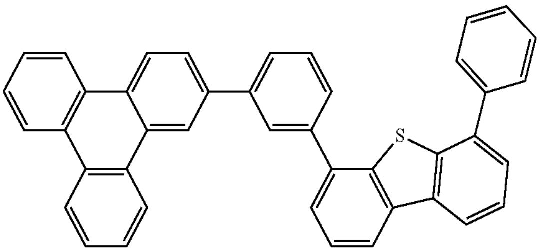
Compound C74



);

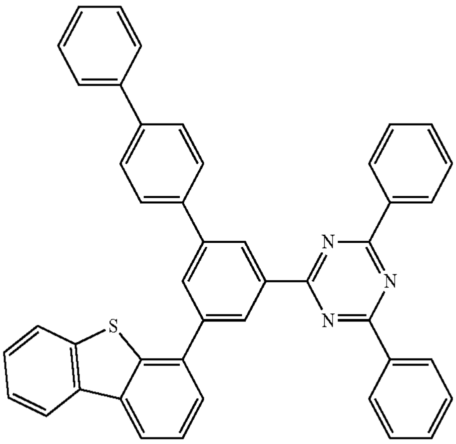
-continued

Compound E8



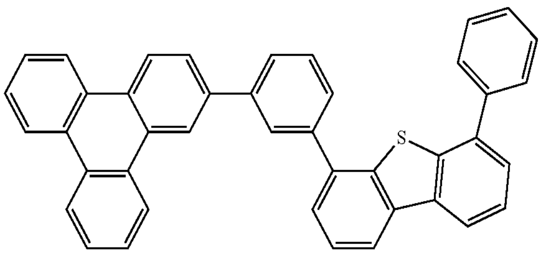
(,

Compound A5



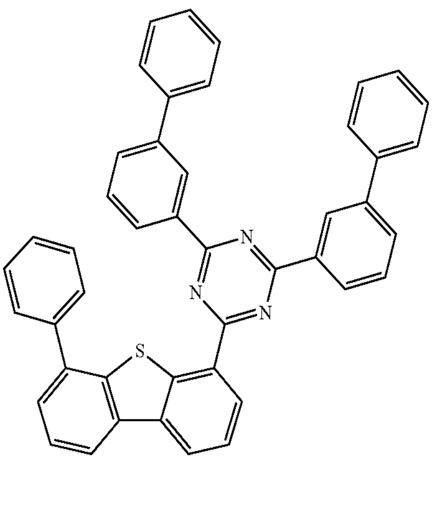
);

Compound E8



(,

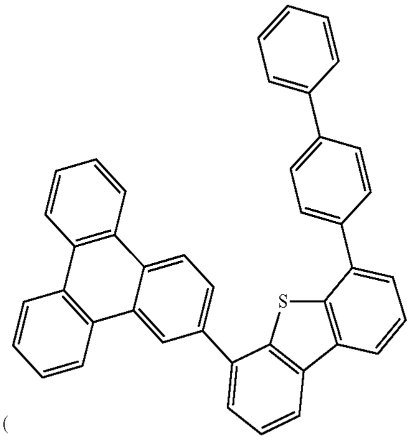
Compound C17



);

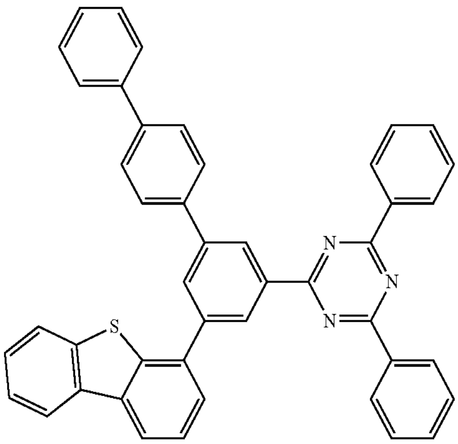
-continued

Compound E17



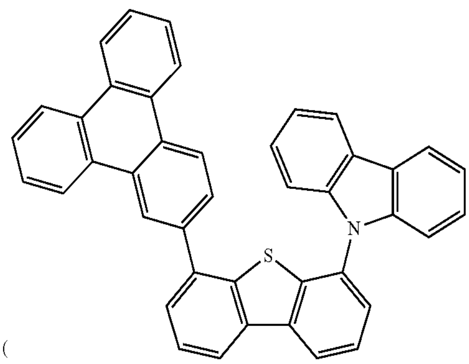
(,

Compound A5



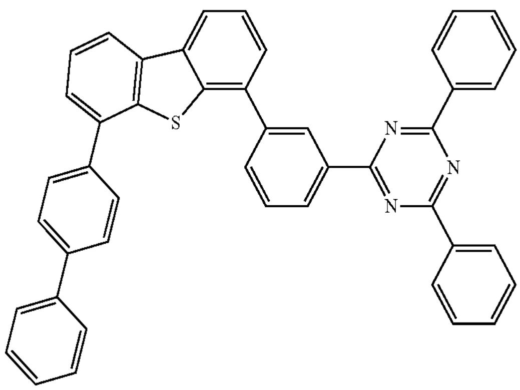
);

Compound E26



(,

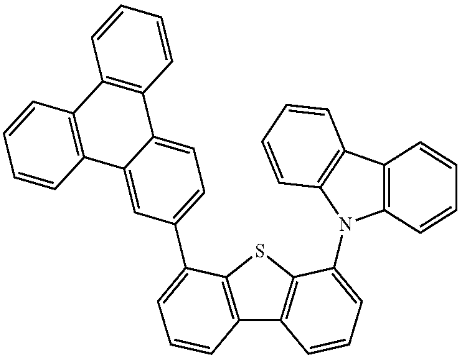
Compound C74



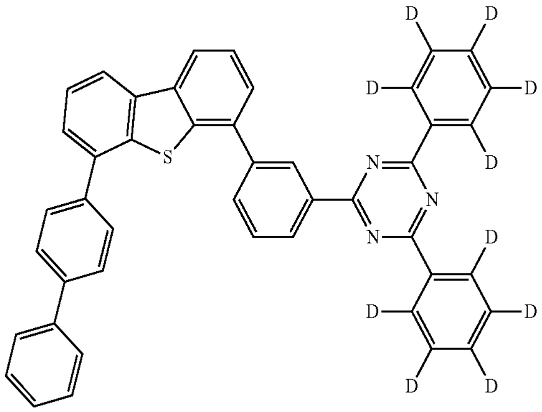
);

-continued

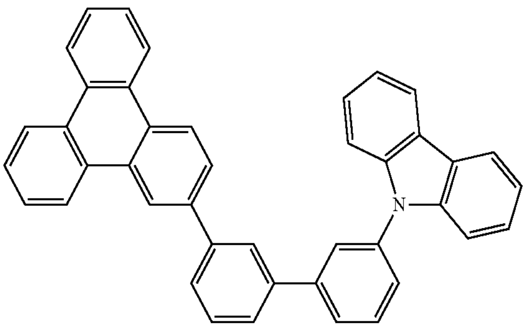
Compound E26

( ,

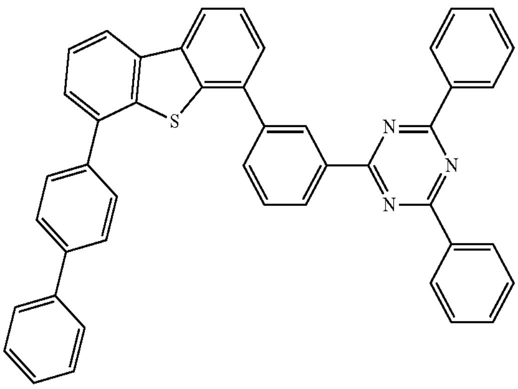
Compound C248

);

Compound E28

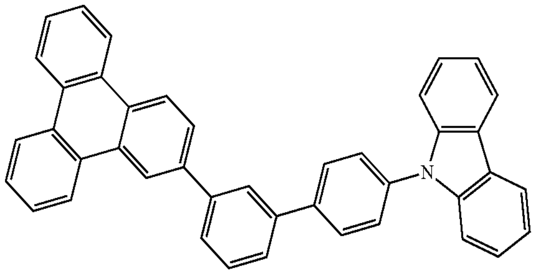


Compound C74

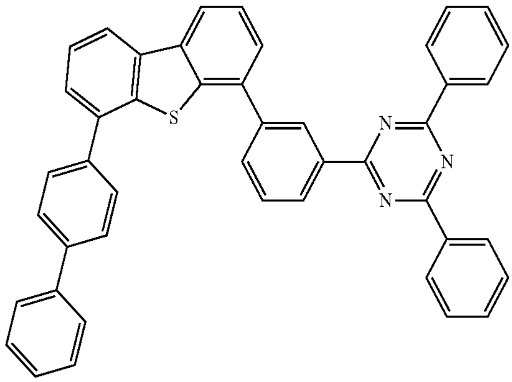
);

-continued

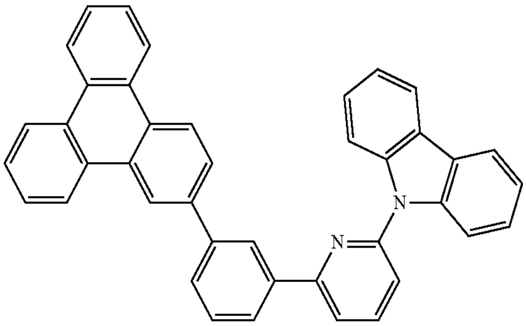
Compound E29

( ,

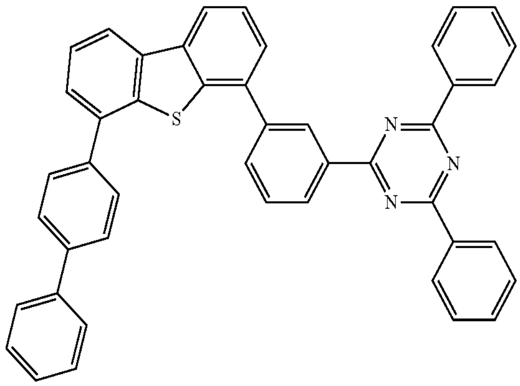
Compound C74

); and

Compound E30

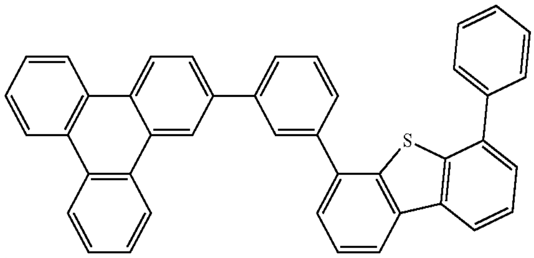
( ,

Compound C74

).

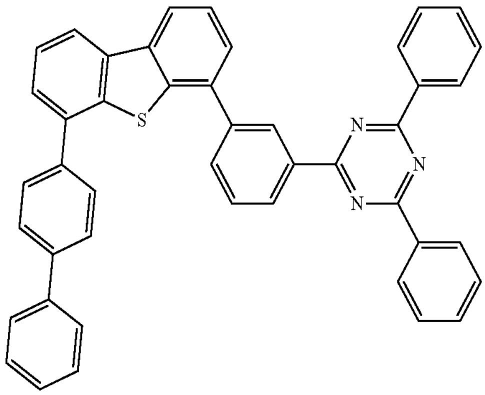
In some embodiments, the mixture of the first compound and the second compound is selected from the group consisting of:

Compound E8



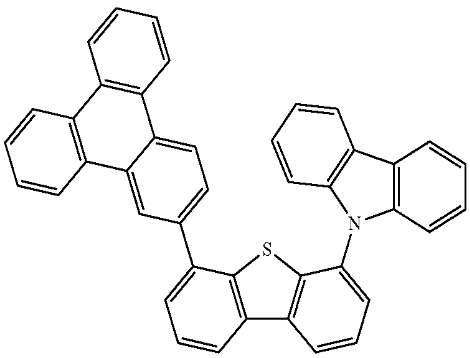
(,

Compound C74



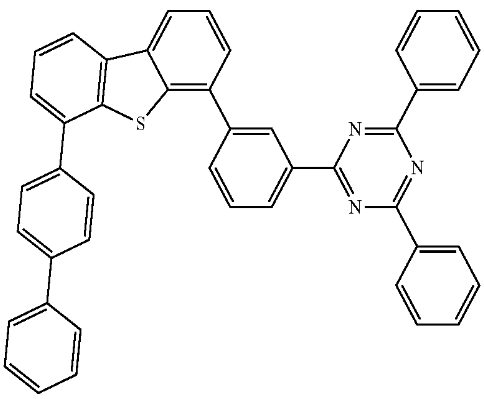
),

Compound E26



(,

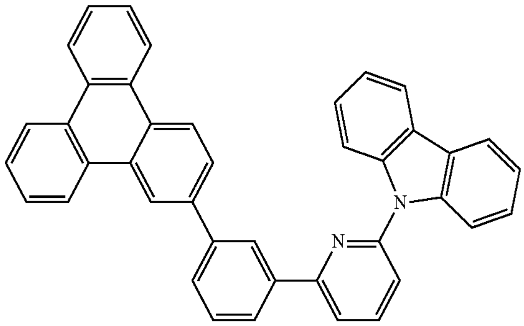
Compound C74



), and

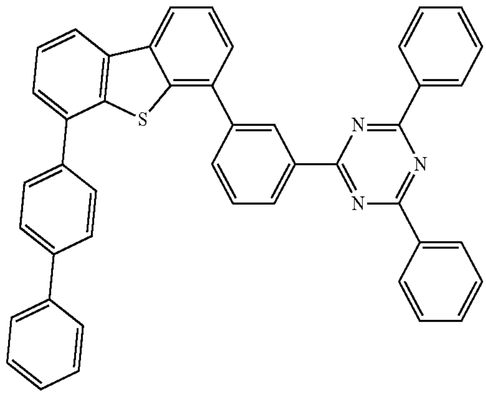
-continued

Compound E30



(,

Compound C74

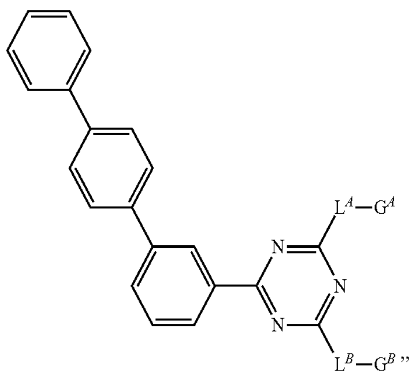


).

In some embodiments, the composition comprises a second compound, where the second compound is a phosphorescent emissive Ir complex having at least one substituent selected from the group consisting of alkyl, cycloalkyl, partially or fully deuterated variants thereof, partially or fully fluorinated variants thereof, and combinations thereof.

According to another embodiment of the resent disclosure, a composition of materials comprising a first compound having a structure of:

Formula III



is disclosed. In the structure of Formula III,

L^A and L^B are selected from a group consisting of direct bond, phenyl, biphenyl, pyridine, and combinations thereof;

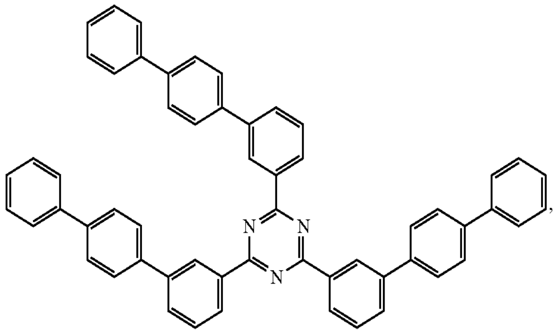
G^A and G^B are selected from a group consisting of phenyl, biphenyl, pyridine, dibenzothiophene, dibenzofuran, dibenzoselenophene, and fluorene; and

G^A and G^B are each optionally further substituted with one or more unfused substituents selected from the group consisting of deuterium, alkyl, alkoxyl, cycloalkyl, cycloalkoxyl, halogen, nitro, nitrile, silyl, phenyl, biphenyl, terphenyl, pyridine, and combinations thereof.

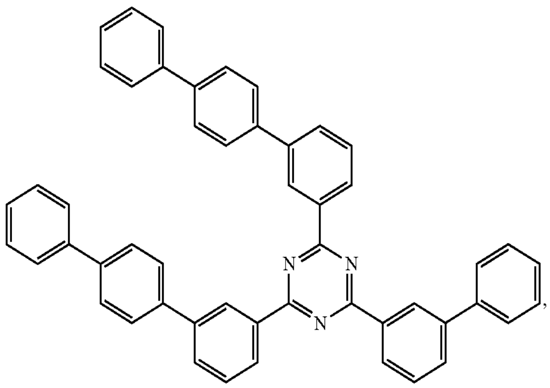
In some embodiments, one or more of L^A and L^B can be a direct bond, and the direct bond can be a single bond or a double bond.

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

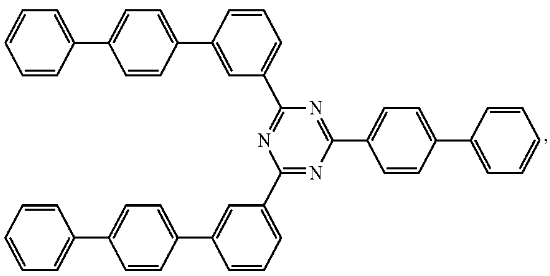
Compound F1



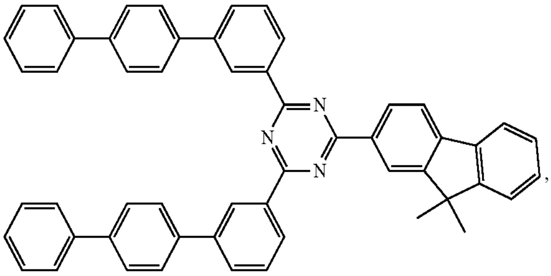
Compound F2



Compound F3



Compound F4



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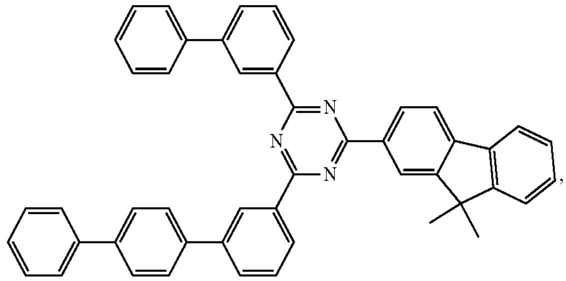
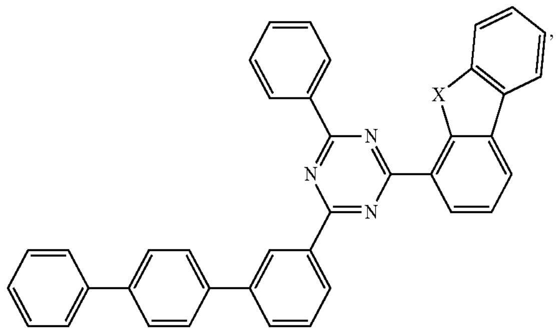
Compound F5

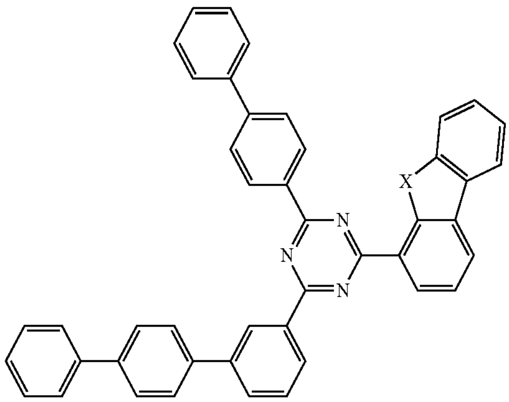


Compound F6 through F8, each represented by the formula



wherein in Compound F6: X = O,
in Compound F7: X = S
in Compound F8: X = Se

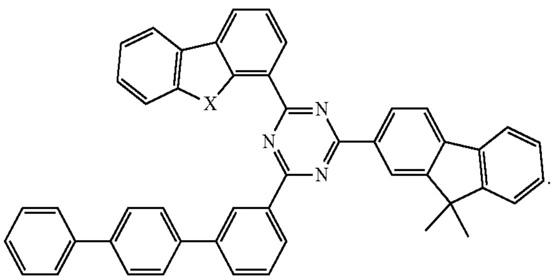
Compound F9 through F11, each represented by the formula



and

wherein in Compound F9: X = O,
in Compound F10: X = S
in Compound F11: X = Se

Compound F12 through F14, each represented by the formula



wherein in Compound F12: X = O,
in Compound F13: X = S
in Compound F14: X = Se

In some embodiments, the first compound has an evaporation temperature T1 of 150 to 350° C.; the second compound has an evaporation temperature T2 of 150 to 350° C.; an absolute value of T1-T2 is less than 20° C.; the first compound has a concentration C1 in said mixture and a concentration C2 in a film formed by evaporating the mixture in a vacuum deposition tool at a constant pressure between 1×10^{6} Torr to 1×10^{9} Torr, at a 2 Å/sec deposition rate on a surface position at a predefined distance away from the mixture being evaporated; and the absolute value of (C1-C2)/C1 is less than 5%.

In some embodiments, the first compound has a vapor pressure of P1 at T1 at 1 atm, the second compound has a vapor pressure of P2 at T2 at 1 atm; and the ratio of P1/P2 is within the range of 0.90 to 1.10.

In some embodiments, the first compound has a first mass loss rate and the second compound has a second mass loss rate, wherein the ratio between the first mass loss rate and the second mass loss rate is within the range of 0.90 to 1.10.

In some embodiments, the first compound and the second compound each has a purity in excess of 99% as determined by high pressure liquid chromatography.

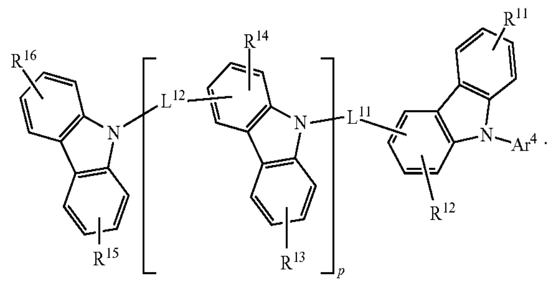
In some embodiments, the composition also comprises a third compound. In some embodiments, the third compound has a different chemical structure than the first and second compounds. In some embodiments, the third compound has a third mass loss rate and the ratio between the first mass loss rate and third mass loss rate is within the range of 0.90 to 1.10. In some embodiments, the third compound has an evaporation temperature T3 of 150 to 350° C., and the absolute value of T1-T3 is less than 20° C.

In some embodiments, the composition is in liquid form at a temperature less than T1 and T2.

In some embodiments, the composition comprises a second compound, where the second compound has the formula IV of

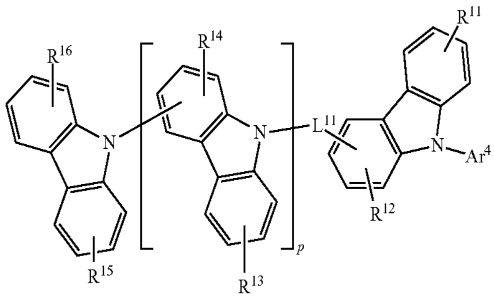
$$G^8 - [G^7]_p - G^6 - Ar^4,$$

having the structure:

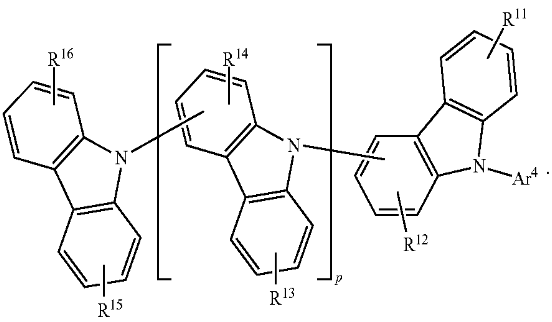


In such embodiments, Ar^4 is selected from the group consisting of aryl, heteroaryl, alkyl, cycloalkyl and combinations thereof; L^{11} and L^{12} are each independently selected from the group consisting of a direct bond, aryl, heteroaryl, alkyl, alkoxyl, and combinations thereof; p is an integer from 0 to 20; when p is greater than 1, each G^7 can be same or different; R^{11}, R^{13}, R^{15}, and R^{16} each independently represents mono, di, tri, or tetra substitution, or no substitution; R^{12} and R^{14} each independently represent mono, di, or tri substitution, or no substitution; R^{11}, R^{12}, R^{13}, R^{14}, R^{15}, and R^{16} are each independently selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, silyl, carbonyl, alkyloxyl, nitrile, isonitrile, aryl, heteroaryl, and combinations thereof; and L^{11}, L^{12}, and Ar^4 are each independently optionally further substituted by one or more substituents selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, silyl, carbonyl, alkyloxyl, nitrile, isonitrile, aryl, heteroaryl, and combinations thereof.

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

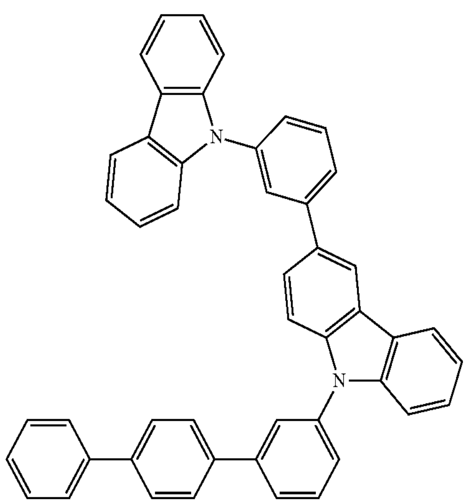


and



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

Compound G1



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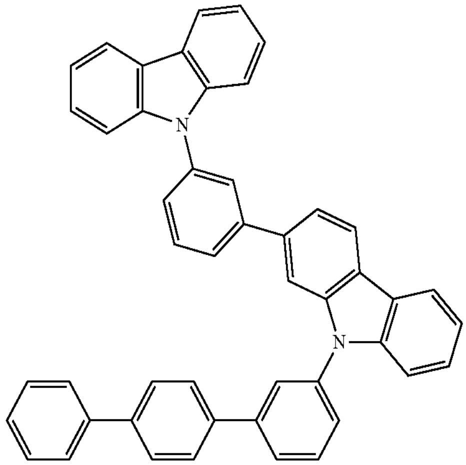
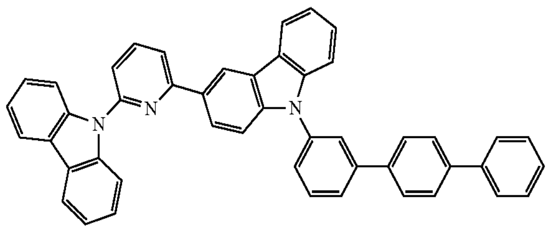
-continued

Compound G2



,

Compound G3



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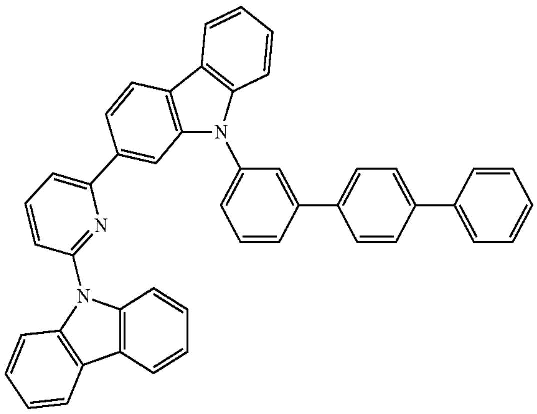
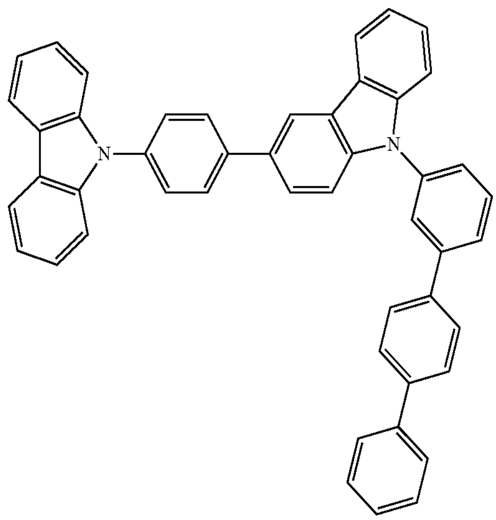
Compound G4



,

Compound G5



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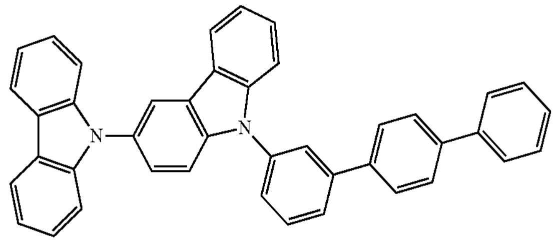
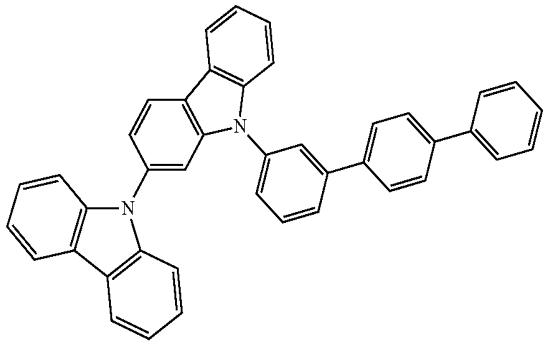
Compound G6



,

Compound G7



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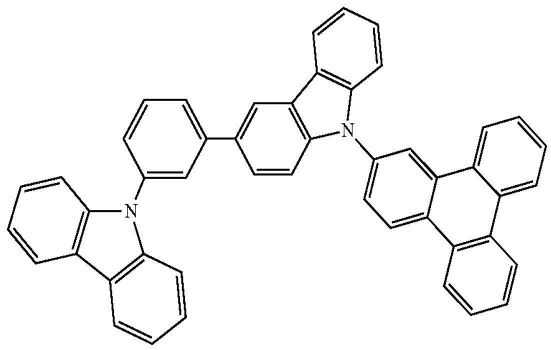
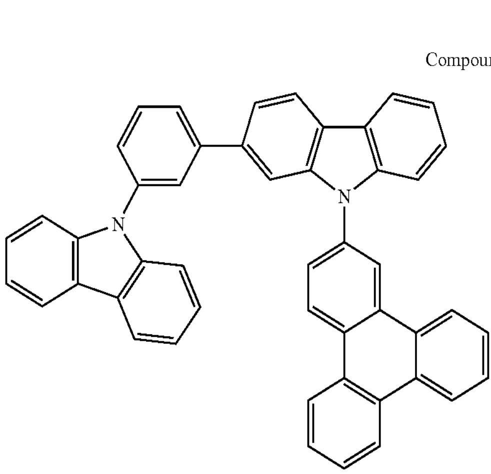
Compound G8



,

Compound G9



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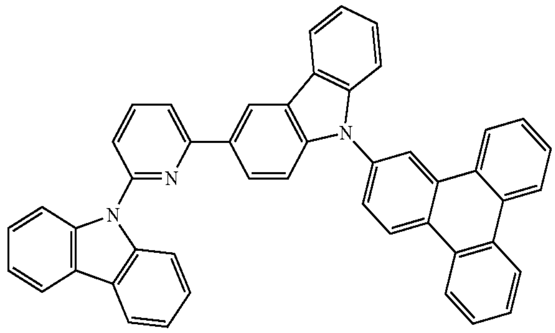
Compound G10



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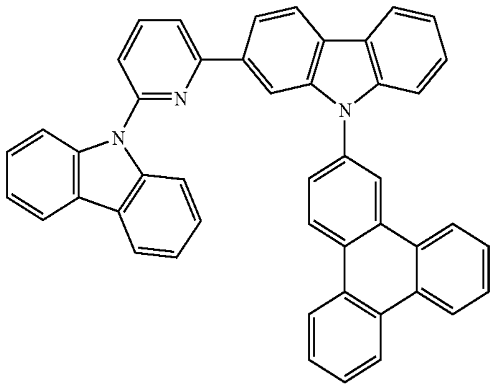
Compound G11



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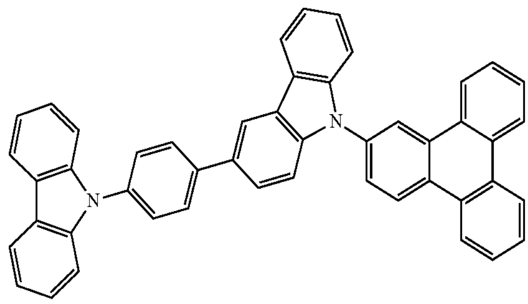
Compound G12



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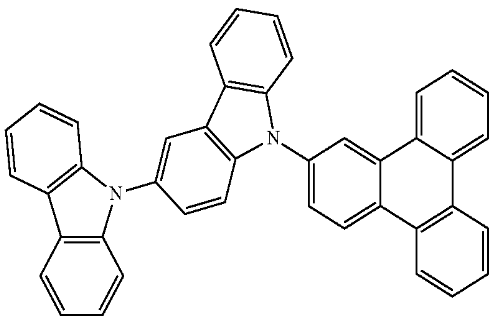
Compound G13



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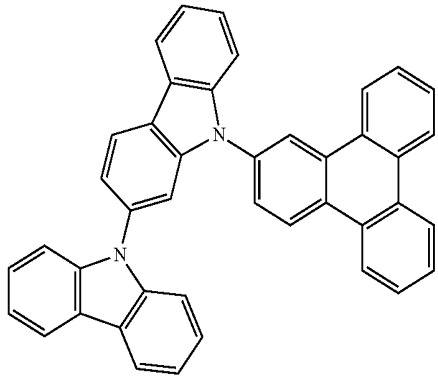
Compound G14



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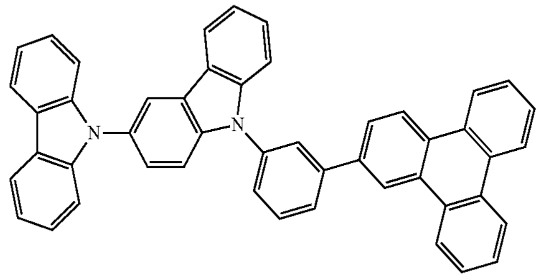
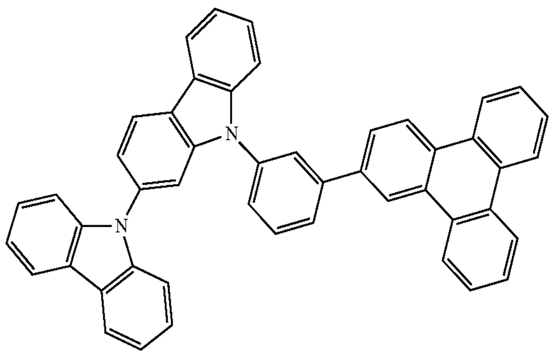
Compound G15



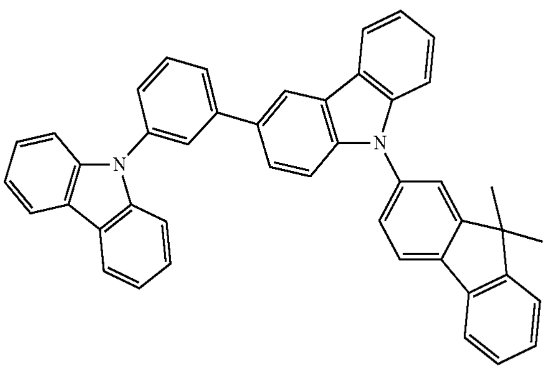
,

Compound G16



,

Compound G17



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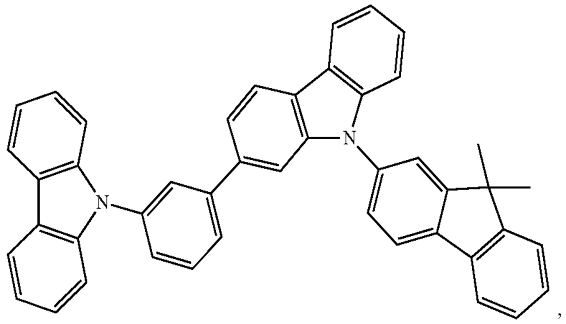
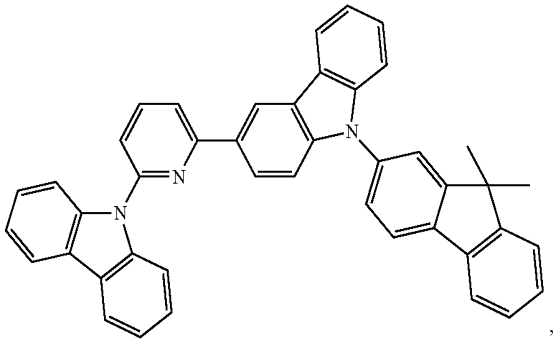
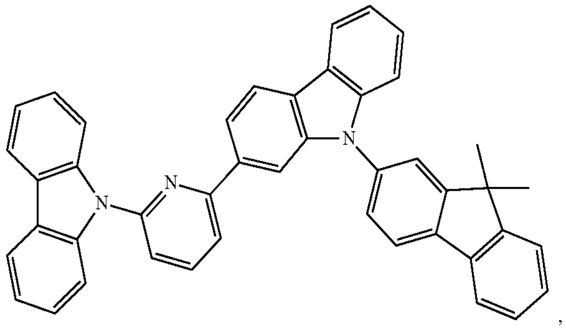
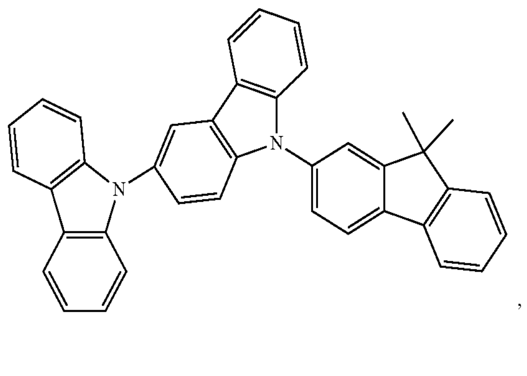

Compound 18


Compound G19


Compound G20


Compound G21

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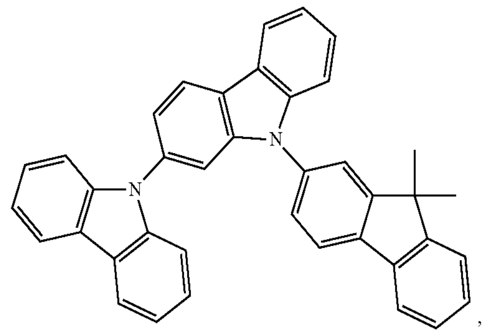
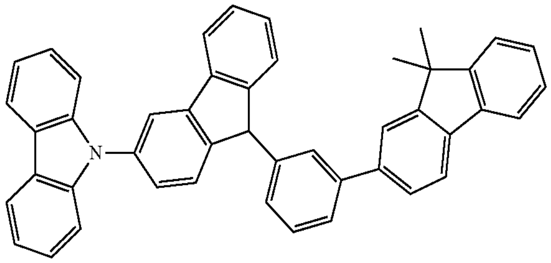
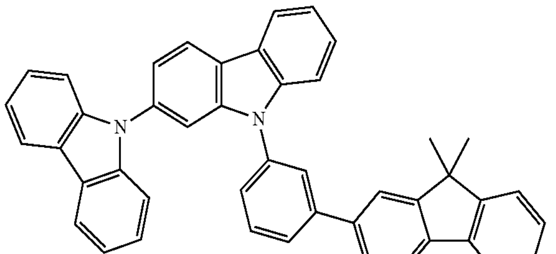
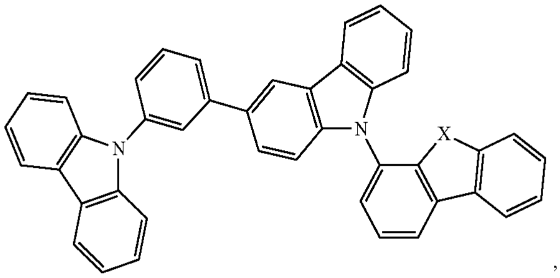

Compound G22


Compound G23


Compound G24

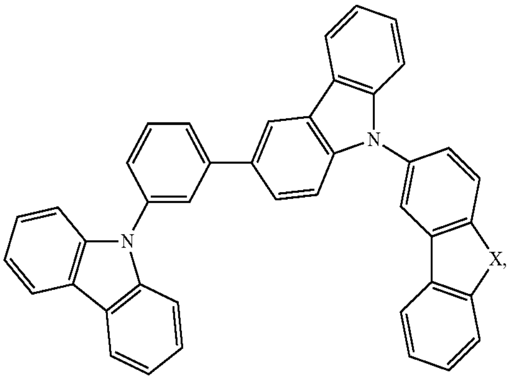
Compound G25 through G27, each represented by the formula



wherin in Compound G25: X = O,
in Compound G26: X = S,
in Compound G27: X = Se

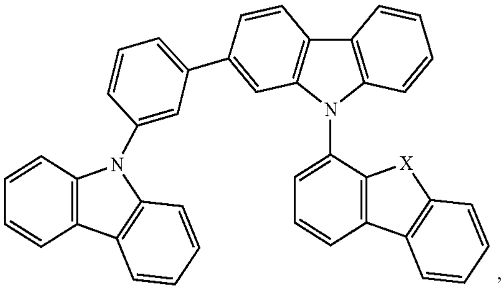
-continued

Compound G28 through G30, each represented by the formula



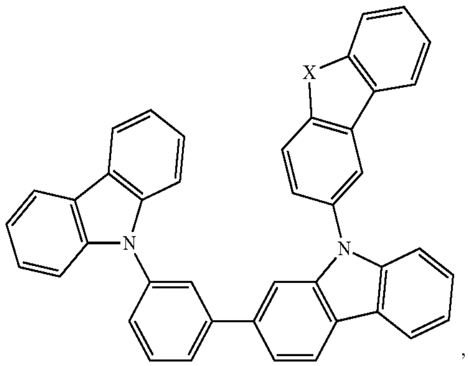
wherin in Compound G28: X = O,
in Compound G29: X = S,
in Compound G30: X = Se

Compound G31 through G33, each represented by the formula



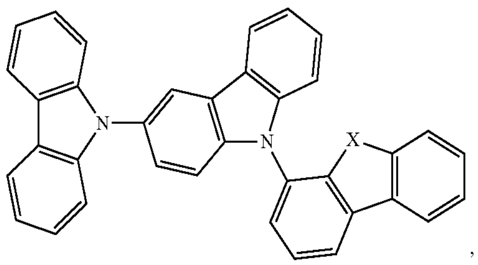
wherin in Compound G31: X = O,
in Compound G32: X = S,
in Compound G33: X = Se

Compound G34 through G36, each represented by the formula



wherin in Compound G34: X = O,
in Compound G35: X = S,
in Compound G36: X = Se

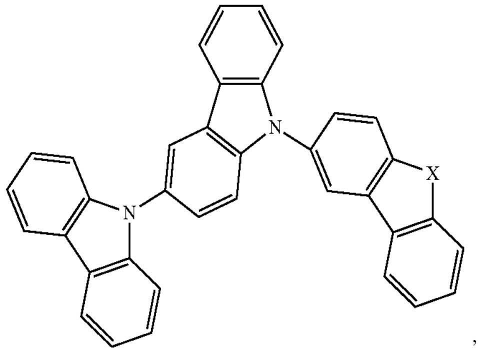
Compound G37 through G39, each represented by the formula



wherin in Compound G37: X = O,
in Compound G38: X = S,
in Compound G39: X = Se

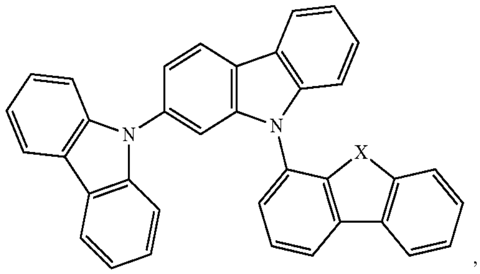
-continued

Compound G40 through G42, each represented by the formula



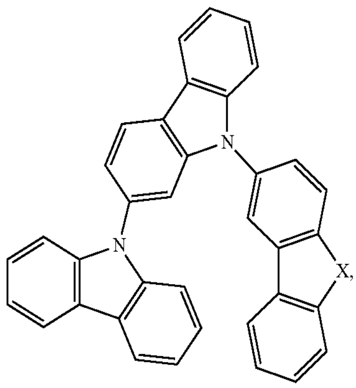
wherin in Compound G40: X = O,
in Compound G41: X = S,
in Compound G42: X = Se

Compound G43 through G45, each represented by the formula



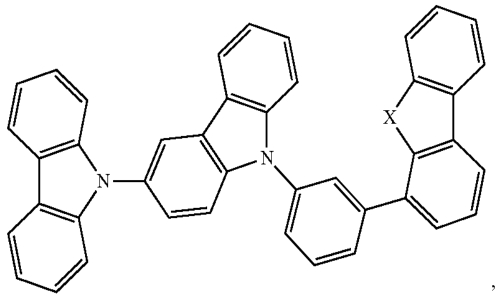
wherin in Compound G43: X = O,
in Compound G44: X = S,
in Compound G45: X = Se

Compound G46 through G48, each represented by the formula



wherin in Compound G46: X = O,
in Compound G47: X = S,
in Compound G48: X = Se

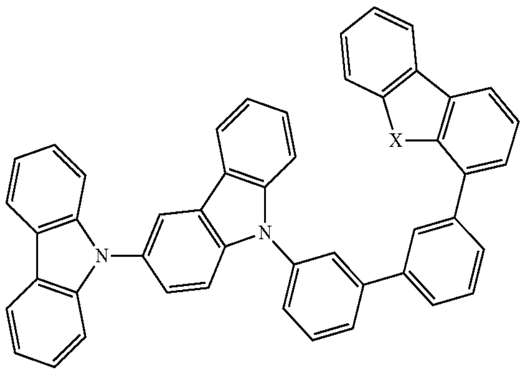
Compound G49 through G51, each represented by the formula



wherin in Compound G49: X = O,
in Compound G50: X = S,
in Compound G51: X = Se

-continued

Compound G52 through G54, each represented by the formula



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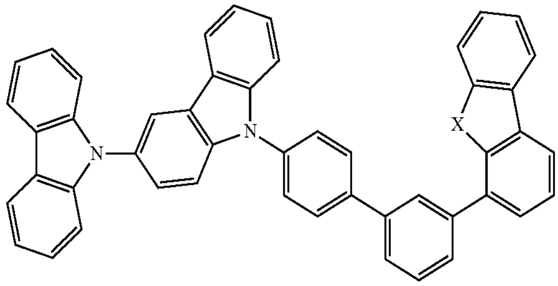
wherin in Compound G52: X = O,
in Compound G53: X = S,
in Compound G54: X = Se

Compound G55 through G57, each represented by the formula



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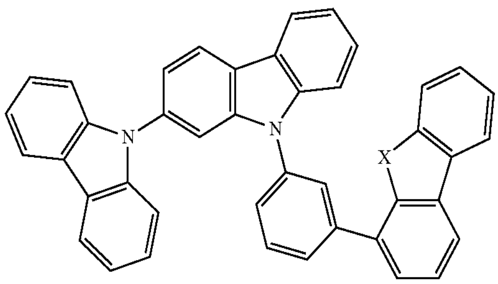
wherin in Compound G55: X = O,
in Compound G56: X = S,
in Compound G57: X = Se

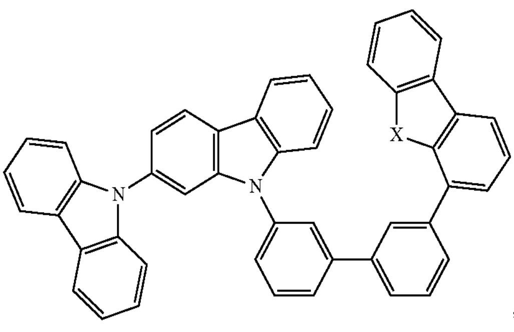
Compound G58 through G60, each represented by the formula



,

wherin in Compound G58: X = O,
in Compound G59: X = S,
in Compound G60: X = Se

Compound G61 through G63, each represented by the formula

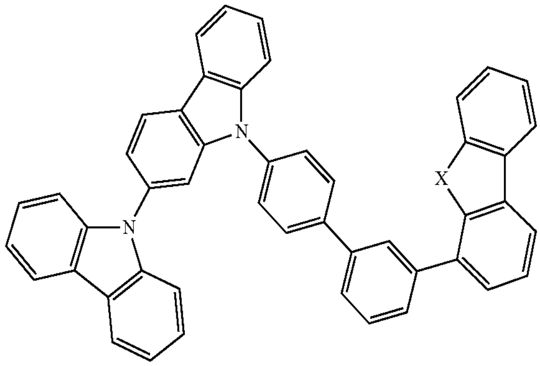


, and

wherin in Compound G61: X = O,
in Compound G62: X = S,
in Compound G63: X = Se

-continued

Compound G64 through G66, each represented by the formula



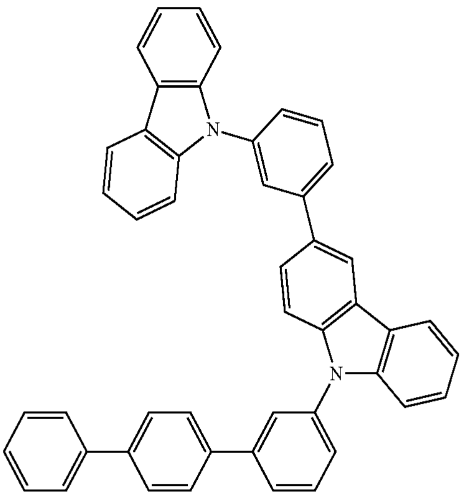
.

wherin in Compound G64: X = O,
in Compound G65: X = S,
in Compound G66: X = Se

In some embodiments, the mixture of the first compound and the second compound is selected from the group consisting of:

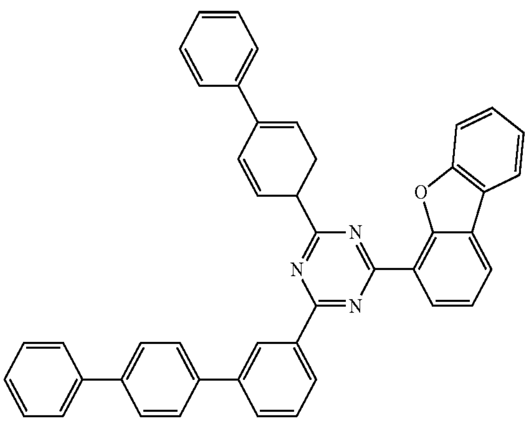
Compound G1

(



,

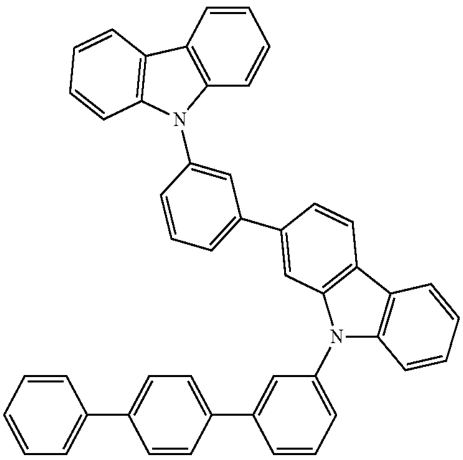
Compound F9



);

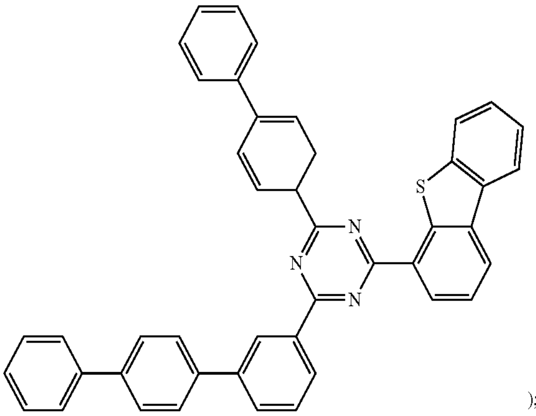
-continued

Compound G2



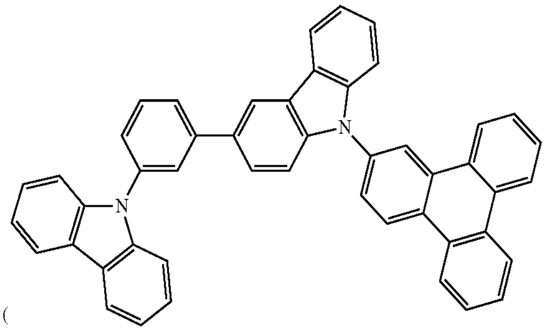
(,

Compound F10



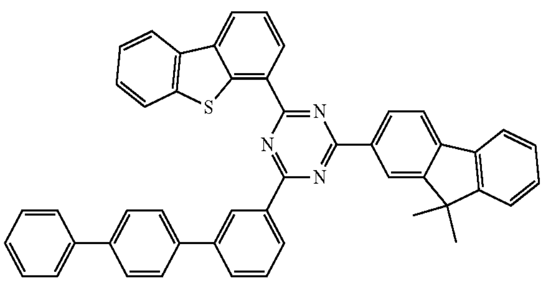
);

Compoung G8



(,

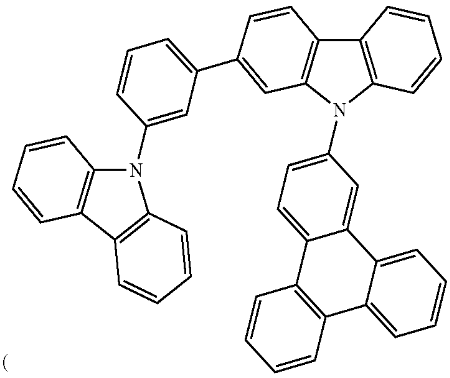
Compound F13



);

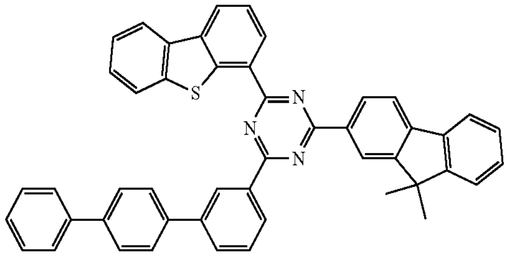
-continued

Compound G9



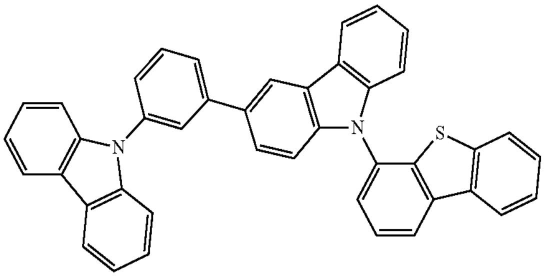
(,

Compound F13



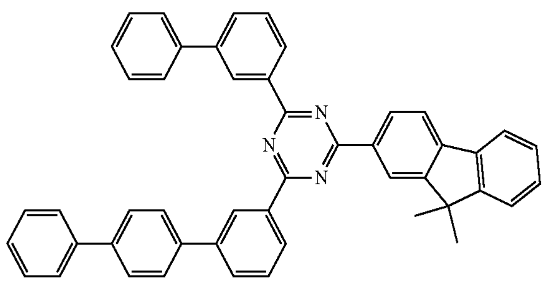
); and

Compound G26



(,

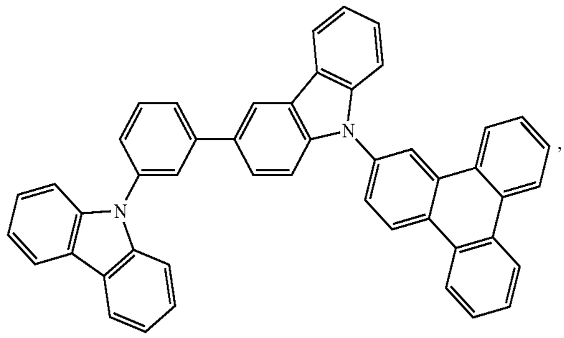
Compound F5



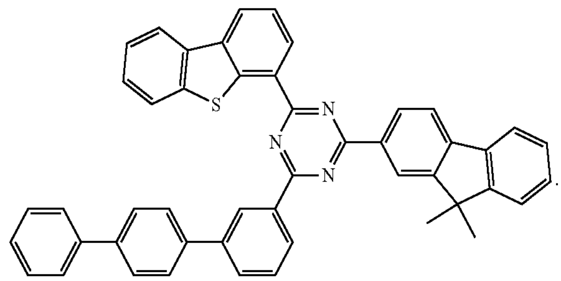
).

In some embodiments, the mixture of the first compound and the second compound is

(Compound G8



Compound F13)



In some embodiments, the first compound has an evaporation temperature T1 of 150 to 350° C., the second compound has an evaporation temperature T2 of 150 to 350° C., or both. In some embodiments, the absolute value of T1-T2 is less than 20° C. In some embodiments, the first compound has a concentration C1 in said mixture and a concentration C2 in a film formed by evaporating the mixture in a vacuum deposition tool at a constant pressure between 1×10^{-6} Torr to 1×10^{-9} Torr, at a 2 Å/sec deposition rate on a surface positioned at a predefined distance away from the mixture being evaporated. In some embodiments, the absolute value of (C1-C2)/C1 is less than 5%.

In some embodiments, the first compound has a vapor pressure of P1 at T1 at 1 atm, the second compound has a vapor pressure of P2 at T2 at 1 atm; and the ratio of P1/P2 is within the range of 0.90 to 1.10.

In some embodiments, the first compound has a first mass loss rate and the second compound has a second mass loss rate, where the ratio between the first mass loss rate and the second mass loss rate is within the range of 0.90 to 1.10.

In some embodiments, the first compound and the second compound each has a purity in excess of 99% as determined by high pressure liquid chromatography.

