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JOSEPH et al.(10) **Pub. No.: US 2015/0243893 A1**(43) **Pub. Date: Aug. 27, 2015**(54) **ORGANIC ELECTROLUMINESCENT
MATERIALS AND DEVICES**(22) Filed: **Feb. 24, 2014**(71) Applicant: **Universal Display Corporation**, Ewing,
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(2013.01); **H01L 51/5016** (2013.01)(73) Assignee: **Universal Display Corporation**, Ewing,
NJ (US)(57) **ABSTRACT**(21) Appl. No.: **14/188,025**

The present disclosure provides novel compounds based on azadibenzothiophenes, azadibenzofurans and azadibenzoselenophenes with at least two nitrogen atoms in the aza rings. The compounds can be used in green, red, yellow and white emitting devices as electron-transporting hosts.

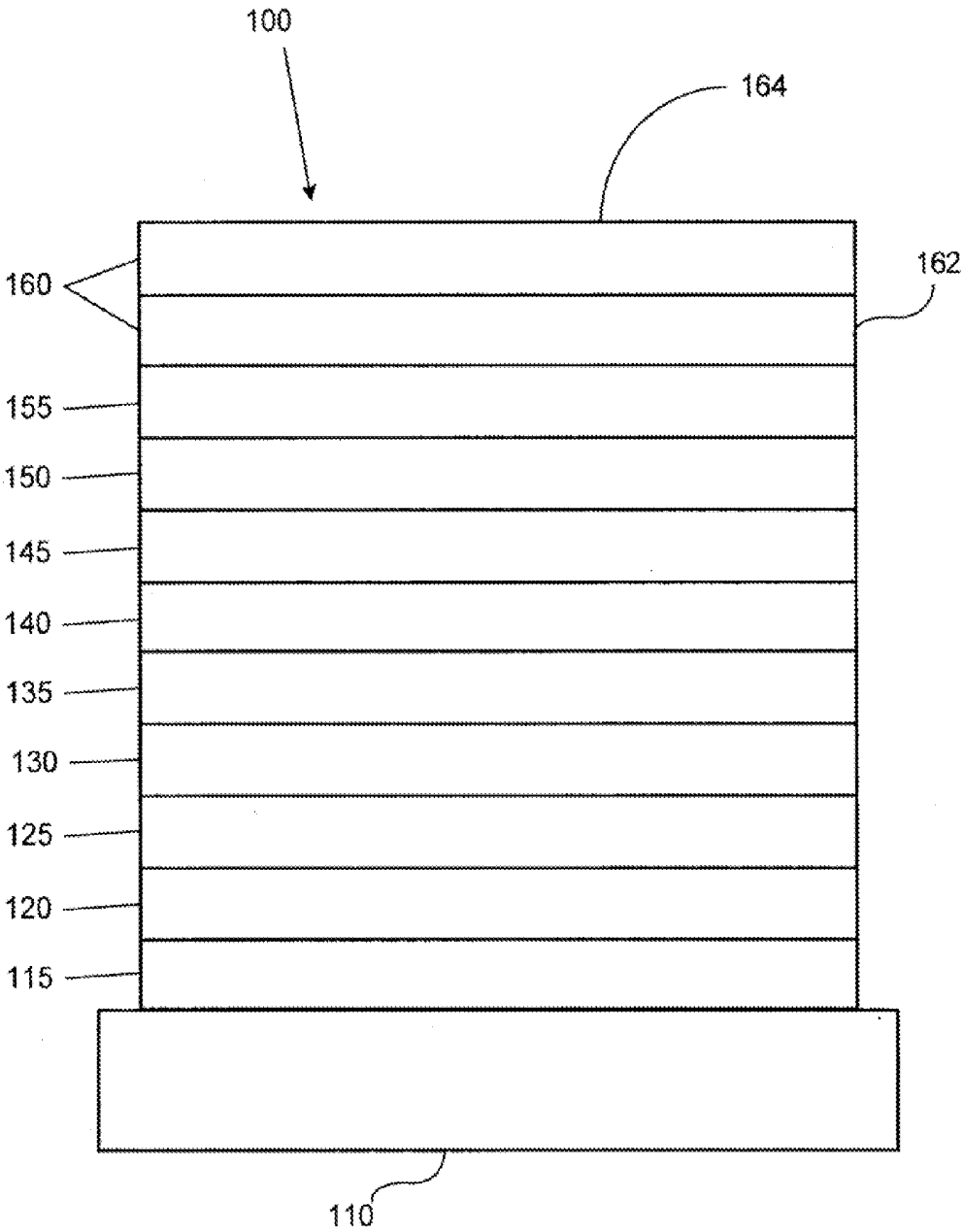


FIG. 1

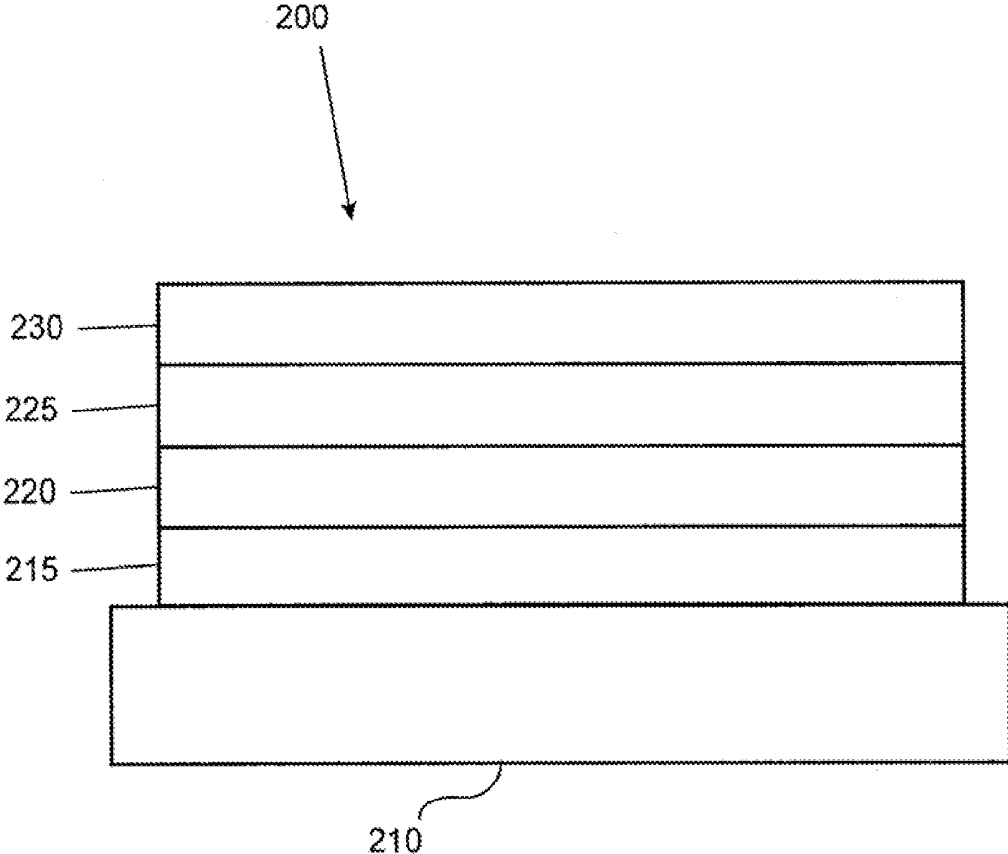


FIG. 2

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

PARTIES TO A JOINT RESEARCH AGREEMENT

[0001] 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

[0002] The present invention relates to organic light emitting devices (OLEDs), and to organic materials used in such devices. More specifically, the present invention relates to novel host compounds based on azadibenzothiophenes, azadibenzofurans and azadibenzoselenophenes with at least two nitrogen atoms in the aza rings useful for phosphorescent OLEDs.

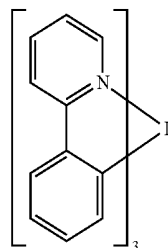
BACKGROUND

[0003] 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.

[0004] 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.

[0005] 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.

[0006] One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)₃, which has the following structure:



[0007] In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

[0008] 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.

[0009] 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.

[0010] As used herein, "solution processible" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

[0011] 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.

[0012] 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.

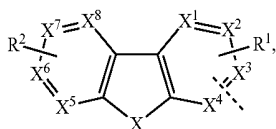
[0013] As used herein, and as would be generally understood by one skilled in the art, a first work function is “greater than” or “higher than” a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to 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.

[0014] 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.

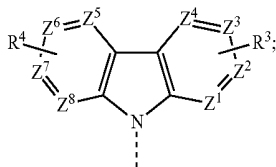
SUMMARY OF THE INVENTION

[0015] The present disclosure provides novel compounds based on azadibenzothiophenes, azadibenzofurans and azadibenzoselenophenes with at least two nitrogen atoms in the aza rings. The new compounds are useful as electron-transporting hosts for phosphorescent emitters in green, red, yellow and white phosphorescent OLEDs to provide low-voltage, high-efficiency and high-stability devices. These materials can be vapor-evaporated or solution processed.

[0016] According to an embodiment of the present disclosure, a novel compound having a formula, G^1 -L- G^2 , Formula I is disclosed. In Formula I, G^1 has the structure:



and G^2 has the structure:



[0017] wherein L is selected from the group consisting of a direct bond, an aryl group having from 6-30 carbon atoms, a heteroaryl group having from 3-30 carbon atoms, and combinations thereof; wherein the aryl group and the heteroaryl group are optionally further substituted with one or more groups independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

[0018] wherein X is selected from the group consisting of O, S, and Se;

[0019] wherein each of $X^1, X^2, X^3, X^4, X^5, X^6, X^7, X^8, Z^1, Z^2, Z^3, Z^4, Z^5, Z^6, Z^7,$ and Z^8 is carbon or nitrogen;

[0020] wherein at least two of $X^1, X^2, X^3, X^4, X^5, X^6, X^7,$ and X^8 are nitrogen;

[0021] wherein at least one of $X^1, X^2, X^3,$ and X^4 is carbon and bonded to L;

[0022] wherein G^2 bonds to L at N;

[0023] wherein each $R^2, R^3,$ and R^4 represent mono, di, tri, tetra substitutions or no substitution;

[0024] wherein R^1 represents mono, di, tri substitutions or no substitution;

[0025] wherein $R^1, R^2, R^3,$ and R^4 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;

[0026] wherein the substitution is optionally fused to G^1 or G^2 ; and

[0027] wherein when R^3 or R^4 is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G^2 at 9-N.

[0028] According to an aspect of the present disclosure, a device comprising a phosphorescent organic light-emitting device incorporating the novel compound is also disclosed. The phosphorescent organic light-emitting device comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises the novel compound having the formula, G^1 -L- G^2 , Formula I, disclosed herein.

[0029] A formulation comprising the novel compound of the present disclosure is also disclosed.

BRIEF DESCRIPTION OF THE DRAWINGS

[0030] FIG. 1 shows an organic light emitting device that can incorporate the inventive compound disclosed herein.

[0031] FIG. 2 shows an inverted organic light emitting device that can incorporate the inventive compound disclosed herein.

DETAILED DESCRIPTION

[0032] 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.

[0033] 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.

[0034] More recently, OLEDs having emissive materials that emit light from triplet states (“phosphorescence”) have been demonstrated. Baldo et al., “Highly Efficient Phospho-

rescent 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.

[0035] 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.

[0036] 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 F₄-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.

[0037] 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.

[0038] 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.

[0039] 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.

[0040] 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.

[0041] 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.

[0042] Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, 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.

[0043] 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.

[0044] The term "halo" or "halogen" as used herein includes fluorine, chlorine, bromine, and iodine.

[0045] 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.

[0046] 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.

[0047] 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.

[0048] The term "alkynyl" as used herein contemplates both straight and branched chain alkyne radicals. Preferred alkyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group may be optionally substituted.

[0049] 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.

[0050] The term "heterocyclic group" as used herein contemplates non-aromatic cyclic radicals. Preferred heterocyclic groups are those containing 3 or 7 ring atoms which includes at least one hetero atom, and includes cyclic amines such as morpholino, piperidino, pyrrolidino, and the like, and cyclic ethers, such as tetrahydrofuran, tetrahydropyran, and the like. Additionally, the heterocyclic group may be optionally substituted.

[0051] 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.

[0052] 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.

[0053] 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.

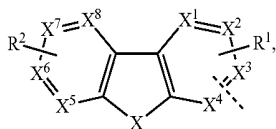
[0054] As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant position, such as carbon. Thus, for example, where R¹ is mono-substituted, then one R¹ must be other than H. Similarly, where R¹ is

di-substituted, then two of R¹ must be other than H. Similarly, where R¹ is unsubstituted, R¹ is hydrogen for all available positions.

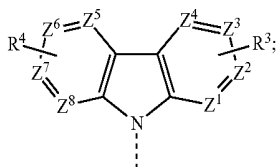
[0055] The “aza” designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzonethiophene, etc. means that one or more of the C—H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[f,h]quinoxaline 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.

[0056] 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. naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[0057] According to an aspect of the present disclosure, a novel compound having a formula: G¹-L-G², Formula I, is disclosed. In Formula I, G¹ has the structure:



and G² has the structure:



[0058] wherein L is selected from the group consisting of a direct bond, an aryl group having from 6-30 carbon atoms, a heteroaryl group having from 3-30 carbon atoms, and combinations thereof; wherein the aryl group and the heteroaryl group are optionally further substituted with one or more groups 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;

[0059] wherein X is selected from the group consisting of O, S, and Se;

[0060] wherein each of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, X⁸, Z¹, Z², Z³, Z⁴, Z⁵, Z⁶, Z⁷, and Z⁸ is carbon or nitrogen;

[0061] wherein at least two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen;

[0062] wherein at least one of X¹, X², X³, and X⁴ is carbon and bonded to L;

[0063] wherein the dashed lines represent the bonds between G¹ and L and between G² and L;

[0064] wherein each R², R³, and R⁴ represent mono, di, tri, tetra substitutions or no substitution;

[0065] wherein R¹ represents mono, di, tri substitutions or no substitution;

[0066] wherein R¹, R², R³, and R⁴ 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;

[0067] wherein the substitution is optionally fused to G¹ or G²; and

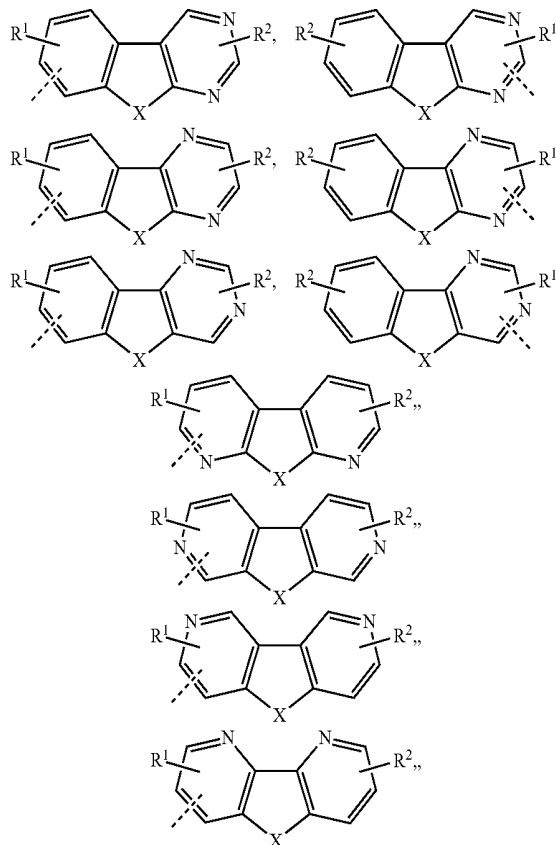
[0068] wherein when R³ or R⁴ is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G² by N.

[0069] In one embodiment, when R¹ or R² is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G¹ by N.

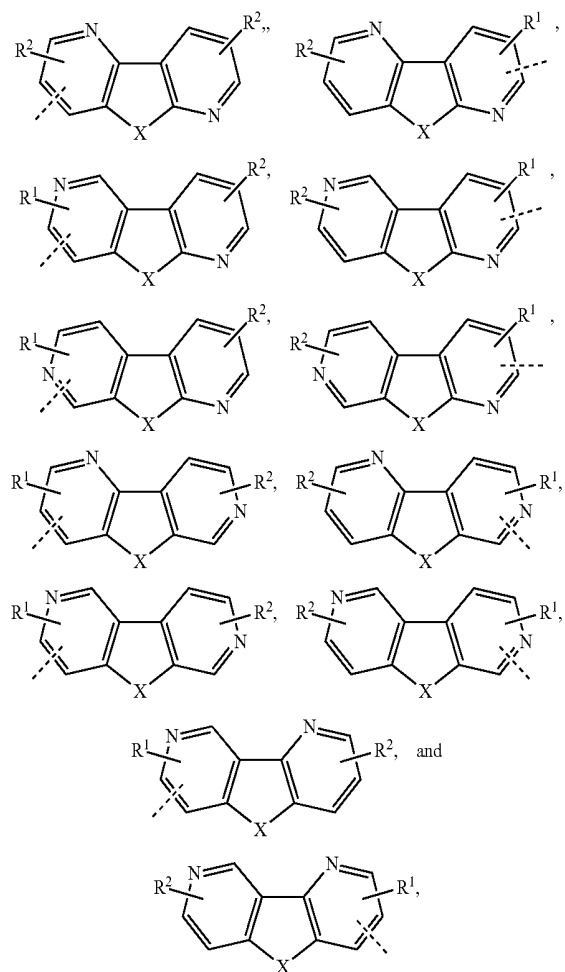
[0070] In one embodiment, X is O or S. In one embodiment, only two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen. In one embodiment, only two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen and on the same ring. In one embodiment, only two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen and on the same ring that is bonded to L.

[0071] In one embodiment, each Z¹, Z², Z³, Z⁴, Z⁵, Z⁶, Z⁷, and Z⁸ is carbon. In one embodiment, R¹, and R² are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, phenyl, pyridyl, carbazolyl, and combinations thereof. In one embodiment, R³, and R⁴ are each independently selected from the group consisting of hydrogen, deuterium, phenyl, pyridyl, 9-carbazolyl, and combinations thereof.

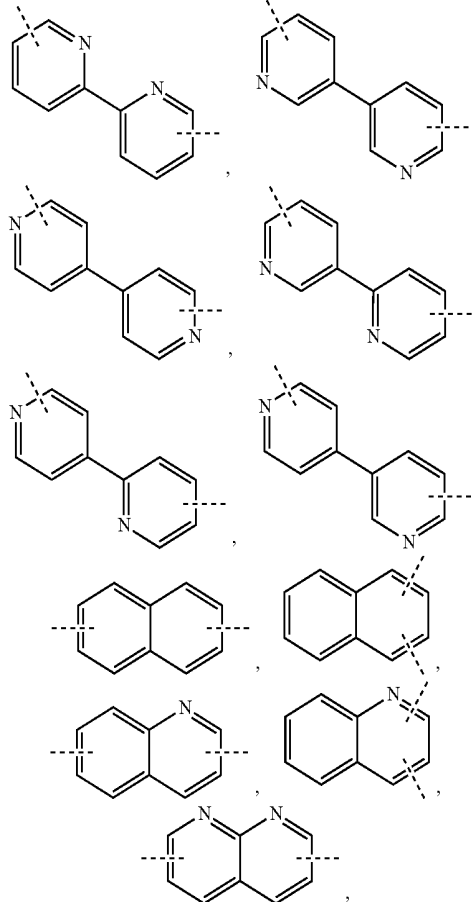
[0072] In another embodiment, G¹ is selected from the group consisting of:



-continued



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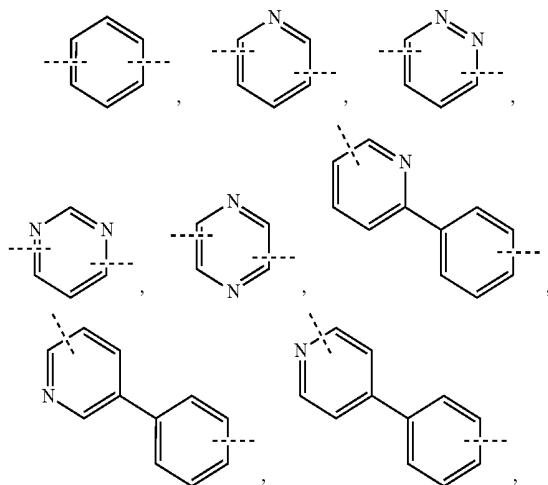
and combinations thereof.

[0074] In another embodiment, G¹ is selected from the group consisting of:

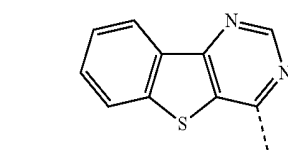
wherein X is selected from the group consisting of O, S, and Se.

[0073] In another embodiment, L is selected from the group consisting of:

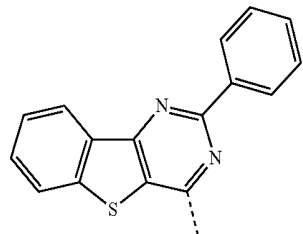
a direct bond,



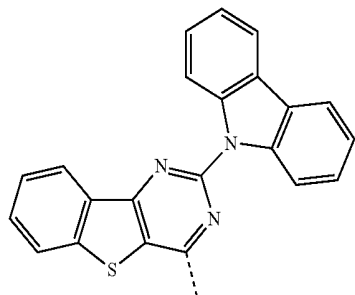
D1



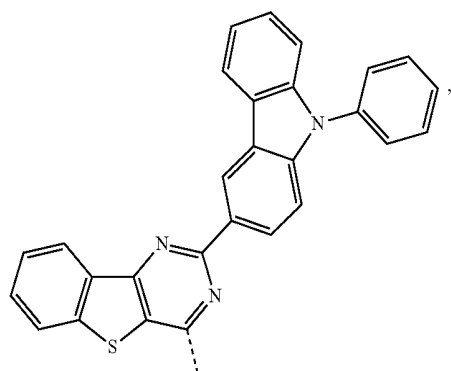
D2



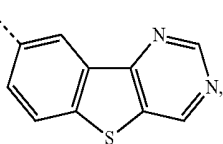
D3



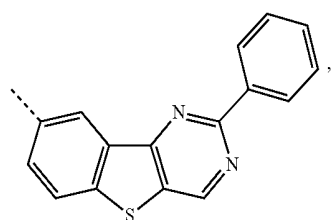
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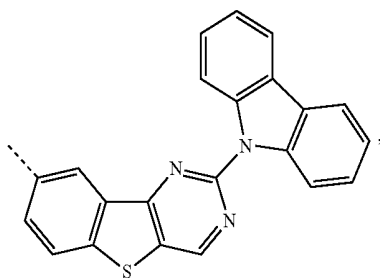
D4



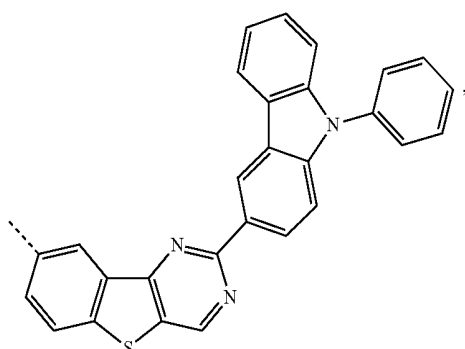
D5



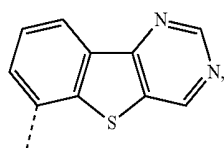
D6



D7

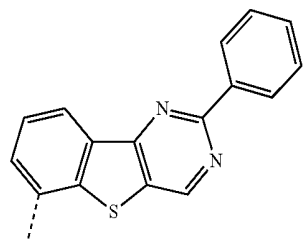


D8

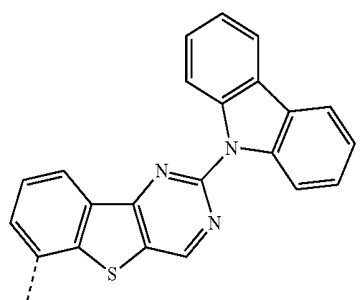


D9

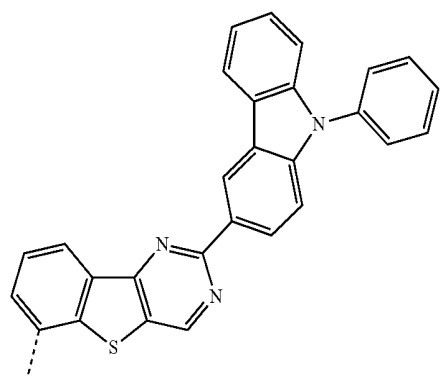
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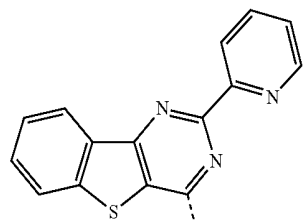
D10



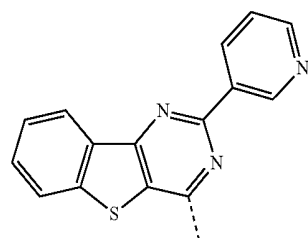
D11



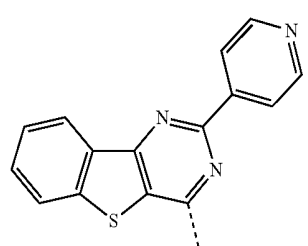
D12



D13

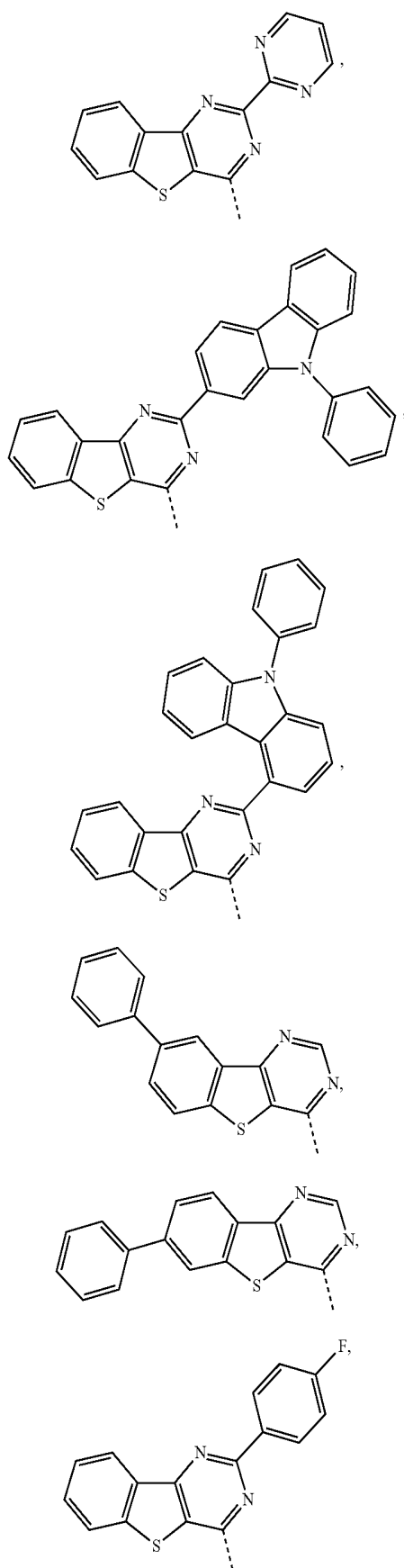


D14



D15

-continued



D16

D17

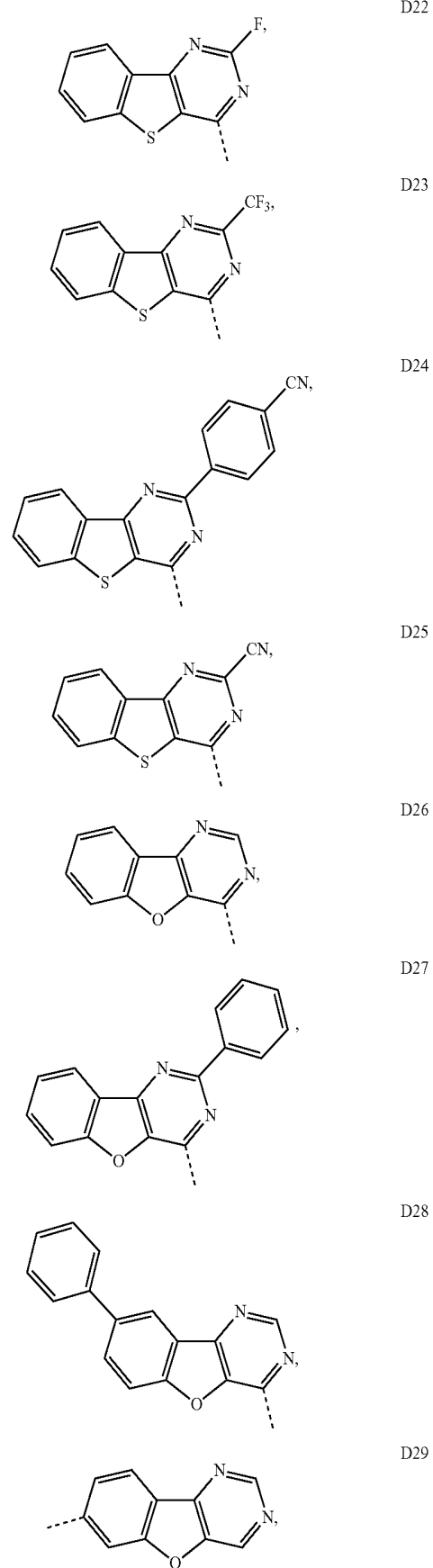
D18

D19

D20

D21

-continued



D22

D23

D24

D25

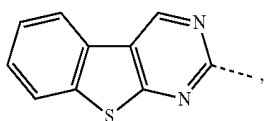
D26

D27

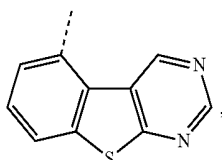
D28

D29

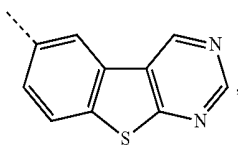
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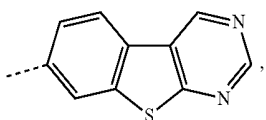
D30



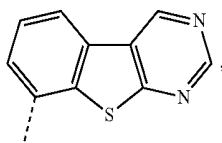
D31



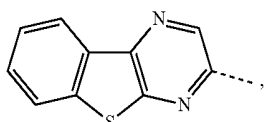
D32



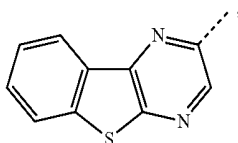
D33



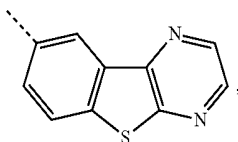
D34



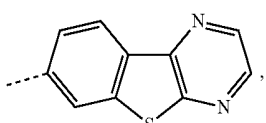
D35



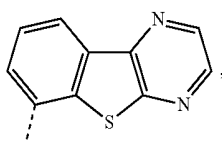
D36



D37

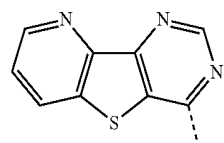


D38

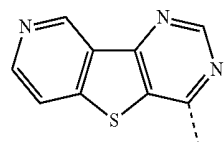


D39

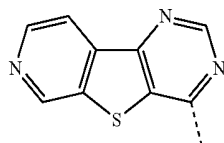
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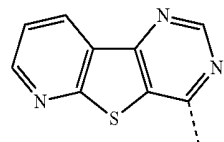
D40



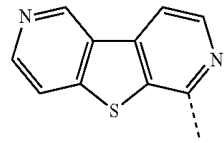
D41



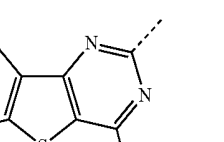
D42



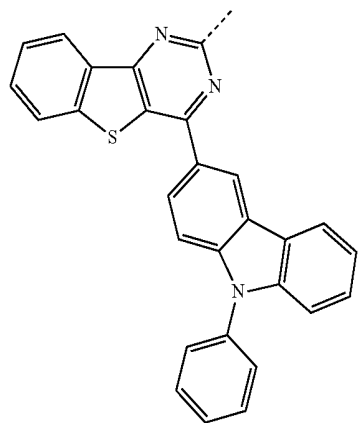
D43



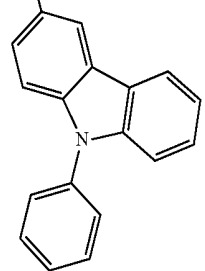
D44



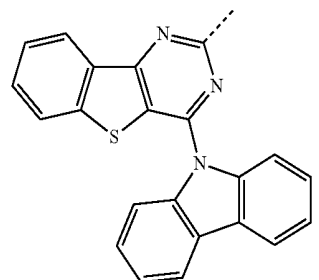
D45



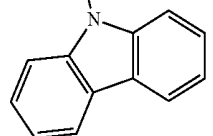
D35



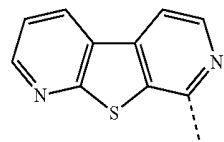
D36



D46

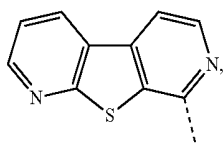


D38

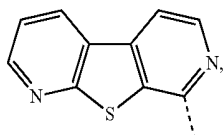


D47

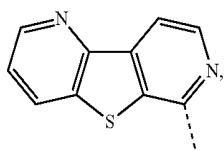
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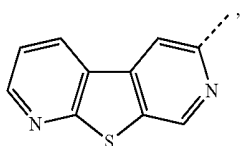
D48



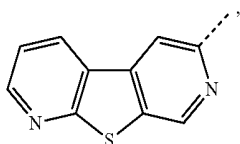
D49



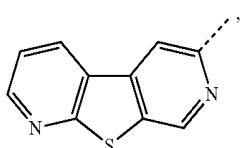
D50



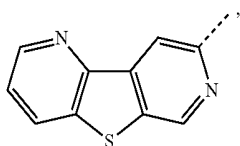
D51



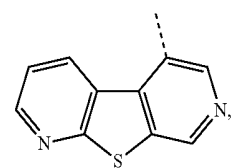
D52



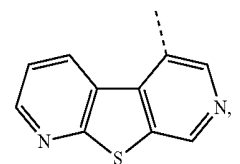
D53



D54

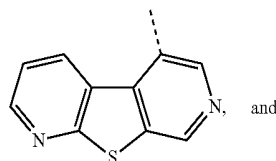


D55

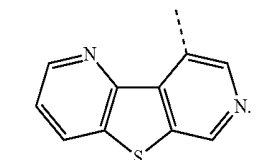


D56

-continued

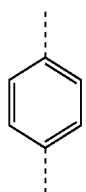


D57

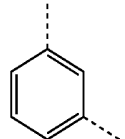


D58

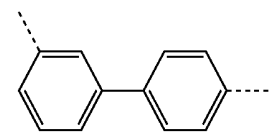
[0075] In another embodiment, L is selected from the group consisting of:
a direct bond (L1),



