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

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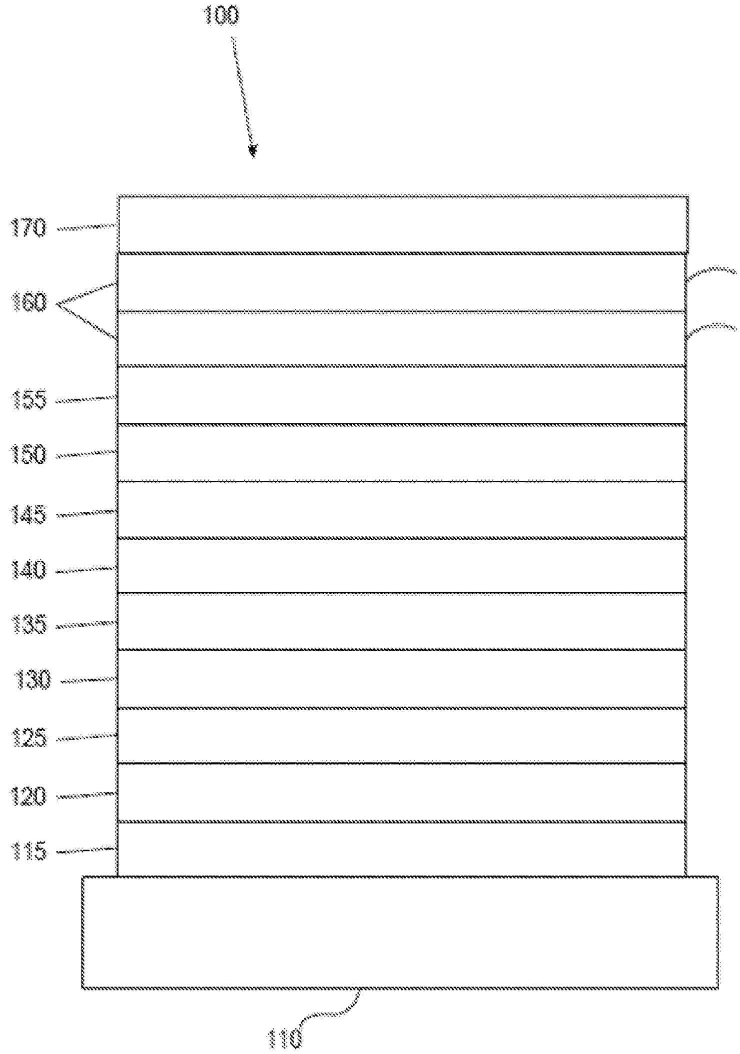
(57) **ABSTRACT**

Novel compounds including at least two donor groups G^D and at least two acceptor groups G^A are disclosed. In these compounds, each donor group G^D and acceptor group G^A can be the same or different; any pair of donor groups G^D is separated by at least one acceptor group G^A; any pair of acceptor groups G^A is separated by at least one donor group G^D; and the total number of the donor groups G^D is equal to the total number of the acceptor groups G^A. Organic light emitting devices, consumer products, formulations, and chemical structures containing the compounds are also disclosed.



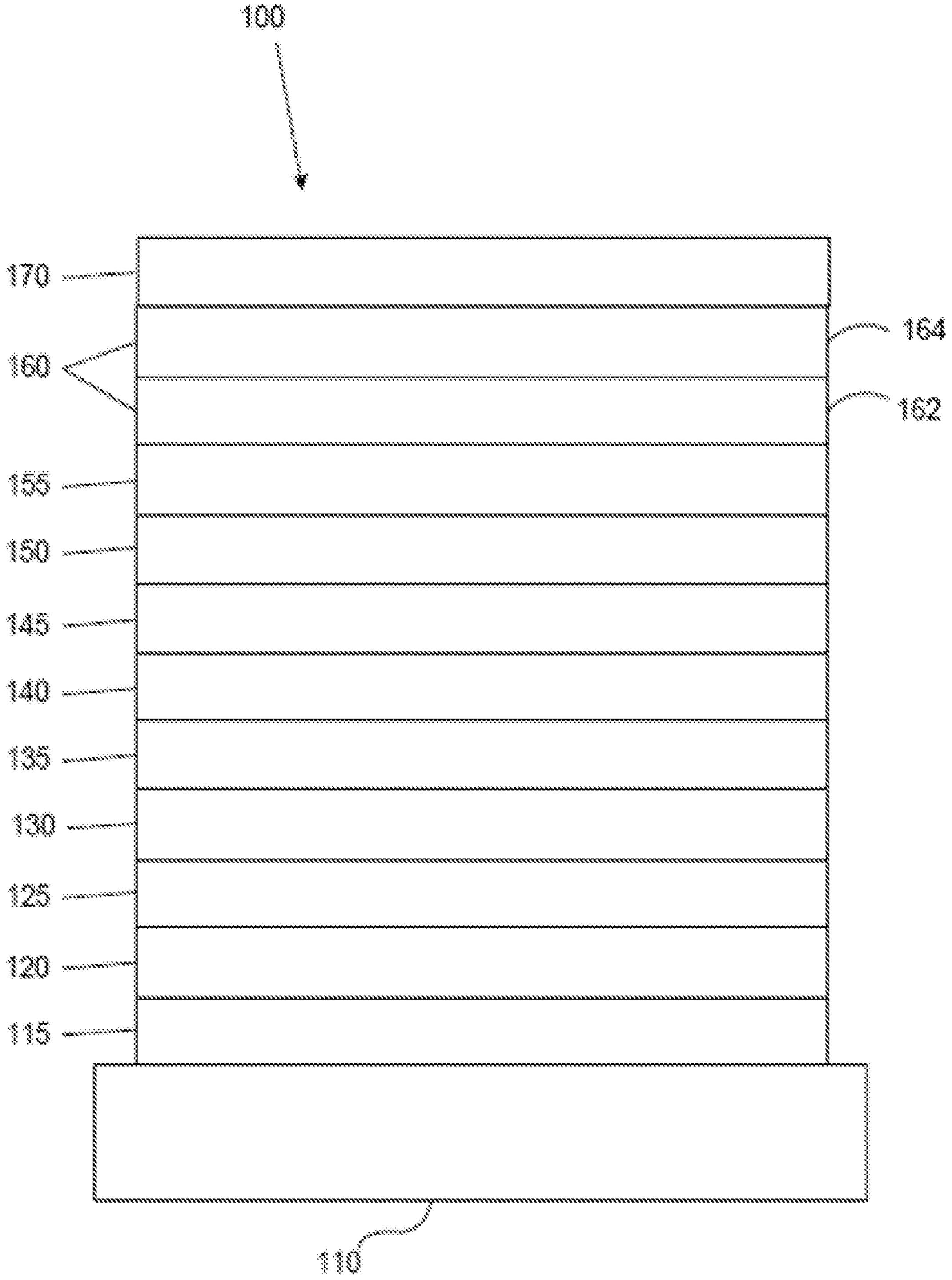


FIG. 1

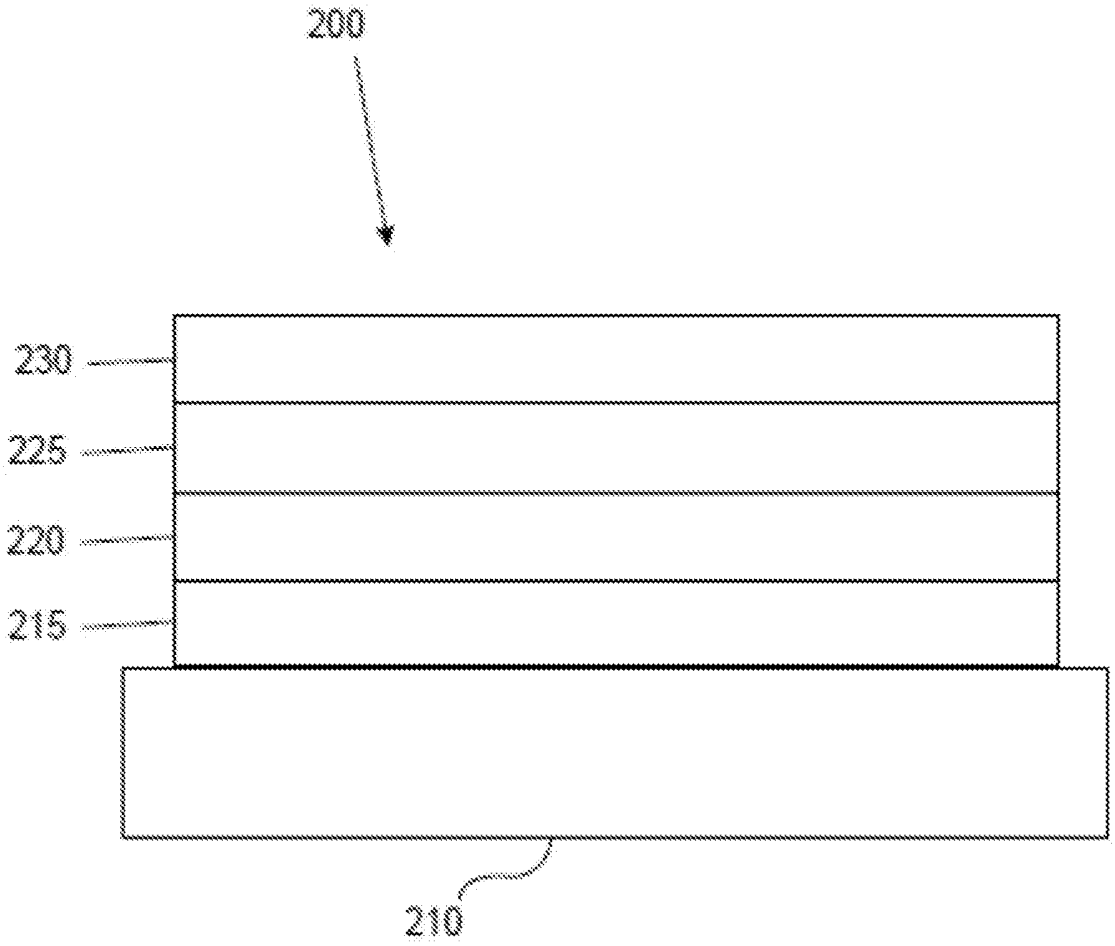


FIG. 2

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application is a continuation-in-part application of the co-pending U.S. patent application Ser. No. 16/439,921, filed on Jun. 13, 2019, which claims priority under 35 U.S.C. § 119(e) to U.S. Provisional Application No. 62/697,464, filed Jul. 13, 2018, the entire contents of which are incorporated herein by reference.

FIELD

[0002] The present invention relates to compounds for use as hosts and devices, such as organic light emitting diodes, including the same.

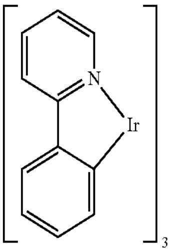
BACKGROUND

[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 diodes/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. Alternatively the OLED can be designed to emit white light. In conventional liquid crystal displays emission from a white backlight is filtered using absorption filters to produce red, green and blue emission. The same technique can also be used with OLEDs. The white OLED can be either a single EML device or a stack structure. 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

[0015] According to an aspect of the present disclosure, a compound including at least two donor groups G^D, and at least two acceptor groups G^A is disclosed. In these compounds, each donor group G^D and acceptor group G^A can be the same or different; any pair of donor groups G^D is separated by at least one acceptor group G^A; any pair of acceptor groups G^A is separated by at least one donor group G^D; and the total number of the donor groups G^D is equal to the total number of the acceptor groups G^A. In some embodiments, the compound has exactly two donor groups G^D and exactly two acceptor groups G^A.

[0016] An OLED comprising the compound of the present disclosure in an organic layer therein is also disclosed.

[0017] A consumer product comprising the OLED is also disclosed.

BRIEF DESCRIPTION OF THE DRAWINGS

[0018] FIG. **1** shows an organic light emitting device.

[0019] FIG. **2** shows an inverted organic light emitting device that does not have a separate electron transport layer.

DETAILED DESCRIPTION

[0020] 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.

[0021] 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.

[0022] More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), 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.

[0023] 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.

[0024] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F_4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

[0025] 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**.

[0026] 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**.

[0027] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. **1** and **2**. For example, the substrate may include an angled reflective surface to improve outcoupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

[0028] 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 organic vapor jet printing (OVJP). 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.