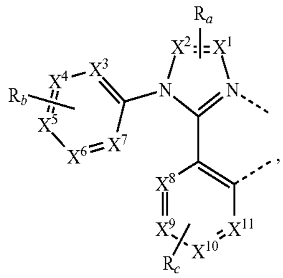
In some embodiments, the composition further comprises a third compound, where the third compound has a different chemical structure than the first and second compounds. In some embodiments, the third compound has an evaporation temperature T3 of 150 to 350° C., and wherein absolute value of T1-T3 is less than 20° C. In some embodiments, the third compound has a third mass loss rate and the ratio between the first mass loss rate and third mass loss rate is within the range of 0.90 to 1.10.

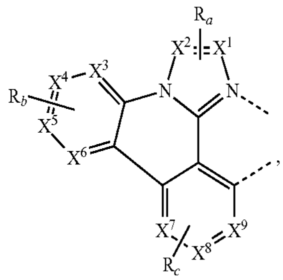
In some embodiments, the composition is in liquid form at a temperature less than T1 and T2.

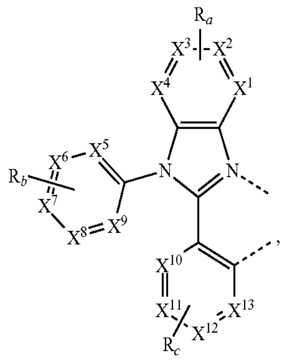
According to another aspect of the present disclosure, a device that includes one or more organic light emitting devices is also provided. At least one of the one or more organic light emitting devices can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer can include a composition comprising a compound according to a structure of Formula I or Formula III, or any of the variations thereof described herein.

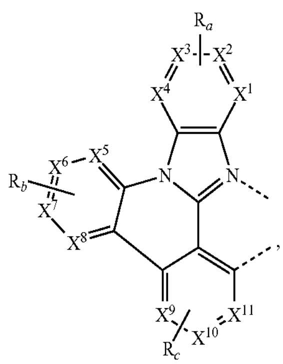
In some embodiments, the organic layer is an emissive layer and the composition comprises a host.

In some embodiments, the organic layer also includes a phosphorescent emissive dopant. In some embodiments, the phosphorescent emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:









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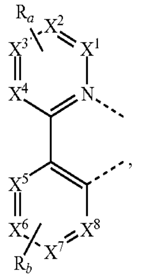

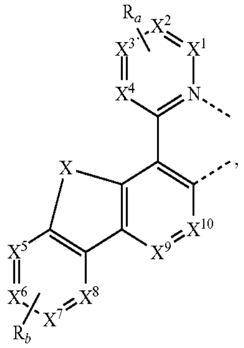

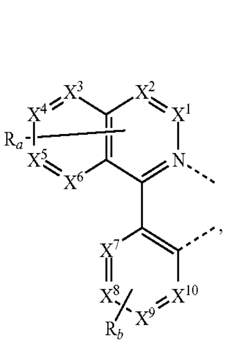

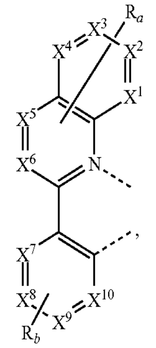

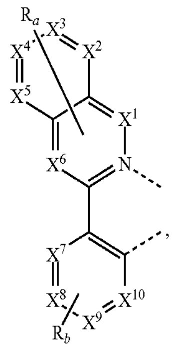

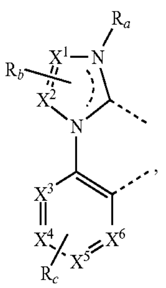

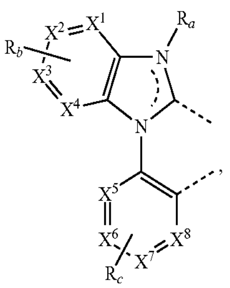

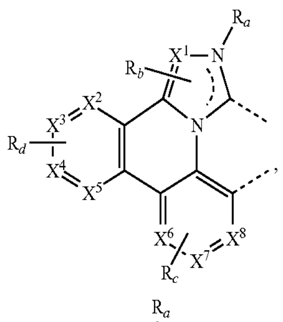

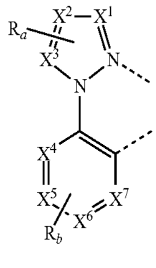

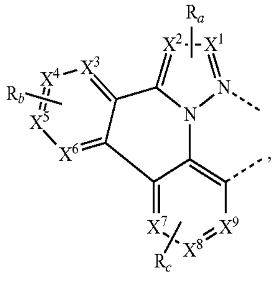

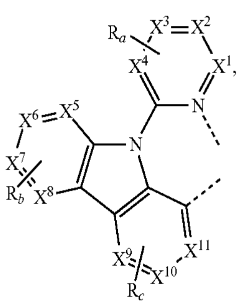

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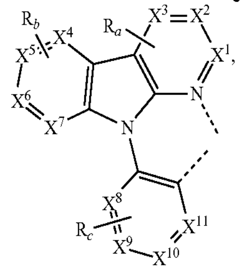
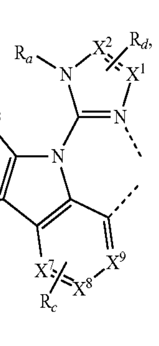


and



each X^1 to X^{13} are independently selected from the group consisting of carbon and nitrogen;

X is selected from the group consisting of BR', NR', PR', O, S, Se, C=O, S=O, SO_2, CR'R', SiR'R", and GeR'R";

R' and R" are optionally fused or joined to form a ring;

each R_a, R_b, R_c, and R_d may represent from mono substitution to the possible maximum number of substitution, or no substitution;

R', R", R_a, R_b, R_c, and R_d are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

any two adjacent substitutents of R_a, R_b, R_c, and R_d are optionally fused or joined to form a ring or form a multidentate ligand.

In some embodiments, the organic layer is a blocking layer and the composition is a blocking material in the organic layer. In some embodiments, the organic layer is an electron transporting layer and the composition is an electron transporting material in the organic layer.

In some embodiments, the first device is selected from the group consisting of a consumer product, an electronic component module, an organic light-emitting device, and a lighting panel.

In some embodiments, at least one of R_a, R_b, R_c, and R_d is selected from the group consisting of alkyl, cycloalkyl, partially or fully deuterated variants thereof, partially or fully fluorinated variants thereof, and combinations thereof.

In yet another aspect of the present disclosure, a method for fabricating an organic light emitting device is provided. The organic light emitting device can include a first electrode, a second electrode, and a first organic layer disposed between the first electrode and the second electrode, where the first organic layer comprises a first composition comprising a mixture of a first compound and a second compound.

In some embodiments, the method includes providing a substrate having the first electrode disposed thereon; depositing the first composition over the first electrode; and depositing the second electrode over the first organic layer. In some embodiments, the first composition is selected from the group consisting of Formulation I and Formulation II, where Formulation I comprises a first compound of Formula I and a second compound of Formula II, and where Formulation II comprises a first compound of Formula III and a second compound of Formula IV.

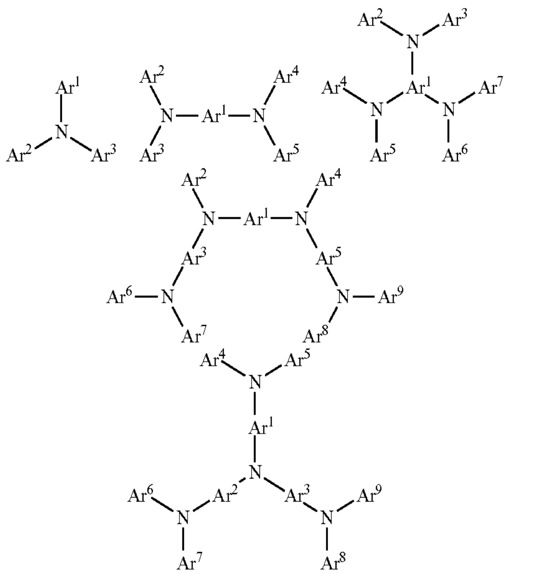
Combination with Other Materials

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

HIL/HTL:

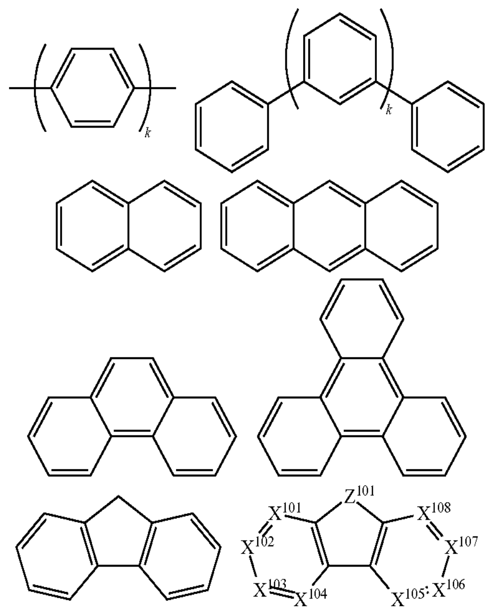
A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but are not limited to: a phthalocyanine or porphyrin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

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



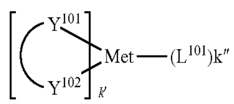
Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

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



wherein k is an integer from 1 to 20; X^{101} to X^{108} is C (including CH) or N; Z^{101} is NAr^1, O, or S; Ar^1 has the same group defined above.

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



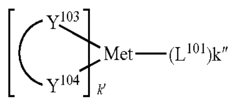
wherein Met is a metal, which can have an atomic weight greater than 40; (Y^{101}-Y^{102}) is a bidentate ligand, Y^{101} and Y^{102} are independently selected from C, N, O, P, and S; L^{101} is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached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

In one aspect, (Y^{101}-Y^{102}) is a 2-phenylpyridine derivative. In another aspect, (Y^{101}-Y^{102}) is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

Host:

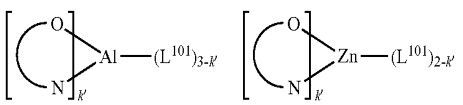
The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. While the Table below categorizes host materials as preferred for devices that emit various colors, any host material may be used with any dopant so long as the triplet criteria is satisfied.

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



wherein Met is a metal; (Y^{103}-Y^{104}) is a bidentate ligand, Y^{103} and Y^{104} are independently selected from C, N, O, P, and S; L^{101} is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

In one aspect, the metal complexes are:

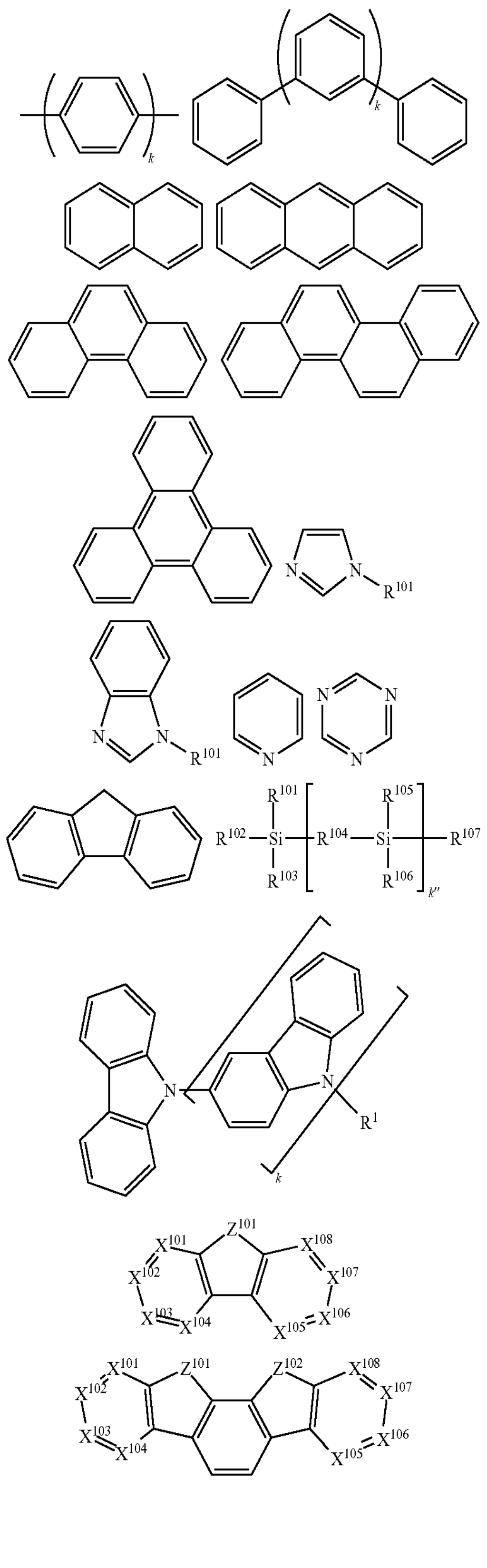


wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

In another aspect, Met is selected from Ir and Pt. In a further aspect, (Y^{103}-Y^{104}) is a carbene ligand.

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

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



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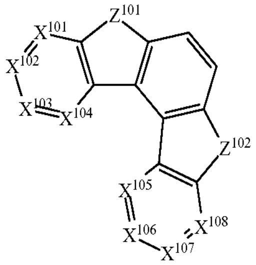
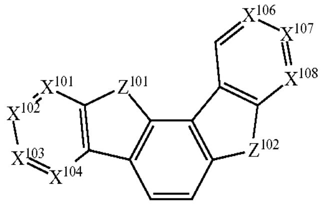
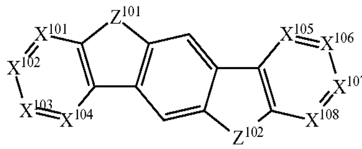
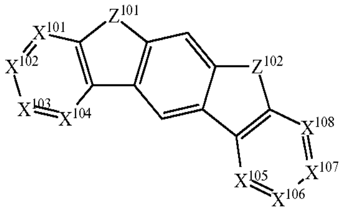








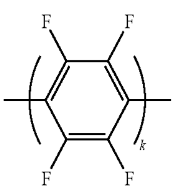
wherein R^{110} to R^{107} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. k is an integer from 0 to 20 or 1 to 20; k''' is an integer from 0 to 20. X^{101} to X^{108} is selected from C (including CH) or N. Z^{101} and Z^{102} is selected from NR^{101}, O, or S.

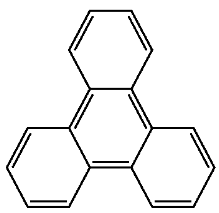
HBL:

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

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

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





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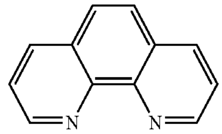
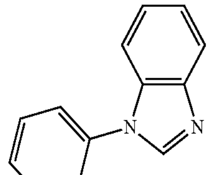
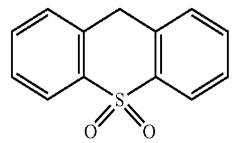
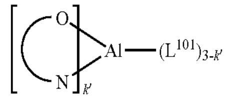






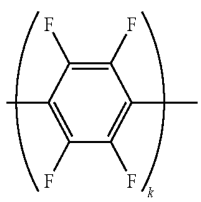


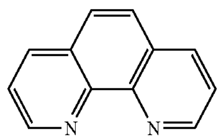
wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

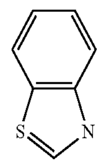
ETL:

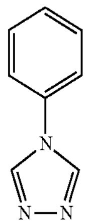
Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may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

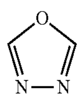
In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

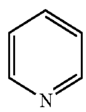


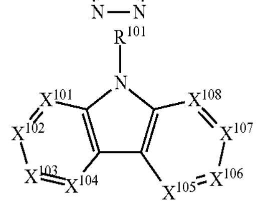


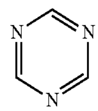


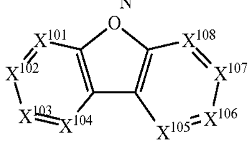


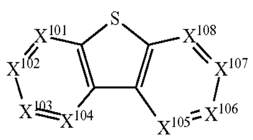


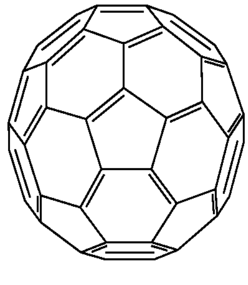


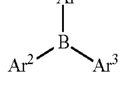






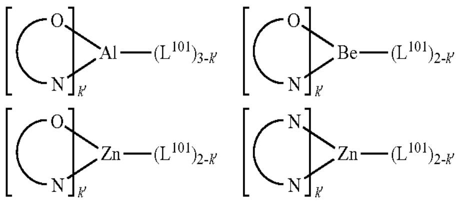






wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. Ar^1 to Ar^3 has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X^{101} to X^{108} is selected from C (including CH) or N.

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



wherein (O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L^{101} is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated. Thus, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. encompasses undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also encompass undeuterated, partially deuterated, and fully deuterated versions thereof.

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

TABLE A

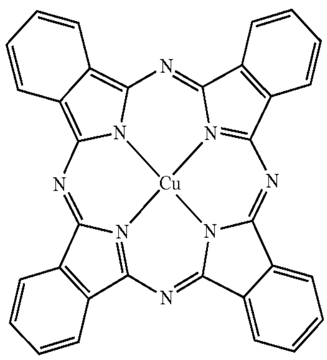
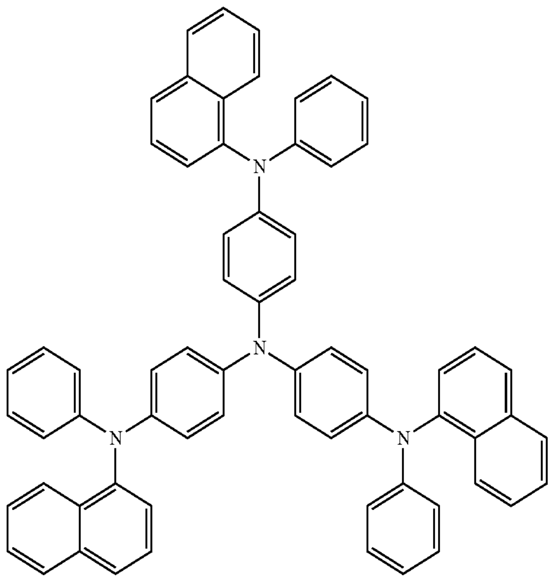
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphyrin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydrocarbon polymer	$-[CH_xF_y]_n-$	Appl. Phys. Lett. 78, 673 (2001)

TABLE A-continued

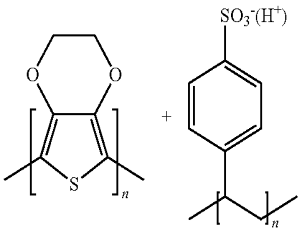
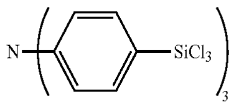
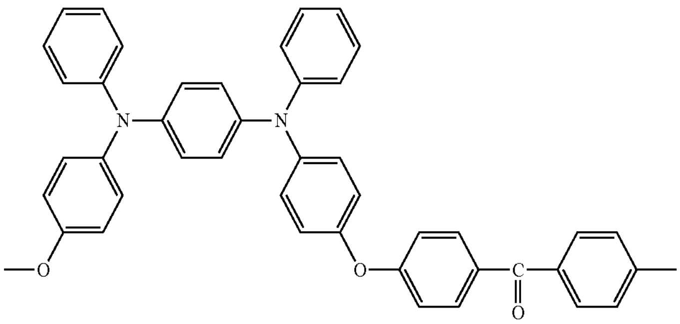
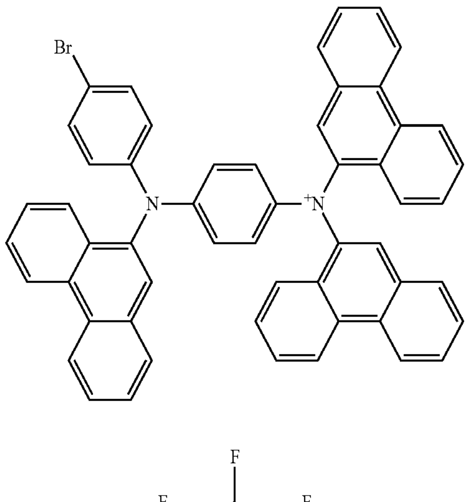
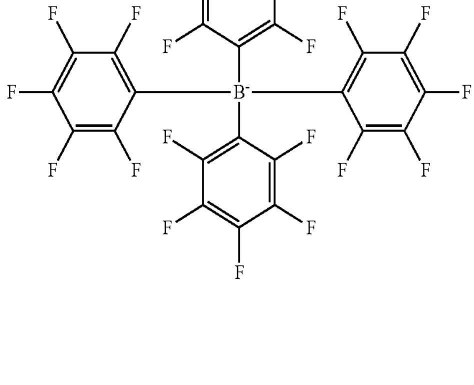
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and silane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants	 and  	EP1725079A1

TABLE A-continued

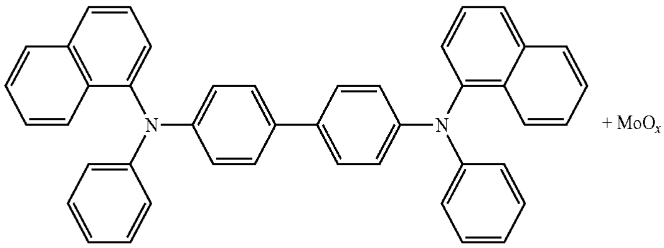
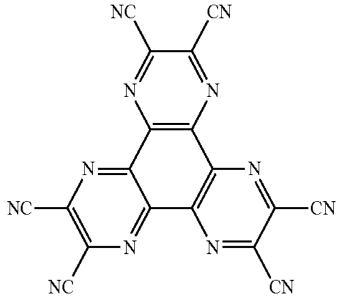
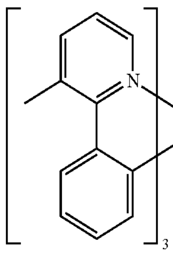
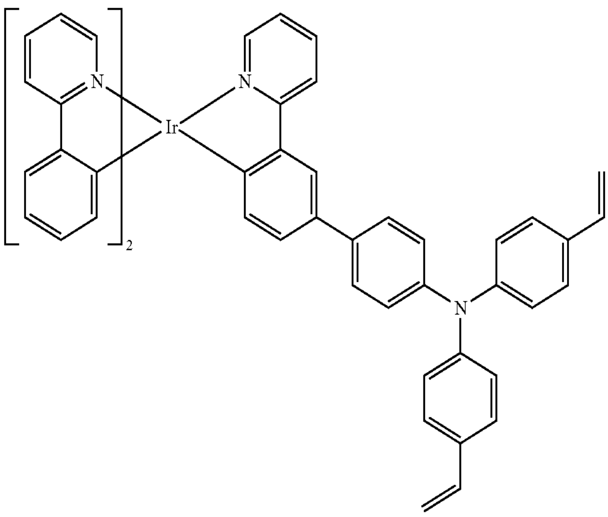
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides		US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009
n-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265

TABLE A-continued

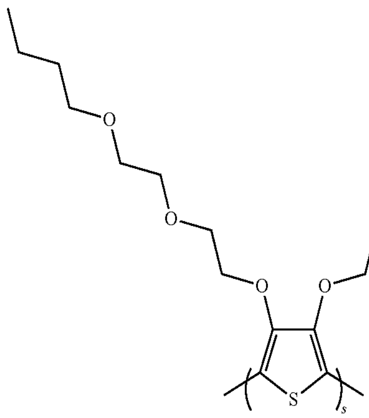
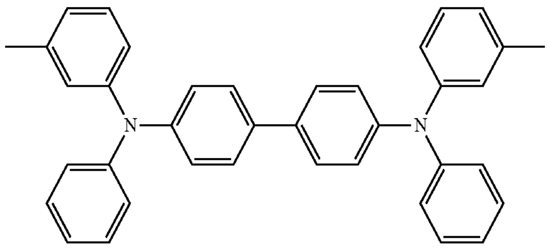
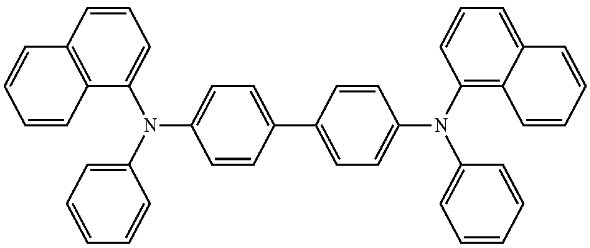
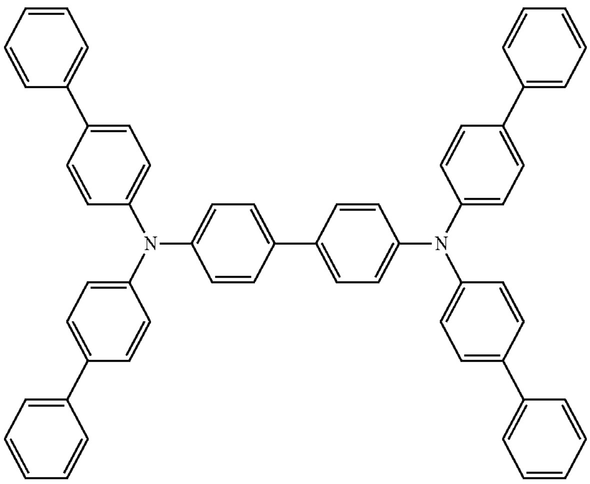
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216
	Hole transporting materials	
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5,061,569
		EP650955

TABLE A-continued

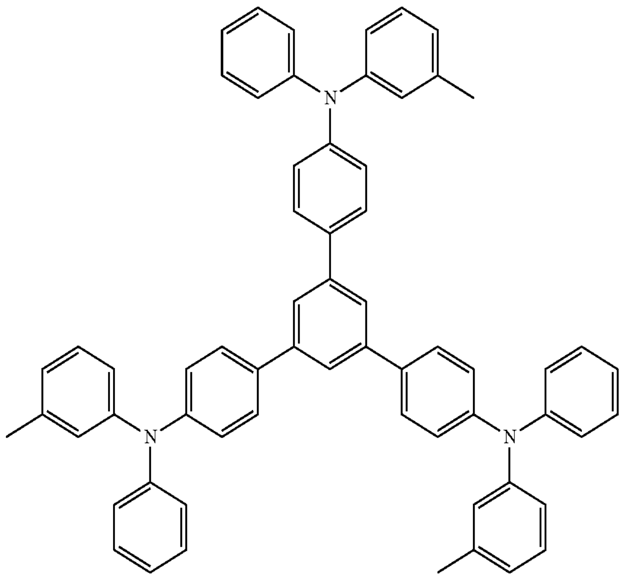
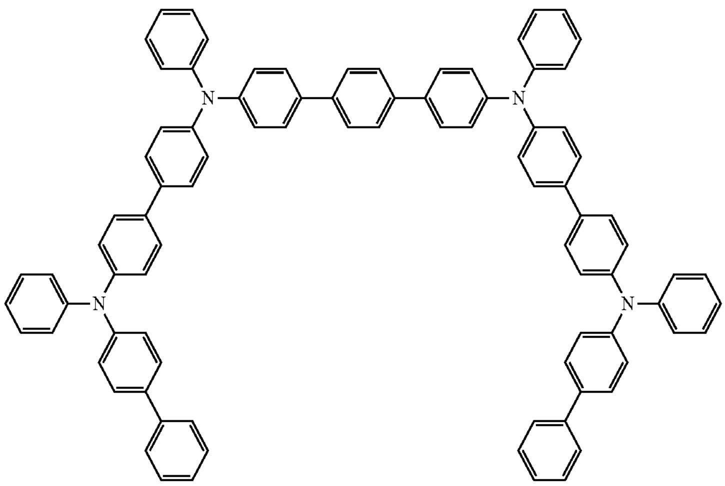
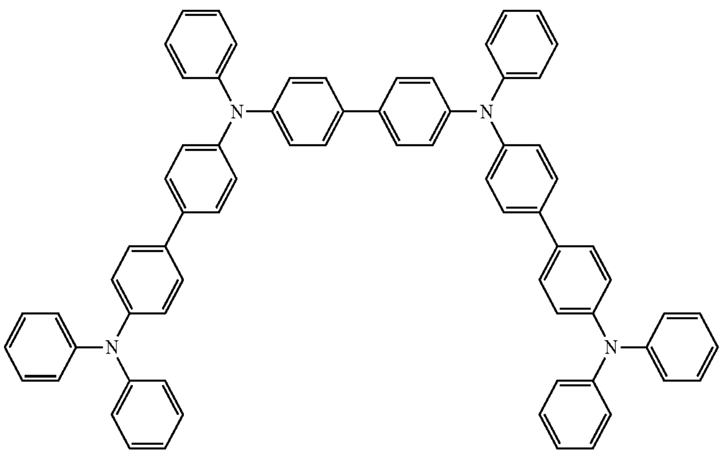
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		J. Mater. Chem. 3, 319 (1993)
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE A-continued

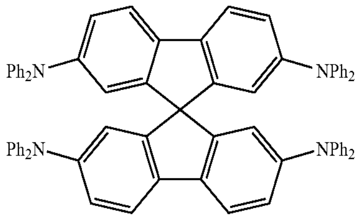
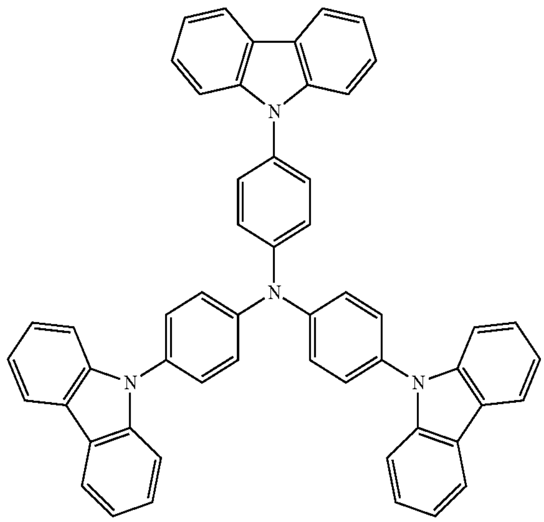
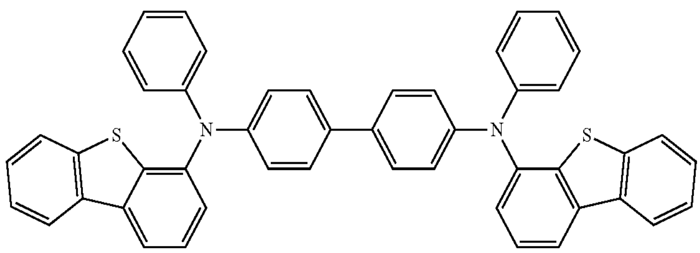
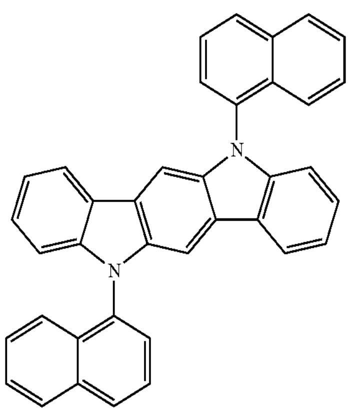
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/(di)-benzofuran		US20070278938, US20080106190 US20110163302
Indolocarbazoles		Synth. Met. 111, 421 (2000)

TABLE A-continued

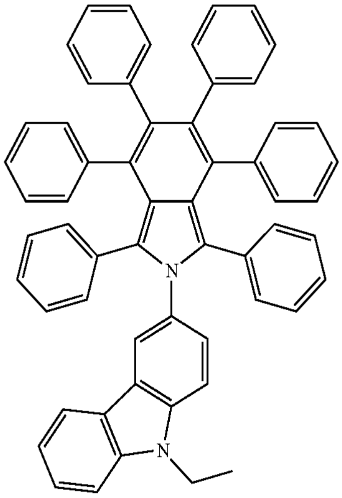
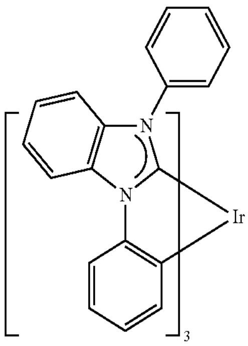
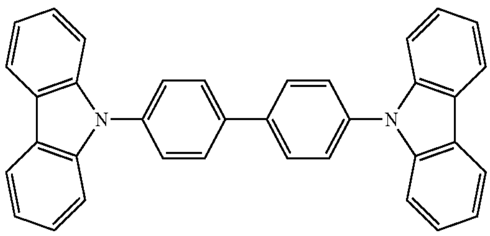
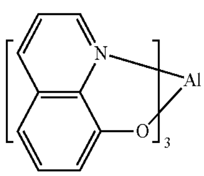
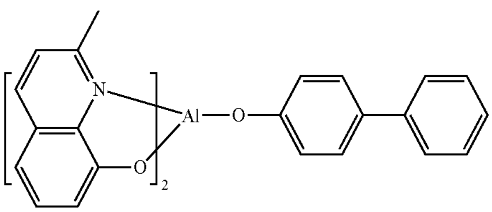
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED host materials Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194

TABLE A-continued

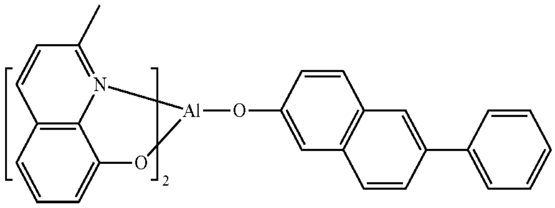
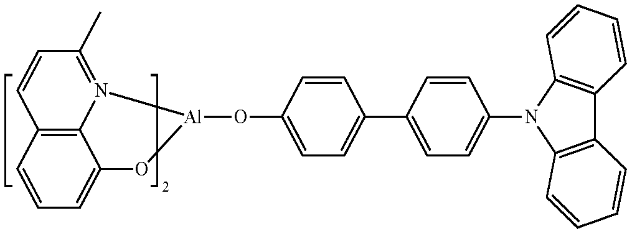
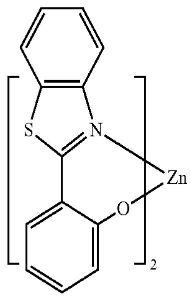
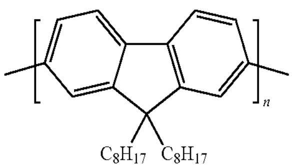
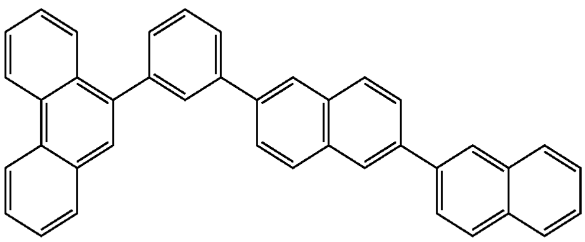
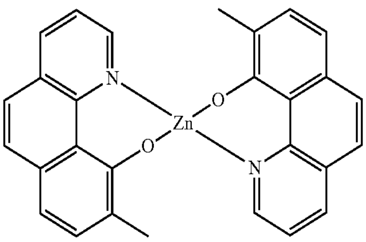
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2010056066

TABLE A-continued

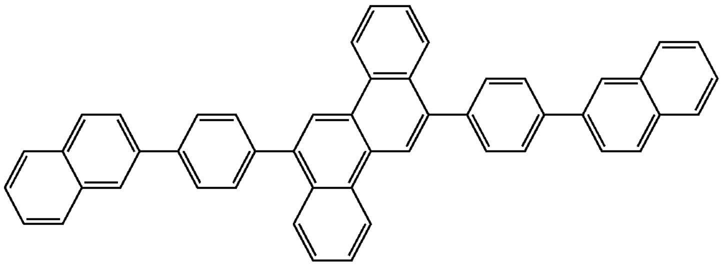
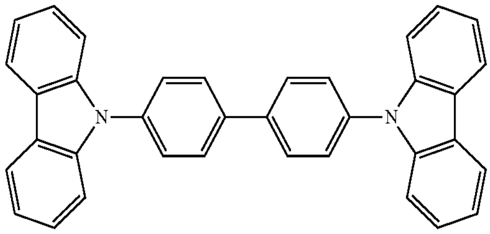
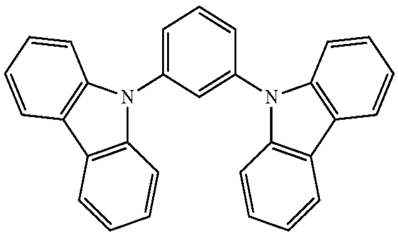
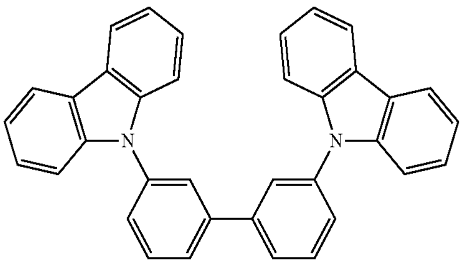
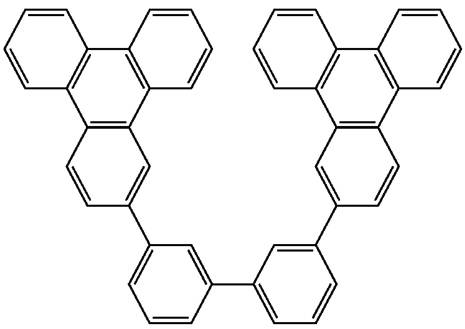
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Chrysene based compounds		WO2011086863
	Green hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE A-continued

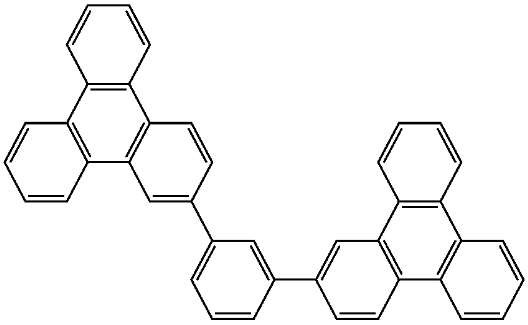
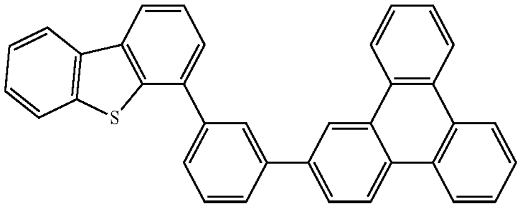
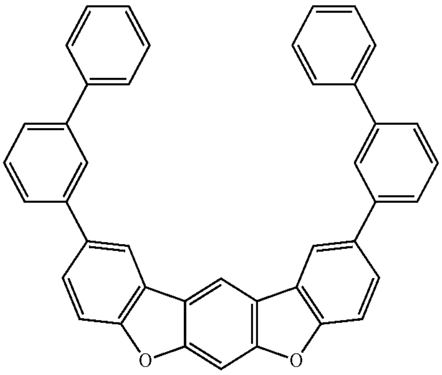
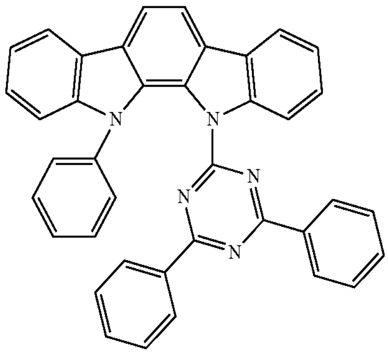
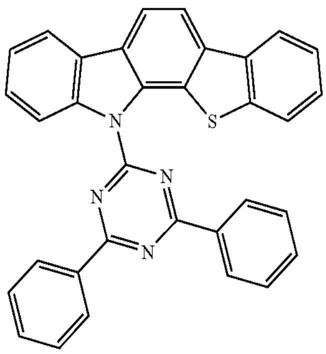
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060280965
		WO2009021126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931
Donor acceptor type molecules		WO2008056746
		WO2010107244

TABLE A-continued

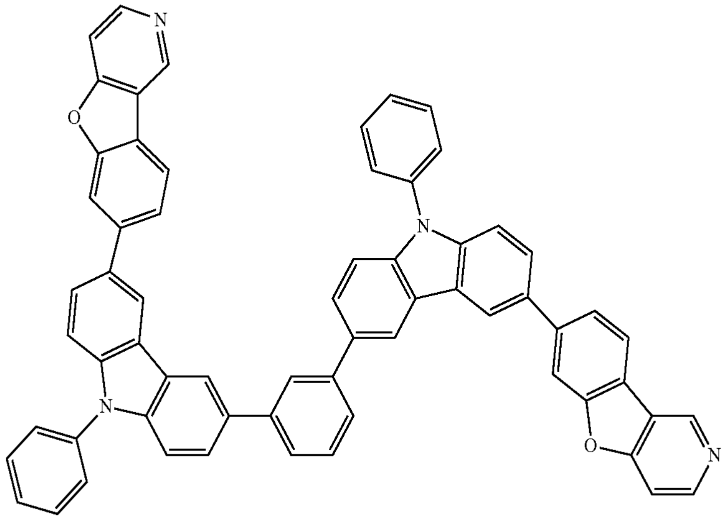
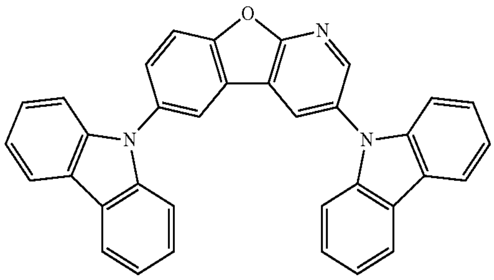
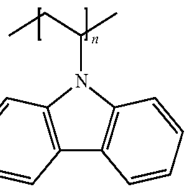
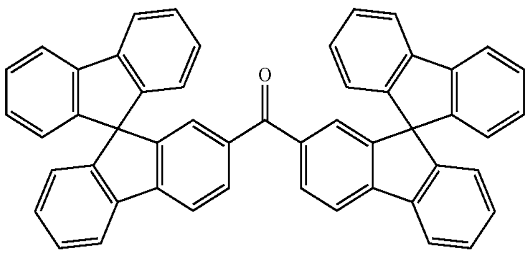
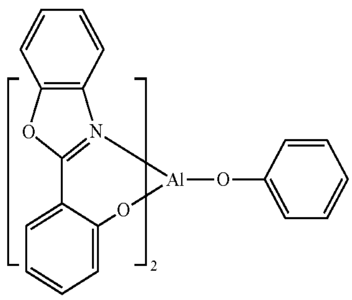
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza-carbazole/DBT/DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207
Metal phenoxybenzooxazole compounds		WO2005089025

TABLE A-continued

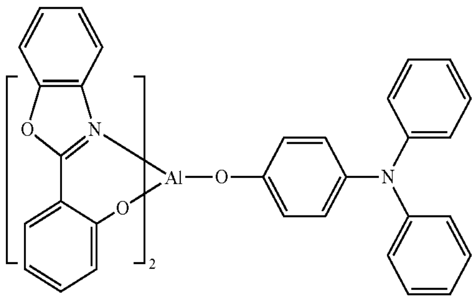
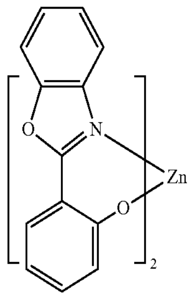
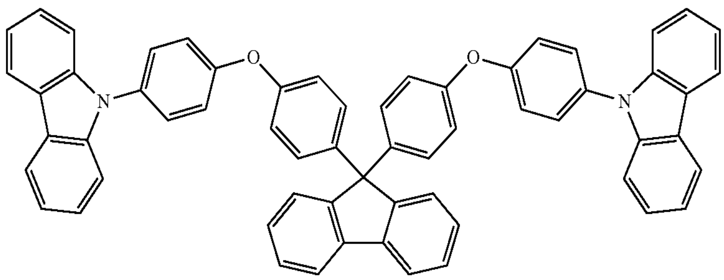
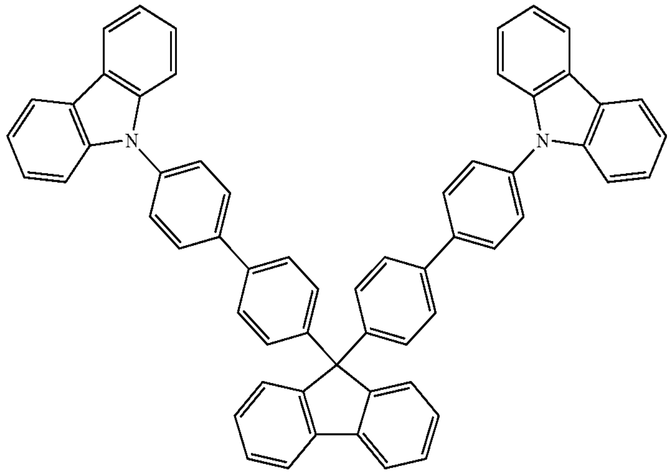
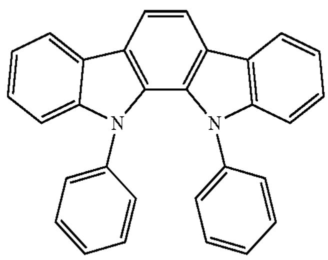
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297
Indolocarbazoles		WO2007063796

TABLE A-continued

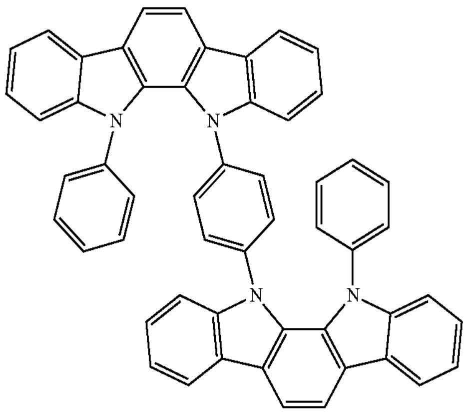
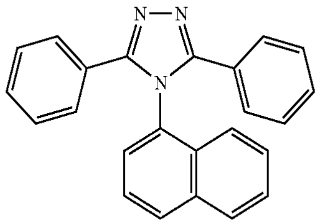
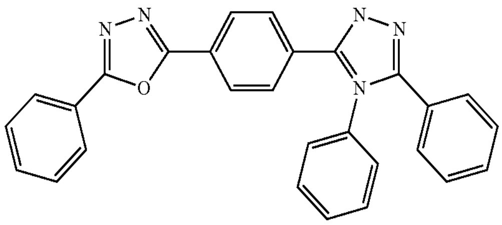
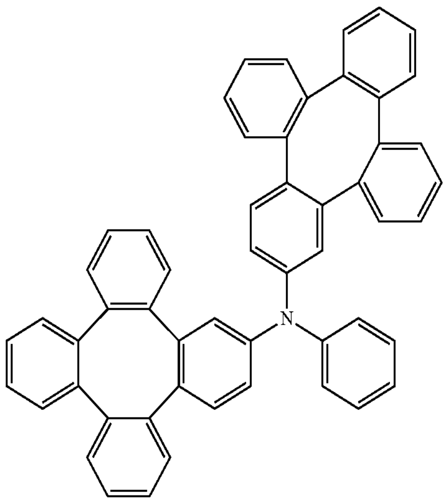
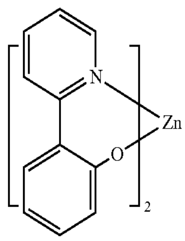
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822
Tetraphenylene complexes		US20050112407
Metal phenoxypyridine compounds		WO2005030900

TABLE A-continued

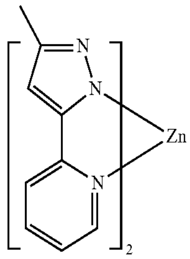
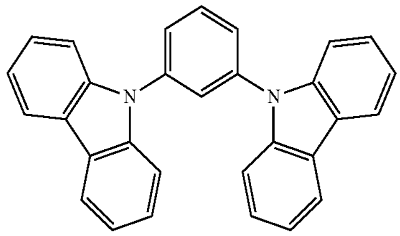
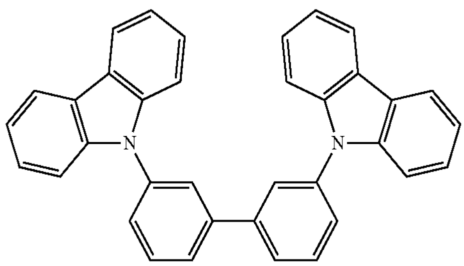
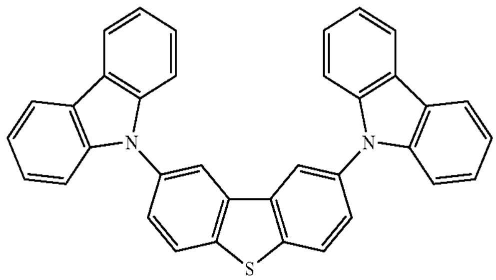
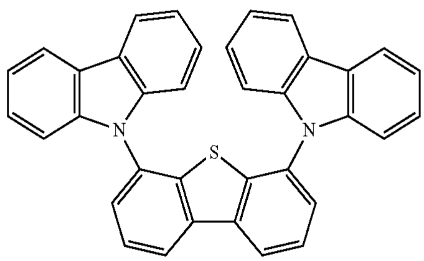
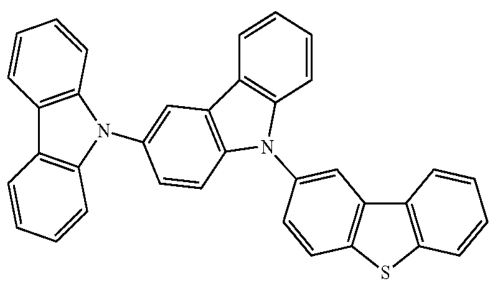
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162
		WO2009086028

TABLE A-continued

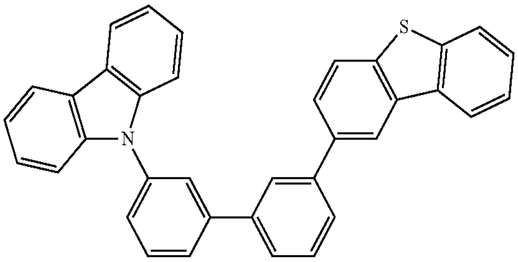
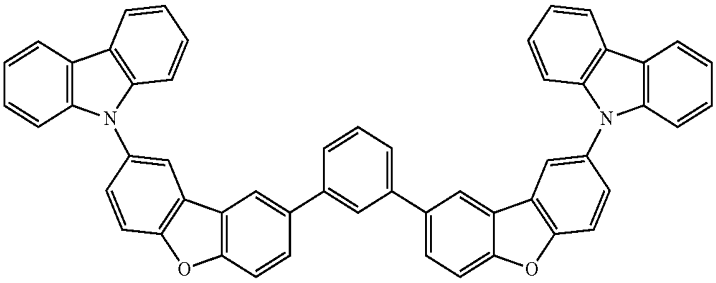
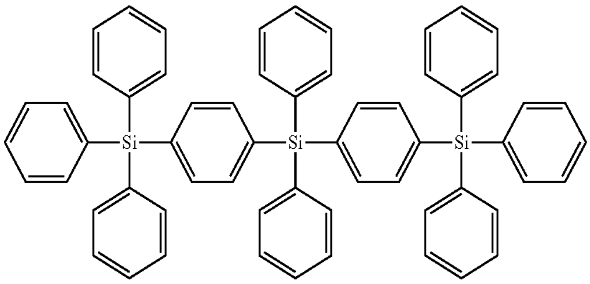
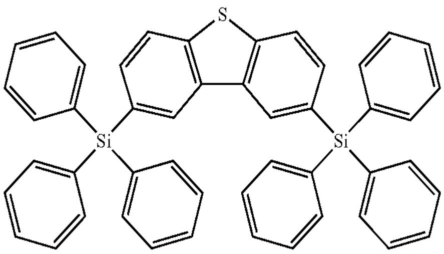
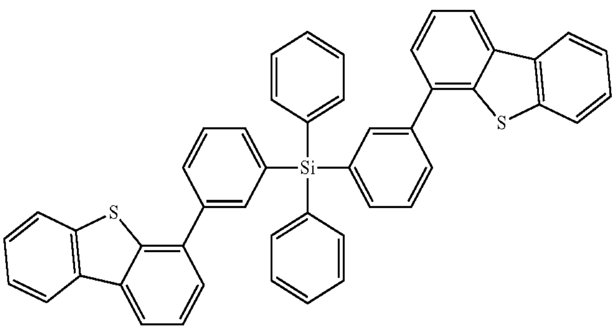
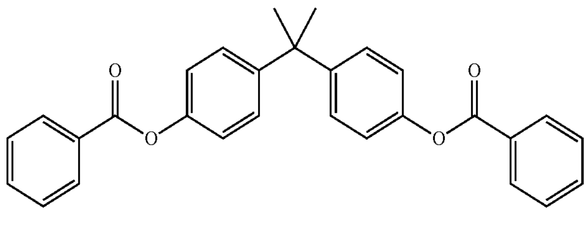
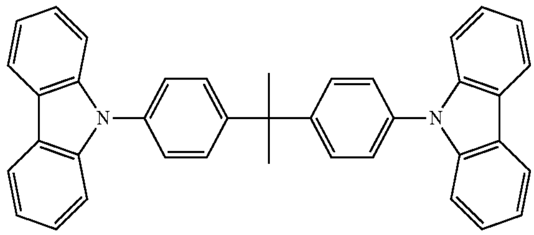
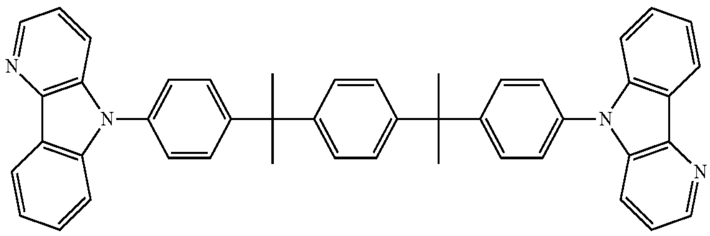
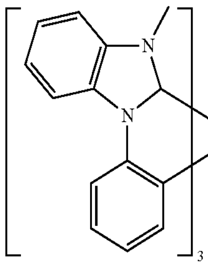
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090030202, US20090017330
		US20100084966
Silicon aryl compounds		US20050238919
		WO2009003898
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298

TABLE A-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114

Phosphorescent dopants
Red dopants

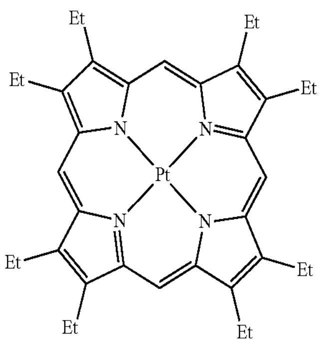
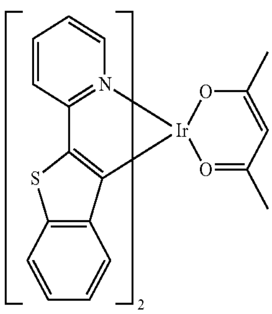
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)

TABLE A-continued

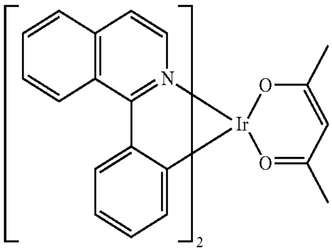
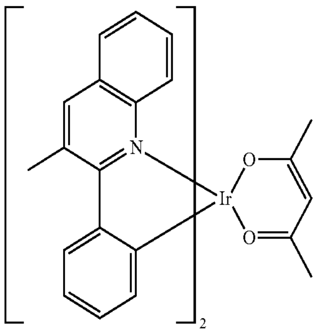
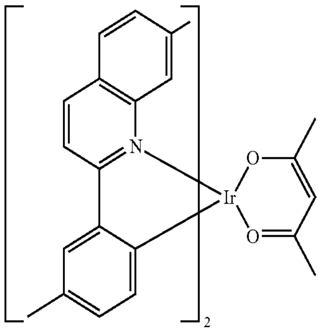
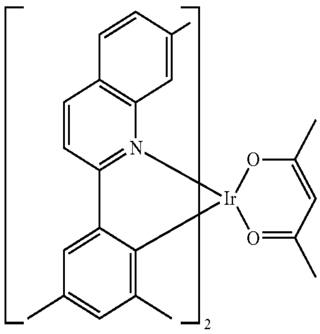
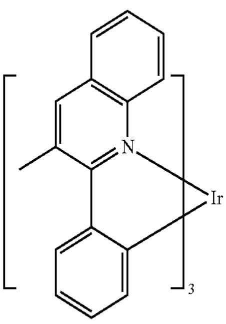
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20030072964
		US20030072964
		US20060202194
		US20060202194
		US20070087321

TABLE A-continued

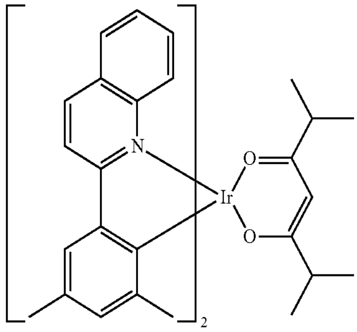
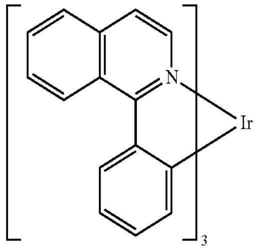
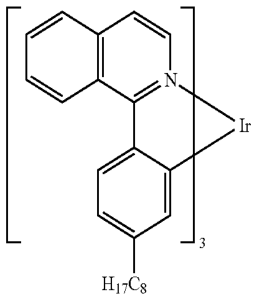
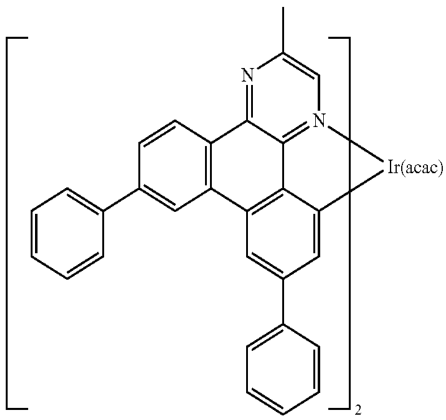
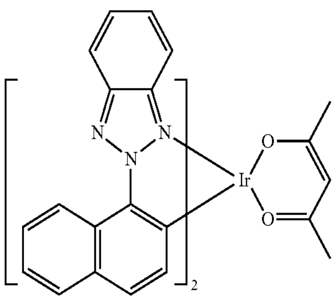
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20080261076 US20100090591
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991
		WO2008101842