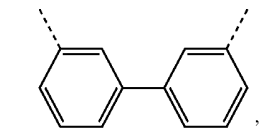
L2



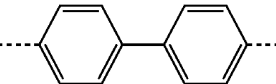
L3



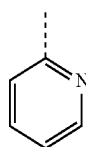
L4



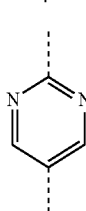
L5



L6

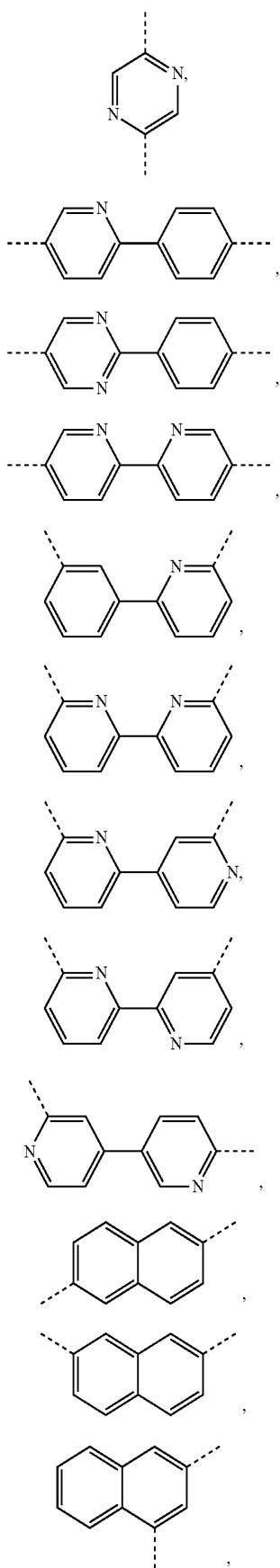


L7

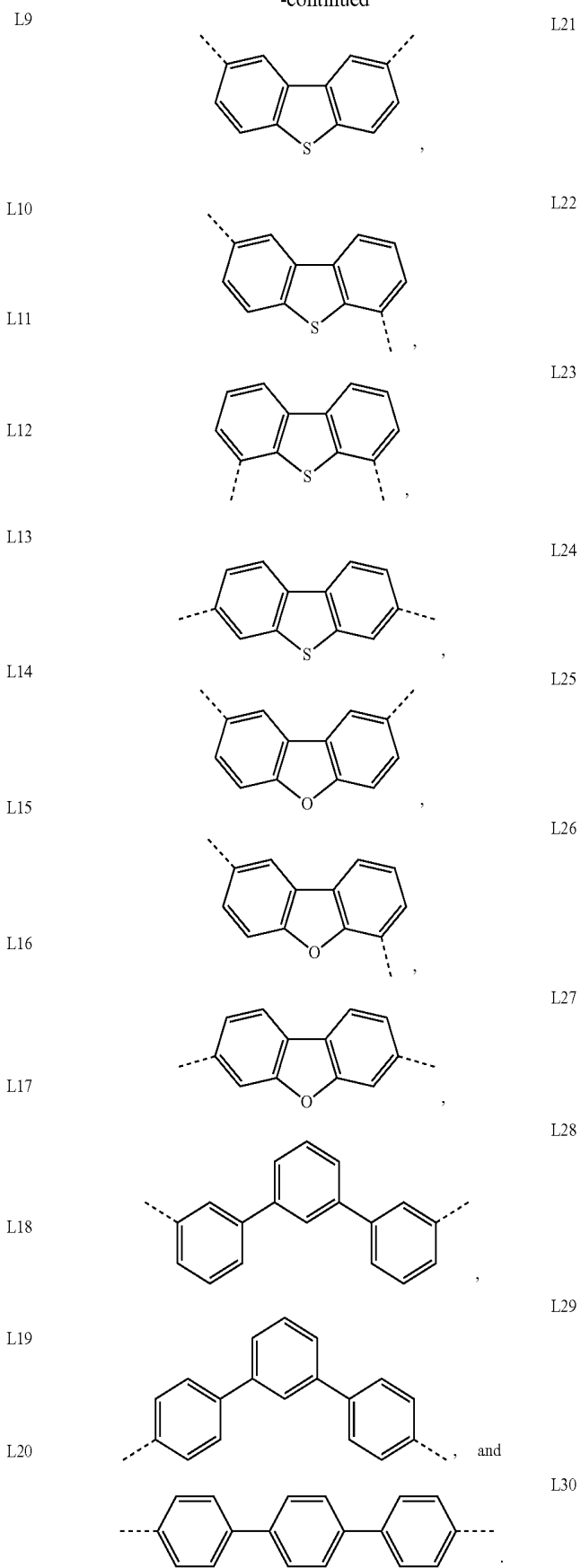


L8

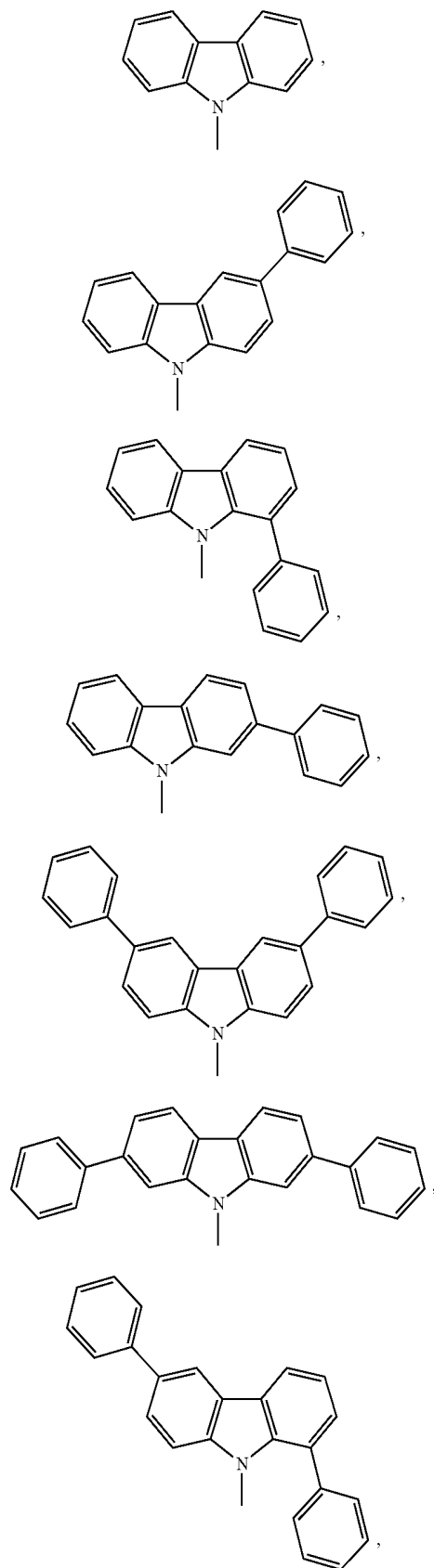
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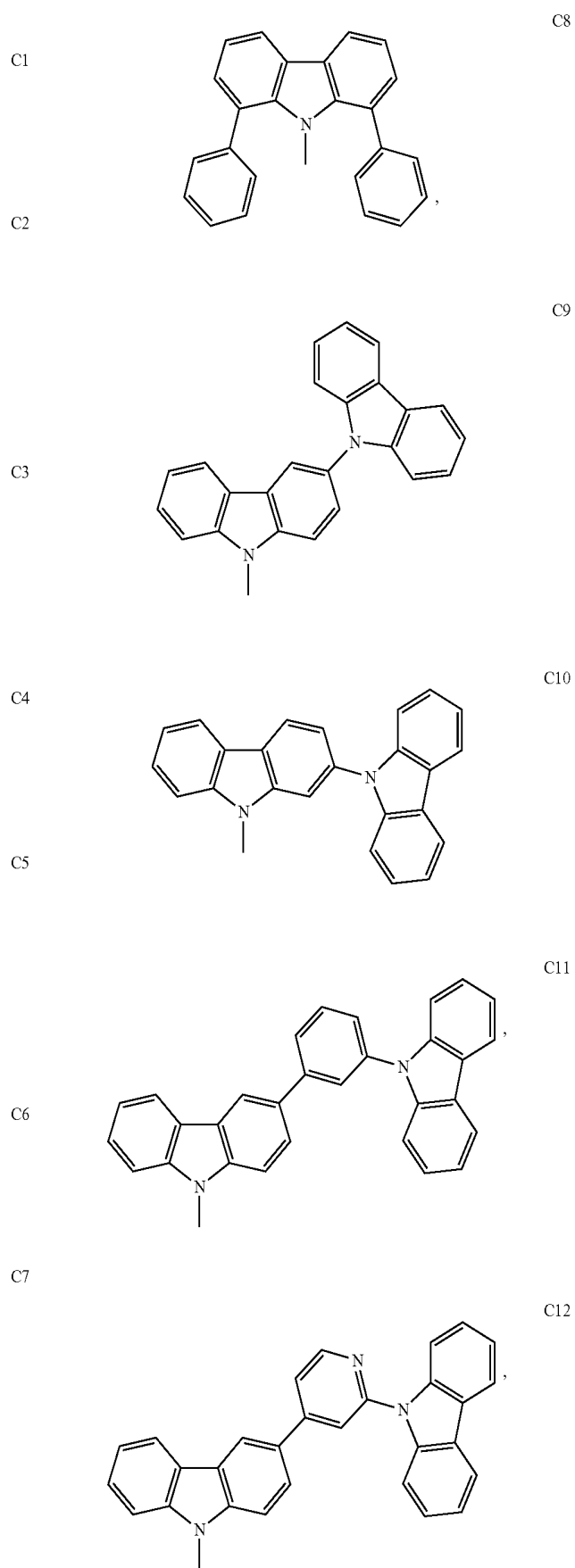
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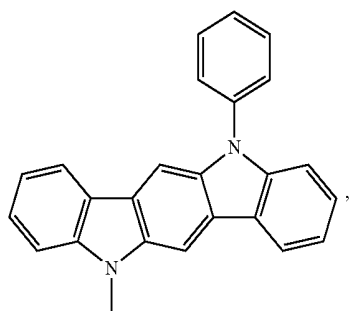
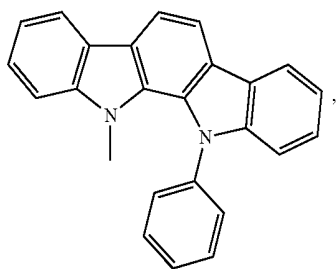
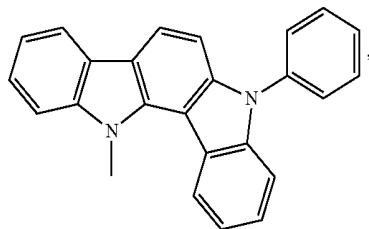
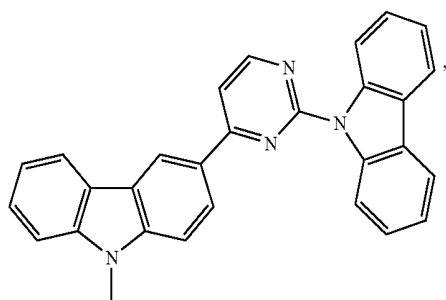
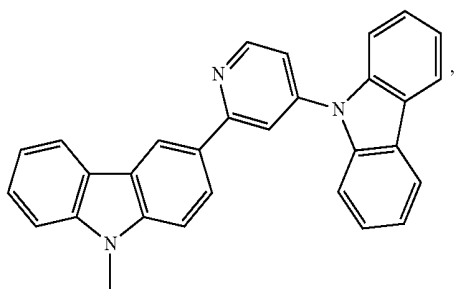
[0076] In another embodiment, G² is selected from the group consisting of:



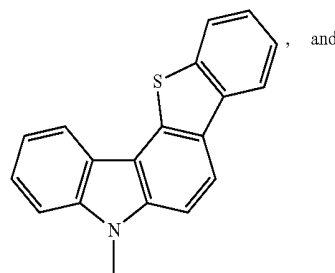
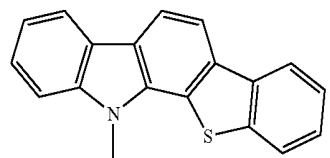
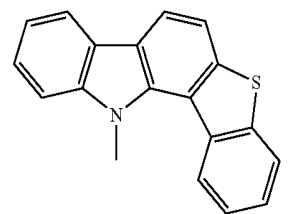
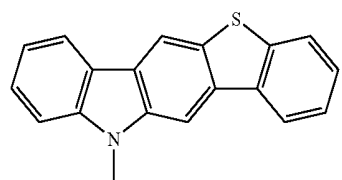
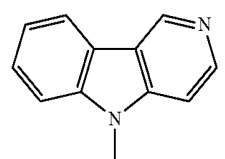
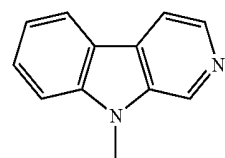
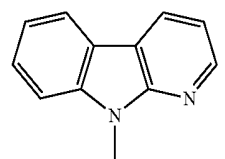
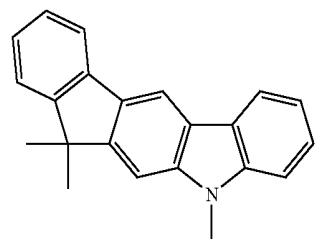
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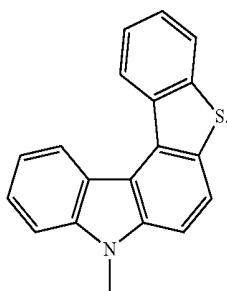


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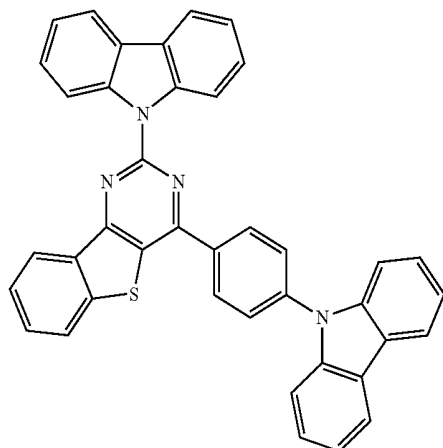
and

-continued



C26

-continued



Compound 61

[0077] According to another embodiment, the novel compound having the formula: G^1-L-G^2 Formula I, is selected from the group of compounds Compound x defined by the formula $Di-L_j-Ck$;

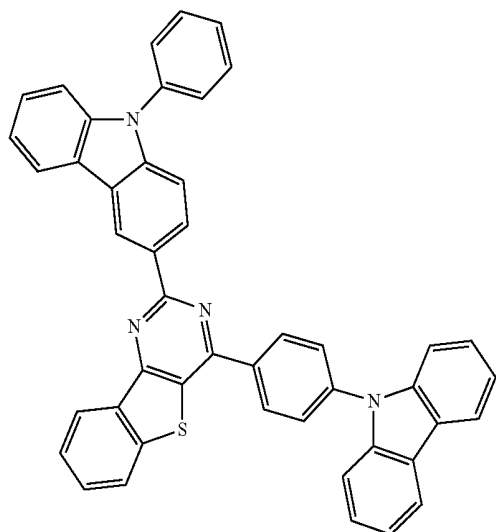
[0078] wherein $x=1740k+58j+i-1798$,

[0079] wherein i is an integer from 1 to 58, j is an integer from 1 to 30, and k is an integer from 1 to 26; and

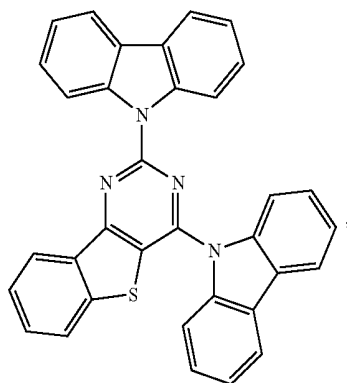
[0080] wherein D1 to D58, L1 to L30, and C1 to C26 have the chemical structures as defined herein.

[0081] According to another embodiment, the novel compound having a formula: G^1-L-G^2 , Formula I, is selected from the group of compounds consisting of:

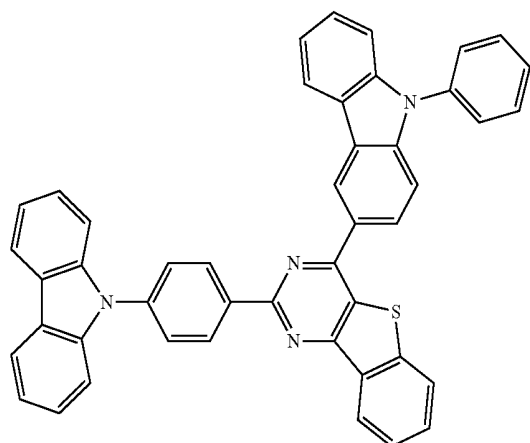
Compound 62



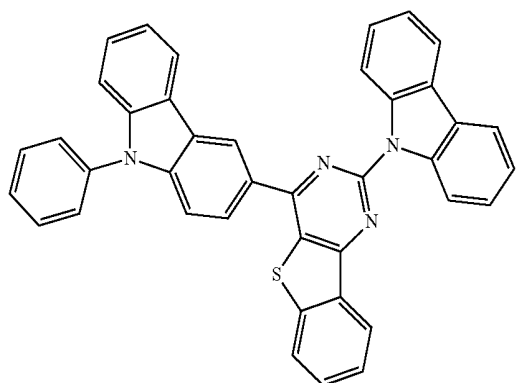
Compound 3



Compound 103

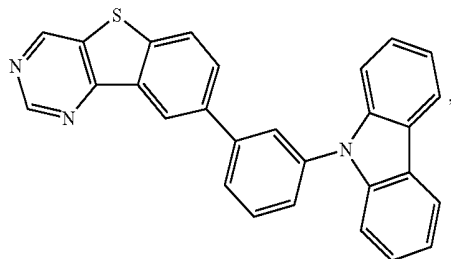


Compound 45



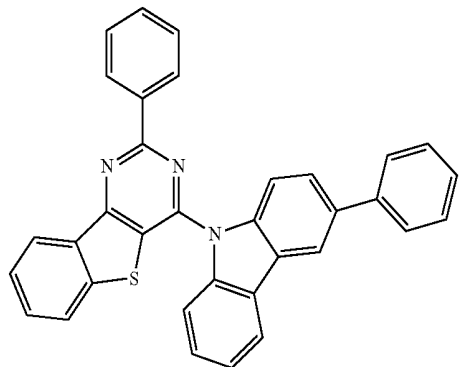
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Compound 121

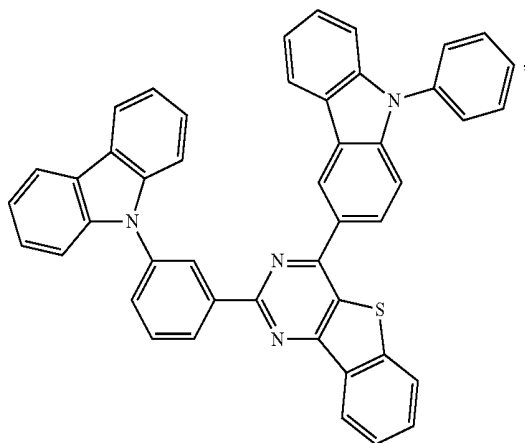


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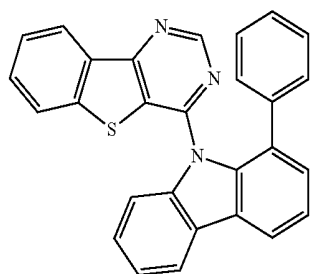
Compound 1742



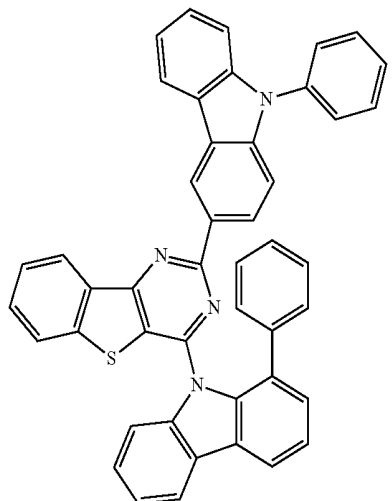
Compound 161



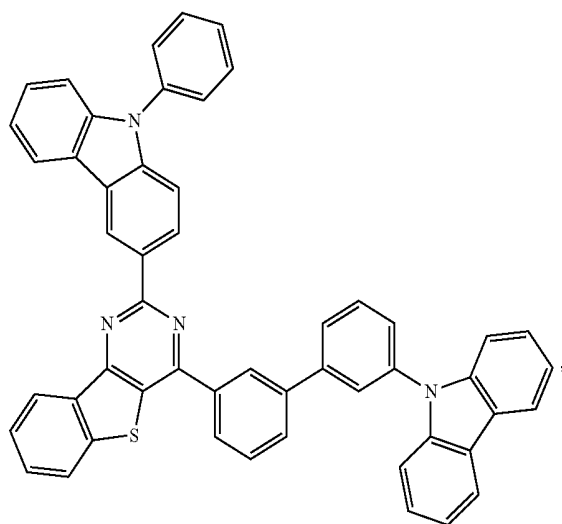
Compound 3481



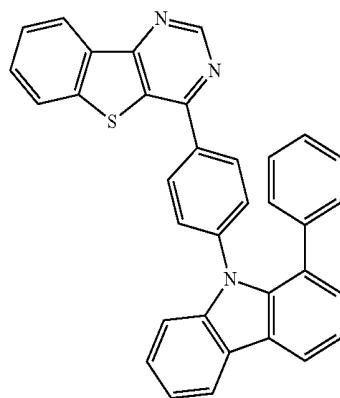
Compound 3484



Compound 236

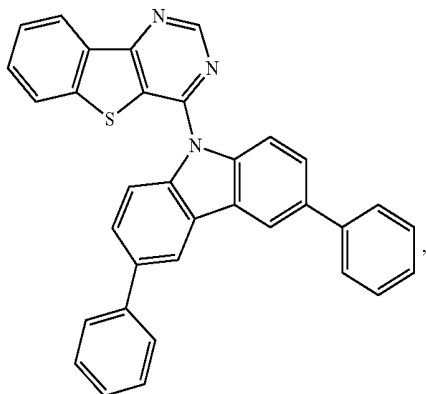


Compound 3539



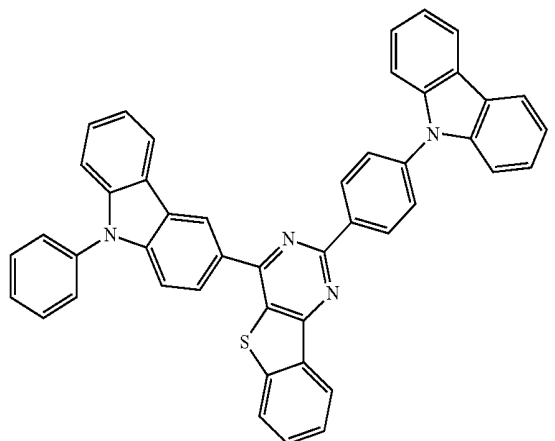
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Compound 6961

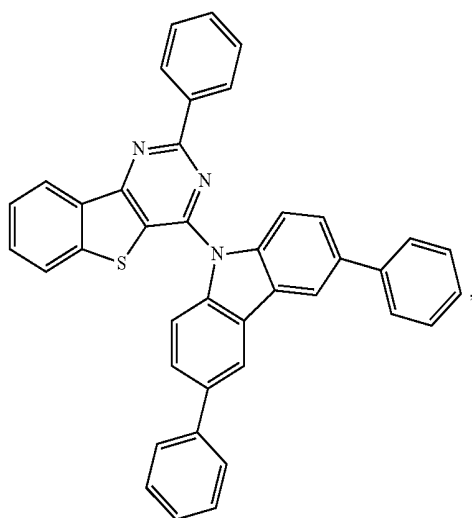


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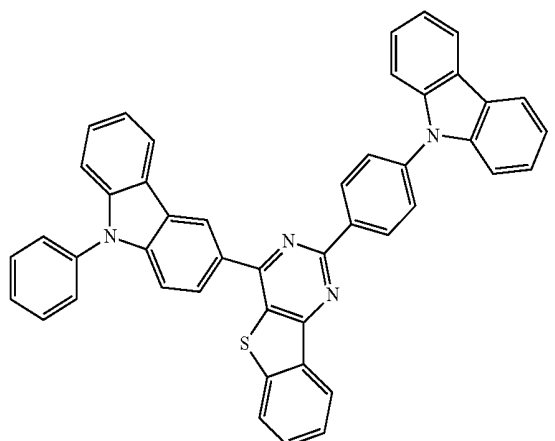
Compound 7063



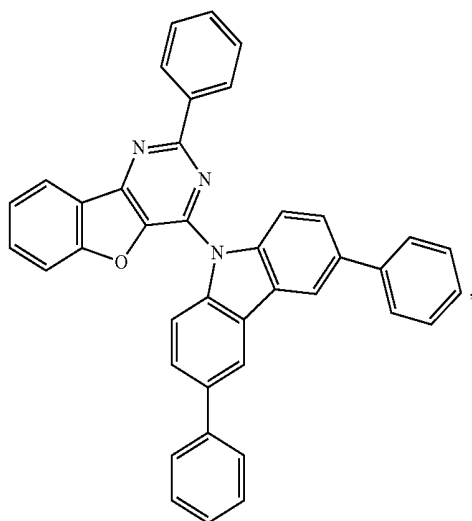
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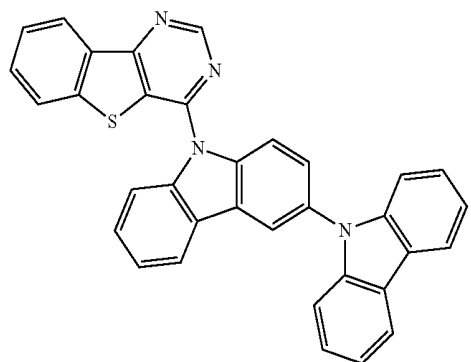
Compound 7121



Compound 6987

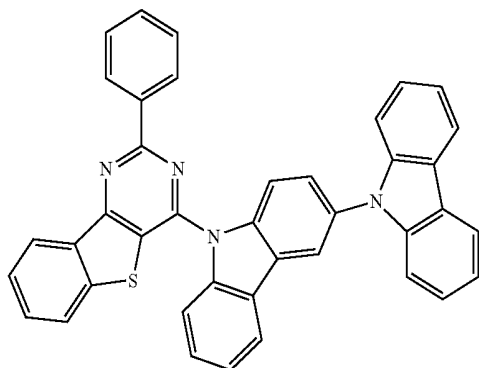


Compound 13921



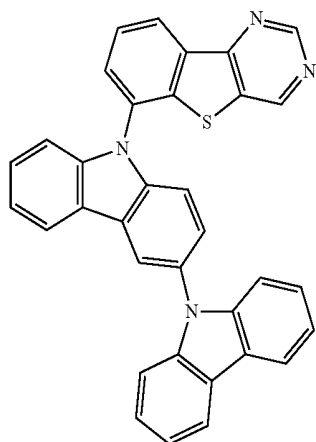
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Compound 13922

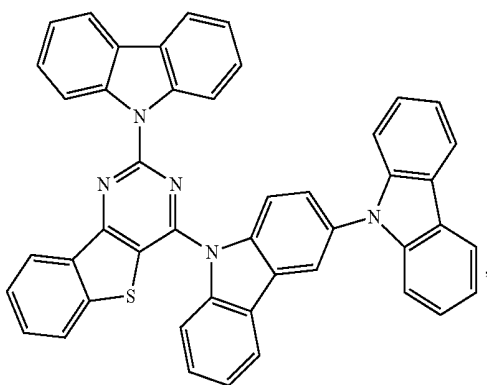


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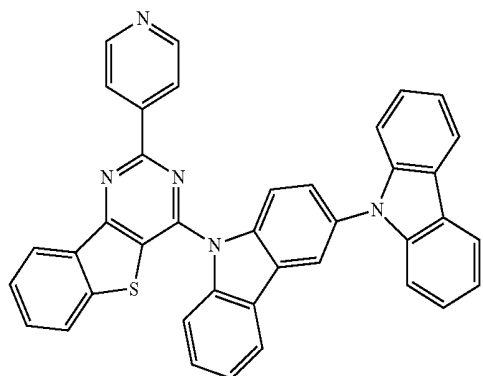
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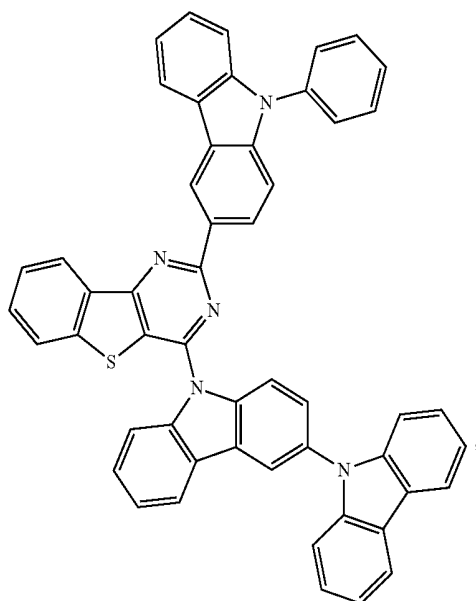
Compound 13923



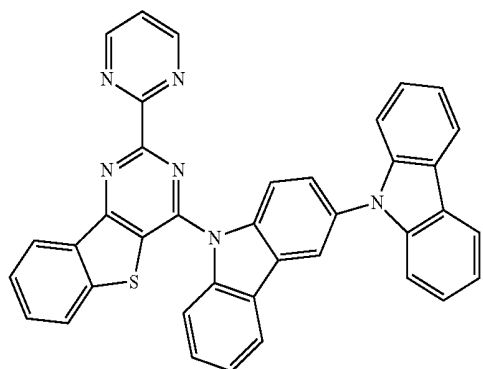
Compound 13935



Compound 13924

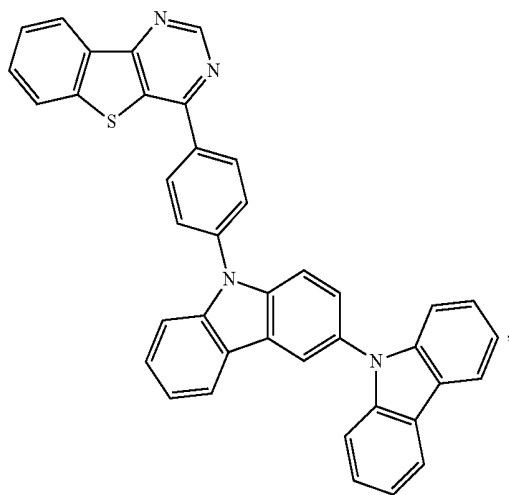


Compound 13936



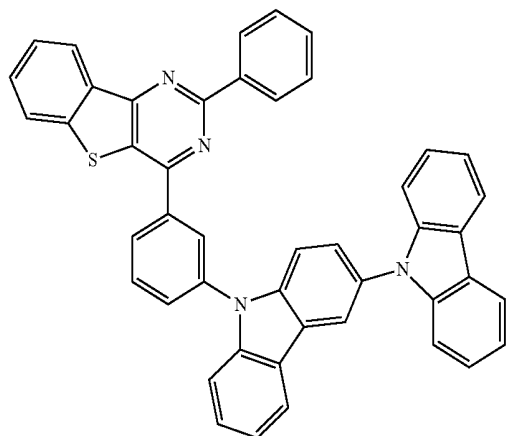
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Compound 13979

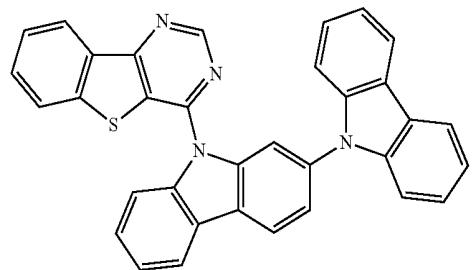


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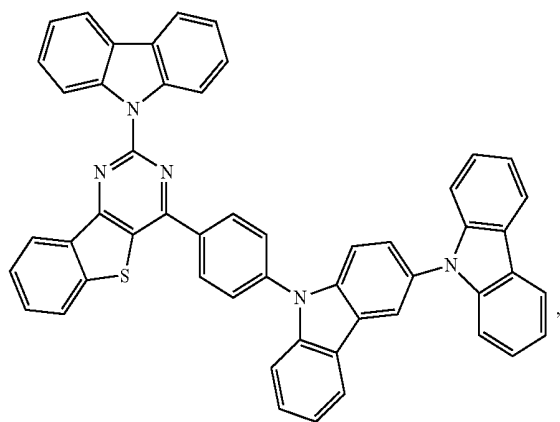
Compound 14038



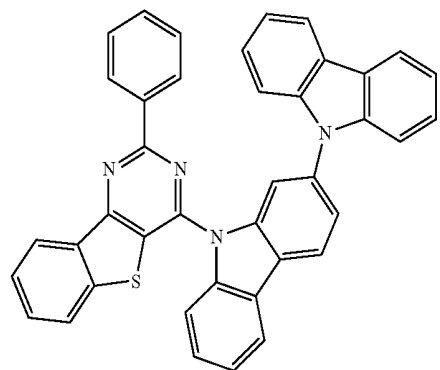
Compound 15661



Compound 13981

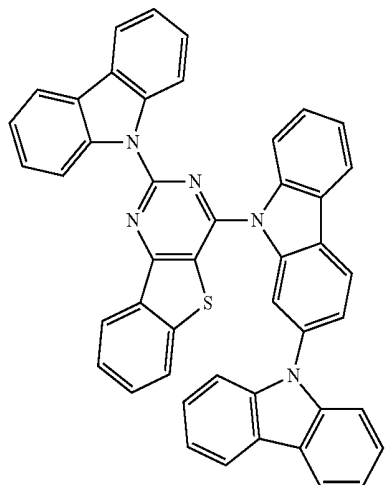
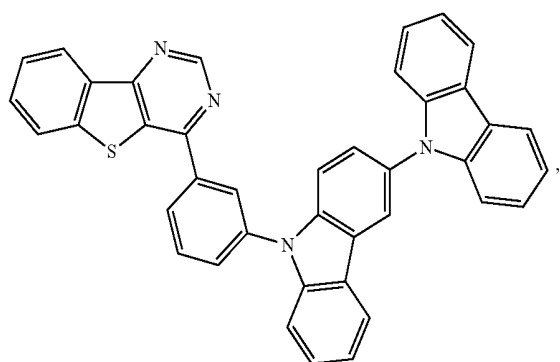


Compound 15662



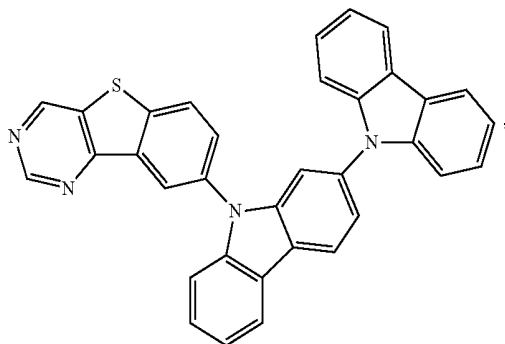
Compound 15663

Compound 14037



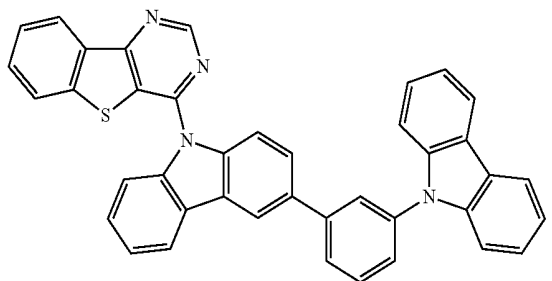
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Compound 15665



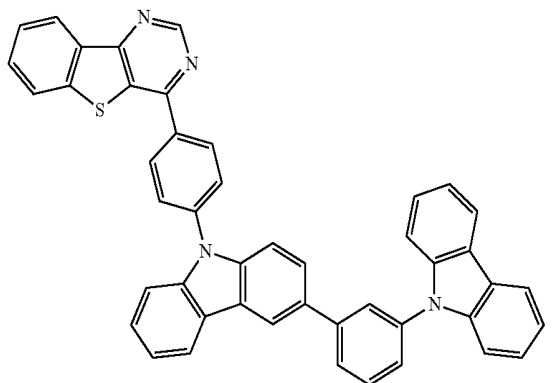
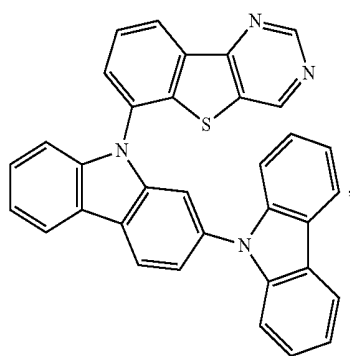
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Compound 17401

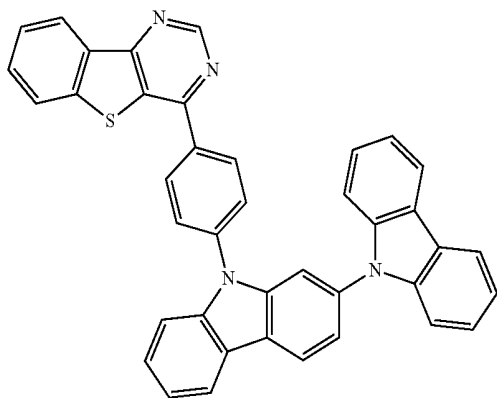


Compound 17459

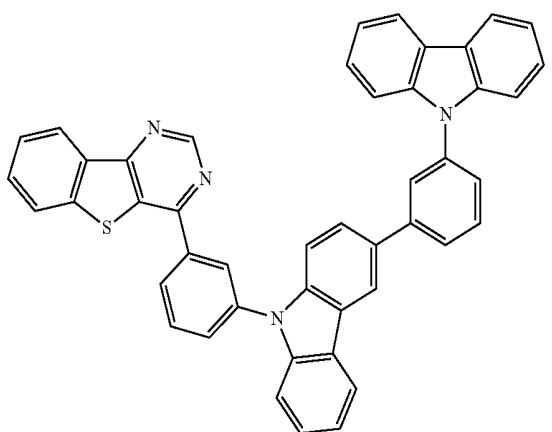
Compound 15669



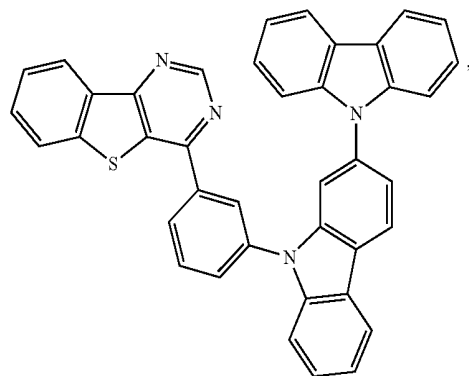
Compound 15719



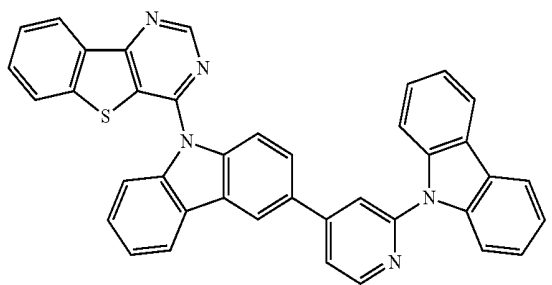
Compound 17517



Compound 15777

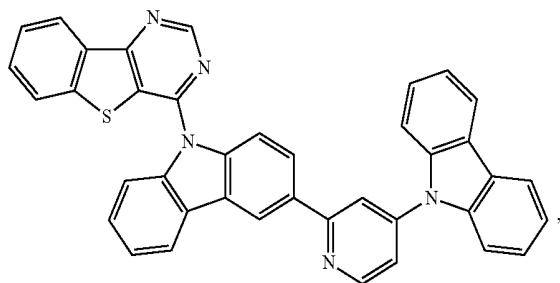


Compound 19141

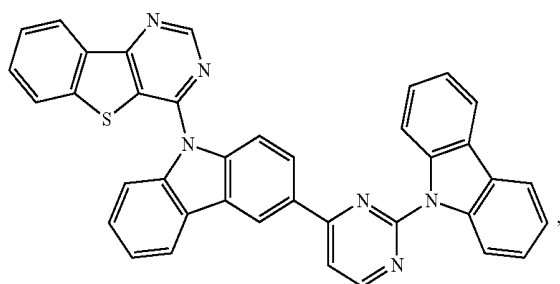


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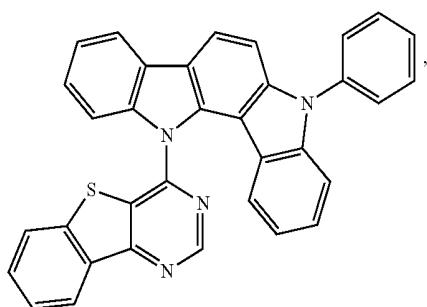
Compound 20881



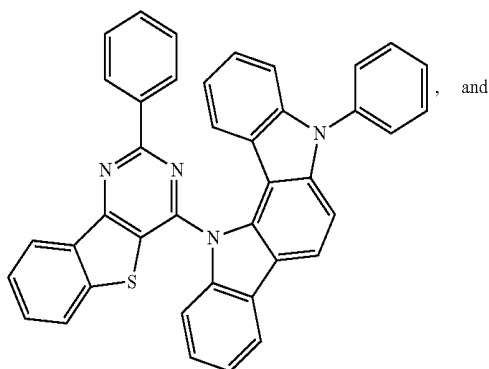
Compound 22621



Compound 24361

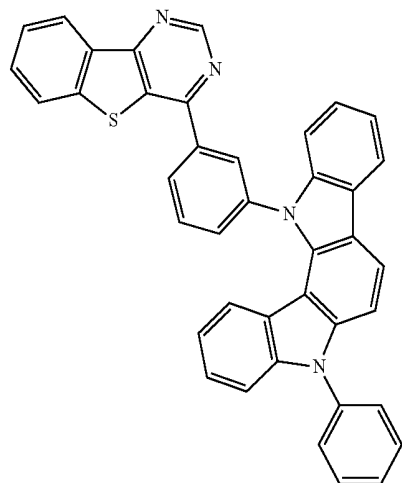


Compound 24362

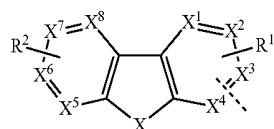


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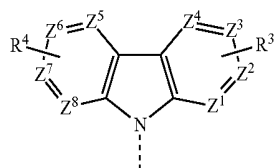
Compound 24477



[0082] According to another aspect of the present disclosure, a first device comprising a first phosphorescent organic light-emitting device is disclosed. The phosphorescent organic light-emitting device comprises an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer comprises a compound having the formula G^1-L-G^2 , Formula I; wherein G^1 has the structure:



and
 G^2 has the structure:



[0083] wherein L is selected from the group consisting of a direct bond, an aryl group having from 6-30 carbon atoms, a heteroaryl group having from 3-30 carbon atoms, and combinations thereof; wherein the aryl group and the heteroaryl group are optionally further substituted with one or more groups 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;

[0084] wherein X is selected from the group consisting of O, S, and Se;

[0085] wherein each of $X^1, X^2, X^3, X^4, X^5, X^6, X^7, X^8, Z^1, Z^2, Z^3, Z^4, Z^5, Z^6, Z^7,$ and Z^8 is carbon or nitrogen;

[0086] wherein at least two of X^1 , X^2 , X^3 , X^4 , X^5 , X^6 , X^7 , and X^8 are nitrogen;

[0087] wherein at least one of X^1 , X^2 , X^3 , and X^4 is carbon and bonded to L;

[0088] wherein the dashed lines represent the bonds between G^1 and L and between G^2 and L;

[0089] wherein each R^2 , R^3 , and R^4 represent mono, di, tri, tetra substitutions or no substitution;

[0090] wherein R^1 represents mono, di, tri substitutions or no substitution;

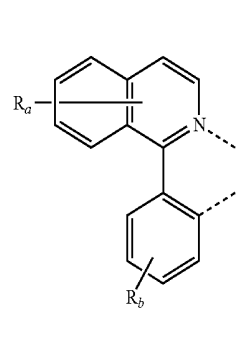
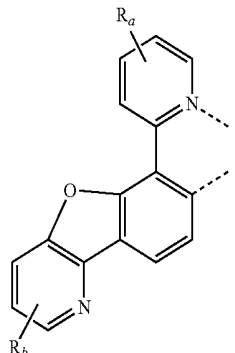
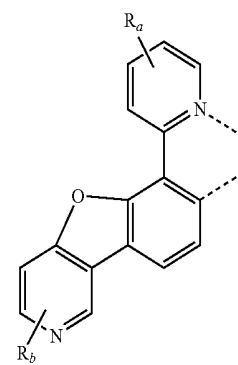
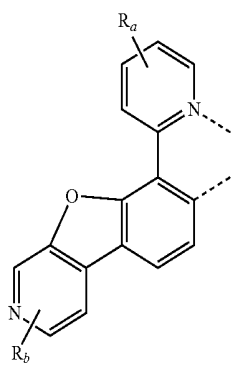
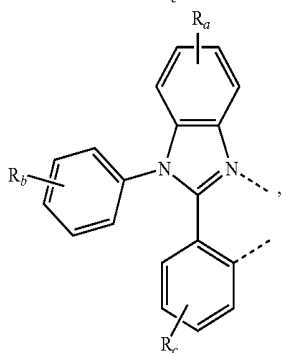
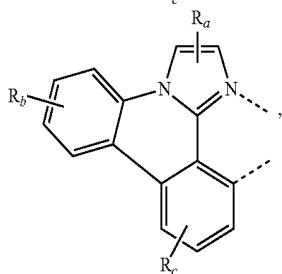
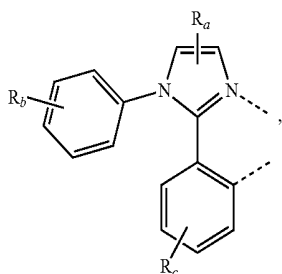
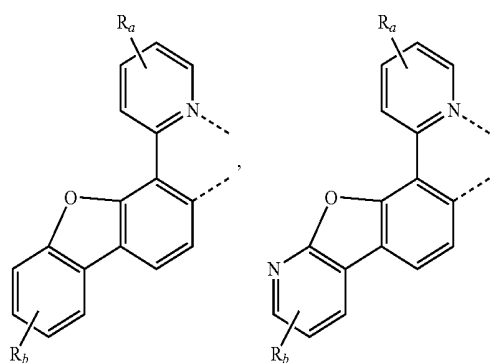
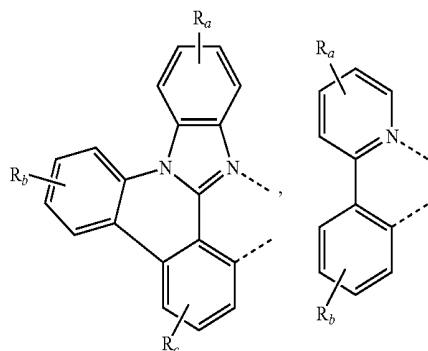
[0091] wherein R^1 , R^2 , R^3 , and R^4 are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkenyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

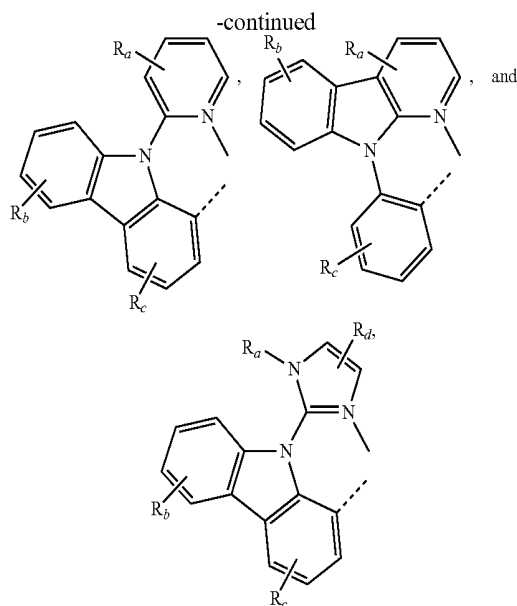
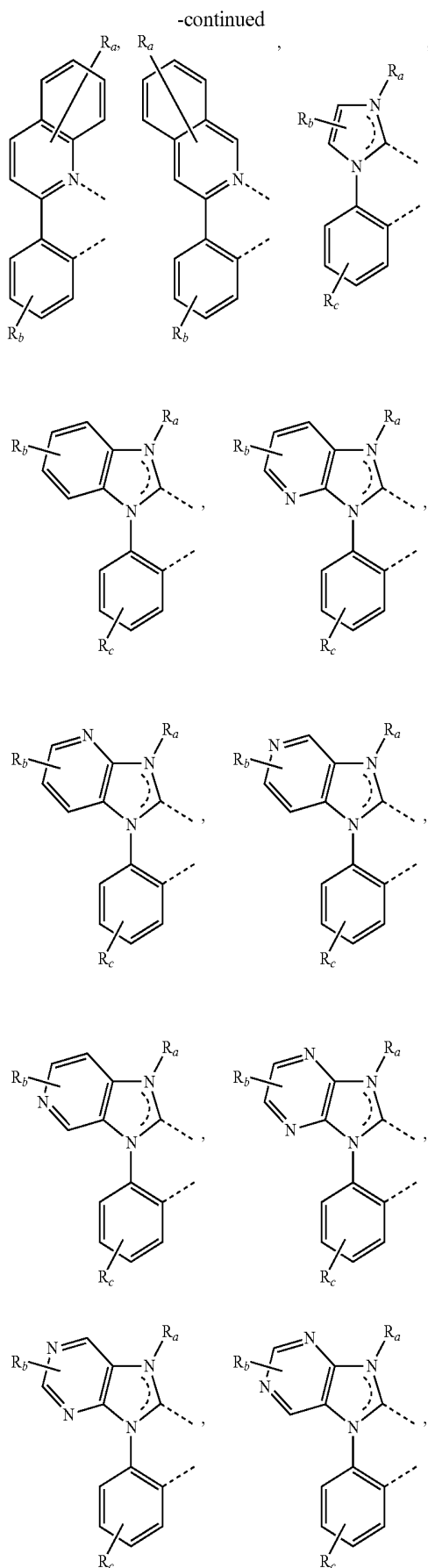
[0092] wherein the substitution is optionally fused to G^1 or G^2 ; and

[0093] wherein when R^3 or R^4 is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G^2 by N.