[0029] 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.

[0030] Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of electronic component modules (or units) that can be incorporated into a variety of electronic products or intermediate components. Examples of such electronic products or intermediate components include display screens, lighting devices such as discrete light source devices or lighting panels, etc. that can be utilized by the end-user product manufacturers. Such electronic component modules can optionally include the driving electronics and/or power source(s). Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of consumer products that have one or more of the electronic component modules (or units) incorporated therein. A consumer product comprising an OLED that includes the compound of the present disclosure in the organic layer in the OLED is disclosed. Such consumer products would include any kind of products that include one or more light source(s) and/or one or more of some type of visual displays. Some examples of such consumer products include flat panel displays, curved displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads-up displays, fully or partially transparent displays, flexible displays, rollable displays, foldable displays, stretchable displays, laser printers, telephones, mobile phones, tablets, phablets, personal digital assistants (PDAs), wearable devices, laptop computers, digital cameras, camcorders, viewfinders, micro-displays (displays that are less than 2 inches diagonal), 3-D displays, virtual reality or augmented reality displays, vehicles, video walls comprising multiple displays tiled together, theater or stadium screen, a light therapy device, and 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.

[0031] 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.

[0032] The terms "halo," "halogen," or "halide" as used interchangeably and refer to fluorine, chlorine, bromine, and iodine.

[0033] The term "acyl" refers to a substituted carbonyl radical (C(O)—R_s).

[0034] The term "ester" refers to a substituted oxycarbonyl (—O—C(O)—R_s or —C(O)—O—R_s) radical.

[0035] The term "ether" refers to an —OR_s radical.

[0036] The terms "sulfanyl" or "thio-ether" are used interchangeably and refer to a —SR_s radical.

[0037] The term "sulfinyl" refers to a —S(O)—R_s radical.

[0038] The term "sulfonyl" refers to a —SO_2—R_s radical.

[0039] The term "phosphino" refers to a —$P(R_s)_3$ radical, wherein each R_S can be same or different.

[0040] The term "silyl" refers to a —$Si(R_s)_3$ radical, wherein each R_S can be same or different.

[0041] The term "borane" refers to a —$B(R_s)_2$ radical or its Lewis adduct—$B(R_s)_3$ radical, wherein R_s can be same or different.

[0042] In each of the above, R_s can be hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combination thereof. Preferred R_s is selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combination thereof.

[0043] The term "alkyl" refers to and includes both straight and branched chain alkyl radicals. Preferred alkyl groups are those containing from one to fifteen carbon atoms and includes methyl, ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, and the like. Additionally, the alkyl group may be optionally substituted.

[0044] The term "cycloalkyl" refers to and includes monocyclic, polycyclic, and spiro alkyl radicals. Preferred cycloalkyl groups are those containing 3 to 12 ring carbon atoms and includes cyclopropyl, cyclopentyl, cyclohexyl, bicyclo[3.1.1]heptyl, spiro[4.5]decyl, spiro[5.5]undecyl, adamantyl, and the like. Additionally, the cycloalkyl group may be optionally substituted.

[0045] The terms "heteroalkyl" or "heterocycloalkyl" refer to an alkyl or a cycloalkyl radical, respectively, having at least one carbon atom replaced by a heteroatom. Optionally the at least one heteroatom is selected from O, S, N, P, B, Si and Se, preferably, O, S or N. Additionally, the heteroalkyl or heterocycloalkyl group is optionally substituted.

[0046] The term "alkenyl" refers to and includes both straight and branched chain alkene radicals. Alkenyl groups are essentially alkyl groups that include at least one carbon-carbon double bond in the alkyl chain. Cycloalkenyl groups are essentially cycloalkyl groups that include at least one carbon-carbon double bond in the cycloalkyl ring. The term "heteroalkenyl" as used herein refers to an alkenyl radical having at least one carbon atom replaced by a heteroatom. Optionally the at least one heteroatom is selected from O, S, N, P, B, Si and Se, preferably, O, S or N. Preferred alkenyl, cycloalkenyl, or heteroalkenyl groups are those containing two to fifteen carbon atoms. Additionally, the alkenyl, cycloalkenyl, or heteroalkenyl group is optionally substituted.

[0047] The term "alkynyl" refers to and includes both straight and branched chain alkyne radicals. Preferred alkynyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group is optionally substituted.

[0048] The terms "aralkyl" or "arylalkyl" are used interchangeably and refer to an alkyl group that is substituted with an aryl group. Additionally, the aralkyl group is optionally substituted.

[0049] The term "heterocyclic group" refers to and includes aromatic and non-aromatic cyclic radicals containing at least one heteroatom. Optionally the at least one heteroatom is selected from O, S, N, P, B, Si and Se, preferably, O, S or N. Hetero-aromatic cyclic radicals may be used interchangeably with heteroaryl. Preferred hetero-non-aromatic cyclic groups are those containing 3 to 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/thio-ethers, such as tetrahydrofuran, tetrahydropyran, tetrahydrothiophene, and the like. Additionally, the heterocyclic group may be optionally substituted.

[0050] The term "aryl" refers to and includes both single-ring aromatic hydrocarbyl groups and polycyclic aromatic 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 an aromatic hydrocarbyl group, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Preferred aryl groups are those containing six to thirty carbon atoms, preferably six to twenty carbon atoms, more preferably six to twelve carbon atoms. Especially preferred is an aryl group having six carbons, ten carbons or twelve carbons. Suitable aryl groups include phenyl, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene, preferably phenyl, biphenyl, triphenyl, triphenylene, fluorene, and naphthalene. Additionally, the aryl group may be optionally substituted.

[0051] The term "heteroaryl" refers to and includes both single-ring hetero-aromatic groups and polycyclic aromatic ring systems that include at least one heteroatom. The heteroatoms include, but are not limited to O, S, N, P, B, Si and Se. In many instances, O, S or N are the preferred heteroatoms. Hetero-single ring aromatic systems are preferably single rings with 5 or 6 ring atoms, and the ring can have from one to six heteroatoms. The hetero-polycyclic ring systems can have 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. The hetero-polycyclic aromatic ring systems can have from one to six heteroatoms per ring of the polycyclic aromatic ring system. Preferred heteroaryl groups are those containing three to thirty carbon atoms, preferably three to twenty carbon atoms, more preferably three to twelve carbon atoms. Suitable heteroaryl groups include dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine, preferably dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, triazine, benzimidazole, 1,2-azaborine, 1,3-azaborine, 1,4-azaborine, borazine, and aza-analogs thereof. Additionally, the heteroaryl group may be optionally substituted.

[0052] Of the aryl and heteroaryl groups listed above, the groups of triphenylene, naphthalene, anthracene, dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, pyrazine, pyrimidine, triazine, and benzimidazole, and the respective aza-analogs of each thereof are of particular interest.

[0053] The terms alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aralkyl, heterocyclic group, aryl, and heteroaryl, as used herein, are independently unsubstituted or substituted with one or more general substituents.

[0054] In many instances, the general substituents are selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, 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.

[0055] In some instances, the preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

[0056] In some instances, the preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, alkoxy, aryloxy, amino, silyl, aryl, heteroaryl, sulfanyl, and combinations thereof.

[0057] In yet other instances, the more preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0058] The terms "substituted" and "substitution" refer to a substituent other than H that is bonded to the relevant position, e.g., a carbon or nitrogen. For example, when R^1 represents mono-substitution, then one R^1 must be other than H (i.e., a substitution). Similarly, when R^1 represents di-substitution, then two of R^1 must be other than H. Similarly, when R^1 represents no substitution, R^1, for example, can be a hydrogen for available valencies of ring atoms, as in carbon atoms for benzene and the nitrogen atom in pyrrole, or simply represents nothing for ring atoms with fully filled valencies, e.g., the nitrogen atom in pyridine. The maximum number of substitutions possible in a ring structure will depend on the total number of available valencies in the ring atoms.

[0059] As used herein, "combinations thereof" indicates that one or more members of the applicable list are combined to form a known or chemically stable arrangement that one of ordinary skill in the art can envision from the applicable list. For example, an alkyl and deuterium can be combined to form a partial or fully deuterated alkyl group; a halogen and alkyl can be combined to form a halogenated alkyl substituent; and a halogen, alkyl, and aryl can be combined to form a halogenated arylalkyl. In one instance, the term substitution includes a combination of two to four of the listed groups. In another instance, the term substitution includes a combination of two to three groups. In yet another instance, the term substitution includes a combination of two groups. Preferred combinations of substituent groups are those that contain up to fifty atoms that are not hydrogen or deuterium, or those which include up to forty atoms that are not hydrogen or deuterium, or those that include up to thirty atoms that are not hydrogen or deuterium. In many instances, a preferred combination of substituent groups will include up to twenty atoms that are not hydrogen or deuterium.

[0060] The "aza" designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzothiophene, etc. means that one or more of the C—H groups in the respective aromatic ring 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.

[0061] As used herein, "deuterium" refers to an isotope of hydrogen. Deuterated compounds can be readily prepared using methods known in the art. For example, U.S. Pat. No. 8,557,400, Patent Pub. No. WO 2006/095951, and U.S. Pat. Application Pub. No. US 2011/0037057, which are hereby incorporated by reference in their entireties, describe the making of deuterium-substituted organometallic complexes. Further reference is made to Ming Yan, et al., *Tetrahedron* 2015, 71, 1425-30 and Atzrodt et al., *Angew. Chem. Int. Ed.* (*Reviews*) 2007, 46, 7744-65, which are incorporated by reference in their entireties, describe the deuteration of the methylene hydrogens in benzyl amines and efficient pathways to replace aromatic ring hydrogens with deuterium, respectively.

[0062] It is to be understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it were a fragment (e.g. phenyl, phenylene, naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. benzene, naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[0063] It is believed that the internal quantum efficiency (IQE) of fluorescent OLEDs can exceed the 25% spin statistics limit through delayed fluorescence. As used herein, there are two types of delayed fluorescence, i.e. P-type delayed fluorescence and E-type delayed fluorescence. P-type delayed fluorescence is generated from triplet-triplet annihilation (TTA).

[0064] On the other hand, E-type delayed fluorescence does not rely on the collision of two triplets, but rather on the thermal population between the triplet states and the singlet excited states. Compounds that are capable of generating E-type delayed fluorescence are required to have very small singlet-triplet gaps. Thermal energy can activate the transition from the triplet state back to the singlet state. This type of delayed fluorescence is also known as thermally activated delayed fluorescence (TADF). A distinctive feature of TADF is that the delayed component increases as temperature rises due to the increased thermal energy. If the reverse intersystem crossing rate is fast enough to minimize the non-radiative decay from the triplet state, the fraction of back populated singlet excited states can potentially reach 75%. The total singlet fraction can be 100%, far exceeding the spin statistics limit for electrically generated excitons.

[0065] E-type delayed fluorescence characteristics can be found in an exciplex system or in a single compound. Without being bound by theory, it is believed that E-type delayed fluorescence requires the luminescent material to have a small singlet-triplet energy gap (ΔE_{S-T}). Organic, non-metal containing, donor-acceptor luminescent materials may be able to achieve this. The emission in these materials is often characterized as a donor-acceptor charge-transfer (CT) type emission. The spatial separation of the HOMO and LUMO in these donor-acceptor type compounds often results in small ΔE_{S-T}. These states may involve CT states. Often, donor-acceptor luminescent materials are constructed by connecting an electron donor moiety such as amino- or carbazole-derivatives and an electron acceptor moiety such as N-containing six-membered aromatic rings.

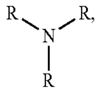
[0066] In some instance, a pair of adjacent substituents can be optionally joined or fused into a ring. The preferred ring is a five, six, or seven-membered carbocyclic or heterocyclic ring, includes both instances where the portion of the ring formed by the pair of substituents is saturated and where the portion of the ring formed by the pair of substituents is unsaturated. As used herein, "adjacent" means that the two substituents involved can be on the same ring next to each other, or on two neighboring rings having the two closest available substitutable positions, such as 2, 2' positions in a biphenyl, or 1, 8 position in a naphthalene, as long as they can form a stable fused ring system.