TABLE A-continued

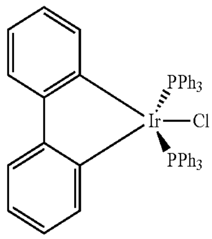
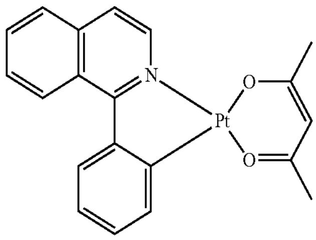
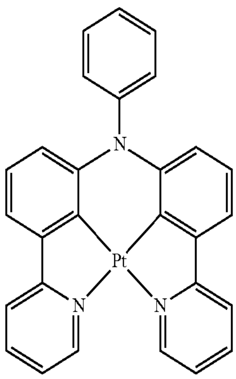
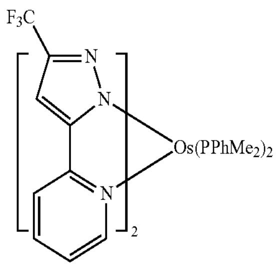
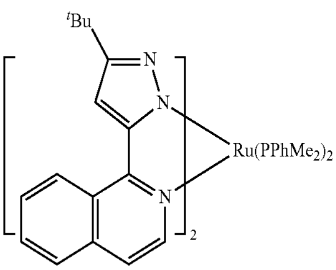
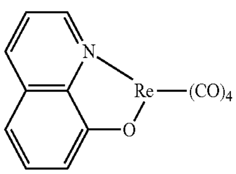
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,232,618
Platinum(II) organometallic complexes		WO2003040257
		US20070103060
Osmium(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673

TABLE A-continued

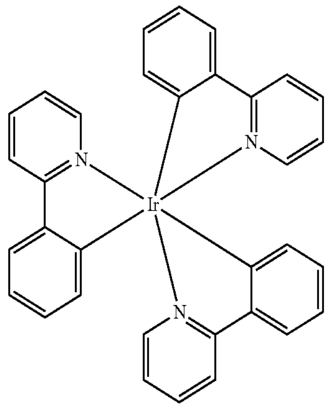
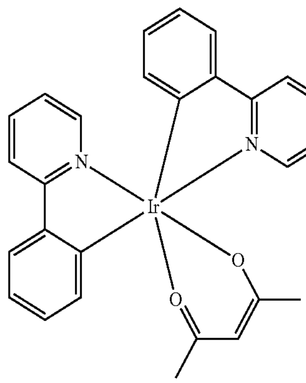
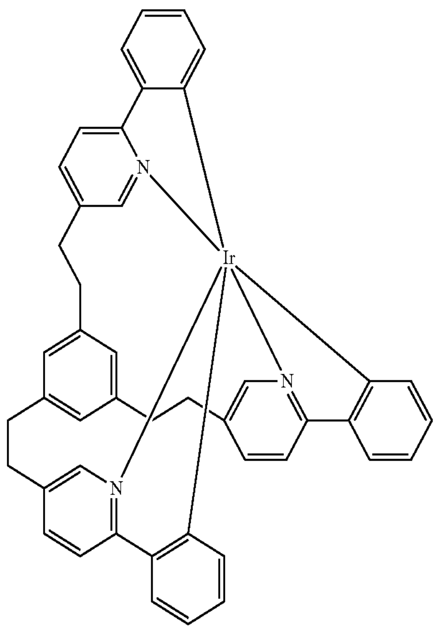
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Green dopants	
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656
		U.S. Pat. No. 7,332,232

TABLE A-continued

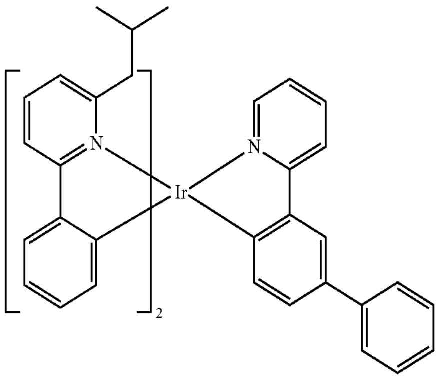
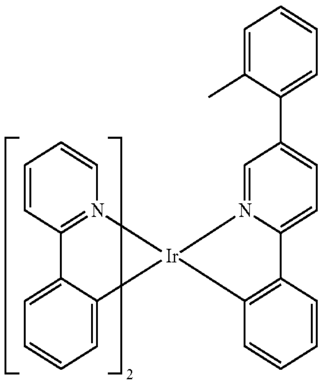
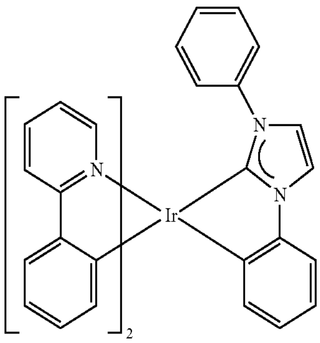
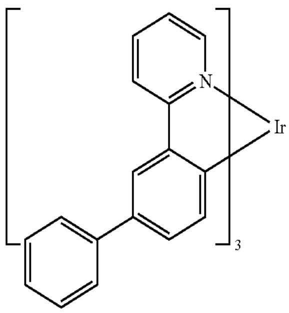
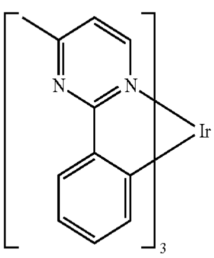
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090108737
		WO2010028151
		EP1841834B
		US20060127696
		US20090039776

TABLE A-continued

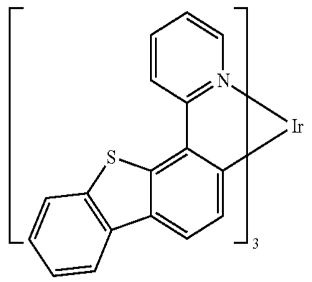
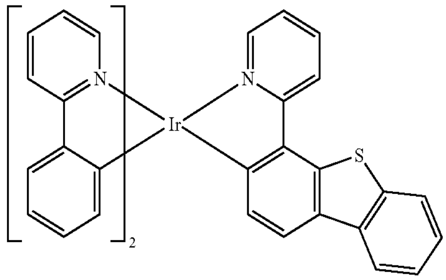
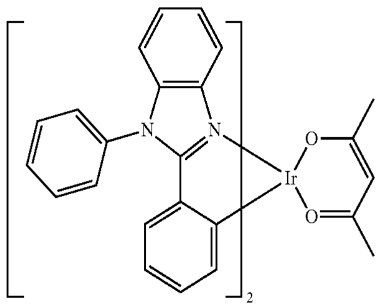
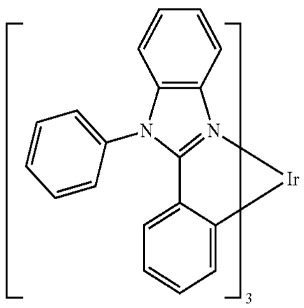
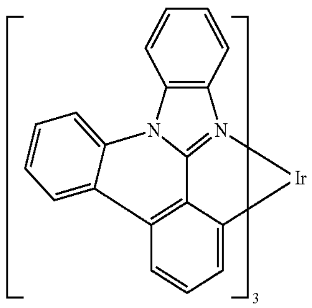
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 6,921,915
		US20100244004
		U.S. Pat. No. 6,687,266
		Chem. Mater. 16, 2480 (2004)
		US20070190359

TABLE A-continued

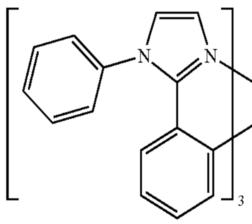
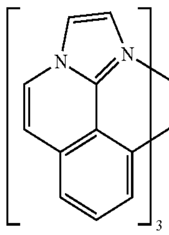
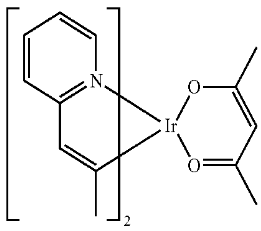
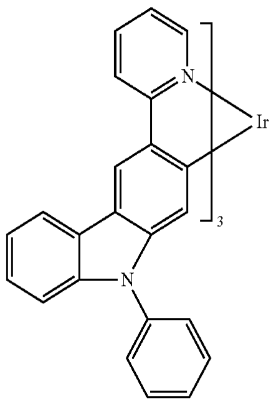
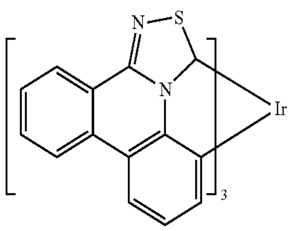
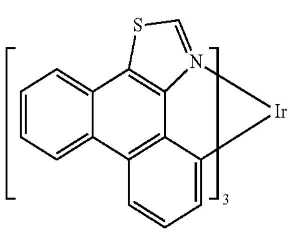
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US 20060008670 JP2007123392
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846

TABLE A-continued

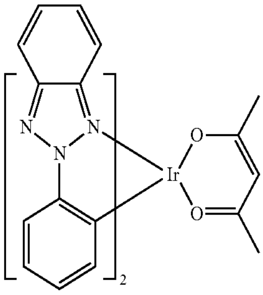
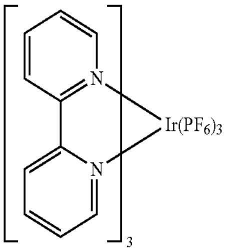
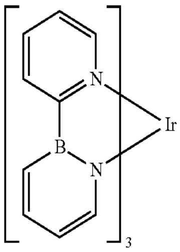
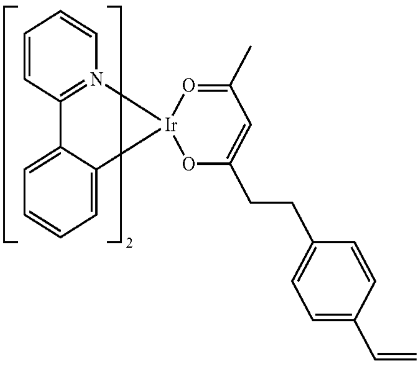
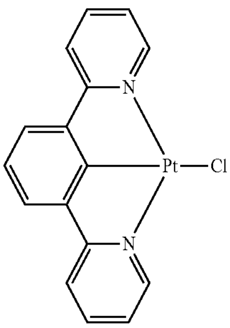
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20080015355
		US20010015432
		US20100295032
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentate ligands		Appl. Phys. Lett. 86, 153505 (2005)

TABLE A-continued

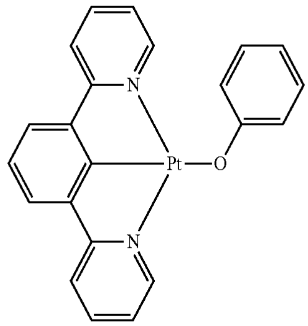
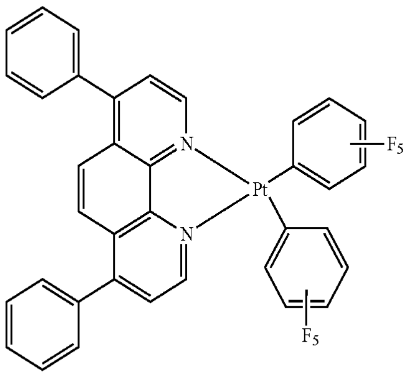
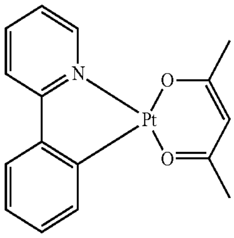
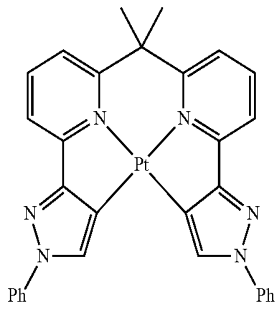
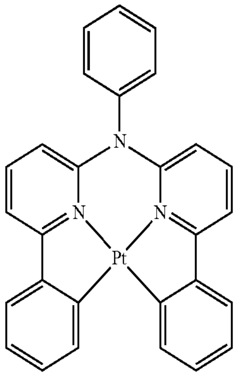
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635
		US20060182992 US20070103060

TABLE A-continued

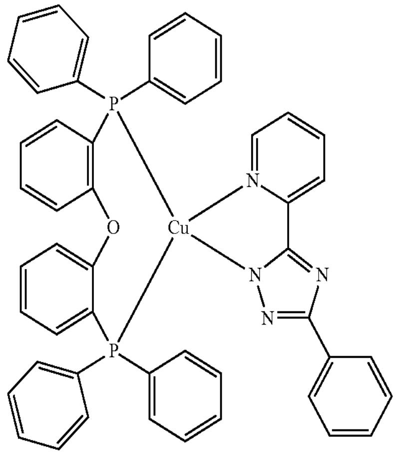
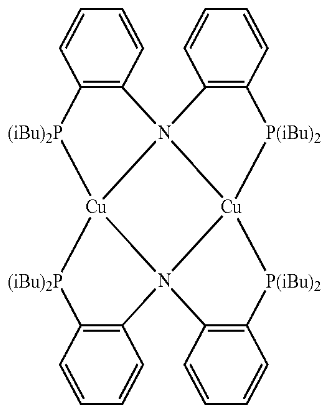
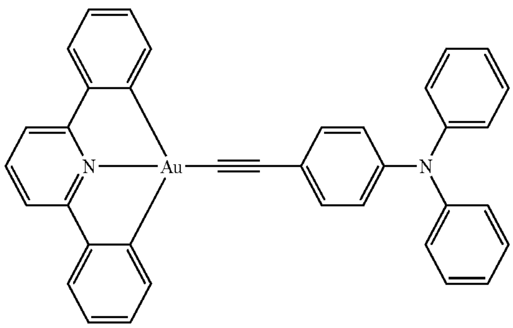
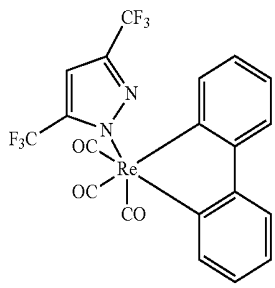
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
		US20070111026
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE A-continued

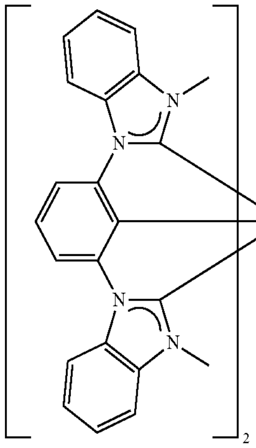
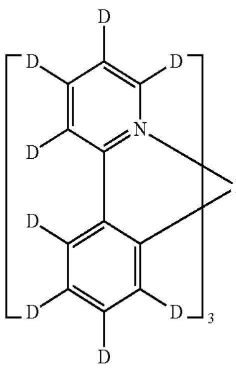
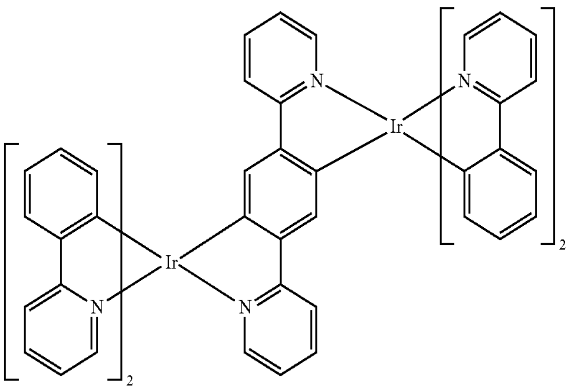
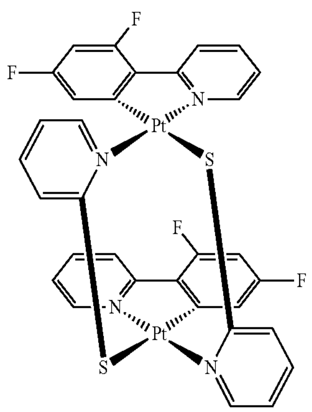
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(II) complexes		U.S. Pat. No. 7,279,704
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928

TABLE A-continued

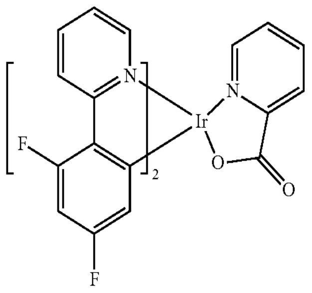
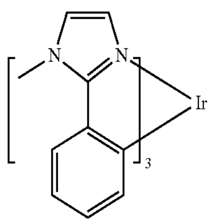
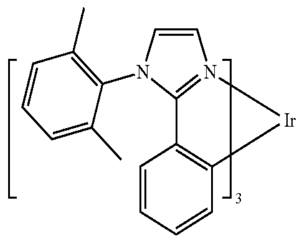
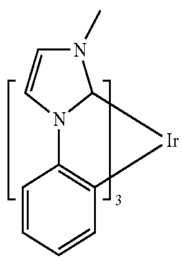
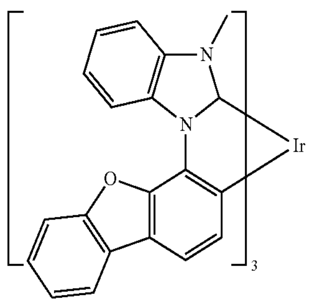
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Blue dopants	
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		U.S. Pat. No. 7,393,599, WO2006056418, US20050260441, WO2005019373
		U.S. Pat. No. 7,534,505

TABLE A-continued

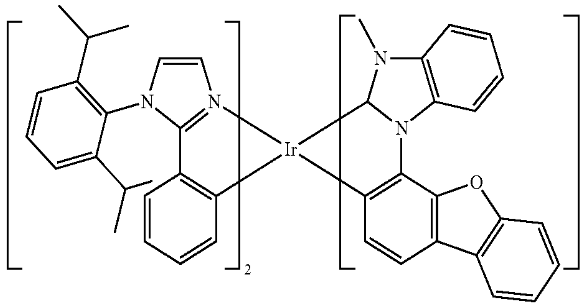
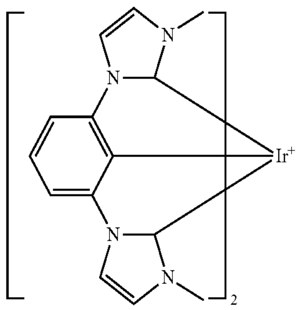
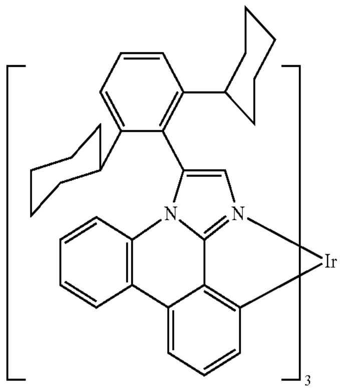
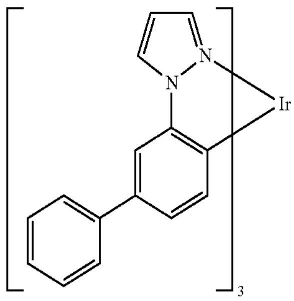
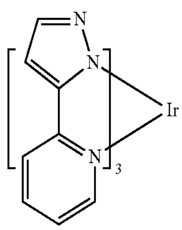
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2011051404
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033 US20100148663
		U.S. Pat. No. 7,338,722
		US20020134984

TABLE A-continued

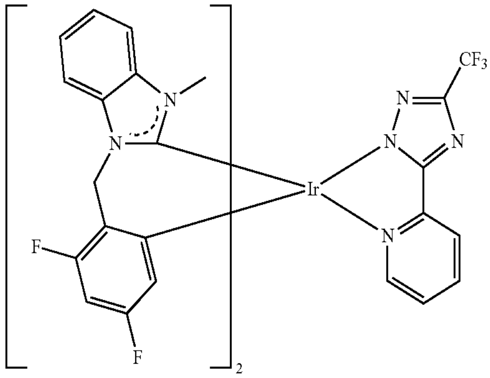
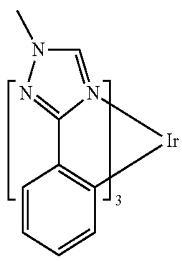
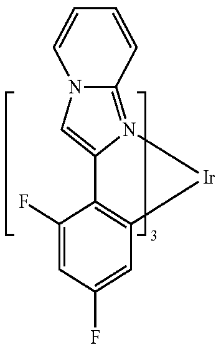
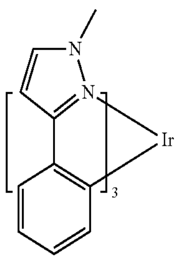
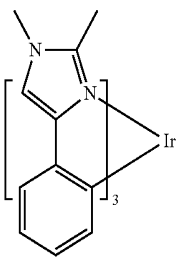
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 47, 4542 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)
		WO2005123873
		WO2005123873

TABLE A-continued

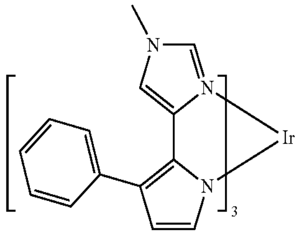
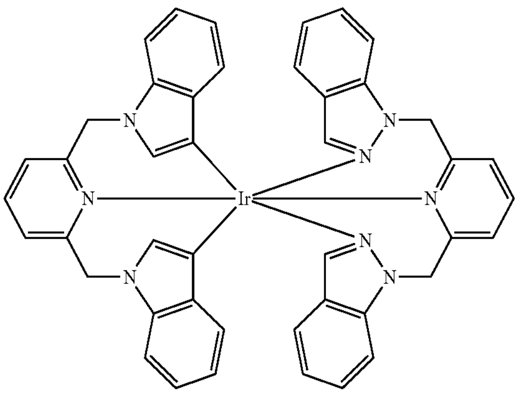
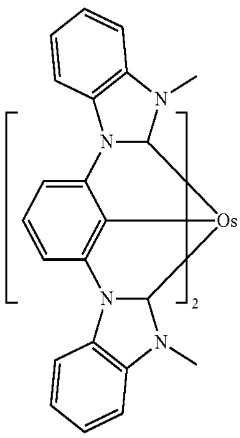
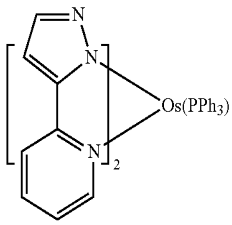
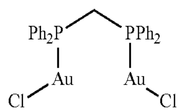
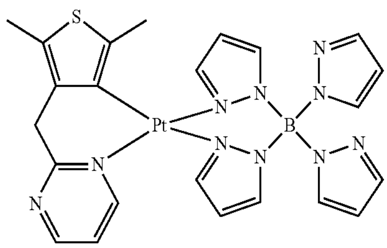
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2007004380
		WO2006082742
Osmium(II) complexes		U.S. Pat. No. 7,279,704
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874

TABLE A-continued

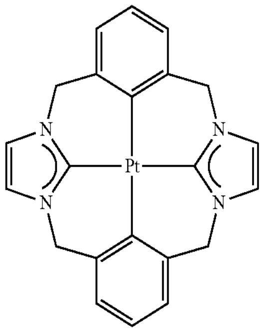
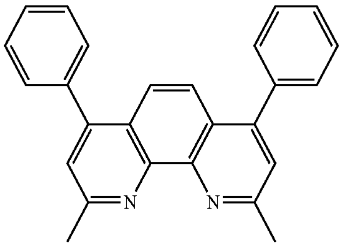
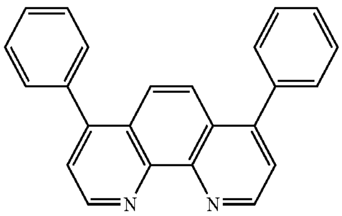
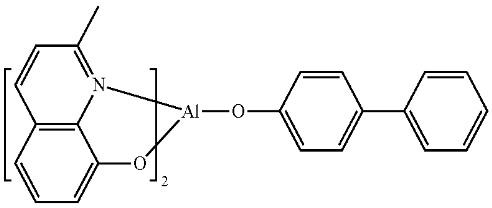
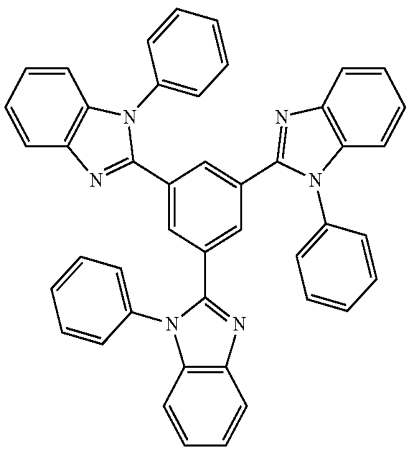
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Pt tetradentate complexes with at least one metal-carbene bond		U.S. Pat. No. 7,655,323
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)

TABLE A-continued

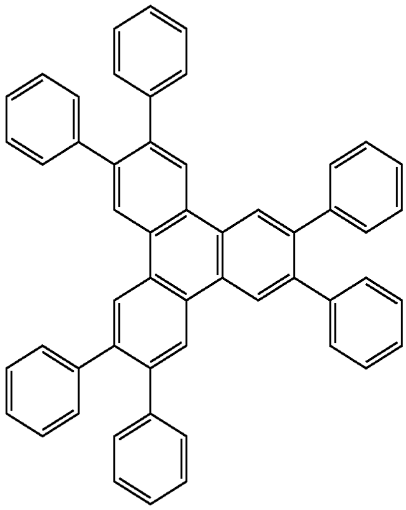
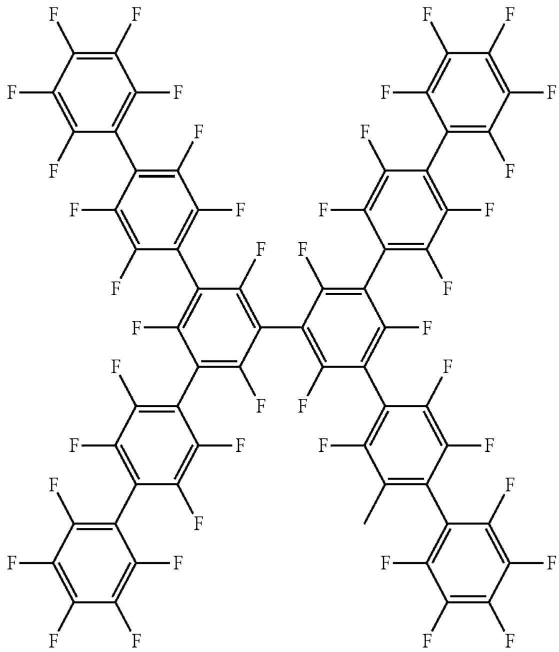
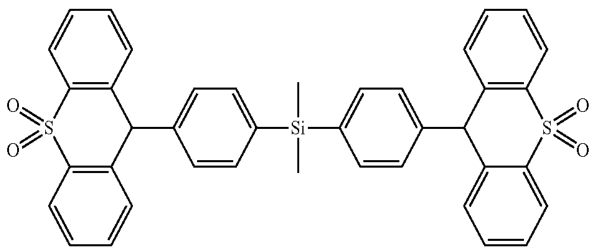
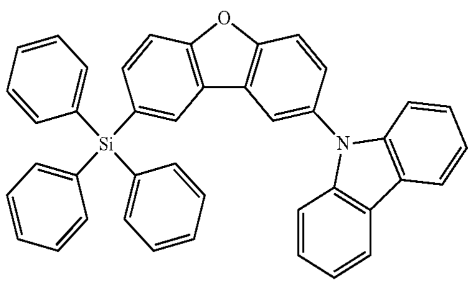
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051

TABLE A-continued

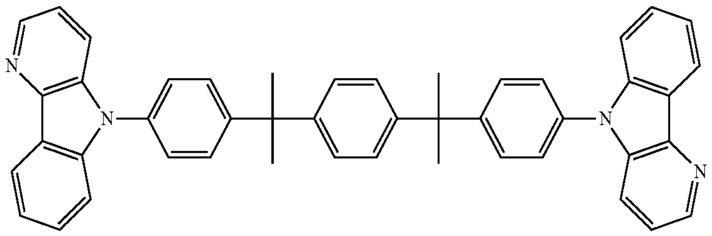
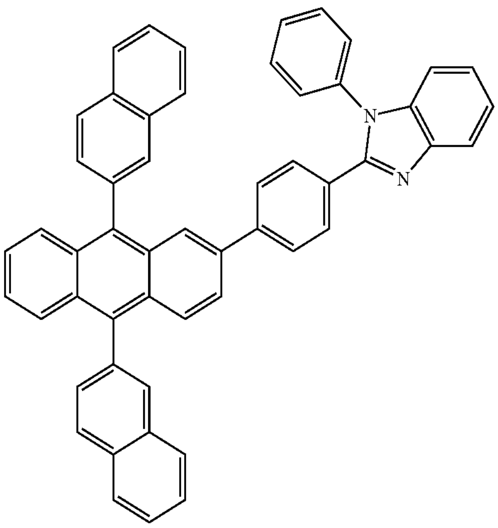
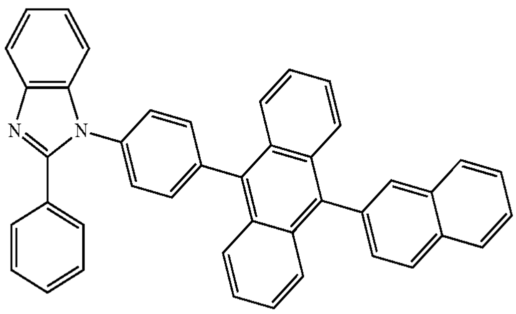
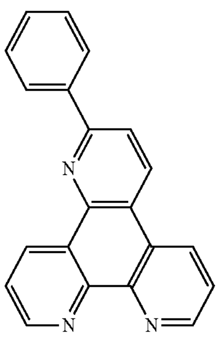
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza-carbazoles		US20060121308
	Electron transporting materials	
Anthracene-benzoimidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives		US20090115316

TABLE A-continued

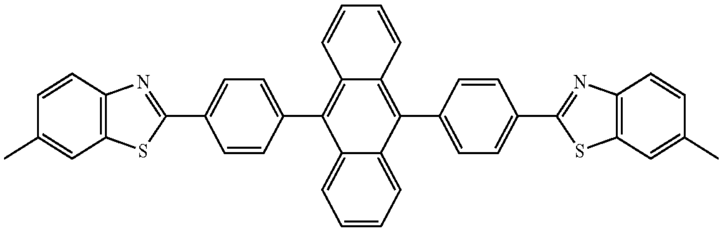
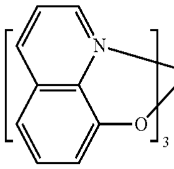
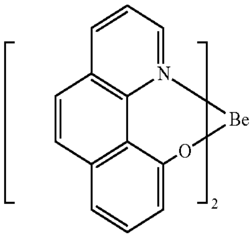
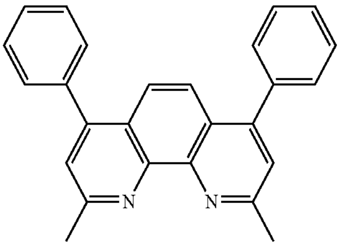
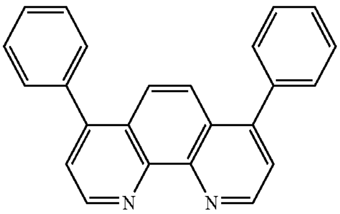
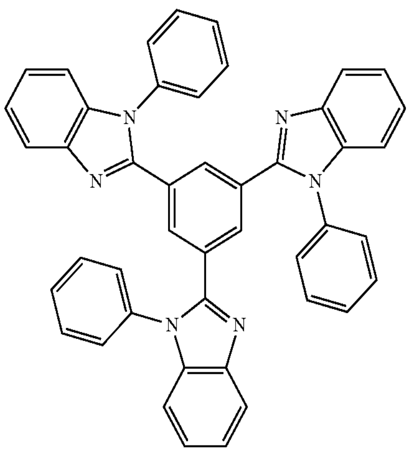
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7,230,107
Metal hydroxybenzoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such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

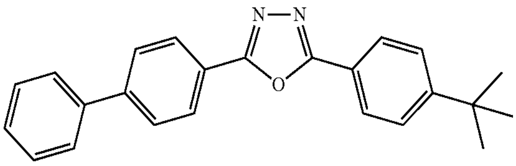
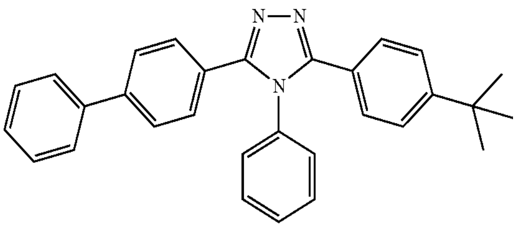
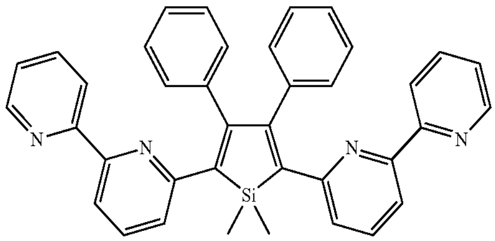
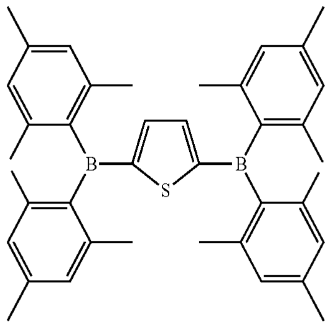
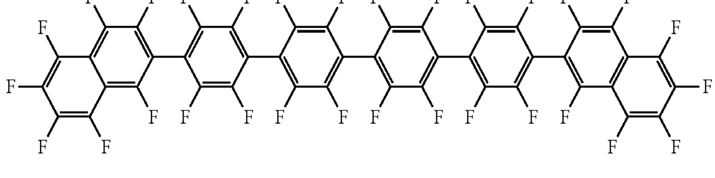
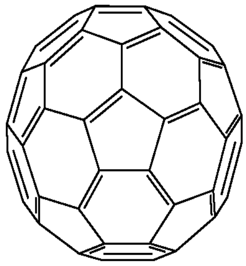
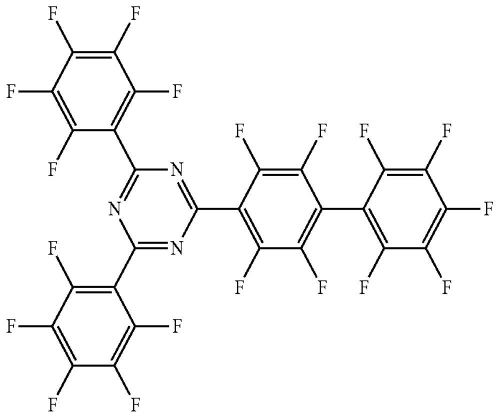
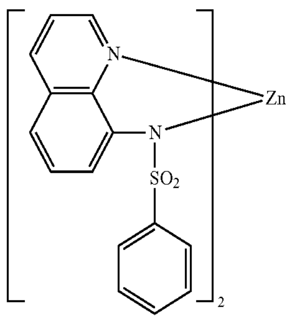
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C_{60})		US20090101870

TABLE A-continued

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

EXPERIMENTAL

Synthesis Examples

Chemical abbreviations used throughout this document are as follows:

SPhos is dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine,

$Pd_2(dba)_3$ is tri(dibenzylideneacetone)dipalladium(0),

$Pd(PPh_3)_4$ is tetrakis(triphenylphosphine) palladium (0),

DCM is dichloromethane,

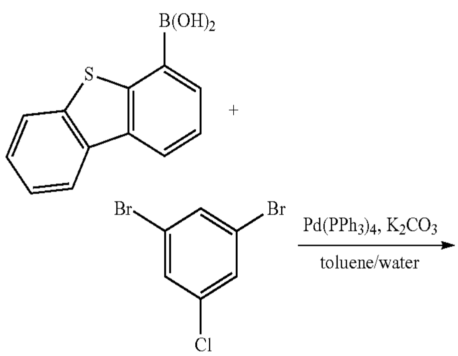
EtOAc is ethyl acetate,

DME is dimethyoxyethane, and

THF is tetrahydrofuran.

Synthesis of Compound A5

Synthesis of 4-(3-bromo-5-chlorophenyl)dibenzo[b,d]thiophene



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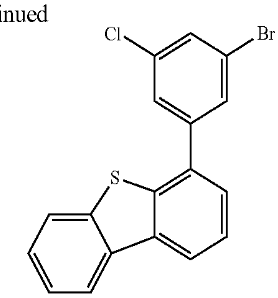
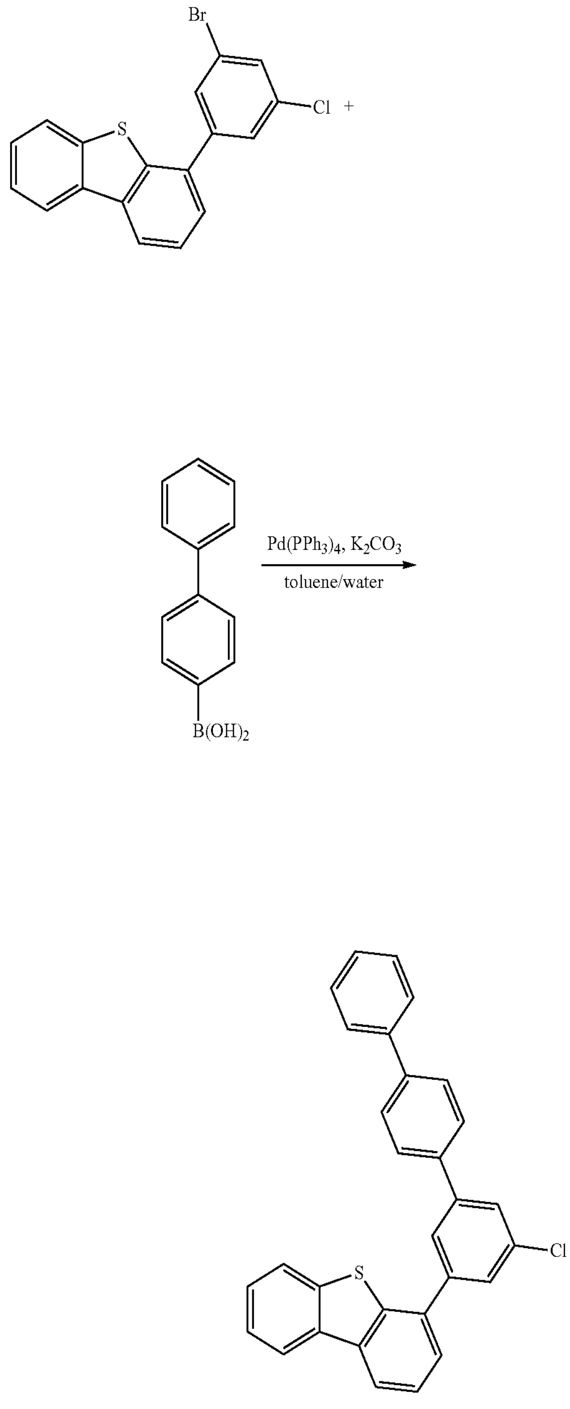


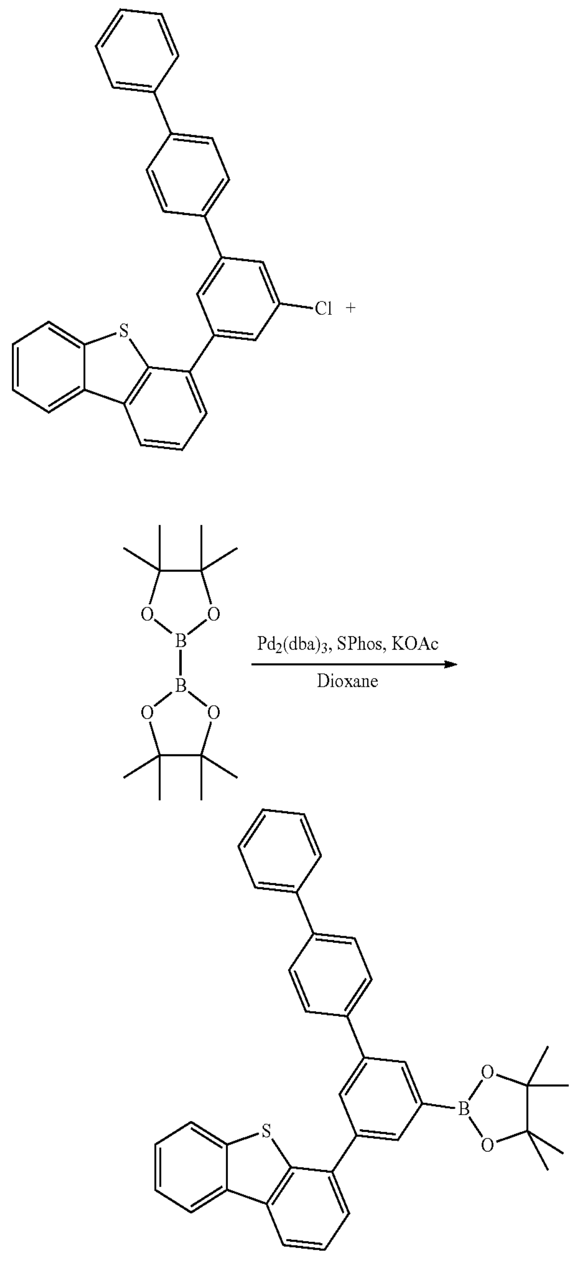
Dibenzo[b,d]thiophen-4-ylboronic acid (3.0 g, 13.15 mmol) and 1,3-dibromo-5-chlorobenzene (10.67 g, 39.5 mmol) were dissolved in toluene (150 ml) under a nitrogen atmosphere in a nitrogen-flushed 250 mL two-necked round-bottomed flask to give a colorless solution. K_2CO_3 (7.27 g, 52.6 mmol) in water (50 ml) was added to the reaction mixture, followed by $Pd(PPh_3)_4$ (0.304 g, 0.263 mmol). The reaction mixture was then heated to reflux under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the organic phase was isolated, the solvent was evaporated, and the unreacted 1,3-dibromo-5-chlorobenzene was distilled off under reduced pressure. The residue was subjected to column chromatography on the silica gel with heptanes/DCM (9/1, v/v) as the eluent, to obtain 4-(3-bromo-5-chlorophenyl)dibenzo[b,d]thiophene (3.5 g, 71.2%) as a white solid.

Synthesis of 4-(5-chloro-[1,1':4',1"-terphenyl]-3-yl)dibenzo[b,d]thiophene



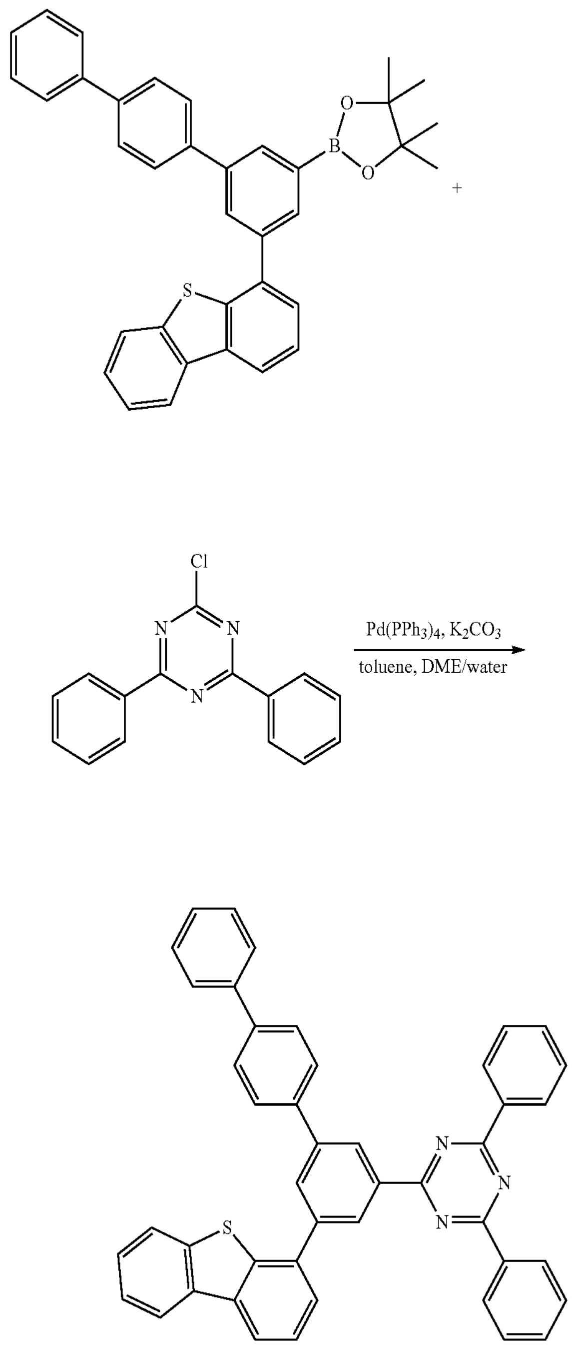
A solution of 4-(3-bromo-5-chlorophenyl)dibenzo[b,d]thiophene (4.0 g, 10.70 mmol), [1,1'-biphenyl]-4-ylboronic acid (2.120 g, 10.70 mmol), K_2CO_3 (3.0 g, 21.4 mmol) and $Pd(PPh_3)_4$ (0.37 g, 0.32 mmol) in toluene (150 ml) and water (50 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the organic layer was isolated and the solvent was evaporated. The residue was purified by column chromatography on silica gel with heptane/DCM (4/1, v/v) as the eluent to isolate 4-(5-chloro-[1,1':4',1"-terphenyl]-3-yl)dibenzo[b,d]thiophene (1.4 g 29%) as a white solid.

Synthesis of 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



A mixture of 4-(5-chloro-[1,1':4',1"-terphenyl]-3-yl)dibenzo[b,d]thiophene (1.40 g, 3.13 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (1.59 g, 6.26 mmol), potassium acetate (0.92 g, 9.40 mmol), SPhos (0.25 g, 0.61 mmol) and $Pd_2(dba)_3$ (0.11 g, 0.12 mmol) in dioxane (150 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was diluted with EtOAc, washed with brine and water, and dried over Na_2SO_4. Upon evaporation of the solvent, the residue was purified by column chromatography on silica gel with heptanes/EtOAc (9/1, v/v) as the eluent to yield 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1.1 g, 65%) as a white solid.

Synthesis of Compound A5

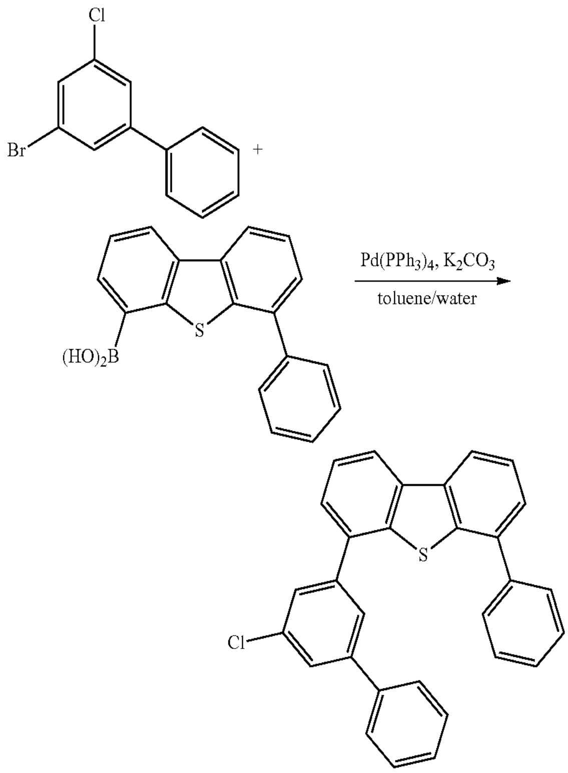


Compound A5

A solution of 2-chloro-4,6-diphenyl-1,3,5-triazine (1.84 g, 6.87 mmol), 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.70 g, 6.87 mmol), $Pd(PPh_3)_4$ (0.16 g, 0.137 mmol), and K_2CO_3 (2.85 g, 20.61 mmol) in DME (150 ml), toluene (100 ml) and water (50 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the solid was isolated by filtration, and washed successively with water, methanol, and EtOAc. The crude product was dissolved in hot toluene, filtered through a short plug of silica gel and recrystallized from toluene to yield Compound A5 (3.1 g, 70%) as a white solid.

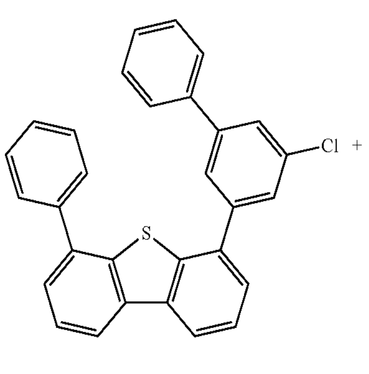
Synthesis of Compound A11

Synthesis of 4-(5-chloro-[1,1'-biphenyl]-3-yl)-6-phenyldibenzol[b,d]thiophene



A solution of 3-bromo-5-chloro-1,1'-biphenyl (10 g, 37.4 mmol), (6-phenyldibenzo[b,d]thiophen-4-yl)boronic acid (11.37 g, 37.4 mmol), $Pd(PPh_3)_4$ (0.432 g, 0.374 mmol), and K_2CO_3 (10.33 g, 74.8 mmol) in toluene (150 ml) and water (30 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the organic phase was isolated and the solvent was evaporated. The residue was purified by column chromatography on silica gel with heptane/DCM (4/1, v/v) as the eluent to yield 4-(5-chloro-[1,1'-biphenyl]-3-yl)-6-phenyldibenzo[b,d]thiophene (12.1 g, 72.4%) as a white solid.

Synthesis of 4,4,5,5-tetramethyl-2-(5-(6-phenyldibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-1,3,2-dioxaborolane



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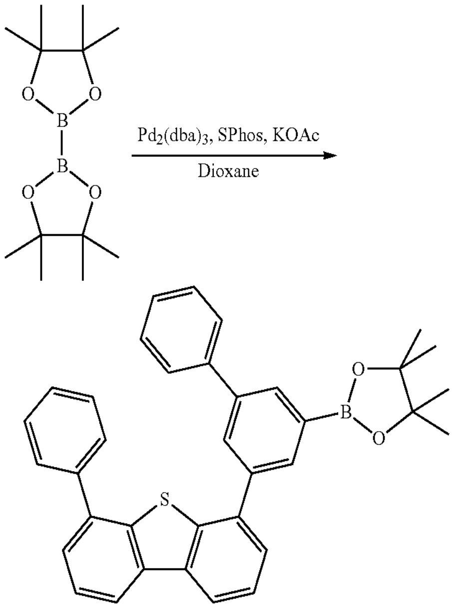
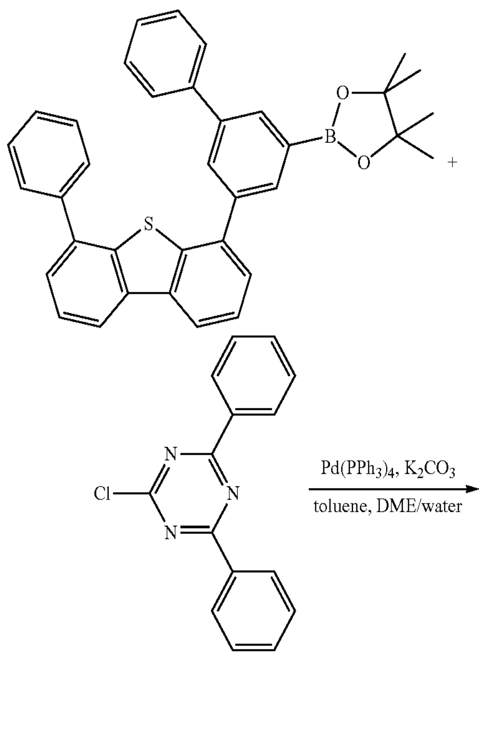


A solution of 4-(5-chloro-[1,1'-biphenyl]-3-yl)-6-phenyldibenzo[b,d]thiophene (13.0 g, 29.1 mmol), 4,4,4',4',5,5,5'5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (14.77 g, 58.2 mmol), $Pd_2(dba)_3$ (0.20 g, 0.22 mmol), SPhos (0.35 g, 0.85 mmol), and potassium acetate (8.56 g, 87 mmol) in dioxane (200 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction solution was quenched with water and extracted with EtOAc. The combined organic extracts were dried over Na_2SO_4 and the solvent was evaporated. The residue was purified by column chromatography on silica gel with heptane/EtOAc (9/1, v/v) as the eluent to yield 4,4,5,5-tetramethyl-2-(5-(6-phenyldibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-1,3,2-dioxaborolane (13.2 g, 84%) as a white solid.

Synthesis of Compound A11



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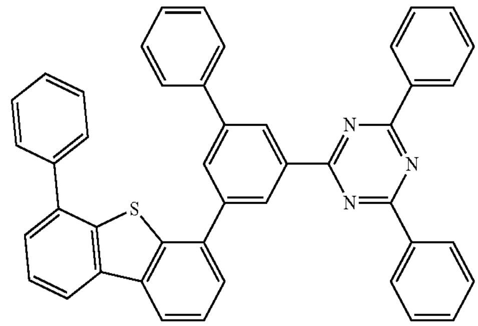
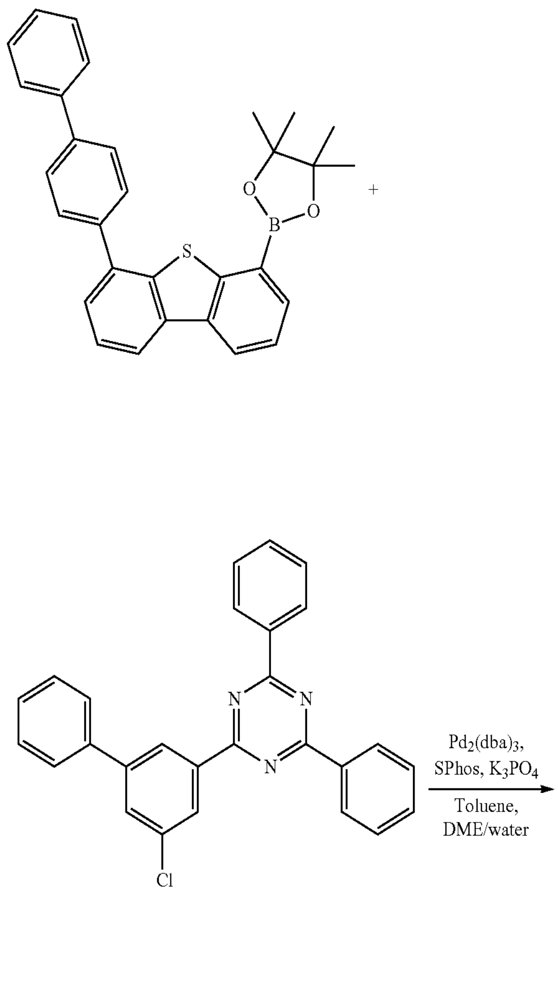


Compound A11

A solution of 4,4,5,5-tetramethyl-2-(5-(6-phenyldibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-1,3,2-dioxaborolane (3.55 g, 6.59 mmol), 2-chloro-4,6-diphenyl-1,3,5-triazine (1.765 g, 6.59 mmol), $Pd(PPh_3)_4$ (0.152 g, 0.132 mmol), and K_2CO_3 (1.822 g, 13.18 mmol) in toluene (100 ml), DME (100 ml) and water (50 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the organic layer was isolated, filtered through a short plug of silica gel and concentrated. The precipitate was collected, washed successively with heptane, ethanol, and heptane to yield Compound A11 (3.9 g, 92%) as a white solid.

Synthesis of Compound A14



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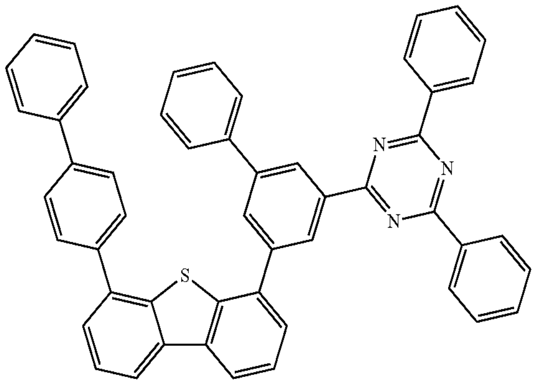
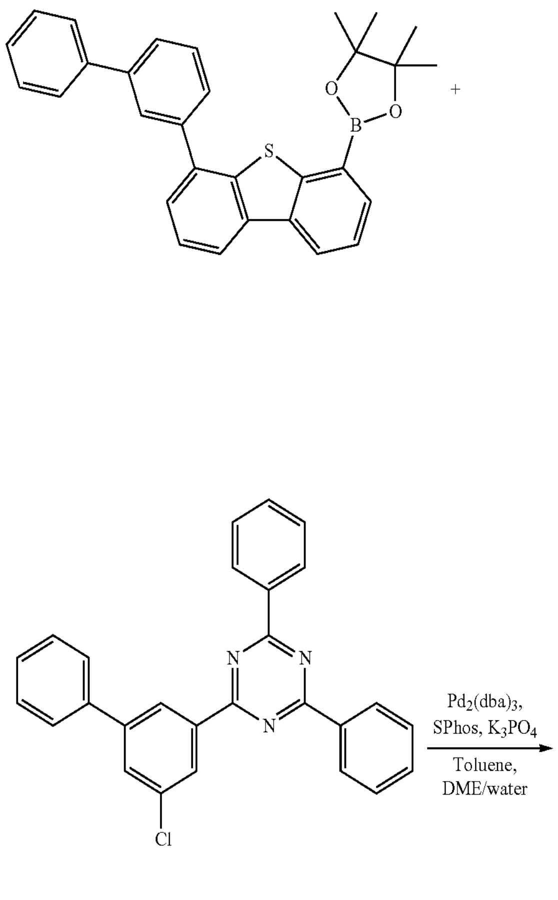


Compound A14

A solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.44 g, 7.44 mmol), 2-(5-chloro-[1,1'-biphenyl]-3-yl)-4,6-diphenyl-1,3,5-triazine (2.92 g, 6.95 mmol), $Pd_2(dba)_3$ (0.159 g, 0.174 mmol), SPhos (0.4 g, 0.976 mmol), and K_3PO_4 (4.80 g, 20.9 mmol) in toluene (125 ml), DME (100 ml) and water (25 ml) was refluxed under nitrogen for 18 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, dissolved in boiling toluene (800 ml), and filtered through a short plug of silica gel. Upon evaporation off the solvent, Compound A14 (3.50 g, 70%) was recrystallized from toluene to yield a white solid.