[0094] In one embodiment of the first device, the organic layer is an emissive layer and the compound of Formula I is a host. In an embodiment, the organic layer further comprises a phosphorescent emissive dopant. In an embodiment, the phosphorescent emissive dopant is a transition metal complex having at least one ligand selected from the group consisting of:

-continued





[0095] wherein R_a , R_b , R_c , and R_d may represent mono, di, tri, or tetra substitution, or no substitution;

[0096] wherein R_a , R_b , R_c , and R_d are 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 two adjacent substituents of R_a , R_b , R_c , and R_d are optionally joined to form a fused ring or form a multidentate ligand.

[0097] In one embodiment of the first device, the organic layer is a blocking layer and the compound is a blocking material in the organic layer. In another embodiment, the organic layer is an electron transporting layer and the compound is an electron transporting material in the organic layer.

[0098] In one embodiment of the first device, the first device is a consumer product. In another embodiment, the first device is an organic light-emitting device. In another embodiment, the first device can comprise a lighting panel.

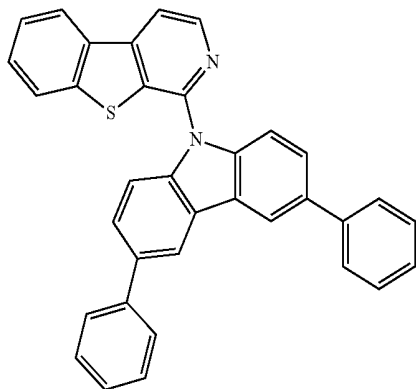
[0099] According to another aspect of the present disclosure, a formulation comprising the compound having the formula G^1 -L- G^2 , Formula I, is disclosed, wherein G^1 , L, and G^2 are as defined above.

[0100] The novel compounds described in this disclosure were used as electron-transporting hosts in the emissive layer of an organic light-emitting device. The molecules of the compounds have two parts: an electron rich part (the substituted or non-substituted carbazole) and an electron poor part (benzothienopyrimidines or benzofurans). Such dual, bipolar, character of the novel compound improves their electron-conducting properties and, thus, the compounds are useful as electron-conducting hosts in red, green, yellow, and white OLED devices. Aza-debenzothiophenes and aza-benzofurans have been used as host materials in phosphorescent OLED devices, however, analogs with two N atoms in one cycle is not known. It is believed that two nitrogen atoms will further lower the LUMO level and provide better stabilized LUMO; as a result such molecules may be more stable to electrons and may have better electron-carrier properties than the analogs with one nitrogen atom. Synthetic approaches to such compounds were widely studied in organic chemistry for preparation of drugs and pesticides. Thus, one can synthesize a variety of diazadibenzothiophenes and diazadibenzofurans with different substituents. Such substituents allow tuning of electronic properties of the material (HOMO, LUMO, etc.) and their physicochemical properties such as T_D , T_G , etc.

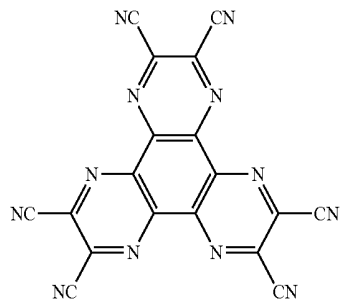
Experimental Results

[0101] The inventors have verified the benefits of the inventive compounds disclosed herein by fabricating experimental OLED devices. Example devices were made using the inventive compounds Compound 3, Compound 45, Compound 6961, and Compound 24361 disclosed herein as the host material in the emissive layer. A comparative device was made using Comparison Compound 1 shown below:

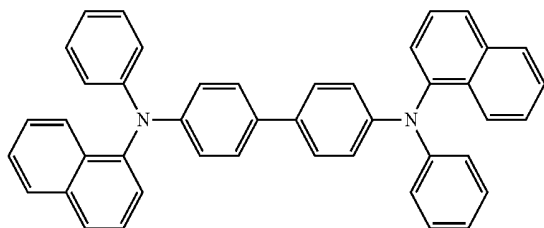
Comparison Compound 1



[0102] HAT-CN was used for hole injection layer ("HIL"). NPD was used for hole transporting layer ("HTL"). Alq₃ was used for electron transporting layer ("ETL").

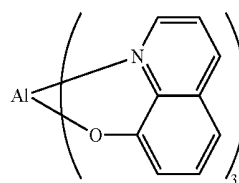


HIL(HAT-CN)



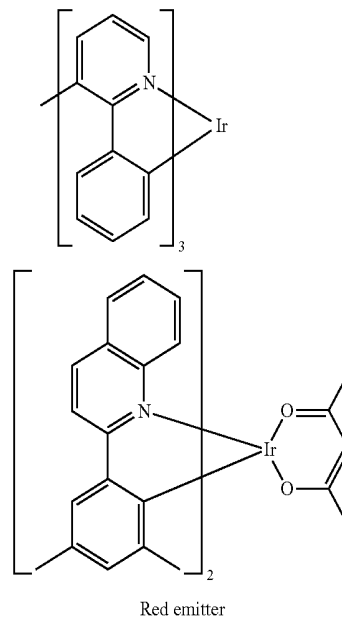
HTL (NPD)

-continued

ETL (Alq₃)

[0103] The compounds used for the hole transporting co-host and red emitter in the emissive layer are shown below.

Compound H



Red emitter

[0104] The organic stack of the Example devices and the Comparative device were fabricated with the following structure: from the ITO surface, 100 Å of HAT-CN as the hole injection layer (HIL), 400 Å of NPD as the hole transporting layer (HTL), 300 Å of the emissive layer (EML) which contains the Host (79%), Compound H (18%), and Red emitter (3%), 100 Å host compound as blocking layer, 550 Å of Alq₃ as the electron transporting layer (ETL) and 10 Å of LiF as the electron injection layer (EIL). The experimental device performance data is presented in Table 1 below.

TABLE 1

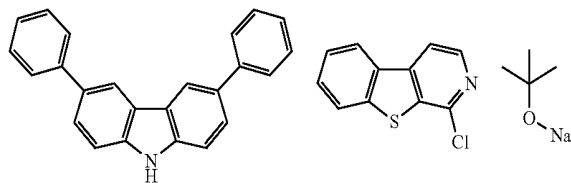
Device performances of the novel host compounds vs. Comparison Compound 1		1931 CIE		At 1,000 nits		At 80 mA/cm ²			
Host	BL	CIE x	CIE y	Voltage %	LE %	EQE %	L ₀ %	LT95% %	
Example Device 1	Compound 3	Compound 3	0.661	0.338	90	122	123	117	288
Example Device 2	Compound 45	Compound 45	0.659	0.340	78	110	112	111	489

TABLE 1-continued

Device performances of the novel host compounds vs. Comparison Compound 1		1931 CIE		At 1,000 nits			At 80 mA/cm ²	
Host	BL	CIE x	CIE y	Voltage %	LE %	EQE %	L ₀ %	LT95% %
Example Device 3	Compound 6961	Compound 6961	0.660 0.339	71	139	136	132	455
Example Device 4	Compound 24361	Compound 24361	0.655 0.343	66	127	121	124	111
Comparison Device	Comparison Compound 1	Comparison Compound 1	0.654 0.343	100	100	100	100	100

[0105] Except for the 1931 CIE coordinates, Table 1 presents relative values using the Comparison Device as the reference, whose relative performance represents 100%. As one can see, all Example Devices 1-4 exhibited superior voltage, luminous efficiency (LE), and external quantum efficiency (EQE) at 1,000 nits. The device operation lifetime measurements were performed at a constant de current of 80 mA/cm² at room temperature with light output monitored as a function of time. La is the initial luminance of the operational lifetime measurement. The operational lifetimes defined at 95% of the initial luminance (LT95%) were shown in the table 1. All Example Devices 1-4 exhibited superior L₀ and LT95 compared to the comparison device.

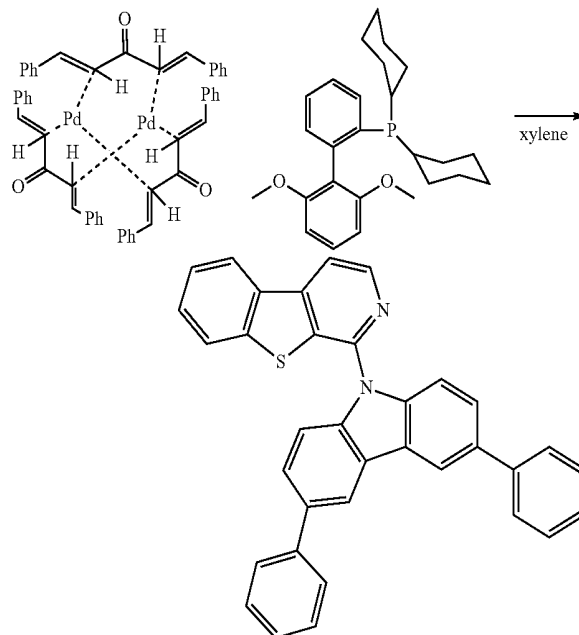
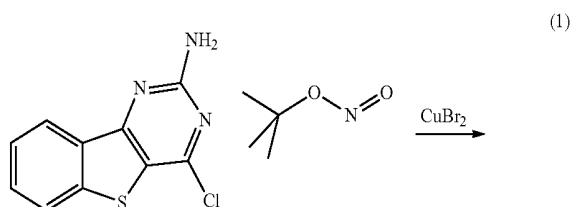
[0106] Synthesis of the Comparison Compound 6961



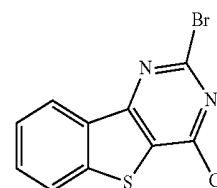
3,6-Diphenyl-9H-carbazole (2.000 g, 6.26 mmol) and 1-chlorobenzo[4,5]thieno[2,3-c]pyridine (1.376 g, 6.26 mmol) were dissolved in xylene (150 ml), then sodium 2-methylpropanoate (1.204 g, 12.52 mmol), Pd₂(dba)₃ (120 mg) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.129 g, 0.313 mmol) were added to the reaction solution. The reaction solution was degassed and heated to reflux under N₂ atm. overnight. Then it was cooled down to room temperature, filtered through celite pad and evaporated. The residue was subjected to column chromatography on silica gel, eluted with hexane/DCM 9/1 to 1/1 (v/v) gradient mixture, providing white solid, which was crystallized from

hexane/DCM. 1-(3,6-Diphenyl-9H-carbazol-9-yl)benzo[4,5]thieno[2,3-c]pyridine to form white crystals of the Comparison Compound 6961 (2.7 g, 5.37 mmol, 86% yield).

[0107] Synthesis of the Novel Compound 3

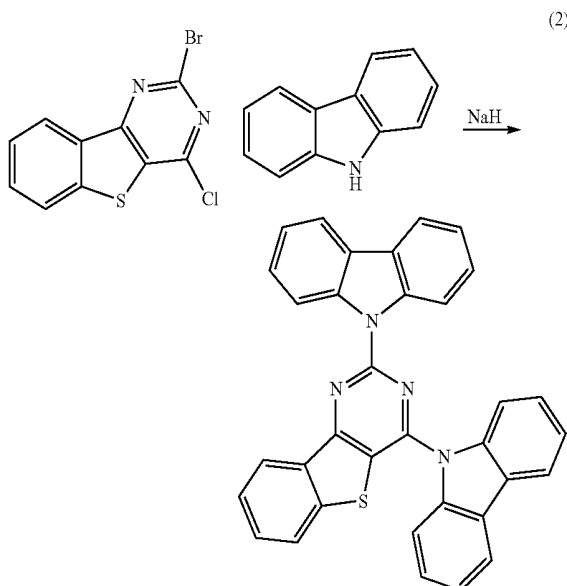


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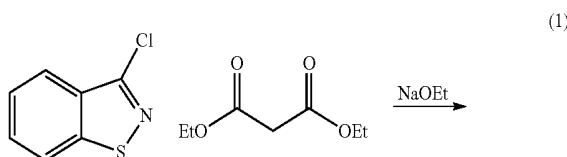
(1) Copper(II) bromide (11.30 g, 50.6 mmol) and tert-butyl nitrite (8.36 ml, 63.3 mmol) were suspended in 170 mL of

acetonitrile and heated to 65° C. 4-Chlorobenzo[4,5]thieno [3,2-d]pyrimidin-2-amine (9.9 g, 42.2 mmol) was added in portions to the reaction solution over the course of 5 minutes and stirred for 30 minutes at 70° C. The reaction solution was cooled to room temperature, quenched with 1M HCl, then filtered and washed with water. The resulting solids were basified with 10% NaOH, extracted 5× with DCM. Acidic aqueous extracted 3× with DCM and combined with other organics. The organic layer was dried over sodium sulfate, filtered and concentrated. The concentrate was redissolved in CHCl₃, washed with 10% NaOH, dried filtered and concentrated to 9.4 g yellow solids. The yellow solids were purified by passing through a plug of Celite/silica with hot toluene then concentrated to 8.7 g (69%) of the 2-bromo-4-chlorobenzo[4,5]thieno[3,2-d]pyrimidine as yellow solid.

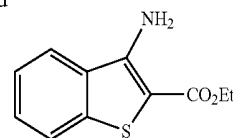


(2) A 250 mL RBF was dried under vacuum and charged with 9H-carbazole (2.79 g, 16.69 mmol) and anhydrous DMF (33 mL). Sodium hydride (0.801 g, 20.03 mmol) was added cautiously to the reaction solution, and stirred until the evolution of hydrogen had stopped. 2-bromo-4-chlorobenzo[4,5]thieno [3,2-d]pyrimidine (2.0 g, 6.68 mmol) was added in one portion to the reaction solution causing an immediate color change from yellow to red. After stirring for ~5 minutes the reaction solution became an unstirring orange suspension then 15 mL of DMF was added to make a thick, stirrable suspension. After ~1 hr, the suspension was quenched with water, filtered and washed with water and EtOH, providing 3.25 g of the 2,4-di(9H-carbazol-9-yl)benzo[4,5]thieno[3,2-d]pyrimidine as off-white solids. The solids were recrystallized twice from toluene and dried in vacuo overnight at 50° C. provided 2.15 g (62% yield) of Compound 3.

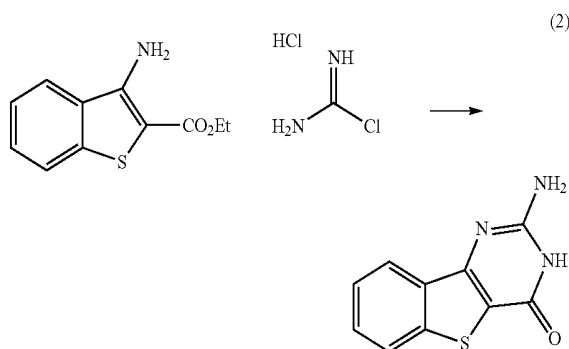
[0108] Synthesis of the Novel Compound 45



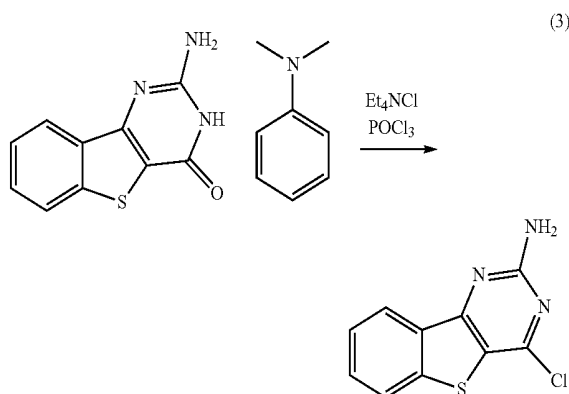
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(1) A dry 2-neck 500 mL RBF was charged with 21% sodium ethanolate (46.2 ml, 124 mmol), diluted with 151 mL absolute EtOH, cooled in an ice bath and treated dropwise with diethyl malonate (18 mL, 118 mmol) under an atmosphere of nitrogen. After stirring for 20 minutes, the ice bath was removed and 3-chlorobenzo[d]isothiazole (20.0 g, 118 mmol) was added in one portion and stirred for 24 hours. The reaction solution was quenched with water, extracted with ether and treated with excess 4M HCl/dioxane. The resulting pinkish-white precipitate was filtered off, suspended in water, basified with Na₂CO₃, extracted with ether, washed with water and brine, dried over sodium sulfate, filtered and concentrated to yellow solids (~20 g) which were recrystallized from ethanol/water and dried in a vacuum oven at 60° C. for 3 hrs affording 19.9 g (76% yield) of the ethyl 3-aminobenzo [b]thiophene-2-carboxylate.

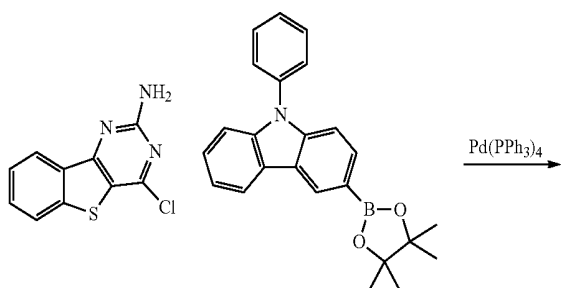
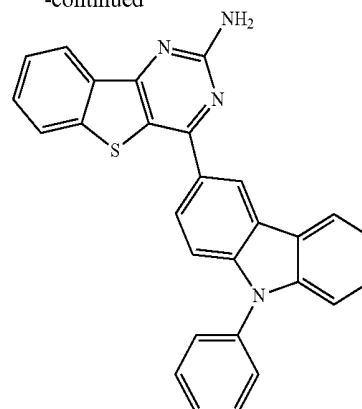


(2) Ethyl 3-aminobenzo[b]thiophene-2-carboxylate (10 g, 45.2 mmol), and carbamimidic chloride hydrochloride (7.27 g, 63.3 mmol) in diglyme (90 mL) were heated to 160° C. for 12 hrs. The reaction solution was cooled to room temperature, filtered, washed with ether and hexanes and dried in vacuo for 3 hrs yielding 10.56 g (108% yield) of crude grey solids of the 2-aminobenzo[4,5]thieno[3,2-d]pyrimidin-4(3H)-one. Used as is without further purification.



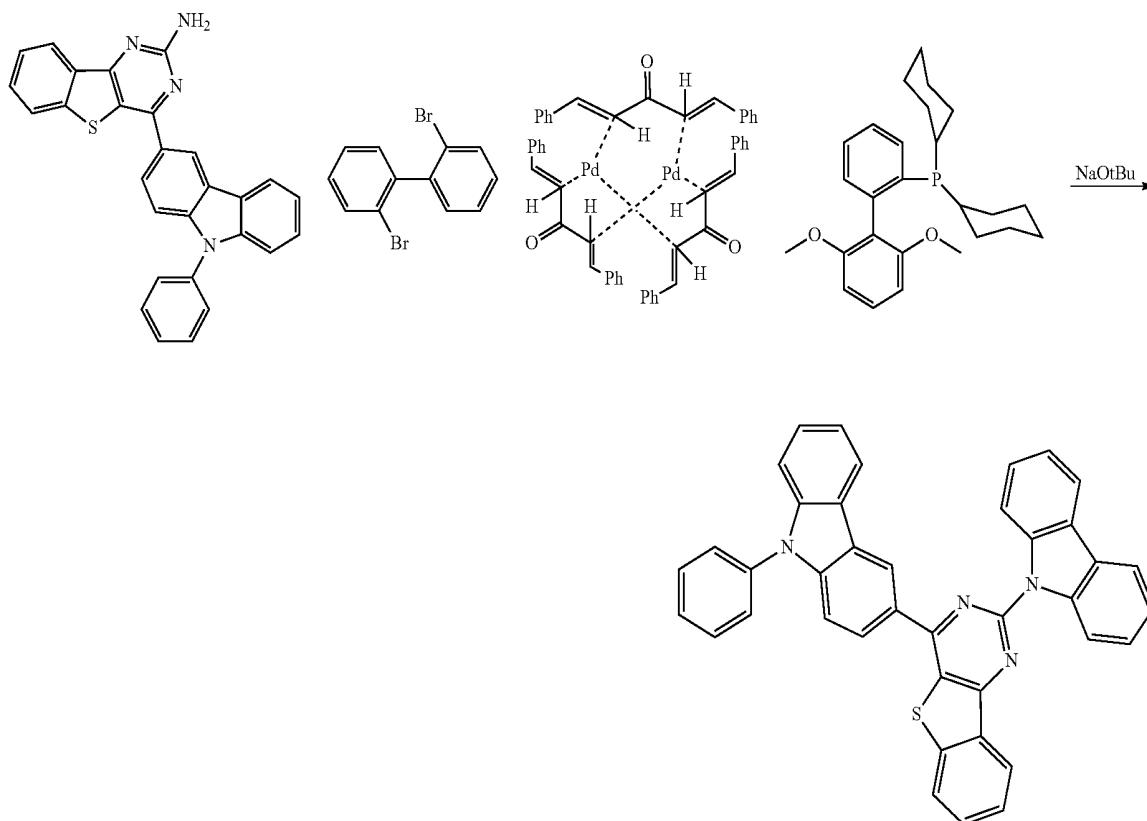
(3) In a 100 mL 3-neck RBF 2-aminobenzo[4,5]thieno[3,2-d]pyrimidin-4(3H)-one (15.30 g, 70.4 mmol) and tetraethylammonium chloride (23.34 g, 141 mmol) were dried under vacuum at 100° C. overnight. Cooled to room temperature and treated with acetonitrile (141 ml) followed by N,N-dimethylaniline (8.9 ml, 70.4 mmol) and phosphoryl trichloride (39.4 ml, 423 mmol). The reaction solution was heated to 110° C. for 15 minutes then cooled to room temperature, transferred to a 500 mL RBF and concentrated on the rotovap. Quenched with addition of ice, and pH adjusted to 7-8 with NaHCO₃ and filtered. Solids washed with water and ether, mascerated with water and filtered, washed with ether and dried in oven overnight yielding 9.4 g (57% yield) of the 4-chlorobenzo[4,5]thieno[3,2-d]pyrimidin-2-amine.

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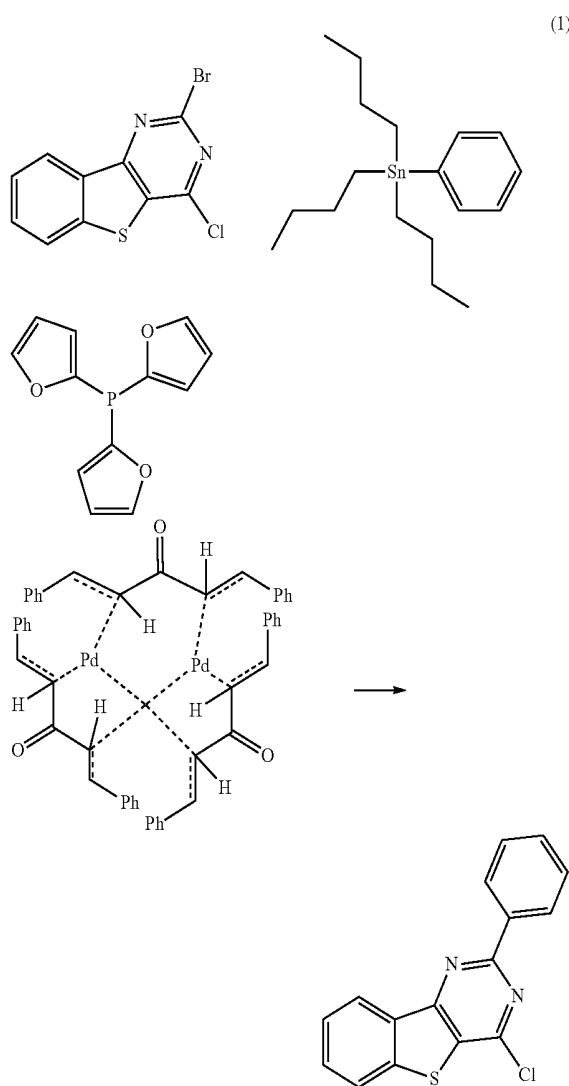
(4) 4-Chlorobenzo[4,5]thieno[3,2-d]pyrimidin-2-amine (2.0 g, 8.49 mmol), 9-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (3.45 g, 9.33 mmol), Pd(PPh₃)₄ (0.588 g, 0.509 mmol) in THF (22.63 ml), and 2M Na₂CO₃ (11.3 ml) were degassed with nitrogen and heated to reflux at 75° C. overnight. The reaction solution was quenched with water, extracted 5× with CHCl₃, dried over sodium sulfate, and filtered and concentrated to yield orange solids. The orange solids were triturated in ~150 mL boiling EtOH and toluene at room temperature afforded 2.65 g (71% yield) of the 4-(9-phenyl-9H-carbazol-3-yl)benzo[4,5]thieno[3,2-d]pyrimidin-2-amine.

(5)



(5) 4-(9-Phenyl-9H-carbazol-3-yl)benzo[4,5]thieno[3,2-d]pyrimidin-2-amine (1.0 g, 2.260 mmol), 2,2'-dibromo-1,1'-biphenyl (0.705 g, 2.260 mmol), Pd(0)2dba3 (0.103 g, 0.113 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.186 g, 0.452 mmol), and sodium 2-methylpropan-2-olate (0.543 g, 5.65 mmol) were suspended in xylene (50 mL), degassed with nitrogen and heated to reflux overnight. Then the reaction solution was cooled down to room temperature and filtered through a plug of Celite, then washed with hot THF and CHCl_3 , and the combined organic solutions were concentrated to orange/brown solids. The solids were dissolved in hot toluene, and filtered through a plug of deactivated alumina yielding a red clear filtrate. The filtrate was concentrated to solids and recrystallized from toluene/ethanol affording 1.8 g of the 2-(9H-carbazol-9-yl)-4-(9-phenyl-9H-carbazol-3-yl)benzo[4,5]thieno[3,2-d]pyrimidine as yellow solids, the Compound 45.

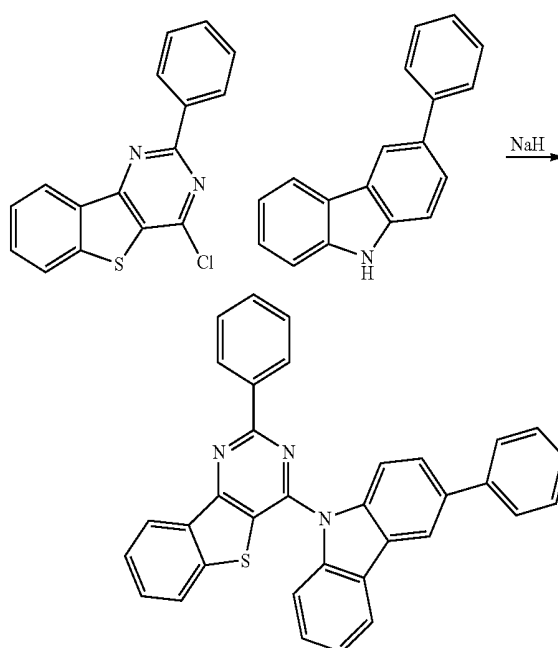
[0109] Synthesis of the Novel Compound 1588



(1) 2-Bromo-4-chlorobenzo[4,5]thieno[3,2-d]pyrimidine (15 g, 50.1 mmol), tri(furan-2-yl)phosphine (2.325 g, 10.01

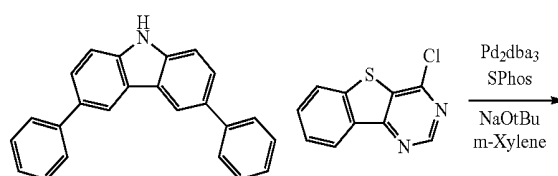
mmol), Pd2dba3 (1.146 g, 1.252 mmol) were dissolved in DMF (295 ml) and degassed by swing purging with nitrogen. Tributyl(phenyl)stannane (17.98 ml, 55.1 mmol) was added in one portion and the reaction was heated to 60° C. After 24 hrs the reaction solution was cooled in an ice bath, filtered and washed with ethanol and heptanes. Gray solids were dissolved in hot DCM and filtered through a plug of Celite/deactivated alumina with DCM to remove color. The filtrate was concentrated to provide 11 g (74%) of 4-chloro-2-phenylbenzo[4,5]thieno[3,2-d]pyrimidine as white solid.

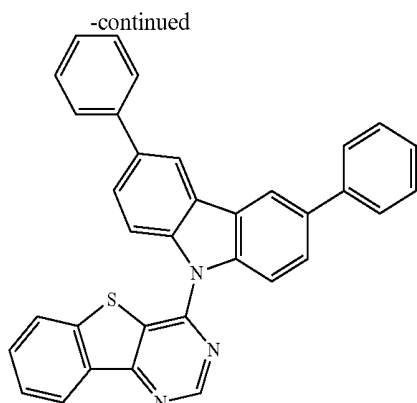
(2)



(2) A 100 mL RBF was dried under vacuum and charged with 3-phenyl-9H-carbazole (2.306 g, 9.48 mmol) and DMF (40 mL). Sodium hydride (0.531 g, 13.27 mmol) (60% in oil) was added to the reaction solution, and stirred until the evolution of hydrogen had stopped. 4-Chloro-2-phenylbenzo[4,5]thieno[3,2-d]pyrimidine (2.25 g, 7.58 mmol) was added in one portion to the reaction solution and stirred overnight at room temperature. The reaction solution was quenched with water, filtered and solid precipitate was washed with water and EtOH. Solids were triturated twice in EtOH, then recrystallized from hot toluene providing 2.9 g (76% yield) of Compound 1742.

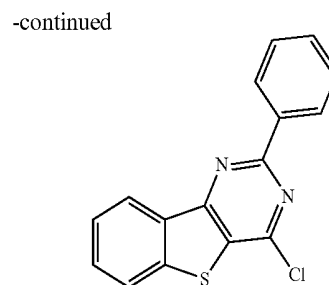
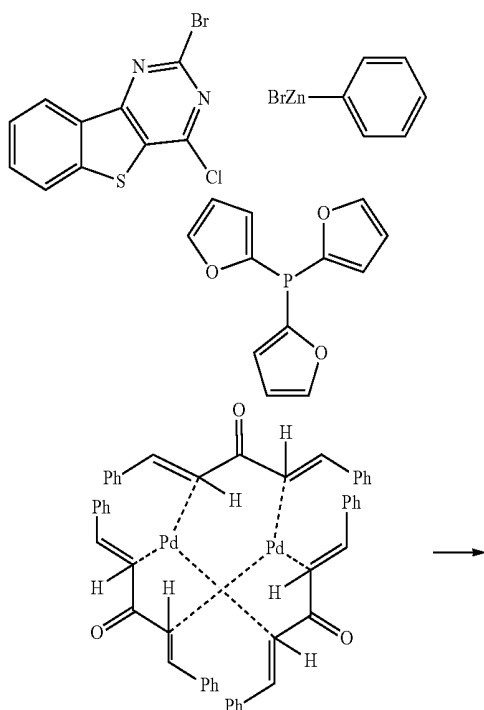
[0110] Synthesis of the Novel Compound 6961



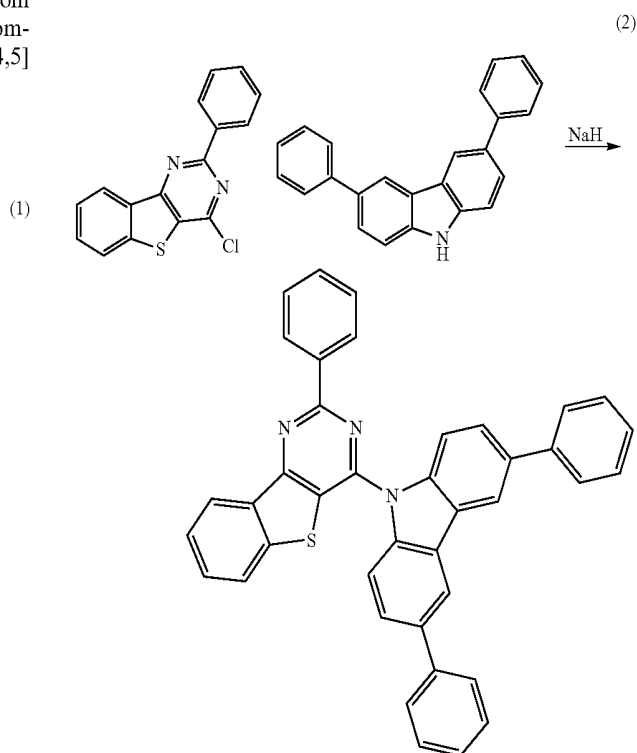


3,6-Diphenyl-9H-carbazole (3.0 g, 9.39 mmol), 4-chlorobenzo[4,5]thieno[3,2-d]pyrimidine (2.280 g, 10.33 mmol), sodium 2-methylpropan-2-olate (2.257 g, 23.48 mmol), Pd₂dba₃ (0.430 g, 0.470 mmol), and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (SPhos) (0.386 g, 0.939 mmol) were charged into a 250-mL round-bottom-flask (RBF), diluted in *m*-xylene (94 ml), degassed and heated to reflux overnight. Then the mixture was cooled down to room temperature and was diluted by DCM, filtered through a pad of Celite and washed with DCM. The solvent was evaporated and the crude solid was purified by column chromatography on silica, eluted with 30-50% DCM in heptanes gradient mixture, then by 50/45/5 (v/v/v) DCM/heptanes/ethyl acetate mixture. After evaporation of the solvent, the yellow solid is triturated in methanol, then the solid was crystallized from heptanes/toluene mixture to provide 1.4 g of the pure Compound 1 (4-(3,6-diphenyl-9H-carbazol-9-yl)benzo[4,5]thieno[3,2-d]pyrimidine).

[0111] Synthesis of the Novel Compound 6962



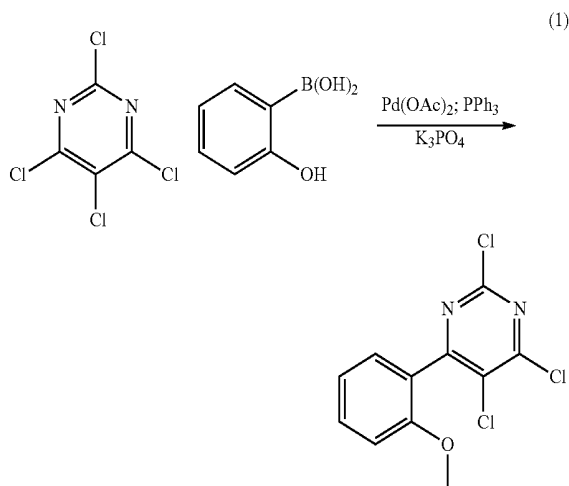
(1) 2-Bromo-4-chlorobenzo[4,5]thieno[3,2-d]pyrimidine (2.5 g, 8.35 mmol), tri(furan-2-yl)phosphine (0.194 g, 0.835 mmol), Pd₂dba₃ (0.191 g, 0.209 mmol) were dissolved in THF (50 mL) and degassed with nitrogen. The reaction solution was heated to 60° C. for 15 minutes, and then phenylzinc (II) bromide (25 mL, 12.52 mmol) was added dropwise. The reaction solution was heated at 60° C. for 2 hrs. An aliquot analyzed by GCMS indicated 13% starting material and 87% of the desired product. 3.8 mL phenylzinc(II) bromide added dropwise to the reaction solution and heating continued overnight. The reaction solution was cooled to room temperature, extracted with DCM, washed with water, dried over sodium sulfate and concentrated in vacuo. The material was purified by column chromatography on silica, eluted with 10-20% DCM/heptanes gradient mixture. The solids were recrystallized from DCM/heptanes affording 0.9 g (36% yield) of the title compound as white needle crystals.