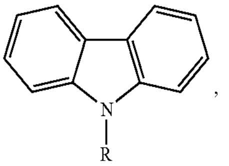
[0067] The novel compounds disclosed herein include at least two electron donor groups and two electron acceptor groups, at least two electron donor groups and one electron acceptor group, or at least one electron donor group and two electron acceptor groups. The at least two donor group are separated by at least one of the at least one or two acceptor group; the at least two acceptor group are separated by at least one of the at least one or two donor group. In some embodiments, and the total number of the donor group is equal to the total number of the acceptor group. In some embodiments, the total number of the donor group is not equal to the total number of the acceptor group. This special configuration provides the molecules unique electronic effects at ground and excited state such as dipole moments, which makes these materials very promising to be used in organic optical electronic applications such as organic electroluminescence devices as hosts, sensitizers, and emitters. When there are multiple moieties that could be donor groups immediately next to each other, these multiple donor groups are counted as one single donor group. Similarly, when there are multiple moieties that could be acceptor groups immediately next to each other, these multiple acceptor groups are counted as one single acceptor group.

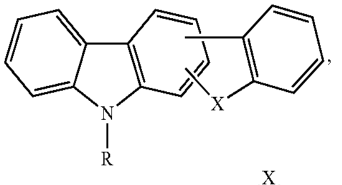
[0068] According to an aspect of the present disclosure, a compound including at least two donor groups G^D, and at least two acceptor groups G^A; at least two donor groups G^D, and at least one acceptor groups G^A; or at least one donor groups G^D, and at least two acceptor groups G^A, is disclosed. In these compounds, each donor group G^D and acceptor group G^A can be the same or different; any pair of donor groups G^D is separated by at least one acceptor group G^A; any pair of acceptor groups G^A is separated by at least one donor group G^D. In some embodiments, the total number of the donor groups G^D is equal to the total number of the acceptor groups G^A. In some embodiments, the total number of the donor groups G^D is not equal to the total number of the acceptor groups G^A. In some embodiments, the compound has exactly two donor groups G^D and exactly two acceptor groups G^A. In some embodiments, the compound comprises at least three donor groups G^D or three acceptor group G^A. In some embodiments, the compound has exactly two donor groups G^D and exactly one acceptor groups G^A. In some embodiments, the compound has exactly one donor groups G^D and exactly two acceptor groups G^A.

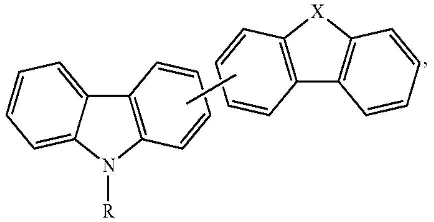
[0069] In some embodiments, each donor group G^D independently comprises at least one moiety selected from the group consisting of amino, indole, carbazole, benzothiophene, benzofuran, benzoselenophene, dibenzothiophene, dibenzofuran, and dibenzoselenophene. In some embodiments, each acceptor group G^A independently comprises at least one moiety selected from the group consisting of nitrile, isonitrile, fluoride, borane, a six-membered aromatic ring having at least one nitrogen, and a 5-membered aromatic ring having at least two heteroatoms. The term "moiety" as used herein refers to a smallest structure that forms a part of a larger structure. The moiety structure can be further substituted in the final form in the larger structure. The moiety structure can be further fused in the final form in the larger structure. For example, in considering the carbazole moiety listed for the donor group G^D above, a structure such as indolocarbazole is considered to contain two carbazole moieties.

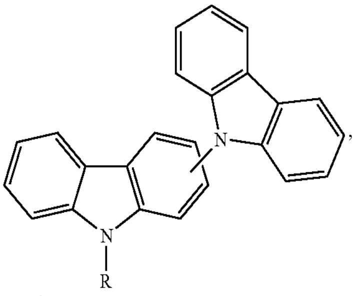
[0070] In some embodiments, each donor group G^D independently comprises at least one moiety selected from the group consisting of:

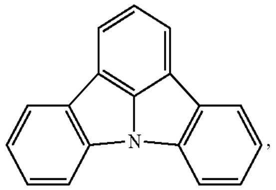


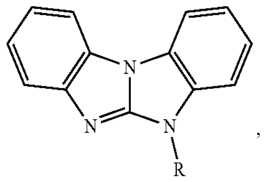


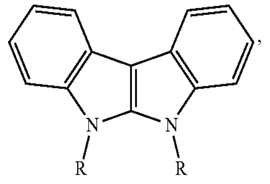












where X is selected from the group consisting of O, S, Se, and NR; and each R is independently selected from (i) an acceptor group G^A, (ii) an organic linker bonded to an acceptor group G^A, and (iii) a terminal group selected from the group consisting of alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, aryl, heteroaryl, and combinations thereof. In some embodiments where more than one R is present, each R is the same. In some embodiments where more than one R is present, at least one R is different. In some embodiments where more than one R is present, all of the Rs are different.

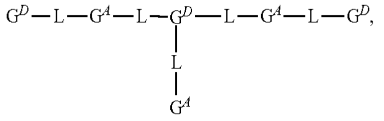
[0071] In some embodiments, each acceptor group G^A independently comprises at least one moiety selected from the group consisting of nitrile, isonitrile, borane, fluoride, pyridine, pyrimidine, pyrazine, triazine, aza-carbazole, aza-dibenzothiophene, aza-dibenzofuran, aza-dibenzoselenophene, aza-triphenylene, imidazole, pyrazole, oxazole, thiazole, isoxazole, isothiazole, triazole, thiadiazole, and oxadiazole.

[0072] In some embodiments, the compound is capable of functioning as an E-type delayed fluorescent emitter at room temperature.

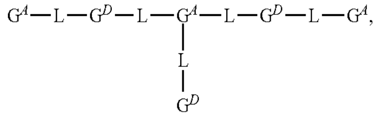
[0073] In some embodiments, the compound has a structure selected from the group consisting of:

$$G^D—L—G^A—L—G^D—L—G^A,$$

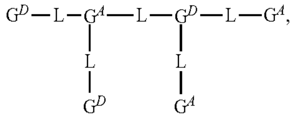
$$G^D—L—G^A—L—G^D—L—G^A—L—G^D—L—G^A,$$



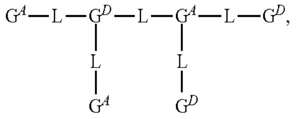
$$G^D—L—G^A—L—\underset{\substack{|\\ L\\ |\\ G^A}}{G^D}—L—G^A—L—G^D,$$



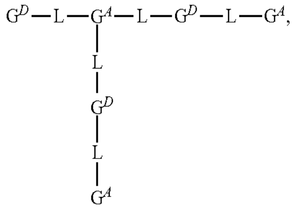
$$G^A—L—G^D—L—\underset{\substack{|\\ L\\ |\\ G^D}}{G^A}—L—G^D—L—G^A,$$



$$G^D—L—\underset{\substack{|\\ L\\ |\\ G^D}}{G^A}—L—\underset{\substack{|\\ L\\ |\\ G^A}}{G^D}—L—G^A,$$

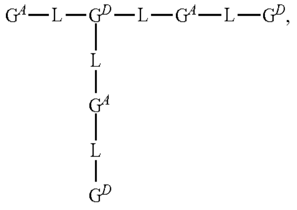


$$G^A—L—\underset{\substack{|\\ L\\ |\\ G^A}}{G^D}—L—\underset{\substack{|\\ L\\ |\\ G^D}}{G^A}—L—G^D,$$



$$G^D—L—\underset{\substack{|\\ L\\ |\\ G^D\\ |\\ L\\ |\\ G^A}}{G^A}—L—G^D—L—G^A,$$

and



$$G^A—L—\underset{\substack{|\\ L\\ |\\ G^A\\ |\\ L\\ |\\ G^D}}{G^D}—L—G^A—L—G^D,$$

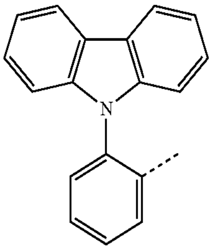
wherein each L is independently a direct bond or an organic linker.

[0074] In some embodiments, each L is the same. In some embodiments, each L is a direct bond. In some embodiments, at least one L is different. In some embodiments, all Ls are different.

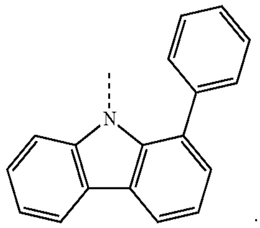
[0075] In some embodiments, each L is independently a direct bond or a conjugated organic linker. In some embodiments, each L is independently selected from the group consisting of a direct bond, aryl, heteroaryl, alkyl, cycloalkyl, silyl, and combinations thereof. In some embodiments, each L is independently selected from the group consisting of a direct bond, an aryl moiety, or a heteroaryl moiety. In some embodiments, each L is a direct bond or an aryl moiety. In some embodiments, each L can be a direct bond or a preferred aryl group described above.

[0076] In some embodiments, at least one L in each formula is a non-conjugated organic linker. In some embodiments, the non-conjugated organic linker can be alkyl, cycloalkyl, or silyl containing moiety. In some embodiments, the non-conjugated organic linker is silyl containing moiety.

[0077] In some embodiments, at least one donor group G^D comprises a moiety selected from the group consisting of



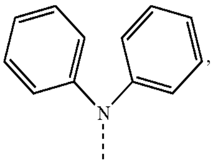
, and



.

[0078] In some embodiments, each donor group G^D is independently selected from the group consisting of:

D1



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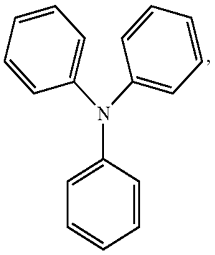

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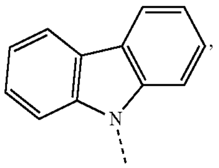

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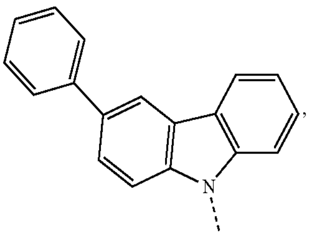

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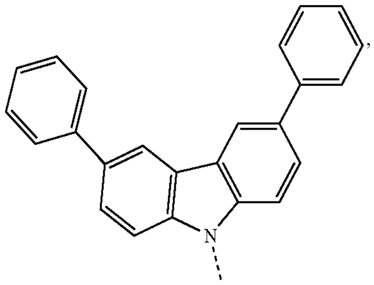

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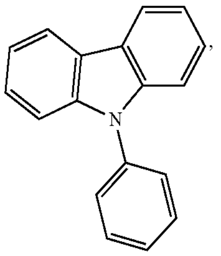

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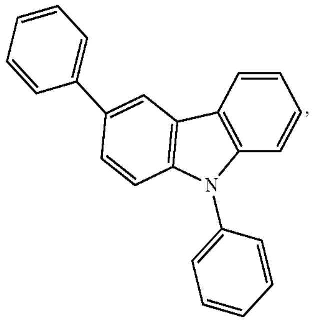

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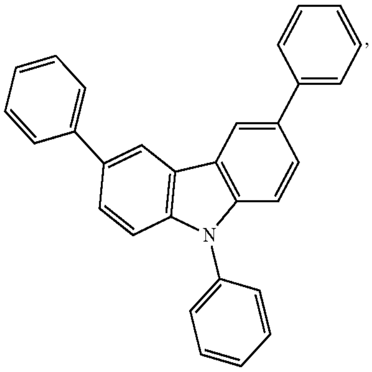

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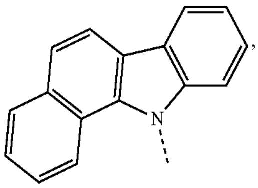

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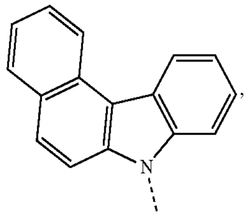

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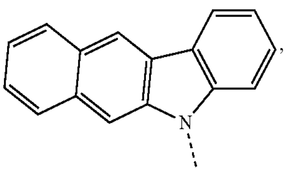

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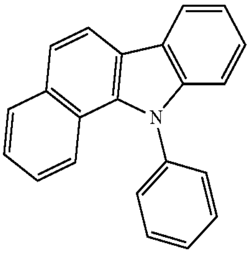

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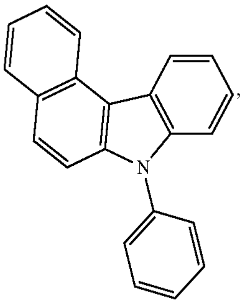