Synthesis of Compound A17



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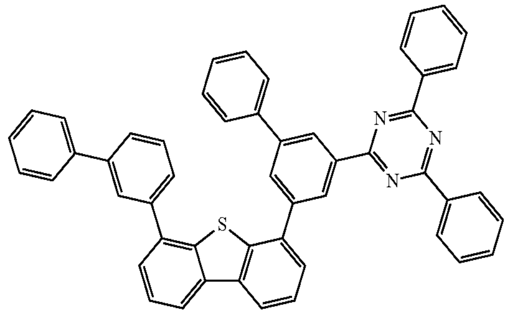
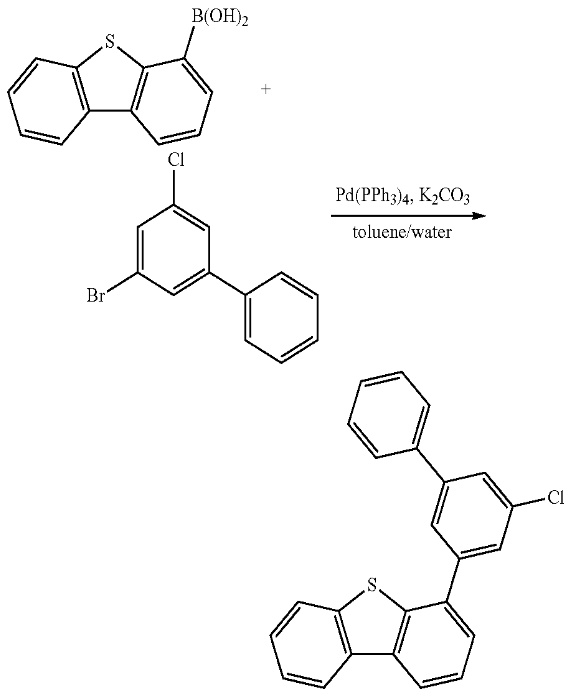


Compound A17

A solution of 2-(6-([1,1'-biphenyl]-3-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.51 g, 7.60 mmol), 2-(5-chloro-[1,1'-biphenyl]-3-yl)-4,6-diphenyl-1,3,5-triazine (2.9 g, 6.91 mmol), $Pd_2(dba)_3$ (0.190 g, 0.207 mmol), SPhos (0.5 g, 1.220 mmol), and K_3PO_4 (4.77 g, 20.7 mmol) in toluene (125 ml), DME (100 ml) and water (20 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, dissolved in boiling toluene (800 ml) and filtered through a short plug of silica gel. Upon evaporation off the solvent, Compound A17 (3.75 g, 76%) was recrystallized from toluene to yield a white solid.

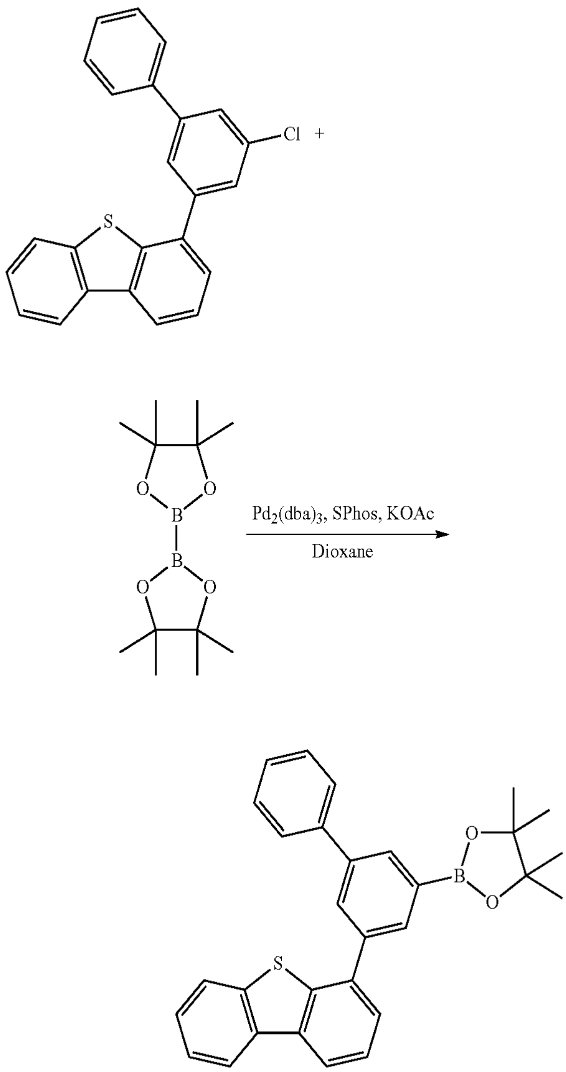
Synthesis of Compound A32

Synthesis of 4-(5-chloro-[1,1'-biphenyl]-3-yl)dibenzo[b,d]thiophene



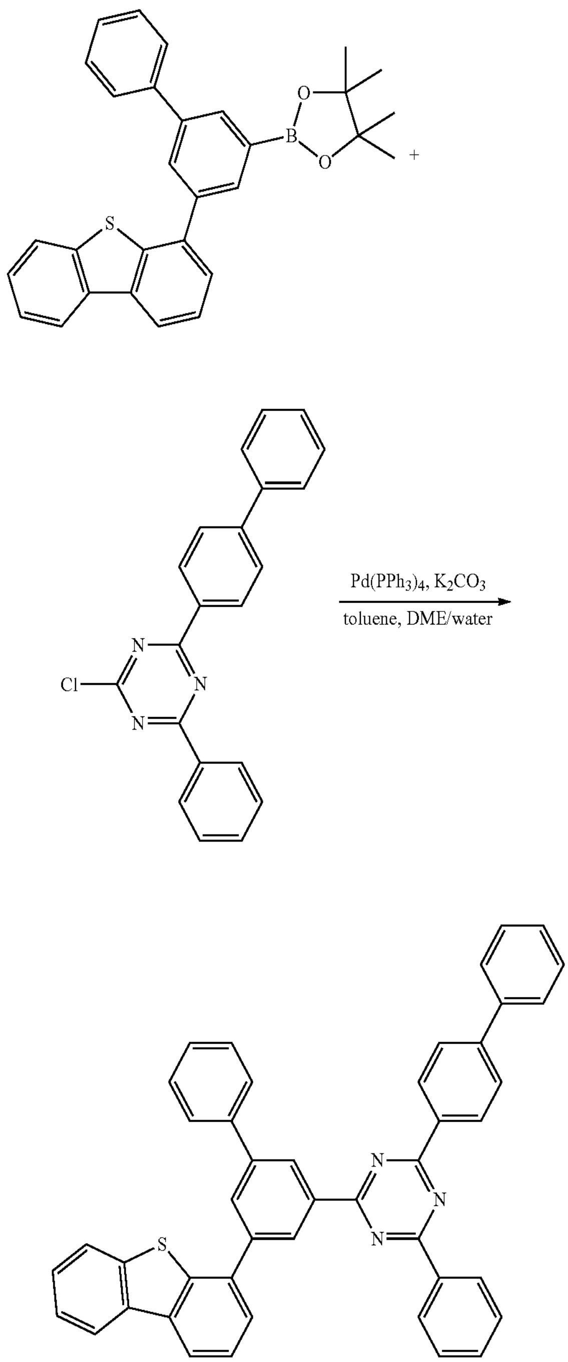
A solution of 3-bromo-5-chloro-1,1'-biphenyl (14.8 g, 55.3 mmol), dibenzo[b,d]thiophen-4-ylboronic acid (12.62 g, 55.3 mmol), $Pd(PPh_3)_4$ (0.639 g, 0.553 mmol) and K_2CO (15.29 g, 111 mmol) in toluene (150 ml) and water (30 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the organic phase was isolated. After evaporating off the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (85/15, v/v) as the eluent to yield 4-(5-chloro-[1,1'-biphenyl]-3-yl)dibenzo[b,d]thiophene (15.4 g, 70%) as a white solid.

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



A solution of 4-(5-Chloro-[1,1'-biphenyl]-3-yl)dibenzo[b,d]thiophene (11.88 g, 32.0 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (16.27 g, 64.1 mmol), $Pd_2(dba)_3$ (280 mg), SPhos (0.32 g, 0.78 mmol), and potassium acetate (9.43 g, 96 mmol) in dioxane (200 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was quenched with water and extracted with EtOAc. After evaporating off the solvent, the residue was purified by column chromatography on silica gel with heptane/EtOAc (9/1, v/v) as the eluent and recrystallization from heptane to yield 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (11.1 g, 74.9%) as a white solid.

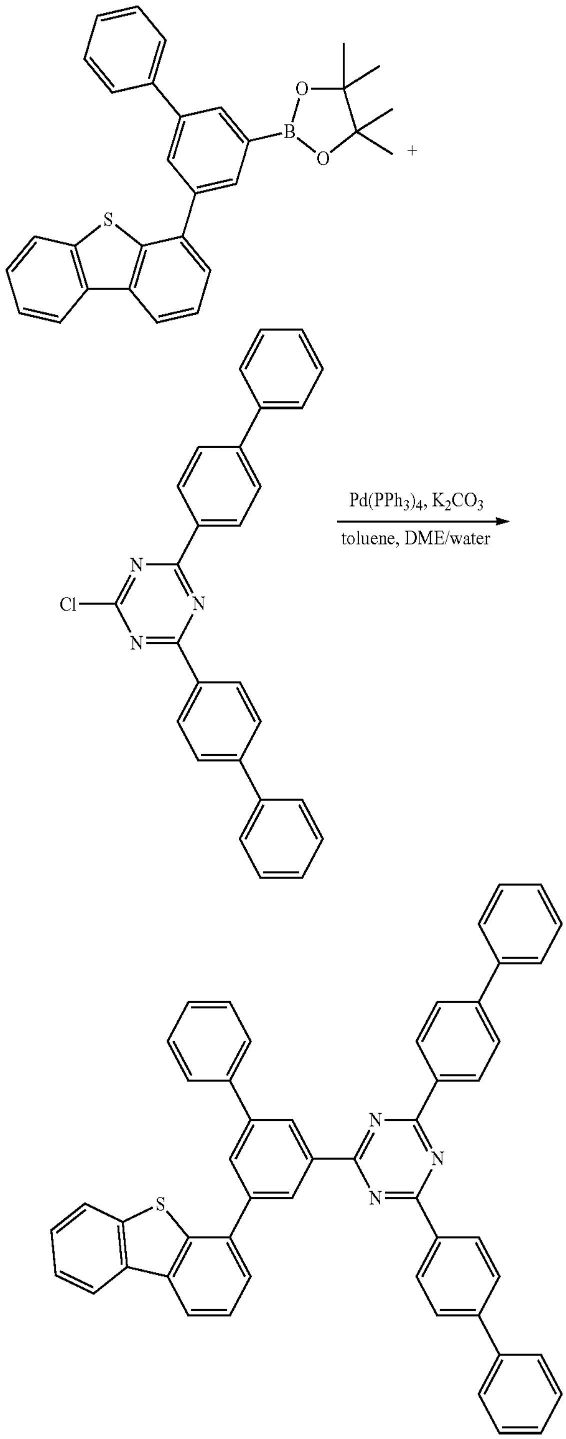
Synthesis of Compound A32



Compound A32

A solution of 2-([1,1'-biphenyl]-4-yl)-4-chloro-6-phenyl-1,3,5-triazine (2.24 g, 6.52 mmol), 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.01 g, 6.52 mmol), $Pd(PPh_3)_4$ (0.151 g, 0.130 mmol) and K_2CO_3 (1.801 g, 13.03 mmol) in toluene (180 ml), DME (30 ml), and water (30 ml) was refluxed under nitrogen for 12 h. After cooling to room temperature (~22° C.), the solid was collected by filtration and washed successively with ethanol, water, and ethanol. The crude product was recrystallized from toluene to yield Compound A32 (2.7 g, 64%) as a white solid.

Synthesis of Compound A35

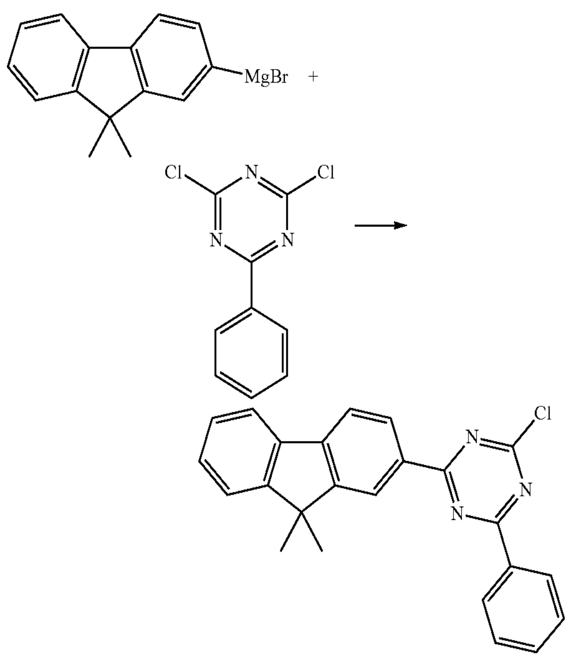


Compound A35

A solution of 2,4-di([1,1'-biphenyl]-4-yl)-6-chloro-1,3,5-triazine (3.0 g, 7.14 mmol) and 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.30 g, 7.14 mmol), $Pd(PPh_3)_4$ (0.164 g, 0.14 mmol), and K_2CO_3 (1.975 g, 14.29 mmol) in toluene (100 ml), DME (100 ml), and water (50 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the solid was collected by filtration and washed successively with ethanol, water, ethanol, and heptane. The crude product was dissolved in hot toluene, filtered through a short plug of silica gel and recrystallized from toluene to yield Compound A35 (3.7 g, 72% yield) as a white solid.

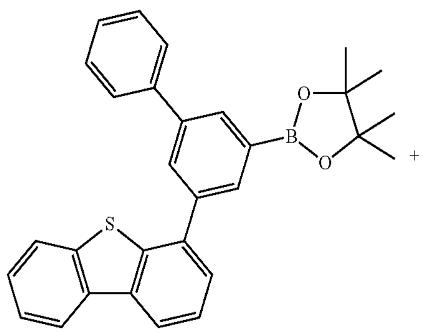
Synthesis of Compound A38

Synthesis of 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine



A Grignard reagent solution prepared by refluxing 2-bromo-9,9-dimethyl-9H-fluorene (19.33 g, 70.8 mmol) and Mg (2.58 g, 106 mmol) in dry THF (100 ml) under nitrogen for 2 h was transferred dropwise into a solution of 2,4-dichloro-6-phenyl-1,3,5-triazine (8.0 g, 35.4 mmol) in dry THF (50 ml) at room temperature (~22° C.). The reaction mixture was stirred under nitrogen overnight (~12 hours), quenched with concentrated HCl solution and extracted with EtOAc. The organic phase was isolated and the solvent was evaporated. The residue was purified by column chromatography on silica gel with heptane/DCM (9/1, v/v) as the eluent and recrystallization from heptane to yield 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (11 g, 81%) as yellow crystals.

Synthesis of Compound A38



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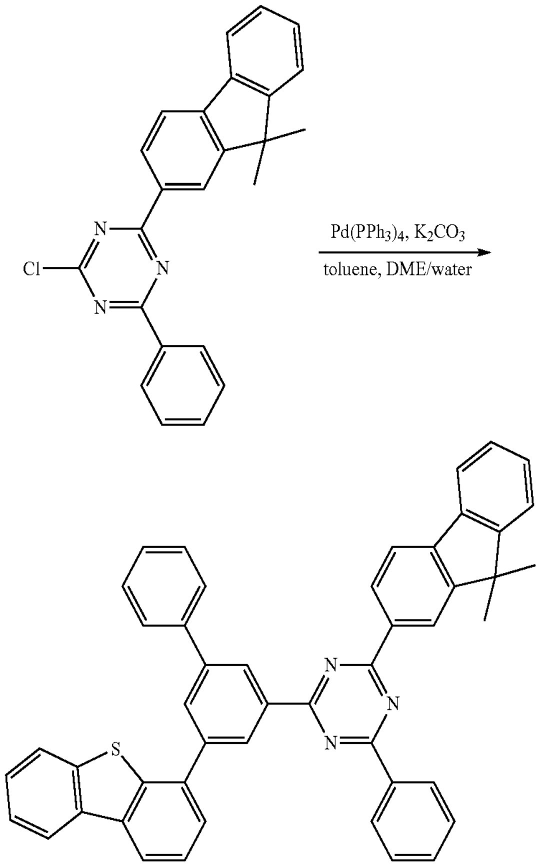
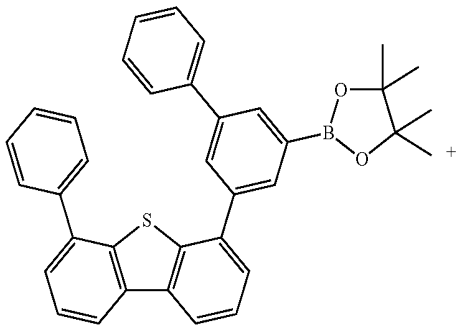


Compound A38

A solution of 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (3.0 g, 7.82 mmol), 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.61 g, 7.82 mmol), $Pd(PPh_3)_4$ (0.18 g, 0.156 mmol) and K_2CO_3 (2.16 g, 15.63 mmol) in toluene (100 ml), DME (100 ml) and water (50 ml) was refluxed under nitrogen for 12 h. After cooling to room temperature (~22° C.), the organic phase was isolated and the solvent was evaporated. The residue was purified by column chromatography on silica gel with heptane/DCM (6/4, v/v) as the eluent and trituration with heptane to yield Compound A38 (4.3 g, 80%) as a white solid.

Synthesis of Compound A41



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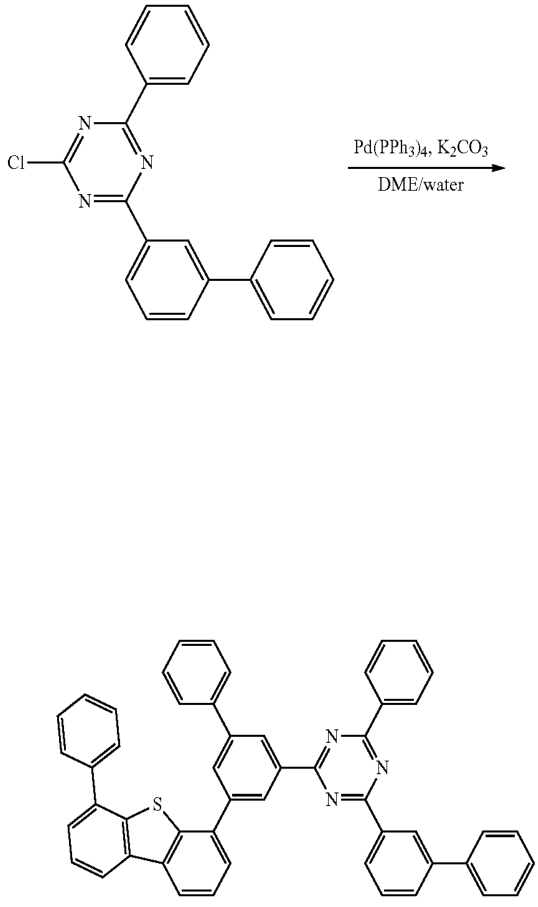
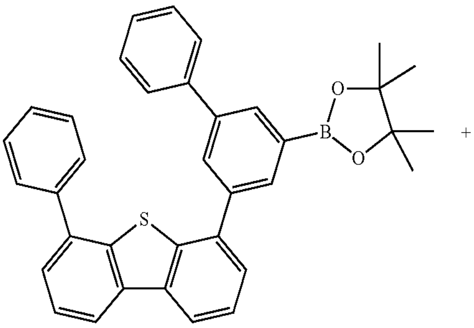


Compound A41

A solution of 4,4,5,5-tetramethyl-2-(5-(6-phenyldibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-1,3,2-dioxaborolane (1.98 g, 3.68 mmol), 2-([1,1'-biphenyl]-3-yl)-4-chloro-6-phenyl-1,3,5-triazine (1.264 g, 3.68 mmol), $Pd(PPh_3)_4$ (0.085 g, 0.074 mmol), and K_2CO_3 (1.016 g, 7.35 mmol) in DME (150 ml) and water (5 ml) was refluxed under nitrogen for 12 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed successively with ethanol, water, ethanol, and heptane, then dissolved in boiling toluene and filtered through a short plug of silica gel. Upon evaporation off the solvent, Compound A41 (2.3 g, 87%) was recrystallized from toluene to yield a white solid.

Synthesis of Compound A47



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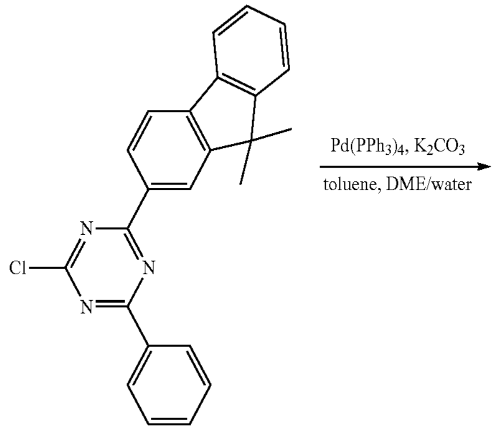
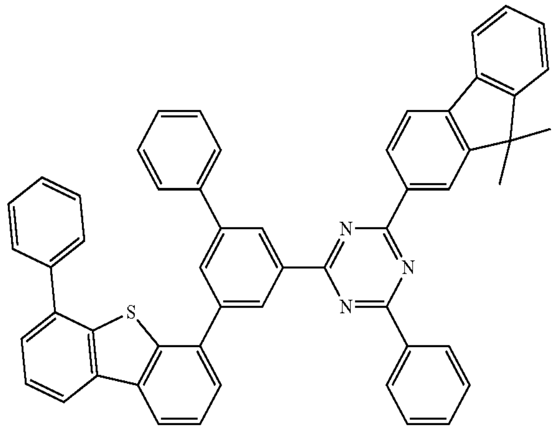
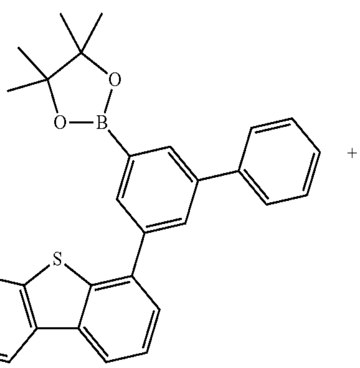




Compound A47

A solution of 4,4,5,5-tetramethyl-2-(5-(6-phenyldibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-1,3,2-dioxaborolane (3.18 g, 5.91 mmol), 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (2.267 g, 5.91 mmol) $Pd(PPh_3)_4$ (0.136 g, 0.118 mmol) and potassium carbonate (1.632 g, 11.81 mmol) in toluene (30 ml), DME (100 ml) and water (20 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the organic layer was isolated and the solvent was evaporated. The residue was purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent to yield Compound A47 (2.1 g, 47%) as a white solid.

Synthesis of Compound A110



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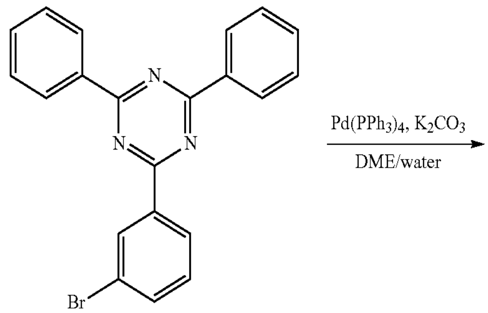
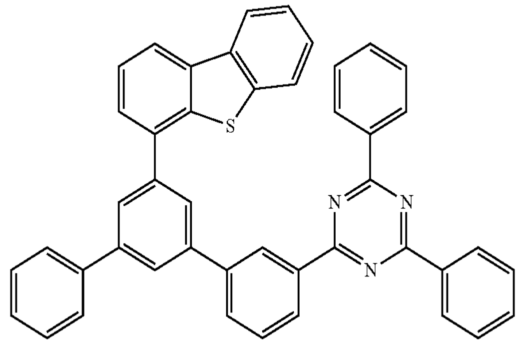
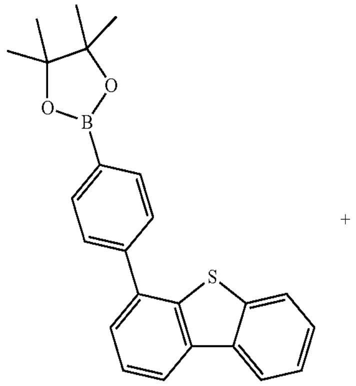




Compound A110

A solution of 2-(5-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1.70 g, 3.68 mmol), 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (1.43 g, 3.68 mmol), $Pd(PPh_3)_4$ (0.085 g, 0.074 mmol), and K_2CO_3 (1.02 g, 7.35 mmol) in DME (120 ml) and water (20 ml) was refluxed under nitrogen for 14 h. After cooling to room temperature (~22° C.), the precipitate was collected by filtration, washed successively with ethanol, water, ethanol and heptane to yield Compound A110 (2.1 g, 89% yield). as a white solid.

Synthesis of Compound A113



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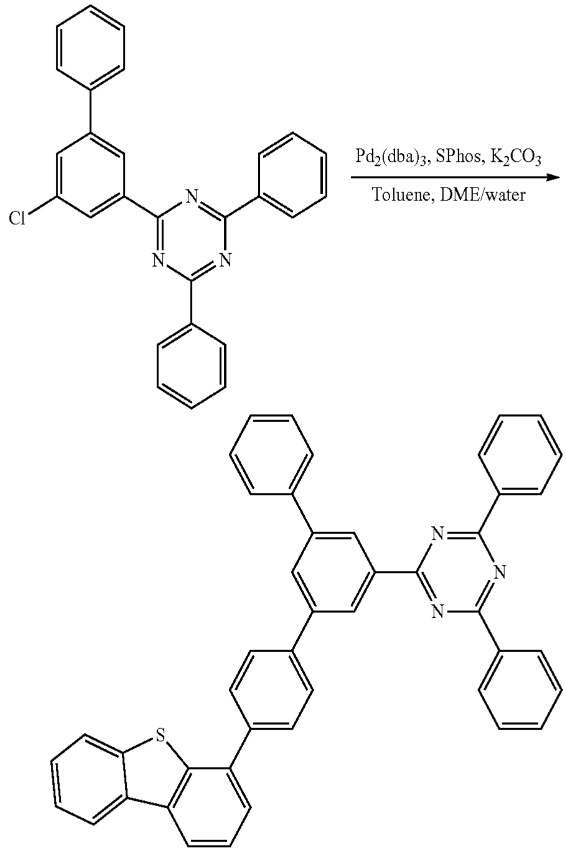
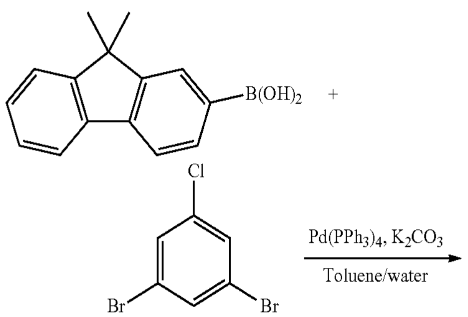


Compound A113

A solution of 2-(5-chloro-[1,1'-biphenyl]-3-yl)-4,6-diphenyl-1,3,5-triazine (3.4 g, 8.10 mmol), 2-(4-(dibenzo[b,d]thiophen-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.28 g, 8.50 mmol), $Pd_2(dba)_3$ (0.222 g, 0.243 mmol), SPhos (0.199 g, 0.486 mmol), and K_2CO_3 (3.36 g, 24.29 mmol) in toluene (16 ml), DME (48 ml), and water (16 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was collected by filtration and triturated with ethanol. The crude product was dissolved in boiling toluene, then filtered through a short plug of silica gel, and recrystallized from toluene to yield Compound A113 (4.25 g, 82%) as a white solid.

Synthesis of Compound A116

Synthesis of 2-(3-bromo-5-chlorophenyl)-9,9-dimethyl-9H-fluorene



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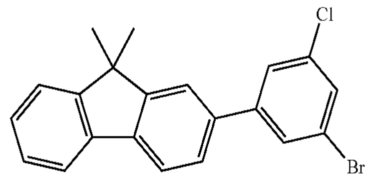
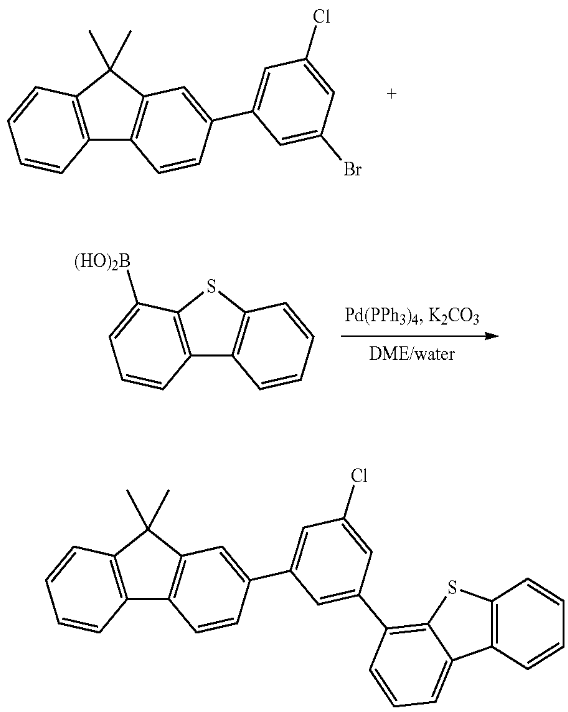


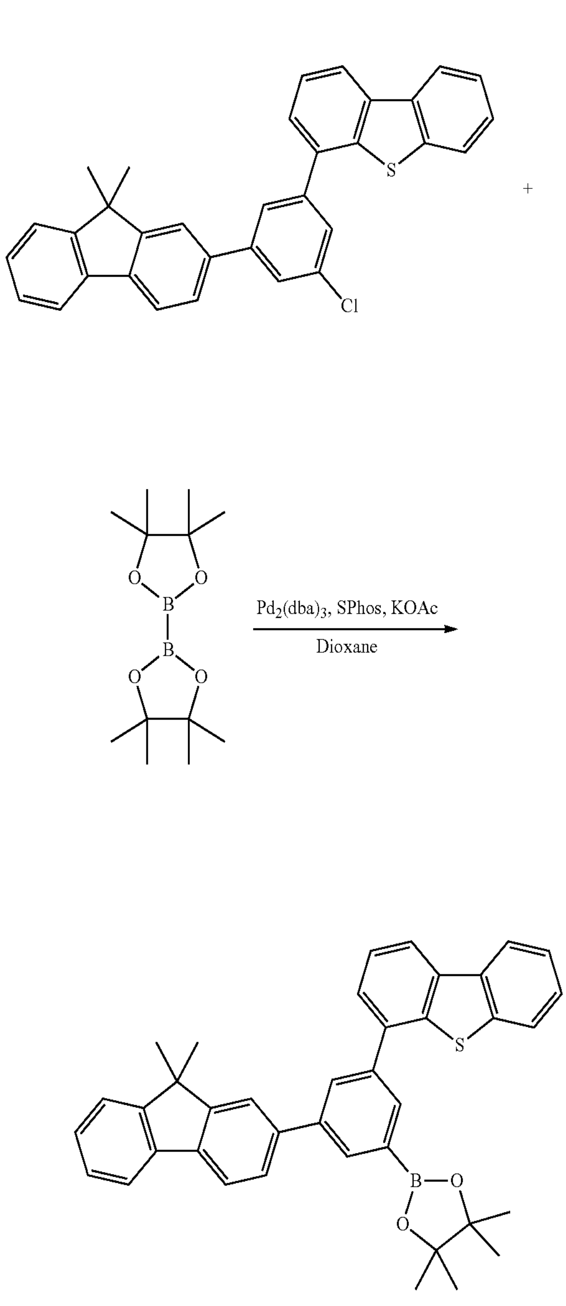
A solution of (9,9-Dimethyl-9H-fluoren-2-yl)boronic acid (5.0 g, 21.0 mmol), 1,3-dibromo-5-chlorobenzene (14.19 g, 52.5 mmol), $Pd(PPh_3)_4$ (0.49 g, 0.42 mmol), and K_2CO_3 (5.80 g, 42.0 mmol) in toluene (200 ml) and water (50 ml) was refluxed under nitrogen for 18 h. After cooling to room temperature (~22° C.), the organic layer was isolated and the excess of 1,3-dibromo-5-chlorobenzene was distilled off. The residue was purified by column chromatography on silica gel with heptane/DCM (9/1, v/v) as the eluent to yield 2-(3-bromo-5-chlorophenyl)-9,9-dimethyl-9H-fluorene (6.2 g, 77%) as a colorless crystalline solid.

Synthesis of 4-(3-chloro-5-(9,9-dimethyl-9H-fluoren-2-yl)phenyl)dibenzo[b,d]thiophene



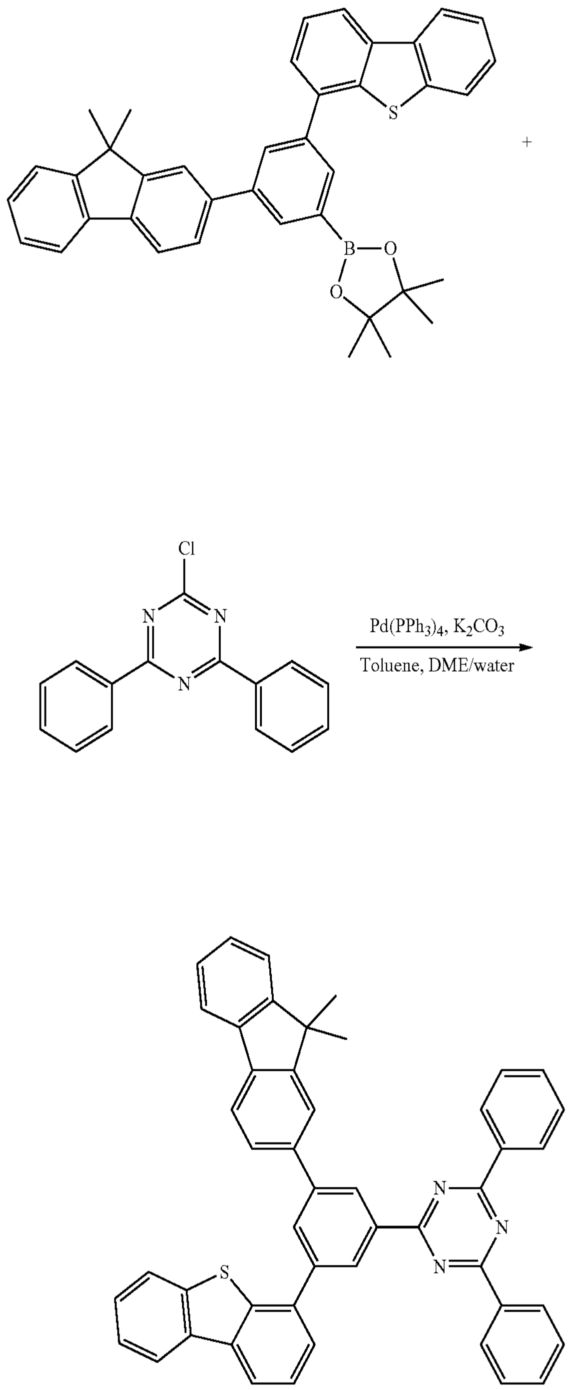
A solution of 2-(3-bromo-5-chlorophenyl)-9,9-dimethyl-9H-fluorene (7.7 g, 20.07 mmol), dibenzo[b,d]thiophen-4-ylboronic acid (4.58 g, 20.07 mmol), $Pd(PPh_3)_4$ (0.464 g, 0.401 mmol), and K_2CO_3 (5.55 g, 40.1 mmol) in DME (150 ml) and water (20 ml) was refluxed under nitrogen for 12 h. After cooling to room temperature (~22° C.), the organic phase was isolated and the solvent was evaporated. The crude product was purified by column chromatography on silica gel with heptane/DCM (9/1 to 4/1, v/v) as the eluent to yield 4-(3-chloro-5-(9,9-dimethyl-9H-fluoren-2-yl)phenyl)dibenzo[b,d]thiophene (9.0 g, 92%) as a white crystalline solid.

Synthesis of 2-(3-(dibenzo[b,d]thiophen-4-yl)-5-(9,9-dimethyl-9H-fluoren-2-yl)phenyl)-4,4,5,5-tetramethyl-1,32-dioxaborolane



A solution of 4-(3-chloro-5-(9,9-dimethyl-9H-fluoren-2-yl)phenyl)dibenzo[b,d]thiophene (9.5 g, 19.51 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (9.91 g, 39.0 mmol), $Pd_2(dba)_3$ (0.268 g, 0.293 mmol), SPhos (0.240 g, 0.585 mmol), and potassium acetate (5.74 g, 58.5 mmol) in dioxane was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the reaction mixture was diluted with water and extracted with ethyl acetate. The combined organic extracts were filtered and evaporated. The crude product was purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent to yield 2-(3-(dibenzo[b,d]thiophen-4-yl)-5-(9,9-dimethyl-9H-fluoren-2-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7.8 g, 69.1%) as a white crystalline solid.

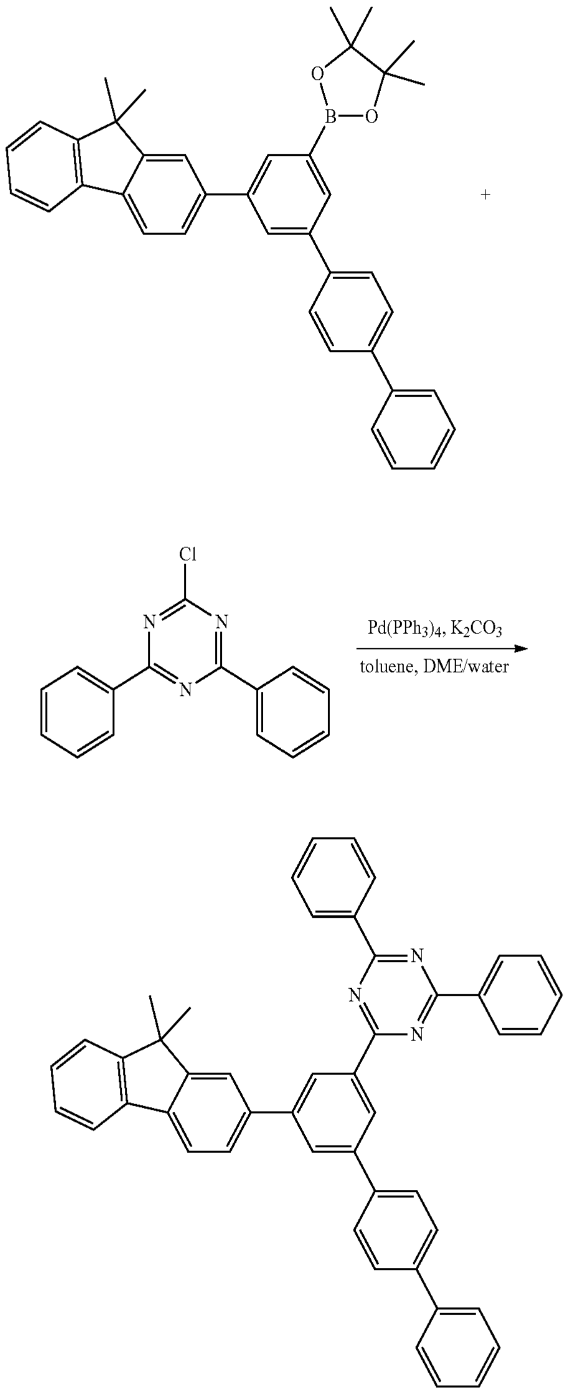
Synthesis of Compound A116



Compound A116

A solution of 2-(3-(dibenzo[b,d]thiophen-4-yl)-5-(9,9-dimethyl-9H-fluoren-2-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5.84 g, 10.09 mmol), 2-chloro-4,6-diphenyl-1,3,5-triazine (2.70 g, 10.09 mmol), $Pd(PPh_3)_4$ (0.233 g, 0.202 mmol), and K_2CO_3 (3.49 g, 25.2 mmol) in DME (100 ml), toluene (100 ml), and water (50 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the precipitate was collected by filtration, then washed successively with water, ethanol, and heptane to yield Compound A116 (5.5 g, 80%) as a white solid.

Synthesis of Compound B3

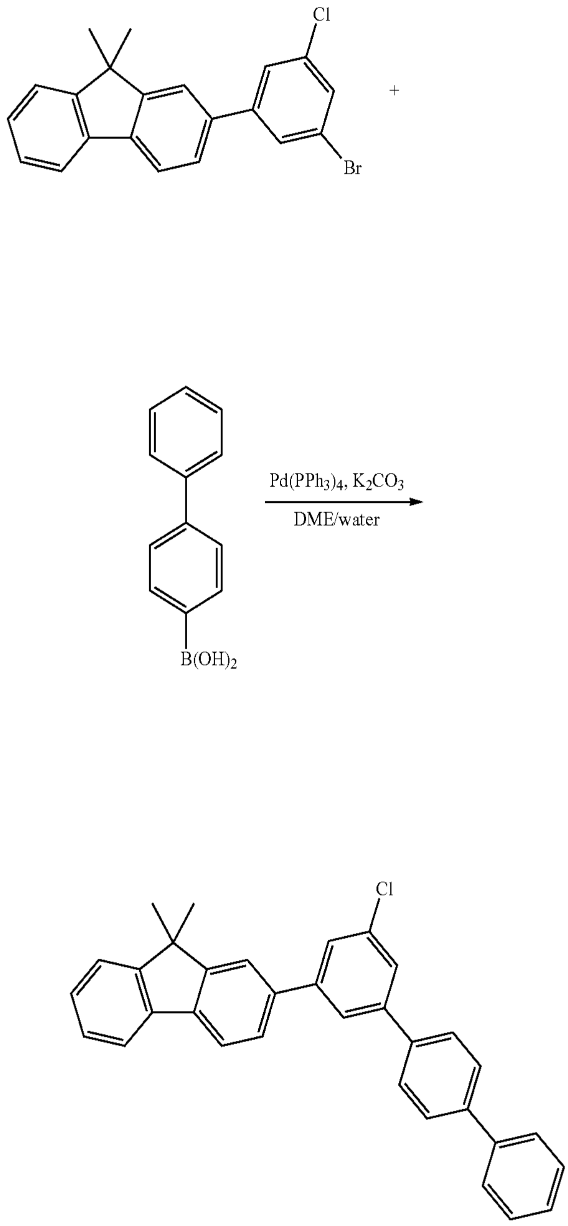


Compound B3

A solution of 2-(5-(9,9-dimethyl-9H-fluoren-2-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3 g, 5.47 mmol), 2-chloro-4,6-diphenyl-1,3,5-triazine (1.464 g, 5.47 mmol), $Pd(PPh_3)_4$ (0.126 g, 0.109 mmol), and K_2CO_3 (1.512 g, 10.94 mmol) in toluene (75 ml), DME (75 ml), and water (20 ml) was refluxed under nitrogen for 6 h. After cooling to room temperature (~22° C.), the precipitate was collected by filtration, then washed successively with water, ethanol, heptanes, and ethanol to yield Compound B3 (2.8 g, 78%) as a white solid.

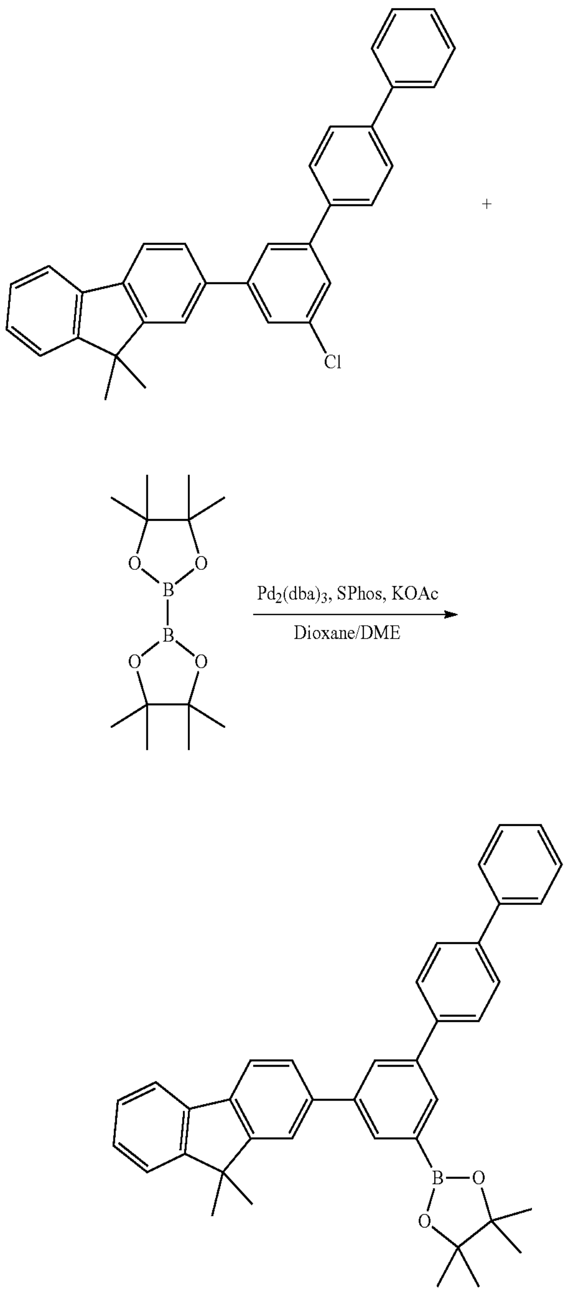
Synthesis of Compound B6

Synthesis of 2-(5-chloro-[1,1':4',1"-terphenyl]-3-yl)-9,9-dimethyl-9H-fluorene



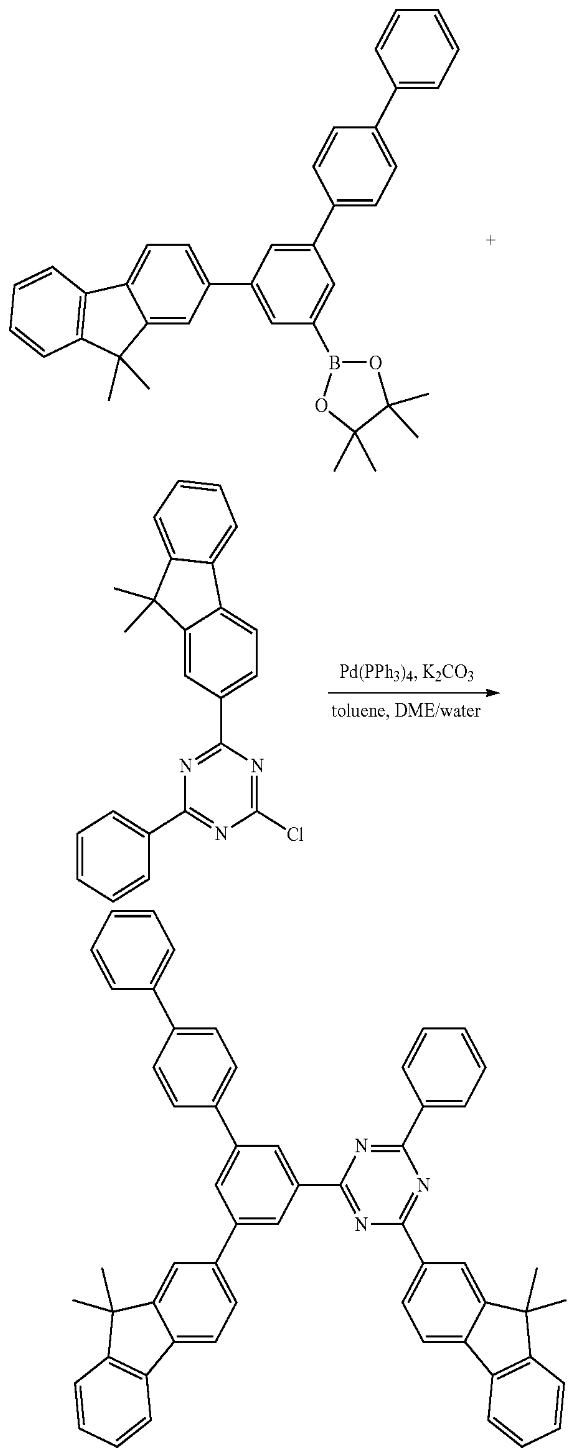
A solution of 2-(3-bromo-5-chlorophenyl)-9,9-dimethyl-9H-fluorene (5 g, 13.03 mmol), [1,1'-biphenyl]-4-ylboronic acid (2.58 g, 13.03 mmol), $Pd(PPh_3)_4$ (0.301 g, 0.261 mmol), and K_2CO (5.40 g, 39.1 mmol) in DME (150 ml) and water (25 ml) was refluxed under nitrogen for 12 h. After cooling to room temperature (~22° C.), the organic phase was isolated and the solvent was evaporated. The crude product was purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent and recrystallized from heptane to yield 2-(5-chloro-[1,1':4',1"-terphenyl]-3-yl)-9,9-dimethyl-9H-fluorene (3.6 g, 60.5%) as colorless crystals.

Synthesis of 2-(5-(9,9-dimethyl-9H-fluoren-2-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



A solution of 2-(5-chloro-[1,1':4',1"-terphenyl]-3-yl)-9,9-dimethyl-9H-fluorene (6.8 g, 14.88 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (7.56 g, 29.8 mmol), $Pd_2(dba)_3$ (0.273 g, 0.298 mmol), SPhos (0.244 g, 0.595 mmol), and potassium acetate (2.92 g, 29.8 mmol) in dioxane (100 ml) and DME (100 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was filtered off. Upon evaporating off the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent to yield 2-(5-(9,9-dimethyl-9H-fluoren-2-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5.0 g, 61.3%) as a white solid.

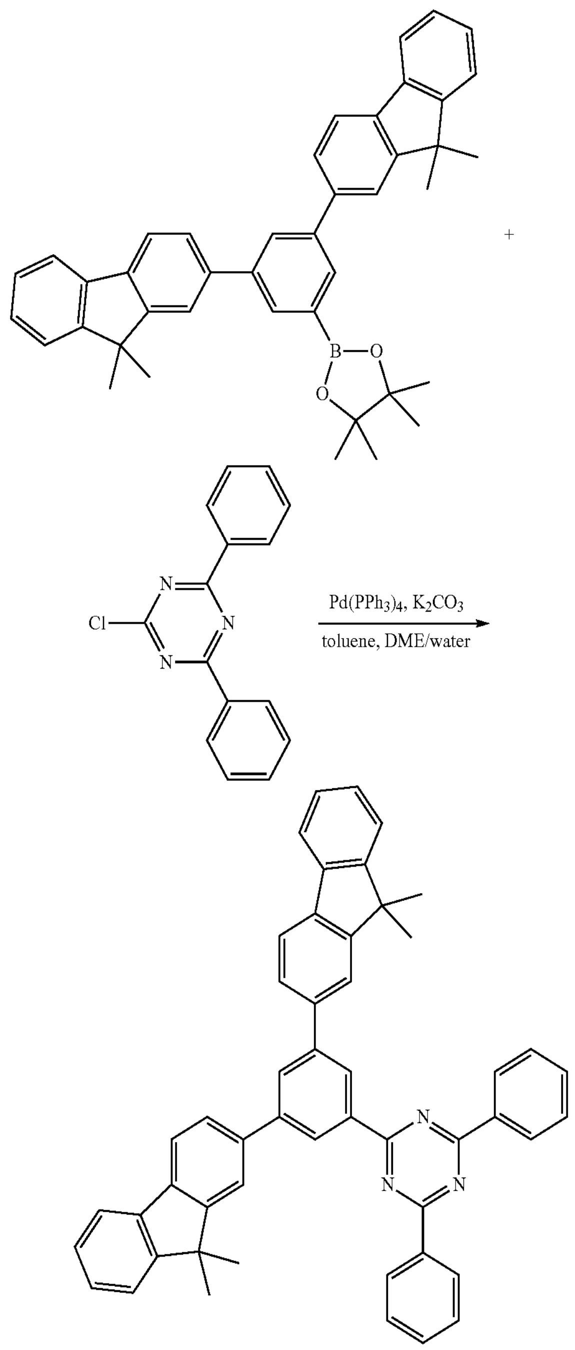
Synthesis of Compound B6



Compound B6

A solution of 2-(5-(9,9-Dimethyl-9H-fluoren-2-yl)-[1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5.17 g, 9.43 mmol), 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (3.62 g, 9.43 mmol), $Pd(PPh_3)_4$ (0.218 g, 0.189 mmol), and potassium carbonate (2.61 g, 18.85 mmol) in DME (75 ml), toluene (75 ml), and water (10 ml) was refluxed under nitrogen for 15 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, then washed successively with ethanol, water, ethanol, and heptane to yield Compound B6 (4.2 g, 58%) as a white crystalline solid.

Synthesis of Compound B7

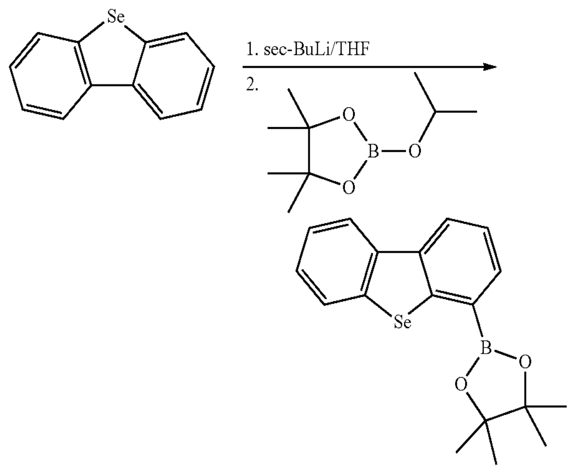


Compound B7

A solution of 2-(3,5-bis(9,9-dimethyl-9H-fluoren-2-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4 g, 6.80 mmol), 2-chloro-4,6-diphenyl-1,3,5-triazine (1.819 g, 6.80 mmol), $Pd(PPh_3)_4$ (0.079 g, 0.068 mmol), and K_2CO_3 (1.878 g, 13.59 mmol) in DME (75 ml), toluene (75 ml), and water (10 ml) was refluxed under nitrogen for 18 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, then washed successively with ethanol, water, ethanol and heptane to yield Compound B7 (3.5 g, 74%) as a white crystalline solid.

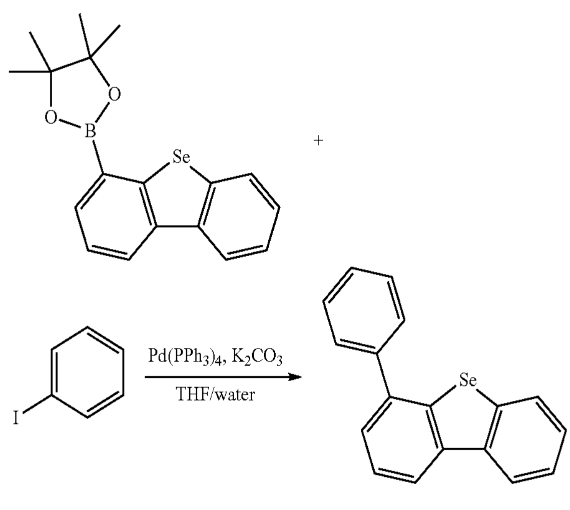
Synthesis of Compound C21

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



Into a solution of dibenzo[b,d]selenophene (7 g, 30.3 mmol) in anhydrous THF (151 ml) a solution of sec-butyllithium (23.79 ml, 33.3 mmol) was added dropwise at −78° C. The resulting mixture was stirred at this temperature for 2 h and warmed to room temperature (~°22° C.). After cooling the mixture to −78° C., the mixture was quenched with 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7.72 ml, 37.9 mmol) by syringe over ~1 minute, then gradually warmed to room temperature (~22° C.) and stirred overnight (~12 hours). The resulting mixture was quenched with methanol and the solvent was removed in vacuo. The crude product was purified by column chromatography on silica gel with heptane/DCM (4/1 to 1/1, v/v) as the eluent to yield 2-(dibenzo[b,d]selenophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7 g, 65%) as a yellow oil.