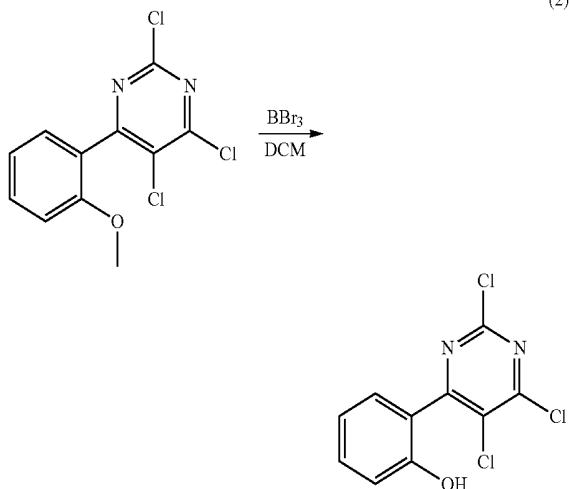
(2) 3,6-Diphenyl-9H-carbazole (1.117 g, 3.50 mmol) was dissolved in DMF (15 mL) and a 60% dispersion of sodium hydride (0.168 g, 4.20 mmol) was added as one portion. The reaction solution was stirred under nitrogen for 30 minutes at room temperature, then 4-chloro-2-phenylbenzo[4,5]thieno

[3,2-d]pyrimidine (0.83 g, 2.80 mmol) was added in one portion and stirring continued at room temperature for 2 hrs. The reaction solution was quenched with water, filtered and triturated three times with EtOH. The product was recrystallized from toluene/EtOH yielding 1.1 g (68%) of the title compound 99.9% pure.

[0112] Synthesis of the Novel Compound 6987

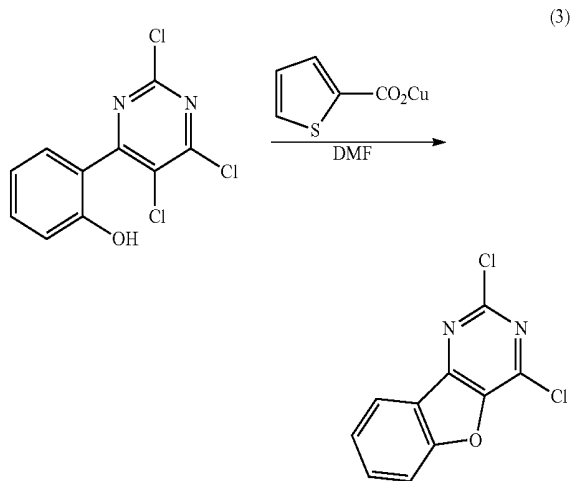


(1) A mixture of perchloropyrimidine (15 g, 65.4 mmol), (2-methoxyphenyl)boronic acid (10.14 g, 65.4 mmol), triphenylphosphine (1.716 g, 6.54 mmol), palladium acetate (0.734 g, 3.27 mmol) and potassium phosphate, H₂O (45.2 g, 196 mmol) in acetonitrile (300 ml)/water (90 ml) was degassed at room temperature. The mixture was stirred at room temperature for 1 hr. before heated at 60° C. for 1 hr. Upon completion of the reaction, the reaction was diluted with ethyl acetate, washed with sodium chloride saturated solution, filtered and evaporated. The crude material was purified by silica gel column chromatography using heptanes/AcOEt: 93/7 to 8/2 as eluent to afford a white solid (10.6 g, 56% yield).

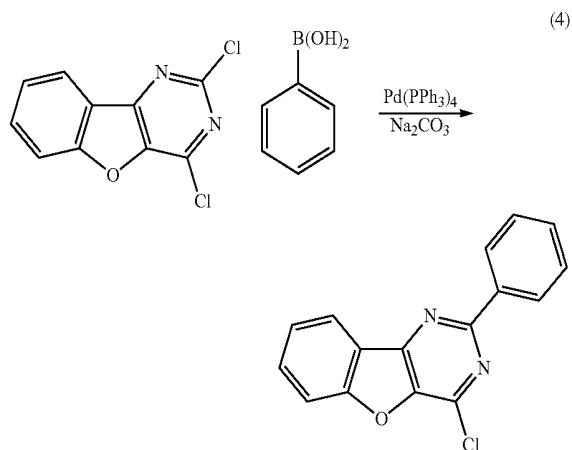


(2) Tribromoborane (84 ml, 84 mmol) was added into a 0° C., stirred solution of 2,4,5-trichloro-6-(2-methoxyphenyl)pyrimidine (10.6 g, 36.6 mmol) in CH₂Cl₂ (330 ml) under N₂ over a period of 1 hr. The mixture was warmed up and stirred at 20° C. overnight. The reaction solution was poured slowly into the ice water with stirring. Aqueous mixture was extracted

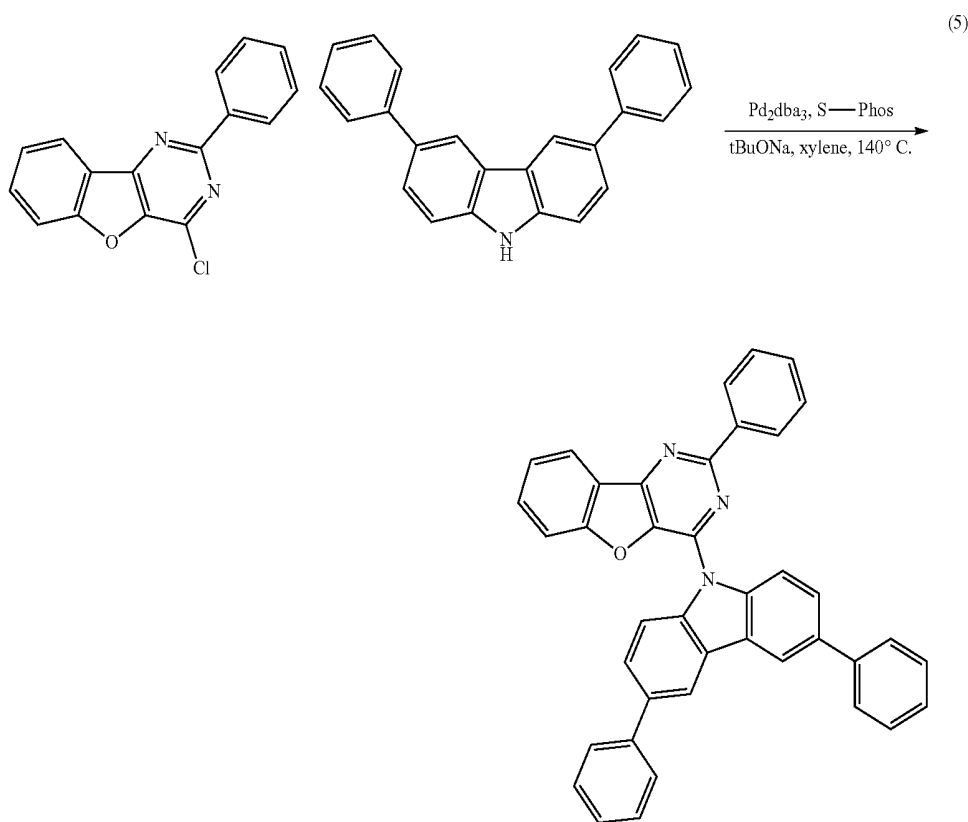
with ethyl acetate (75 mL×2 times). Organic solution was washed with water, aqueous NaHCO₃, water and brine, and then dried over anhydrous Na₂SO₄. The crude material was purified by silica gel column chromatography eluted with heptane/ethyl acetate 92/8 to 8/2 gradient mixture to afford 2-(2,5,6-trichloropyrimidin-4-yl)phenol as yellow solid (7.3 g, 72.4% yield).



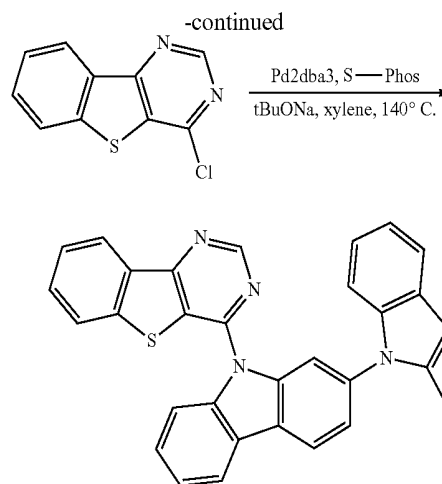
(3) A mixture of 2-(2,5,6-trichloropyrimidin-4-yl)phenol (6.5 g, 23.59 mmol) and ((thiophene-2-carbonyl)oxy)copper (5.40 g, 28.3 mmol) in DMF (130 ml) was heated at 100° C. for 2.5 hours. The reaction was cooled down and filtered through a bed of Celite. Water was added and the light green solid was filtered off. This crude material was purified by silica gel column chromatography eluted with heptane/ethyl acetate 95/5 to 9/1 gradient mixture to afford a yellow solid (1.43 g 25.4% yield).



(4) A mixture of phenylboronic acid (1.530 g, 12.55 mmol), 2,4-dichlorobenzofuro[3,2-d]pyrimidine (3.0 g, 12.55 mmol) and sodium carbonate (2.66 g, 25.10 mmol) in THF (120 ml)/water (24 mL) was degassed for 20 min, then Pd(PPh₃)₄ (0.435 g, 0.376 mmol) was added and the mixture was heated at 60° C. under N₂ overnight. Upon completion, organic phase was separated and evaporated. The crude was purified by silica gel column chromatography with heptane/DCM/ethyl acetate 7/3/0.2 to 4/6/0.2 (v/v/v) as eluent to afford a yellow solid (2.0 g, 56.8% yield).

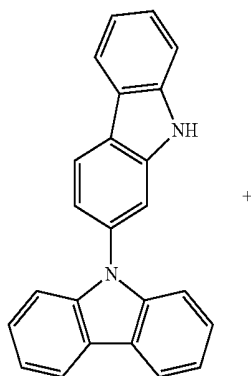


(5) A mixture of 4-chloro-2-phenylbenzofuro[3,2-d]pyrimidine (2 g, 7.12 mmol), 3,6-diphenyl-9H-carbazole (2.276 g, 7.12 mmol) and sodium 2-methylpropan-2-olate (1.369 g, 14.25 mmol) in xylene (120 mL) was degassed, then $\text{Pd}_2(\text{dba})_3$ (0.130 g, 0.142 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (SPhos) (0.234 g, 0.570 mmol) were then added and heated at 140° C. overnight. The reaction solution was purified by silica gel column chromatography using heptane/DCM/ethyl acetate 80/20/2 to 4/6/0.2 (v/v/v) gradient mixture to afford Compound 6987 as a light yellow solid. (1.25 g, 31.1%).



Synthesis of the Novel Compound 15661

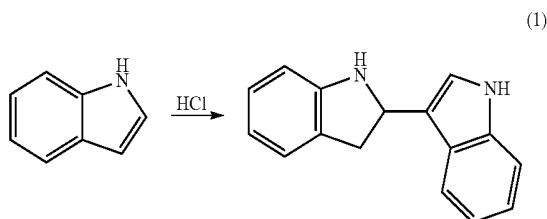
[0113]



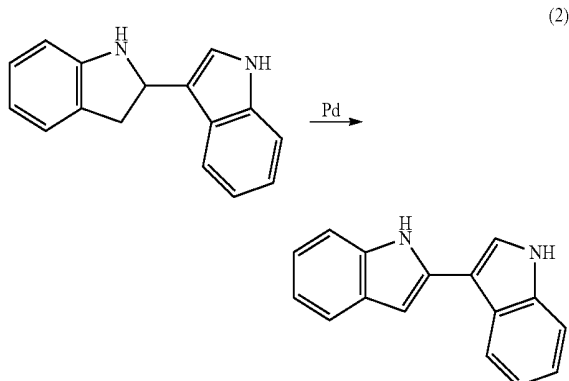
A mixture of 4-chlorobenzo[4,5]thieno[3,2-d]pyrimidine (3.09 g, 13.99 mmol), 9H-2,9'-bicarbazole (3.1 g, 9.33 mmol), sodium 2-methylpropan-2-olate (1.793 g, 18.65 mmol), $\text{Pd}_2(\text{dba})_3$ (0.342 g, 0.373 mmol) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (S-Phos, 0.613 g, 1.492 mmol) in 140 mL of xylene was degassed for 30 min. and the reaction mixture was heated to reflux under nitrogen atmosphere overnight. Upon completion, the reaction cooled down to room temperature, and solid material was filtered off. Then it was dissolved in hot toluene, filtered and evaporated. The crude material was recrystallized from DCM and DCM/THF to afford a yellow solid (1.8 g, 37.4% yield).

[0114] Synthesis of the Novel Compound 24361

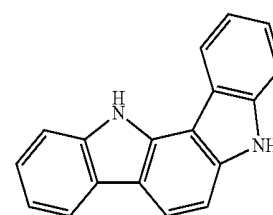
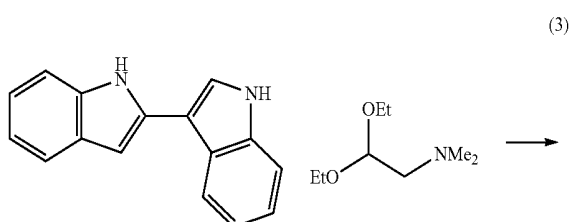
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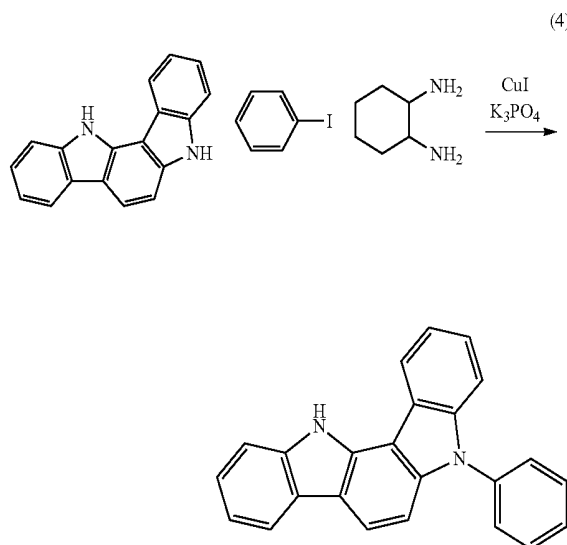
(1) A dry 500 mL RBF was charged with 1H-indole (29.0 g, 248 mmol) and ether (165 ml). The mixture was cooled to -20°C . and treated with 2M HCl in ether (260 ml, 520 mmol) over the course of 30 minutes. The cooling bath was removed and the reaction solution was stirred at room temperature for 24 hours. The reaction solution was filtered to get white powder and washed with ether. The solid was then washed with NaHCO_3 aq. and extracted with EtOAc. The solid was then washed with saturated NaHCO_3 and brine, dried over Na_2SO_4 , filtered, and concentrated to afford 30.9 g of the 3-(indolin-2-yl)-1H-indole as clear, pink, viscous oil.



(2) 3-(Indolin-2-yl)-1H-indole (29 g, 124 mmol) in toluene (248 ml) was treated with 10 wt. % palladium (3.29 g, 3.09 mmol) on carbon. The reaction was heated to reflux at 115°C . for 3 hrs. The suspension was filtered hot, through a plug of Celite, which was then extracted 5x with hot toluene. The filtrate was concentrated in vacuo to half volume, cooled to room temperature and filtered to afford pink solids. The pink solids were washed with toluene and hexanes and dried in vacuo at 50°C . yielding 16.4 g (57% yield) of the 1H,1'H-2,3'-biindole as off-white solid.

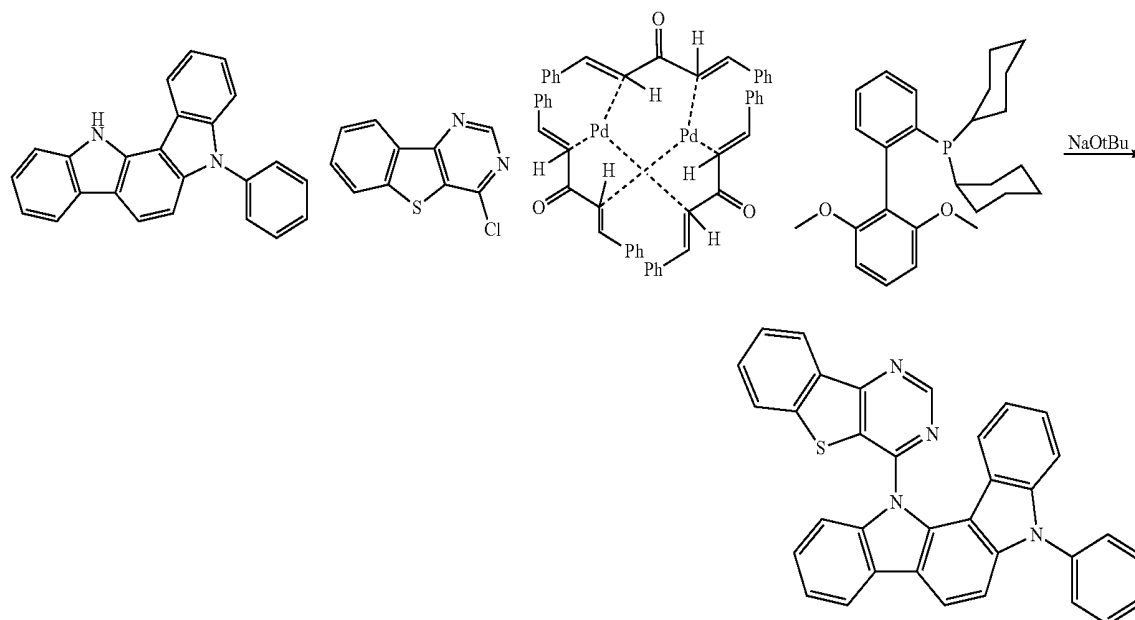


(3) 1H,1'H-2,3'-biindole (16.4 g, 70.6 mmol) and 2,2-diethoxy-N,N-dimethylethanamine (14.18 ml, 78 mmol) in glacial acetic acid (160 mL) were refluxed at 130°C . overnight under nitrogen. The reaction solution was cooled to room temperature and filtered. The filtrate was washed with small amount of acetic acid and excess of water. The filtrate was dried in the oven at 65°C . overnight affording 10.79 g (60%) of the 5,12-dihydroindolo[3,2-a]carbazole as gray solid.



(4) Iodobenzene (2.278 ml, 20.39 mmol) and cyclohexane-1,2-diamine (0.901 ml, 3.71 mmol) were added to a degassed suspension of 5,12-dihydroindolo[3,2-a]carbazole (4.75 g, 18.53 mmol), copper(I) iodide (0.353 g, 1.853 mmol) and K_3PO_4 (8.26 g, 38.9 mmol) in m-xylene (93 ml). The reaction solution was refluxed at 155°C . for 48 hours. Based on TLC analysis after 24 hrs the reaction was not complete; the reaction mixture was cooled to room temperature, treated with more CuI (0.35 g) and cyclohexane-1,2-diamine (0.9 mL) and heated to reflux overnight. The suspension was filtered through Celite with THF and DCM. The filtrate was concentrated and purified by column chromatography with hexane:DCM gradient mixture (4:1 to 1:1 v/v). The filtrate was evaporated and dried in vacuo yielding 6.02 g (98% yield) of the 5-phenyl-5,12-dihydroindolo[3,2-a]carbazole as white solid.

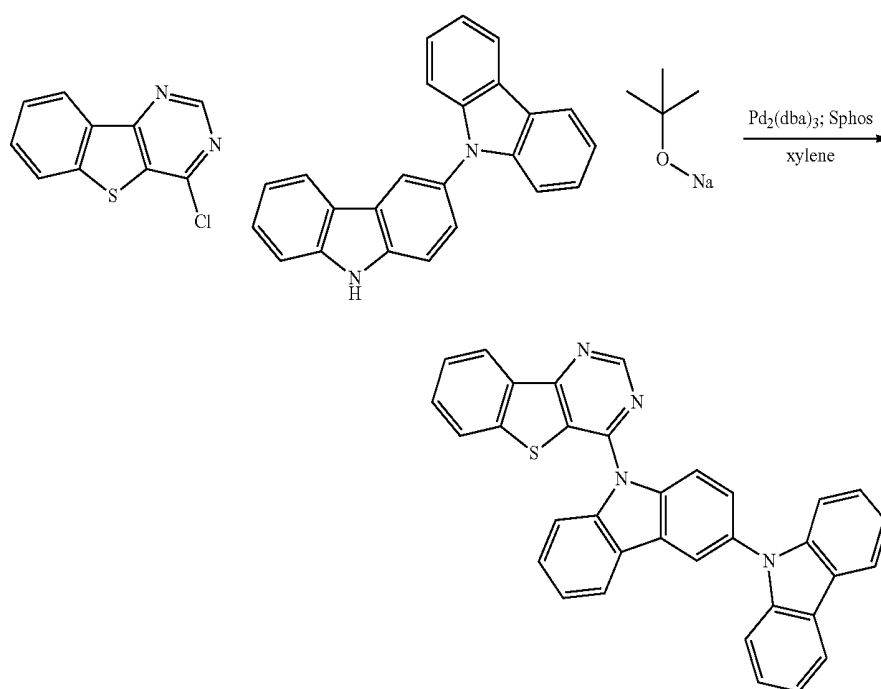
(5)



(5) 5-Phenyl-5,12-dihydroindolo[3,2-a]carbazole (2.83 g, 8.51 mmol), 4-chlorobenzo[4,5]thieno[3,2-d]pyrimidine (3.29 g, 14.90 mmol), Pd₂dba₃ (0.390 g, 0.426 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.699 g, 1.703 mmol), sodium 2-methylpropan-2-olate (2.046 g, 21.28 mmol) were suspended in xylene (120 mL), degassed with nitrogen, then heated to reflux at 155° C. overnight. After 15 hrs, additional 0.2 g of Pd₂dba₃ and 0.35 g of dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phos-

phine were added. The suspension was degassed with nitrogen and heated to reflux at 155° C. for 24 hrs. The reaction was filtered through a plug of Celite and evaporated. The residue was purified by column chromatography eluted with 20% DCM, 5% EtOAc in heptanes. Fractions containing product were further purified by trituration in EtOH and recrystallized from toluene/heptanes to provide 2.5 g of Compound 24361.

[0115] Synthesis of the Novel Compound 13361



4-Chlorobenzo[4,5]thieno[3,2-d]pyrimidine (1.992 g, 9.03 mmol) and 9H-3,9'-bicarbazole (2.000 g, 6.02 mmol), sodium 2-methylpropan-2-olate (1.156 g, 12.03 mmol), Pd2 (dba)3 (250 mg) and dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (SPhOS) (310 mg) were suspended in xylene (100 ml), degassed and heated to reflux for 18 hr. The reaction solution was cooled down, filtered through celite plug and evaporated. Column chromatography on silica gel column, eluted with hexane/DCM 1/1 (v/v), then hexane/EtOAc 4/1 (v/v), followed by crystallization from hexane/DCM provided yellow crystals (2.8 g, 90% yield).

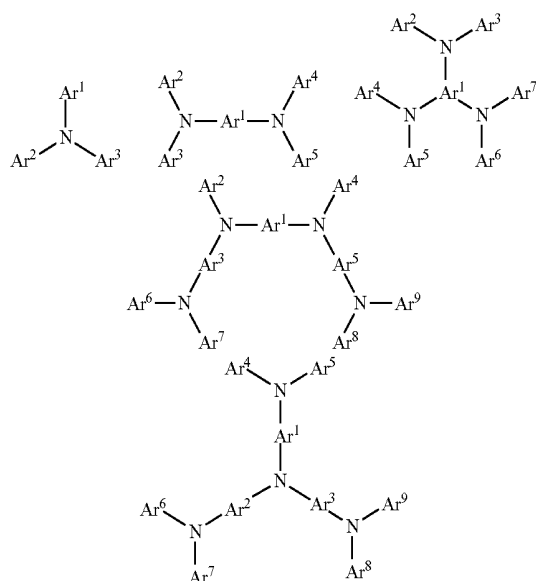
Combination with Other Materials

[0116] 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:

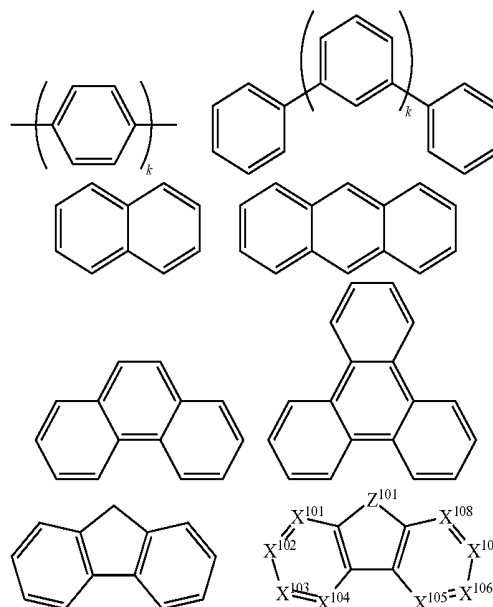
[0117] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluoro-hydrocarbon; 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 MoO₃; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

[0118] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:



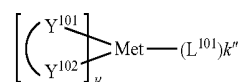
[0119] Each of Ar¹ to Ar⁹ is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysenes, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyrindine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuro-pyridine, furodipyrindine, benzothienopyridine, thienodipyrindine, benzoselenophenopyridine, and selenophenodipyrindine; 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.

[0120] In one aspect, Ar¹ to Ar⁹ is independently selected from the group consisting of:



wherein k is an integer from 1 to 20; X¹⁰¹ to X¹⁰⁸ is C (including CH) or N; Z¹⁰¹ is NAr¹, O, or S; Ar¹ has the same group defined above.

[0121] Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:



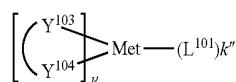
wherein Met is a metal, which can have an atomic weight greater than 40; (Y¹⁰¹-Y¹⁰²) is a bidentate ligand, Y¹⁰¹ and Y¹⁰² are independently selected from C, N, O, P, and S; L¹⁰¹ is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k'' is the maximum number of ligands that may be attached to the metal.

[0122] In one aspect, (Y¹⁰¹-Y¹⁰²) is a 2-phenylpyridine derivative. In another aspect, (Y¹⁰¹-Y¹⁰²) 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. Fe³⁺/Fe couple less than about 0.6 V.

Host:

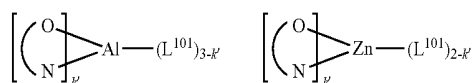
[0123] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any 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.

[0124] Examples of metal complexes used as host are preferred to have the following general formula:



wherein Met is a metal; (Y¹⁰³-Y¹⁰⁴) is a bidentate ligand, Y¹⁰³ and Y¹⁰⁴ are independently selected from C, N, O, P, and S; L¹⁰¹ is 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.

[0125] In one aspect, the metal complexes are:



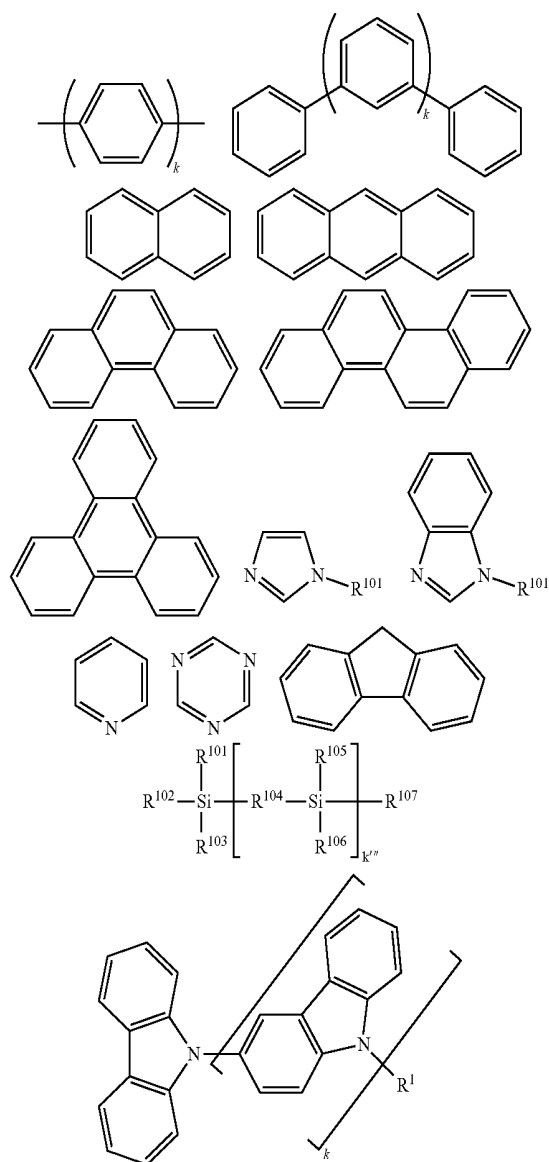
wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

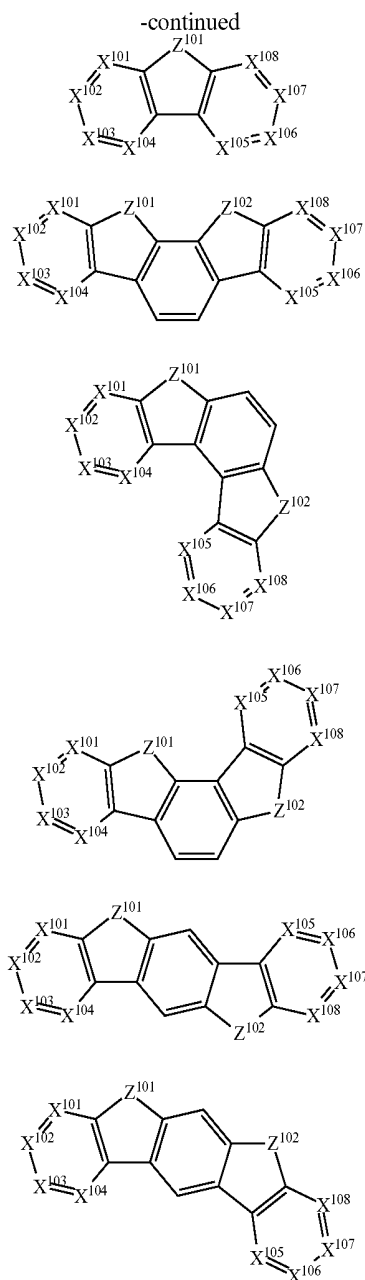
[0126] In another aspect, Met is selected from Ir and Pt. In a further aspect, (Y¹⁰³-Y¹⁰⁴) is a carbene ligand.

[0127] 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, naphthyr-

dine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofurofuryridine, furodipyridine, benzothienopyridine, thienodipyridine, benzosele-nophenopyridine, 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, cycloalk-enyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0128] In one aspect, host compound contains at least one of the following groups in the molecule:





wherein R¹⁰¹ to R¹⁰⁷ 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^m is an integer from 0 to 20. X¹⁰¹ to X¹⁰⁸ is selected from C (including CH) or N. Z¹⁰¹ and Z¹⁰² is selected from NR¹⁰¹, O, or S.

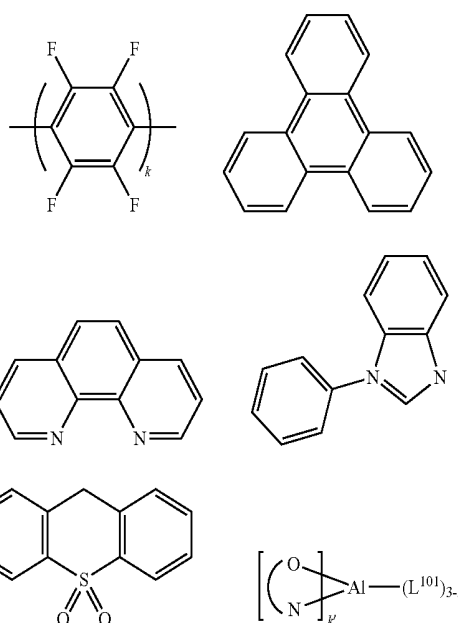
HBL:

[0129] 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.

[0130] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

[0131] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

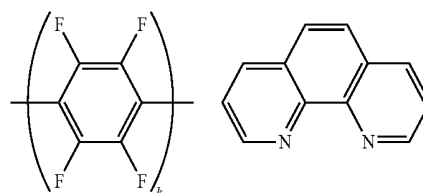


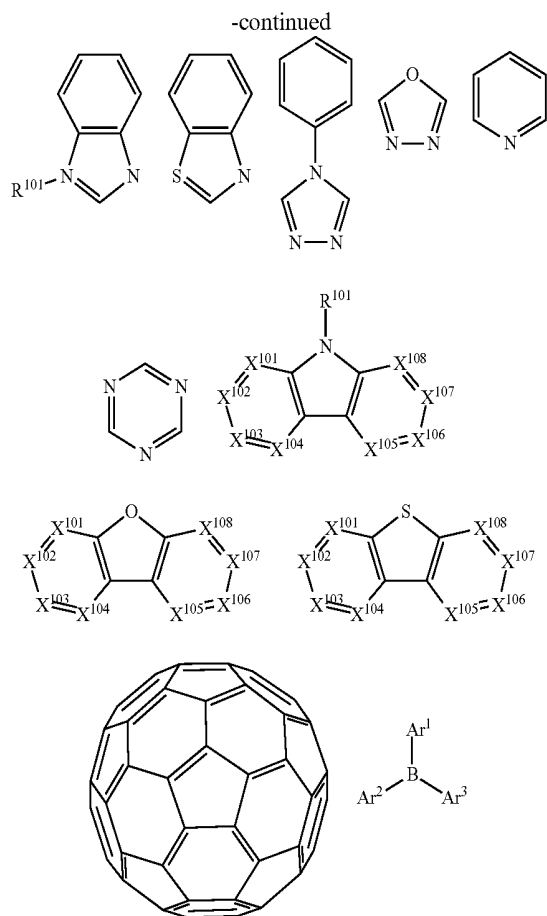
wherein k is an integer from 1 to 20; L¹⁰¹ is an another ligand, k' is an integer from 1 to 3.

ETL:

[0132] 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.

[0133] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

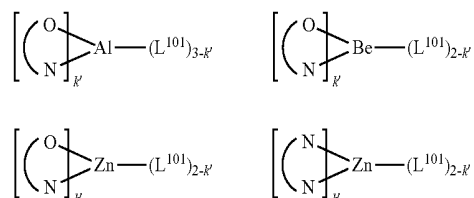




wherein R¹⁰¹ is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned

above. Ar¹ to Ar³ has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X¹⁰¹ to X¹⁰⁸ is selected from C (including CH) or N.

[0134] In another aspect, the metal complexes used in ETL contains, but not limit 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; L¹⁰¹ is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

[0135] 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.