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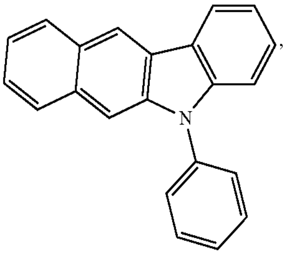

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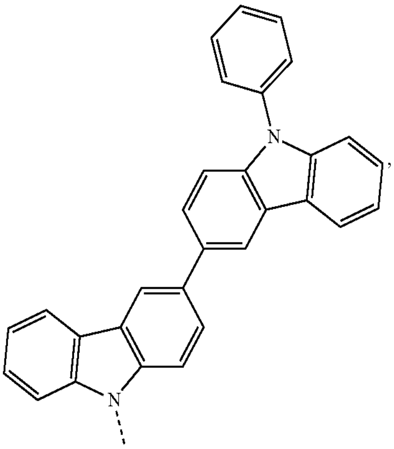

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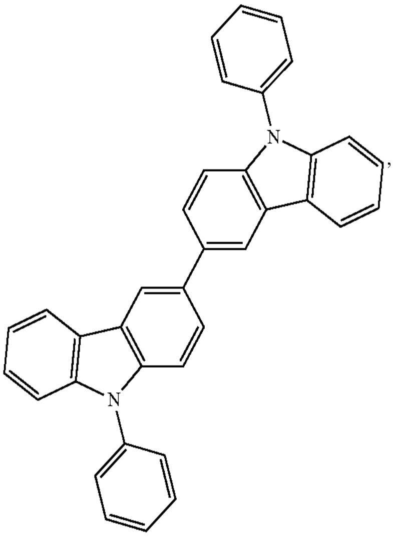

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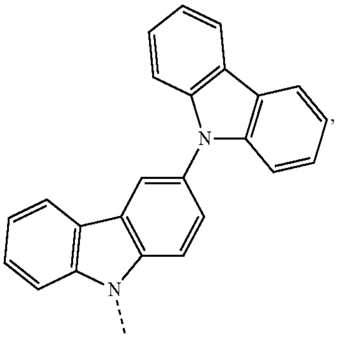

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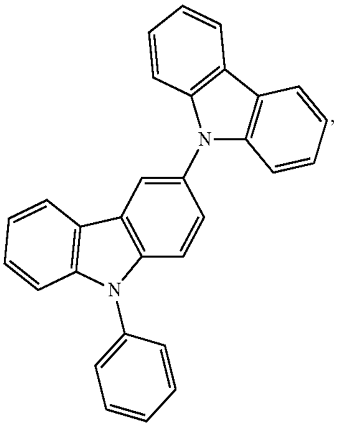

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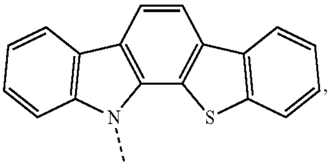

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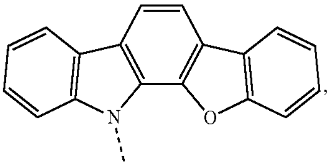

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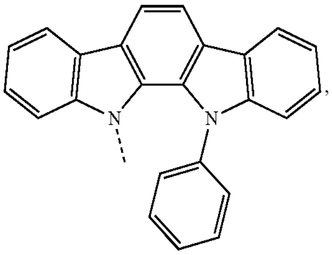

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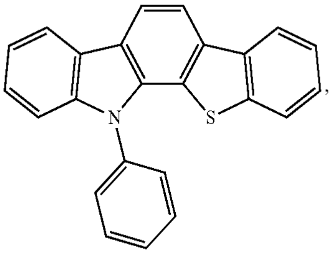

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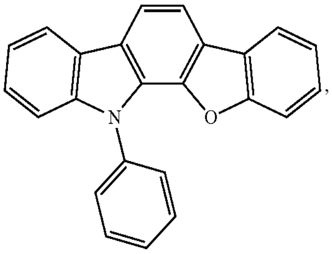

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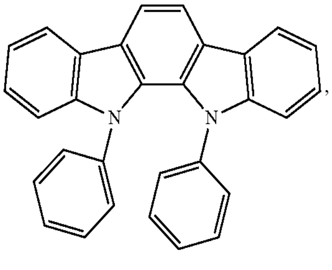

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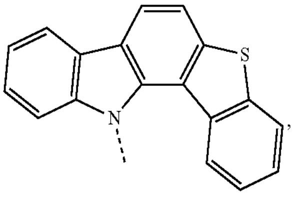

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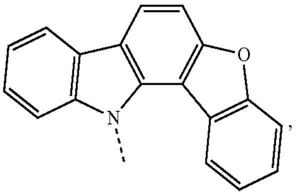

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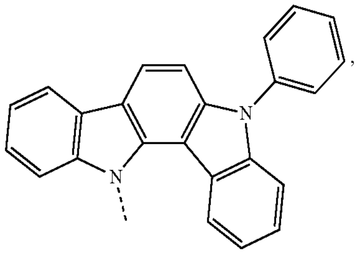
D27



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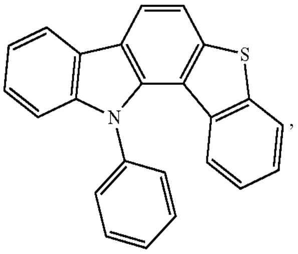

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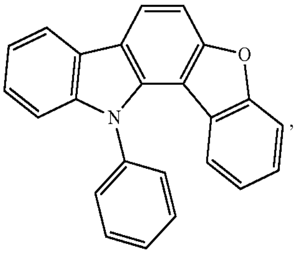

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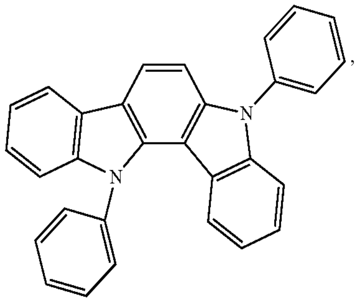

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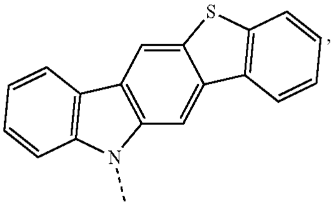

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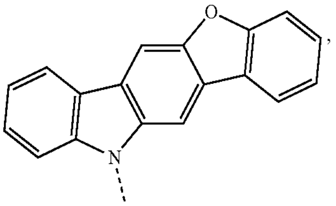

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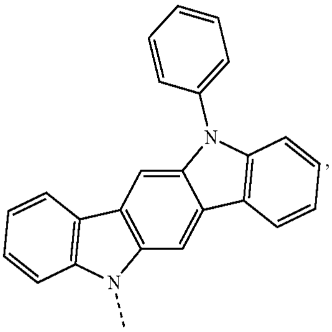

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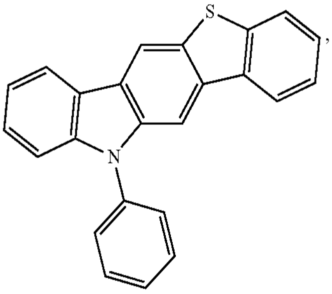

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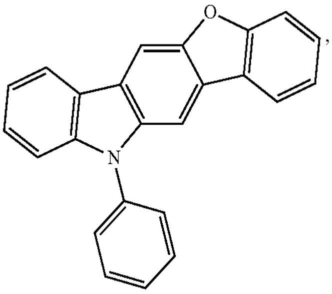

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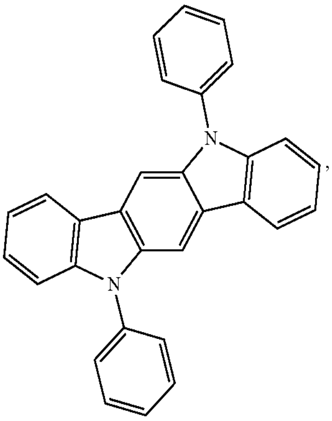

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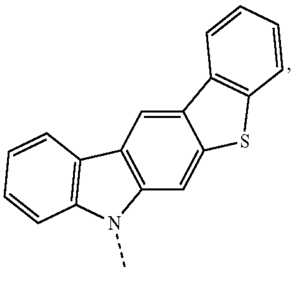

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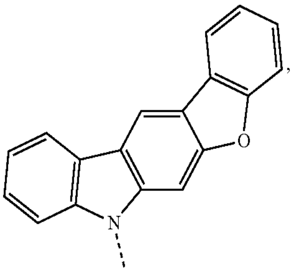

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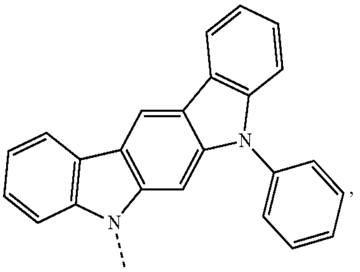

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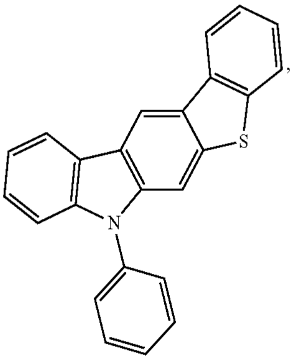

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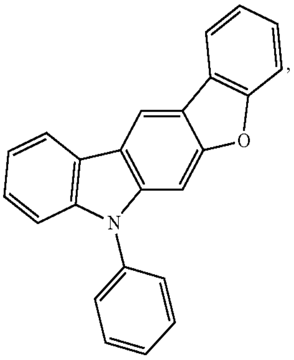

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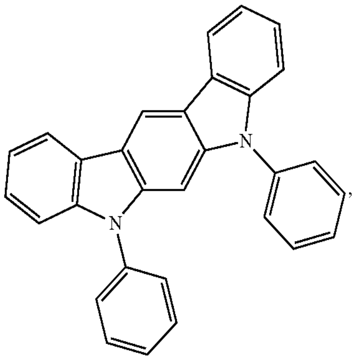

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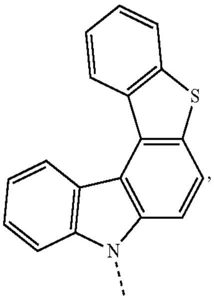

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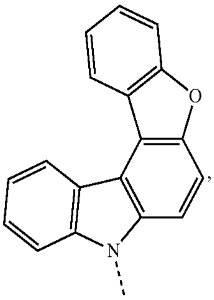

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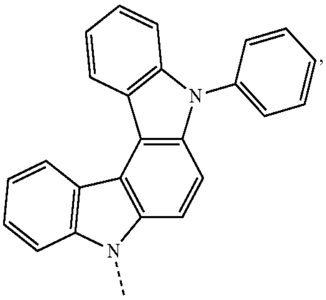

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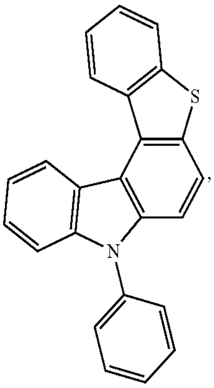

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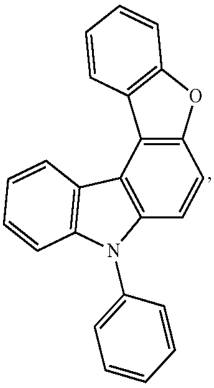

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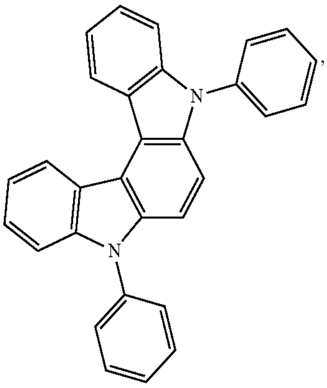

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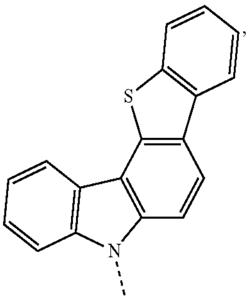

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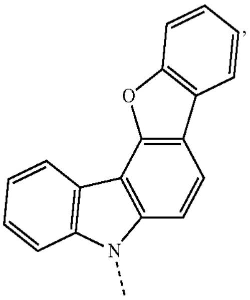