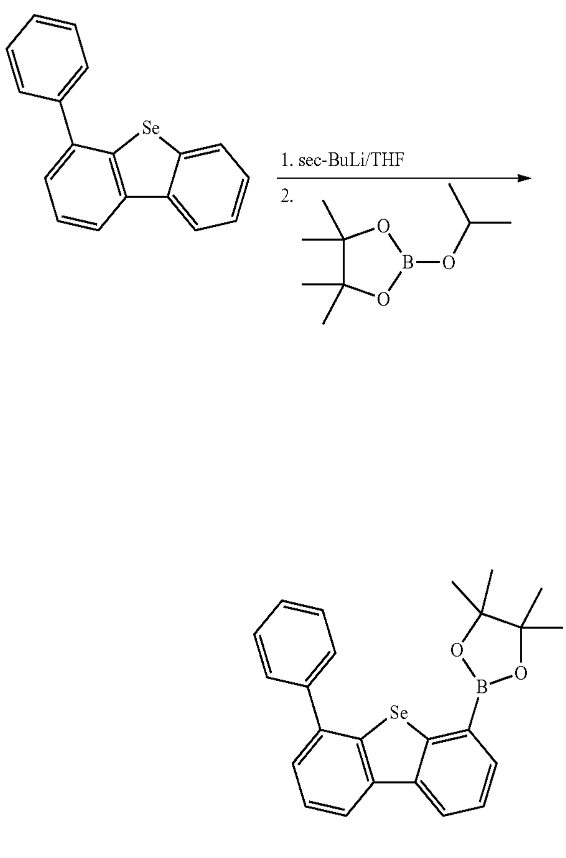
Synthesis of 4-phenyldibenzo[b,d]selenophene



A solution of 2-(dibenzo[b,d]selenophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7.0 g, 19.60 mmol), iodobenzene (2.62 ml, 23.52 mmol), $Pd(PPh_3)_4$ (0.453 g, 0.392

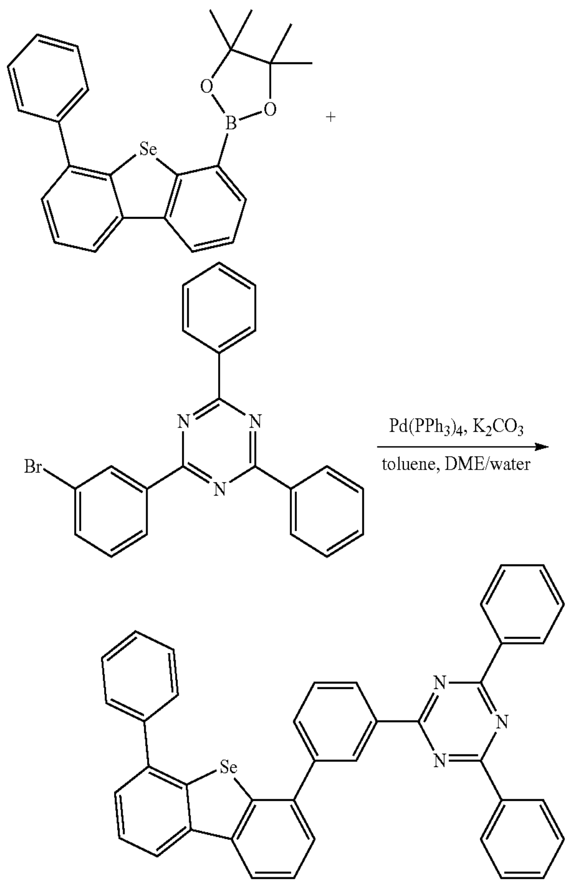
mmol), and K_2CO_3 (8.13 g, 58.8 mmol) in THF (78 ml) and water (19.60 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the reaction mixture was partitioned with ethyl acetate and water. The organic phase was isolated, then washed with brine and dried over Na_2SO_4. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (9/1, v/v) as the eluent to yield 4-phenyldibenzo[b,d]selenophene (5.3 g, 88%) as a colorless oil.

Synthesis of 4,4,5,5-tetramethyl-2-(6-phenyldibenzo[b,d]selenophen-4-yl)-1,3,2-dioxaborolane



A solution of 4-phenyldibenzo[b,d]selenophene (5.3 g, 17.25 mmol) in THF (108 ml) was cooled to −78° C. and treated slowly with a solution of sec-butyllithium 1.4 M (16.63 ml, 23.29 mmol) in cyclohexane. The resulting mixture was stirred at this −78° C. for h before being allowed to warm to room temperature (~22° C.). The dark red solution was cooled to −78° C. and quenched with 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5.28 ml, 25.9 mmol) by syringe. The reaction mixture was allowed to warm gradually to room temperature (~22° C.) and stirred for 16 h. The resulting mixture was quenched with methanol, then the solvent was removed in vacuo. The residue was dissolved in DCM, washed with water and brine, and then dried over Na_2SO_4. After evaporating the solvent, the crude product was recrystallized from heptane to yield 4,4,5,5-tetramethyl-2-(6-phenyldibenzo[b,d]selenophen-4-yl)-1,3,2-dioxaborolane (5 g, 67%) as a pale yellow solid.

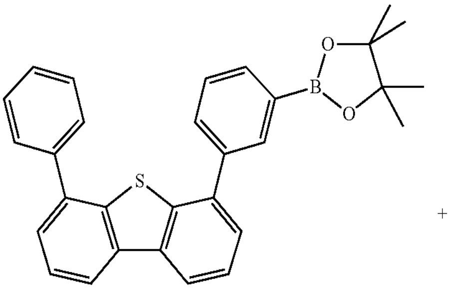
Synthesis of Compound C21



Compound C21

A solution of 4,4,5,5-tetramethyl-2-(6-phenyldibenzo[b,d]selenophen-4-yl)-1,3,2-dioxaborolane (2.0 g, 4.62 mmol), 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (1.882 g, 4.85 mmol), $Pd(PPh_3)_4$ (0.160 g, 0.139 mmol), and K_2CO_3 (1.914 g, 13.85 mmol) in DME (28 ml), toluene (9 ml), and water (9 ml) was refluxed under nitrogen for 8 h. After cooling to room temperature (~22° C.), the solids were collected by filtration, then washed with water and ethanol, dissolved in boiling toluene, and finally filtered through a short plug of silica gel. After evaporating the solvent, Compound C21 (2.6 g, 74%) recrystallized from toluene as a white solid.

Synthesis of Compound C23



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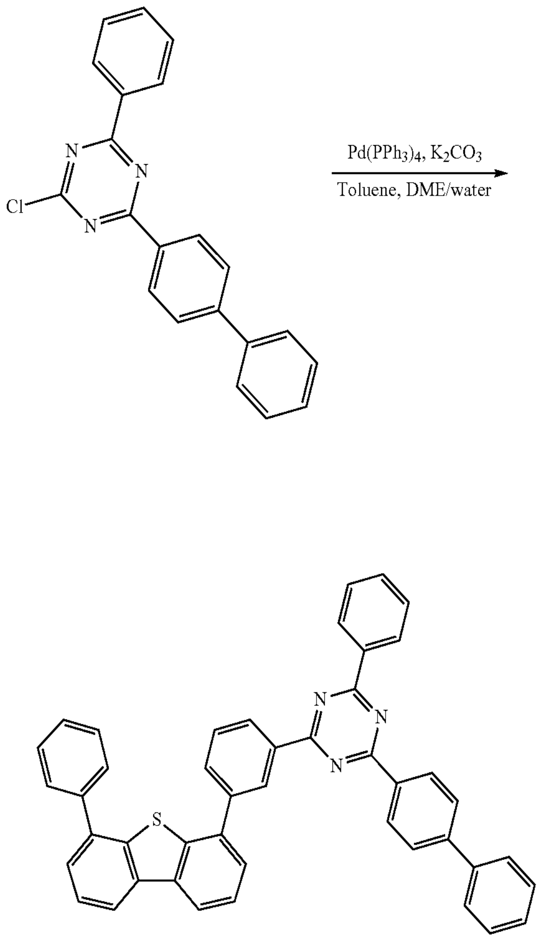
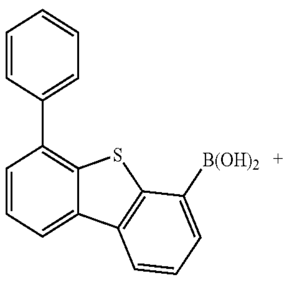


Compound C23

A solution of 4,4,5,5-tetramethyl-2-(3-(6-phenyldibenzo[b,d]thiophen-4-yl)phenyl)-1,3,2-dioxaborolane (3.0 g, 6.49 mmol), 2-([1,1'-biphenyl]-4-yl)-4-chloro-6-phenyl-1,3,5-triazine (2.454 g, 7.14 mmol), $Pd(PPh_3)_4$ (0.375 g, 0.324 mmol), and K_2CO_3 (2.69 g, 19.46 mmol) in toluene (13 ml), DME (39 ml), and water (13 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solids were collected by filtration, then triturated with ethanol, dissolved in boiling toluene, and filtered through a short plug of silica gel. After evaporating the solvent, Compound C23 (3.78 g, 91%) recrystallized from toluene as a white solid.

Synthesis of Compound C29



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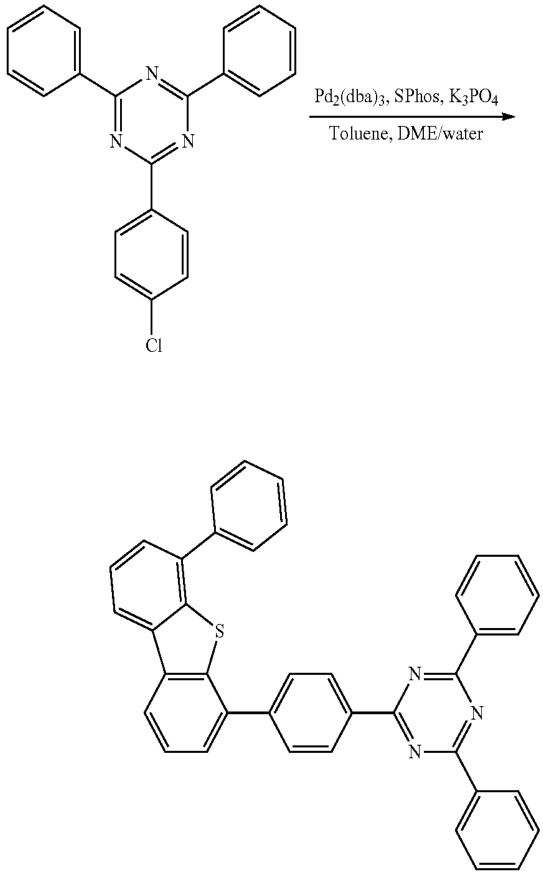
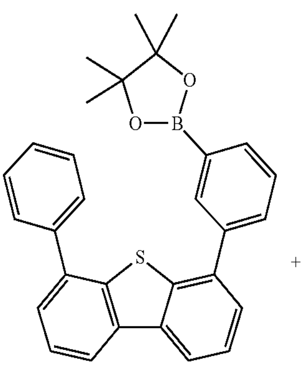


Compound C29

A solution of 2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (2.75 g, 8.00 mmol), 6-phenyl-dibenzo[b,d]thiophen-4-yl boronic acid (2.68 g, 8.80 mmol), $Pd_2(dba)_3$ (0.20 g, 0.22 mmol) and SPhos (0.40 g, 0.98 mmol), and K_3PO_4 (5.52 g, 24.00 mmol) in toluene (150 ml), DME (125 ml) and water (30 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the precipitate was collected by filtration and washed with water and DCM, before being dissolved in boiling toluene and filtered through a short plug of silica gel. After evaporating the solvent, Compound C29 (2.42 g, 53%) was recrystallized from toluene to give a white solid.

Synthesis of Compound C47



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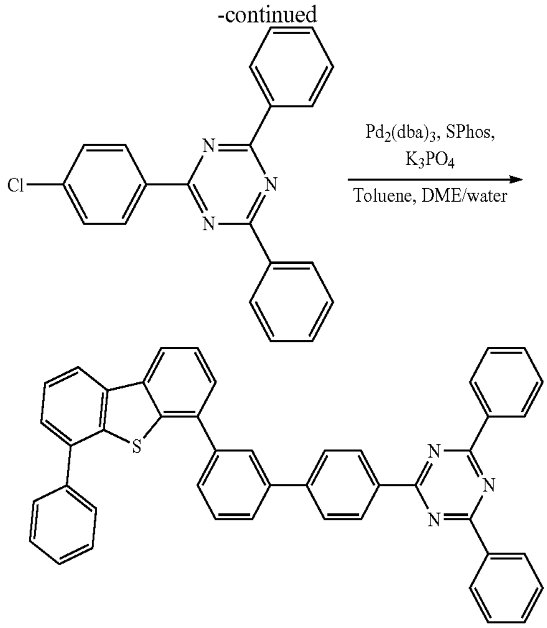
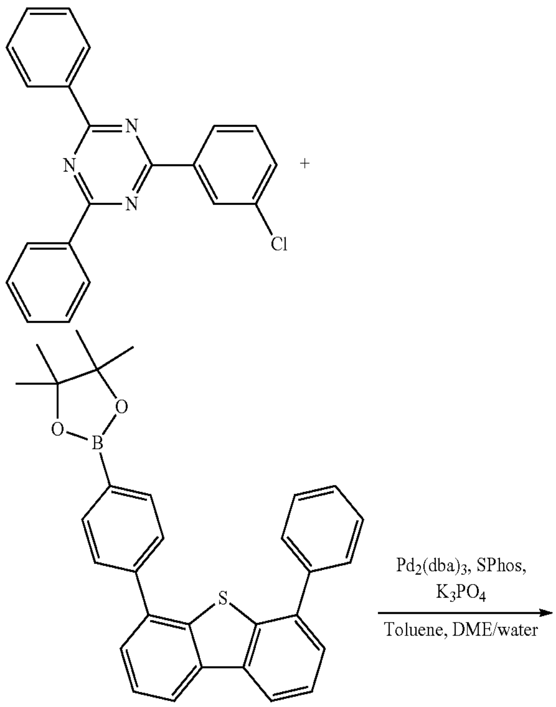


Compound C47

A suspension of 4,4,5,5-tetramethyl-2-(3-(6-phenyldibenzo[b,d]thiophen-4-yl)phenyl)-1,3,2-dioxaborolane (3.09 g, 6.69 mmol), 2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (2.3 g, 6.69 mmol), $Pd_2(dba)_3$ (0.123 g, 0.134 mmol), and SPhos (0.110 g, 0.268 mmol) and K_3PO_4 (4.26 g, 20.07 mmol) in toluene (20 ml), DME (30 ml), and water (10 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, then dissolved in boiling toluene, filtered through a short plug of silica, and recrystallized from toluene to yield Compound C47 (3.51%, 81%) as a white solid.

Synthesis of Compound C56



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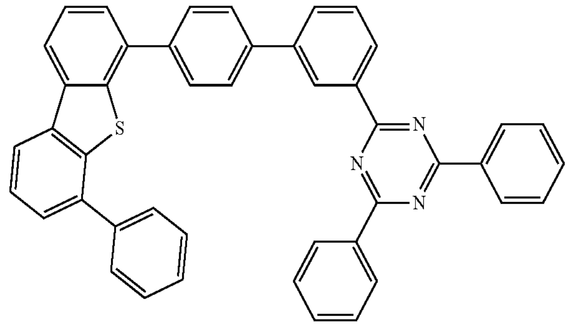
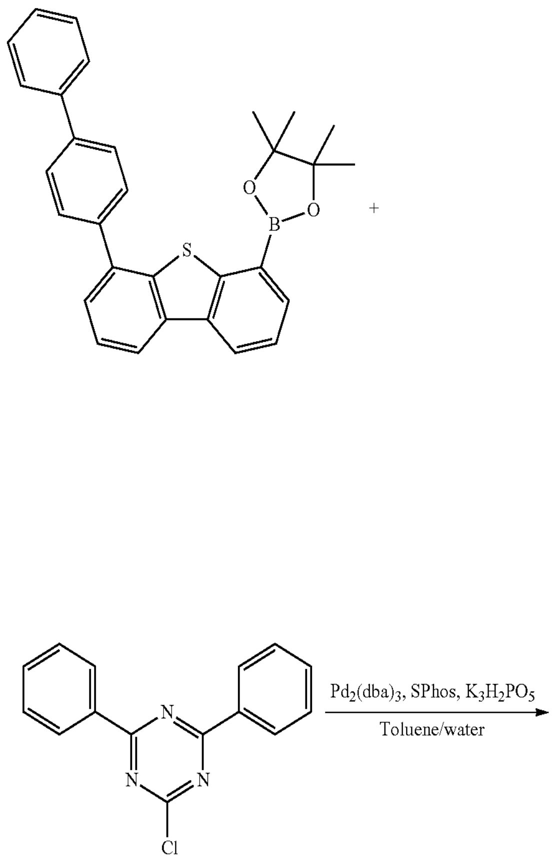


Compound C56

A solution of 4,4,5,5-tetramethyl-2-(4-(6-phenyldibenzo[b,d]thiophen-4-yl)phenyl)-1,3,2-dioxaborolane (3.5 g, 7.57 mmol), 2-(3-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (2.169 g, 6.31 mmol), $Pd_2(dba)_3$ (0.17 g, 0.19 mmol), SPhos (0.23 g, 0.57 mmol), and K_3PO_4 (4.02 g, 18.9 mmol) in toluene (100 ml), DME (100 ml), and water (10 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was filtered through a plug of silica gel. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (9/1 to 4/1, v/v) as eluent and recrystallization from DCM to yield Compound C56 (2.2 g, 54%) as a white solid.

Synthesis of Compound C65



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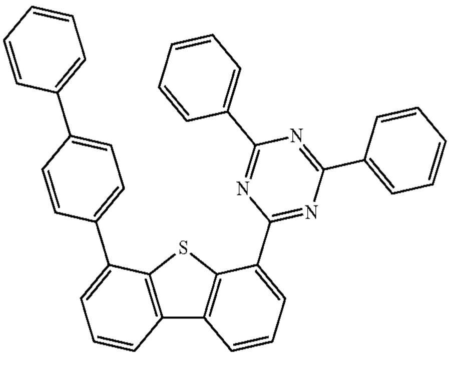
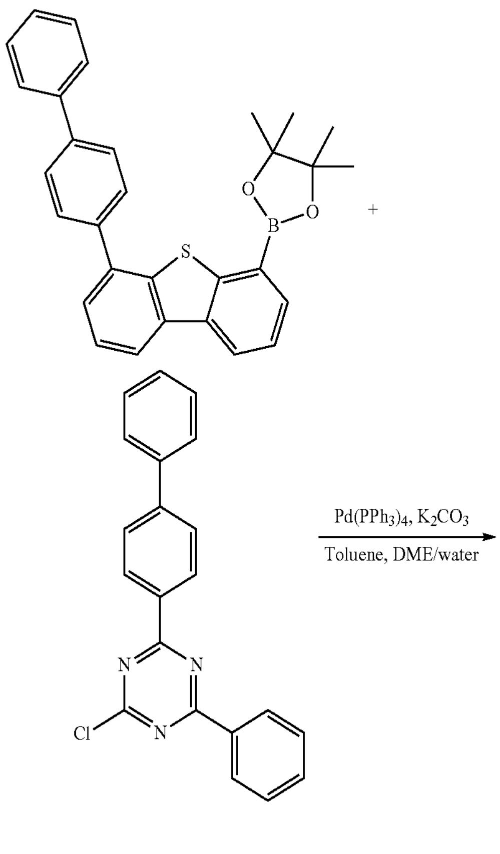


Compound C65

A mixture solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.75 g, 8.11 mmol), 2-chloro-4,6-diphenyl-1,3,5-triazine (2.61 g, 9.73 mmol), $Pd_2(dba)_3$ (0.149 g, 0.162 mmol), SPhos (0.266 g, 0.649 mmol), and potassium phosphate hydrate (3.74 g, 16.22 mmol) in toluene (90 mL) and water (10 mL) was refluxed under nitrogen overnight (~12 hours). Upon completion, the toluene was evaporated and the mixture was extracted with dichloromethane (not completely soluble) and washed with brine and water. The organic layers were combined, dried over Na_2SO_4, and concentrated under vacuum. The crude materials was triturated with ethanol and then with toluene to yield Compound C65 (3.0 g, 65%) as a light-yellow solid.

Synthesis of Compound C68



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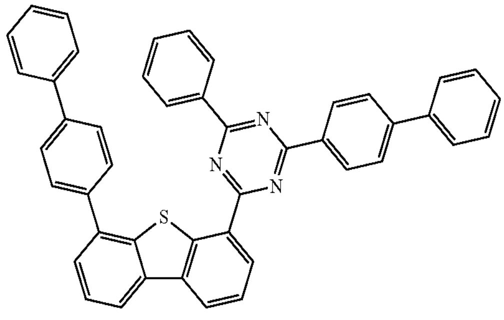
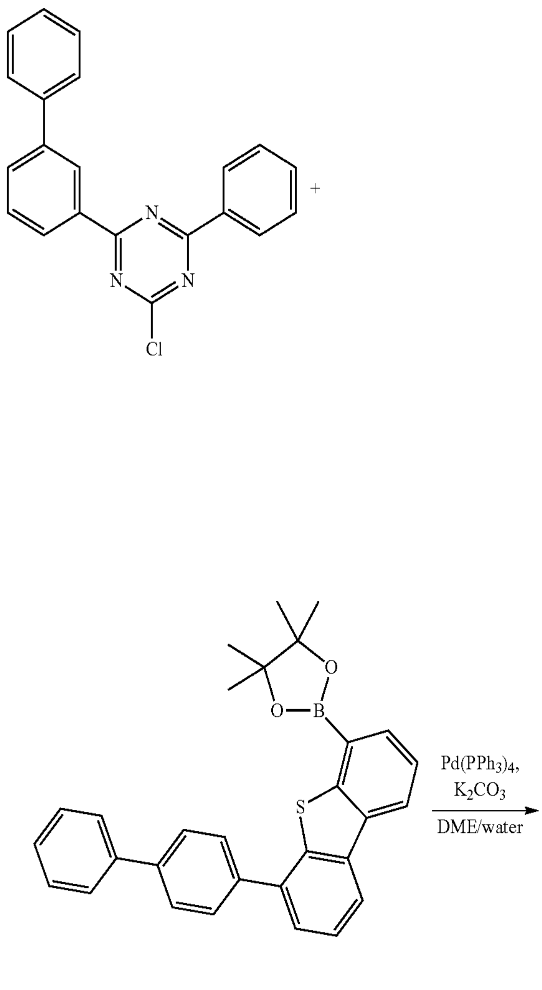


Compound C68

A solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4 g, 8.65 mmol), 2-([1,1'-biphenyl]-4-yl)-4-chloro-6-phenyl-1,3,5-triazine (2.75 g, 8.00 mmol), $Pd(PPh_3)_4$ (0.28 g, 0.24 mmol), and K_2CO_3 (3.31 g, 24 mmol) in toluene (125 ml), DME (100 ml) and water (25 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the precipitate was collected by filtration then rinsed with toulene. The crude product was triturated successively with toluene and methanol, then sublimed under vacuum to yield Compound C68 (4.25 g, 83%) as a white solid.

Synthesis of Compound C71



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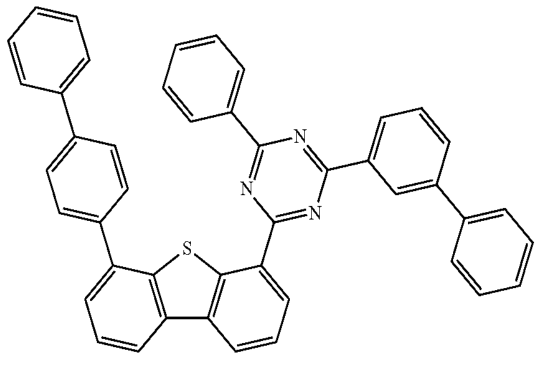
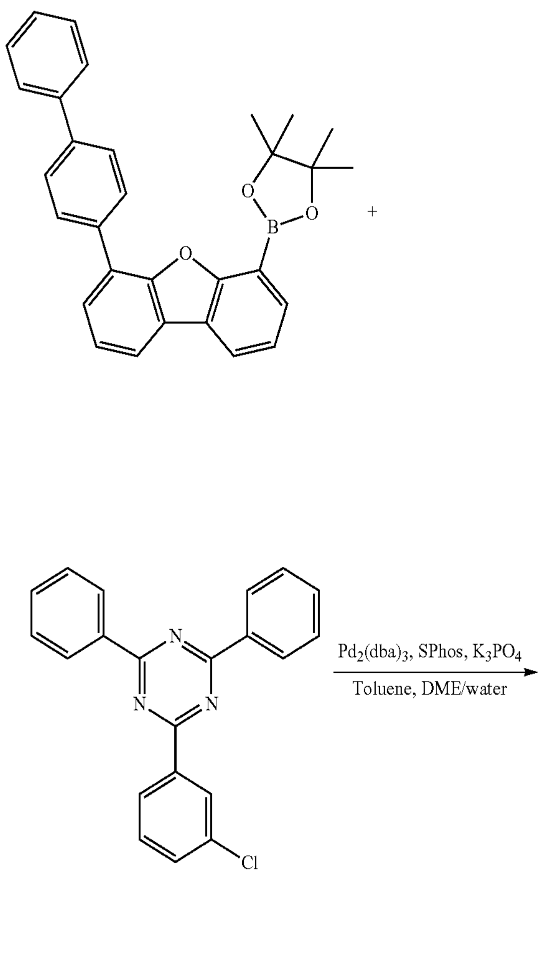


Compound C71

A suspension of 2-([1,1'-biphenyl]-3-yl)-4-chloro-6-phenyl-1,3,5-triazine (2.1 g, 6.11 mmol), 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.82 g, 6.11 mmol), $Pd(PPh_3)_4$ (0.141 g, 0.122 mmol), and K_2CO_3 (2.53 g, 18.32 mmol) in DME (150 ml) and water (20 ml) was refluxed under nitrogen for 3 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, then washed with water and ethanol. The solid was dissolved in boiling toluene, filtered through a short plug of silica gel. After evaporating the solvent, the crude product was recrystallized from toluene to yield Compound C71 (2.9 g, 74%) as a light-yellow solid.

Synthesis of Compound C73



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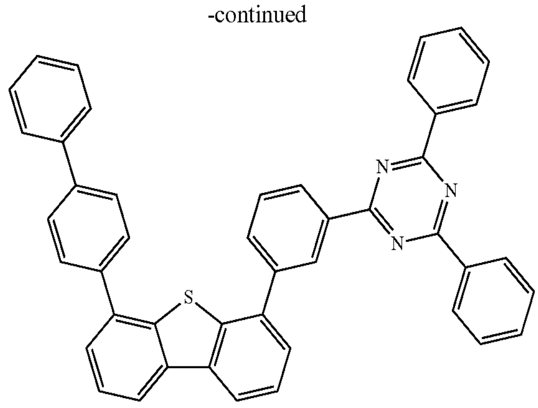
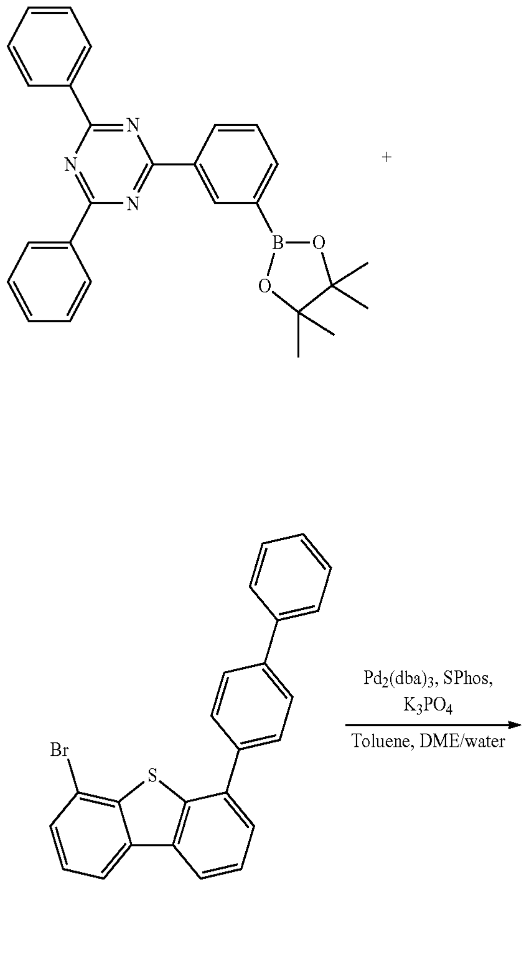


Compound C73

A solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]furan-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.2 g, 9.41 mmol), 2-(3-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (3.46 g, 10.07 mmol), $Pd_2(dba)_3$ (0.258 g, 0.282 mmol), SPhos (0.463 g, 1.129 mmol), and K_3PO_4 (6.49 g, 28.2 mmol) in toluene (125 ml), DME (100 ml), and water (25 ml) was refluxed under nitrogen for 18 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, dissolved in boiling toluene, filtered through a short plug of silica gel, and recrystallized from toluene to yield Compound C73 (4.5 g, 76%) as a white solid.

Synthesis of Compound C74



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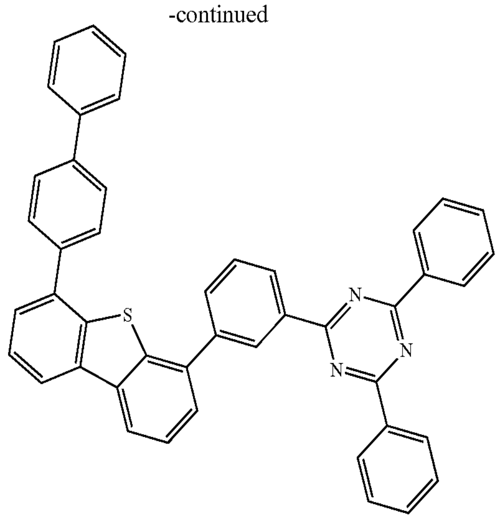
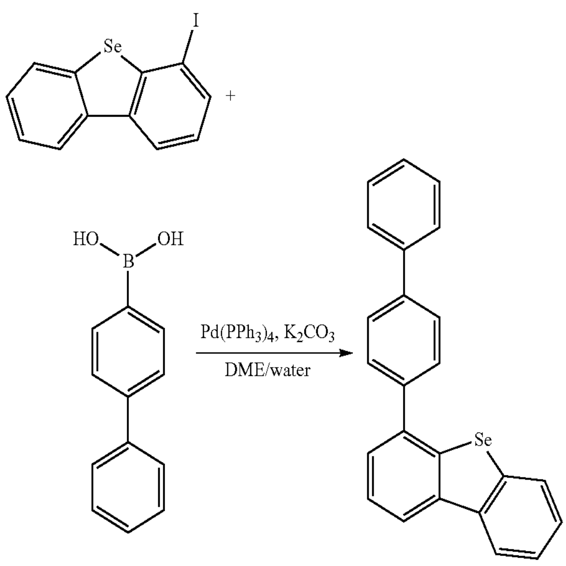


Compound C74

A solution of 2,4-diphenyl-6-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1,3,5-triazine (2.64 g, 6.07 mmol), 4-([1,1'-biphenyl]-4-yl)-6-bromodibenzo[b,d]thiophene (2.53 g, 6.10 mmol), $Pd_2(dba)_3$ (0.139 g, 0.152 mmol), SPhos (0.187 g, 0.455 mmol), and K_3PO_4 (2.146 g, 10.11 mmol) in toluene (75 ml), DME (75 ml), and water (7.50 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the solid was collected by filtration, purified by column chromatography on silica gel with heptane/DCM (4/1 to 7/3, v/v) as eluent and recrystallization from heptane to yield Compound C74 (2.0 g, 61%) as a white solid.

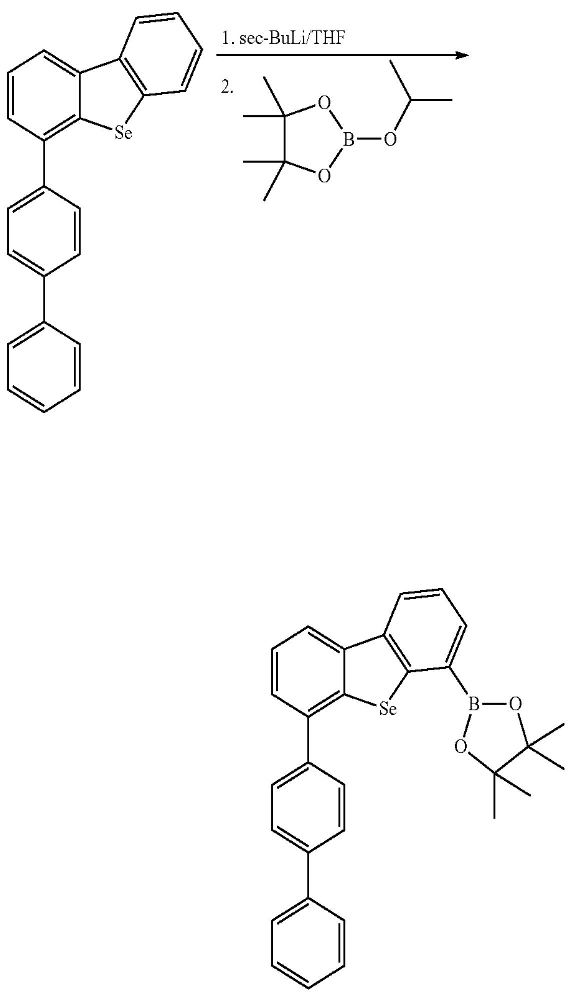
Synthesis of Compound C75

Synthesis of 4-([1,1'-biphenyl]-4-yl)dibenzo[b,d]selenophene



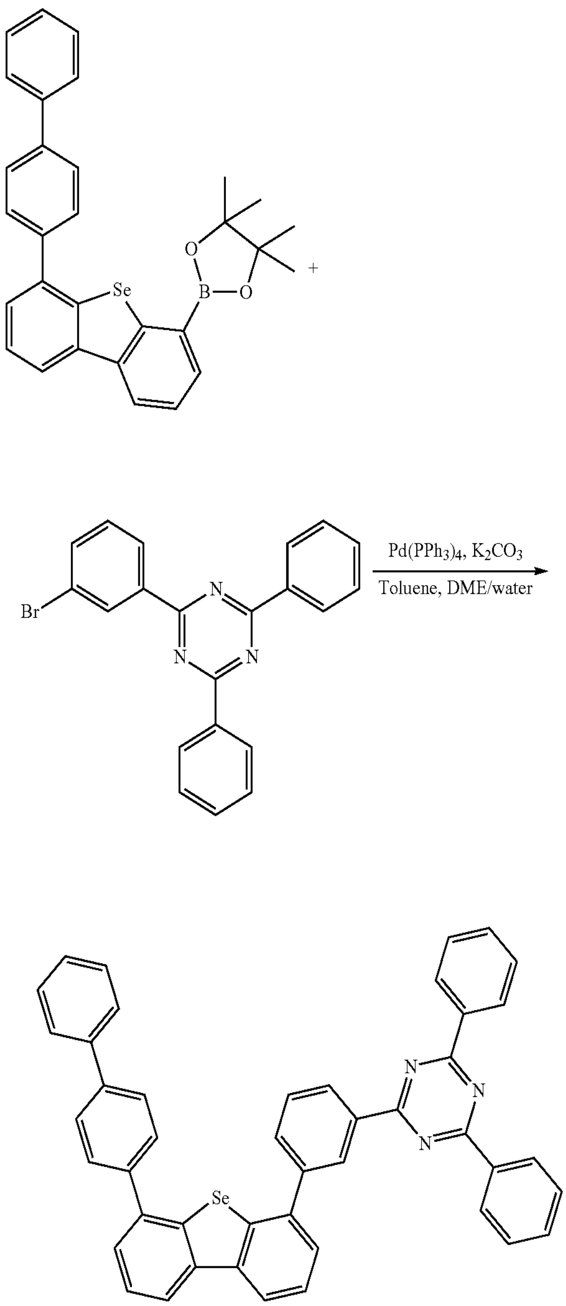
A solution of 4-iodo-dibenzo[b,d]selenophene (10 g, 28.0 mmol), [1,1'-biphenyl]-4-ylboronic acid (8.32 g, 42.0 mmol), $Pd(PPh_3)_4$ (1.624 g, 1.400 mmol), and K_2CO_3 (7.74 g, 56.0 mmol) in DME (200 ml) and water (40 ml) was refluxed under nitrogen for 24 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed with water and heptane, then dissolved in boiling toluene and filtered through a short plug of silica gel. After evaporating the solvent, 4-([1,1'-biphenyl]-4-yl)dibenzo[b,d]selenophene (8.0 g, 74%) was recrystallized from toluene as a white solid.

Synthesis of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]selenophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



Into a solution of 4-([1,1'-biphenyl]-4-yl)dibenzo[b,d]selenophene (5.5 g, 14.35 mmol) in THF (150 ml) a solution of sec-butyl lithium (18.45 ml, 25.8 mmol) was added dropwise at −78° C. The resulting mixture was stirred at −78° C. for 5 h before 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5.12 ml, 25.1 mmol) was added in one portion. The reaction mixture was gradually warmed to room temperature (~22° C.) and stirred for 16 h before quenching with water. The resulting mixture was extracted with ethyl acetate, then dried over Na_2SO_4. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (4/1 to 3/2, v/v) as the eluent to yield 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]selenophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.6 g, 36%) as a white solid.

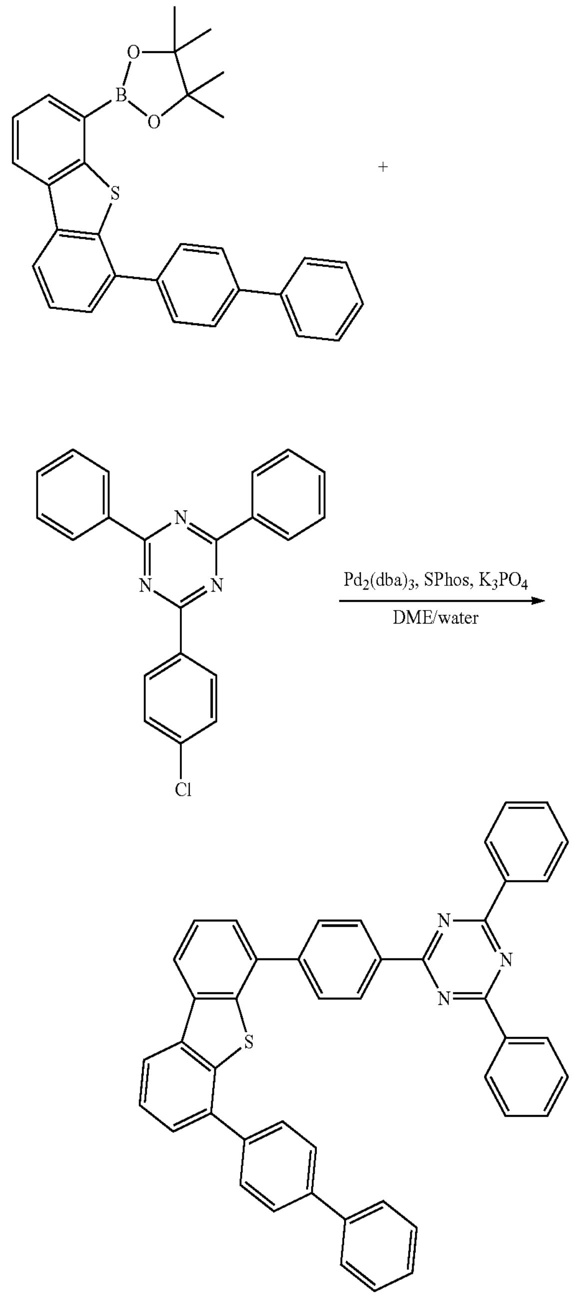
Synthesis of Compound C75



Compound C75

A solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]selenophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.62 g, 5.15 mmol), 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (2 g, 5.15 mmol), $Pd(PPh_3)_4$ (0.179 g, 0.155 mmol), and K_2CO_3 (1.424 g, 10.30 mmol) in DME (150 ml), toluene (50 ml), and water (40 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed successively with water and heptane, then dissolved in boiling toluene and filtered through a short plug of silica gel. The crude product further purified by recrystallized successively from heptane and toluene to yield Compound C75 (2.1 g, 59%) as white crystals.

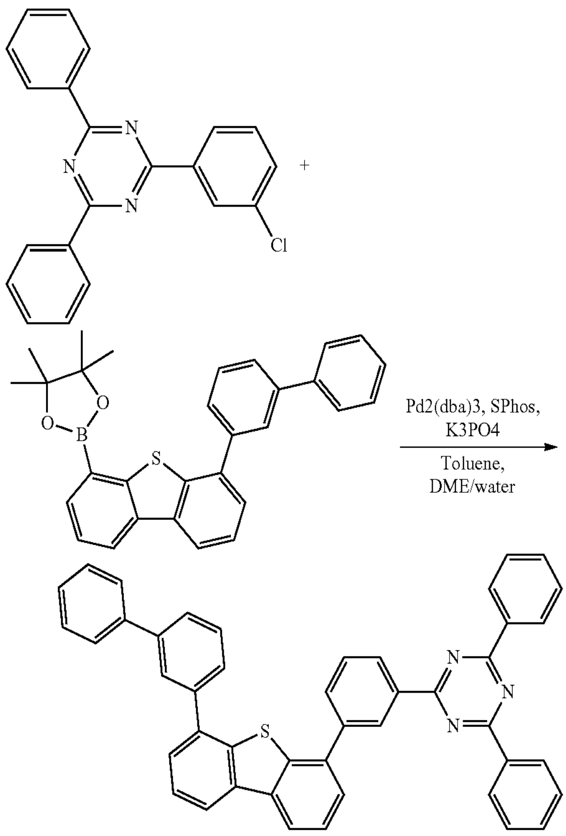
Synthesis of Compound C83



Compound C83

A suspension of 2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (2.409 g, 7.01 mmol), 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.7 g, 5.84 mmol), $Pd_2(dba)_3$ (0.107 g, 0.117 mmol), SPhos (0.096 g, 0.234 mmol), and K_2CO_3 (2.421 g, 17.52 mmol) in toluene (20 ml), DME (65 ml), and water (15 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was diluted with water. The solid was collected by filtration, washed with water and ethanol, redissolved in hot toluene, and filtered through a short plug of silica gel. After evaporating the solvent, the residue was recrystallized from EtOAc to yield Compound C83 (3.2 g, 85%) as a white solid.

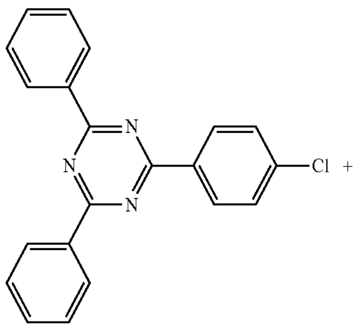
Synthesis of Compound C101



Compound C101

A solution of 2-(6-([1,1'-biphenyl]-3-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.03 g, 8.73 mmol), 2-(3-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (2.50 g, 7.27 mmol), $Pd_2(dba)_3$ (0.20 g, 0.22 mmol), SPhos (0.27 g, 0.65 mmol), and K_3PO_4 (4.63 g, 21.8 mmol) in toluene (100 ml). DME (100 ml), and water (10 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was diluted with DCM and filtered through a plug of silica gel. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (4/1 to 3/2, v/v) as the eluent and recrystallization from DCM to yield Compound C101 (1.6 g, 43%) as a white solid.

Synthesis of Compound C110



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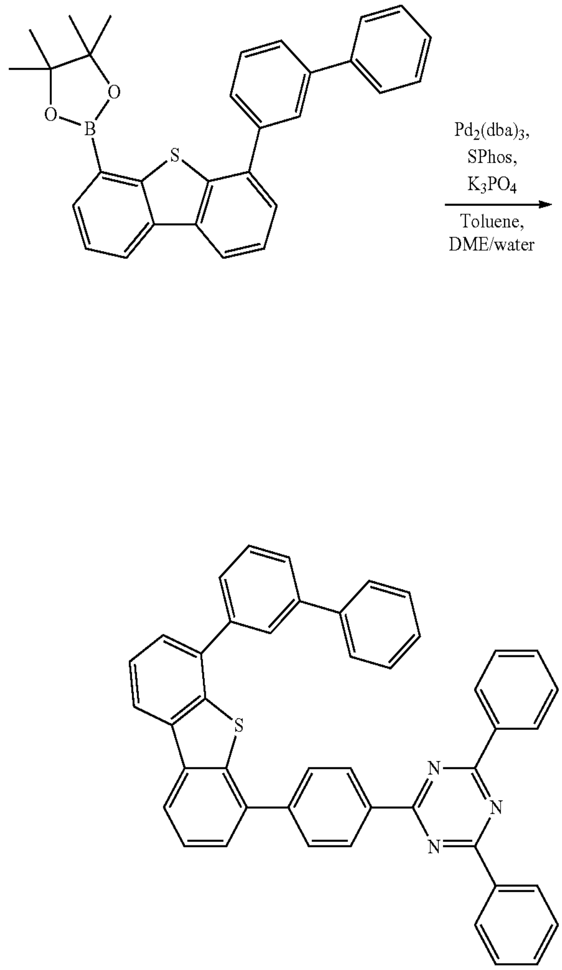
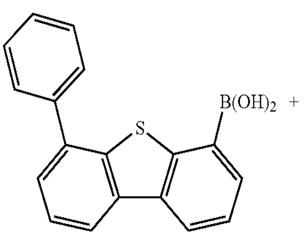


Compound C110

A suspension of 2-(6-([1,1'-biphenyl]-3-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.1 g, 6.70 mmol), 2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (2.54 g, 7.37 mmol), Pd2(dba)3 (0.123 g, 0.134 mmol), and SPhos (0.110 g, 0.268 mmol), and K_3PO_4 (4.27 g, 20.11 mmol) in toluene (20.00 ml), DME (30.0 ml) and water (10 ml) was refluxed under nitrogen overnight. After cooling to room temperature, it was diluted with water and the solid was collected by filtration and washed with ethanol. The crude product was dissolved in boiling toluene and filtered through a short plug of silica gel. Upon evaporation off the solvent, Compound C110 (4.2 g, 97%) was recrystallized from toluene as a white solid.

Synthesis of Compound C119



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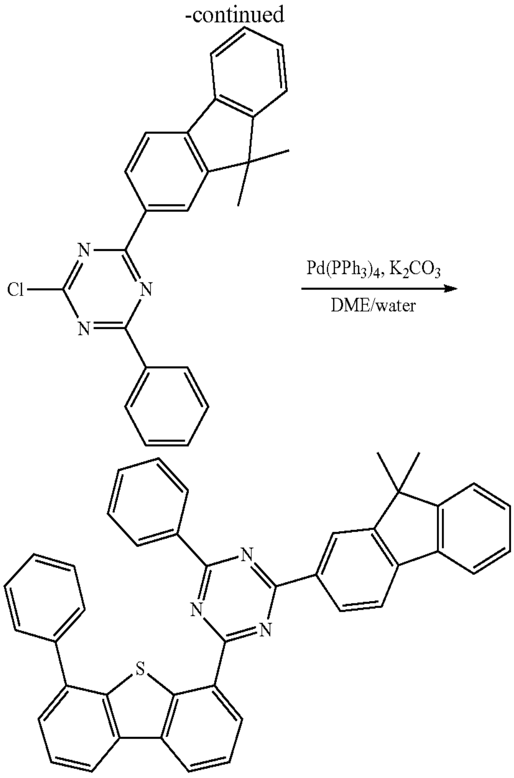
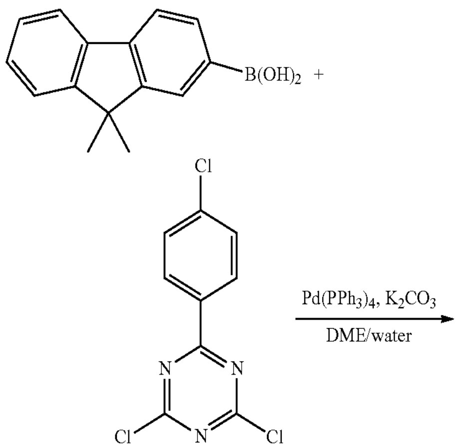


Compound C119

A solution of (6-phenyldibenzo[b,d]thiophen-4-yl)boronic acid (3.14 g, 10.32 mmol), 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (3.6 g, 9.38 mmol), $Pd(PPh_3)_4$ (0.217 g, 0.188 mmol), and K_2CO_3 (3.89 g, 28.1 mmol) in DME (180 ml) in water (50 ml) was refluxed under nitrogen for 14 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed successively with methanol, water, ethanol, ethyl acetate and heptane, then dissolved in dichloromethane and filtered through a short plug of silica gel. After evaporating the solvent, the crude product was triturated with ethanol and heptane to yield Compound C119 (4.0 g, 70%) as a white solid.

Synthesis of Compound C131

Synthesis of 2-(4-chlorophenyl)-4,6-bis(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine



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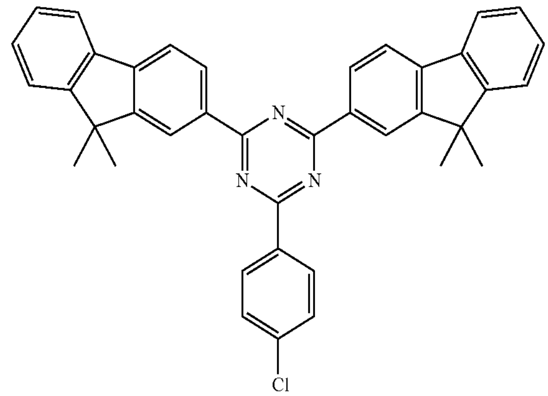
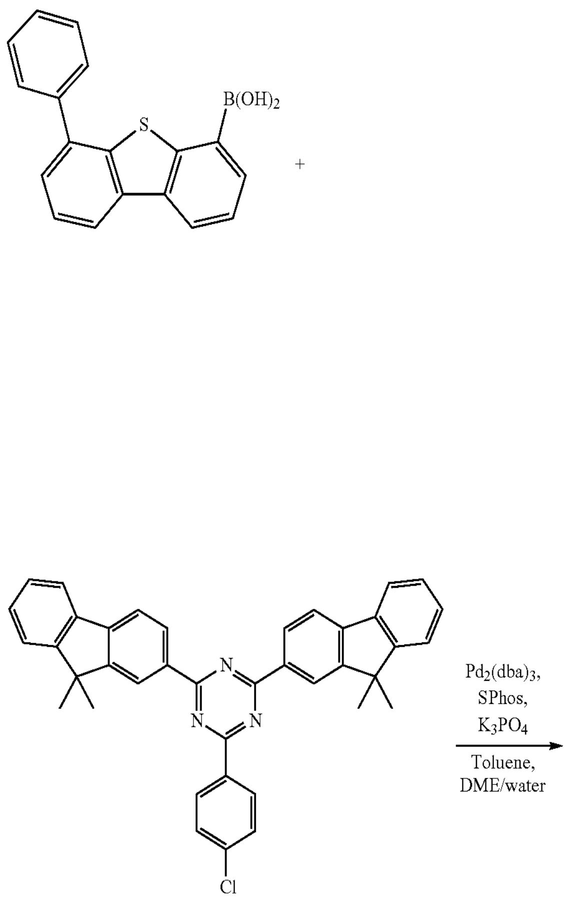


A solution of 2,4-dichloro-6-(4-chlorophenyl)-1,3,5-triazine (5 g, 19.19 mmol), (9,9-dimethyl-9H-fluoren-2-yl)boronic acid (9.14 g, 38.4 mmol), $Pd(PPh_3)_4$ (0.444 g, 0.384 mmol), and K_2CO_3 (7.96 g, 57.6 mmol) in DME (150 ml) and water (15 ml) was refluxed under nitrogen for 13 h. After cooling to room temperature (~22° C.), the organic phase was isolated. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (4/1, v/v) as the eluent to yield 2-(4-chlorophenyl)-4,6-bis(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (5.43 g, 49.1%) as a white solid.

Synthesis of Compound C131



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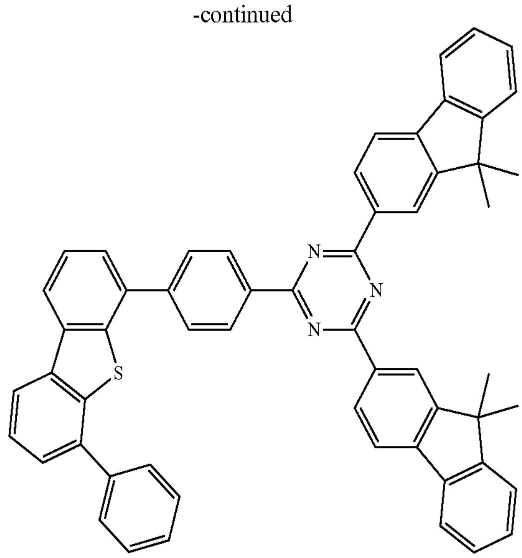
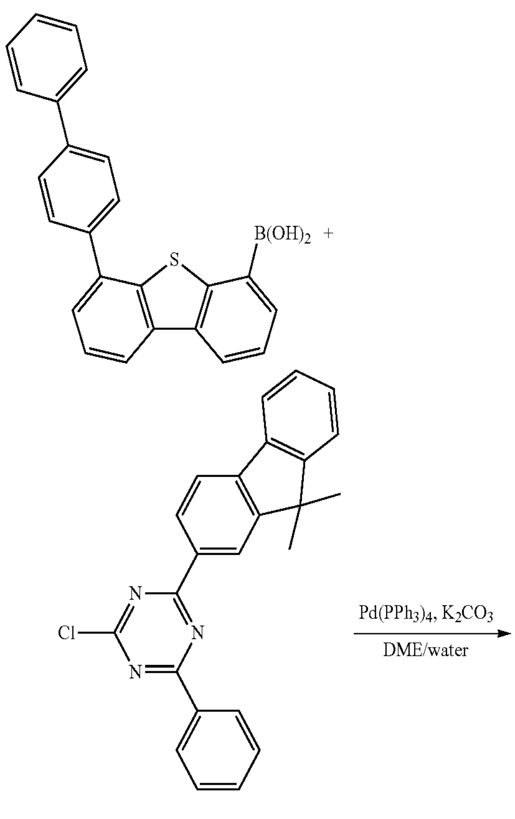


Compound C131

A solution of 2-(4-chlorophenyl)-4,6-bis(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (5.43 g, 9.42 mmol), (6-phenyldibenzo[b,d]thiophen-4-yl)boronic acid (2.87 g, 9.42 mmol), $Pd_2(dba)_3$ (0.129 g, 0.141 mmol), SPhos (0.116 g, 0.283 mmol), and K_3PO_4 (4.34 g, 18.85 mmol) in DME (200 ml) and water (25 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the organic phase was isolated and purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent to yield Compound C131 as a white solid.

Synthesis of Compound C134



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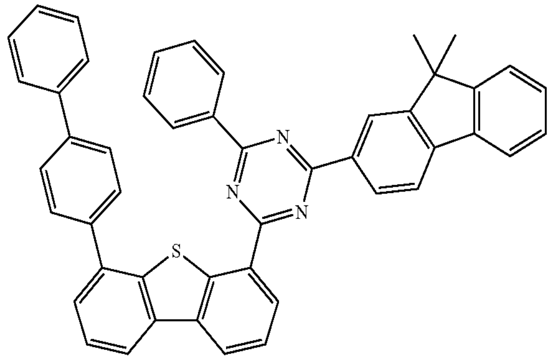
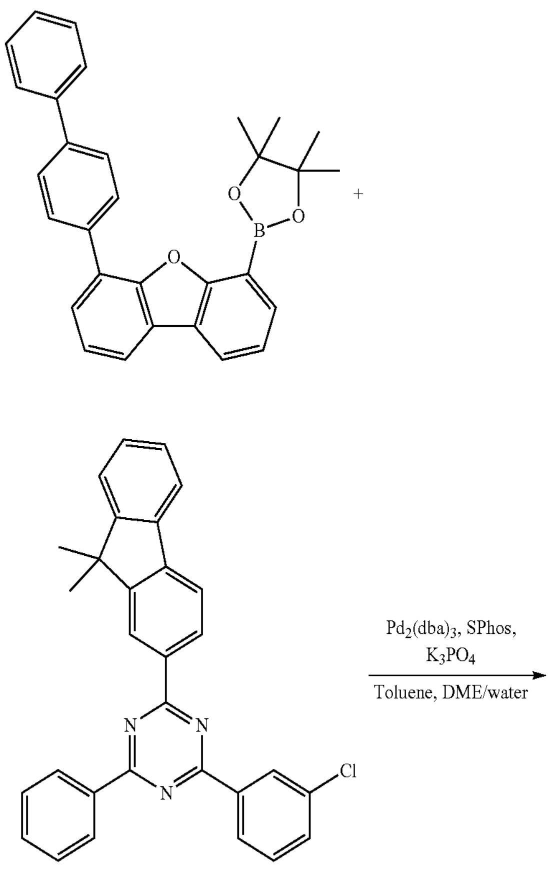


Compound C134

A solution of (6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)boronic acid (2.25 g, 5.92 mmol), 2-chloro-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (2.4 g, 6.25 mmol), $Pd(PPh_3)_4$ (0.137 g, 0.118 mmol), and K_2CO_3 (2.453 g, 17.75 mmol) in DME (200 ml) and water (50 ml) was refluxed under nitrogen for 14 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed successively with methanol, water, ethanol, ethyl acetate and heptane, then dissolved in boiling toulene and filtered through a short plug of silica gel. After evaporating the solvent, the crude product was triturated with ethanol and heptane to yield Compound C134 (3.0 g, 75%)

Synthesis of Compound C139



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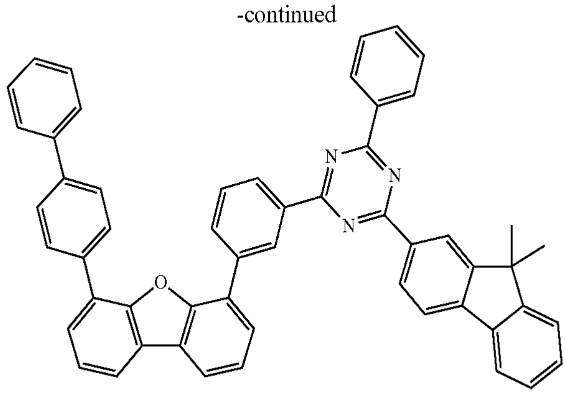
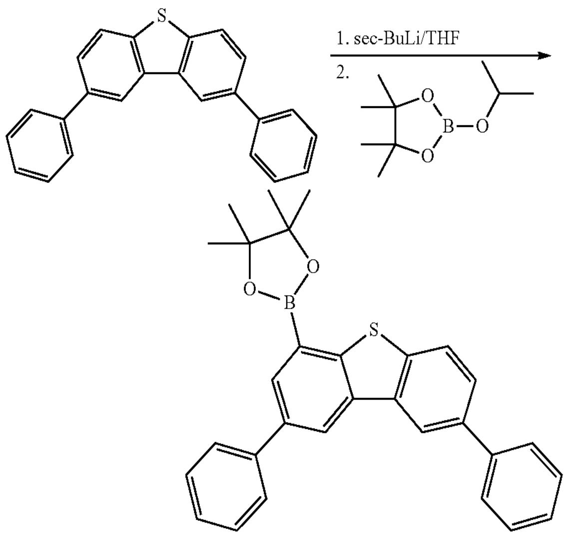


Compound C139

A solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]furan-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.41 g, 9.89 mmol), 2-(3-chlorophenyl)-4-(9,9-dimethyl-9H-fluoren-2-yl)-6-phenyl-1,3,5-triazine (4.25 g, 9.24 mmol), $Pd_2(dba)_3$ (0.211 g, 0.231 mmol), SPhos (0.379 g, 0.924 mmol), and K_3PO_4 (6.38 g, 27.7 mmol) in toluene (125 ml), DME (100 ml), and water (30 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the reaction mixture was extracted with toluene. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/toluene (4/1 to 1/1, v/v) as eluent to yield Compound C139 (4.1 g, 59.7%) as a white solid.