[0136] 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 2 below. Table 2 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 2

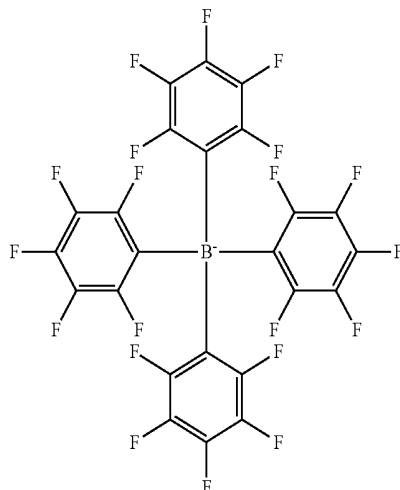
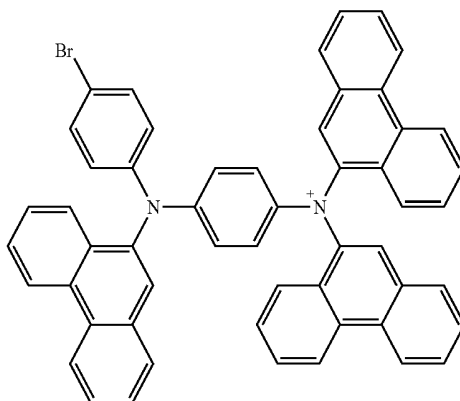
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphyrin compounds		Appl. Phys. Lett. 69, 2160 (1996)

TABLE 2-continued

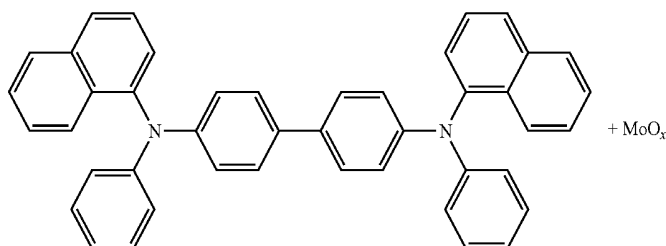
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF _x Fluorohydrocarbon polymer	$\text{-(CH}_x\text{F}_y\text{)-}_n$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and silane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants		EP1725079A1 and

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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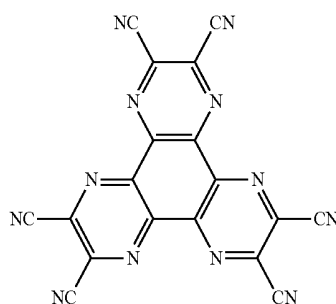


Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides



US20050123751
SID Symposium
Digest, 37, 923
(2006)
WO2009018009

n-type
semiconducting
organic complexes



US20020158242

TABLE 2-continued

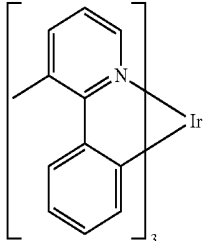
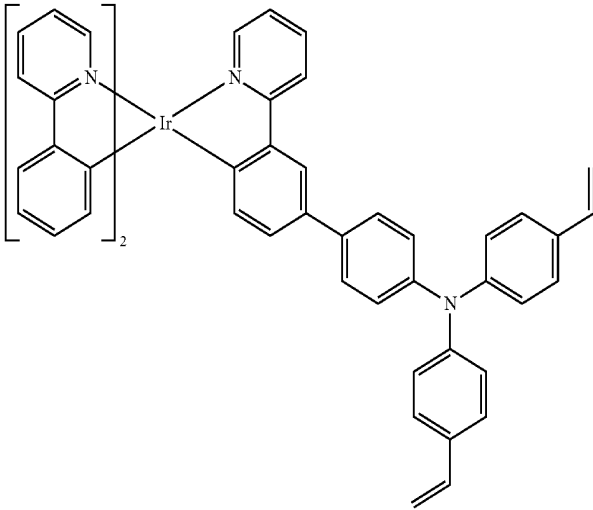
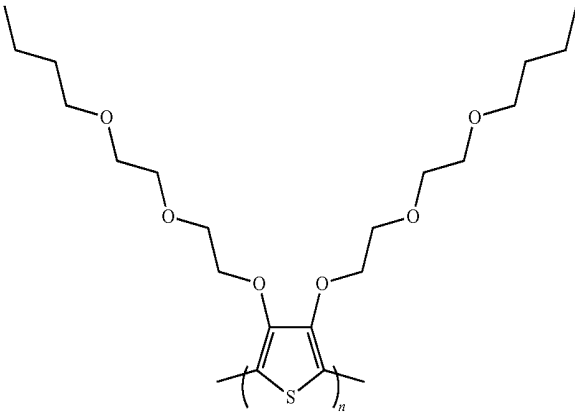
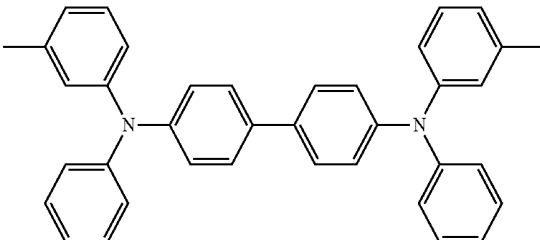
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216
Hole transporting materials		
Triarylamines (e.g., TPD, α -NPD)		Appl. Phys. Lett. 51, 913 (1987)

TABLE 2-continued

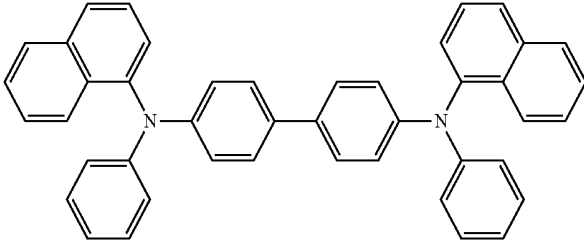
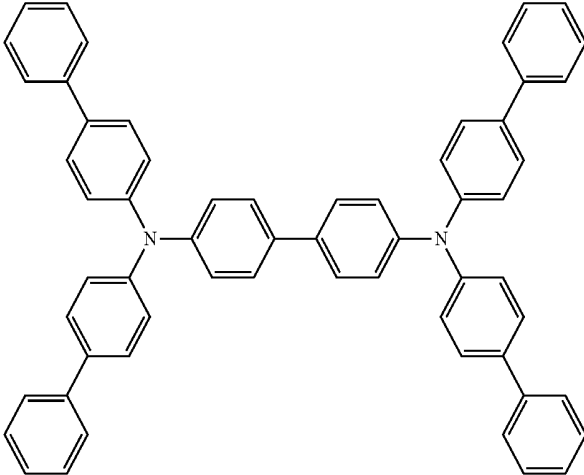
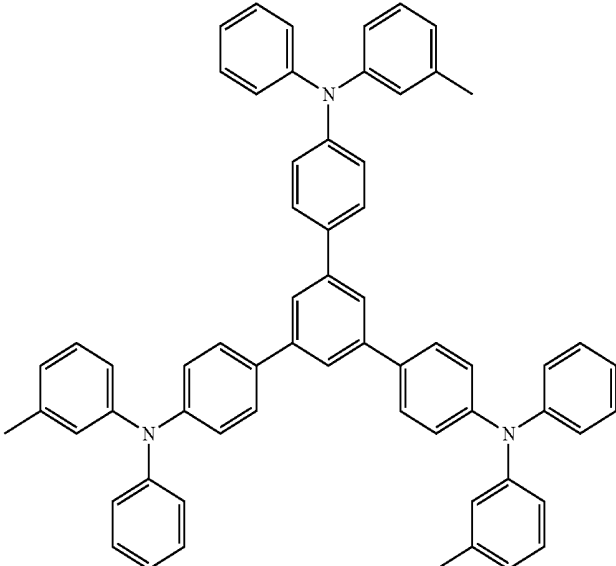
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 5,061,569
		EP650955
		J. Mater. Chem. 3, 319 (1993)

TABLE 2-continued

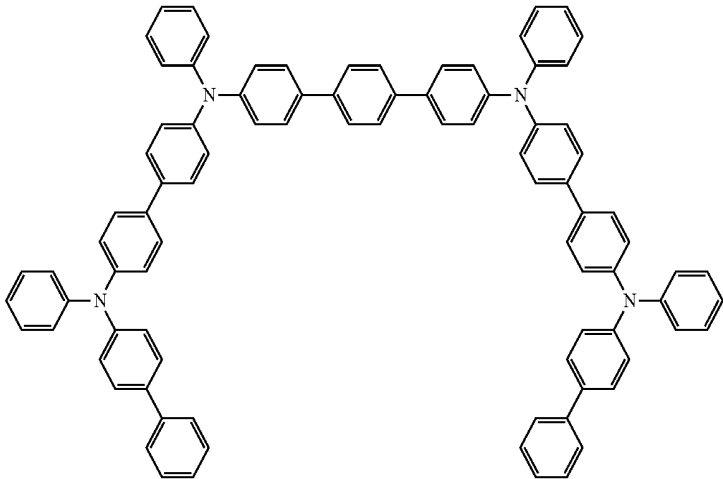
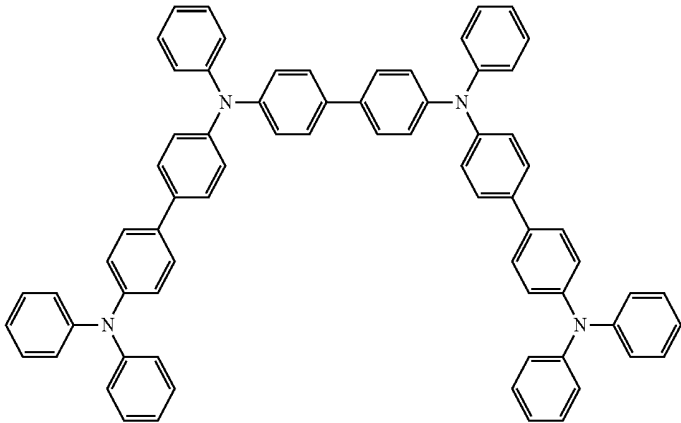
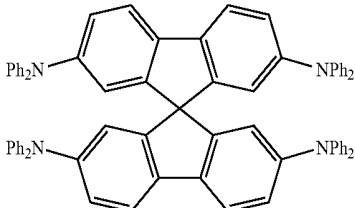
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)

TABLE 2-continued

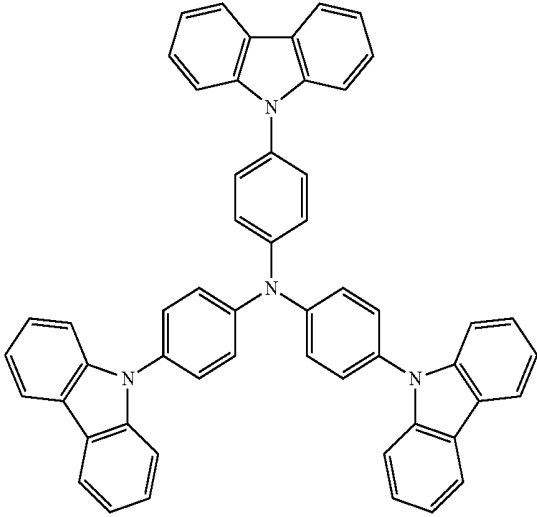
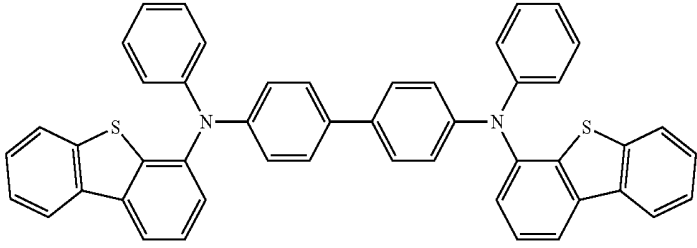
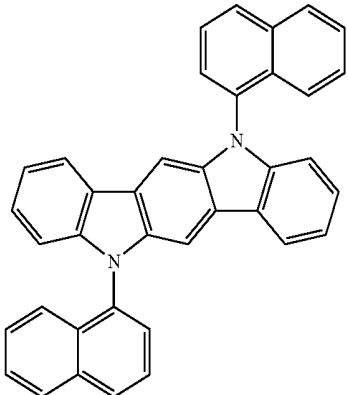
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190 US20110163302
Indolocarbazoles		Synth. Met. 111, 421 (2000)

TABLE 2-continued

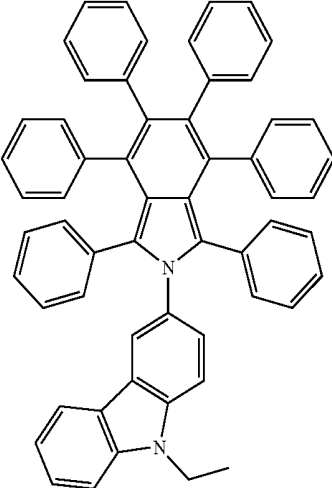
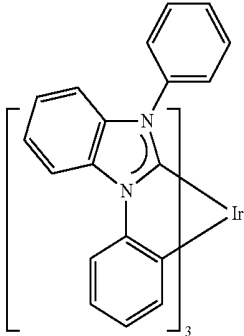
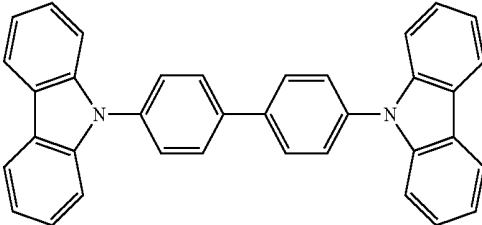
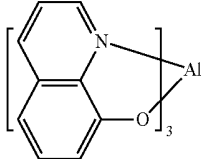
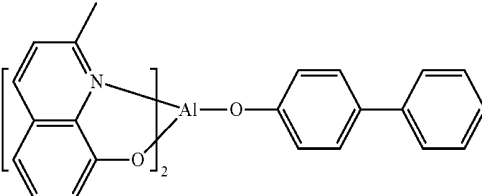
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221
Phosphorescent OLED hosts materials Red hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq ₃ , BALq)		Nature 395, 151 (1998)
		US20060202194

TABLE 2-continued

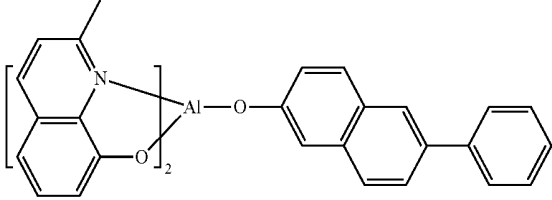
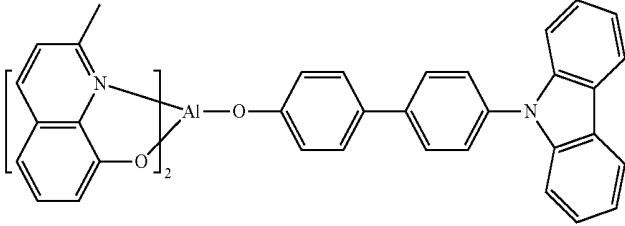
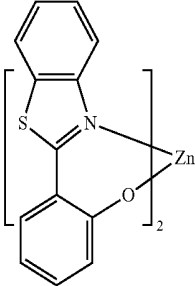
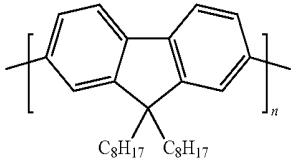
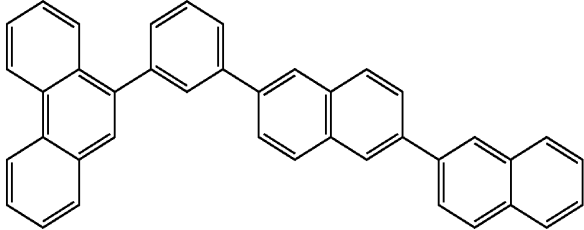
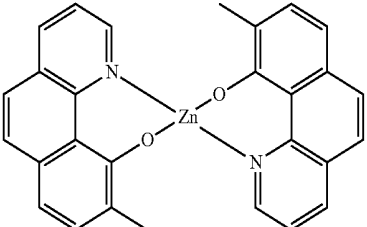
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2005014551
		WO2006072002
Metal phenoxy-benzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US2009008605, US20090009065
Zinc complexes		WO2010056066

TABLE 2-continued

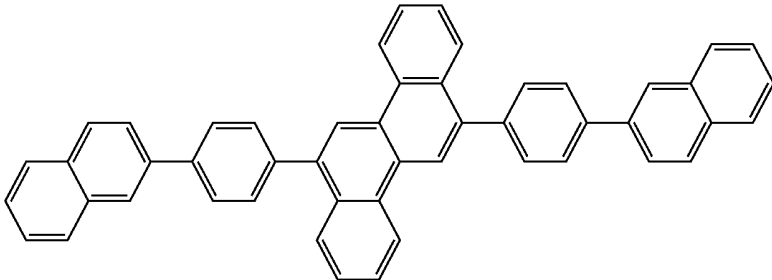
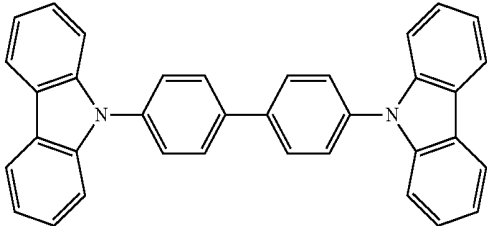
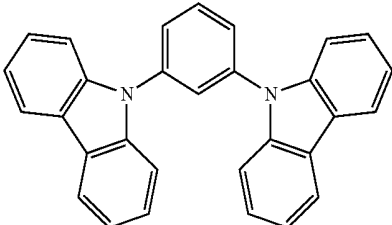
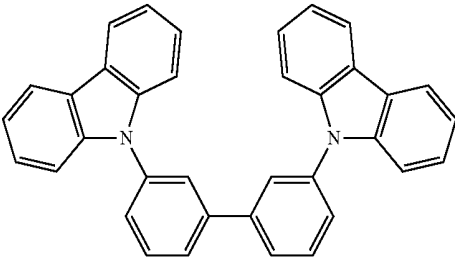
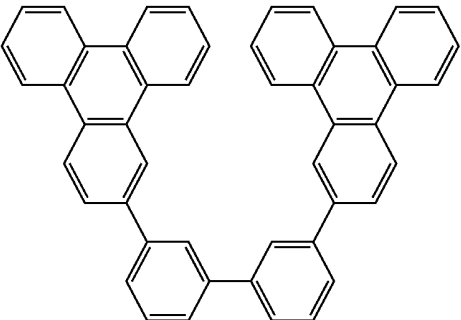
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Chrysene based compounds		WO2011086863
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE 2-continued

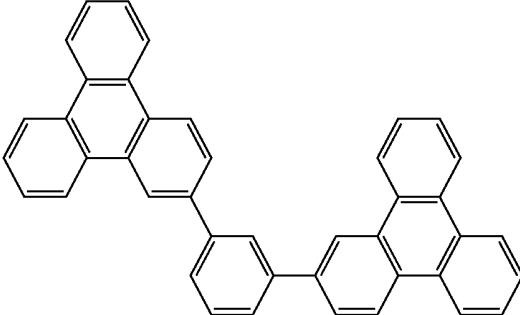
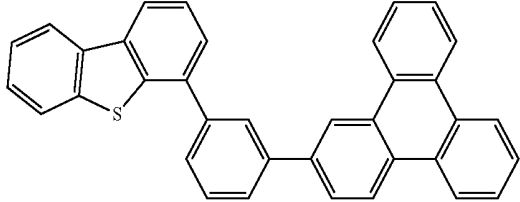
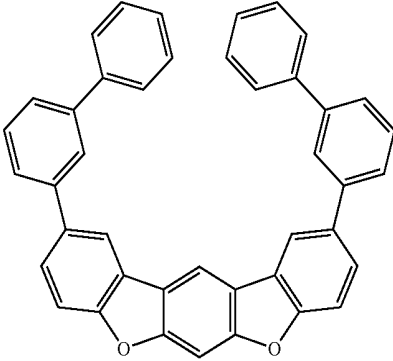
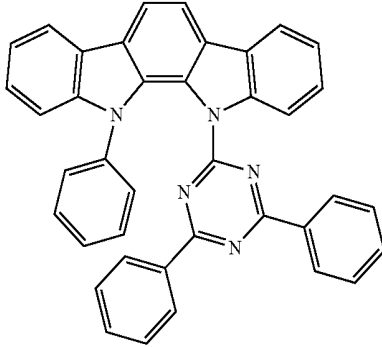
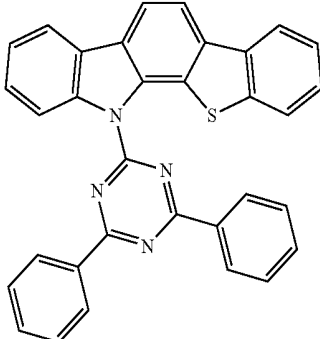
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Poly-fused heteroaryl compounds		US20060280965
		WO2009021126
Donor acceptor type molecules		US20090309488 US20090302743 US20100012931
Donor acceptor type molecules		WO2008056746
		WO2010107244

TABLE 2-continued

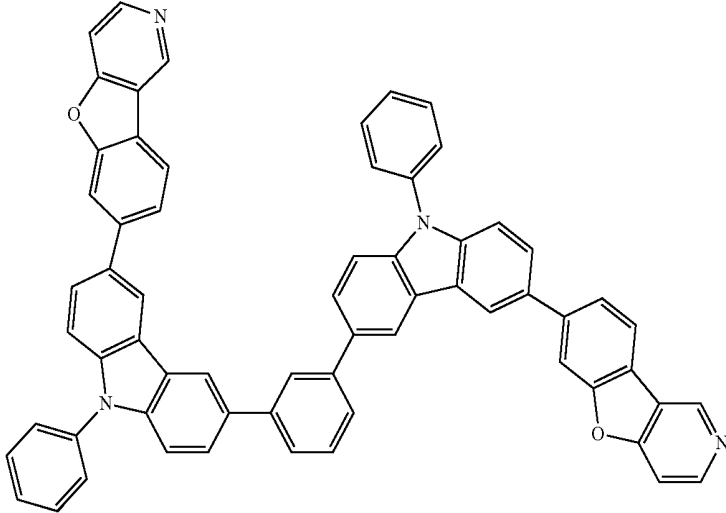
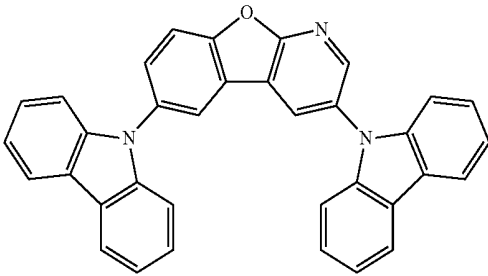
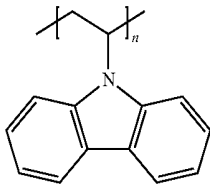
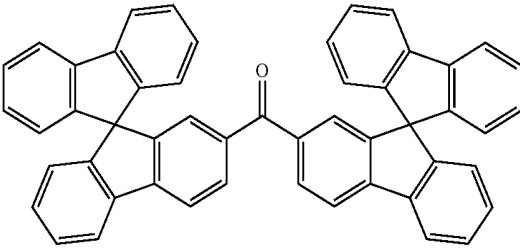
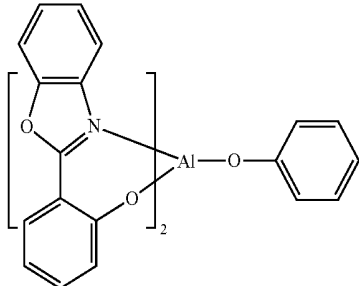
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza-carbazole/ DBT/DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207
Metal phenoxy- benzoxazole compounds		WO2005089025

TABLE 2-continued

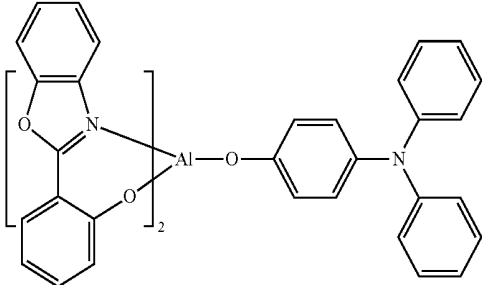
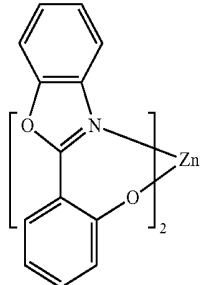
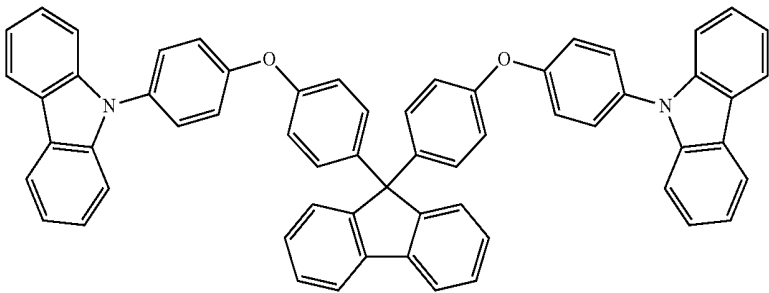
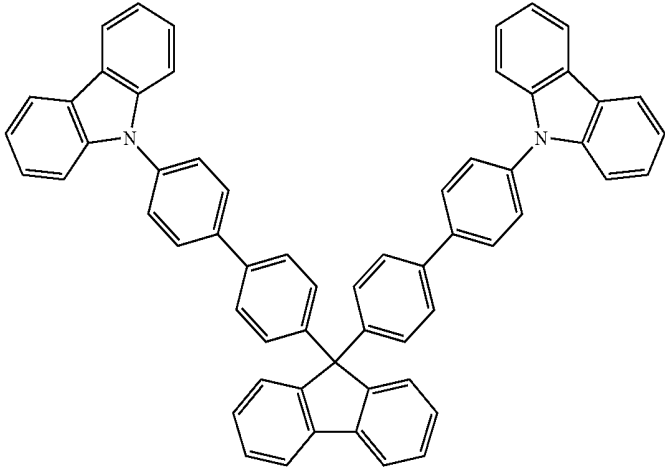
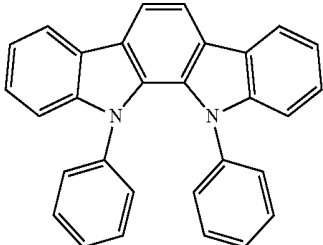
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297
Indolocarbazoles		WO2007063796

TABLE 2-continued

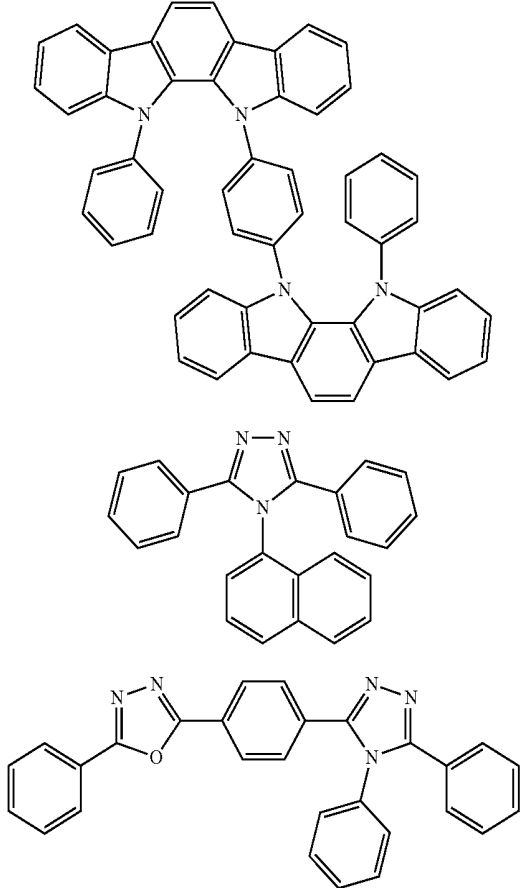
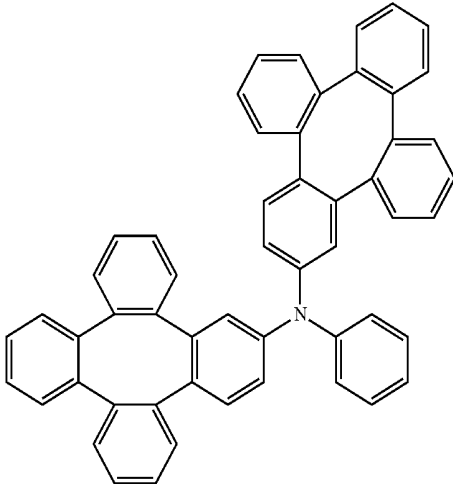
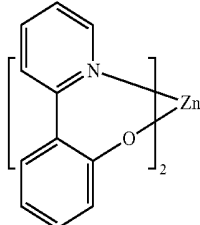
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		<p>WO2007063754</p> <p>J. Appl. Phys. 90, 5048 (2001)</p> <p>WO2004107822</p>
Tetraphenylene complexes		US20050112407
Metal phenoxy pyridine compounds		WO2005030900

TABLE 2-continued

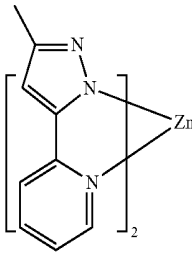
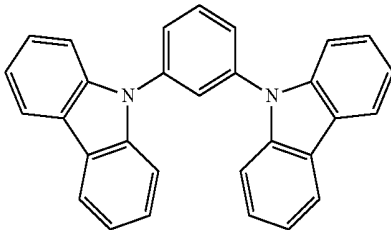
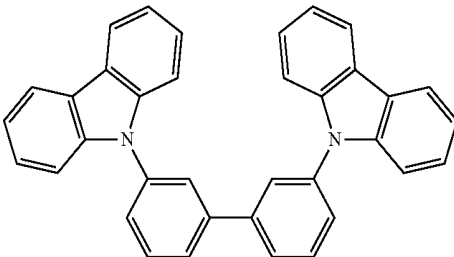
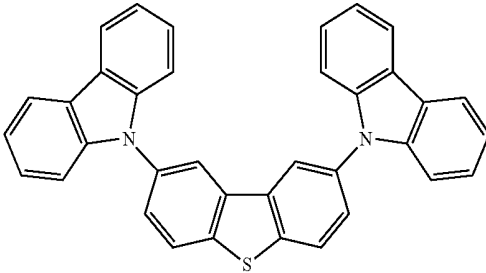
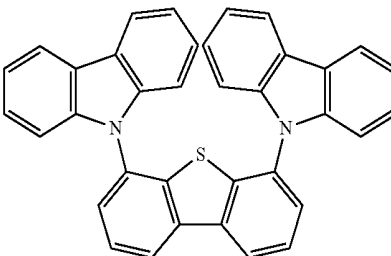
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal coordination complexes (e.g., Zn, Al with N N ligands)		US20040137268, US20040137267
Blue hosts		
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/ Dibenzofuran- carbazole compounds		WO2006114966, US20090167162
		US20090167162

TABLE 2-continued

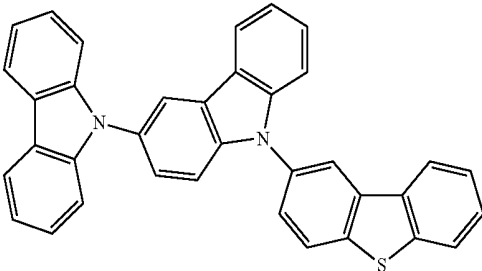
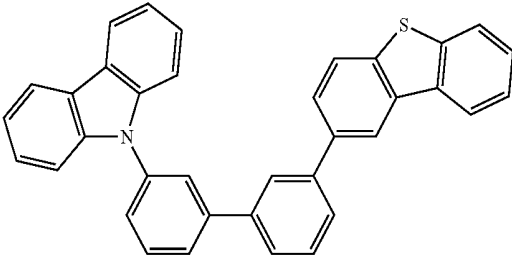
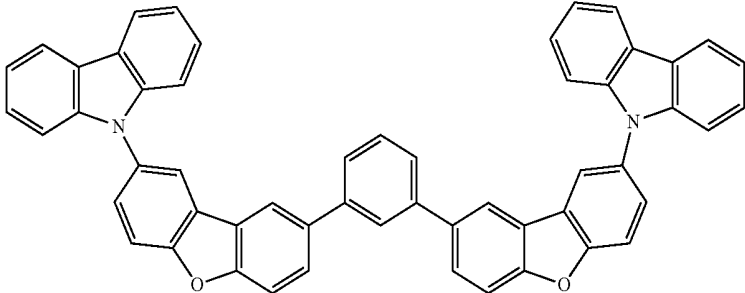
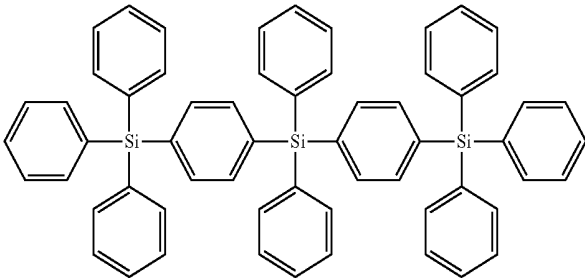
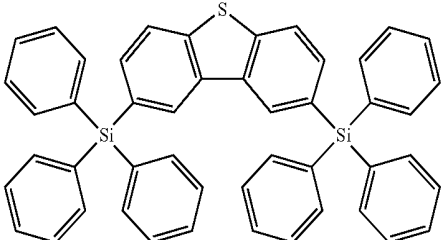
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	 <p>A chemical structure consisting of two indole rings connected at their 3-positions to a central benzene ring. The 2-positions of the indole rings are also substituted with phenyl groups.</p>	WO2009086028
	 <p>A chemical structure consisting of two indole rings connected at their 3-positions to a biphenyl bridge (two benzene rings connected at the para positions). The 2-positions of the indole rings are also substituted with phenyl groups.</p>	US20090030202, US20090017330
	 <p>A chemical structure consisting of two indole rings connected at their 3-positions to a benzofuran bridge (a benzene ring fused to a furan ring). The 2-positions of the indole rings are also substituted with phenyl groups.</p>	US20100084966
Silicon aryl compounds	 <p>A linear chain of three silicon atoms connected by phenyl rings. Each silicon atom is also bonded to two phenyl groups, one above and one below the chain.</p>	US20050238919
	 <p>A chemical structure consisting of two silicon atoms connected by a benzothienyl bridge (a benzene ring fused to a thiophene ring). Each silicon atom is also bonded to two phenyl groups, one above and one below the bridge.</p>	WO2009003898

TABLE 2-continued

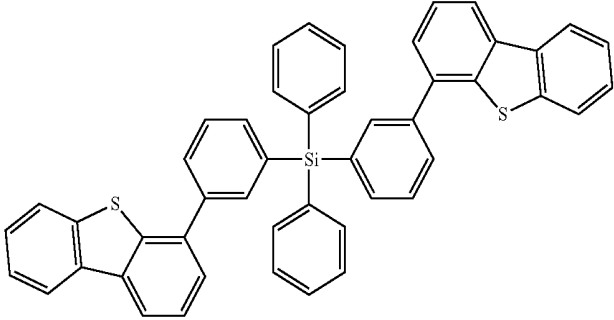
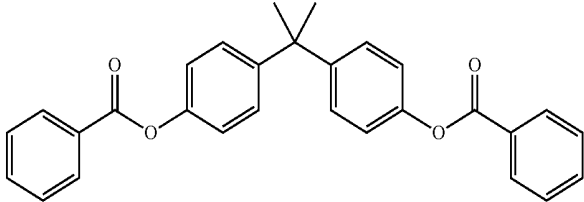
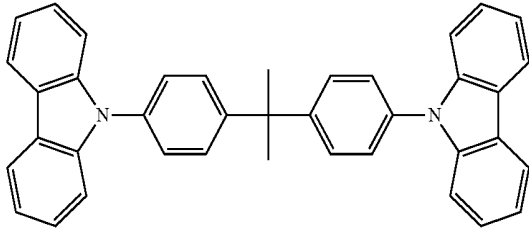
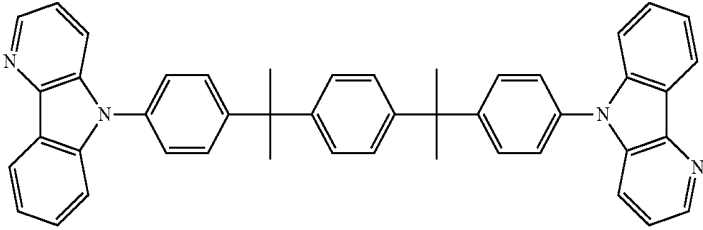
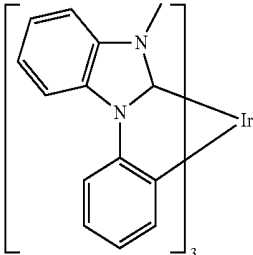
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114

TABLE 2-continued

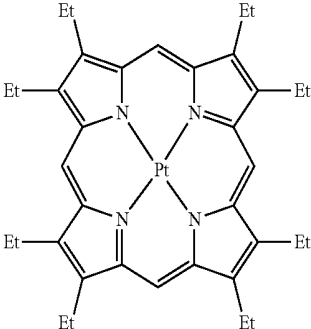
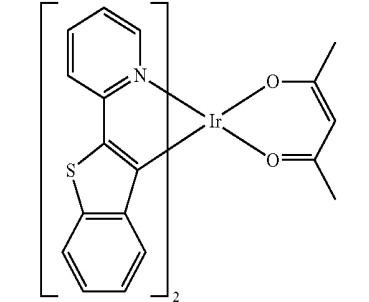
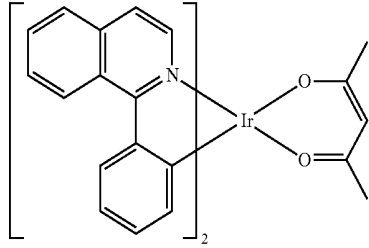
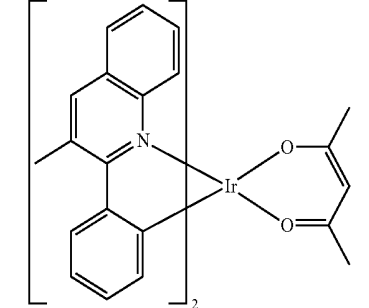
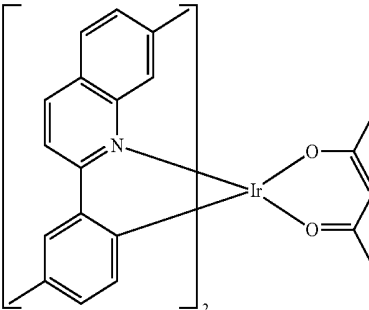
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Heavy metal porphyrins (e.g., PtOEP)	<p style="text-align: center;">Phosphorescent dopants Red dopants</p> 	Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US2006835469
		US2006835469
		US20060202194

TABLE 2-continued

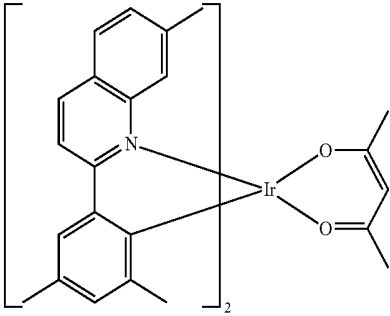
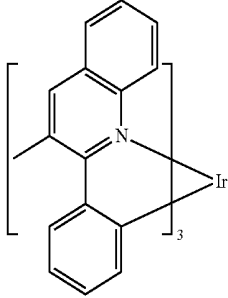
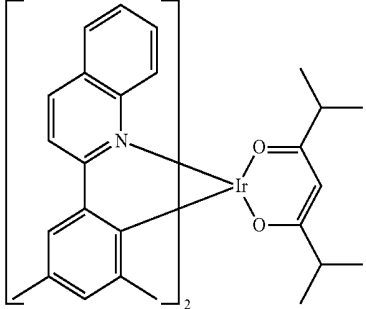
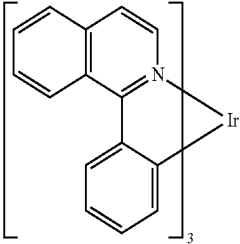
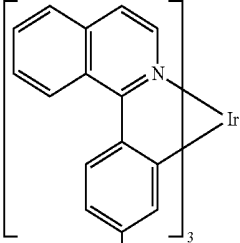
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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		US20070087321
		US20080261076 US20100090591
		US20070087321
	 <p data-bbox="738 2033 791 2065">H₁₇C₈</p>	Adv. Mater. 19, 739 (2007)

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Platinum(II) organometallic complexes		WO2009100991
		WO2008101842
		U.S. Pat. No. 7,232,618
		WO2003040257
		US20070103060

TABLE 2-continued

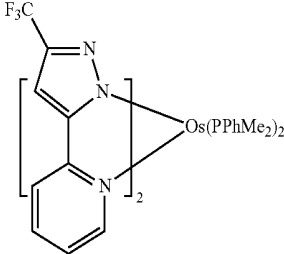
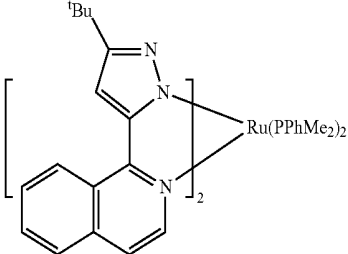
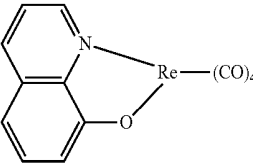
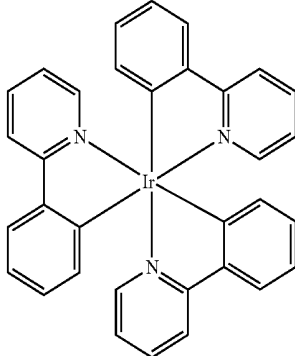
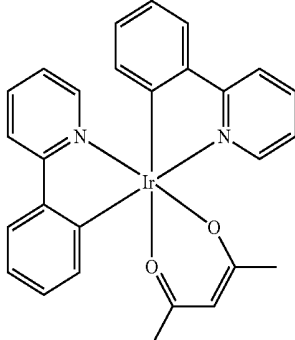
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
Green dopants		
Iridium(III) organometallic complexes	 <p data-bbox="707 1653 839 1675" style="text-align: center;">and its derivatives</p>	Inorg. Chem. 40, 1704 (2001)
		US20020034656

TABLE 2-continued

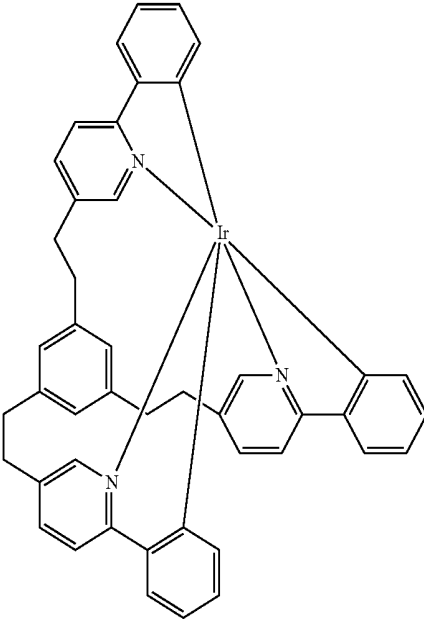
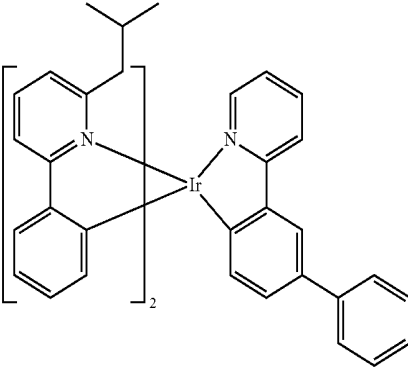
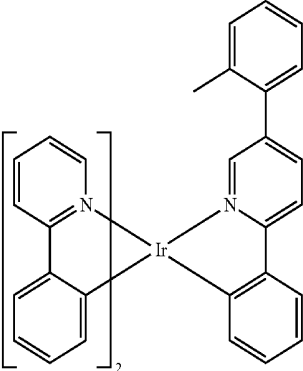
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		U.S. Pat. No. 7,332,232
		US20090108737
		WO2010028151

TABLE 2-continued

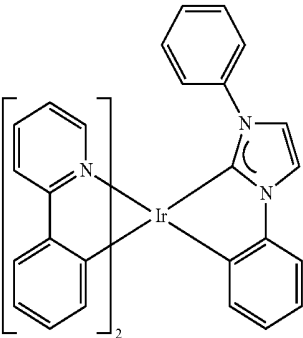
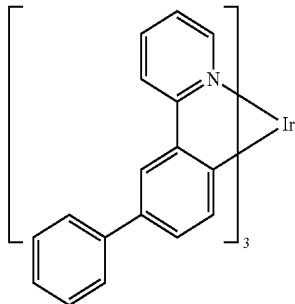
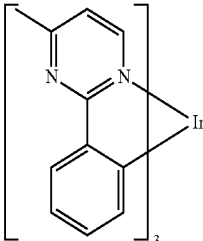
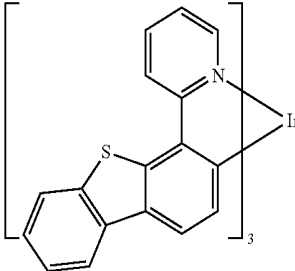
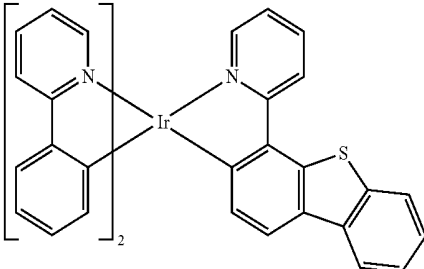
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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		US20060127696
		US20090039776
		U.S. Pat. No. 6,921,915
		US20100244004