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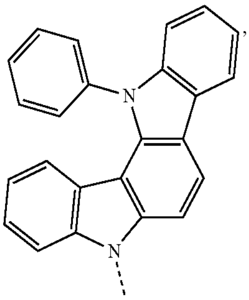

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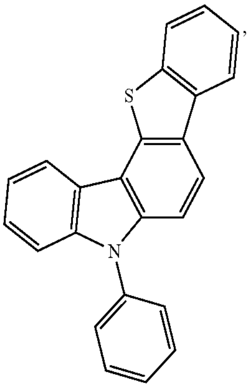

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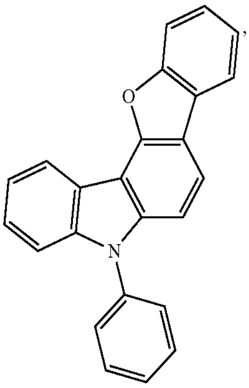

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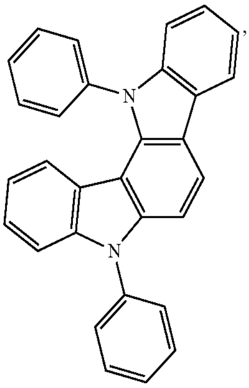

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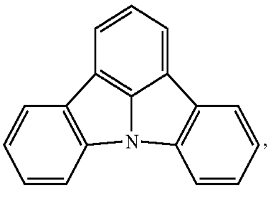

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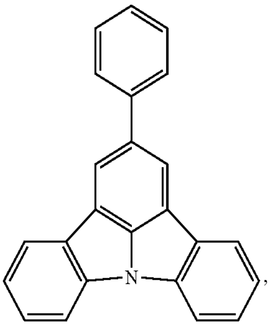

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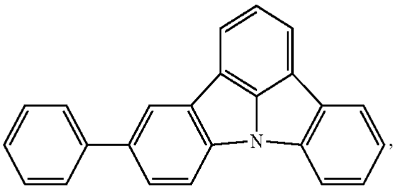

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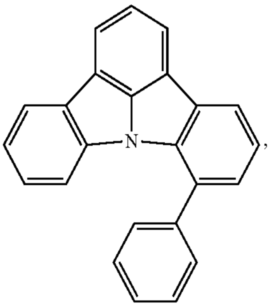

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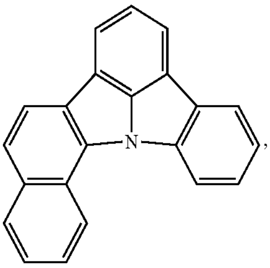

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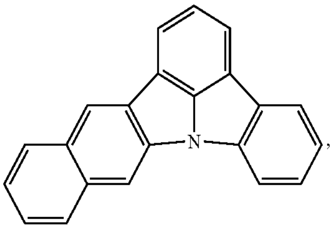

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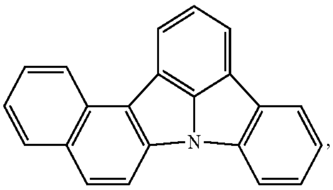

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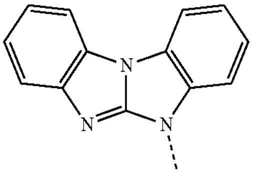

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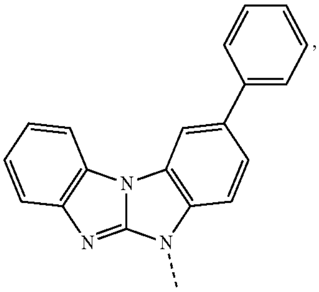

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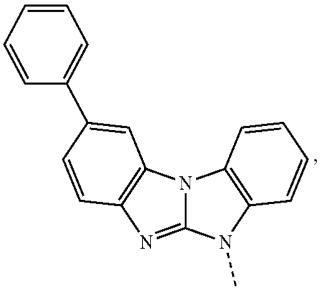

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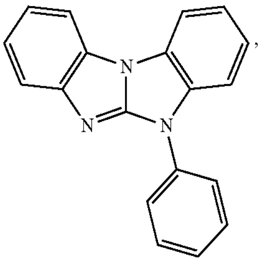

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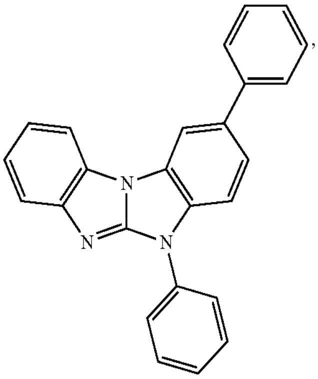

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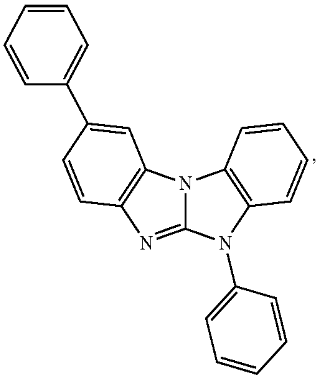

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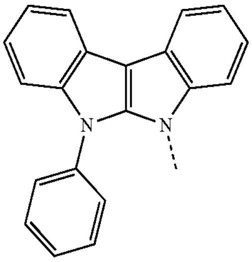
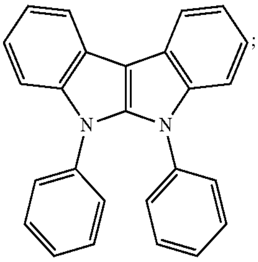


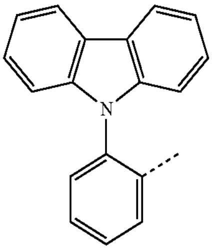
, and

D69

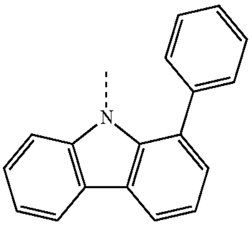


wherein each donor group G^D is at least divalent unless the donor group G^D is a monovalent end group; and wherein, in structures containing a dashed line, the dashed line represents a bond to a linker or an acceptor group G^A.

[0079] In some embodiments, at least one donor group G^D comprises a moiety selected from the group consisting of



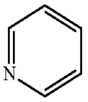
, and



.

[0080] In some embodiments, each acceptor group G^A is independently selected from the group consisting of:

A1



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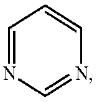
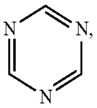
A2



A3



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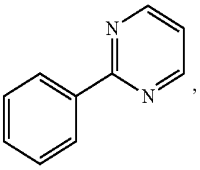
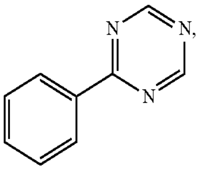


A5



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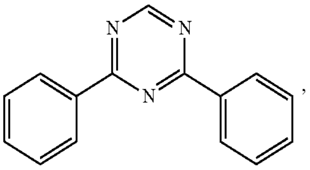

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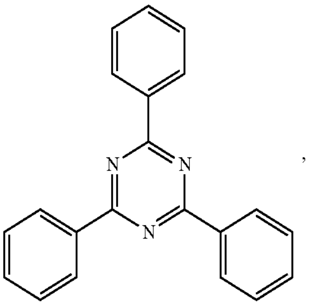

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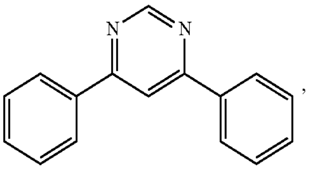

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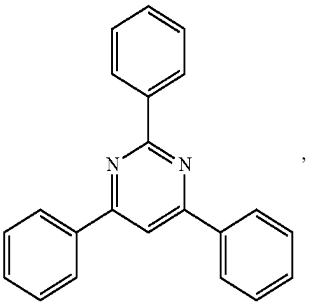

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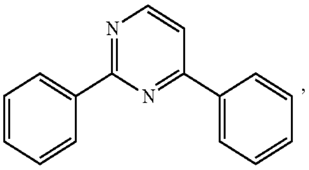

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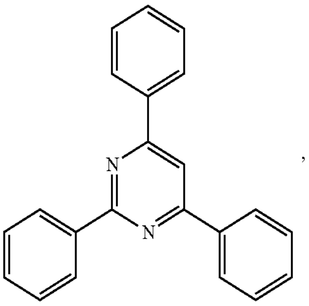

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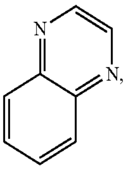

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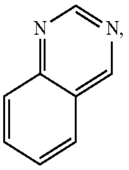

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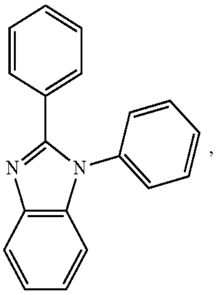

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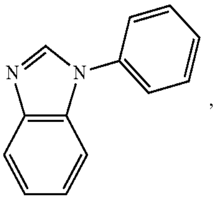

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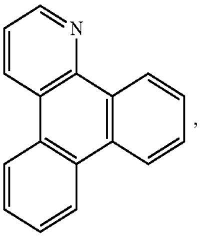

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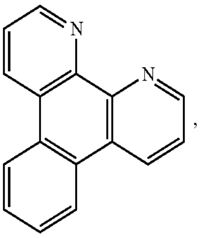

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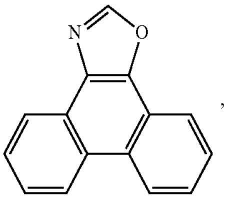

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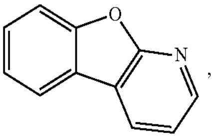

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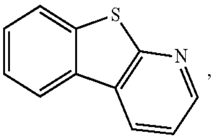

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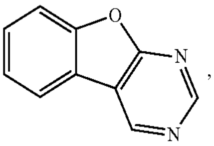

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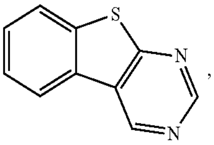

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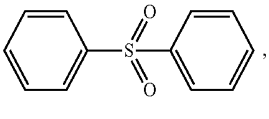

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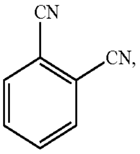

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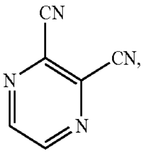

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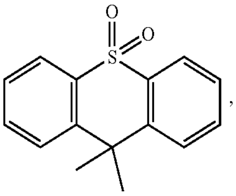

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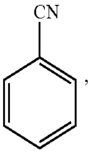

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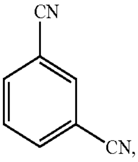
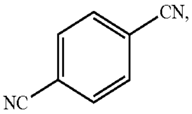
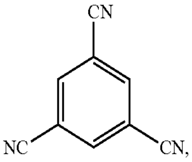


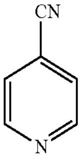
B7



B8



B9



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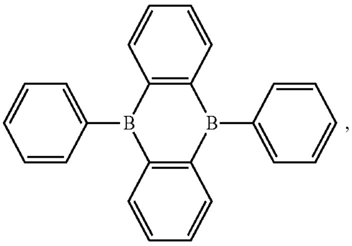

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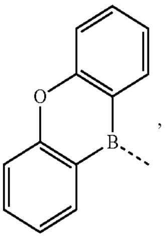

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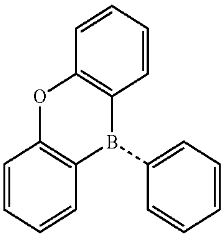

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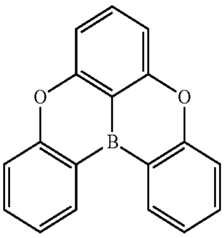

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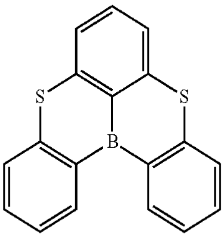

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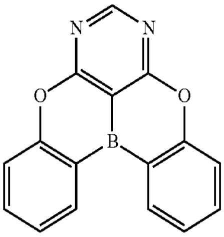

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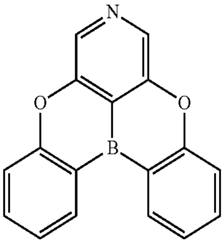