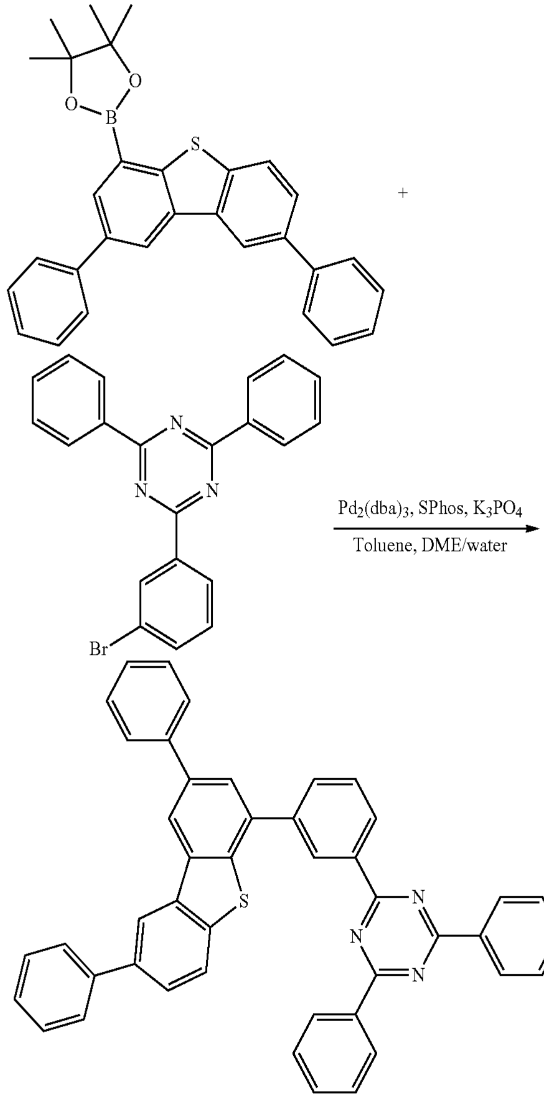
Synthesis of Compound C173

Synthesis of 2-(2,8-diphenyldibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



A solution of sec-butyllithium in cyclohexane (28.5 ml, 39.9 mmol) was added dropwise into a solution of 2,8-diphenyldibenzo[b,d]thiophene (7.45 g, 22.14 mmol) in anhydrous THF at −78° C. The reaction mixture was stirred at −78° C. for 2 h, while 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7.21 g, 38.8 mmol) was added at a rate of 1 mL/min. The reaction mixture was gradually warmed to room temperature (~22° C.) and stirred for 16 h before quenching with a 10% NH_4Cl aqueous solution. The resulting mixture was extracted with ethyl acetate. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent and then recrystallized from heptane to yield 2-(2,8-diphenyldibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5.5 g, 53.7%) as white crystals.

Synthesis of Compound 173

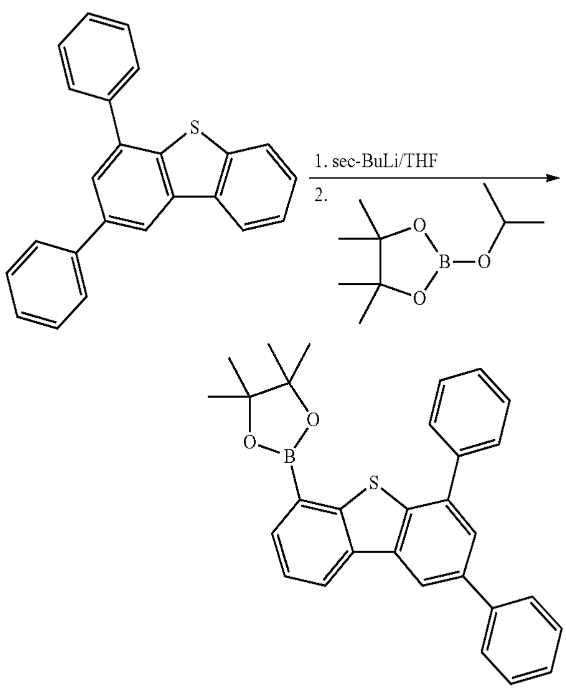


Compound 173

A solution of 2-(2,8-diphenyldibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.03 g, 6.55 mmol), 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (2.54 g, 6.55 mmol), $Pd_2(dba)_3$ (0.090 g, 0.098 mmol), SPhos (0.081 g, 0.197 mmol), and K_3PO_4 (3.02 g, 13.11 mmol) in DME (100 ml), toluene (100 ml), and water (10 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed successively with ethanol, water, ethanol and heptane, and then triturated with boiling toluene to yield Compound 173 (4.0 g, 95%) as a white solid.

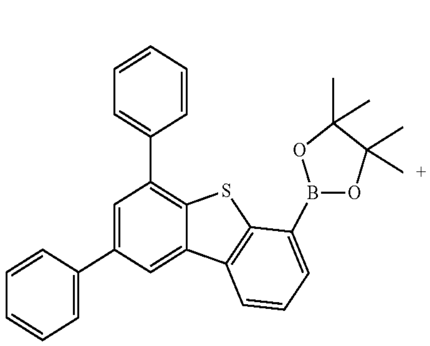
Synthesis of Compound C185

Synthesis of 2-(6,8-diphenyldibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



Sec-butyllithium in cyclohexane (38.2 ml, 53.5 mmol) was added dropwise into a solution of 2,4-diphenyldibenzo[b,d]thiophene (10 g, 29.7 mmol) in anhydrous THF at −78° C. The reaction mixture was stirred at −78° C. for 2 h, while 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (10.61 ml, 52.0 mmol) was added at a rate of 1 mL/min. The reaction mixture was gradually warmed to room temperature (~22° C.) and stirred for 16 h before being quenched with a 10% NH_4Cl aqueous solution. The resulting mixture was extracted with ethyl acetate. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/DCM (4/1 to 0/1, v/v) as the eluent, then recrystallized from heptane to yield 2-(6,8-diphenyldibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (9.5 g, 69%) as white crystals.

Synthesis of Compound C185



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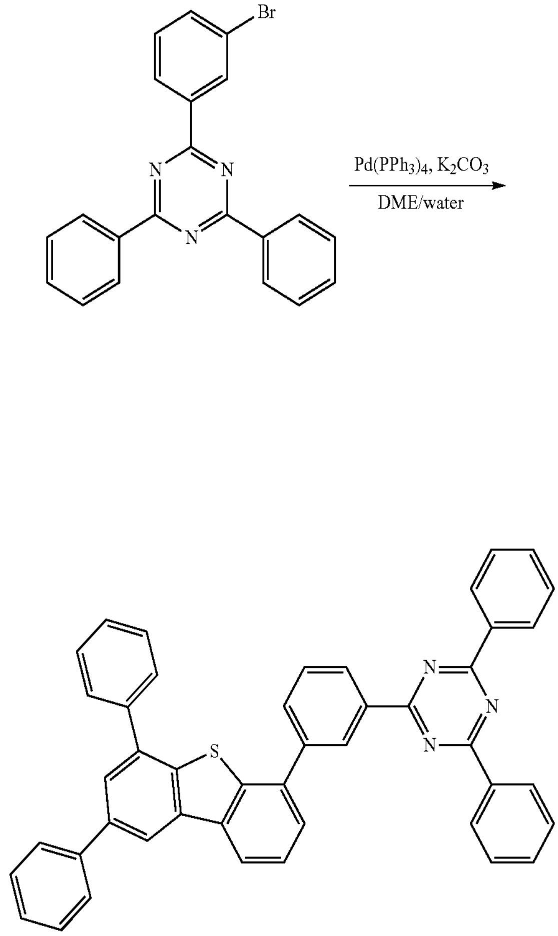
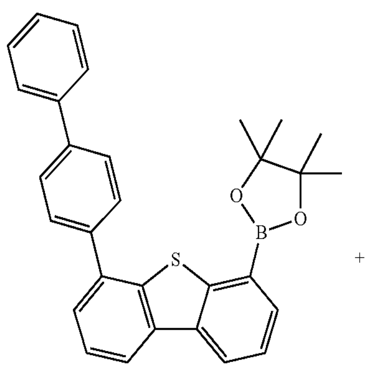


Compound C185

A solution of 2-(6,8-diphenyldibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.29 g, 9.27 mmol), 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (3 g, 7.73 mmol), $Pd(PPh_3)_4$ (0.269 g, 0.232 mmol), and K_2CO_3 (2.14 g, 15.45 mmol) in DME (200 ml) and water (40.0 ml) was refluxed under nitrogen for 5 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, dissolved in boiling xylene, then filtered through a short plug of silica gel and recrystallized from xylene to yield Compound C185 (2.6 g, 52.3%) as a white solid.

Synthesis of Compound C251



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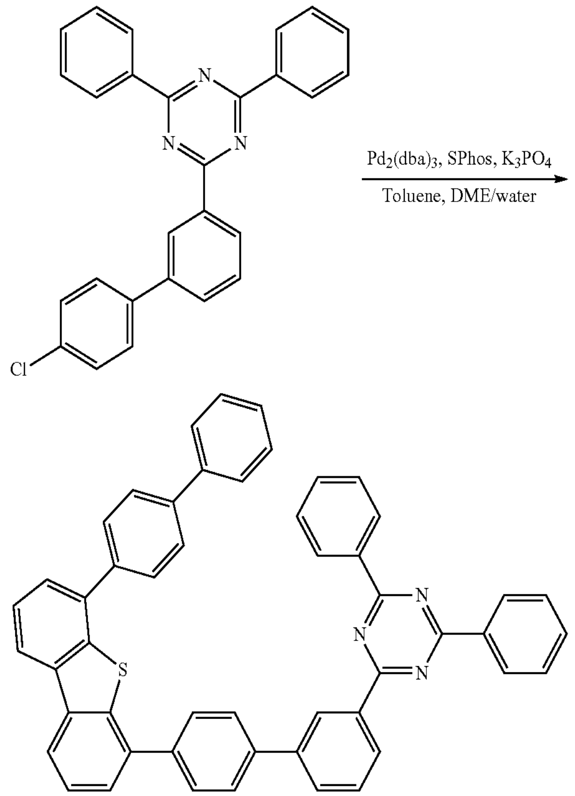
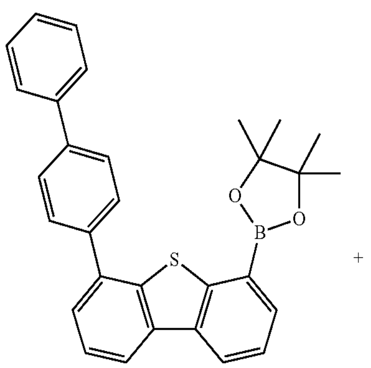


Compound C251

A solution of 2-(4'-chloro-[1,1'-biphenyl]-3-yl)-4,6-diphenyl-1,3,5-triazine (3.0 g, 7.14 mmol), 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.53 g, 7.64 mmol), $Pd_2(dba)_3$ (0.196 g, 0.214 mmol), SPhos (0.40 g, 0.976 mmol), and K_3PO_4 (4.93 g, 21.43 mmol) in DME (80 ml), toluene (160 ml), and water (25 ml) was refluxed for 18 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, washed with water, then dissolved in boiling toluene and filtered through a short plug of silica gel, and recrystallized from toluene to yield Compound C251 (3.43 g, 67%) as a white solid.

Synthesis of Compound C254



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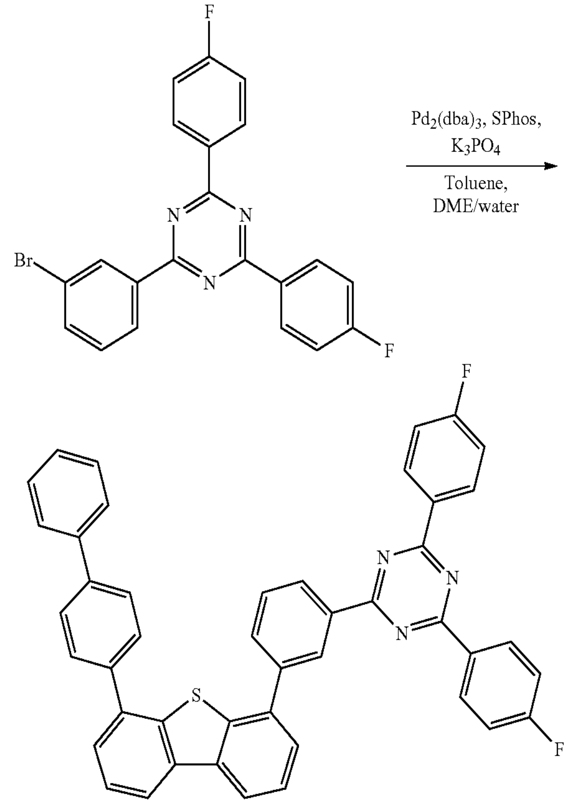
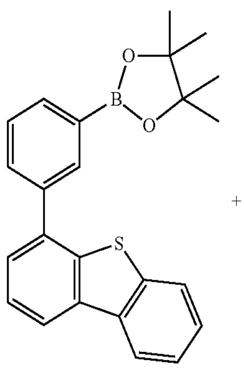


Compound C254

A solution of 2-(6-([1,1'-biphenyl]-4-yl)dibenzo[b,d]thiophen-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.72 g, 5.89 mmol), 2-(3-bromophenyl)-4,6-bis(4-fluorophenyl)-1,3,5-triazine (2.5 g, 5.89 mmol), $Pd_2(dba)_3$ (0.081 g, 0.088 mmol), SPhos (0.073 g, 0.177 mmol), and K_3PO_4 (2.71 g, 11.79 mmol) in DME (200 ml) and water (50 ml) was refluxed under nitrogen for 18 h. After cooling to room temperature (~22° C.), the solid was collected by filtration and purified by column chromatography on silica gel with heptane/DCM (1/1, v/v) as the eluent and recrystallized from heptane to yield Compound C254 (2.5 g, 62%) as white crystals.

Synthesis of Compound D1



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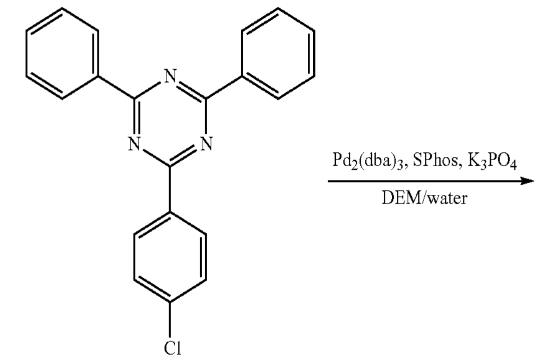
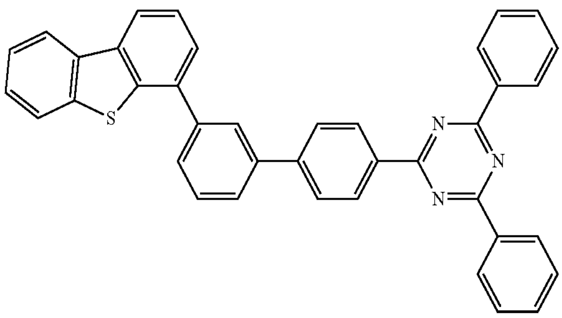
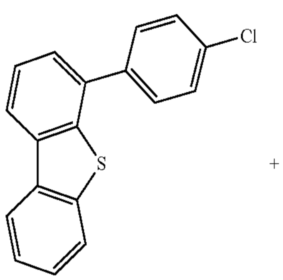




Compound D1

A solution of 2-(3-(dibenzo[b,d]thiophen-4-yl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.5 g, 9.06 mmol), 2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine (3.43 g, 9.97 mmol), $Pd_2(dba)_3$ (0.166 g, 0.181 mmol), SPhos (0.149 g, 0.362 mmol), and K_3PO_4 (5.77 g, 27.2 mmol) in DME (70 ml) and water (15 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was diluted with water. The solid was collected by filtration, washed with methanol, dissolved in hot toluene and filtered through a short plug of silica gel. After evaporating the solvent, Compound D1 (4.20 g, 82%) recrystallized from toluene as a white solid.

Synthesis of Compound D2



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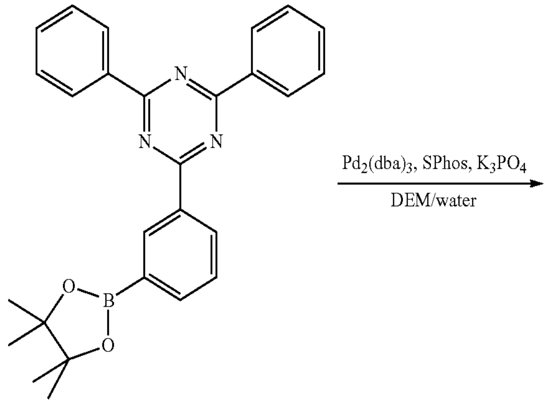
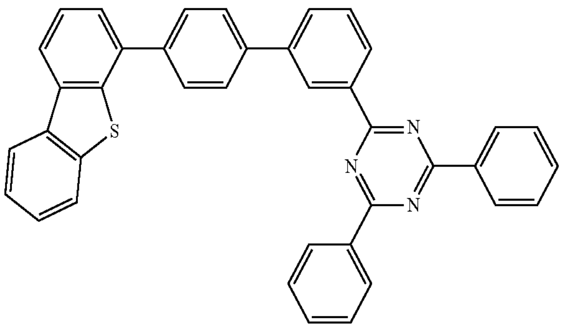
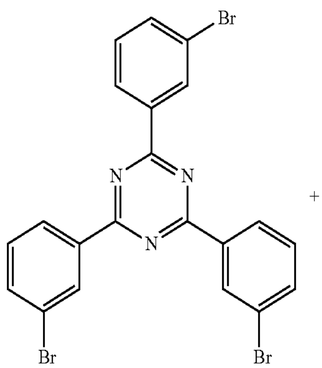




Compound D2

A solution of 4-(4-chlorophenyl)dibenzo[b,d]thiophene (2.46 g, 8.35 mmol), 2,4-diphenyl-6-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1,3,5-triazine (4.0 g, 9.19 mmol), $Pd_2(dba)_3$ (0.15 g, 0.17 mmol), SPhos (0.27 g, 0.67 mmol), and K_3PO_4 (2.89 g, 16.7 mmol) in DME (90 ml) and water (10 ml) was refluxed under nitrogen for 6 h. After cooling to room temperature (~22° C.), the reaction mixture was diluted with water. The solid was collected by filtration, washed successively with water and methanol, re-dissolved in hot toluene, and filtered through a short plug of silica gel. After evaporating the solvent, Compound 248 (2.1 g, 50%) recrystallized from toluene as a white solid.

Synthesis of Compound F1



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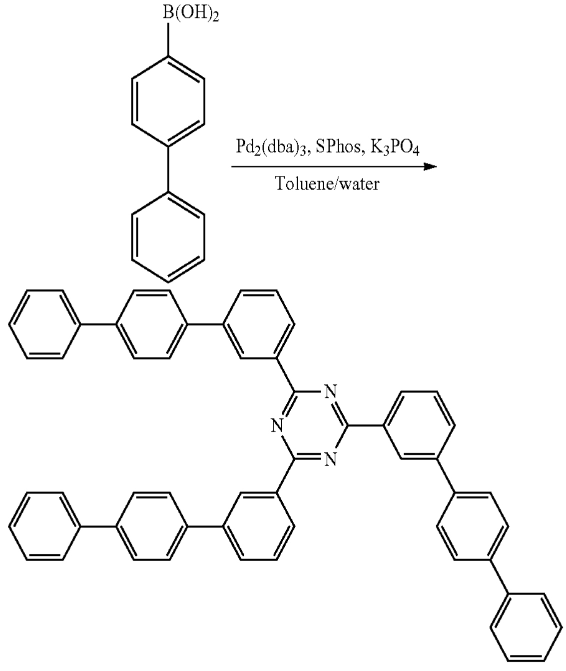
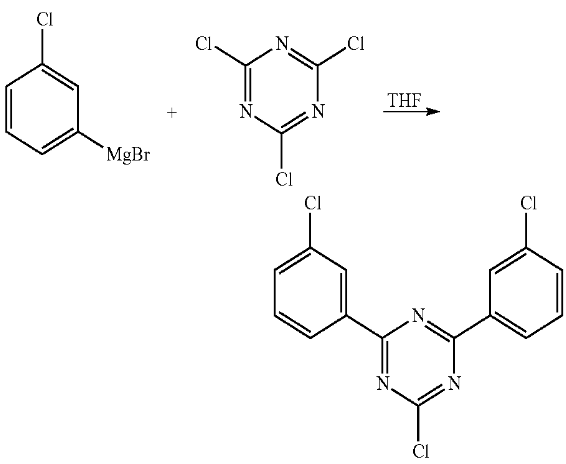


Compound F1

A solution of 2,4,6-tris(3-bromophenyl)-1,3,5-triazine (3 g, 5.49 mmol), [1,1'-biphenyl]-4-ylboronic acid (3.48 g, 17.58 mmol), $Pd_2(dba)_3$ (0.101 g, 0.110 mmol), SPhos (0.180 g, 0.440 mmol), and K_3PO_4 (2.332 g, 10.99 mmol) in toluene (54 ml) and water (6 ml) was refluxed under nitrogen for 12 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, the washed successively with water, methanol, and toluene. The crude product was purified by sublimation to yield Compound F1 (1.7 g, 40%) as a white solid.

Synthesis of Compound F2

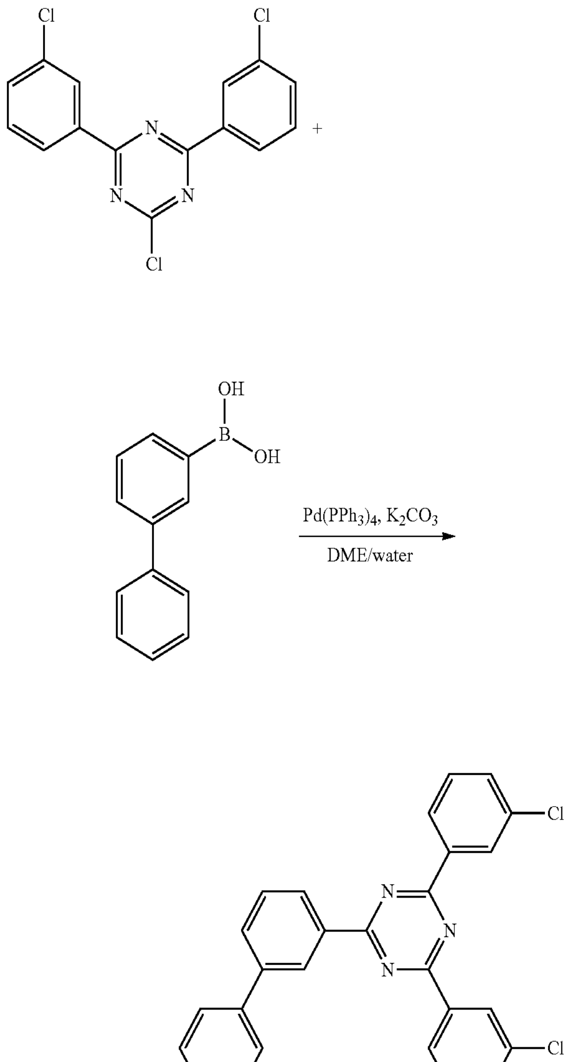
Synthesis of 2-chloro-4,6-bis(3-chlorophenyl)-1,3,5-triazine



A solution of (3-chlorophenyl)magnesium bromide (50 ml, 50.0 mmol) was added dropwise into a solution of 2,4,6-trichloro-1,3,5-triazine (3.1 g, 16.7 mmol) in THF (50 ml) at 0° C. It was slowly warmed to room temperature

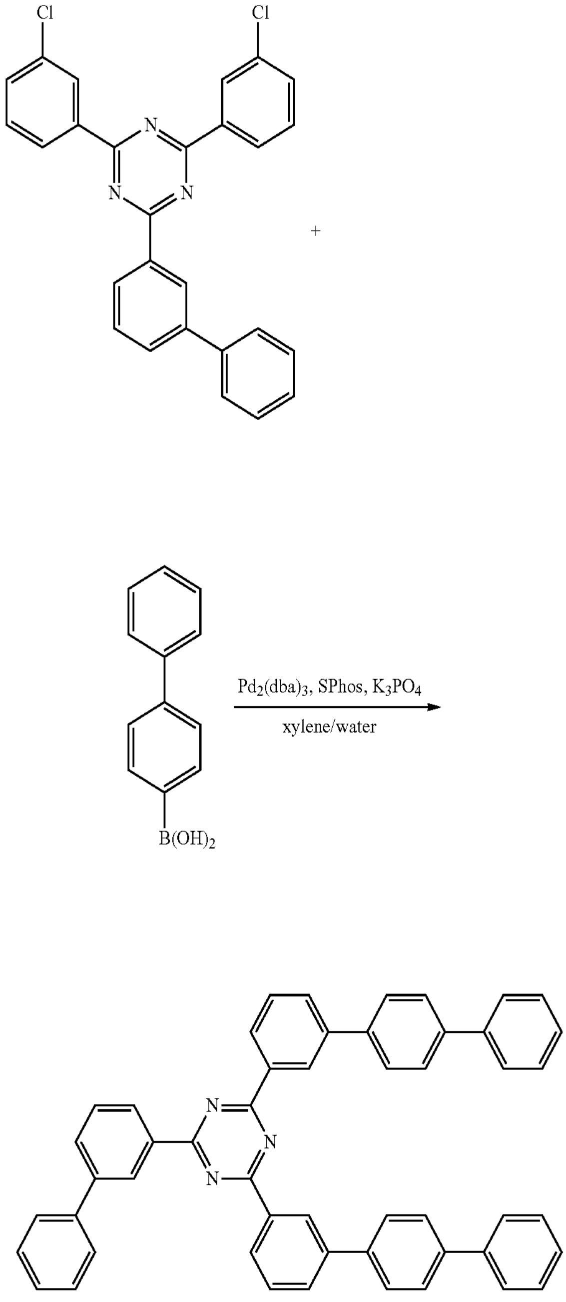
(~22° C.) and stirred for 2 h. The reaction mixture was diluted with toluene and poured into an aqueous solution of HCl (1M, 200 ml). The organic layer was isolated, washed with water, and then dried over Na_2SO_4. After evaporating the solvent, the residue was purified by column chromatography on silica gel to yield 2-chloro-4,6-bis(3-chlorophenyl)-1,3,5-triazine (2.1 g, 37%) as a pale yellow solid.

Synthesis of 2-([1,1'-biphenyl]-3-yl)-4,6-bis(3-chlorophenyl)-1,3,5-triazine



A solution of 2-chloro-4,6-bis(3-chlorophenyl)-1,3,5-triazine (3.6 g, 10.7 mmol), [1,1'-biphenyl]-3-ylboronic acid (3.2 g, 16.0 mmol), K_2CO_3 (4.4 g, 32.1 mmol) and $Pd(PPh_3)_4$ (0.62 g, 0.54 mmol) in DME (60 ml) and water (20 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was filtered through a plug of silica gel. The filtrate was evaporated, and the residue was purified by column chromatography on silica gel with heptane/DCM (9/1 to 7/3, v/v) as the eluent and precipitation from DCM to methanol to give 2-([1,1'-biphenyl]-3-yl)-4,6-bis(3-chlorophenyl)-1,3,5-triazine (3.7 g, 76%) as a white solid.

Synthesis of Compound F2

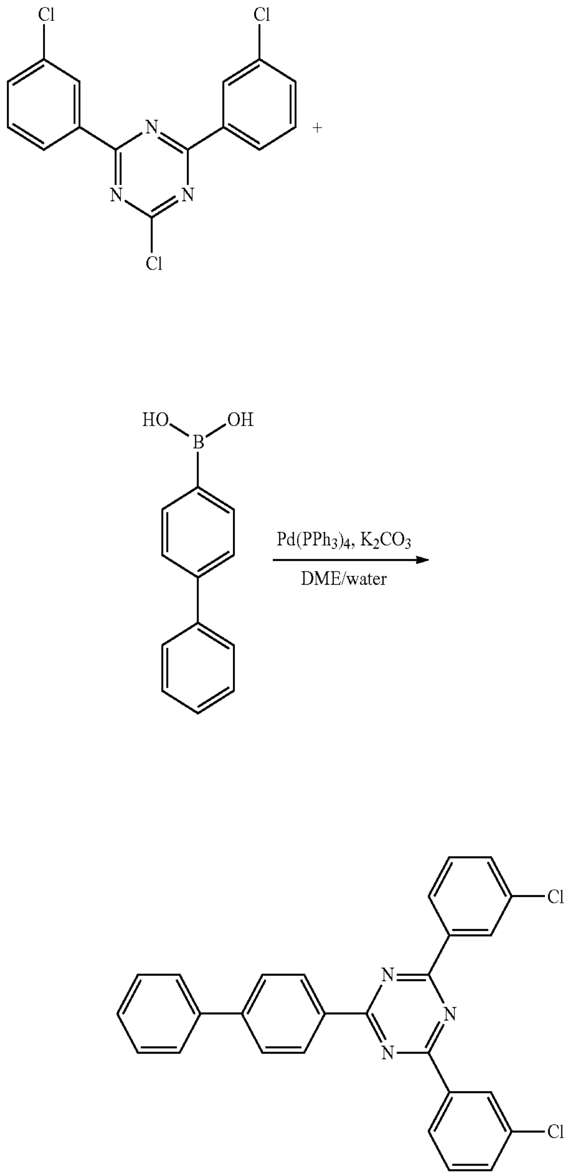


Compound F2

A solution of 2-([1,1'-Biphenyl]-3-yl)-4,6-bis(3-chlorophenyl)-1,3,5-triazine (3.7 g, 8.1 mmol), [1,1'-biphenyl]-4-ylboronic acid (4.0 g, 20.4 mmol), $Pd_2(dba)_3$ (0.15 g, 0.16 mmol), SPhos (0.27 g, 0.65 mmol), and K_3PO_4 monohydrate (5.6 g, 24.4 mmol) in m-xylene (200 ml) and water (20 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the solid was collected by filtration and washed with water and toluene. The solid was then was dissolved in boiling o-xylene and filtered through a short plug of silica gel. After evaporating the solvent, Compound F2 (4.5 g, 80%) recrystallized from o-xylene as white solid.

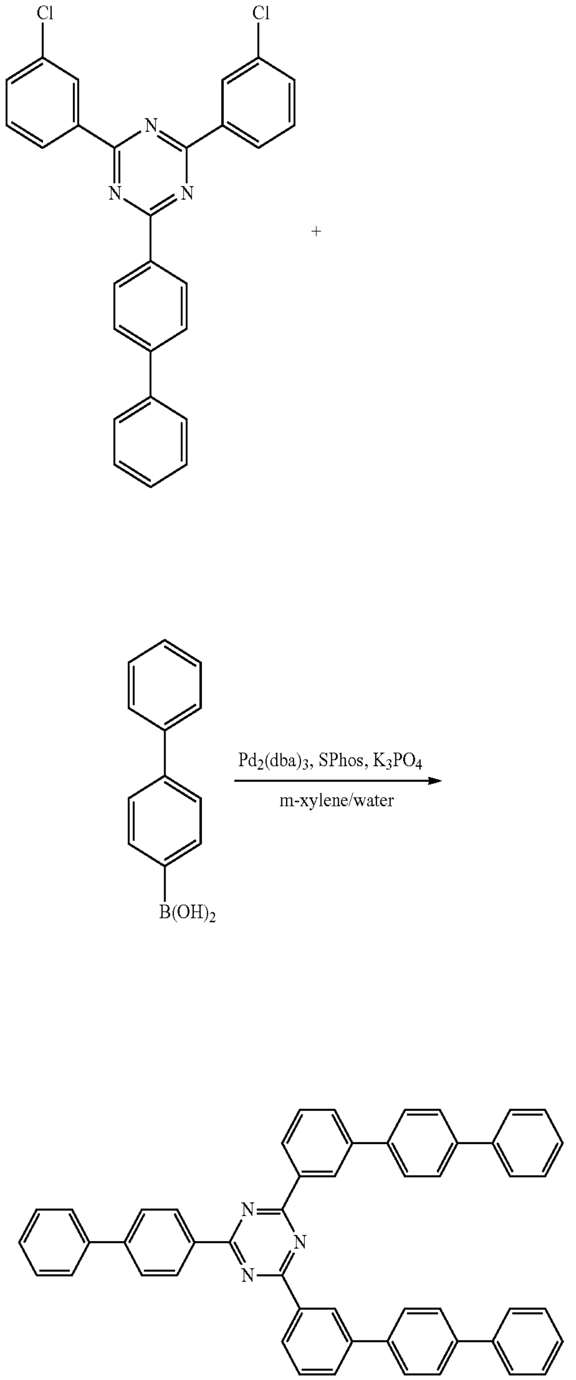
Synthesis of Compound F3

Synthesis of 2-([1,1'-biphenyl]-4-yl)-4,6-bis(3-chlorophenyl)-1,3,5-triazine



A solution of 2-chloro-4,6-bis(3-chlorophenyl)-1,3,5-triazine (0.2 g, 0.59 mmol), [1,1'-biphenyl]-4-ylboronic acid (0.14 g, 0.71 mmol), K_2CO_3 (0.25 g, 1.78 mmol), and $Pd(PPh_3)_4$ (0.034 g, 0.030 mmol) in DME (21 ml) and water (7 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was filtered through a plug of silica gel. The organic layer was isolated, washed with water, and then dried over Na_2SO_4. After evaporating the solvent, the crude product was purified by column chromatography on silica gel with heptane/DCM (9/1 to 7/3, v/v) as eluent to yield 2-([1,1'-biphenyl]-4-yl)-4,6-bis(3-chlorophenyl)-1,3,5-triazine (0.2 g, 74%) as a white solid.

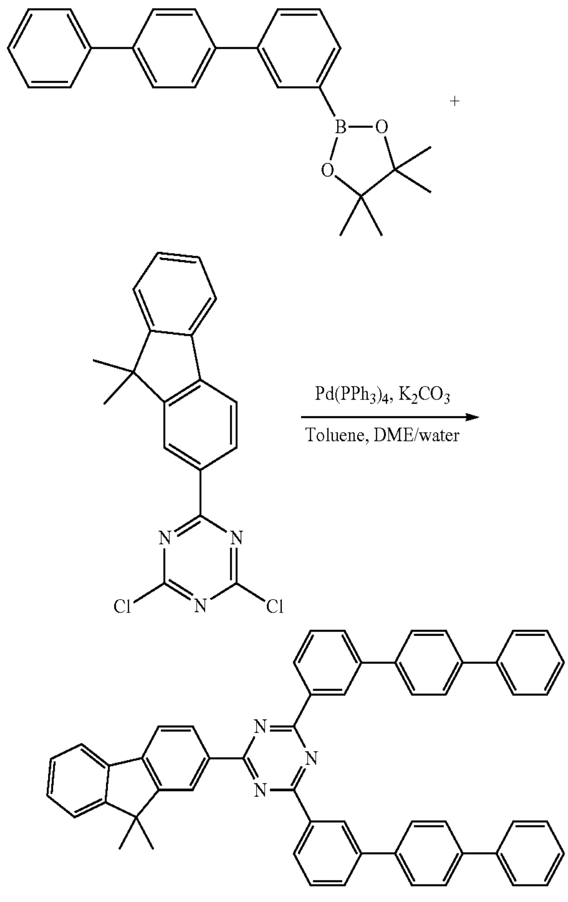
Synthesis of Compound F3



Compound F3

A solution of 2-([1,1'-Biphenyl]-4-yl)-4,6-bis(3-chlorophenyl)-1,3,5-triazine (2.3 g, 5.1 mmol), [1,1'-biphenyl]-4-ylboronic acid (3.0 g, 15.2 mmol), $Pd_2(dba)_3$ (0.093 g, 0.10 mmol), SPhos (0.17 g, 0.41 mmol), and K_3PO_4 monohydrate (3.5 g, 15.2 mmol) in m-xylene (200 ml) and water (20 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the solid was collected by filtration and triturated with boiling o-xylene. The crude product was purified by sublimation to yield Compound F3 (2.1 g, 60%) as a white solid.

Synthesis of Compound F4

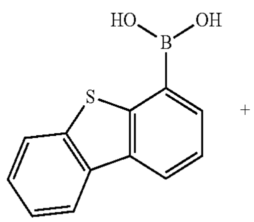


Compound F4

A solution of 2,4-dichloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (2.2 g, 6.43 mmol), 2-([1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.75 g, 7.71 mmol), $Pd(PPh_3)_4$ (0.223 g, 0.193 mmol), and K_2CO_3 (2.67 g, 19.29 mmol) in DME (100 ml), toluene (100 ml), and water (20 ml) was refluxed under nitrogen for 16 h. After cooling to room temperature (~22° C.), the solid was collected by filtration, then washed successively with water and toluene to yield Compound F4 (1.7 g, 36%) as a white solid.

Synthesis of Compound F7

Synthesis of 2-chloro-4-(dibenzo[b,d]thiophen-4-yl)-6-phenyl-1,3,5-triazine



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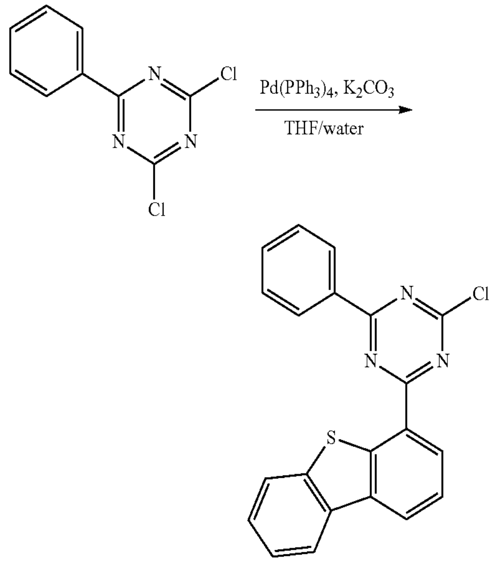
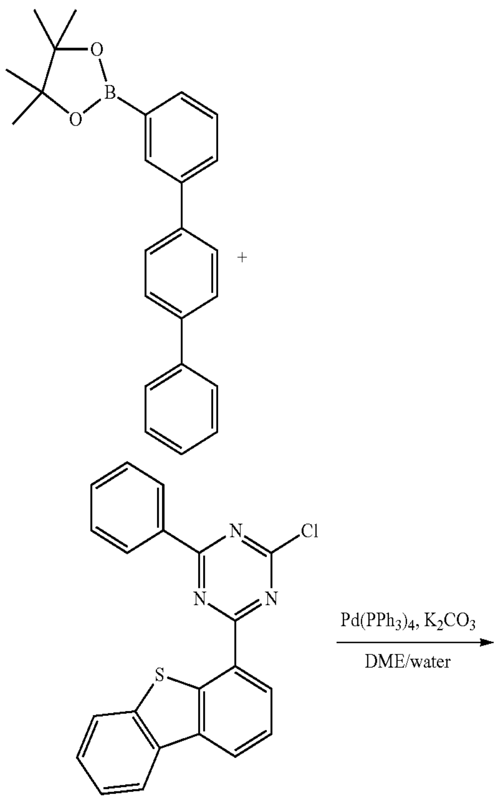


A solution of dibenzo[b,d]thiophen-4-ylboronic acid (5.0 g, 21.92 mmol), 2,4-dichloro-6-phenyl-1,3,5-triazine (12.39 g, 54.8 mmol), $Pd(PPh_3)_4$ (1.267 g, 1.096 mmol), and K_2CO_3 (9.09 g, 65.8 mmol) in THF (Ratio: 10.0, Volume: 199 ml) and water (Ratio: 1.000, Volume: 19.93 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction solution was filtered through a short plug of silica gel. The crude product was purified by column chromatography on silica gel and sublimation to yield 2-chloro-4-(dibenzo[b,d]thiophen-4-yl)-6-phenyl-1,3,5-triazine (7.1 g, 72%) as a yellow solid.

Synthesis of Compound F7



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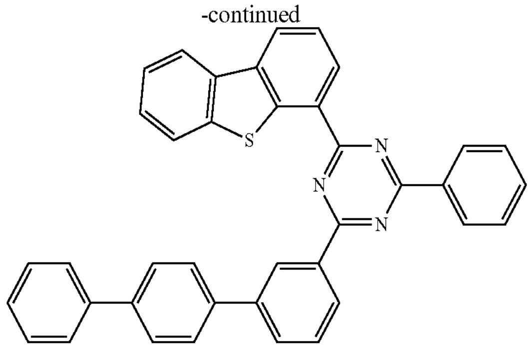
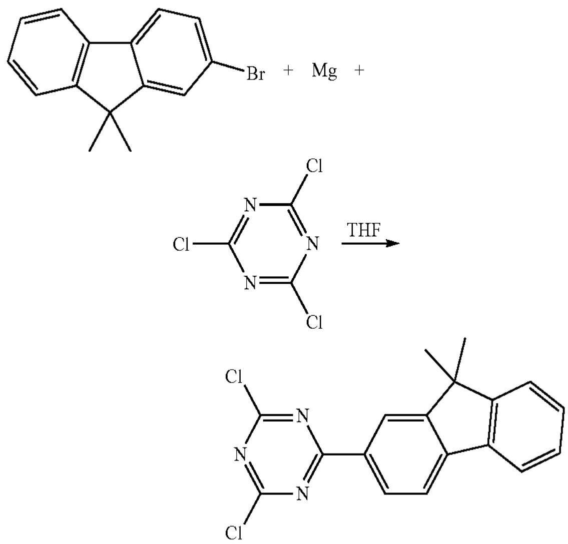


Compound F7

A solution of 2-([1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.359 g, 6.62 mmol), 2-chloro-4-(dibenzo[b,d]thiophen-4-yl)-6-phenyl-1,3,5-triazine (2.25 g, 6.02 mmol), $Pd(PPh_3)_4$ (0.348 g, 0.301 mmol), and K2CO3 (2.495 g, 18.05 mmol) in DME (Ratio: 10.0, Volume: 54.7 ml) and Water (Ratio: 1.000, Volume: 5.47 ml) was refluxed under nitrogen overnight (~12 hours). After cooling to room temperature (~22° C.), the reaction mixture was diluted with water and THF. The solid was collected by filtration, washed successively with water, THF and ethanol, triturated successively with hot ethanol, DCM and toluene, and then sublimed to yield Compound F7 (3.24 g, 77%) as a white solid.

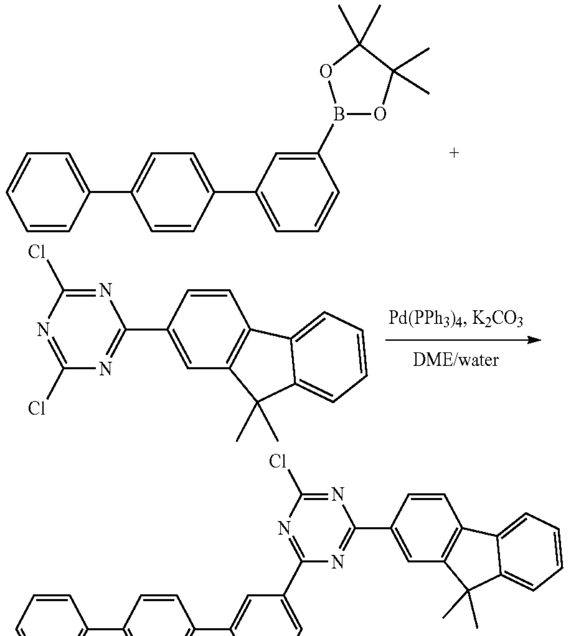
Synthesis of Compound F13

Synthesis of 2,4-dichloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine



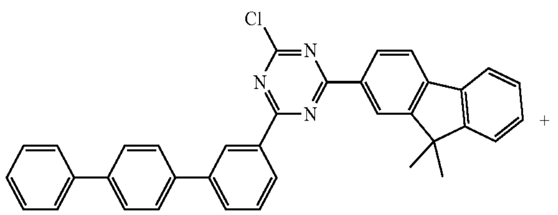
A solution of 2-bromo-9,9-dimethyl-9H-fluorene (12.0 g, 43.9 mmol) in THF (100 ml) was added dropwise into a suspension of Mg (1.6 g, 65.9 mmol) in THF (50 ml) activated with iodine at 60° C. under nitrogen. After addition, the reaction mixture was refluxed for 3 h before transferring it into a solution of 2,4,6-trichloro-1,3,5-triazine (8.10 g, 43.9 mmol) in THF (50 ml) at 0° C. The reaction mixture was then allowed to warm to room temperature (~22° C.) and stirred overnight (~12 hours) before quenching with an aqueous HCl solution. The resulting mixture was extracted with EtOAc. The combined organic extracts were dried over Na_2SO_4. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/EtOAc (9/1, v/v) as the eluent to yield 2,4-dichloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (8.0 g, 53%) as a white solid.

Synthesis of 2-([1,1':4',1"-terphenyl]-3-yl)-4-chloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine



A solution of 2-([1,1':4',1"-terphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.00 g, 11.23 mmol), 2,4-dichloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (10.76 g, 31.4 mmol), $Pd(PPh_3)_4$ (0.259 g, 0.225 mmol), and K_2CO_3 (4.66 g, 33.7 mmol) in DME (150 ml) and water (50 ml) was refluxed under nitrogen for 18 h. After cooling to room temperature (~22° C.), the reaction mixture was diluted with water, then extracted with EtOAc and the organic extracts were dried over Na_2SO_4. After evaporating the solvent, the residue was purified by column chromatography on silica gel with heptane/EtOAc (4/1, v/v) as the eluent to yield 2-([1,1':4',1"-terphenyl]-3-yl)-4-chloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (4.5 g, 8.39 mmol, 74.8% yield) as a white solid.

Synthesis of Compound F13



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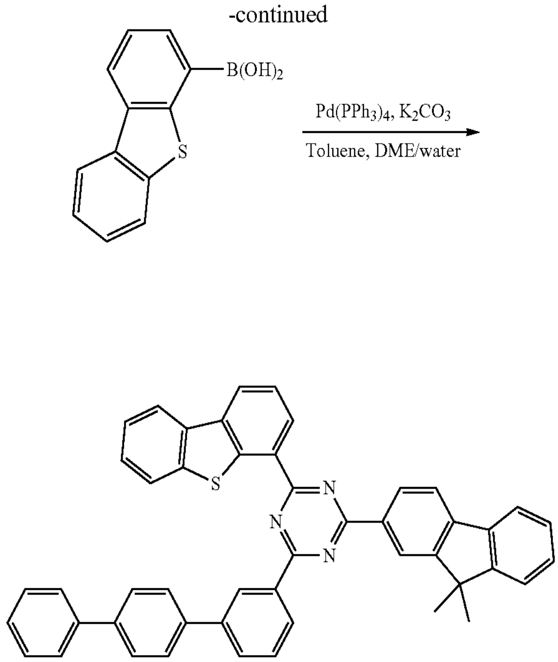


Compound F13

A solution of 2-([1,1':4',1"-terphenyl]-3-yl)-4-chloro-6-(9,9-dimethyl-9H-fluoren-2-yl)-1,3,5-triazine (2.7 g, 5.04 mmol), dibenzo[b,d]thiophen-4-ylboronic acid (1.72 g, 7.56 mmol), $Pd(PPh_3)_4$ (0.116 g, 0.101 mmol), and K_2CO_3 (2.1 g, 15.11 mmol) in toluene (200 ml), DME (300 ml), and water (50 ml) was refluxed under nitrogen for 14 h. After cooling to room temperature (~22° C.), the solid was collected by filtration and washed successively with water, methanol, EtOAc, and heptane. The crude product was dissolved in boiling toluene and filtered through a short plug of silica gel. After evaporating the solvent, the Compound F13 (16.5 g, 48%) precipitated as a white solid.

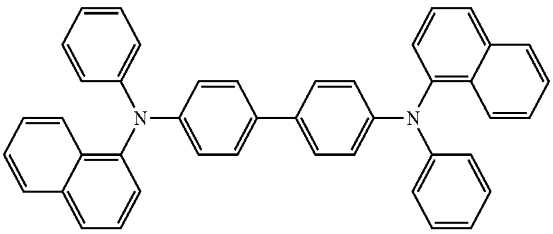
Device Examples

Application in OLED.

All devices were fabricated by high vacuum (~10^{-7} Torr) thermal evaporation. The anode electrode was 80 nm of indium tin oxide (ITO). The cathode electrode consisted of 1 nm of LiF followed by 100 nm of Al. All devices were 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.

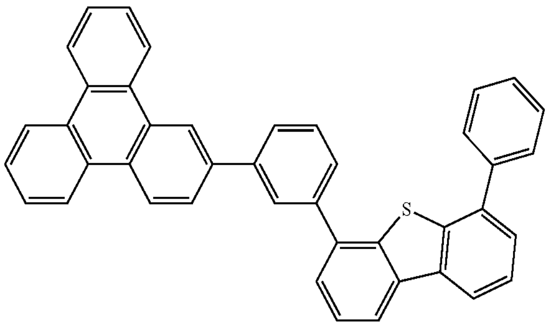
Device Examples—Set 1.

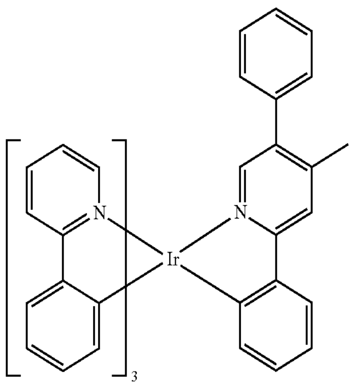
A first set of device examples have organic stacks consisting of, sequentially, from the ITO surface, 10 nm of LG101 (from LG Chem) as the hole injection layer (HIL), 45 nm of 4,4'-bis[N-(1-naphthyl)-N-phenylaminolbiphenyl (NPD) as the hole-transport layer (HTL), and 30 nm of Compound E8 with 20 wt % of inventive compound (Compound C65) or comparative compound (CC-1) and 10 wt % of emitter GD as the emissive layer (EML). On top of the EML, 50 nm of Compound C65 or CC-1 was deposited as the hole blocking layer (HBL), followed by 40 nm of tris(8-hydroxyquinolinato)aluminum (Alq_3) as the electron-transport layer (ETL). The structures of the compounds used are shown below.



NPD

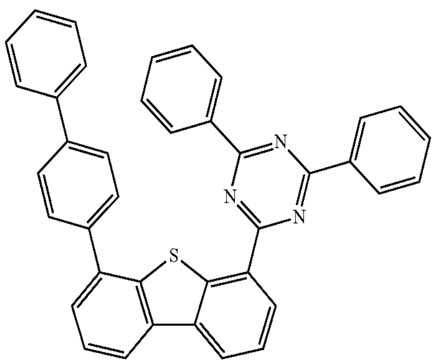
Compound E8





GD

Compound C65



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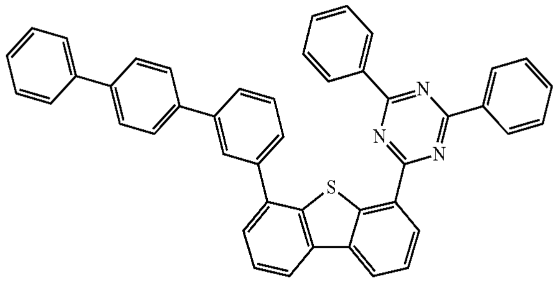
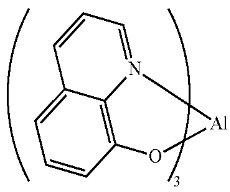


CC-1



Alq_3

Table D1, below, is a summary of the device data, voltage (V), external efficiency (EQE) and power efficiency (PE), recorded at 9000 nits for the Device Example 1.

TABLE D1

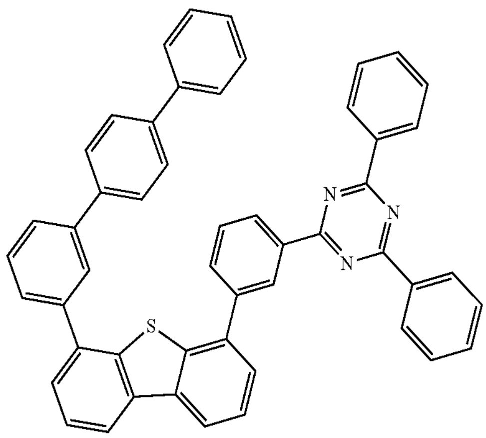
Device	EML	HBL	Color	V (V)	EQE (%)	PE (lm/W)
Device C-1	E8: CC-1: GD	CC-1	Green	8.1	14.5	20.5
Device 1	E8: C65: GD	C65	Green	7.6	15.1	22.5

The data in Table D1 shows that Device 1 using inventive compound C65 as the co-host and HBL achieves higher efficiency at a lower driving voltage than Device C-1 using comparative compound CC-1 as the co-host and HBL.

Device Examples—Set 2.

A second set of device examples have the same structure as that in Device Example 1 except that an inventive Compound C101 or a comparative compound CC-2 doped with 15% of GD is used as a two-component EML. The chemical structures of the inventive and comparative compounds used are presented below.

CC-2



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Compound C101

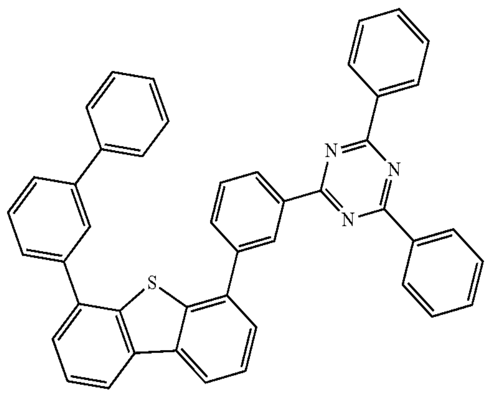


Table D2, below, is a summary of the relative device data recorded at 9000 nits for the Device Example 2. Device lifetime LT97 is defined as the time it takes for devices to decay to 97% of their original luminance under a constant current density with an initial luminance of 9000 nits, and the values are normalized to that of Device C-2.

TABLE D2

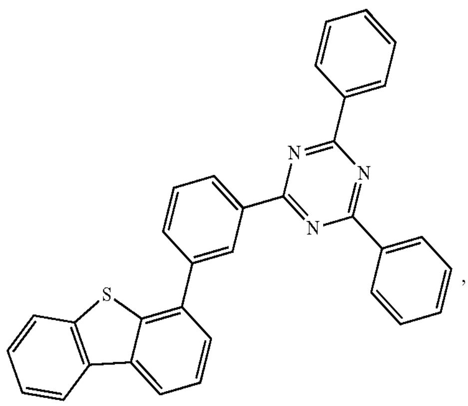
Device	EML	HBL	Color	V (V)	EQE (%)	PE (lm/W)	LT97
Device C-2	CC-2: GD	CC-2	Green	7.5	14.7	22	100
Device 2	C101: GD	C101	Green	7.6	14.7	23	130

The data in Table D2 shows that Device 2 using inventive compound Compound C101 as the host and HBL achieves higher efficiency and longer lifetime than Device C-2 using comparative compound CC-2 as the host and HBL.

Device Examples—Set 3.

A third set of device examples have the same structure as that in Device Example 1. The chemical structures of the inventive and comparative compounds used are presented below.