TABLE 2-continued

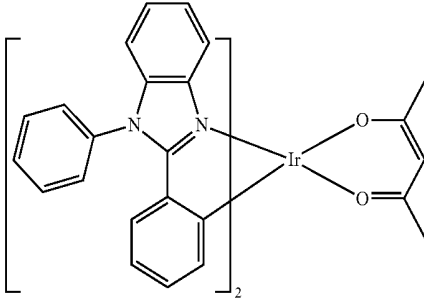
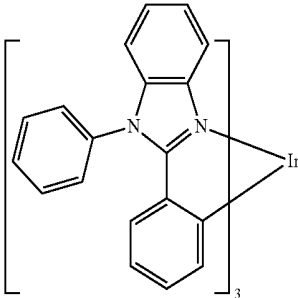
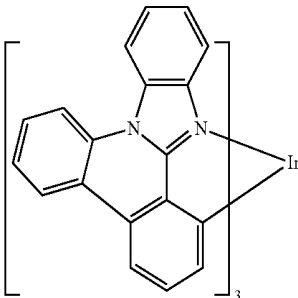
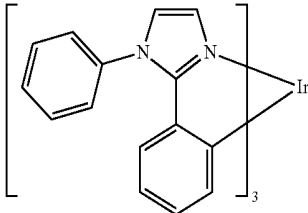
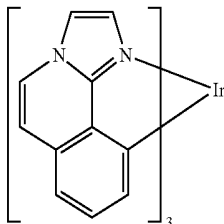
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	 <p>The structure shows an iridium (Ir) center coordinated to two phenylpyridine ligands (each in brackets with a subscript 2) and a chelating diene ligand (1,5-hexadiene derivative). The diene ligand is shown as a six-membered ring with two oxygen atoms and two methyl groups.</p>	U.S. Pat. No. 6,687,266
	 <p>The structure shows an iridium (Ir) center coordinated to three phenylpyridine ligands, each enclosed in brackets with a subscript 3.</p>	Chem. Mater. 16, 2480 (2004)
	 <p>The structure shows an iridium (Ir) center coordinated to three phenylpyridine ligands, each enclosed in brackets with a subscript 3. One of the phenylpyridine ligands is fused to a benzene ring.</p>	US20076190359
	 <p>The structure shows an iridium (Ir) center coordinated to three phenylpyridine ligands, each enclosed in brackets with a subscript 3.</p>	US 20060008670 JP2007123392
	 <p>The structure shows an iridium (Ir) center coordinated to three phenylpyridine ligands, each enclosed in brackets with a subscript 3.</p>	WO2010086089, WO2011044988

TABLE 2-continued

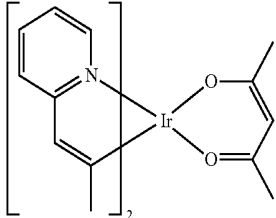
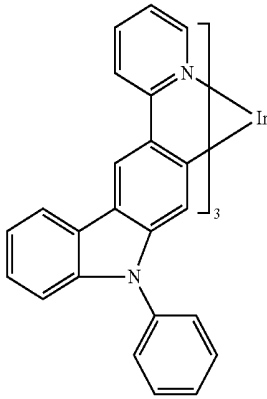
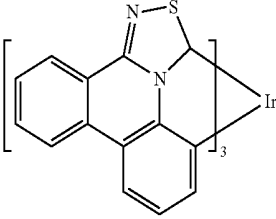
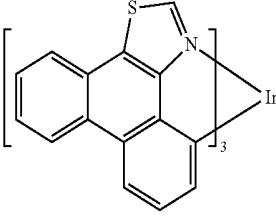
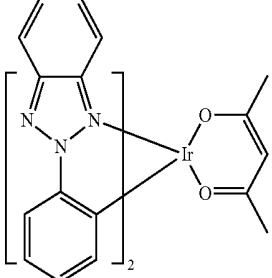
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090065846
		US20080015355

TABLE 2-continued

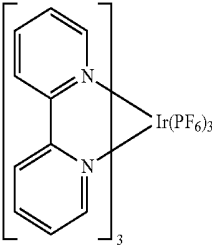
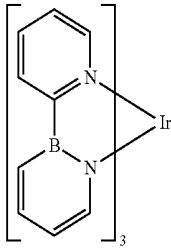
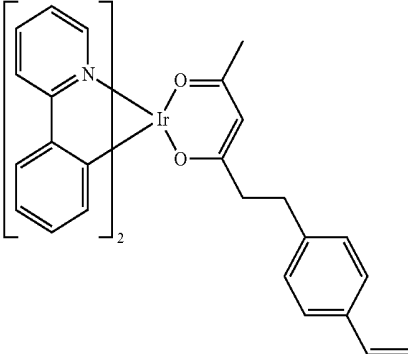
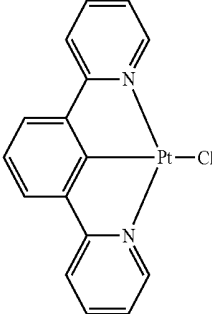
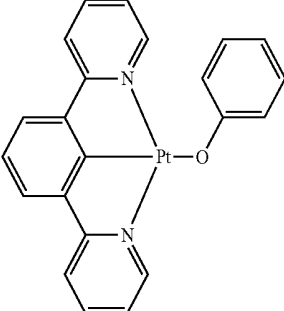
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20010015432
		US20100295032
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentate ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86,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

TABLE 2-continued

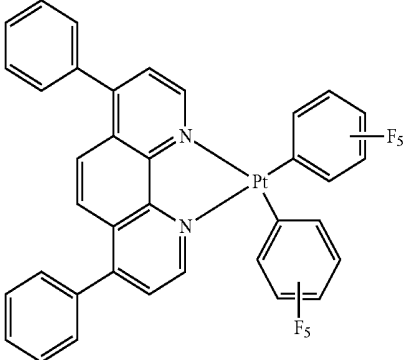
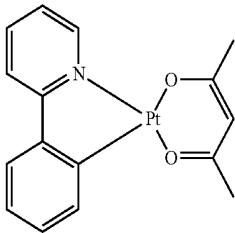
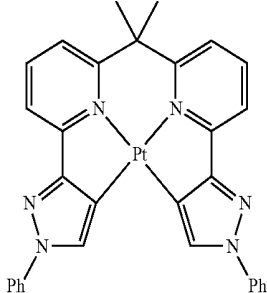
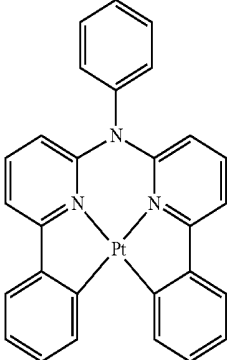
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Chem. Lett. 34, 592 (2005)
		WO2002015645
		US20060263635
		US20060182992 US20070103060

TABLE 2-continued

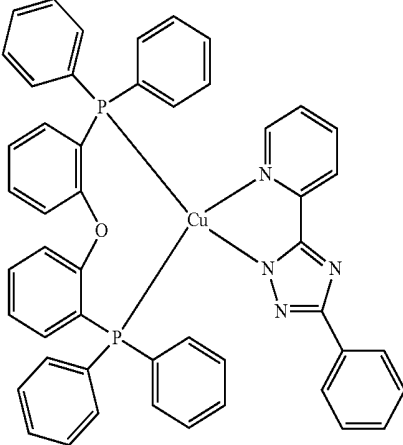
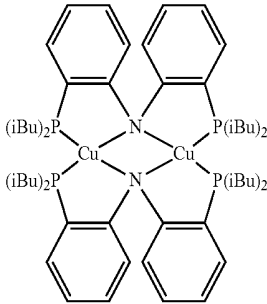
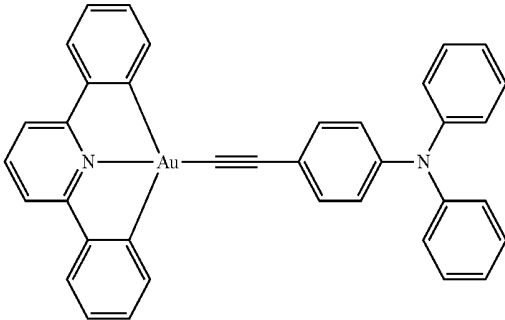
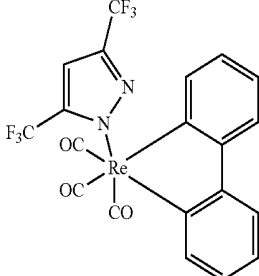
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Cu complexes		WO2009000673
		US20070111026
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE 2-continued

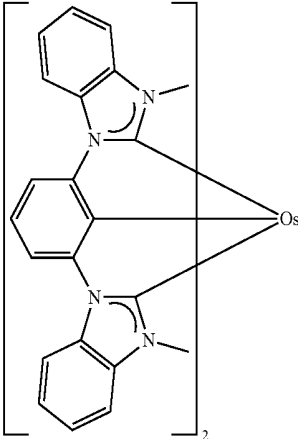
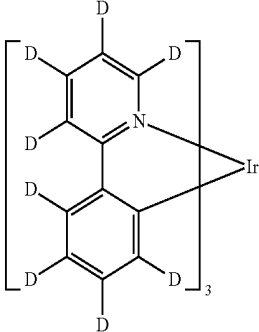
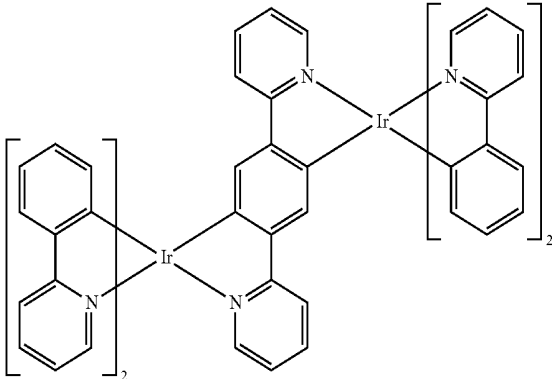
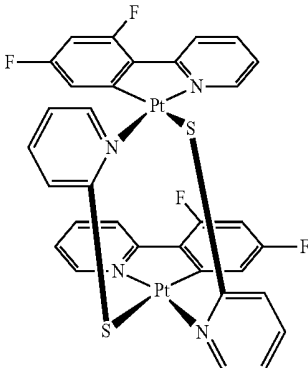
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(II) complexes		U.S. Pat. No. 7,279,704
Deuterated organometallic complexes		US20030138657
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
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 2-continued

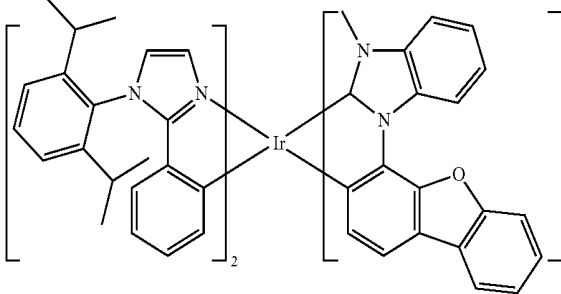
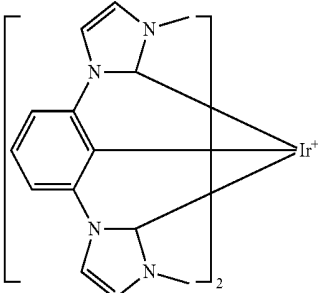
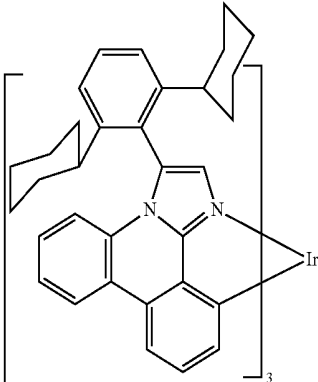
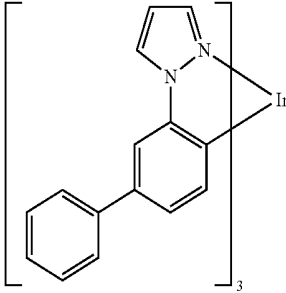
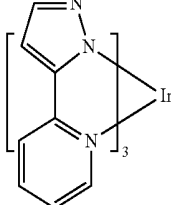
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2011051404
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033 US20100148663
		U.S. Pat. No. 7,338,722
		US20020134984

TABLE 2-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 2-continued

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

TABLE 2-continued

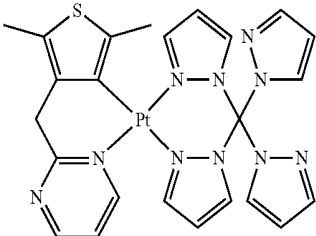
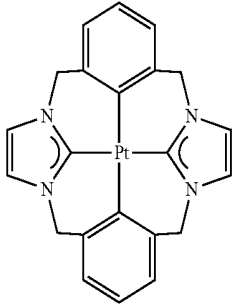
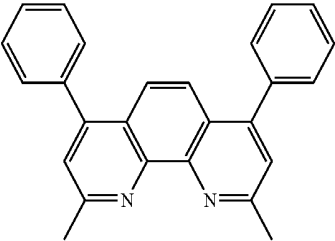
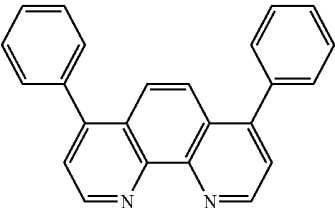
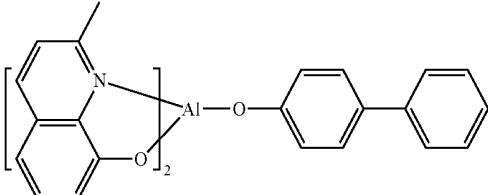
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Platinum(II) complexes		WO2006098120, WO2006103874
Pt tetradentate complexes with at least one metal-carbene bond		U.S. Pat. No. 7,655,323
Exciton/hole blocking layer materials		
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl.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

TABLE 2-continued

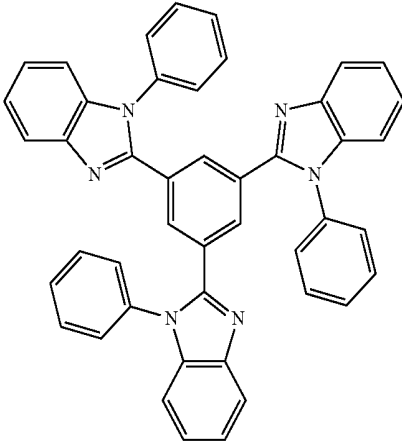
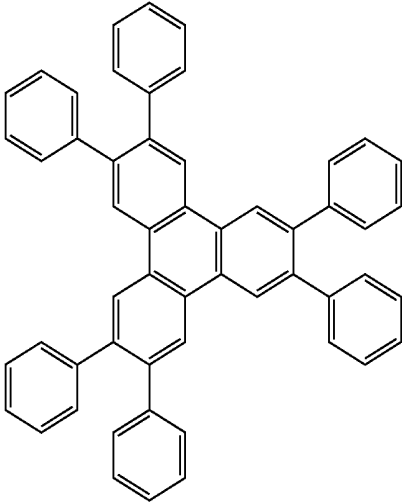
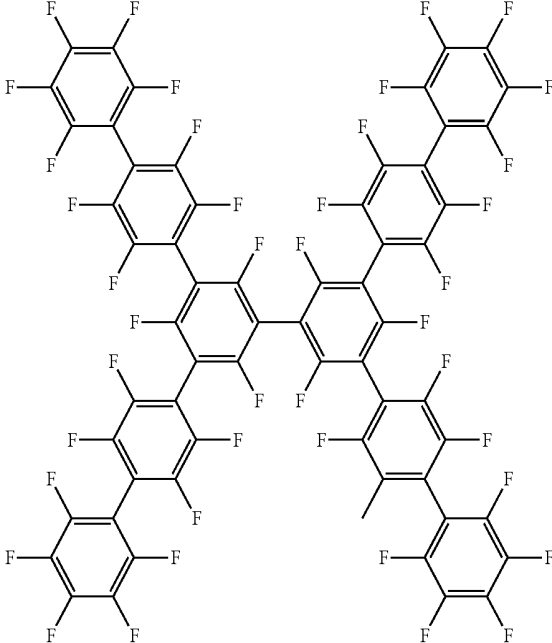
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)

TABLE 2-continued

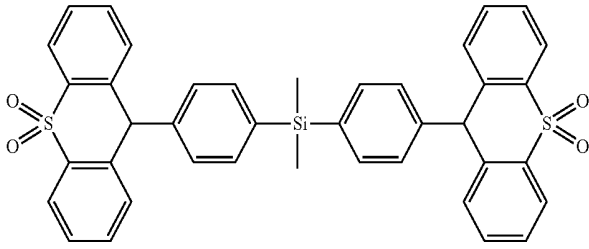
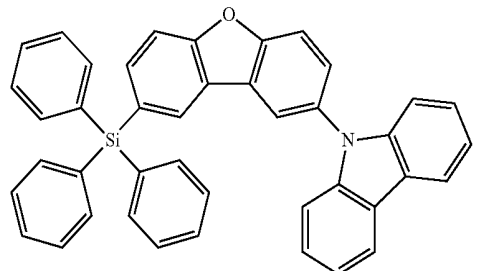
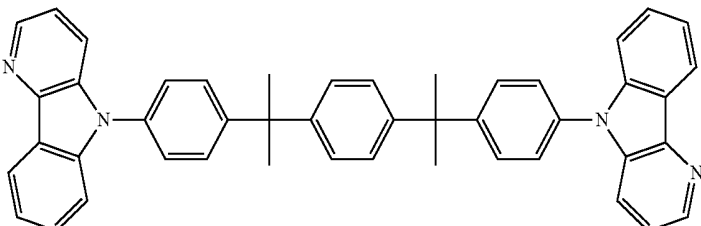
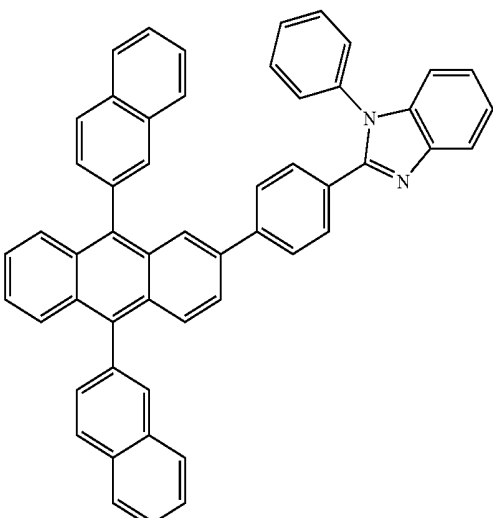
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051
Aza-carbazoles		US20060121308
Electron transporting materials		
Anthracene-benzoimidazole compounds		WO2003060956

TABLE 2-continued

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

TABLE 2-continued

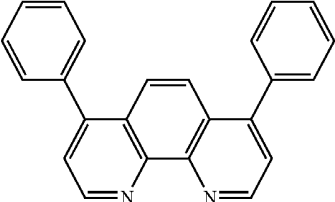
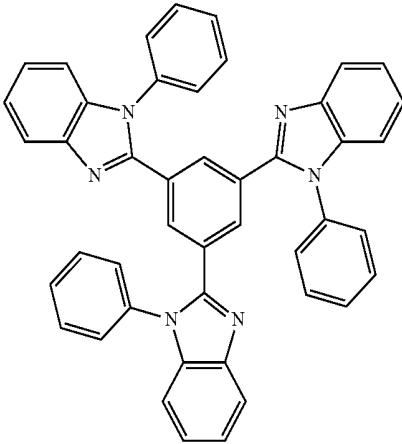
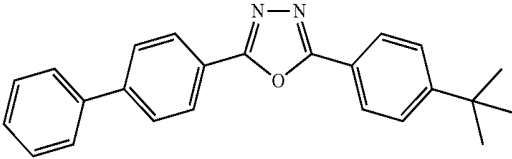
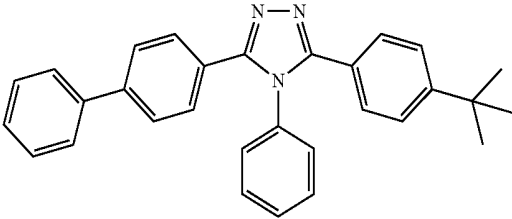
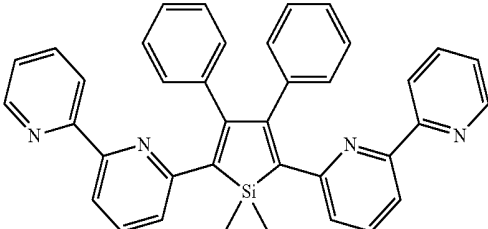
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzimidazole)		Appl. Phys. Lett. 79, 449 (2001)
		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds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

TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g. C60)		US20090101870
Triazine complexes		US20040036077
Zn (N N) complexes		U.S. Pat. No. 6,528,187

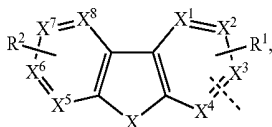
[0137] It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be

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.

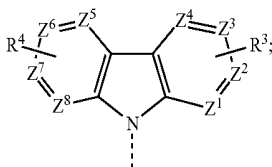
What is claimed is:

1. A compound having a formula:
G¹-L-G², Formula I;
wherein G¹ has the structure:



and

G² has the structure:



wherein L is selected from the group consisting of a direct bond, an aryl group having from 6-30 carbon atoms, a heteroaryl group having from 3-30 carbon atoms, and combinations thereof; wherein the aryl group and the heteroaryl group are optionally further substituted with one or more groups 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;

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

wherein each of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, X⁸, Z¹, Z², Z³, Z⁴, Z⁵, Z⁶, Z⁷, and Z⁸ is carbon or nitrogen;

wherein at least two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen;

wherein at least one of X¹, X², X³, and X⁴ is carbon and bonded to L;

wherein the dashed lines represent the bonds between G¹ and L and G² and L;

wherein each R², R³, and R⁴ represent mono, di, tri, tetra substitutions or no substitution;

wherein R¹ represents mono, di, tri substitutions or no substitution;

wherein R¹, R², R³, and R⁴ 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;

wherein the substitution is optionally fused to G¹ or G²; and

wherein when R³ or R⁴ is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G² by N.

2. The compound of claim 1, wherein when R¹ or R² is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G¹ by N.

3. The compound of claim 1, wherein X is O or S.

4. The compound of claim 1, wherein only two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen.

5. The compound of claim 1, wherein only two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen and on the same ring.

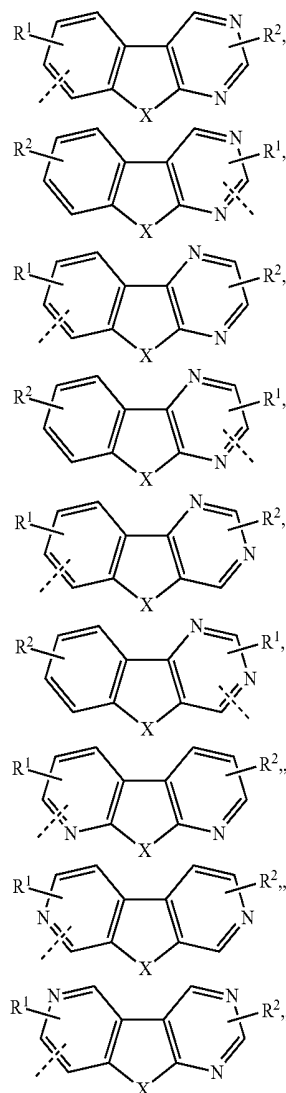
6. The compound of claim 1, wherein only two of X¹, X², X³, X⁴, X⁵, X⁶, X⁷, and X⁸ are nitrogen and on the same ring that is bonded to L.

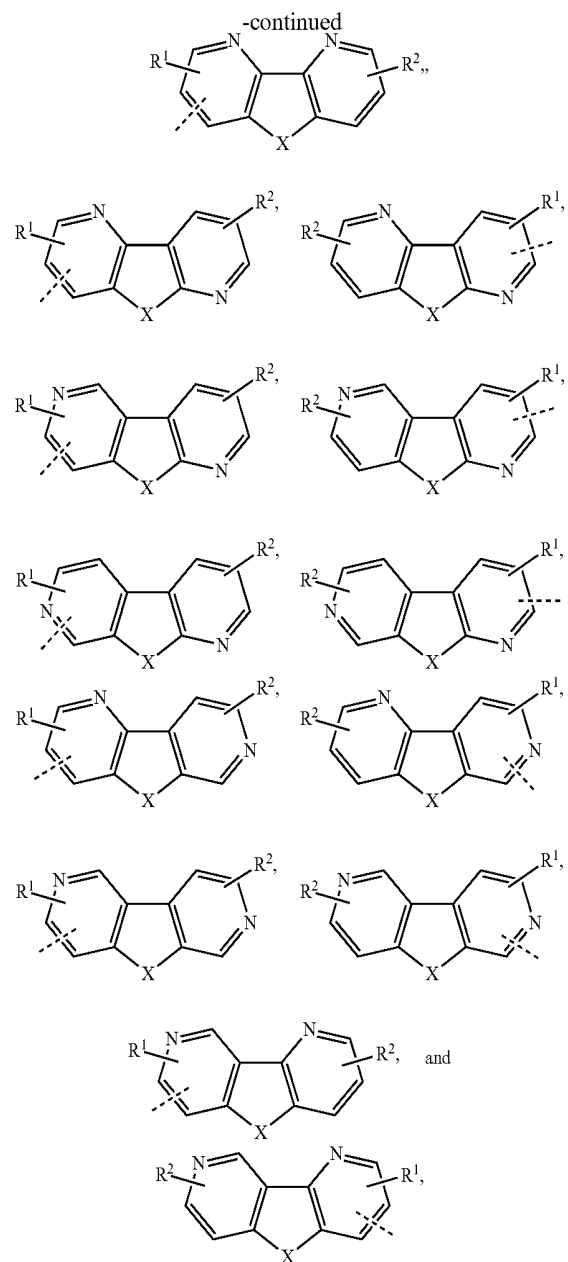
7. The compound of claim 1, wherein each Z¹, Z², Z³, Z⁴, Z⁵, Z⁶, Z⁷, and Z⁸ is carbon.

8. The compound of claim 1, wherein R¹, and R² are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, phenyl, pyridyl, carbazolyl, and combinations thereof.

9. The compound of claim 1, wherein R³, and R⁴ are each independently selected from the group consisting of hydrogen, deuterium, phenyl, pyridyl, 9-carbazolyl, and combinations thereof.

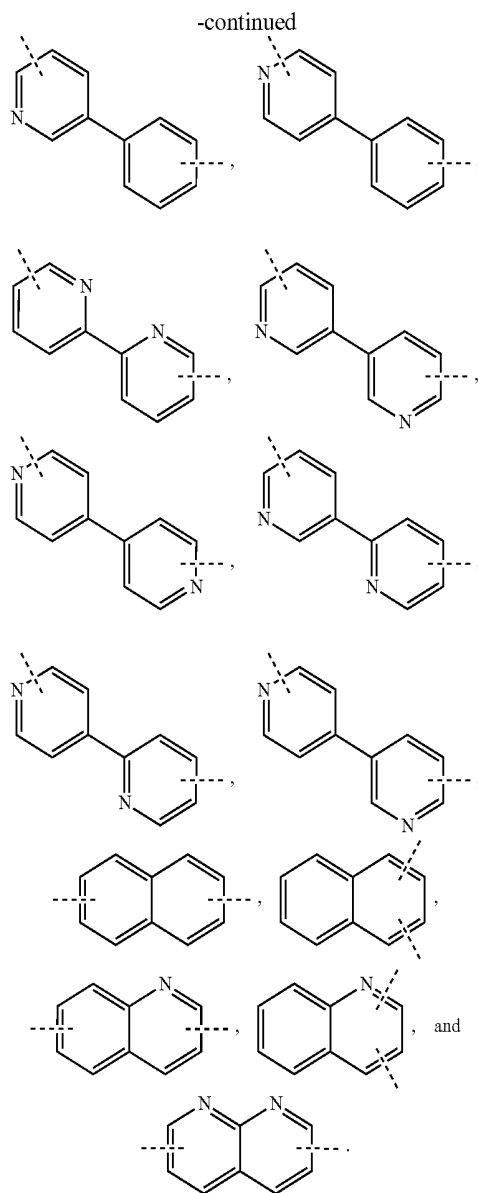
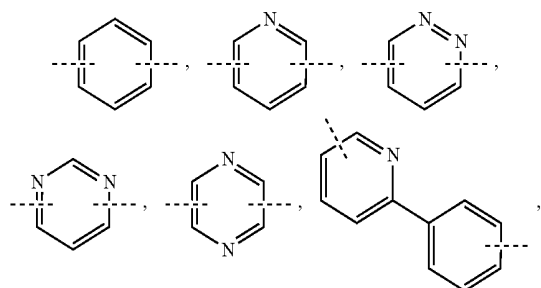
10. The compound of claim 1, wherein G¹ is selected from the group consisting of:



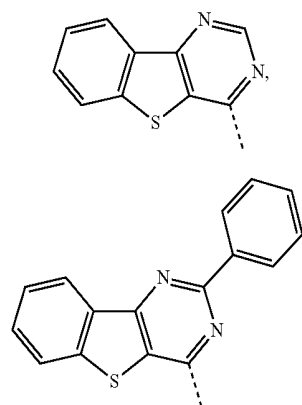


wherein X is selected from the group consisting of O, S, and Se.

11. The compound of claim 1, wherein L is selected from the group consisting of:
a direct bond,



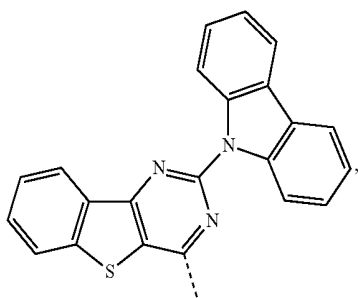
12. The compound of claim 1, wherein G¹ is selected from the group consisting of:



D1

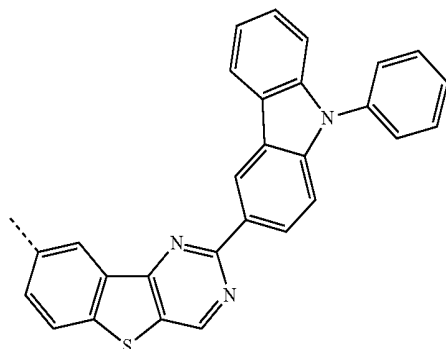
D2

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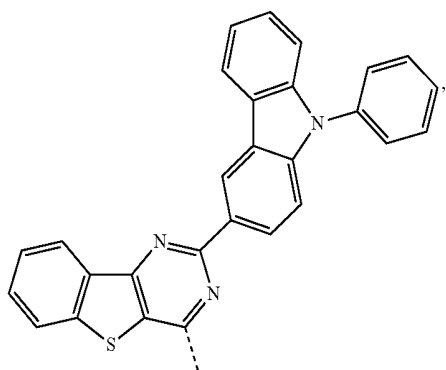


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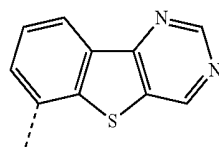
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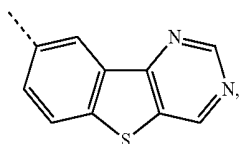
D8



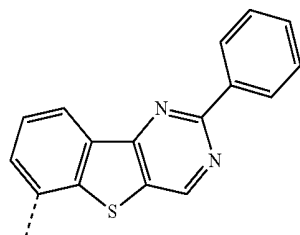
D4



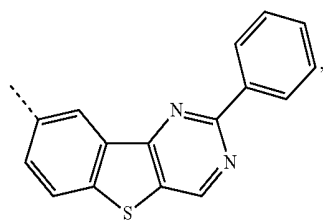
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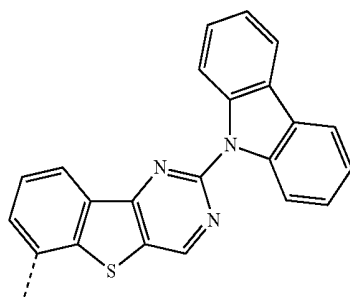
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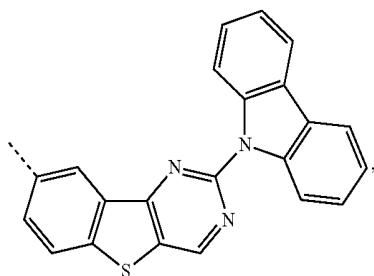
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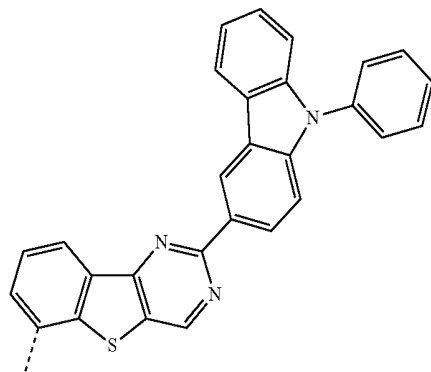
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D11

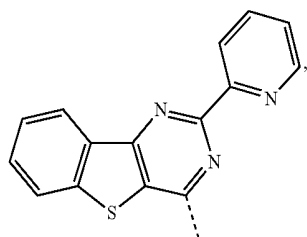


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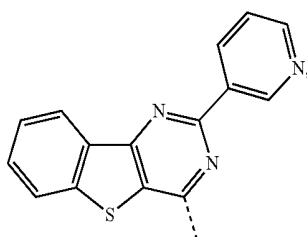


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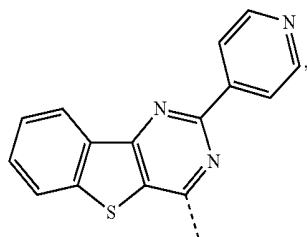
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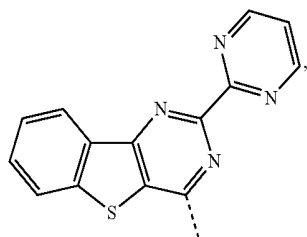
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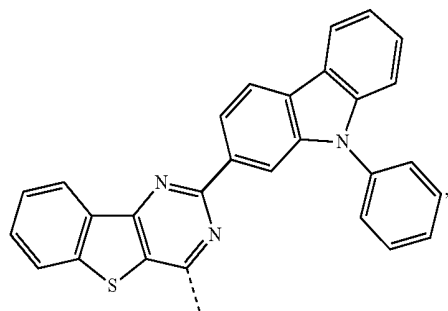
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D15

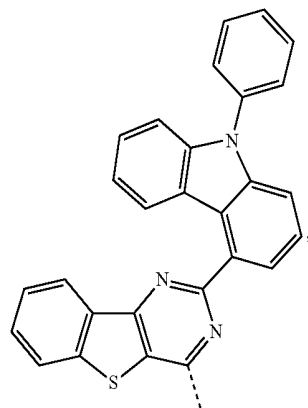


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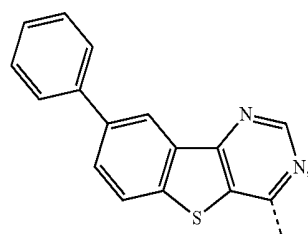


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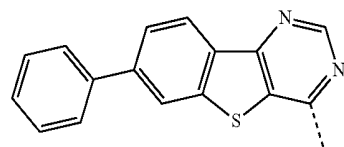
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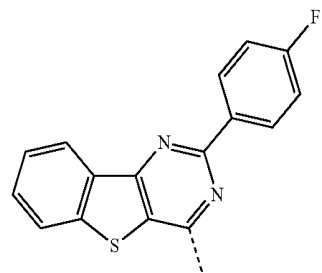
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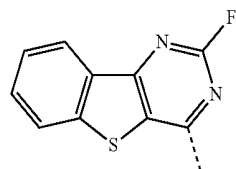
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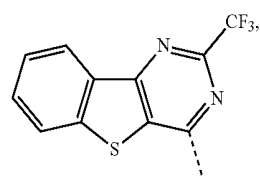
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D21

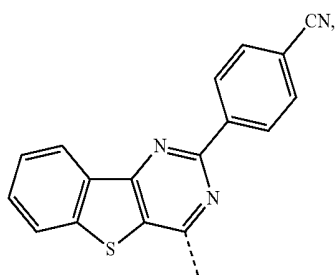


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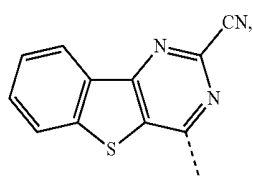


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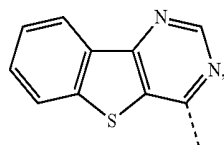
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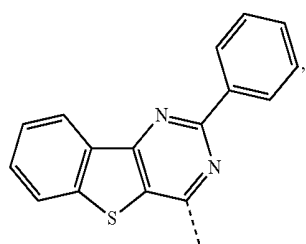
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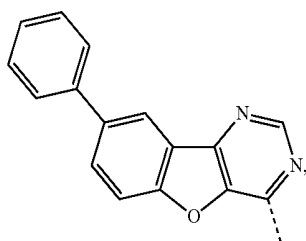
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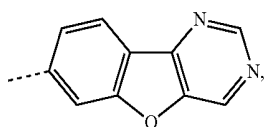
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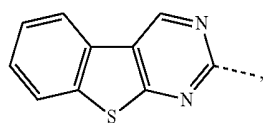
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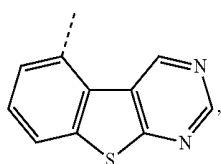
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D29

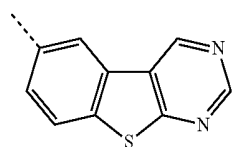


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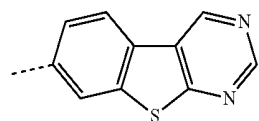


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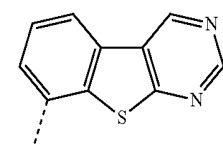
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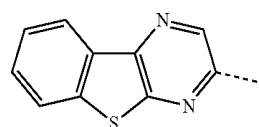
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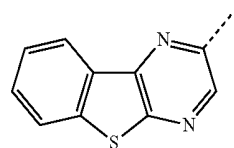
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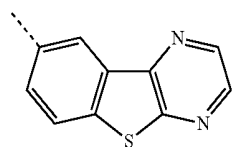
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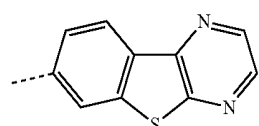
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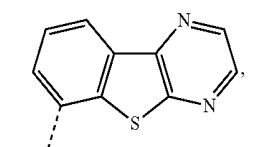
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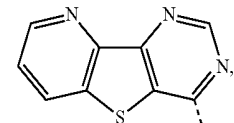
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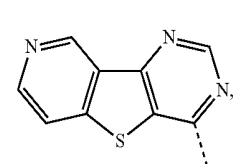
D38



D39

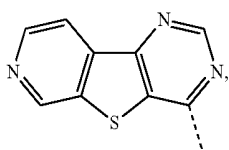


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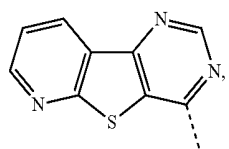


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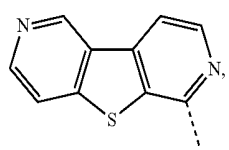
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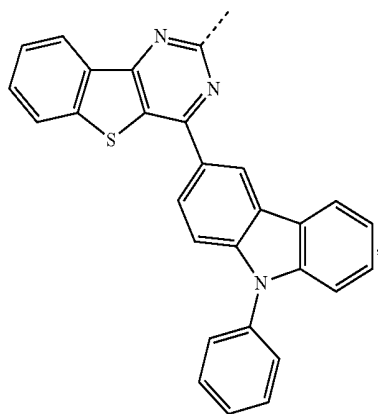
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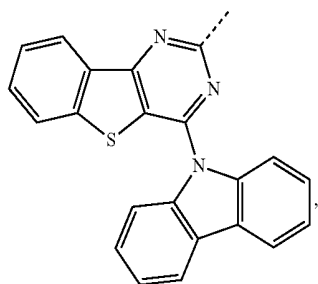
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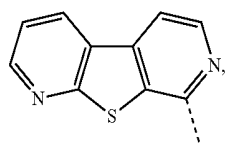
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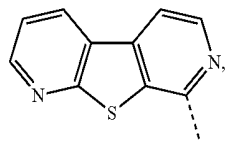
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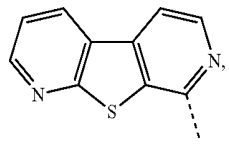
D46