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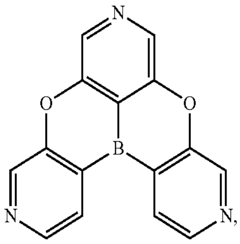

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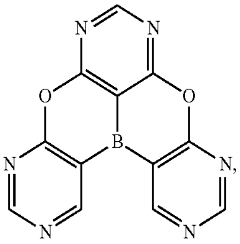

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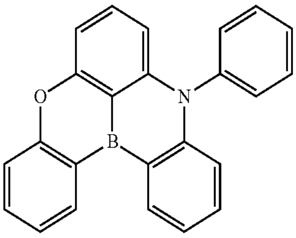

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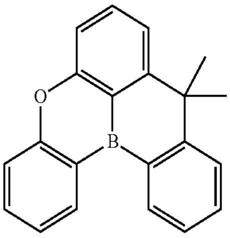

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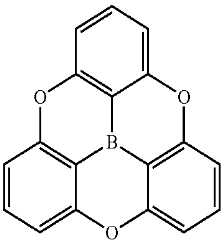

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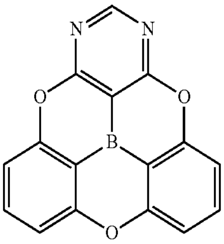

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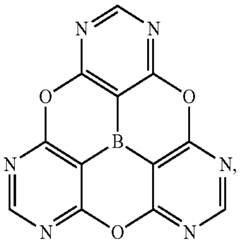

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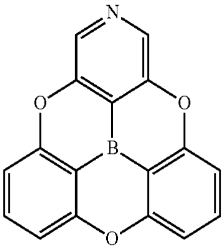

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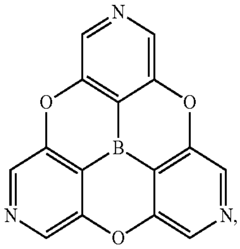

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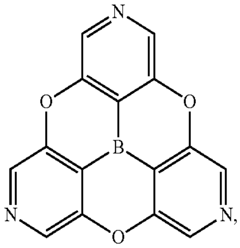
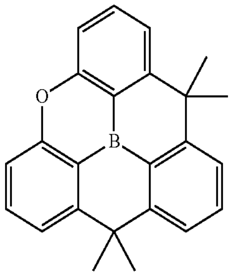


B27



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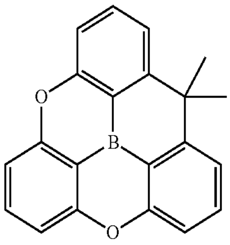
B28



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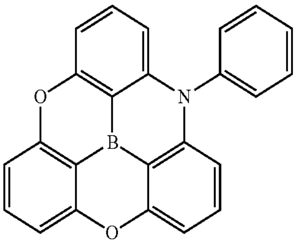

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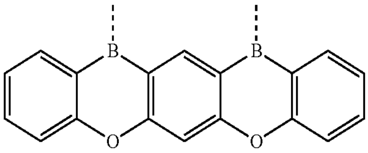
B30



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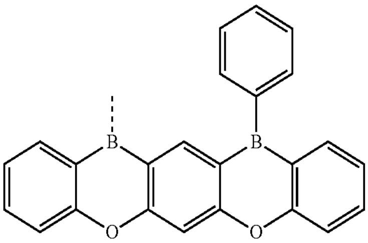
B31



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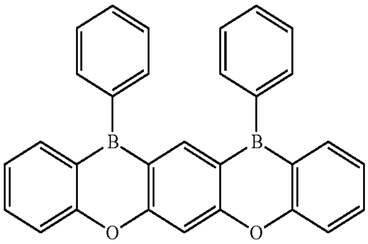
B32



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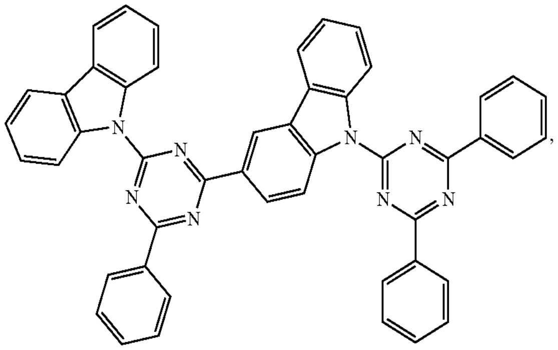
wherein each acceptor group G^A is at least divalent unless the acceptor group G^A is a monovalent end group.

[0081] In some embodiments, the compound is selected from the group consisting of:

Compound A1



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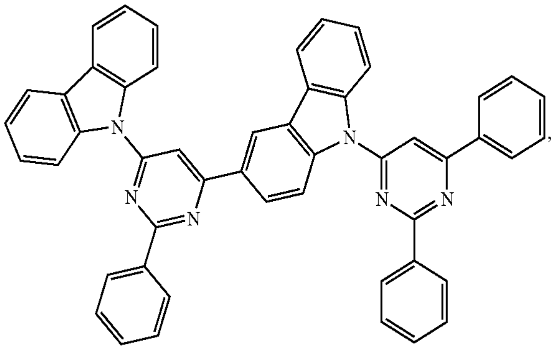
Compound A2



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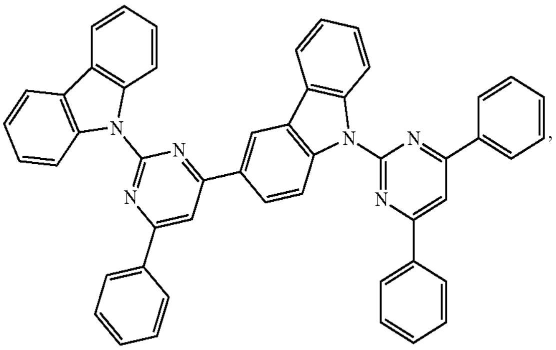
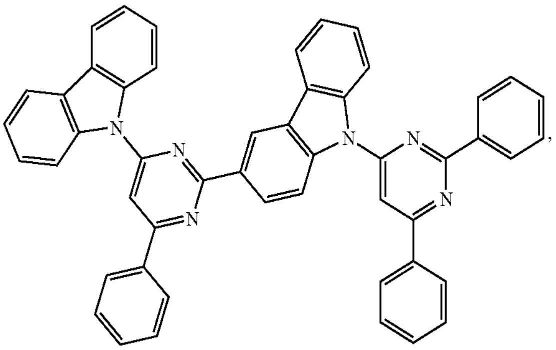
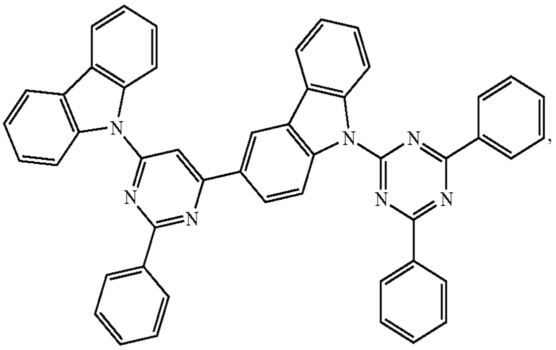
Compound A3



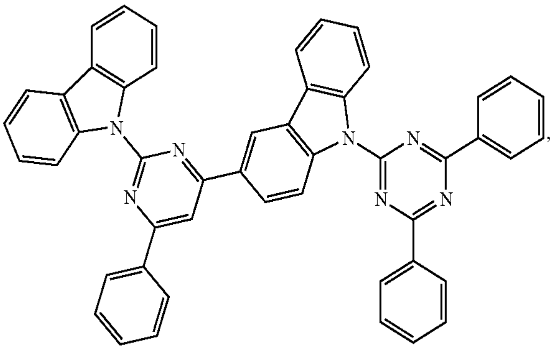
Compound A4



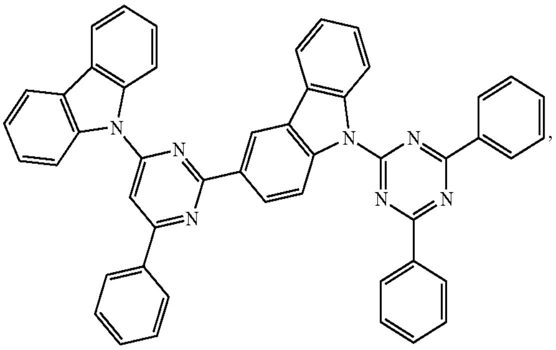
Compound A5



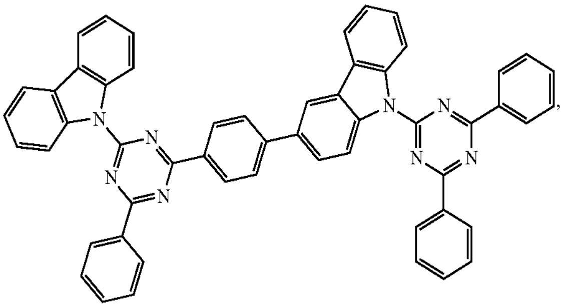
Compound A6



Compound A7



Compound A8



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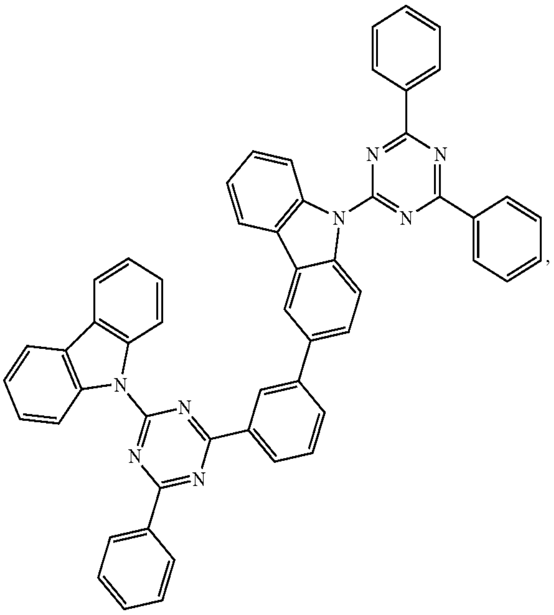
Compound A9



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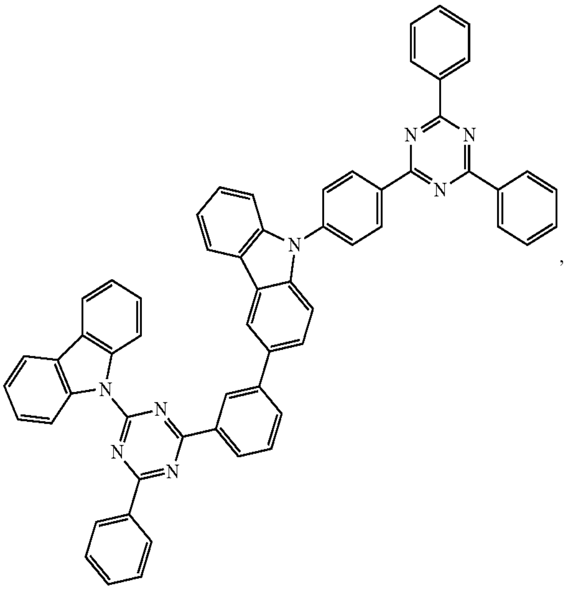
Compound A10



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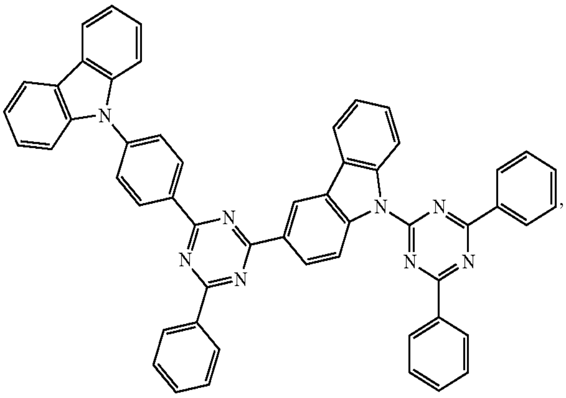
Compound A11