CC-3



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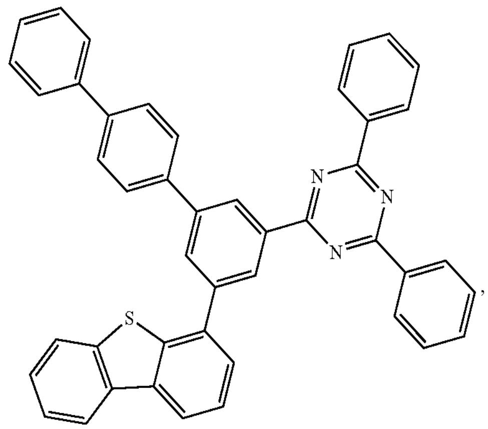
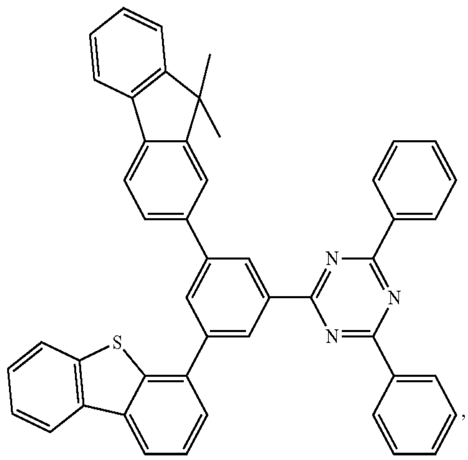
Compound A5



Compound A116



Compound C74

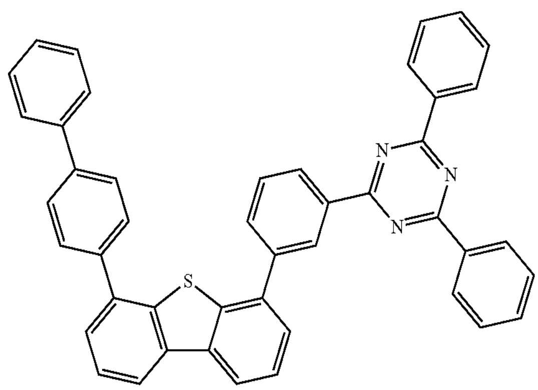


Table D3, below, is a summary of the relative device data recorded at 1000 nits for the Device Examples 3. Device lifetime LT95 defined as the time it takes for devices to decay to 95% of their original luminance under a constant current density with an initial luminance of 1000 nits, was calculated, with an acceleration factor of 1.8, from the values measured at a current density of 50 mA/cm^2, and normalized to that of Device C-3.

TABLE D3

Device	EML	HBL	Color	LT95
Device C-3	E8:CC-3:GD	CC-3	Green	100
Device 3	E8:A5:GD	A5	Green	694

TABLE D3-continued

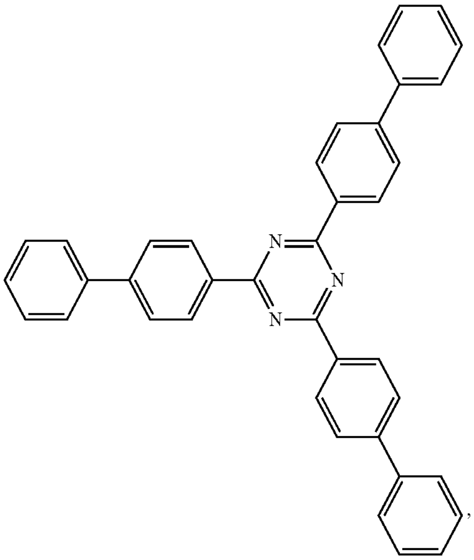
Device	EML	HBL	Color	LT95
Device 4	E8:A116:GD	A116	Green	529
Device 5	E8:C74:GD	C74	Green	537

The data in Table D3 show that, using as cohost with E8 in EML and as EBL, inventive compounds having substitutions on dibenzothiophene or bridging phenyl demonstrate longer lifetime than comparative compound that does not have these substitutions.

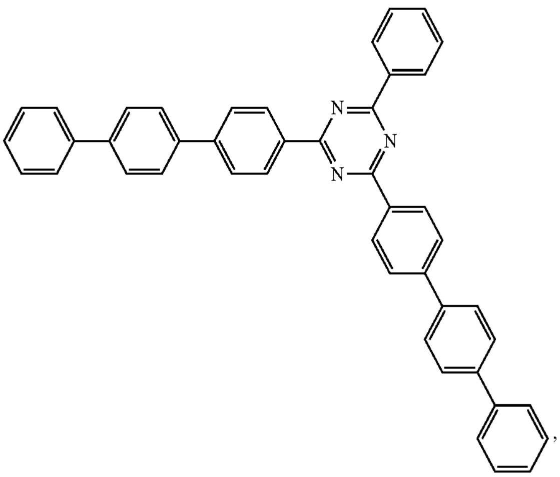
Device Examples—Set 4.

A fourth set of devices have the same structure as that in Device Example 2. The chemical structures of the inventive and comparative compounds used are presented below.

CC-4



CC-5



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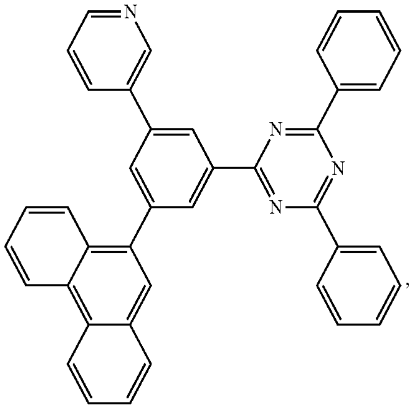
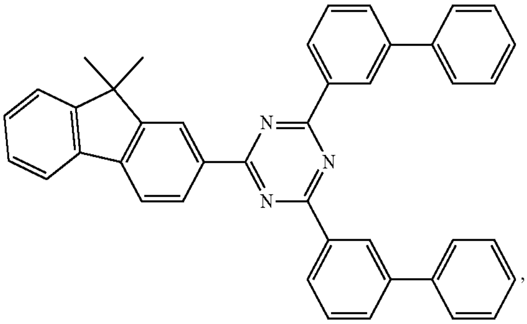
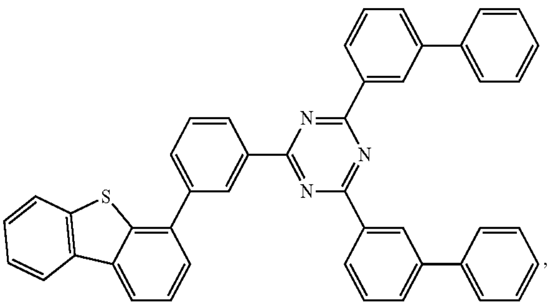
CC-6



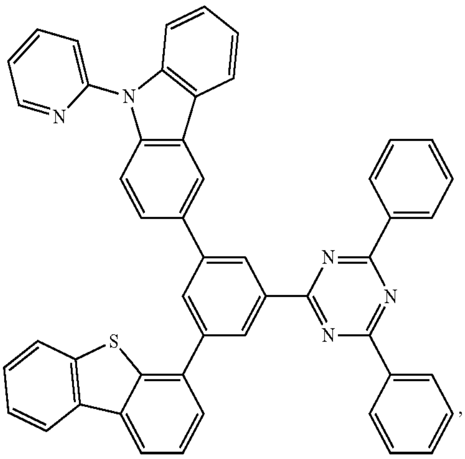
CC-7



CC-8



CC-9



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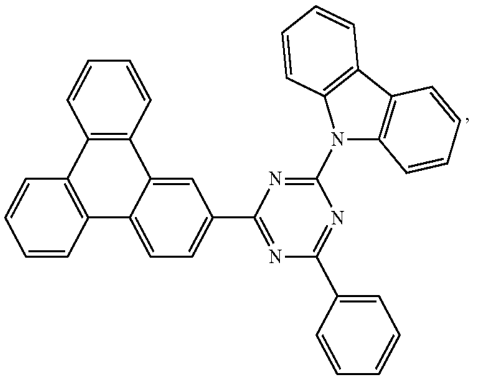
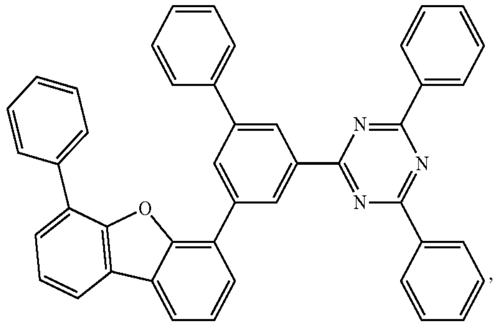
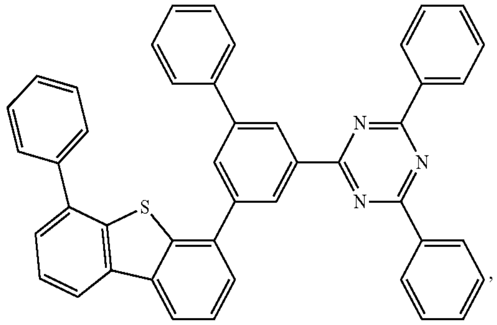
CC-10



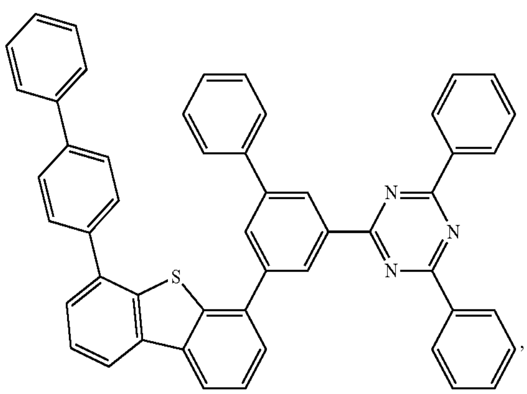
Compound A10



Compound A11



Compound A14



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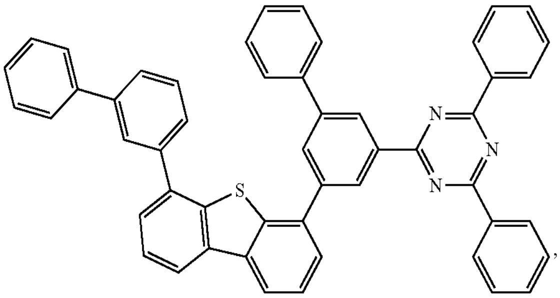
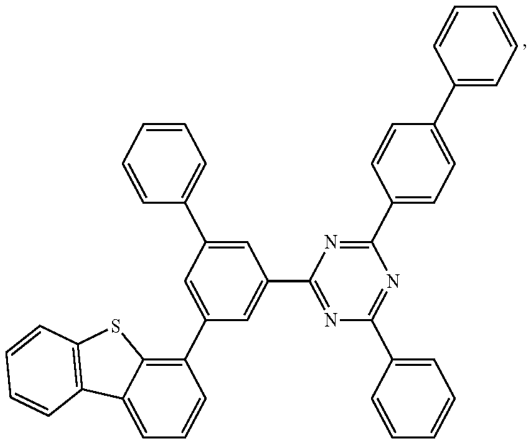
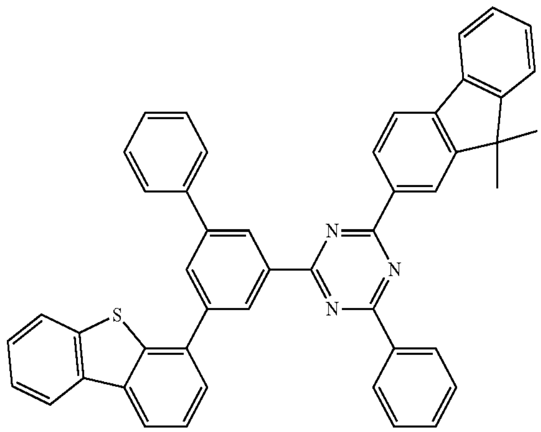
Compound A17



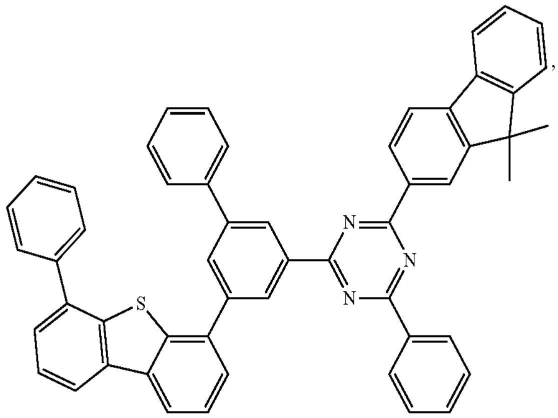
Compound A32



Compound A38



Compound A47



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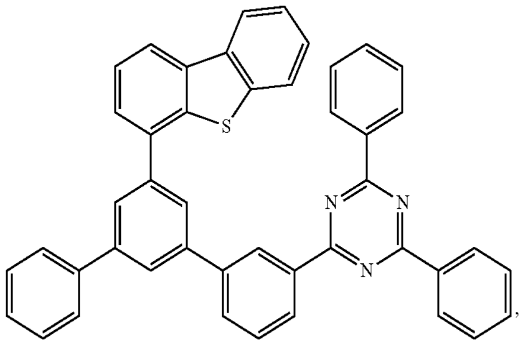
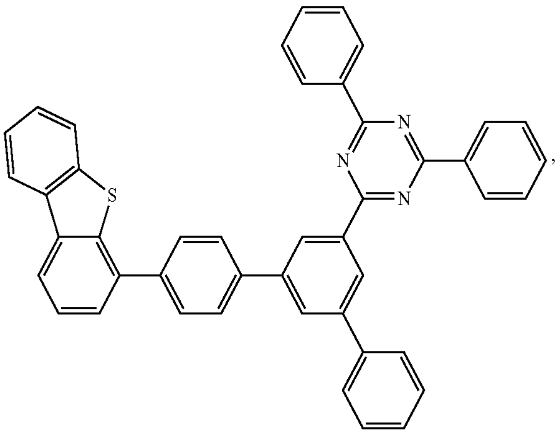
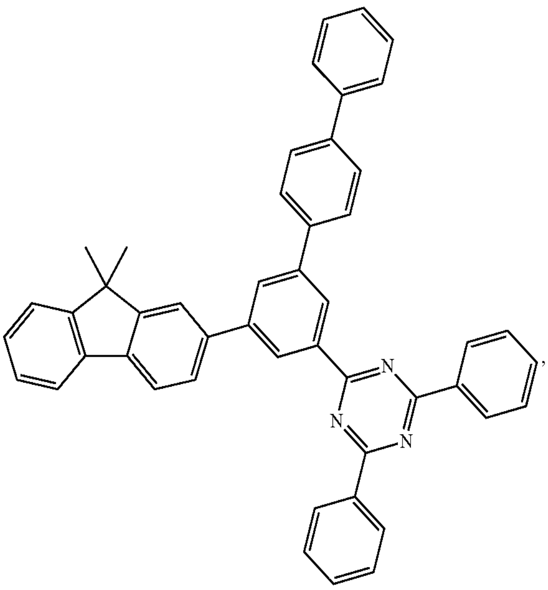
Compound A110



Compound A113



Compound B3



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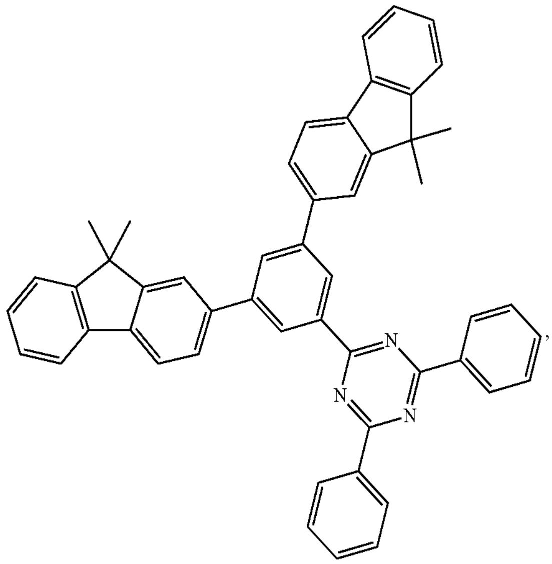
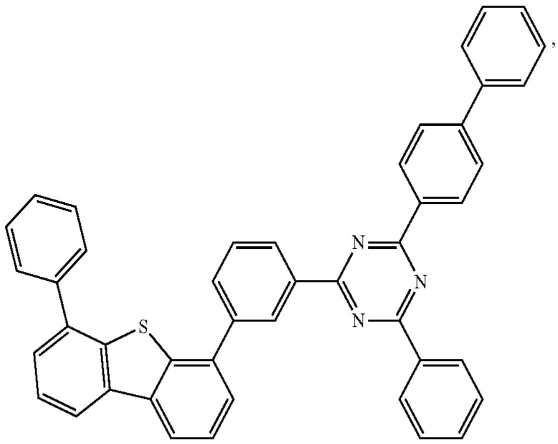
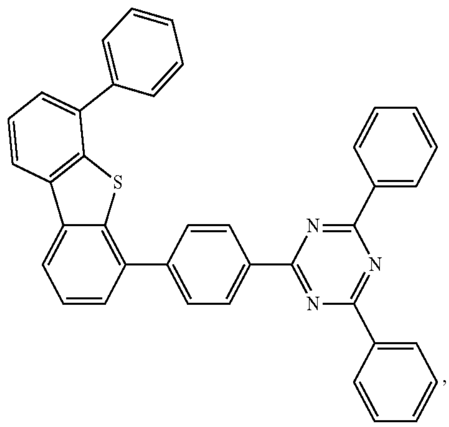
Compound B7



Compound C23



Compound C29



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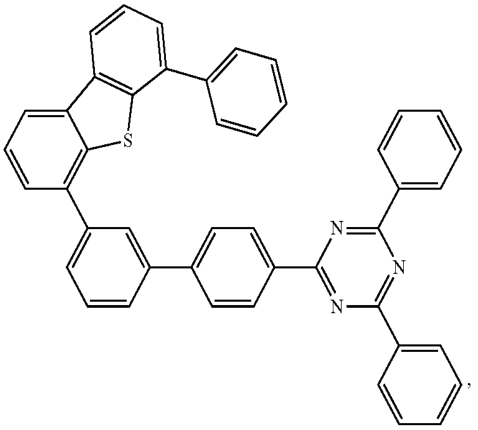
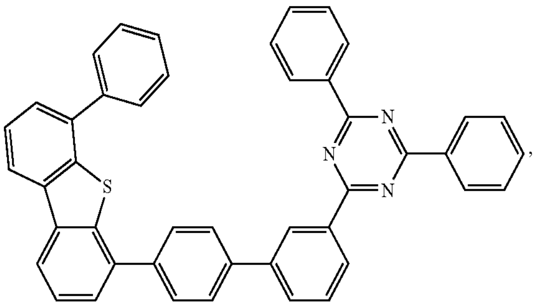
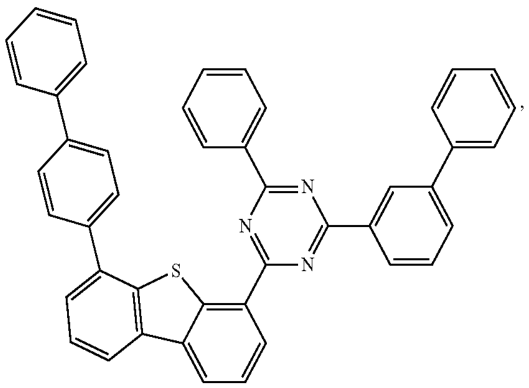
Compound C47



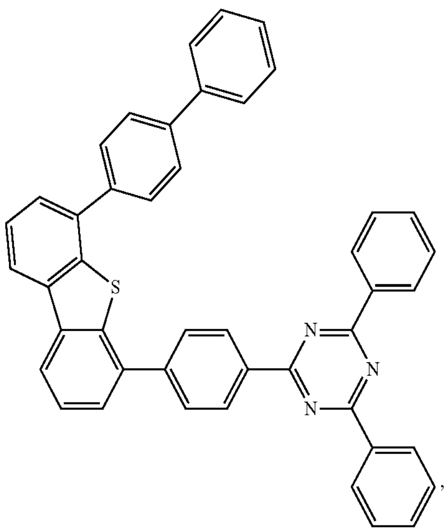
Compound C56



Compound C71



Compound C83



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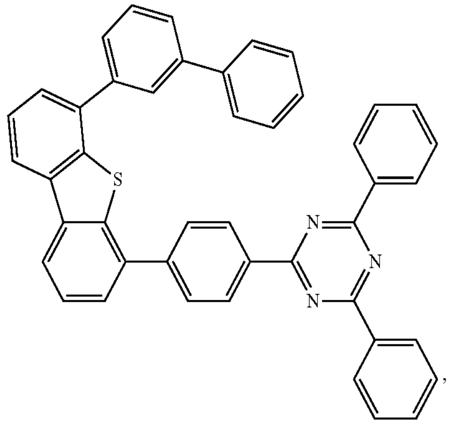
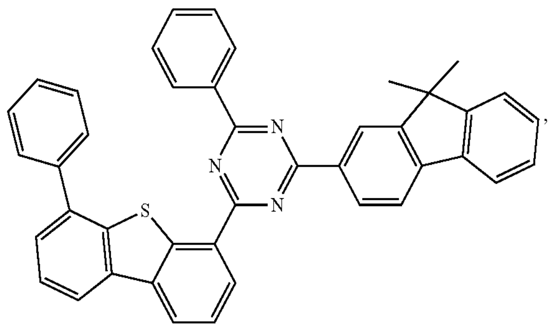
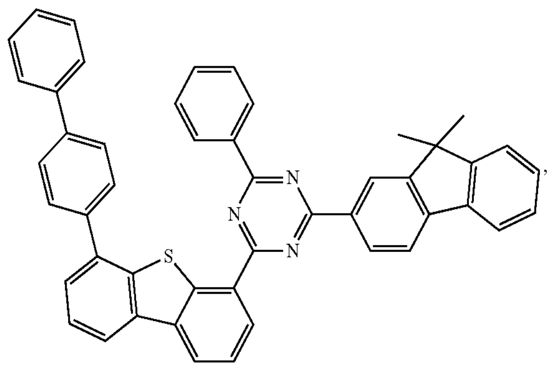
Compound C110



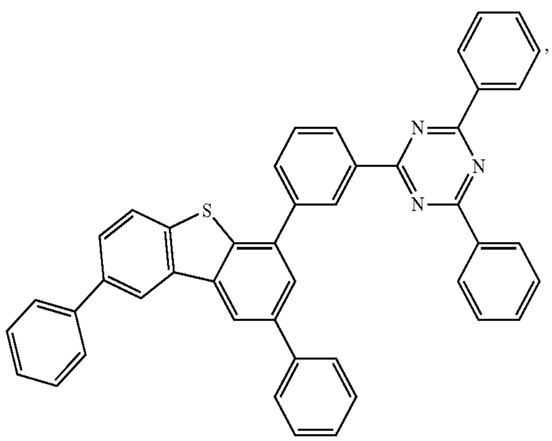
Compound C119



Compound C134



Compound C173



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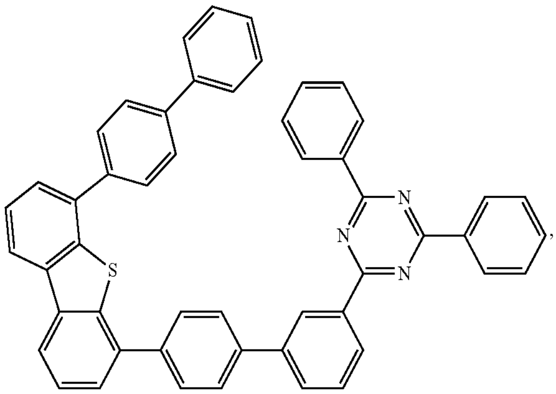
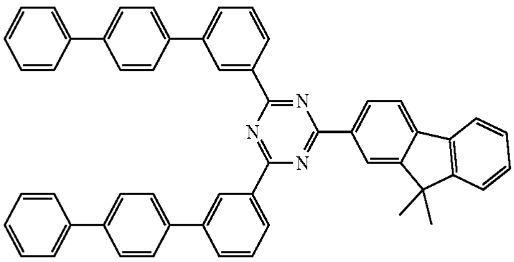
Compound C251



Compound F4



and

Compound F13

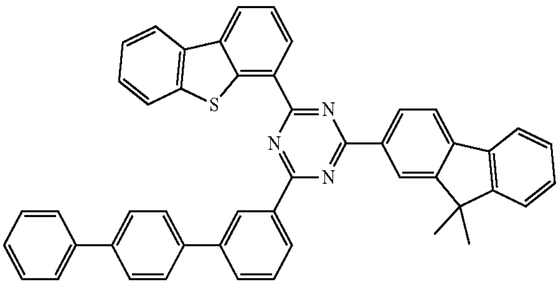


Table D4, below, is a summary of the relative device data recorded at 1000 nits for the Device Example 4. Device lifetime LT95 was normalized to that of Device C-4.

TABLE D4

Device	EML	HBL	Color	LT95
Device C-4	CC-4:GD	CC-4	Green	100
Device C-5	CC-5:GD	CC-5	Green	3
Device C-6	CC-6:GD	CC-6	Green	3
Device C-7	CC-7:GD	CC-7	Green	147
Device C-8	CC-8:GD	CC-8	Green	93
Device C-9	CC-9:GD	CC-9	Green	62
Device C-10	CC-10:GD	CC-10	Green	88
Device 6	A10:GD	A10	Green	899
Device 7	A11:GD	A11	Green	602
Device 8	A14:GD	A14	Green	1029
Device 9	A17:GD	A17	Green	848
Device 10	A32:GD	A32	Green	969
Device 11	A38:GD	A38	Green	721
Device 12	A47:GD	A47	Green	859
Device 13	A110:GD	A110	Green	902
Device 14	A113:GD	A113	Green	1248
Device 15	B3:GD	B3	Green	1136
Device 16	B7:GD	B7	Green	849
Device 17	C23:GD	C23	Green	1466
Device 18	C29:GD	C29	Green	344
Device 19	C47:GD	C47	Green	915
Device 20	C56:GD	C56	Green	287
Device 21	C71:GD	C71	Green	181

TABLE D4-continued

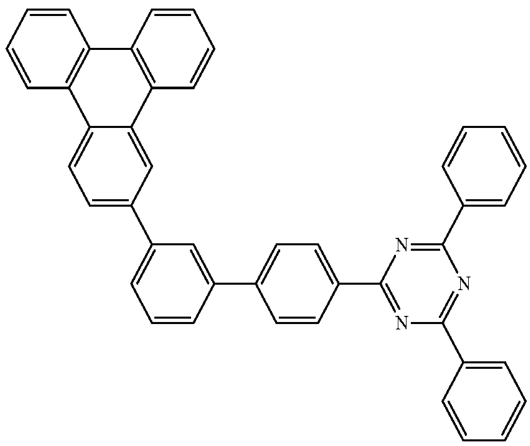
Device	EML	HBL	Color	LT95
Device 22	C83:GD	C83	Green	444
Device 23	C110:GD	C110	Green	477
Device 24	C119:GD	C119	Green	285
Device 25	C134:GD	C134	Green	192
Device 26	C140:GD	C140	Green	824
Device 27	C173:GD	C173	Green	760
Device 28	C251:GD	C251	Green	1830
Device 29	F4:GD	F4	Green	314
Device 30	F13:GD	F13	Green	223

The data in Table D4 show that OLED devices using inventive compounds as hosts and HBL have longer lifetime than that using comparative compounds.

Device Examples—Set 5.

A fifth set of devices have the same structure as that in Device Example 1. The chemical structures of the inventive and comparative compounds used are presented below.

CC-11



Compound D2

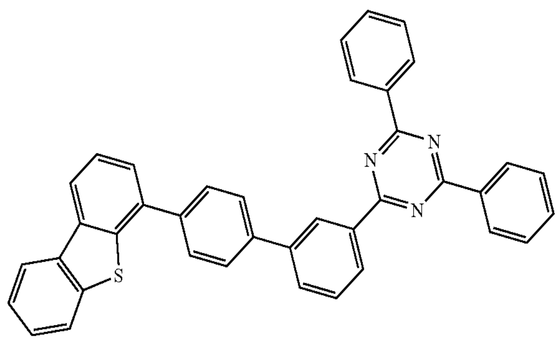


Table D5, below, is a summary of the relative device data recorded at 9000 nits for the Device Example 5. Device lifetime LT97 is defined as the time it takes for devices to decay to 97% of their original luminance under a constant current density with an initial luminance of 9000 nits, and the values are normalized to that of Device C-11.

TABLE D5

Device	EML	HBL	Color	V (V)	EQE (%)	PE (lm/W)	LT97
Device C-11	E8: CC-11: GD	CC-11	Green	8.1	13.9	19.4	100
Device 31	E8: D2: GD	D2	Green	7.7	14.8	21.8	123

The data in Table D5 shows that Device 31 using inventive compound Compound D2 as the host and HBL achieves higher efficiency and longer lifetime than Device C-11 using comparative compound CC-11 as the host and HBL.

The device data in Tables D1 through D5 together show that the inventive compounds having unique chemical structures are superior to comparative compounds when they are used as hosts or co-host and EBL in OLEDs. It is well accepted that OLED device performance is highly dependent on the materials properties, which are attributable to materials chemical structure.

Premixture Examples

The compatibility of selected h- and e-hosts was evaluated by compositional analysis of films fabricated by single-source co-evapoaration of the premixture of these two components. A first set of potential premixtures of selected h- and e-hosts are presented in Table PM1.

TABLE PM1

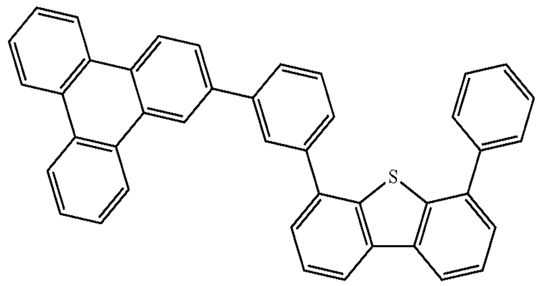
Potential premixtures comprising selected h- and e-hosts

Premixtures	h-hosts	e-hosts
PM-A1	Compound E1	Compound C1
PM-A2	Compound E2	Compound C2
PM-A3	Compound E5	Compound C65
PM-A4	Compound E8	Compound C74
PM-A5	Compound E11	Compound C74
PM-A6	Compound E17	Compound C74
PM-A7	Compound E8	CC-1
PM-A8	Compound E8	Compound A5
PM-A9	Compound E8	Compound C17
PM-A10	Compound E17	Compound A5
PM-A11	Compound E25	CC-1
PM-A12	Compound E26	Compound C74
PM-A13	Compound E26	Compound C248
PM-A14	Compound E28	Compound C74
PM-A15	Compound E29	Compound C74
PM-A16	Compound E30	Compound C74

Premixture Example—Set 1:

For premixture PM-A4, Compound E8 and Compound C74 were provided at a weight ratio of 7:3, then they were physically mixed, grinded and loaded into an evaporation source. The premixed compositions were thermally co-evaporated at a rate of 2 Å/s in a vacuum chamber under a pressure less than 10^{-7} Torr, and deposited onto glass substrates. The substrates were replaced continuously after deposition of 500 Å of film without stopping the deposition and cooling the source. The compositions of films were analyzed by high-performance liquid chromatography (HPLC) and the results are shown in Table 2.

Compound E8



Compound C74

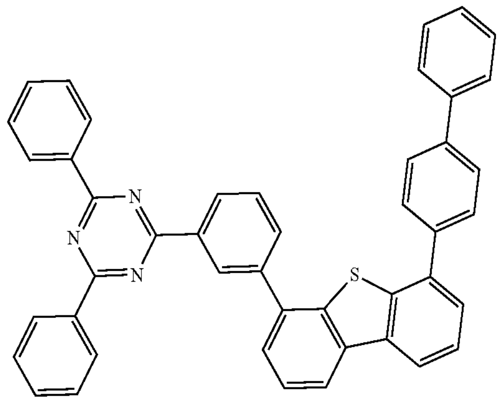


TABLE PM2

HPLC composition (%) of sequentially deposited films from premixture (PM-A4) comprising Compound E8 and Compound C74 with weight ratio 7:3. (HPLC Conditions C18, 100 45 min, Detected wavelength 254 nm) (Due to different absorption coefficients, the HPLC composition may or may not agree with the weight ratio.)

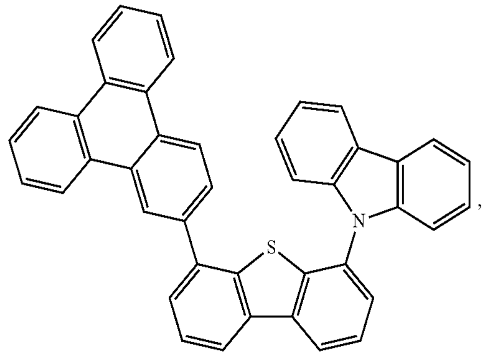
Films	Compound E8	Compound C74
Plate 1	69.5	30.5
Plate 2	68.4	31.6
Plate 3	68.2	31.8
Plate 4	68.2	31.8
Plate 5	68.4	31.6
Plate 6	69.3	30.7
Plate 7	70.6	29.4
Plate 8	71.7	28.3
Plate 9	73.0	27.0

As shown in Table PM2, the composition of the components Compound E8 and Compound C74 did not change significantly from plate 1 through plate 9. The minor fluctuations in the concentrations do not reveal any trend and can be explained by the accuracy of HPLC analysis. Normally, the change of the concentration before and after depositions within 5% throughout the process is considered to be good and useful for commercial OLED application.

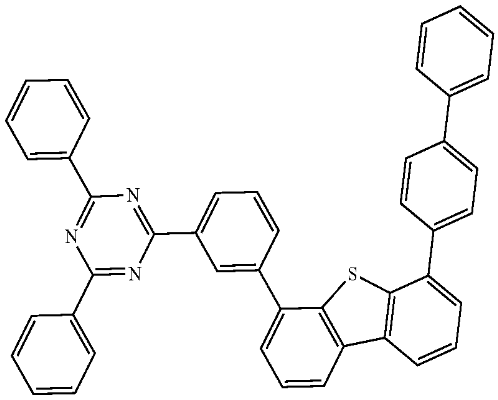
Premixture Example—Set 2:

For premixture PM-A12, Compound E26 and Compound C74 were provided at a weight ratio of 3:2, then they were physically mixed, grinded, and loaded into an evaporation source. The premixed compositions were thermally co-evaporated at a rate of 2 Å/s in a vacuum chamber under a pressure less than 10^{-7} Torr, and deposited onto glass substrates. The substrates were replaced continuously after deposition of 500 Å of film without stopping the deposition and cooling the source. The compositions of films were analyzed by high-performance liquid chromatography (HPLC) and the results are shown in Table PM3.

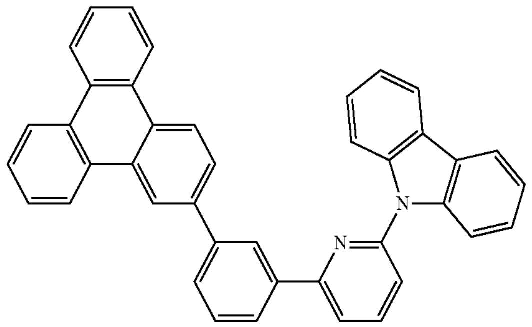
Compound E26



Compound C74



Compound E30



Compound C74

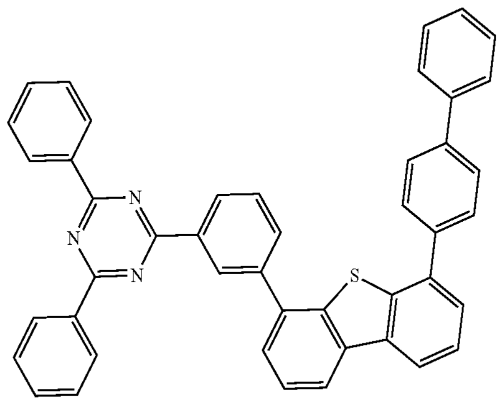


TABLE PM3

HPLC composition (%) of sequentially deposited films from premixture (PM-A12) comprising Compound E26 and Compound C74 with weight ratio 3:2. (HPLC Conditions C18, 100 45 min, Detected wavelength 254 nm) (Due to different absorption coefficients, the HPLC composition may or may not agree with the weight ratio.)

Films	Compound E26	Compound C74
Plate 1	67.1	32.9
Plate 2	67.3	32.7
Plate 3	68.4	31.6
Plate 4	69.6	30.4
Plate 5	70.8	29.2
Plate 6	71.9	28.1
Plate 7	72.9	27.1
Plate 8	73.9	26.1

Again, the results of plates 1 to 8 show only minor variations and would be considered to be good and useful for commercial OLED application.

Premixture Example—Set 3.

For premixture PM-A16, Compound E30 and Compound C74 were provided at a weight ratio of 1:1, then they were physically mixed, grinded and loaded into an evaporation source. The premixed compositions were thermally co-evaporated at a rate of 2 Å/s in a vacuum chamber under a pressure less than 10^{-7} Torr, and deposited onto glass substrates. The substrates were replaced continuously after deposition of 500 Å of film without stopping the deposition and cooling the source. The compositions of films were analyzed by high-performance liquid chromatography (HPLC) and the results are shown in Table PM4.

TABLE PM4

HPLC composition (%) of sequentially deposited films from premixture (PM-A16) comprising Compound E30 and Compound C74 with weight ratio 1:1. (HPLC Conditions C18, 100 45 min, Detected wavelength 254 nm) (Due to different absorption coefficients, the HPLC composition may or may not agree with the weight ratio.)

Films	Compound E30	Compound C74
Plate 1	52.3	47.7
Plate 2	51.6	48.4
Plate 3	52.1	47.9
Plate 4	52.9	47.1
Plate 5	53.9	46.1
Plate 6	54.6	45.4
Plate 7	51.8	48.2

The data in Tables PM2, PM3 and PM4 show that the ratio of the two components in premixtures PM-A4, PM-A12 and PM-A16 does not change significantly over a continuous single-source coevaporation. The minor fluctuations in the concentrations do not reveal any trend and can be explained by the accuracy of HPLC analysis. Normally, the change of the concentration before and after depositions within 5% throughout the process is considered to be good and useful for commercial OLED application. These experiments conclude that PM-A4, PM-A12 and PM-A16 are stable premixtures for coevaporation. The coevaporation stability of these premixtures is believed to tracable to the unique chemical structures associated with these two classes of materials.

A second set of potential premixtures of selected h- and e-hosts are presented in Table PM5.

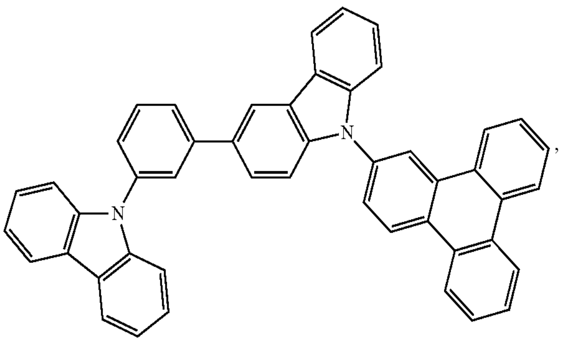
TABLE PM5

Potential premixtures comprising selected h- and e-hosts		
Premixtures	h-hosts	e-hosts
PM-B1	Compound G1	Compound F9
PM-B2	Compound G2	Compound F10
PM-B3	Compound G8	Compound F13
PM-B4	Compound G9	Compound F13
PM-B5	Compound G26	Compound F5

Example 1

For premixture PM-B3, Compound G8 and Compound F13 were provided at a weight ratio of 9:1, then they were physically mixed, grinded and loaded into an evaporation source. The premixed compositions were thermally co-evaporated at a rate of 2 Å/s in a vacuum chamber under a pressure less than 10^{-7} Torr, and deposited onto glass substrates. The substrates were replaced continuously after deposition of 500 Å of film without stopping the deposition or cooling the source. The deposition was stopped upon material depletion. The compositions of films were analyzed by high-performance liquid chromatography (HPLC) and the results are shown in Table PM6.

Compound G8



Compound F13

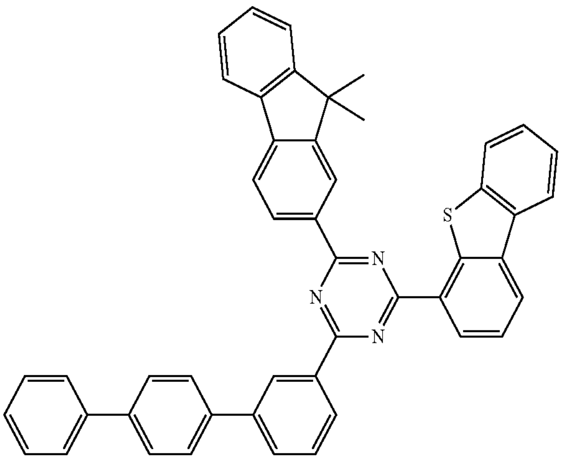


TABLE PM6

Table PM6: HPLC composition (%) of sequentially deposited films from premixture (PM-B3) comprising Compound G8 and Compound F13 with weight ratio 9:1. (HPLC Conditions C18, 100 45 min, Detection wavelength 254 nm) (Due to different absorption coefficients, the HPLC composition may or may not agree with the weight ratio.)

Films	Compound G8	Compound F13
Plate 1	95.9	4.1
Plate 2	96.0	4.0
Plate 3	96.5	3.5
Plate 4	96.8	3.2

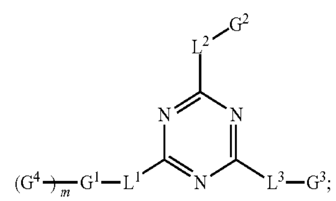
The composition of the components Compound G8 and Compound F13 did not change significantly from plate 1 through plate 4. The minor fluctuations in the concentrations do not reveal any trend and can be explained by the accuracy of HPLC analysis. Normally, the change of the concentration before and after depositions within 5% throughout the process is considered to be good and useful for commercial OLED application. These results demonstrate that PM3 is a stable premixtures for coevaporation. The coevaporation stability of this premixture is believed to be traceable to the unique chemical structures associated with these two classes of materials.

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

We claim:

1. A composition of materials comprising a first compound, wherein the first compound has a formula:

Formula I



wherein G^2, G^3, and, when present, G^4 are each optionally further substituted with one or more unfused substituents selected from the group consisting of deuterium, alkyl, alkoxyl, cycloalkyl, cycloalkoxyl, halogen, nitro, nitrile, silyl, phenyl, biphenyl, terphenyl, pyridine, and combinations thereof; and

wherein

(A) when m=0, L^1 is biphenyl, L^2 is a direct bond, L^3 is a direct bond,

G^1 is selected from the group consisting of dibenzoselenophene and fluorene, and

G^2 and G^3 are each independently selected from the group consisting of phenyl, biphenyl, terphenyl, fluorene, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, aza-fluorene, and combinations thereof; and

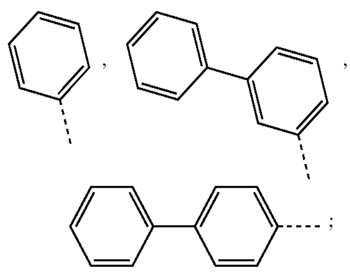
(B) when m is 1 to 7, G^1 is selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and fluorene, and each G^4 is independently selected from the group consisting of phenyl, and biphenyl, and at least one G^4 is biphenyl,

wherein L^1, L^2 and L^3 are each independently selected from the group consisting of direct bond, phenyl, biphenyl, terphenyl, pyridine, pyrimidine, and combinations thereof, and

G^2 and G^3 are each independently selected from the group consisting of phenyl, biphenyl, terphenyl, fluorene, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, aza-fluorene, and combinations thereof.

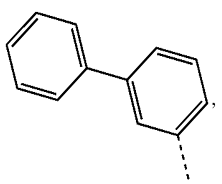
2. The composition of claim **1**, wherein m is 0.

3. The composition of claim **1**, wherein each G^4 is independently selected from the group consisting of:

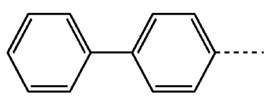


and

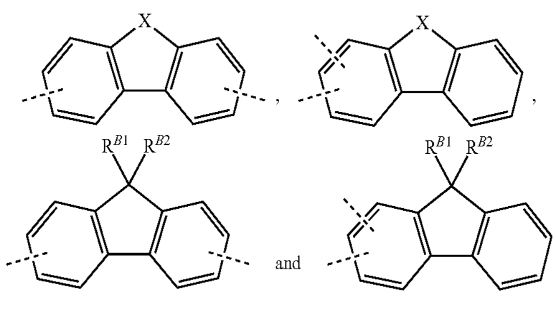
the first G^4 is selected from the group consisting of



and



4. The composition of claim **1**, wherein G' has the structure selected from the group consisting of:

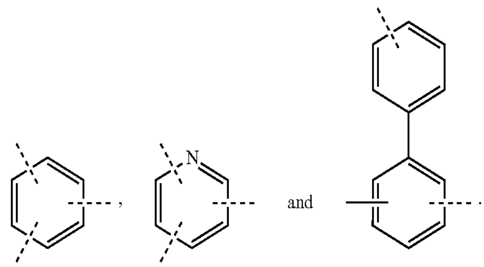


wherein, when m=0, X is Se, and, wherein m is 1 to 7, X is selected from a group consisting of O, S and Se;

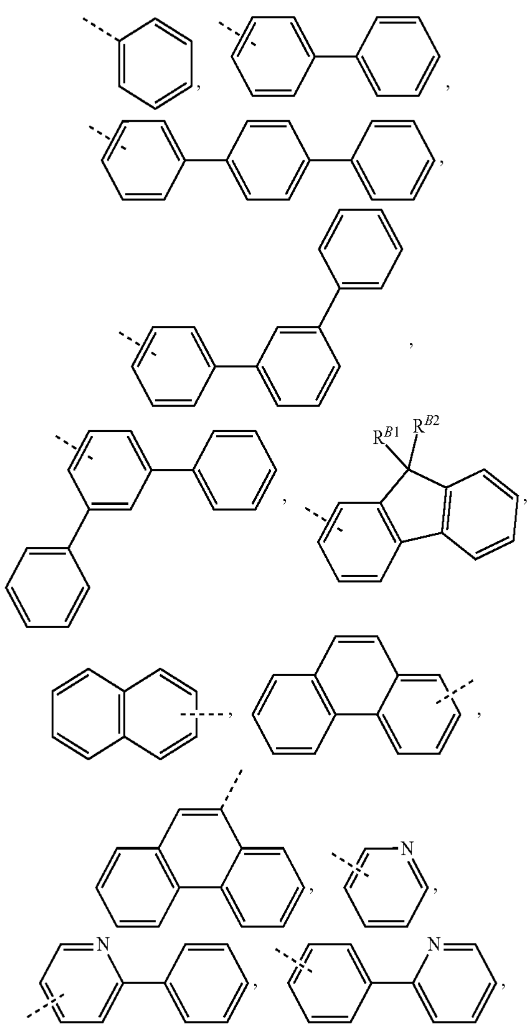
wherein R^{B1} and R^{B2} are independently selected from a group consisting of hydrogen, deuterium, alkyl, cycloalkyl, alkoxyl, aryl, heteroaryl, halogen, and combinations thereof; and

wherein R^{B1} and R^{B2} are optionally joined to form a ring.

5. The composition of claim **1**, wherein m is equal to or greater than 1 and L^1 is selected from the group consisting of:



6. The composition of claim **1**, wherein, consistent with limitation (A) or (B), G^2 and G^3 are independently selected from the group consisting of:



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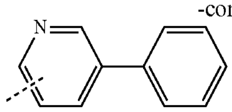
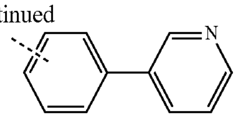
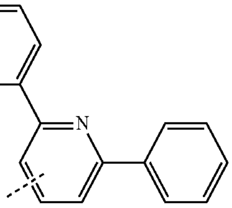
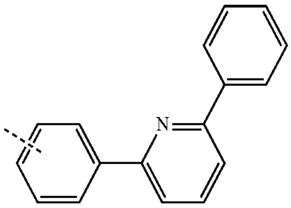
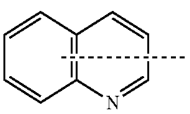
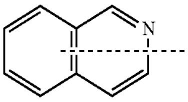
,

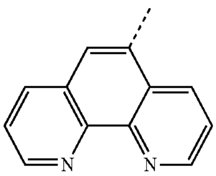
,

,

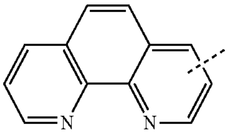
,

,

,



and

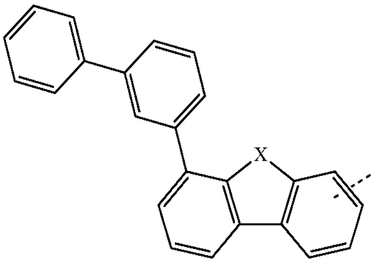
;

wherein R^{B1} and R^{B2} are independently selected from a group consisting of hydrogen, deuterium, alkyl, cycloalkyl, alkoxyl, aryl, heteraryl, halogen, and combinations thereof; and

wherein R^{B1} and R^{B2} are optionally joined to form a ring.

7. The composition of claim **1**, wherein at least one of G^2, G^3, and, when present, G^4 is substituted with at least one fluorine atom.

8. The composition of claim **1**, wherein, when m is 1, G^4-G^1 has a structure selected from the group consisting of:



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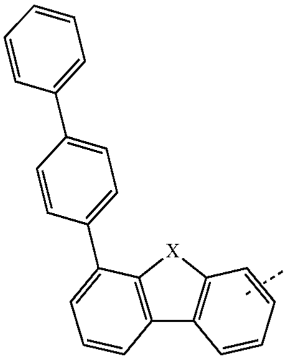

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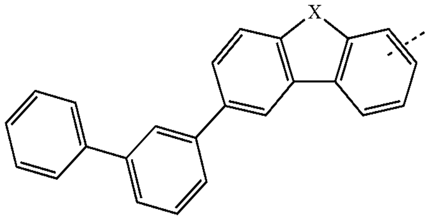

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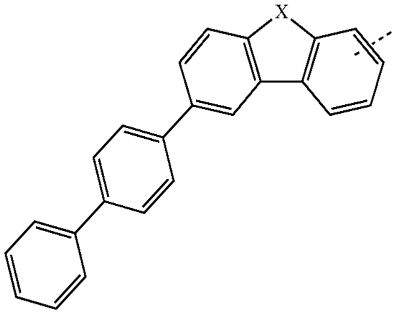

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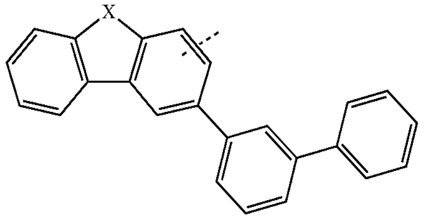

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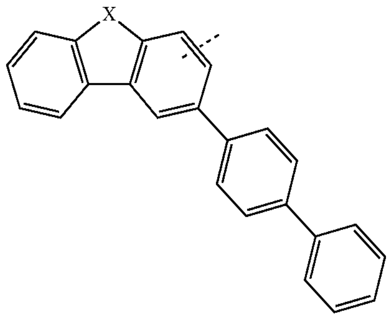

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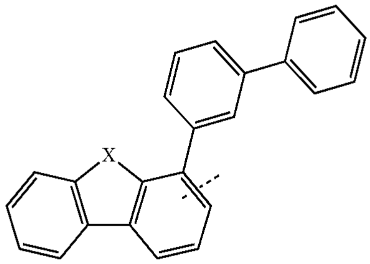
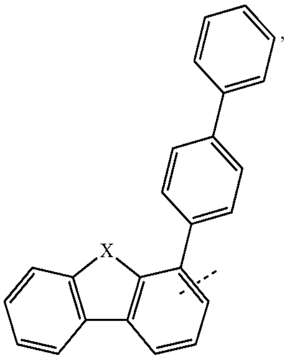


, and

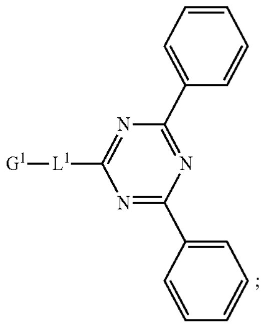


,

wherein X is selected from the group consisting of O, S, Se, and $CR^{B1}R^{B2}$, and wherein R^{B1} and R^{B2} are independently selected from a group consisting of hydrogen, deuterium, alkyl, cycloalkyl, alkoxyl, aryl, heteraryl, halogen, and combinations thereof; and

wherein R^{B1} and R^{B2} are optionally joined to form a ring.

9. The composition of claim **1**, wherein the first compound has a formula:

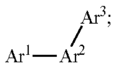


wherein L^1 is biphenyl.

10. The composition of claim **1**, wherein the composition comprises a second compound;

wherein the second compound has the formula II:

Formula II



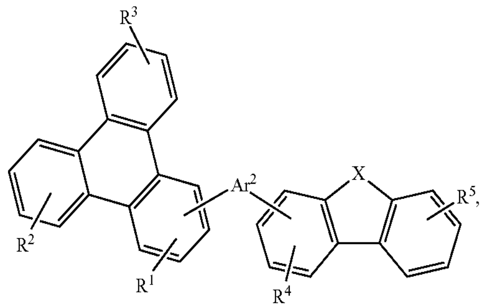
wherein Ar^1 is selected from the group consisting of triphenylene, and aza-triphenylene;

wherein Ar^2 is selected from the group consisting of a direct bond, phenyl, biphenyl, terphenyl, naphthalene, pyridine, dibenzofuran, dibenzothiophene, dibenzoselenophene, aza-dibenzofuran, aza-dibenzothiophene, aza-dibenzoselenophene, and combinations thereof;

wherein Ar^3 is selected from the group consisting of benzene, biphenyl, terphenyl, naphthalene, pyridine, dibenzofuran, dibenzothiophene, dibenzoselenophene, aza-dibenzofuran, aza-dibenzothiophene, aza-dibenzoselenophene, carbazole, aza-carbazole, and combinations thereof; and

wherein Ar^1, Ar^2 and Ar^a are each, independently, optionally further substituted with one or more substitutions selected from the group consisting of deuterium, halogen, alkyl, aryl, heteroaryl, and combinations thereof.

11. The composition of claim **10**, wherein the second compound is selected from the group consisting of



and

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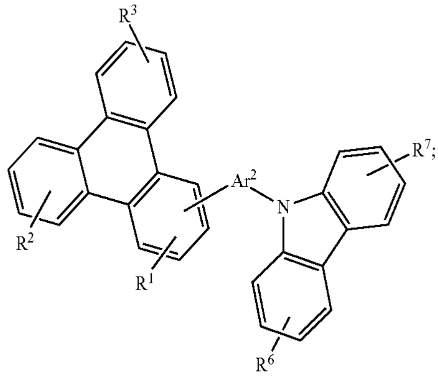


wherein X is selected from the group consisting of O, S and Se;

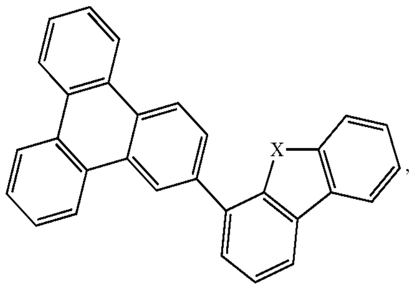
wherein R^1 and R^4 each independently represents mono, di, or tri, substitution, or no substitution;

wherein R^2, R^3, R^5, and R^6 each independently represents mono, di, tri, or tetra substitution, or no substitution; and

wherein R^1 to R^6 are each independently selected from the group consisting of hydrogen, deuterium, benzene, biphenyl, terphenyl, naphthalene, fluorene, triphenylene, phenanthrene, dibenzofuran, dibenzothiophene, carbazole and combinations thereof.