D47

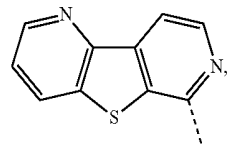


D48

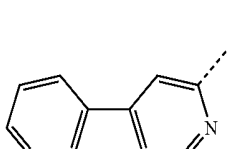


D49

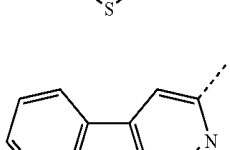
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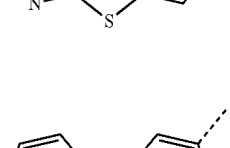
D50



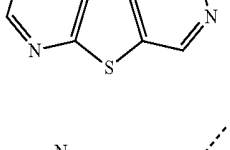
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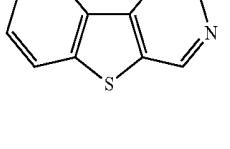
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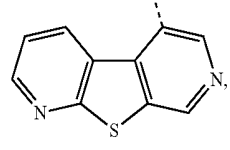
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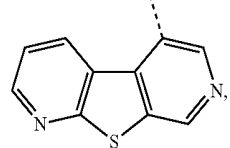
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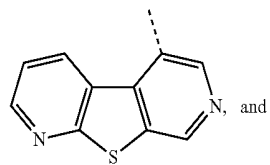
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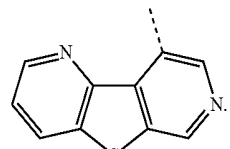
D56



D57

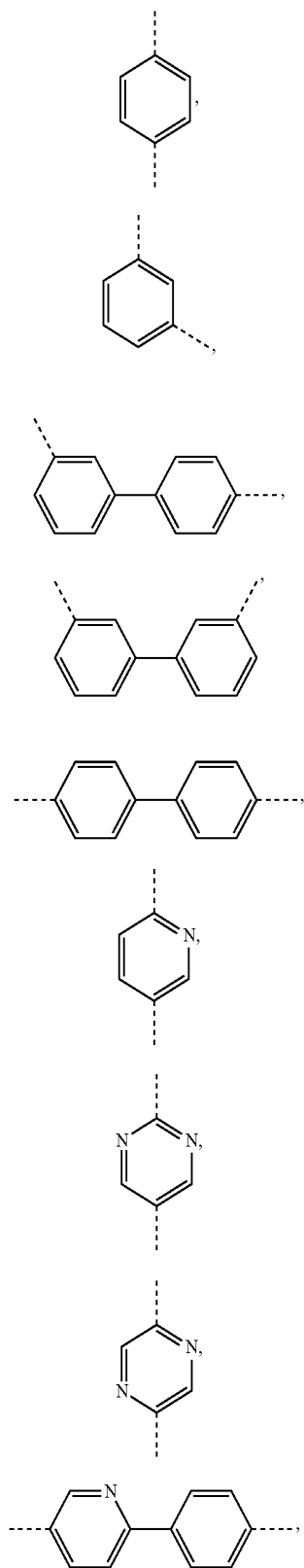


D58



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

a direct bond (L1),



L2

L3

L4

L5

L6

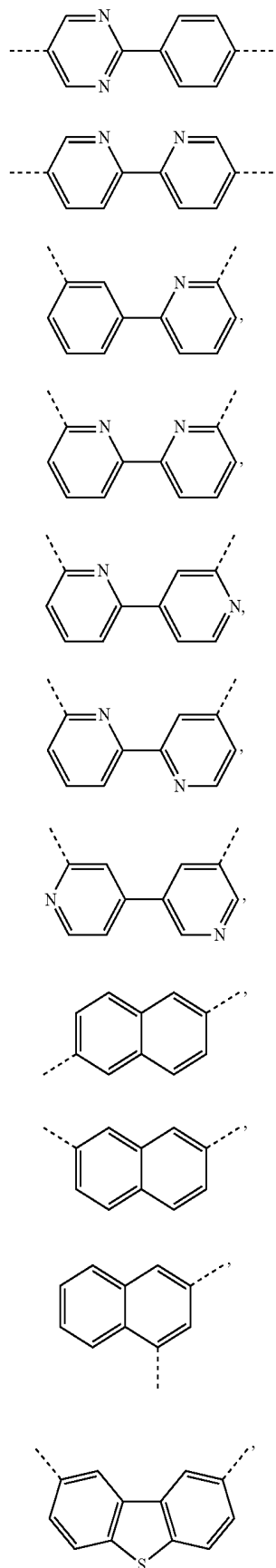
L7

L8

L9

L10

-continued



L11

L12

L13

L14

L15

L16

L17

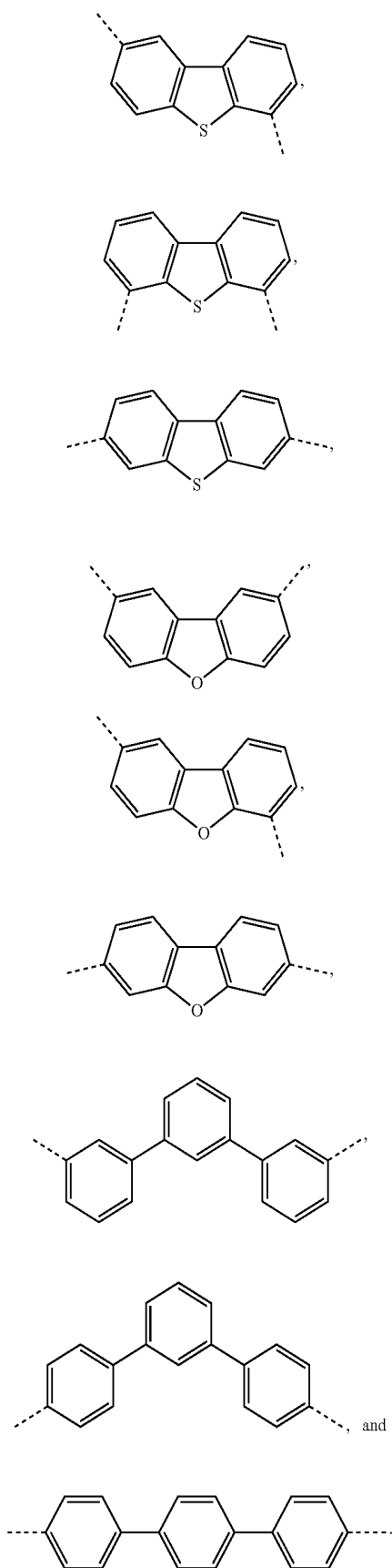
L18

L19

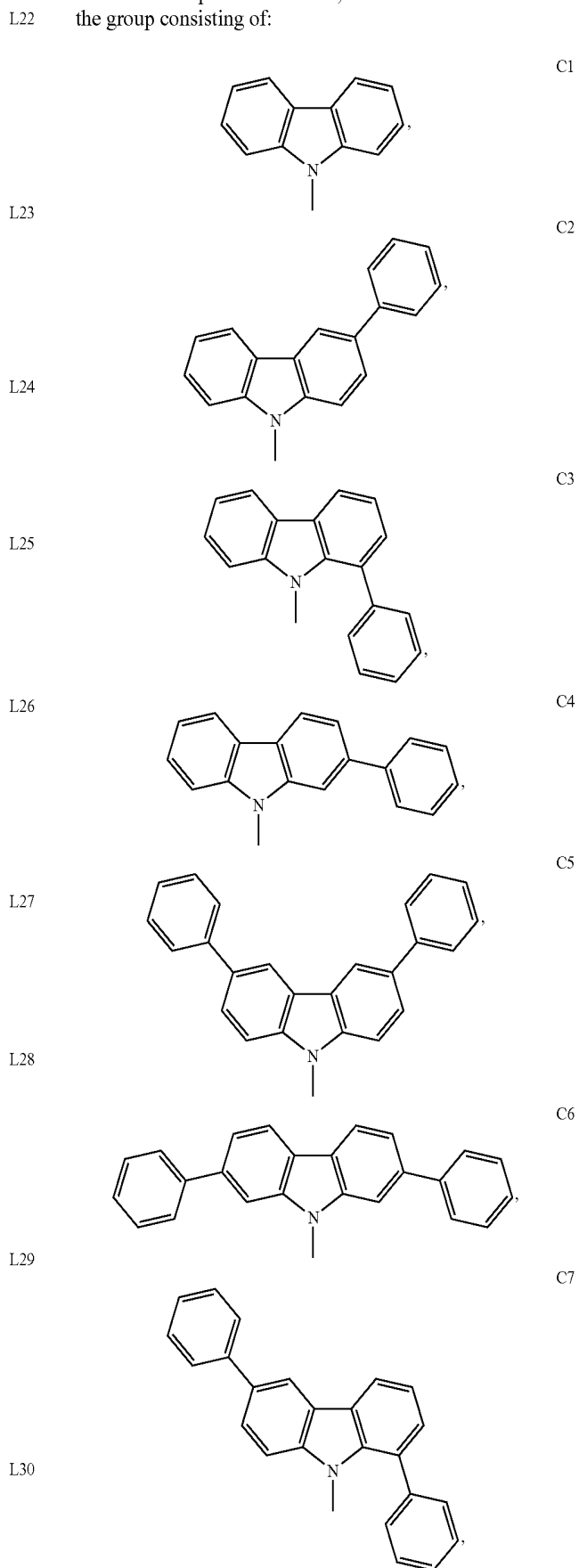
L20

L21

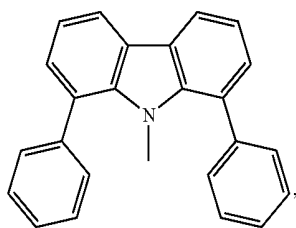
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14. The compound of claim 1, wherein G^2 is selected from the group consisting of:

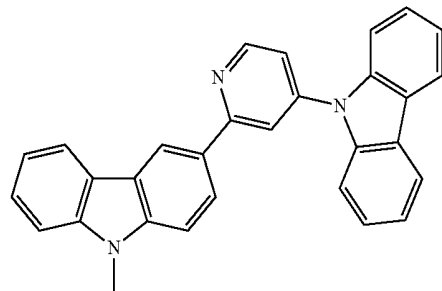


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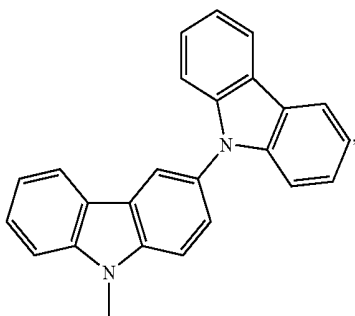
C8

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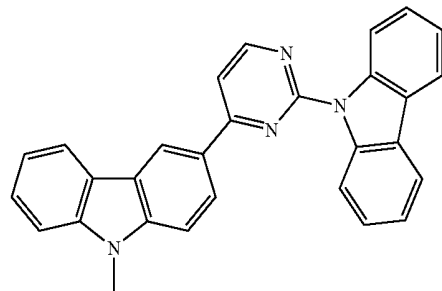


C13

C9

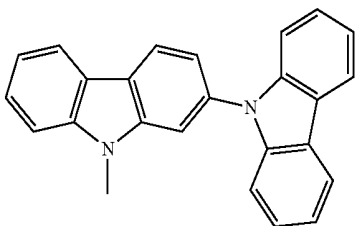


C14

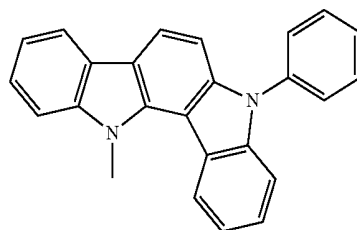


C15

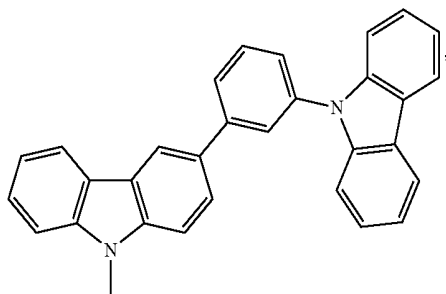
C10



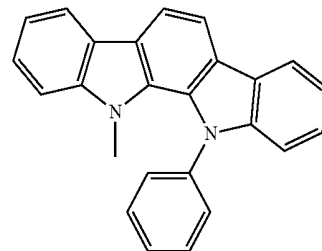
C16



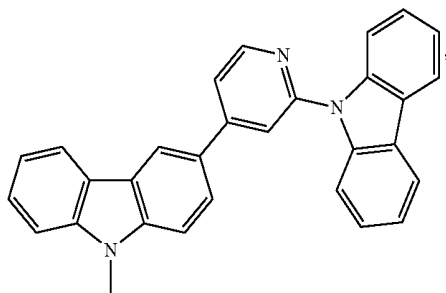
C11



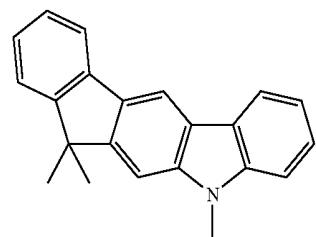
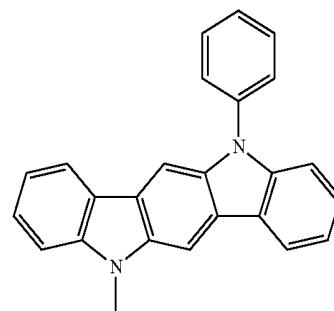
C17



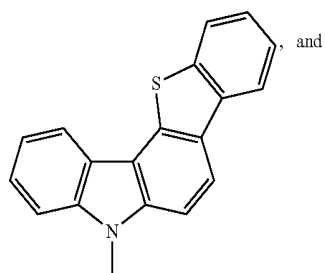
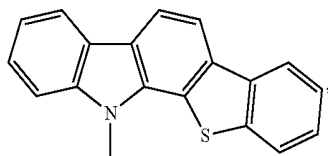
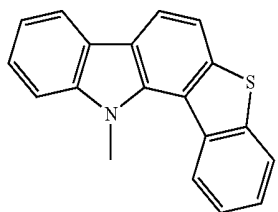
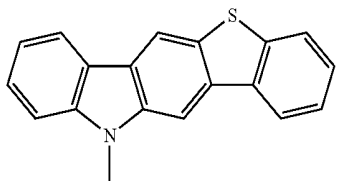
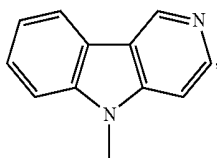
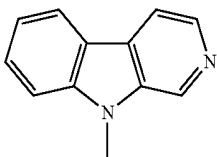
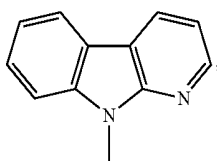
C12



C18



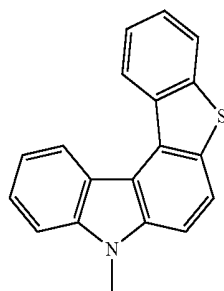
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and

-continued

C19



C26

C20

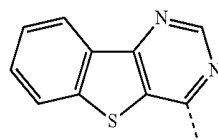
15. The compound of claim 1, wherein the compound is Compound x having the formula Di-Lj-Ck;

C21

wherein $x=1740k+58j+i-1798$, i is an integer from 1 to 58, j is an integer from 1 to 30, and k is an integer from 1 to 26; and

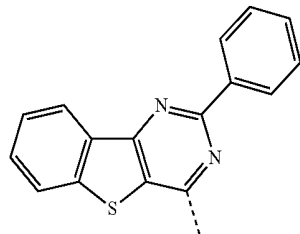
wherein D1 to D58 have the following structures:

C22



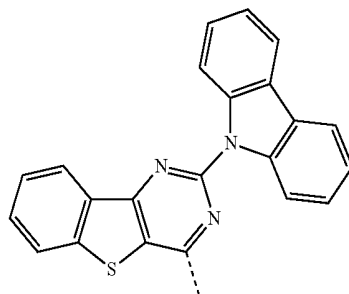
D1

C23



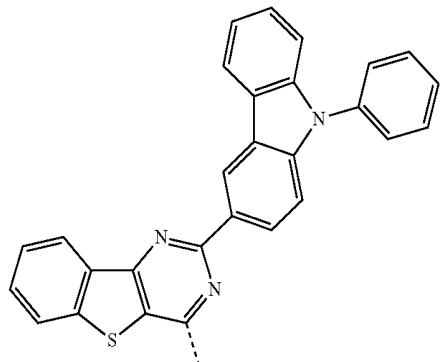
D2

C24



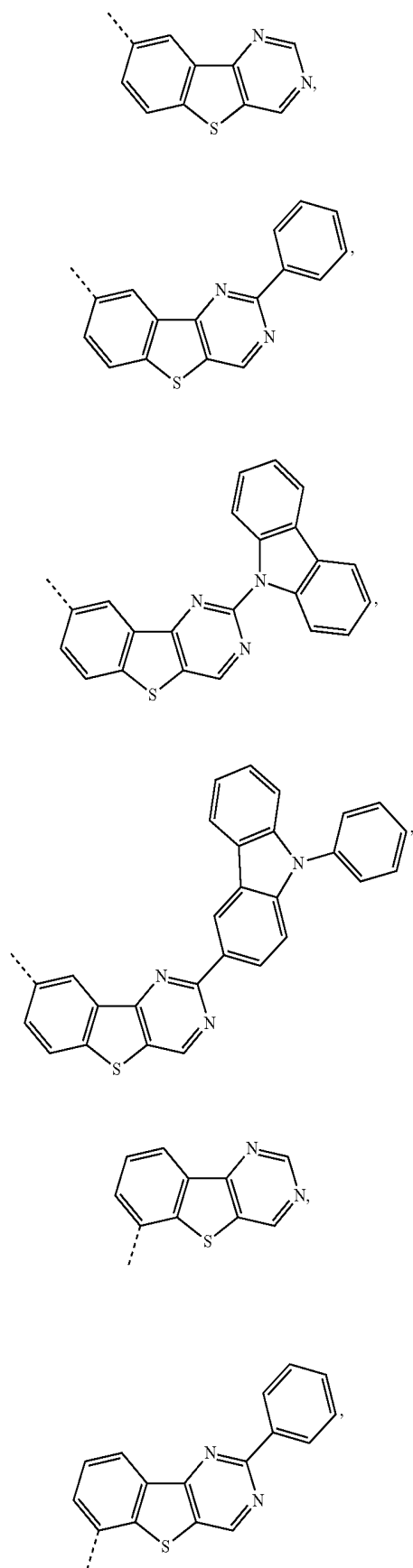
D3

C25

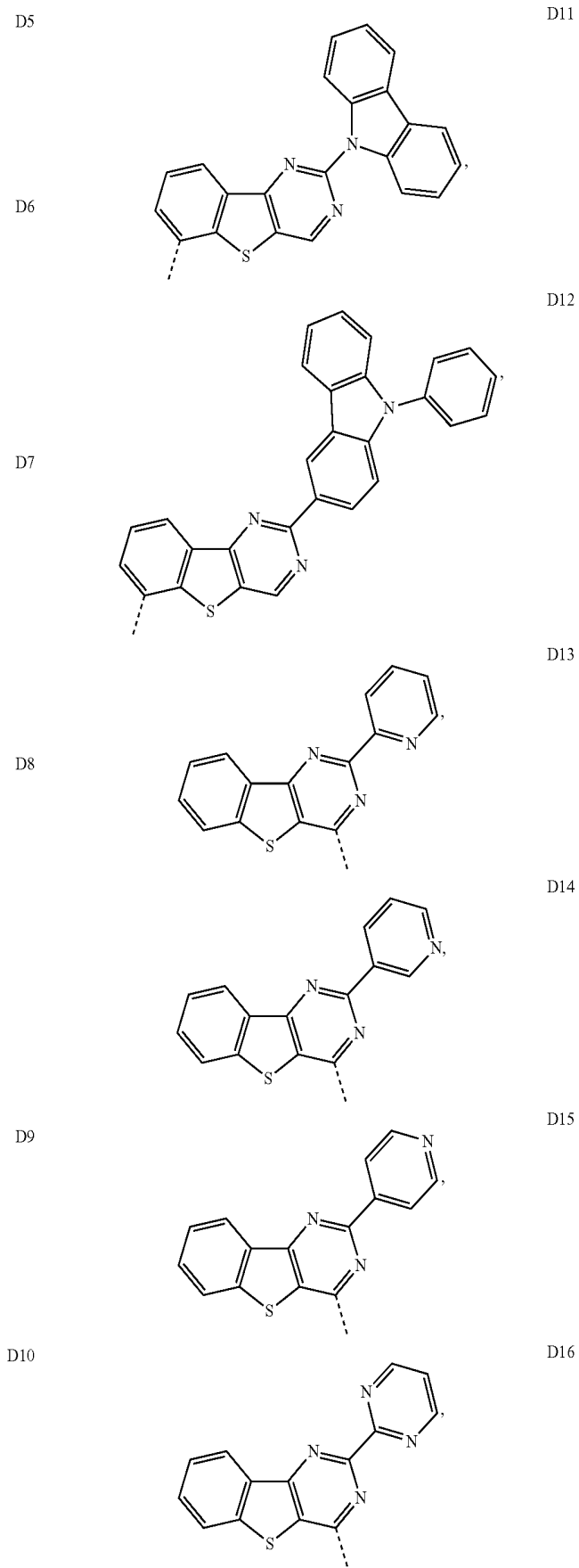


D4

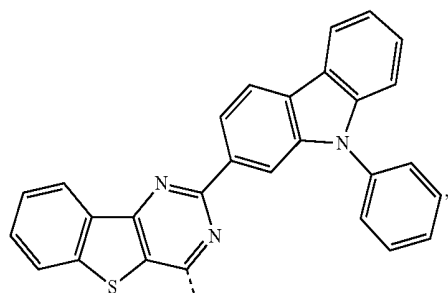
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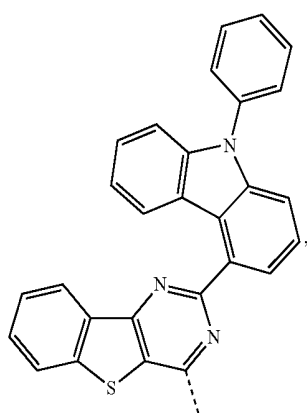
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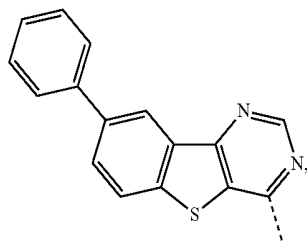
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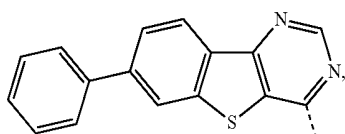
D17



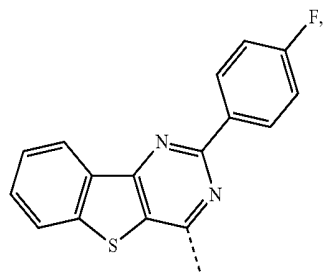
D18



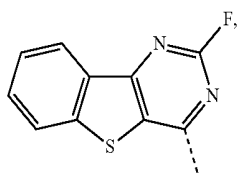
D19



D20

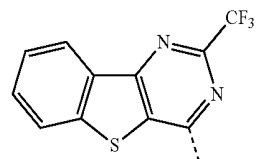


D21

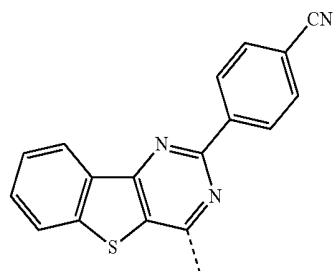


D22

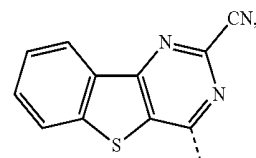
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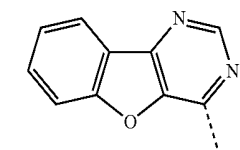
D23



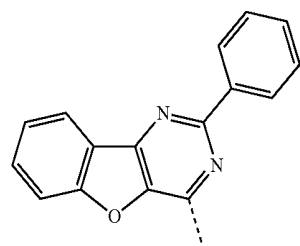
D24



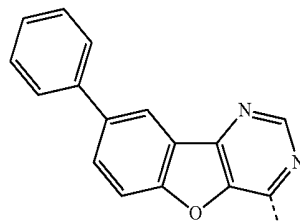
D25



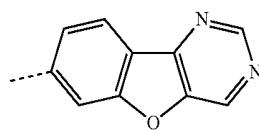
D26



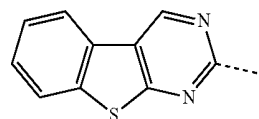
D27



D28

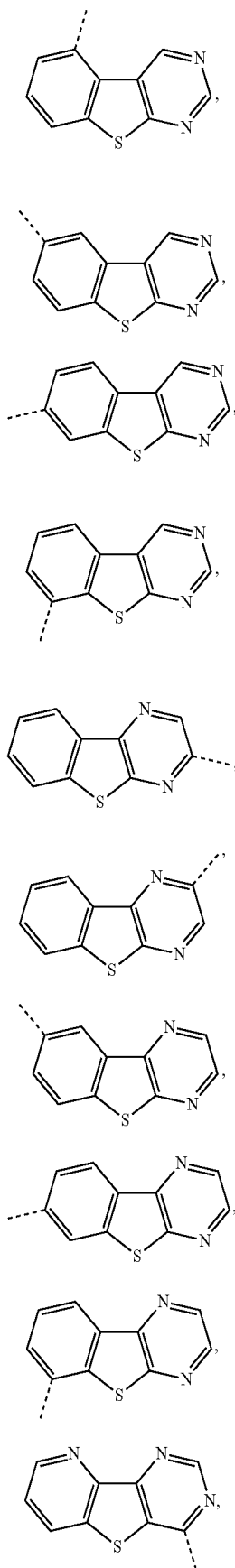


D29

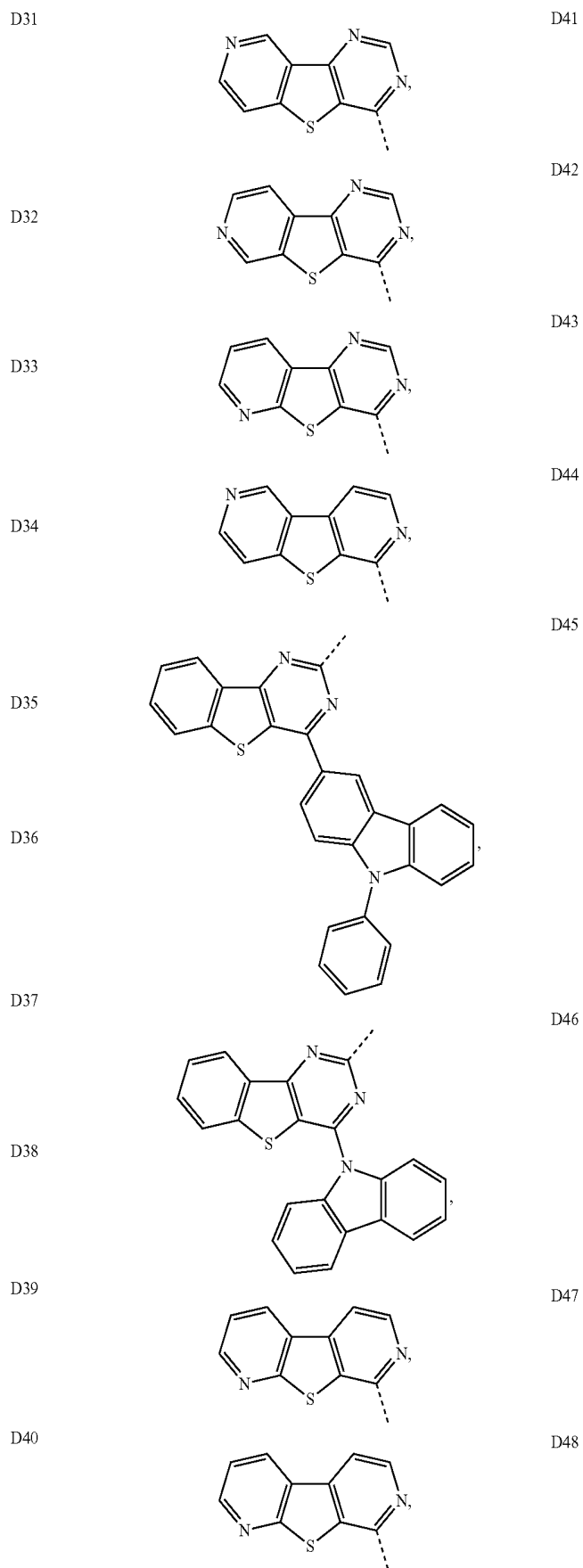


D30

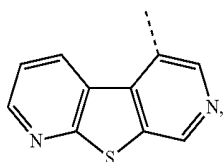
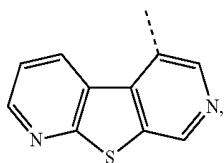
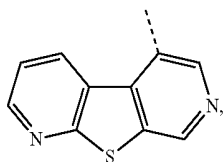
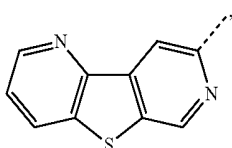
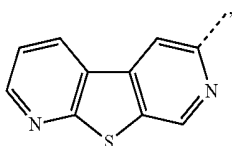
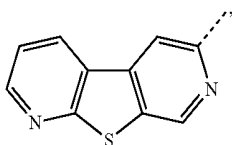
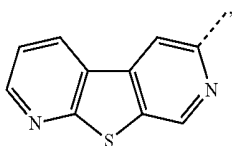
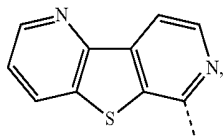
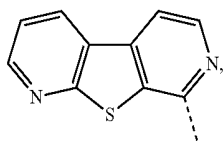
-continued



-continued



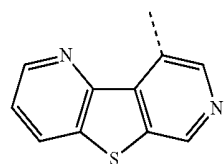
-continued



-continued

D49

D58

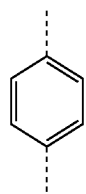


D50

wherein L1 to L30 have the following structures:
L1 is a direct bond,

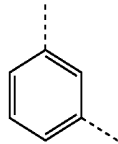
L2

D51



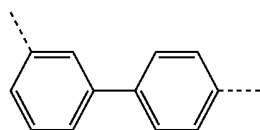
L3

D52



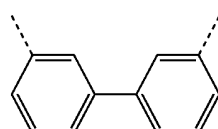
L4

D53



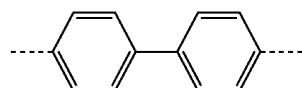
L5

D54



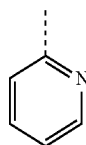
L6

D55



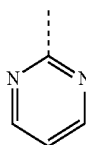
L7

D56

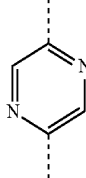


L8

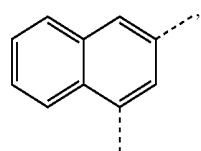
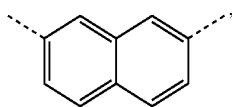
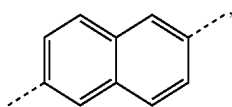
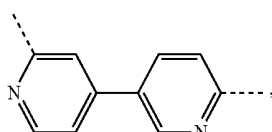
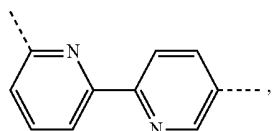
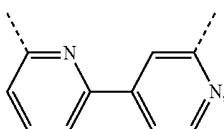
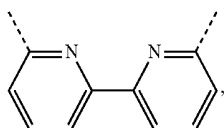
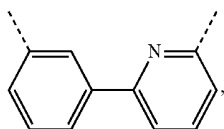
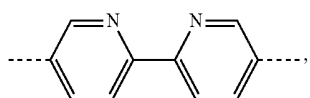
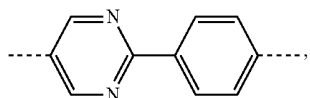
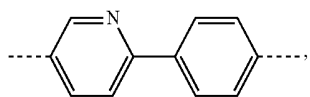
D57



L9



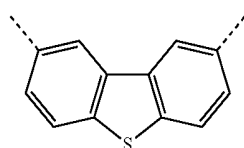
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-continued

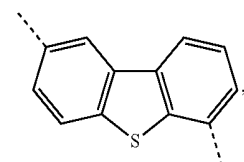
L10

L21



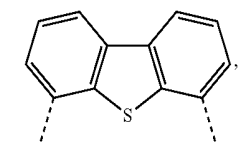
L11

L22



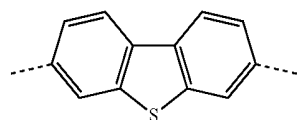
L12

L23



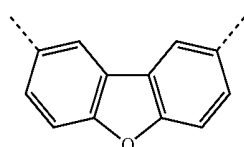
L13

L24



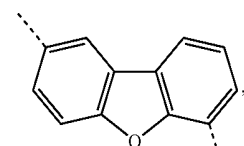
L14

L25



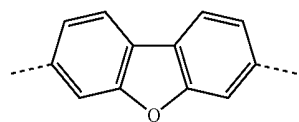
L15

L26



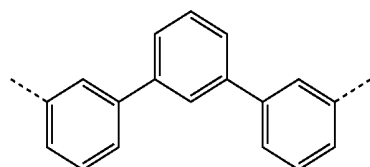
L16

L27



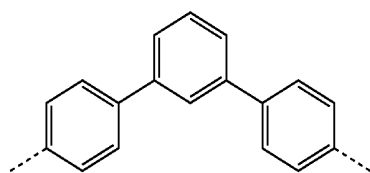
L17

L28



L18

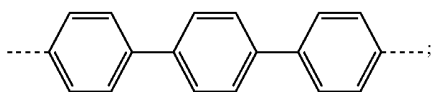
L29



L19

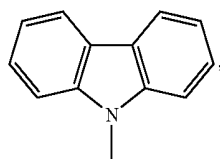
L20

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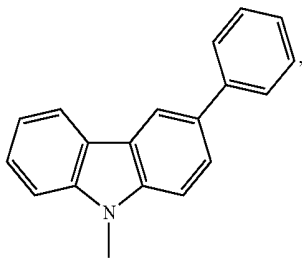


and

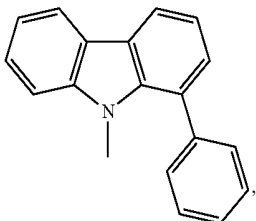
wherein C1 to C26 have the following structures:



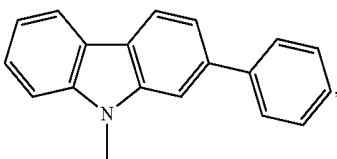
C1



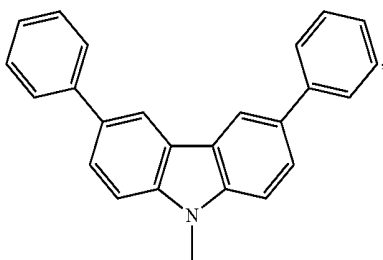
C2



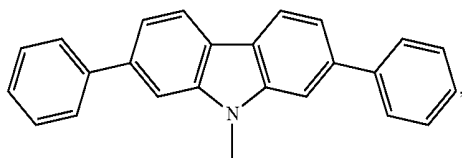
C3



C4

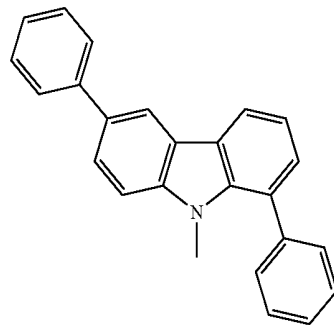


C5

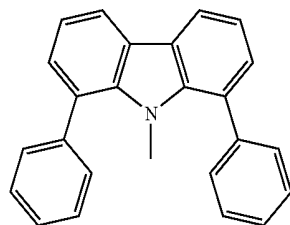


C6

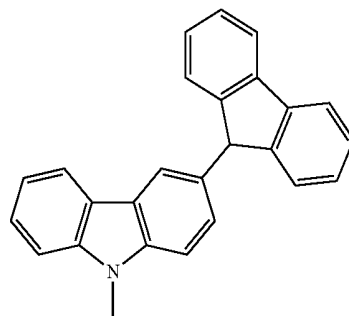
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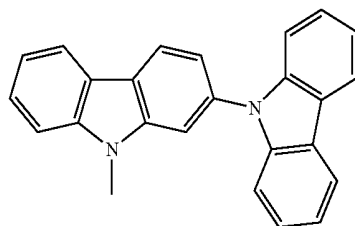
C7



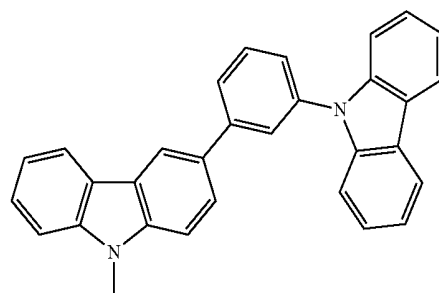
C8



C9



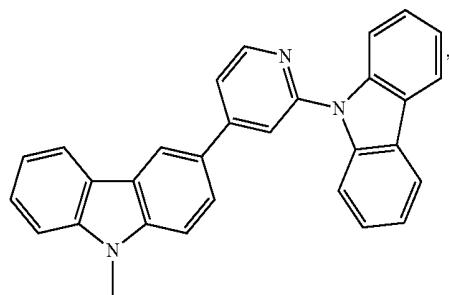
C10



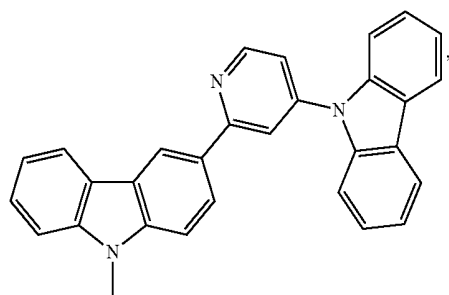
C11

L30

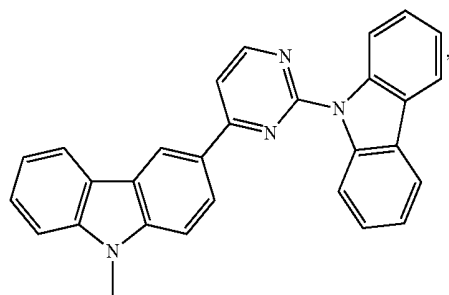
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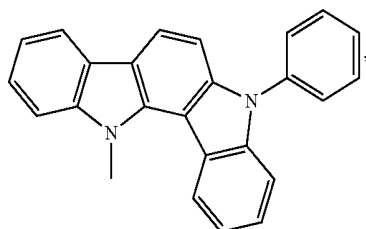
C12



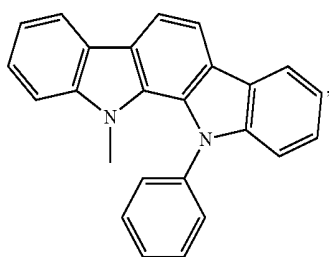
C13



C14

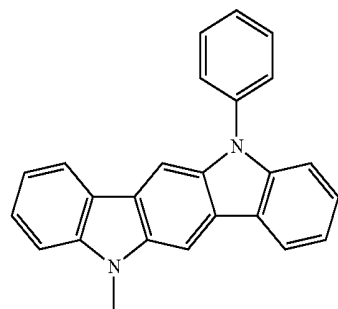


C15

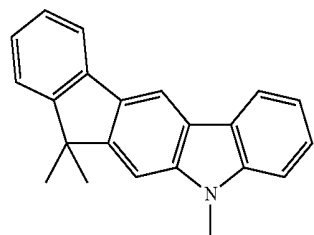


C16

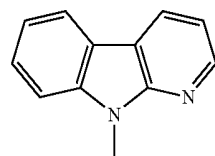
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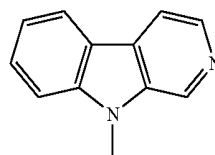
C17