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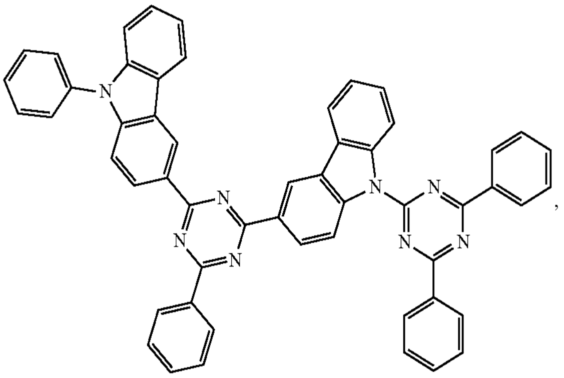
Compound A12



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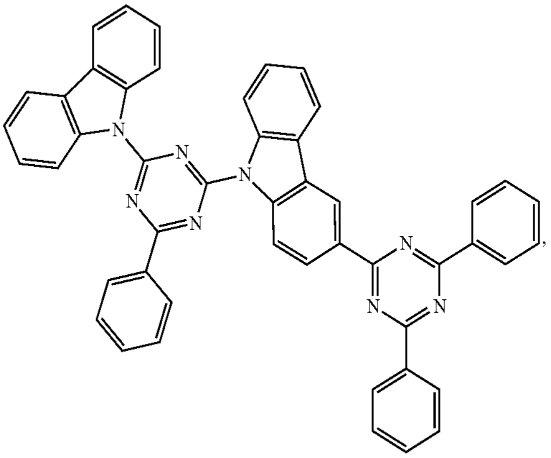
Compound A13



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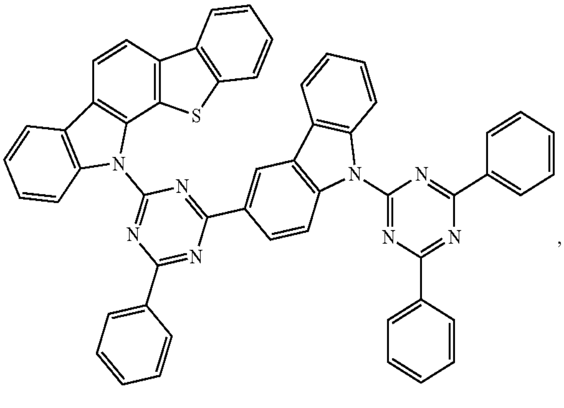
Compound A14



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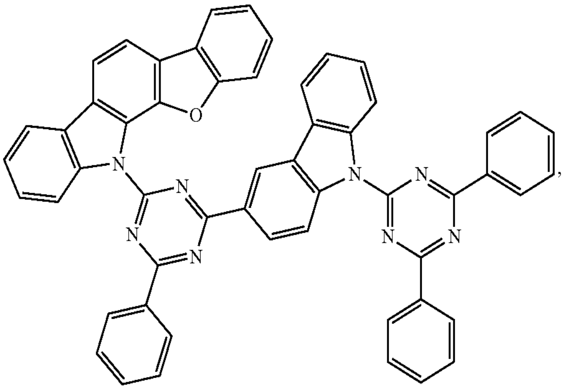
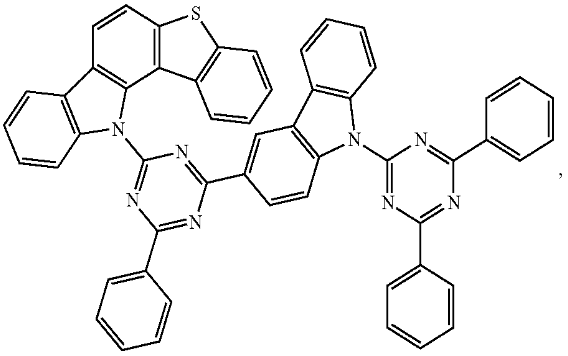
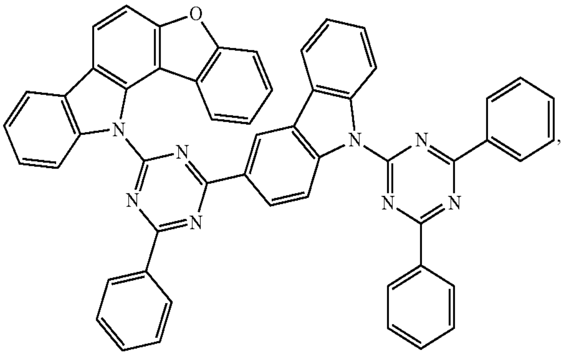
Compound A15



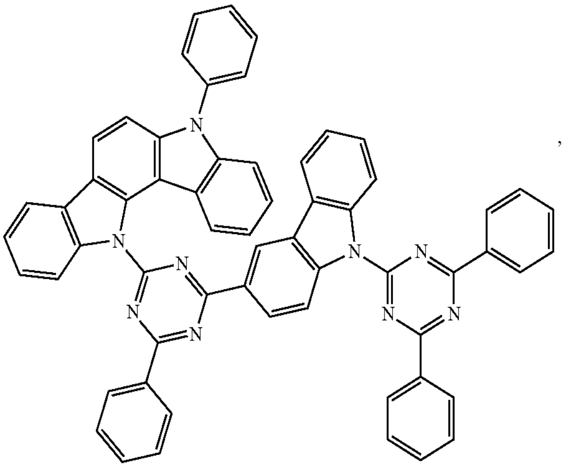
Compound A16



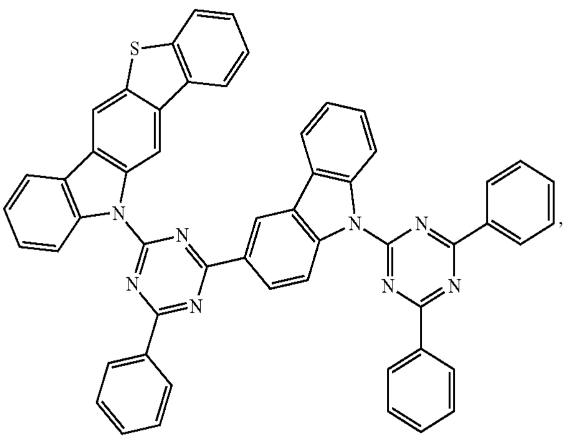
Compound A17



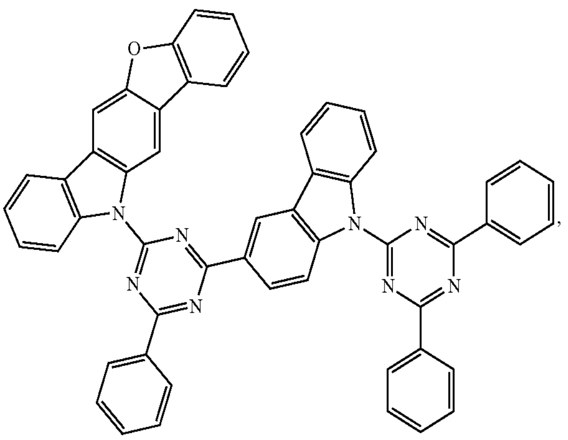
Compound A18



Compound A19



Compound A20



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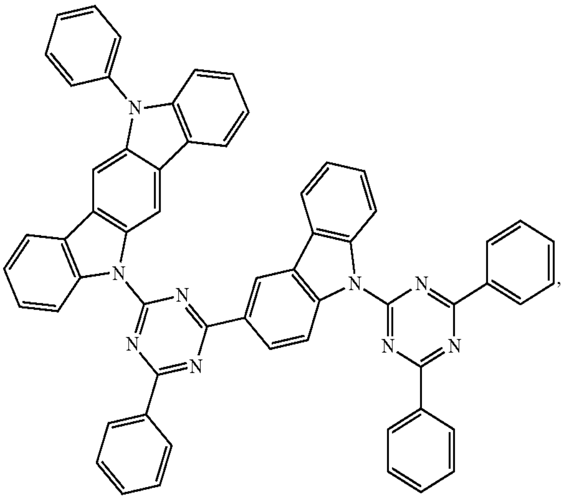
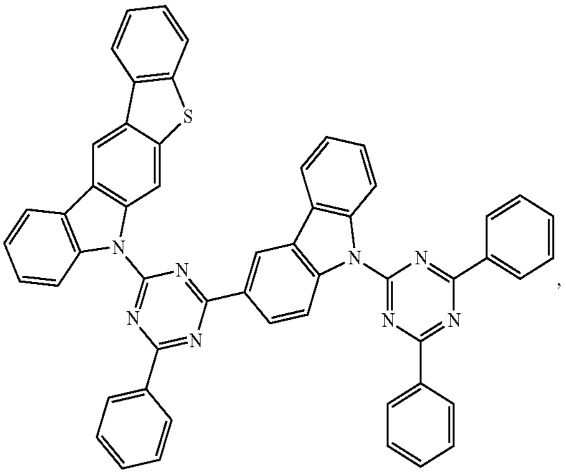
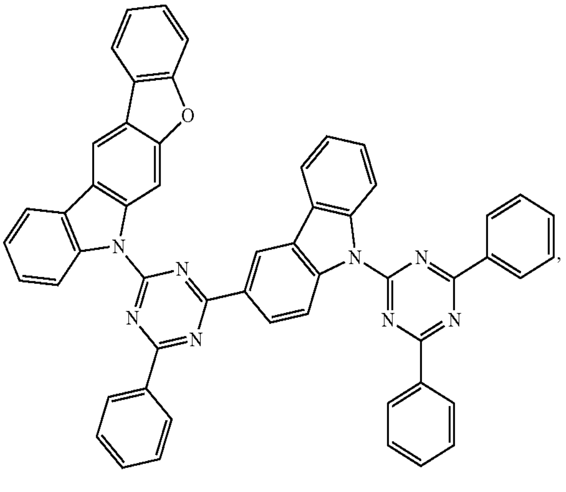
Compound A21