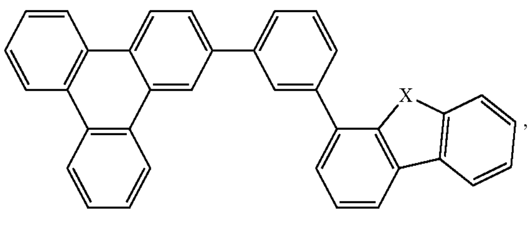
12. The composition of claim **10**, wherein the second compound is selected from the group consisting of

Compound E1 through E3, each repressented by the formula



wherein in Compound E1: X = O,
in Compound E2: X = S,
in Compound E3: X = Se

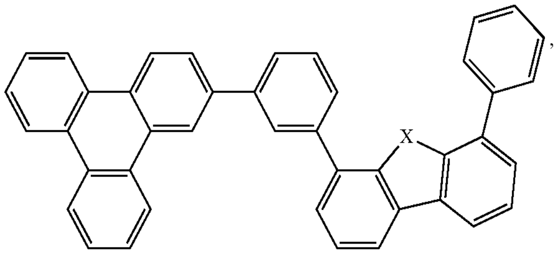
Compound E4 through E6, each represented by the formula



wherein in Compound E4: X = O,
in Compound E5: X = S,
in Compound E6: X = Se

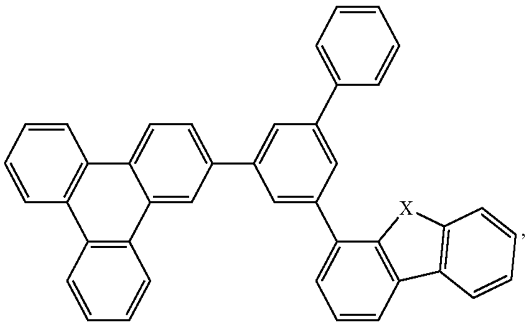
-continued

Compound E7 through E9, each represented by the formula



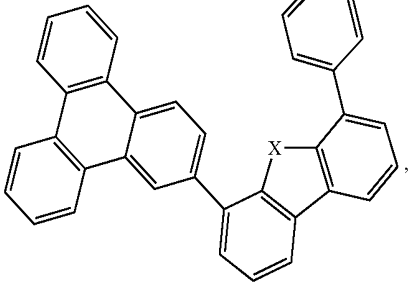
wherein in Compound E7: X = O,
in Compound E8: X = S,
in Compound E9: X = Se

Compound E10 through E12, each represented by the formula



wherein in Compound E10: X = O,
in Compound E11: X = S,
in Compound E12: X = Se

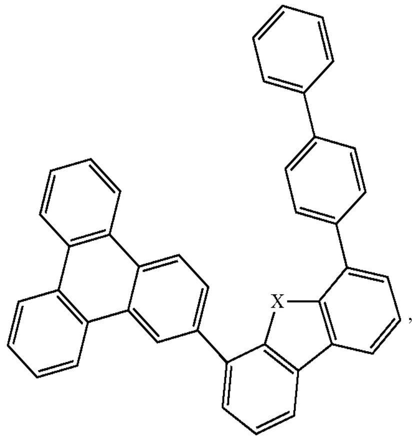
Compound E13 through E15, each represented by the formula



wherein in Compound E13: X = O,
in Compound E14: X = S,
in Compound E15: X = Se

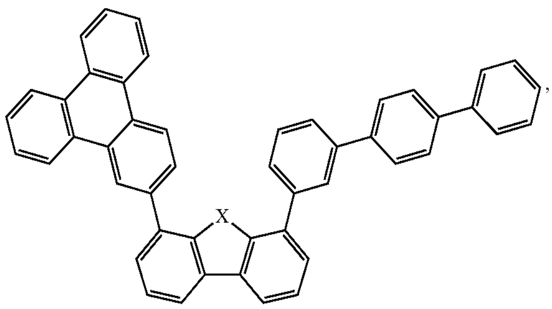
-continued

Compound E16 through E18, each represented by the formula



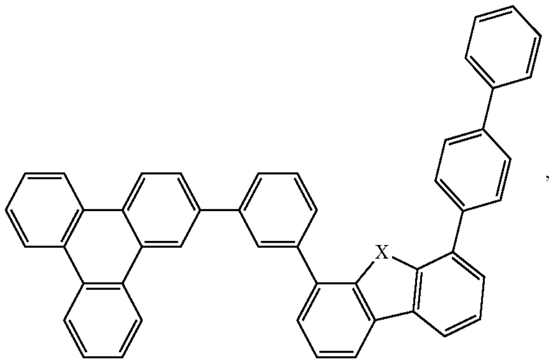
wherein in Compound E16: X = O,
in Compound E17: X = S,
in Compound E18: X = Se

Compound E19 through E21, each represented by the formula



wherein in Compound E19: X = O,
in Compound E20: X = S,
in Compound E21: X = Se

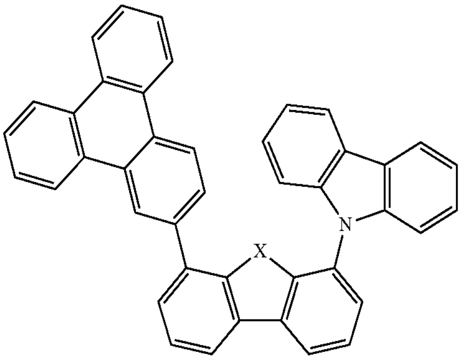
Compound E22 through E24, each represented by the formula



wherein in Compound E22: X = O,
in Compound E23: X = S,
in Compound E24: X = Se

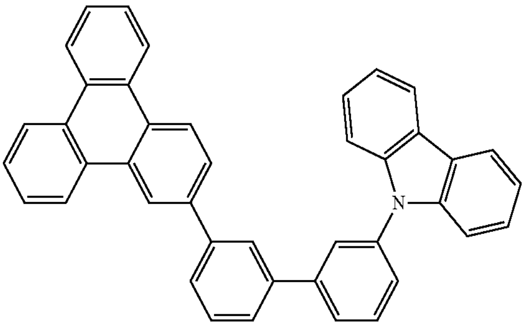
-continued

Compound E25 through E27, each represented by the formula



wherein in Compound E25: X = O,
in Compound E26: X = S,
in Compound E27: X = Se

Compound E28



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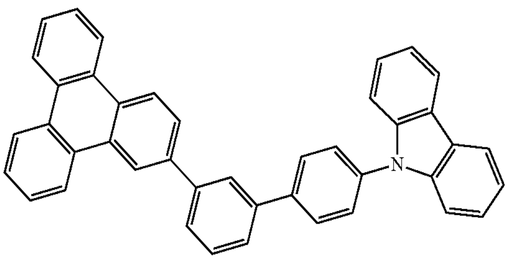
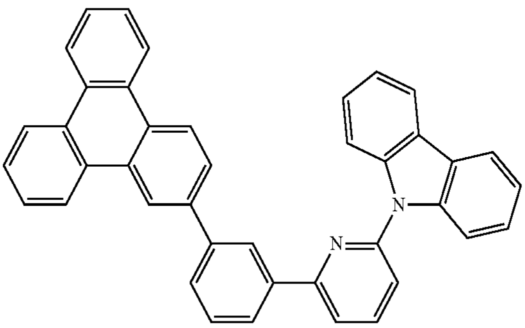
Compound E29



, and

Compound E30



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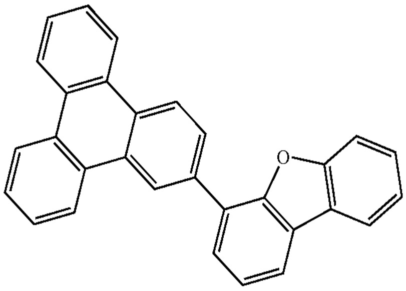
13. A composition comprising a mixture of a first compound and a second compound selected from the group consisting of:

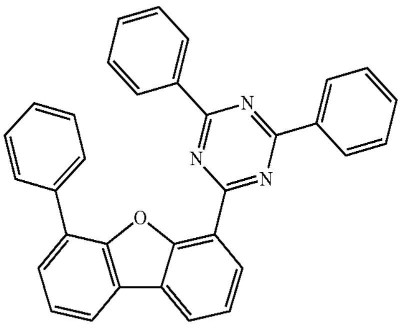
Compound E1

(



,

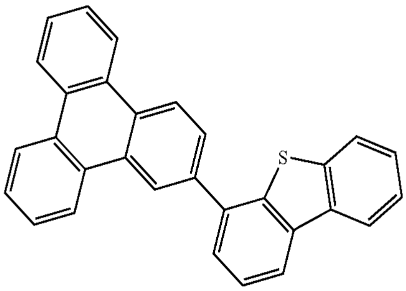
Compound C1



);

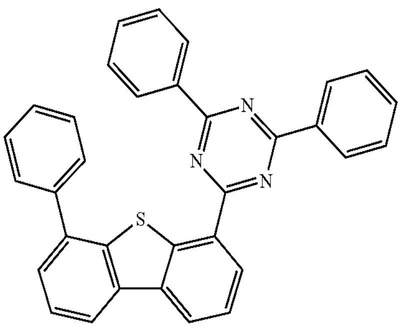
Compound E2

(



,

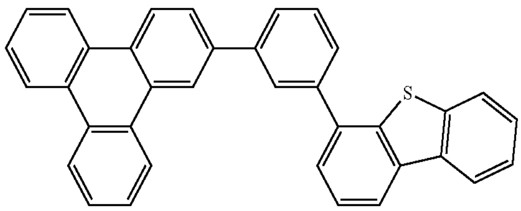
Compound C2



);

Compound E5

(



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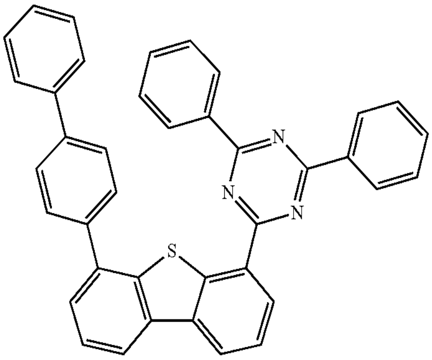
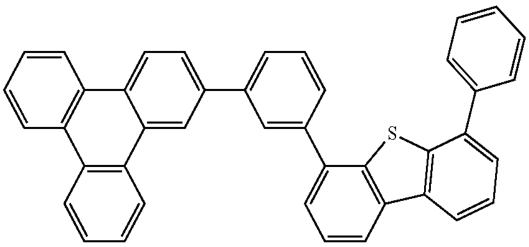
Compound C65



);

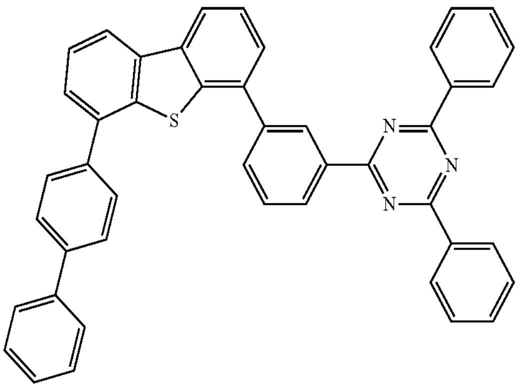
Compound E8

(



,

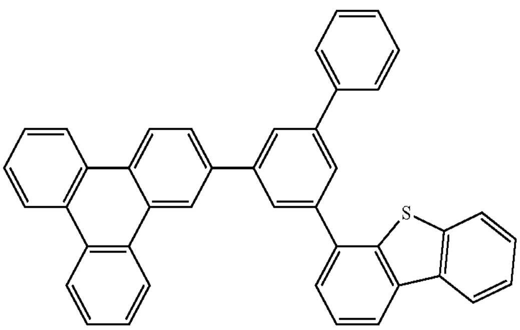
Compound C74



);

Compound E11

(



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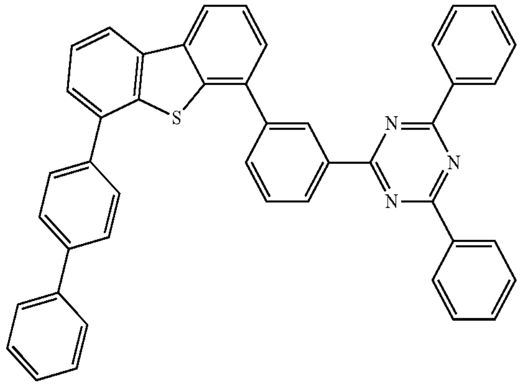
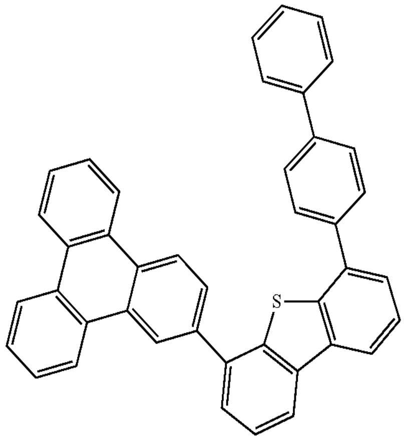
Compound C74



);

Compound E17

(



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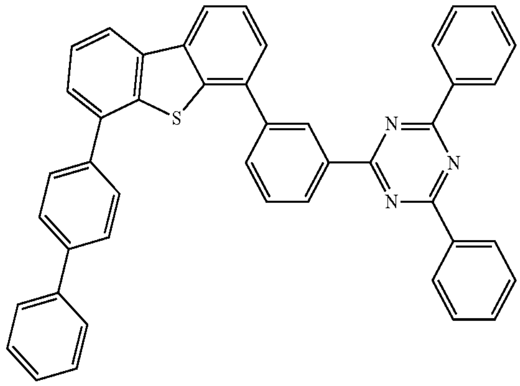
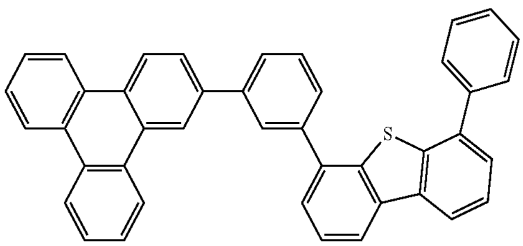
Compound C74



);

Compound E8

(



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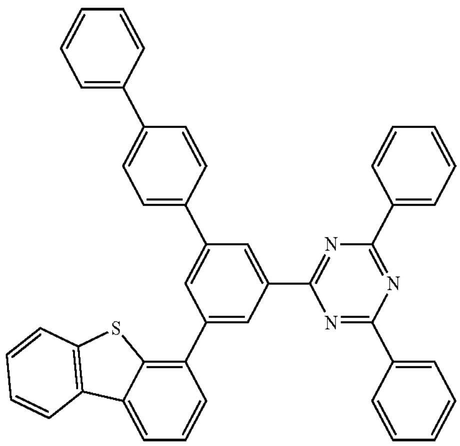
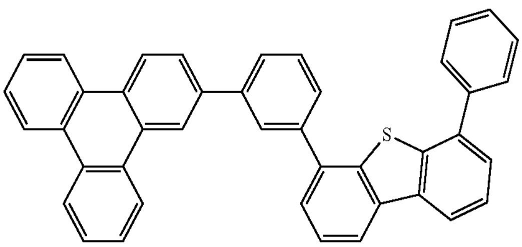
Compound A5



);

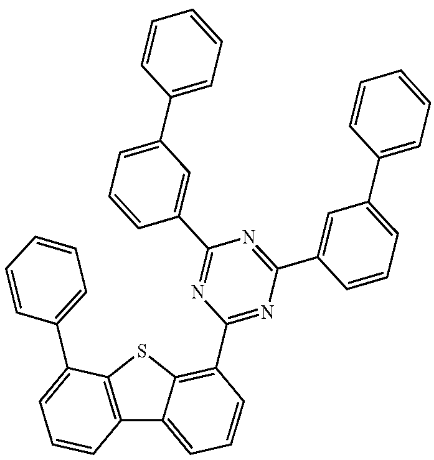
Compound E8

(



,

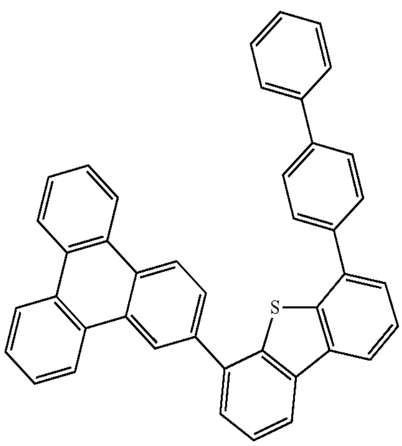
Compound C17



);

Compound E17

(



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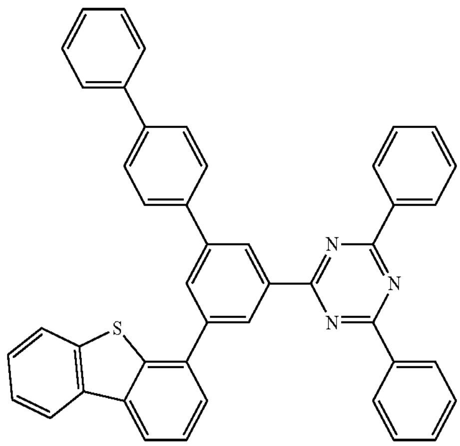
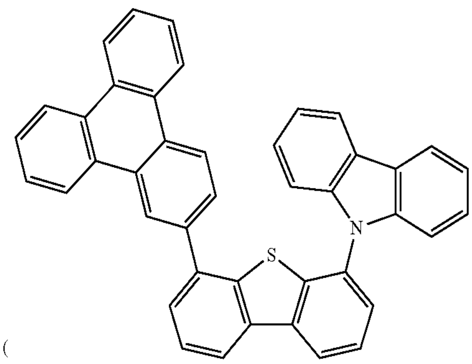
Compound A5



);

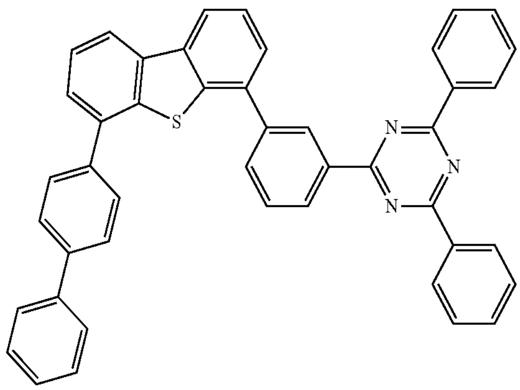
Compound E26

(



,

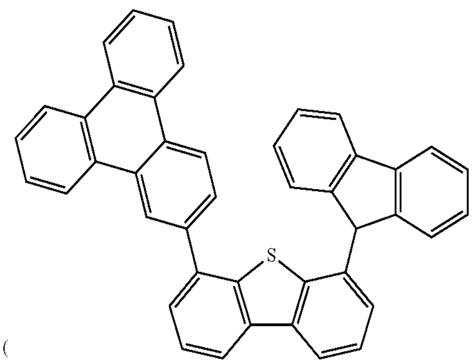
Compound C74



);

Compound E26

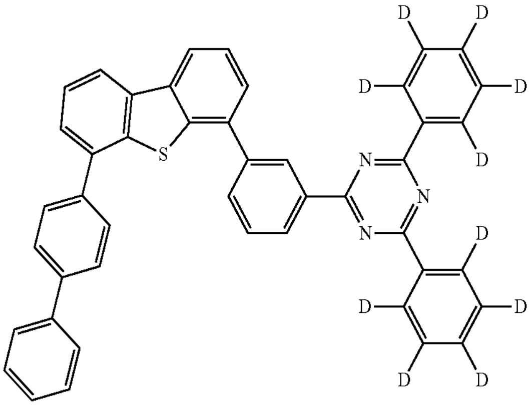
(



,

-continued

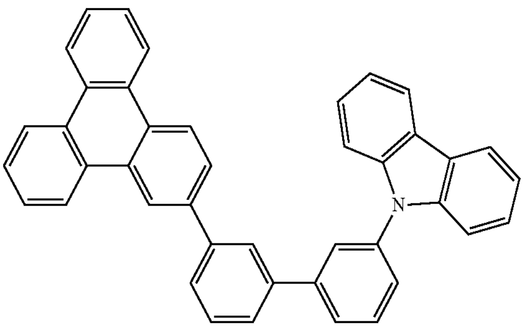
Compound C248



);

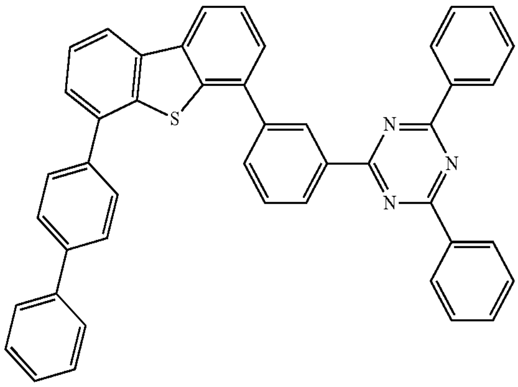
Compound E28

(



,

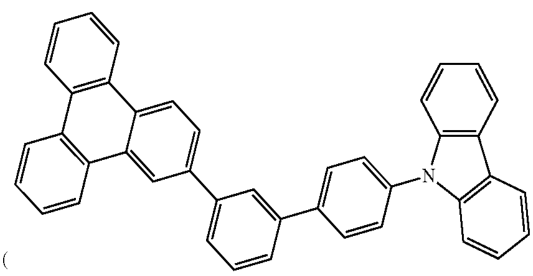
Compound C74



);

Compound E29

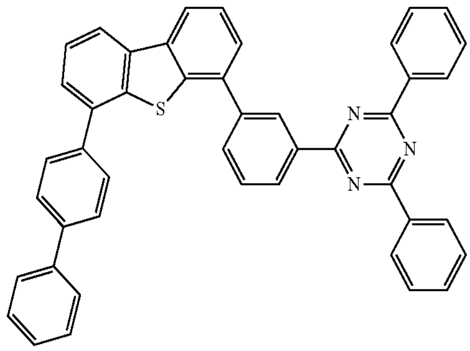
(



,

-continued

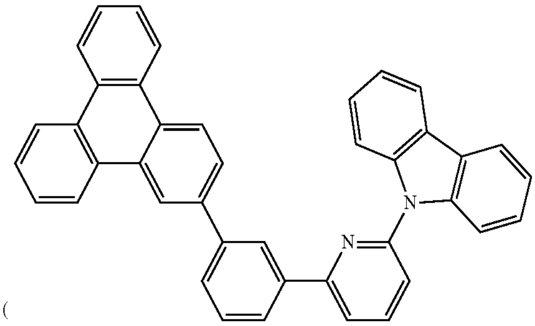
Compound C74



); and

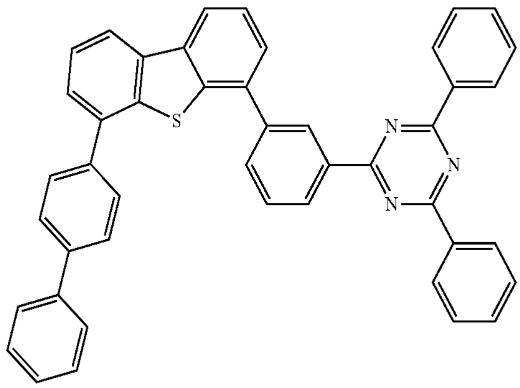
Compound E30

(



,

Compound C74



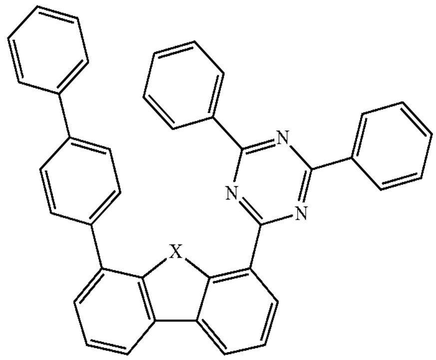
).

14. The composition of claim **1**, wherein the composition comprises a second compound; wherein the second compound is a phosphorescent emissive Ir complex having at least one substituent selected from the group consisting of alkyl, cycloalkyl, partially or fully deuterated variants thereof, partially or fully fluorinated variants thereof, and combinations thereof.

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

-continued

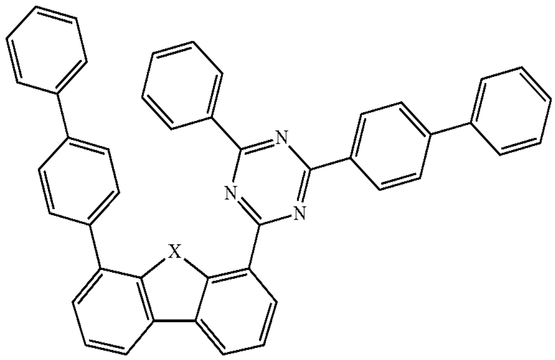
Compound C64 through C66, each represented by the formula



,

wherein in Compound C64: X = O,
in Compound C65: X = S,
in Compound C66: X = Se

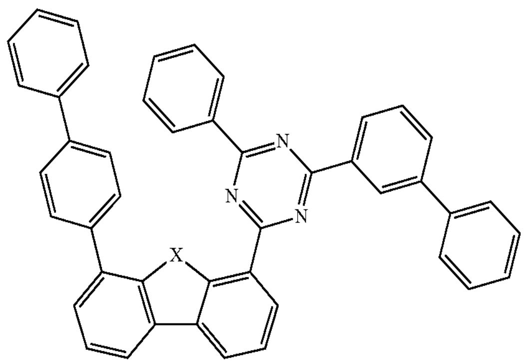
Compound C67 through C69, each represented by the formula



,

wherein in Compound C67: X = O,
in Compound C68: X = S,
in Compound C69: X = Se

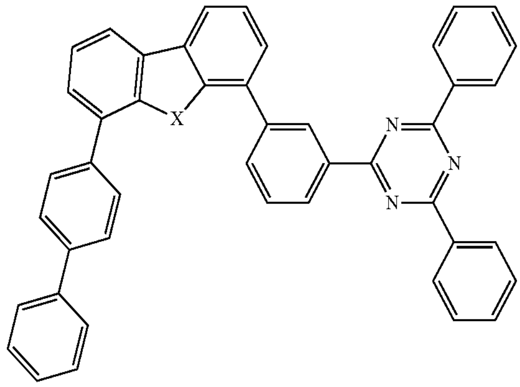
Compound C70 through C72, each represented by the formula



,

wherein in Compound C70: X = O,
in Compound C71: X = S,
in Compound C72: X = Se

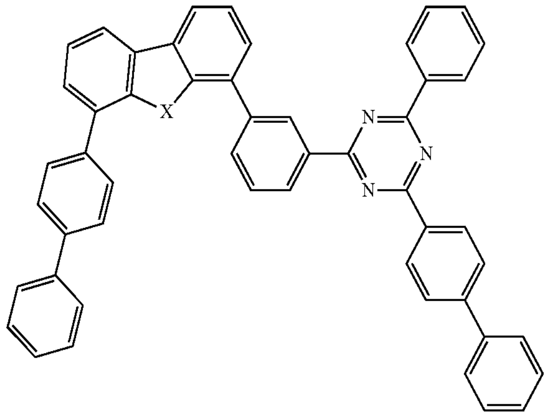
Compound C73 through C75, each represented by the formula



,

wherein in Compound C73: X = O,
in Compound C74: X = S,
in Compound C75: X = Se

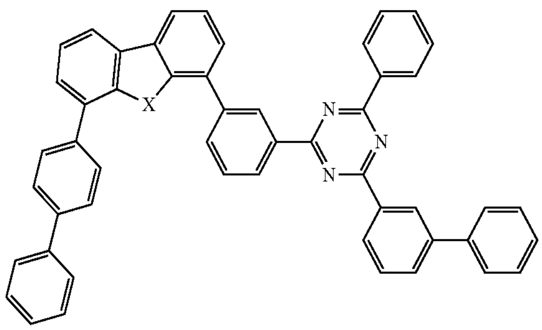
Compound C76 through C78, each represented by the formula



,

wherein in Compound C76: X = O,
in Compound C77: X = S,
in Compound C78: X = Se

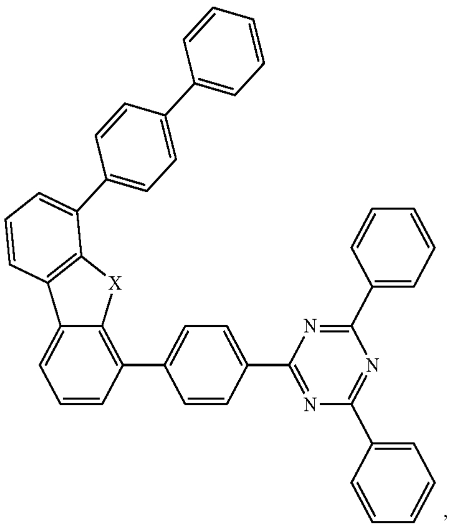
Compound C79 through C81, each represented by the formula



,

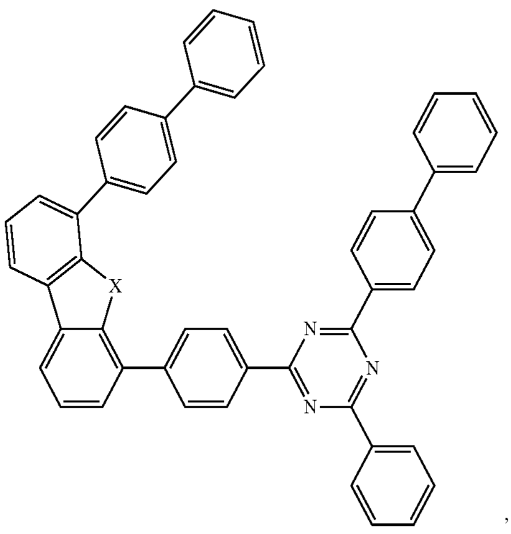
wherein in Compound C79: X = O,
in Compound C80: X = S,
in Compound C81: X = Se

Compound C82 through C84, each represented by the formula



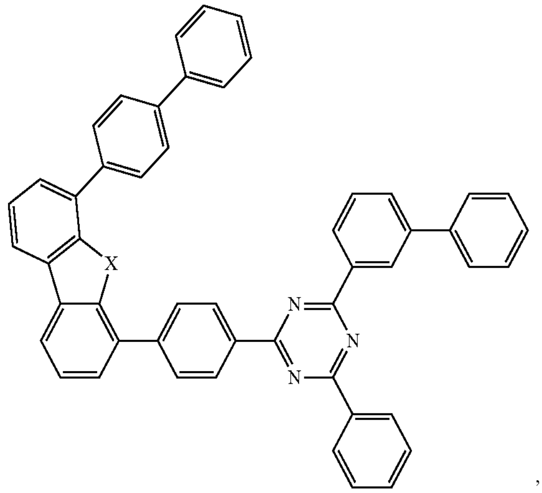
wherein in Compound C82: X = O,
in Compound C83: X = S,
in Compound C84: X = Se

Compound C85 through C87, each represented by the formula



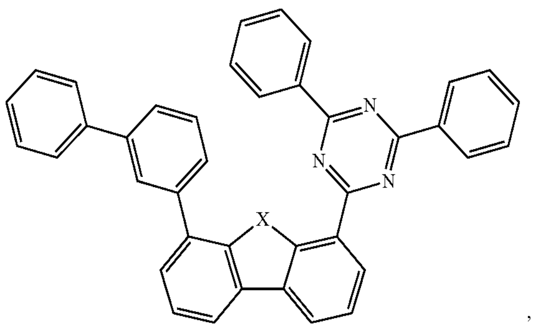
wherein in Compound C85: X = O,
in Compound C86: X = S,
in Compound C87: X = Se

Compound C88 through C90, each represented by the formula



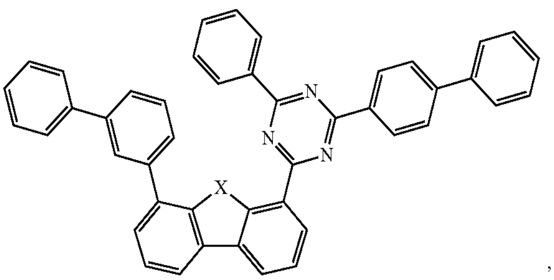
wherein in Compound C88: X = O,
in Compound C89: X = S,
in Compound C90: X = Se

Compound 91 through 93, each represented by the formula



wherein in Compound C91: X = O,
in Compound C92: X = S,
in Compound C93: X = Se

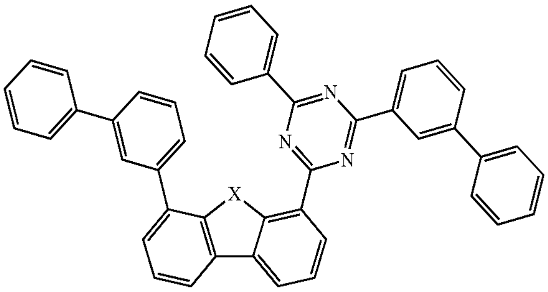
Compound C94 through C96, each represented by the formula



wherein in Compound C94: X = O,
in Compound C95: X = S,
in Compound C96: X = Se

-continued

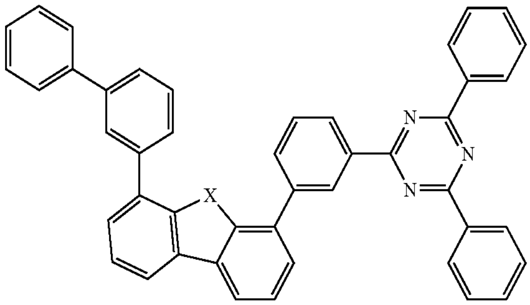
Compound C97 through C99, each represented by the formula



,

wherein in Compound C97: X = O,
in Compound C98: X = S,
in Compound C99: X = Se

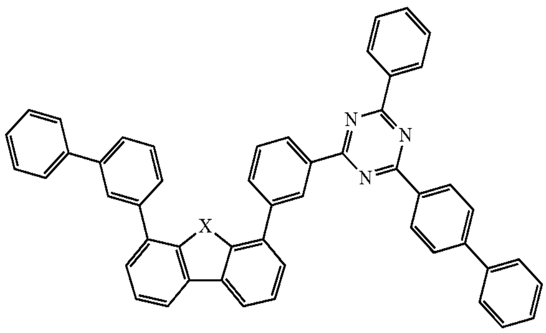
Compound C100 through C102, each represented by the formula



,

wherein in Compound C100: X = O,
in Compound C101: X = S,
in Compound C102: X = Se

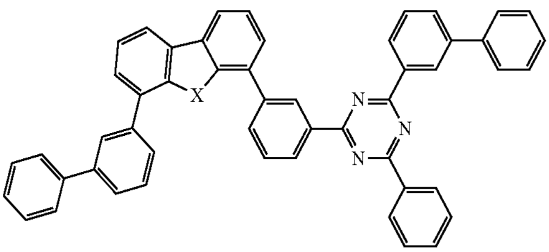
Compound C103 through C105, each represented by the formula



,

wherein in Compound C103: X = O,
in Compound C104: X = S,
in Compound C105: X = Se

Compound C106 through C108, each represented by the formula

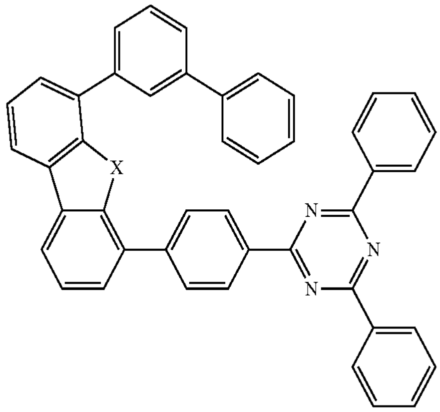


,

wherein in Compound C106: X = O,
in Compound C107: X = S,
in Compound C108: X = Se

-continued

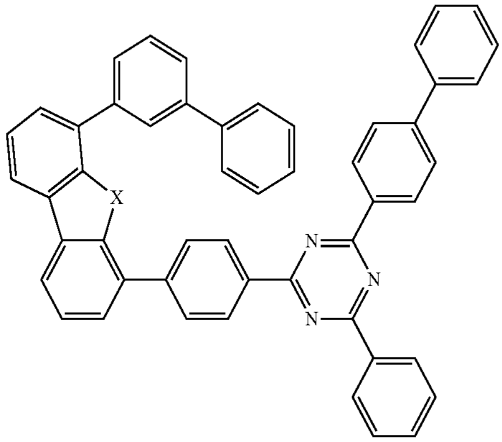
Compound C109 through C111, each represented by the formula



,

wherein in Compound C109: X = O,
in Compound C110: X = S,
in Compound C111: X = Se

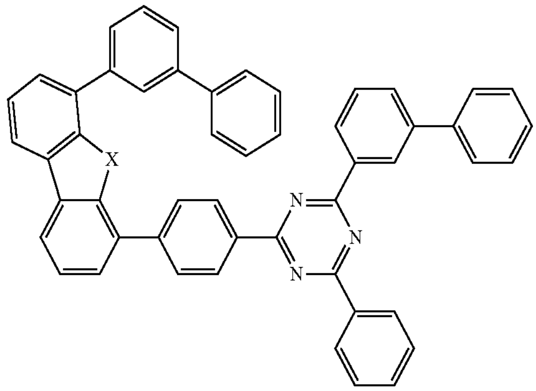
Compound C112 through C114, each represented by the formula



,

wherein in Compound C112: X = O,
in Compound C113: X = S,
in Compound C114: X = Se

Compound C115 through C117, each represented by the formula

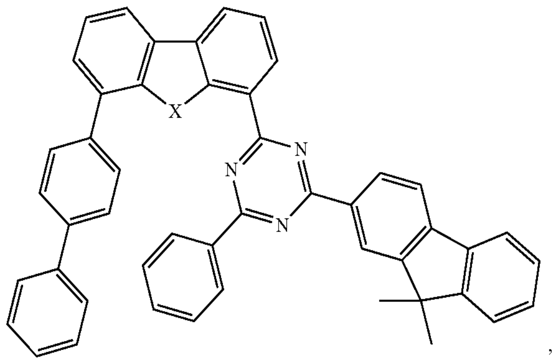


,

wherein in Compound C115: X = O,
in Compound C116: X = S,
in Compound C117: X = Se

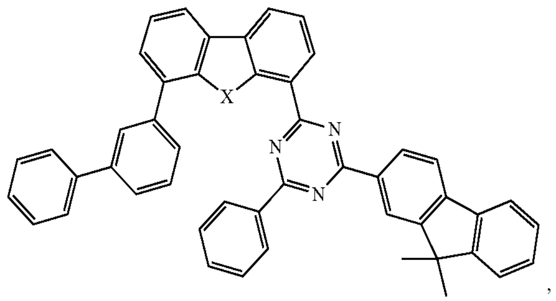
-continued

Compound C133 through C135, each represented by the formula



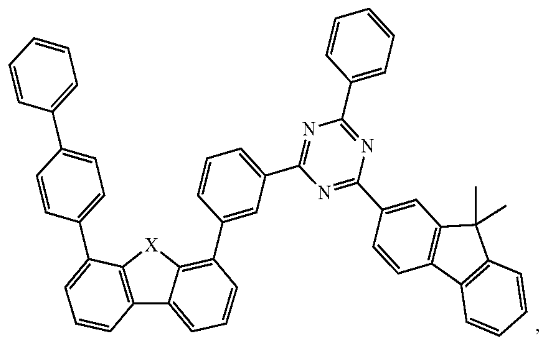
wherein in Compound C133: X = O,
in Compound C134: X = S,
in Compound C135: X = Se

Compound C136 through C138, each represented by the formula



wherein in Compound C136: X = O,
in Compound C137: X = S,
in Compound C138: X = Se

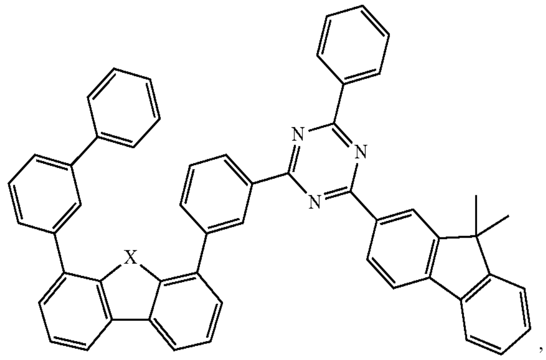
Compound C139 through C141, each represented by the formula



wherein in Compound C139: X = O,
in Compound C140: X = S,
in Compound C141: X = Se

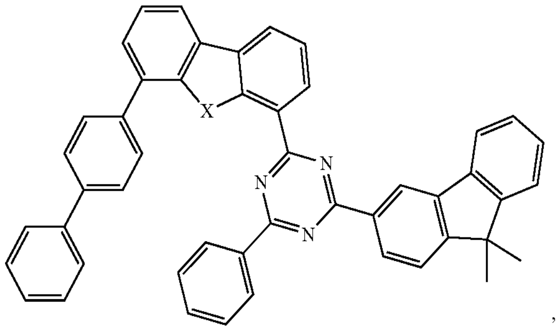
-continued

Compound C142 through C144, each represented by the formula



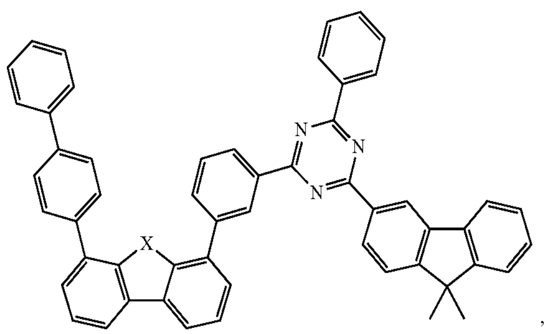
wherein in Compound C142: X = O,
in Compound C143: X = S,
in Compound C144: X = Se

Compound C151 through C153, each represented by the formula



wherein in Compound C151: X = O,
in Compound C152: X = S,
in Compound C153: X = Se

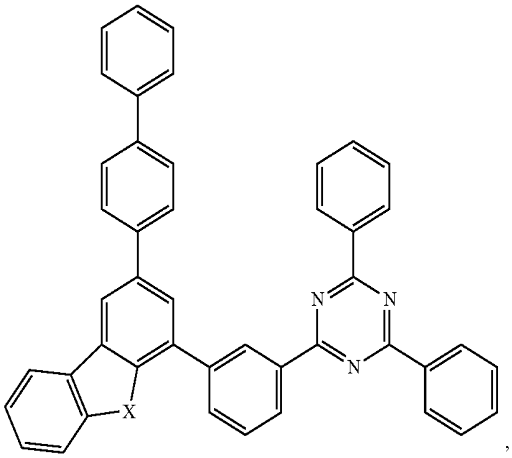
Compound C154 through C156, each represented by the formula



wherein in Compound C154: X = O,
in Compound C155: X = S,
in Compound C156: X = Se

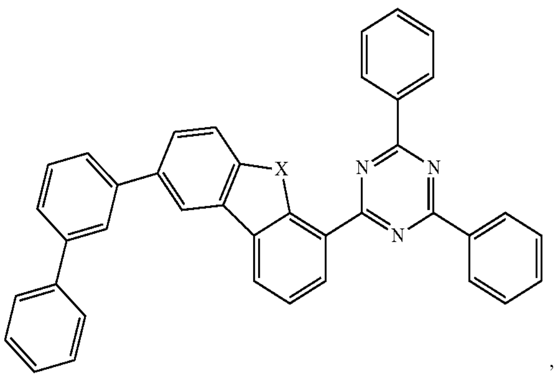
-continued

Compound C169 through C171, each represented by the formula



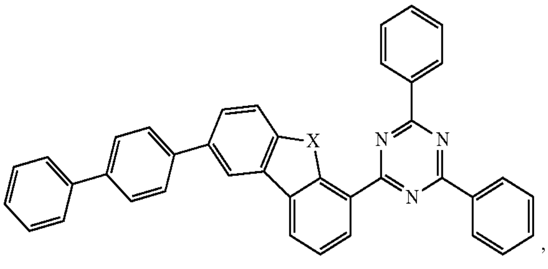
wherein in Compound C169: X = O,
in Compound C170: X = S,
in Compound C171: X = Se

Compound C178 through C180, each represented by the formula



wherein in Compound C178: X = O,
in Compound C179: X = S,
in Compound C180: X = Se

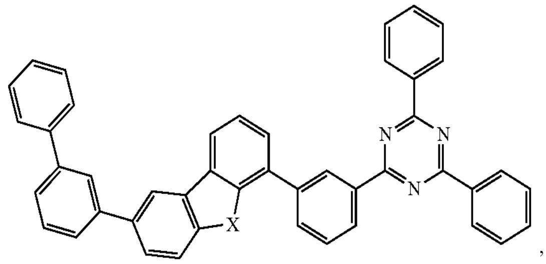
Compound C181 through C183, each represented by the formula



wherein in Compound C181: X = O,
in Compound C182: X = S,
in Compound C183: X = Se

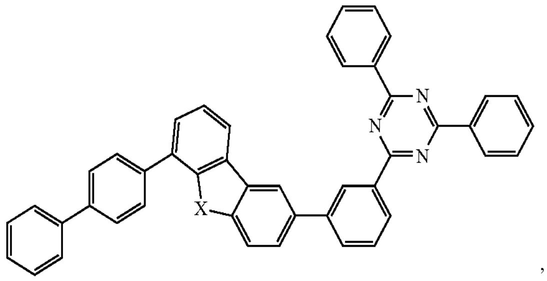
-continued

Compound C187 through C189, each represented by the formula



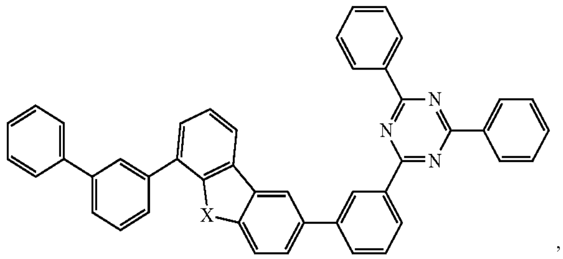
wherein in Compound C187: X = O,
in Compound C188: X = S,
in Compound C189: X = Se

Compound C199 through C201, each represented by the formula



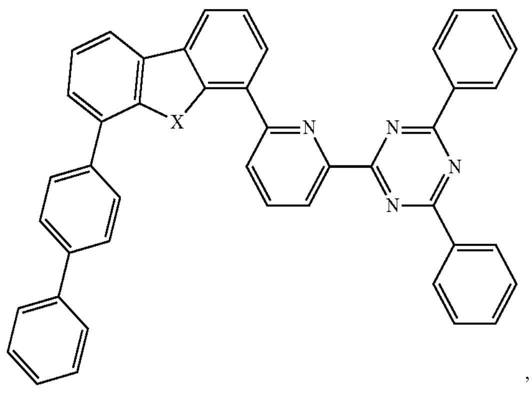
wherein in Compound C199: X = O,
in Compound C200: X = S,
in Compound C201: X = Se

Compound C202 through C204, each represented by the formula



wherein in Compound C202: X = O,
in Compound C203: X = S,
in Compound C204: X = Se

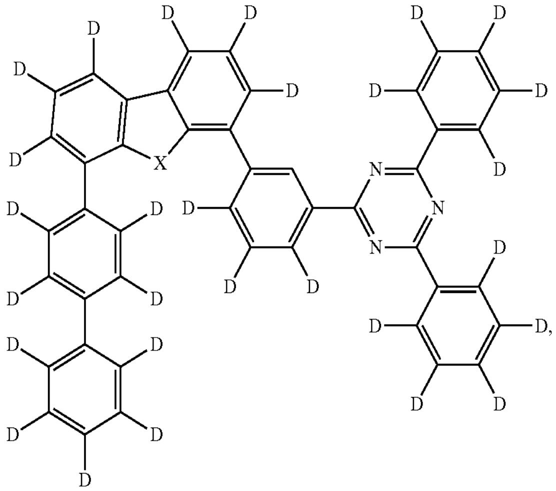
Compound C217 through C219, each represented by the formula



wherein in Compound C217: X = O,
in Compound C218: X = S,
in Compound C219: X = Se

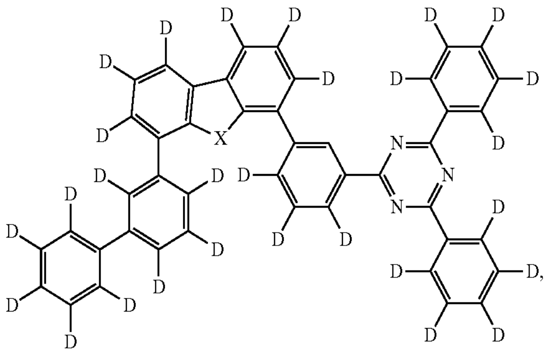
-continued

Compound C238 through C240, each represented by the formula



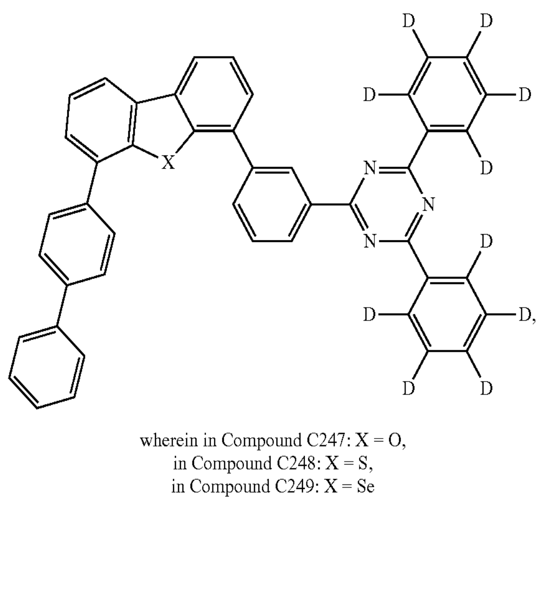
wherein in Compound C238: X = O,
in Compound C239: X = S,
in Compound C240: X = Se

Compound C244 through C246, each represented by the formula



wherein in Compound C244: X = O,
in Compound C245: X = S,
in Compound C246: X = Se

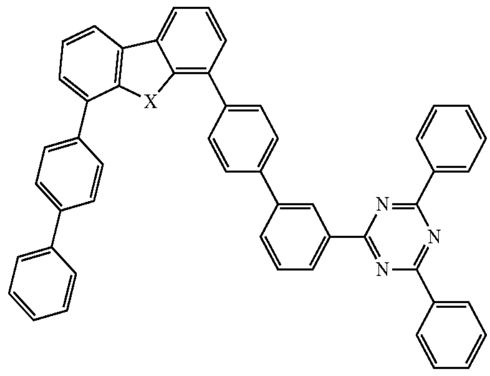
Compound C247 through C249, each represented by the formula



wherein in Compound C247: X = O,
in Compound C248: X = S,
in Compound C249: X = Se

-continued

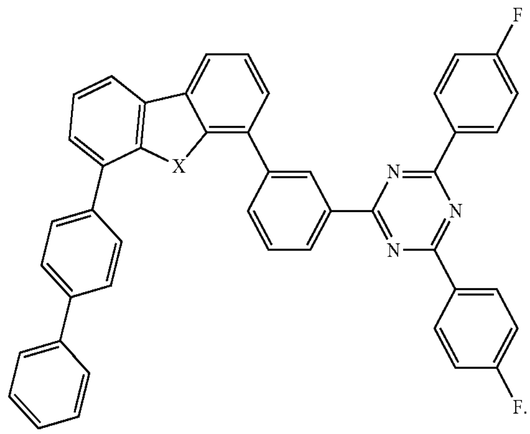
Compound C250 through C252, each represented by the formula



, and

wherein in Compound C250: X = O,
in Compound C251: X = S,
in Compound C252: X = Se

Compound C253 through C255, each represented by the formula



wherein in Compound C253: X = O,
in Compound C254: X = S,
in Compound C255: X = Se

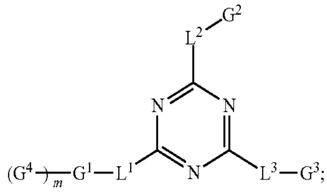
16. A first device comprising a first organic light emitting device, the first organic light emitting device comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a composition of materials comprising a first compound, wherein the first compound has a formula:

Formula I



wherein G^2, G^3, and, when present, G^4 are each optionally further substituted with one or more unfused substituents selected from the group consisting of deuterium, alkyl, alkoxyl, cycloalkyl, cycloalkoxyl, halogen, nitro, nitrile, silyl, phenyl, biphenyl, terphenyl, pyridine, and combinations thereof; and wherein

(A) when m=0, L^1 is biphenyl, L^2 is a direct bond, L^3 is a direct bond,

G^1 is selected from the group consisting of dibenzoselenophene and fluorene, and

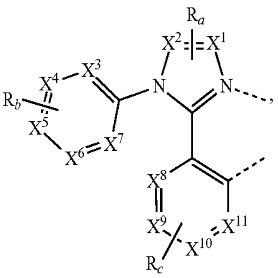
G^2 and G^3 are each independently selected from the group consisting of phenyl, biphenyl, terphenyl, fluorene, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, aza-fluorene, and combinations thereof; and

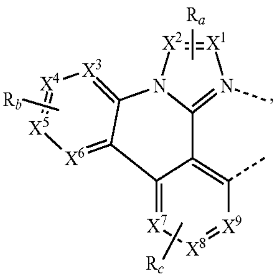
(B) when m is 1 to 7, G^1 is selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and fluorene, and each G^4 is independently selected from the group consisting of phenyl, and biphenyl, and at least one G^4 is biphenyl,

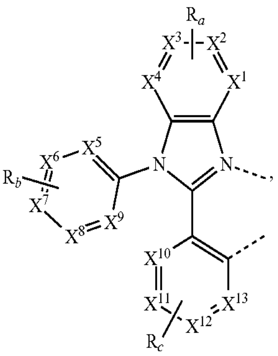
wherein L^1, L^2 and L^3 are each independently selected from the group consisting of direct bond, phenyl, biphenyl, terphenyl, pyridine, pyrimidine, and combinations thereof, and

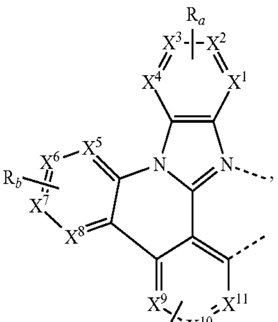
G^2 and G^3 are each independently selected from the group consisting of phenyl, biphenyl, terphenyl, fluorene, naphthalene, phenanthrene, pyridine, pyrimidine, pyrazine, quinoline, isoquinoline, phenanthroline, aza-fluorene, and combinations thereof.

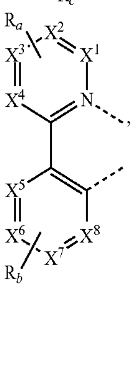
17. The first device of claim **16**, wherein the organic layer further comprises a phosphorescent emissive dopant; wherein the phosphorescent emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:

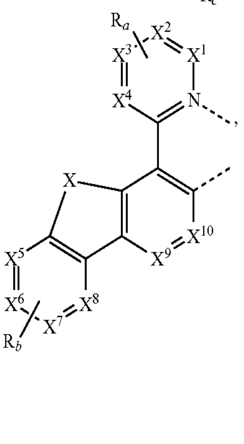












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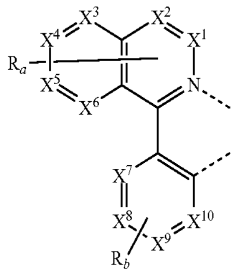
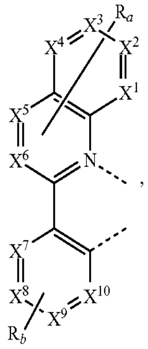
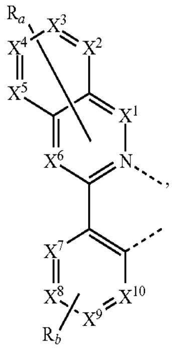
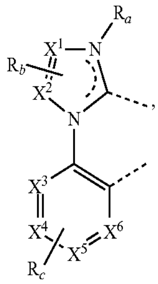
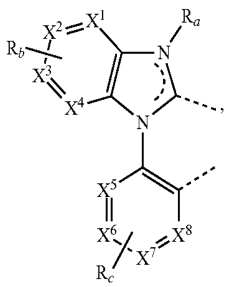
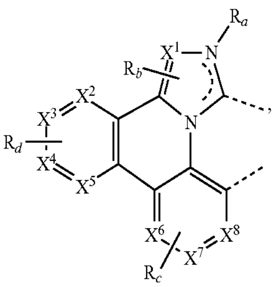


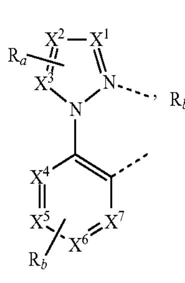


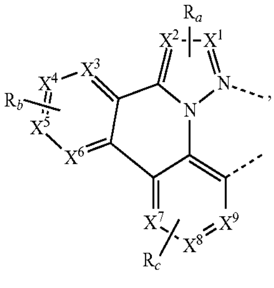


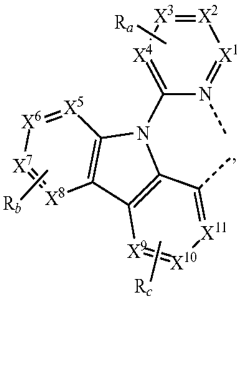


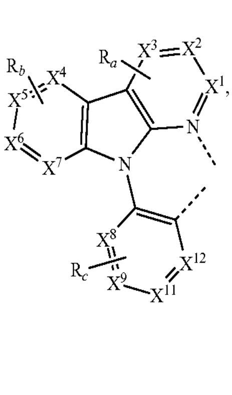






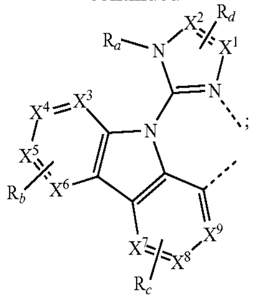






and

-continued



wherein each X^1 to X^{13} are independently selected from the group consisting of carbon and nitrogen;

wherein X is selected from the group consisting of BR', NR', PR', O, S, Se, C=O, S=O, SO_2, CR'R", SiR'R", and GeR'R";

wherein R' and R" are optionally fused or joined to form a ring;

wherein each R', R", R_a, R_b, R_c, and R_d may represent from mono substitution to the possible maximum number of substitution, or no substitution;

wherein R', R", R_a, R_b, R_e, and R_d are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein any two adjacent substitutents of R_a, R_b, R_e, and R_d are optionally fused or joined to form a ring or form a multidentate ligand.

18. The first device of claim **16**, wherein the organic layer is a blocking layer and the composition is a blocking material in the organic layer.

19. The first device of claim **16**, wherein the organic layer is an electron transporting layer and the composition is an electron transporting material in the organic layer.

20. The composition of claim **1**, wherein wherein m is equal to or greater than 1.

* * * * *

patsnap

专利名称(译)	有机电致发光材料和器件		
公开(公告)号	US10297762	公开(公告)日	2019-05-21
申请号	US14/734712	申请日	2015-06-09
[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	ZENG LICHANG LAYEK SUMAN BOUDREAULT PIERRE LUC T ELSHENAWY ZEINAB KOTTAS GREGG DYATKIN ALEXEY BORISOVICH JOSEPH SCOTT ADAMOVICH VADIM XIA CHUANJUN WANG TING CHIH YEAGER WALTER		
发明人	ZENG, LICHANG LAYEK, SUMAN BOUDREAULT, PIERRE-LUC T. ELSHENAWY, ZEINAB KOTTAS, GREGG DYATKIN, ALEXEY BORISOVICH JOSEPH, SCOTT ADAMOVICH, VADIM XIA, CHUANJUN WANG, TING-CHIH YEAGER, WALTER		
IPC分类号	H01L51/00 C07D251/24 C07D409/10 C09K11/02 C09K11/06 C07D421/10 C07D405/10 C07D409/04 H01L51/50		
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代理机构(译)	DUANE MORRIS LLP		
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优先权	62/022300 2014-07-09 US 62/038925 2014-08-19 US 62/060192 2014-10-06 US 62/083490 2014-11-24 US		
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外部链接	Espacenet		

摘要(译)

描述了包含第一化合物和第二化合物的组合物。该组合物可以是具有式I结构的第一化合物的混合物， 和具有式II结构的第二化合物， 该组合物也可以是具有式III结构的第一化合物的混合物， 和具有式IV结构的第二化合物， 还描述了包括用于式I和II或式III和IV的组合物的装置，例如OLED，以及制备它们的方法。