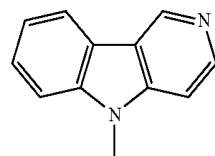
C18



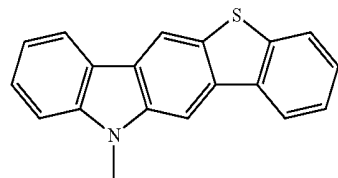
C19



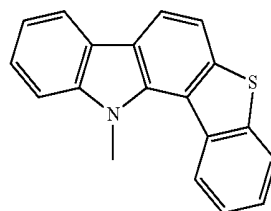
C20



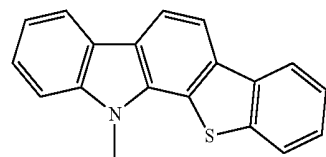
C21



C22

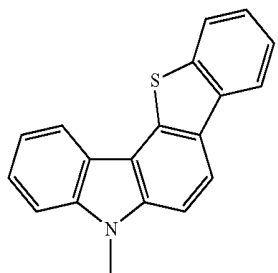


C23



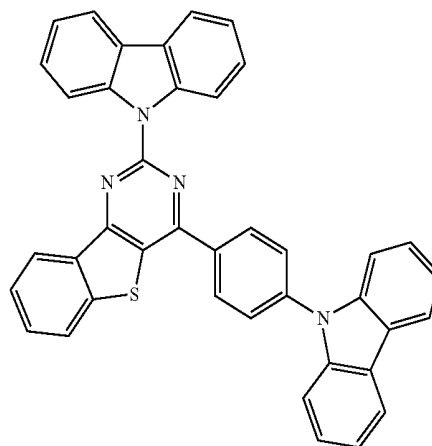
C24

-continued



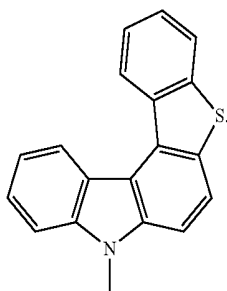
C25

-continued



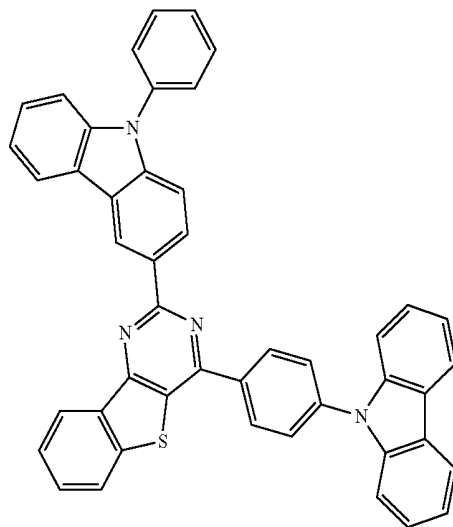
Compound 61

C26

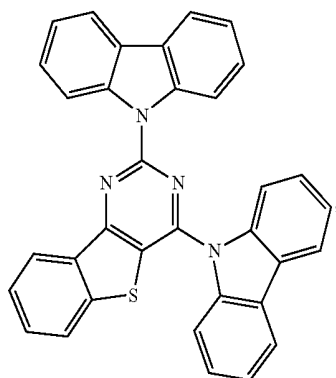


Compound 62

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

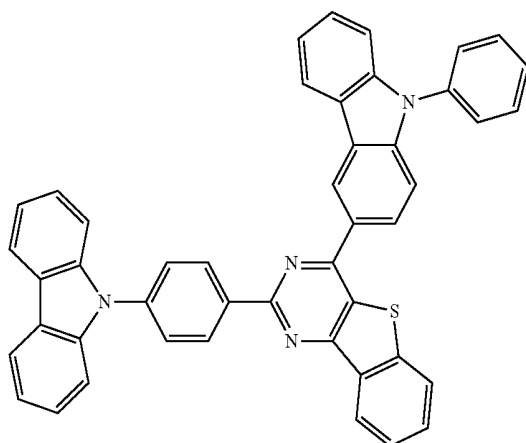
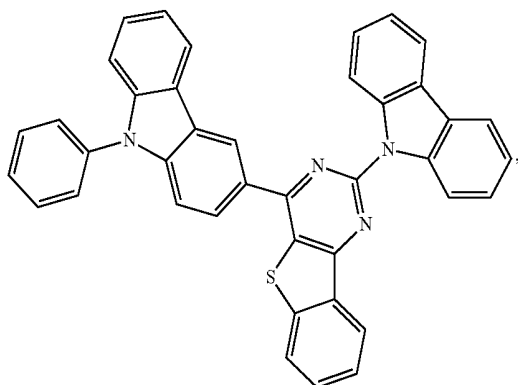


Compound 3



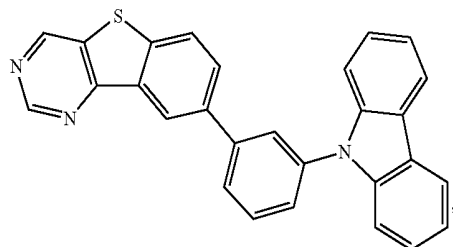
Compound 103

Compound 45

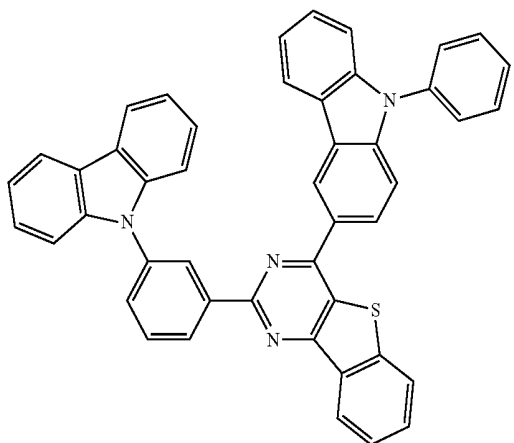


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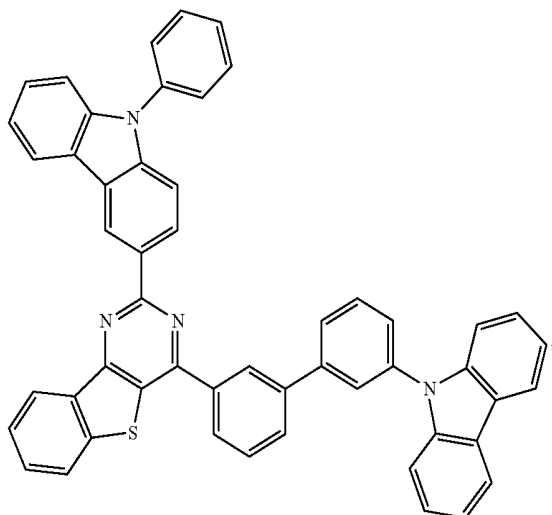
Compound 121



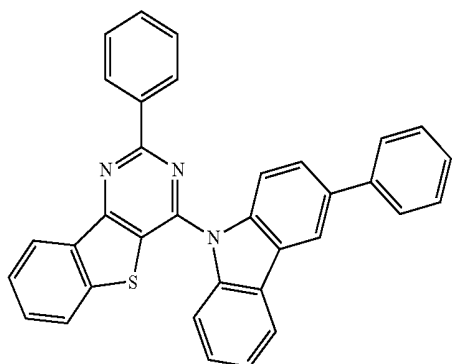
Compound 161



Compound 236

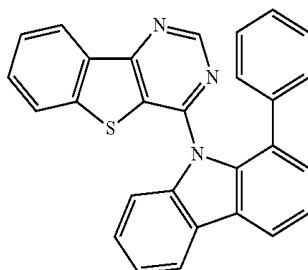


Compound 1742

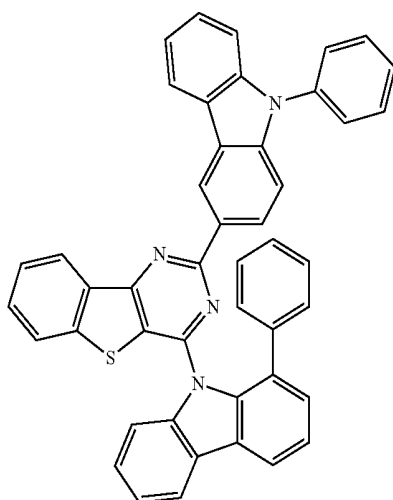


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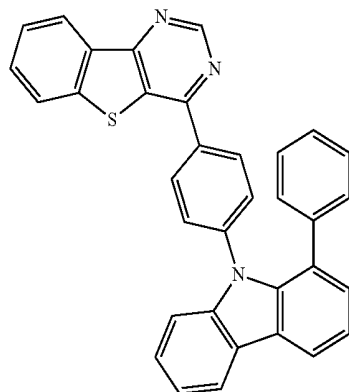
Compound 3481



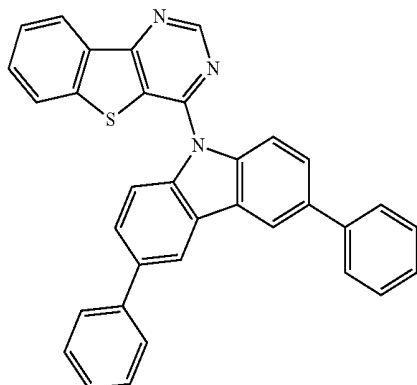
Compound 3484



Compound 3539

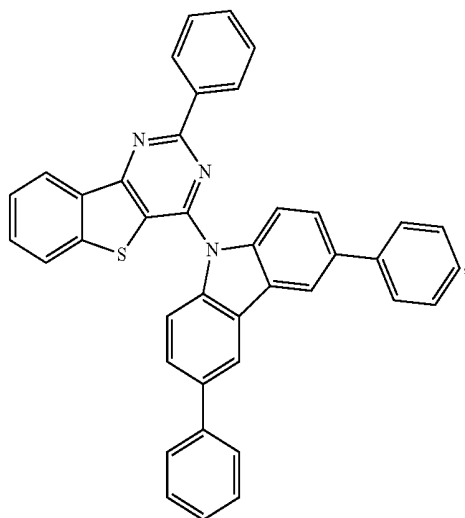


Compound 6961



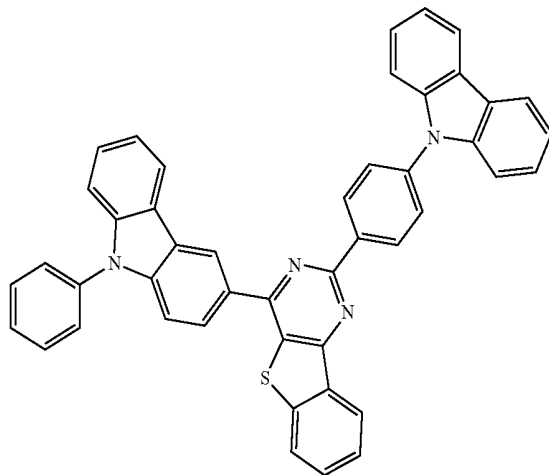
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Compound 6962

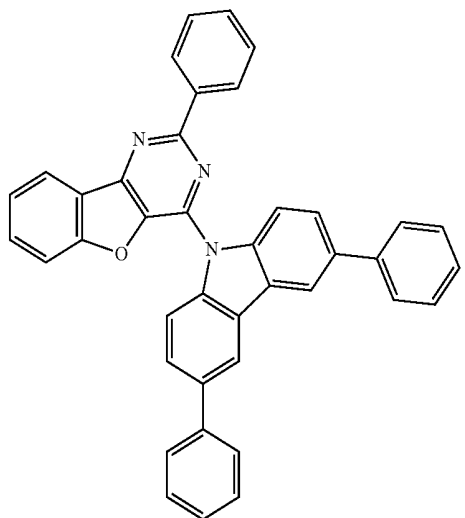


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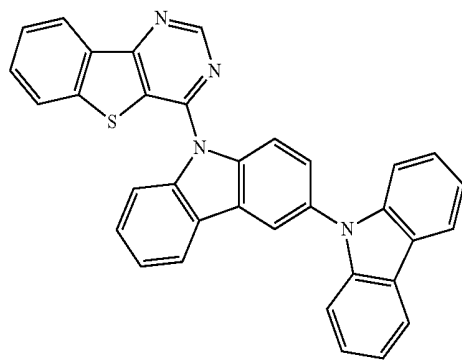
Compound 7121



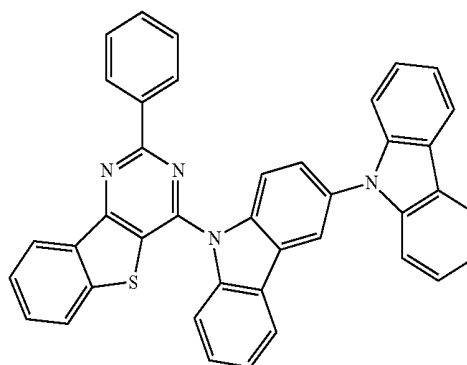
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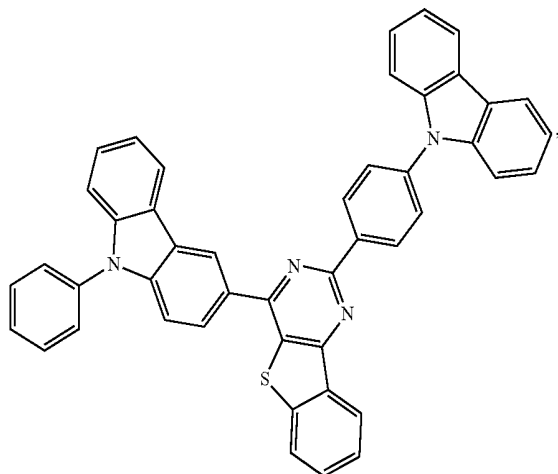
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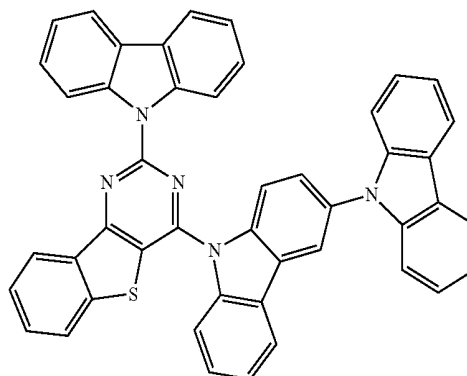
Compound 13922



Compound 7063

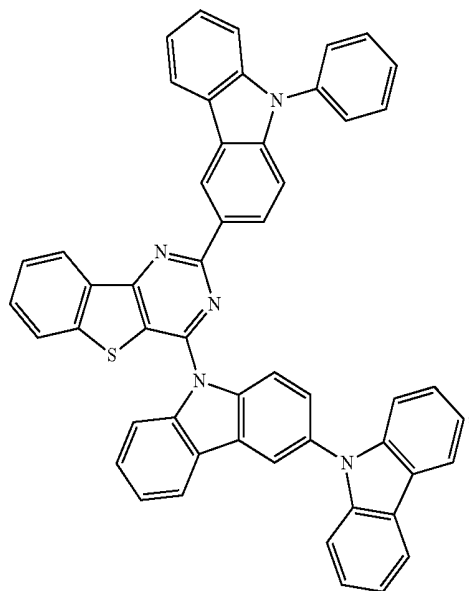


Compound 13923



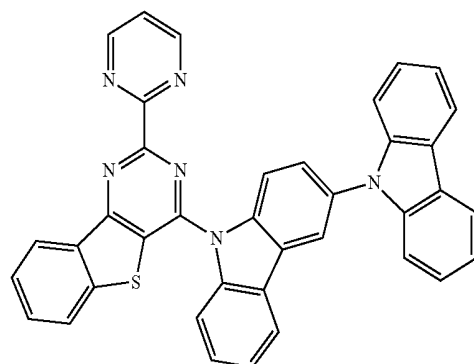
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Compound 13924



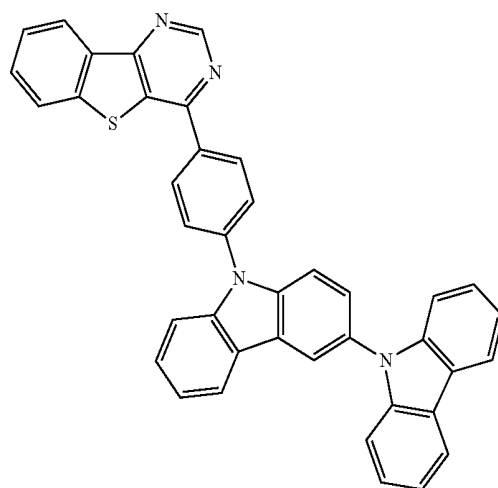
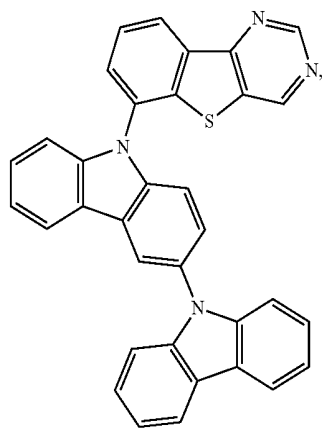
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Compound 13936

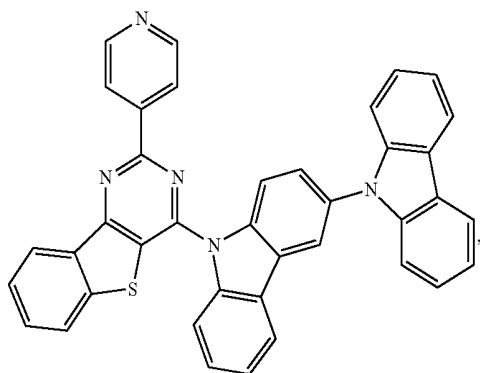


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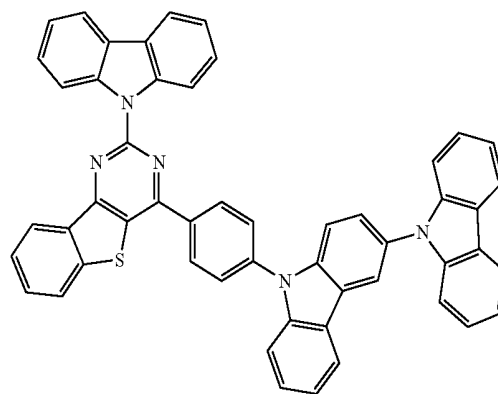
Cp.[pimd 13929



Compound 13935

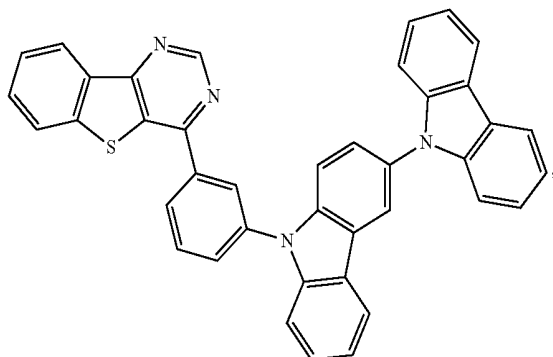


Compound 13981

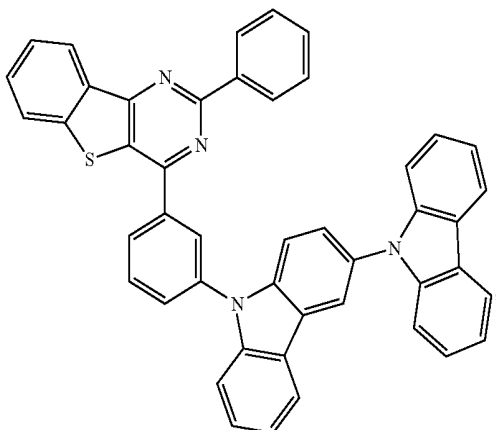


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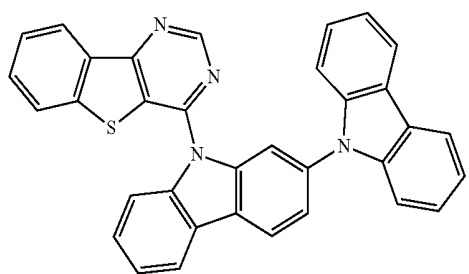
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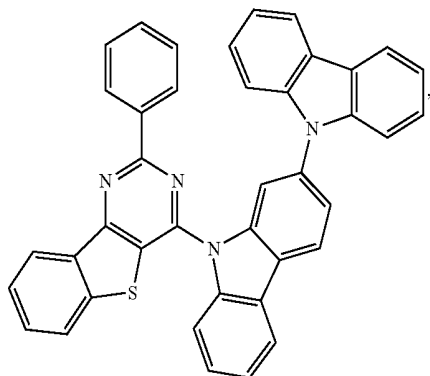
Compound 14038



Compound 15661

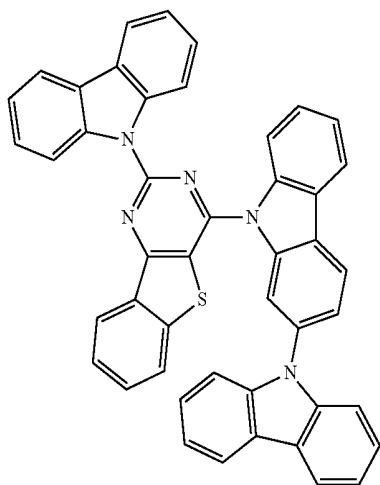


Compound 15662

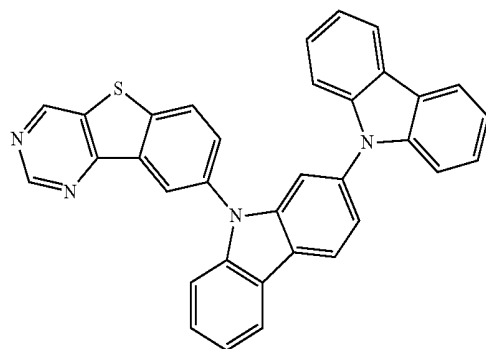


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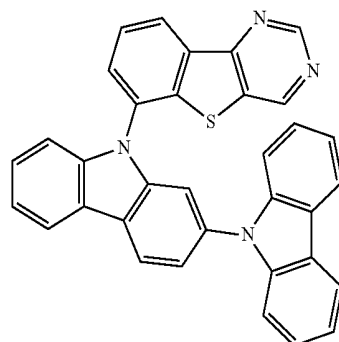
Compound 15663



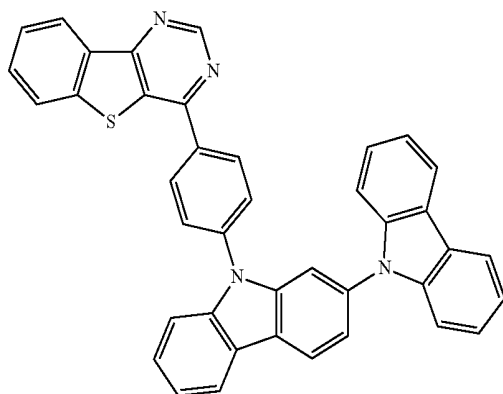
Compound 15665



Compound 15669

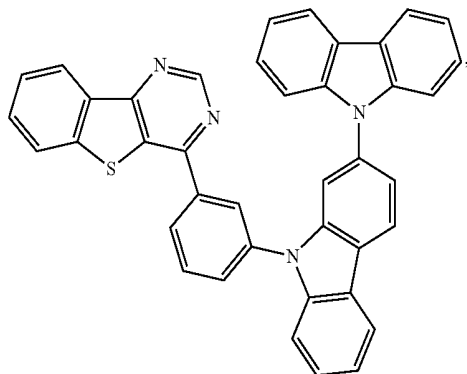


Compound 15719



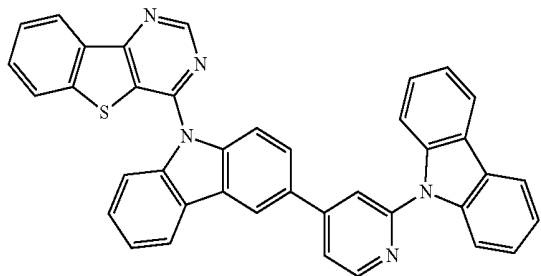
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Compound 15777

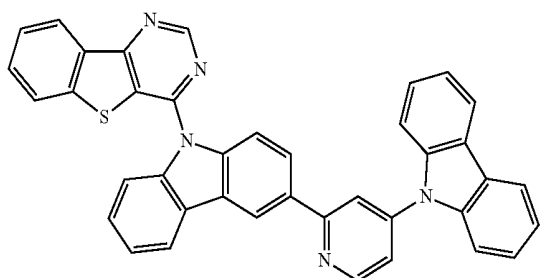


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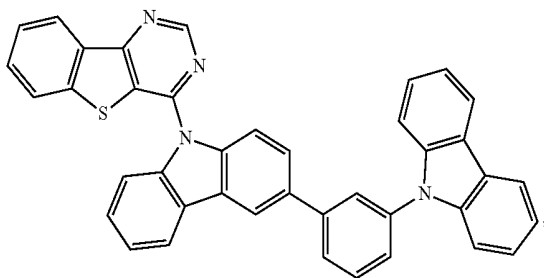
Compound 19141



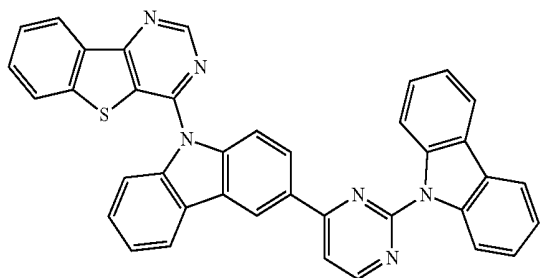
Compound 20881



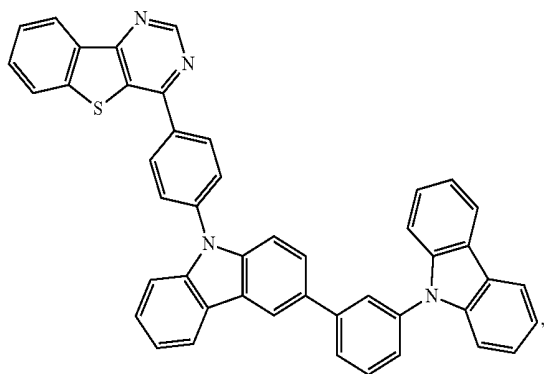
Compound 17401



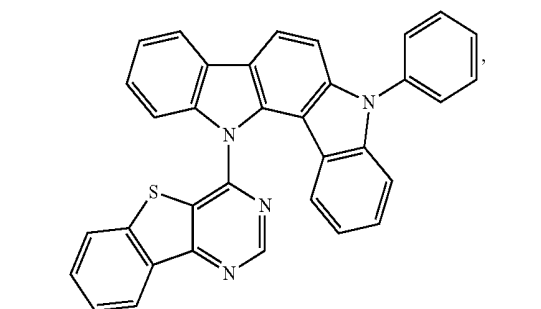
Compound 22621



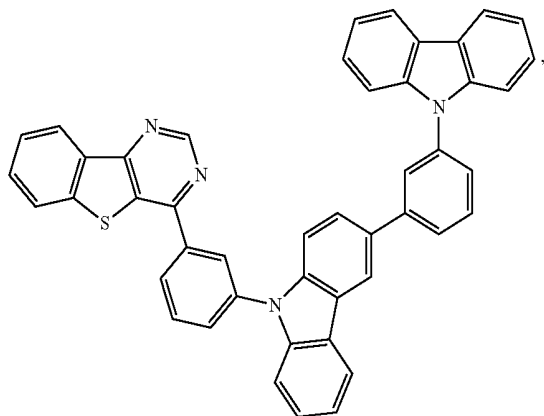
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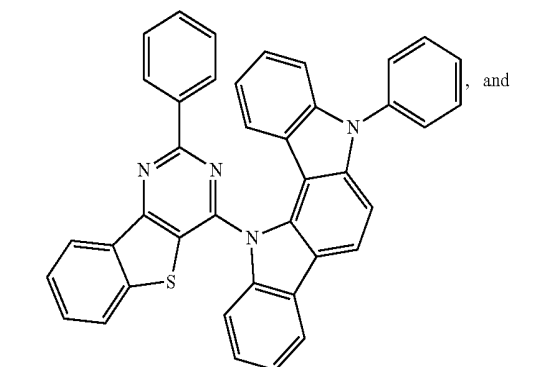
Compound 24361



Compound 17517



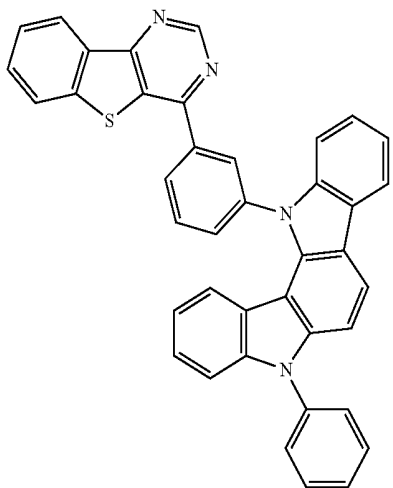
Compound 24362



, and

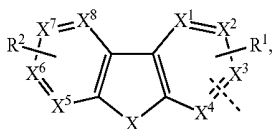
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Compound 24477



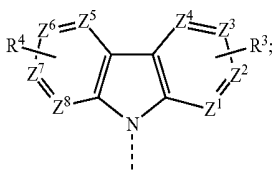
17. A first device comprising a first phosphorescent organic light-emitting device, the phosphorescent organic light-emitting device comprising:

- an anode;
 - a cathode; and
 - an organic layer, disposed between the anode and the cathode, comprising a compound having a formula G^1 -L- G^2 , Formula I;
- wherein G^1 has the structure:



and

G^2 has the structure:



wherein L is selected from the group consisting of a direct bond, an aryl group having from 6-30 carbon atoms, a heteroaryl group having from 3-30 carbon atoms, and combinations thereof; wherein the aryl group and the heteroaryl group are optionally further substituted with one or more groups 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;

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

wherein each of X^1 , X^2 , X^3 , X^4 , X^5 , X^6 , X^7 , X^8 , Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , Z^7 , and Z^8 is carbon or nitrogen;

wherein at least two of X^1 , X^2 , X^3 , X^4 , X^5 , X^6 , X^7 , and X^8 are nitrogen;

wherein at least one of X^1 , X^2 , X^3 , and X^4 is carbon and bonded to L;

wherein the dashed lines represent the bonds between G^1 and L and G^2 and L;

wherein each R^2 , R^3 , and R^4 represent mono, di, tri, tetra substitutions or no substitution;

wherein R^1 represents mono, di, tri substitutions or no substitution;

wherein R^1 , R^2 , R^3 , and R^4 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;

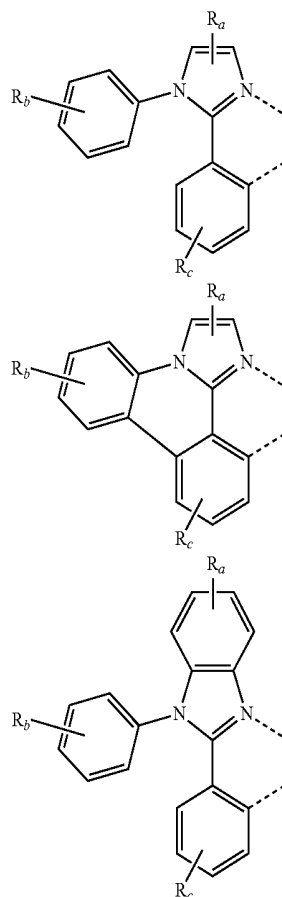
wherein the substitution is optionally fused to G^1 or G^2 ; and

wherein when R^3 or R^4 is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G^2 by N.

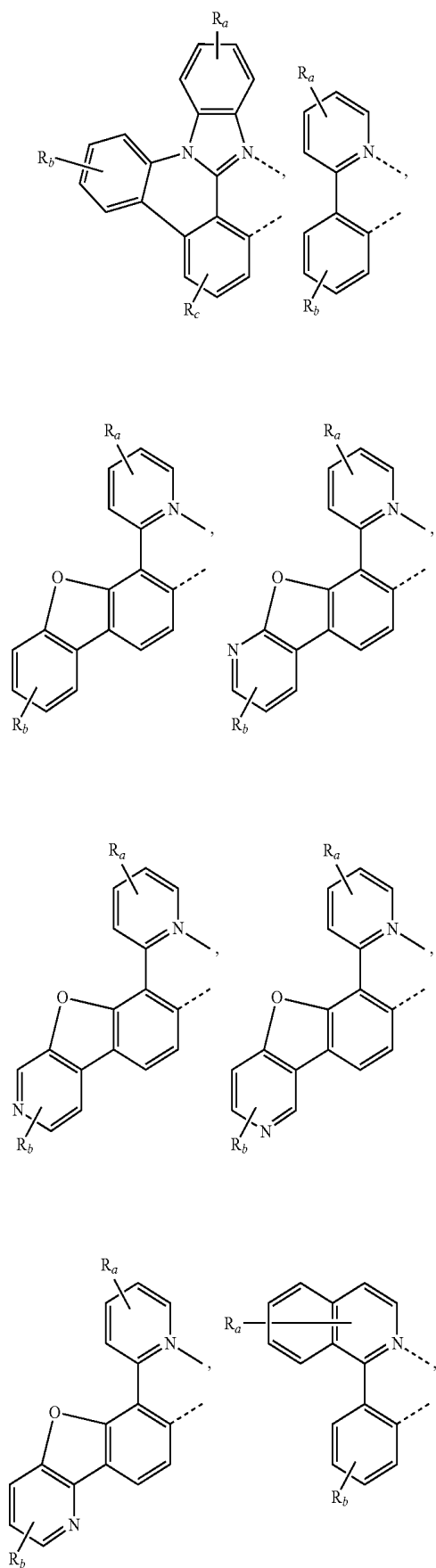
18. The first device of claim 17, wherein the organic layer is an emissive layer and the compound of Formula I is a host.

19. The first device of claim 17, wherein the organic layer further comprising a phosphorescent emissive dopant.

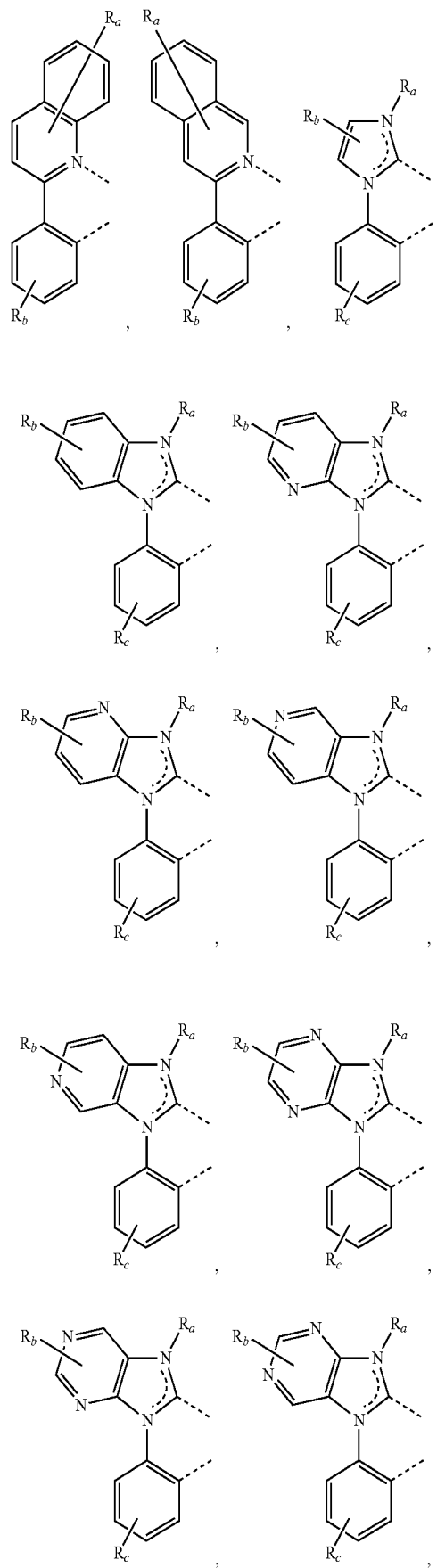
20. The first device of claim 19, wherein the phosphorescent emissive dopant is a transition metal complex having at least one ligand selected from the group consisting of:

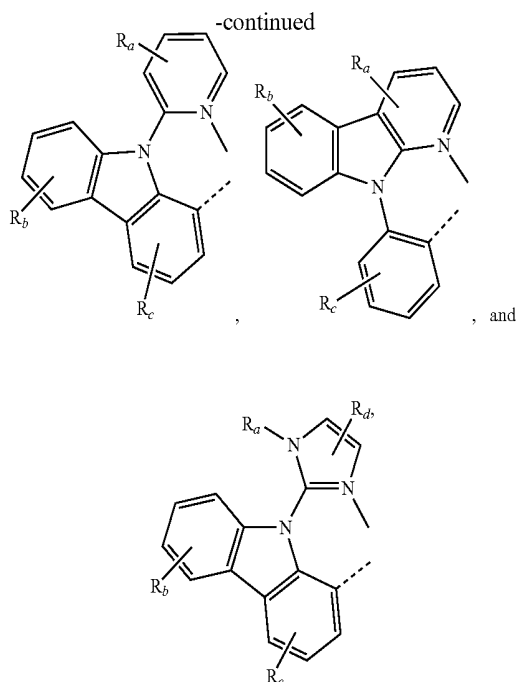


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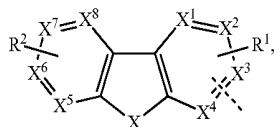
wherein R_a , R_b , R_c , and R_d may represent mono, di, tri, or tetra substitution, or no substitution;

wherein R_a , R_b , R_c , and R_d are 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 two adjacent substituents of R_a , R_b , R_c , and R_d are optionally joined to form a fused ring or form a multi-dentate ligand.

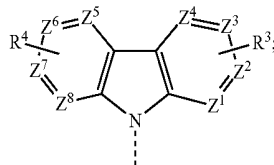
21. A formulation comprising a compound having a formula G^1-L-G^2 , Formula I;

wherein G^1 has the structure:



and

G^2 has the structure:



wherein L is selected from the group consisting of a direct bond, an aryl group having from 6-30 carbon atoms, a heteroaryl group having from 3-30 carbon atoms, and combinations thereof; wherein the aryl group and the heteroaryl group are optionally further substituted with one or more groups 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;

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

wherein each of X^1 , X^2 , X^3 , X^4 , X^5 , X^6 , X^7 , X^8 , Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , Z^7 , and Z^8 is carbon or nitrogen;

wherein at least two of X^1 , X^2 , X^3 , X^4 , X^5 , X^6 , X^7 , and X^8 are nitrogen;

wherein at least one of X^1 , X^2 , X^3 , and X^4 is carbon and bonded to L;

wherein the dashed lines represent the bonds between G^1 and L and G^2 and L;

wherein each R^2 , R^3 , and R^4 represent mono, di, tri, tetra substitutions or no substitution;

wherein R^1 represents mono, di, tri substitutions or no substitution;

wherein R^1 , R^2 , R^3 , and R^4 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;

wherein the substitution is optionally fused to G^1 or G^2 ; and

wherein when R^3 or R^4 is carbazole or substituted carbazole, the carbazole or substituted carbazole is connected to G^2 by N.

* * * * *

专利名称(译)	有机电致发光材料和器件		
公开(公告)号	US20150243893A1	公开(公告)日	2015-08-27
申请号	US14/188025	申请日	2014-02-24
[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	JOSEPH SCOTT BOUDREAUULT PIERRE LUC T DYATKIN ALEXEY BORISOVICH LI DAVID ZENAN XIA CHUANJUN YAMAMOTO HITOSHI		
发明人	JOSEPH, SCOTT BOUDREAUULT, PIERRE-LUC T. DYATKIN, ALEXEY BORISOVICH LI, DAVID ZENAN XIA, CHUANJUN YAMAMOTO, HITOSHI		
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CPC分类号	H01L51/0032 H01L51/5016 H01L51/5024 C07D491/04 C07D495/04		
其他公开文献	US9502656		
外部链接	Espacenet USPTO		

摘要(译)

本公开内容提供了基于氮杂二苯并噻吩，氮杂二苯并咪唑和氮杂二苯并硒蒽的新化合物，其在氮杂环中具有至少两个氮原子。该化合物可用作绿色，红色，黄色和白色发光器件作为电子传输主体。