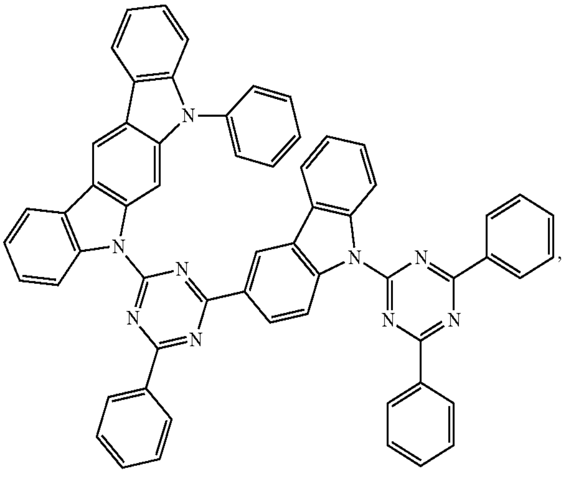
Compound A22



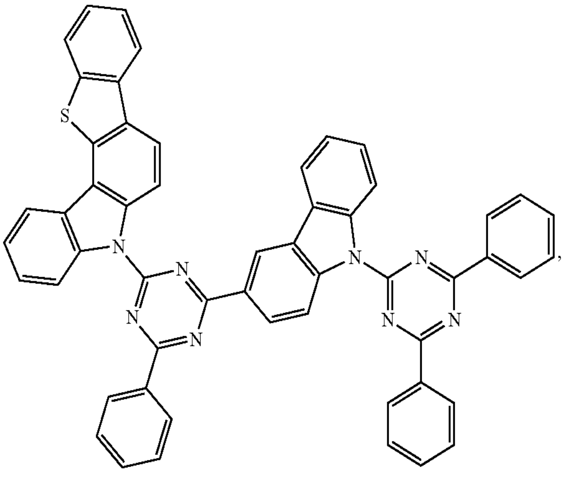
Compound A23



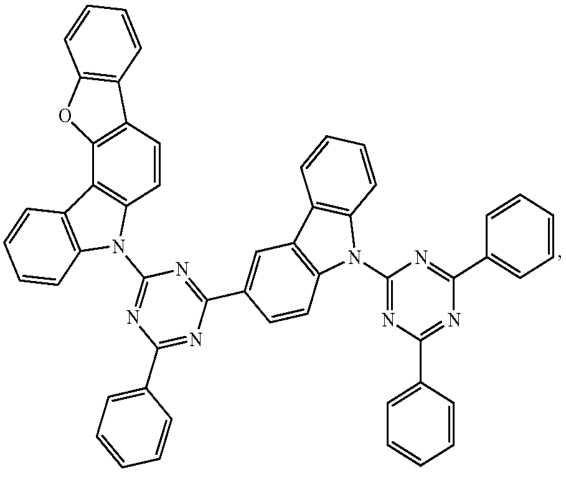
Compound A24



Compound A25



Compound A26



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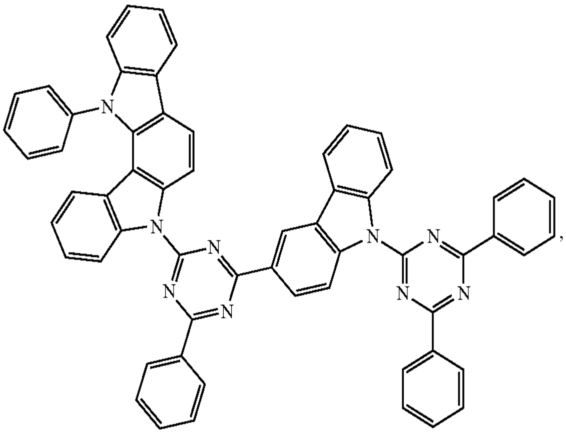
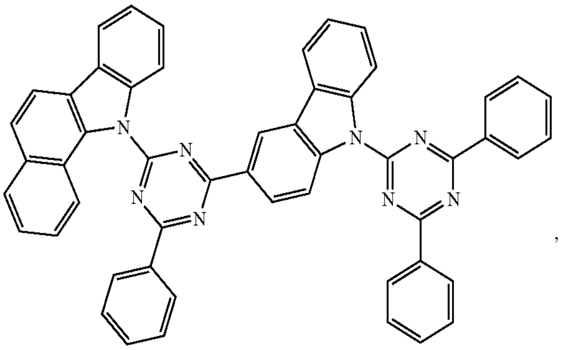
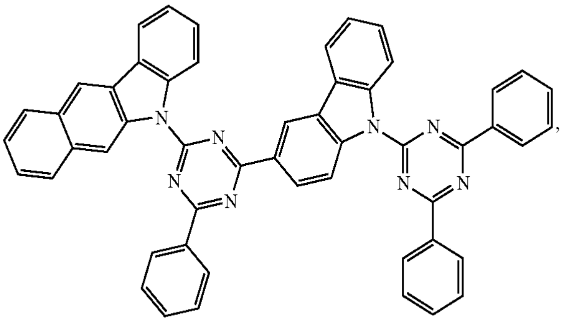
Compound A27



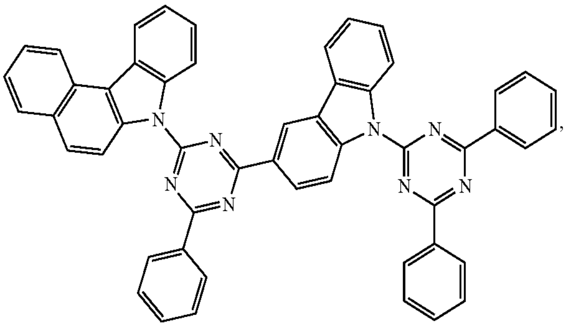
Compound A28



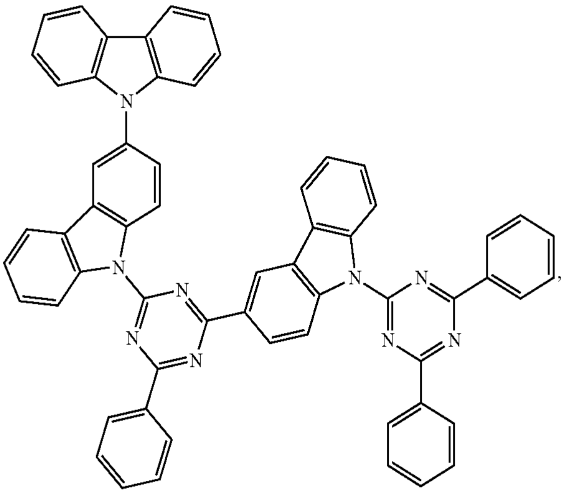
Compound A29



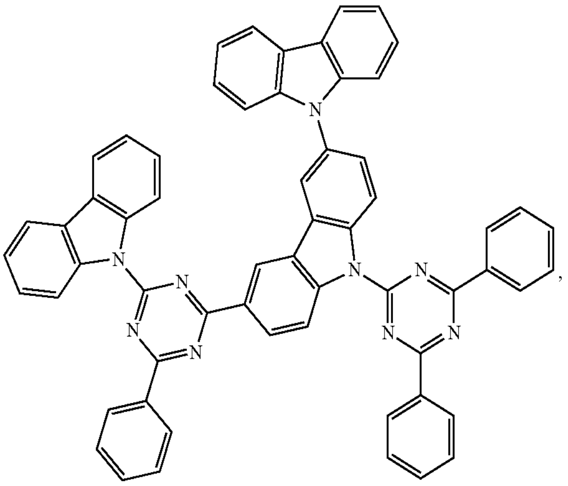
Compound A30



Compound A31



Compound A32



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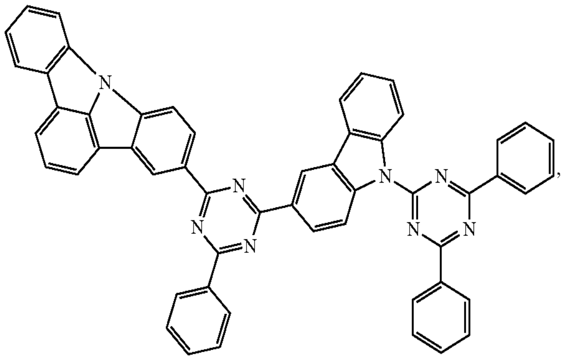
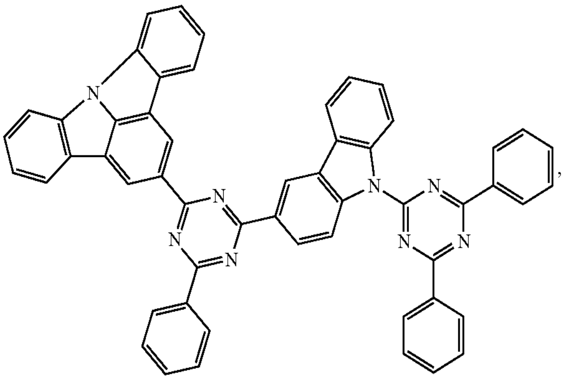
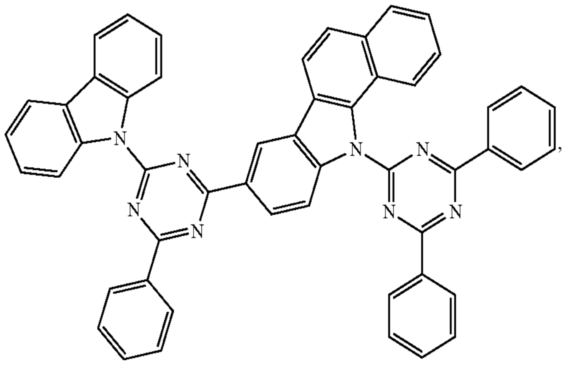
Compound A33



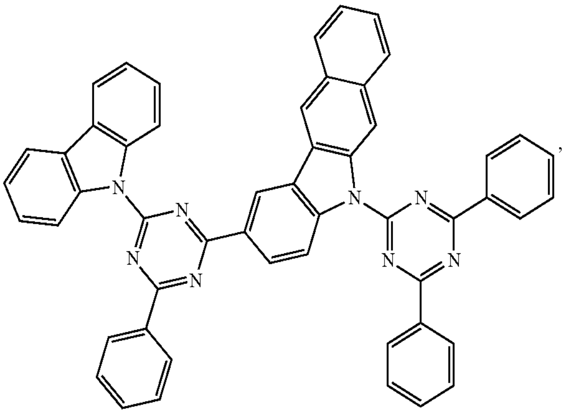
Compound A34



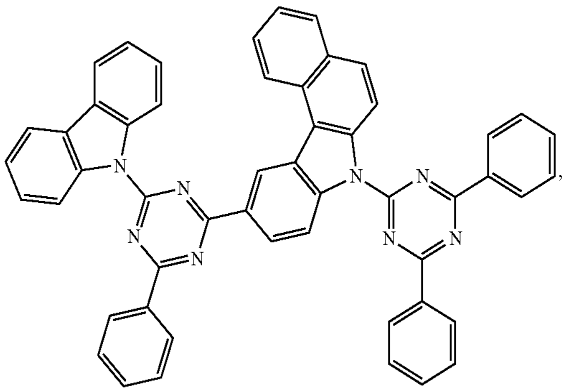
Compound A35



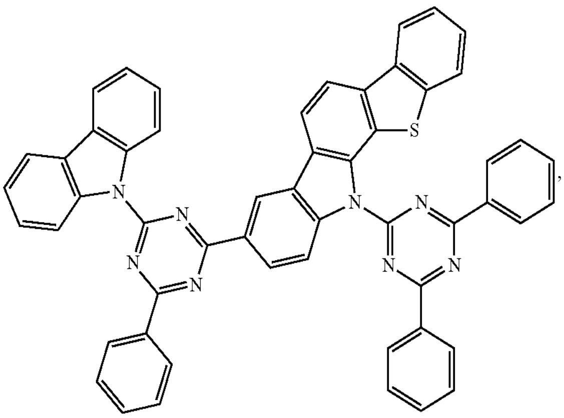
Compound A36



Compound A37



Compound A38



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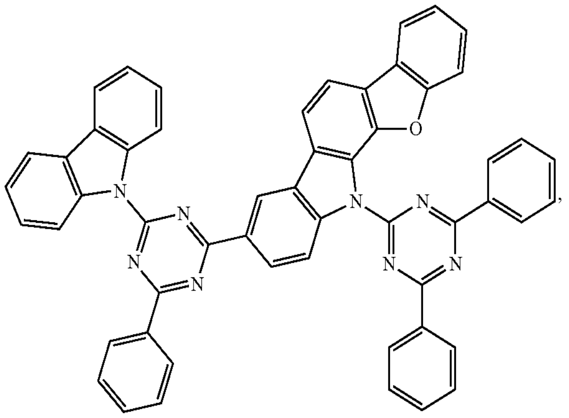
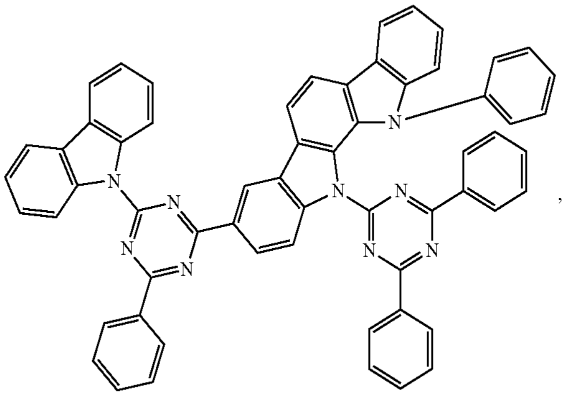
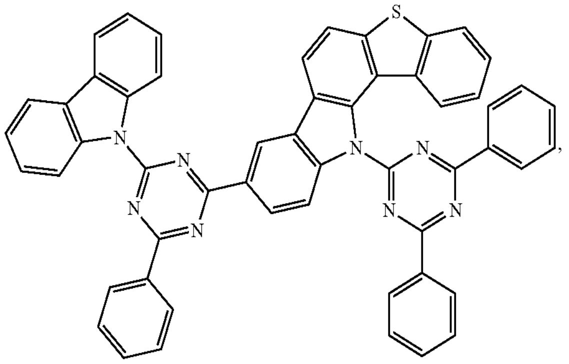
Compound A39



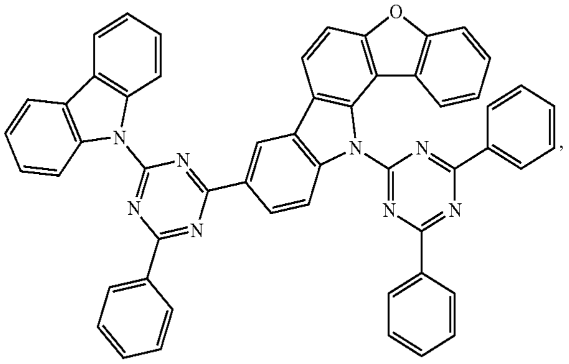
Compound A40



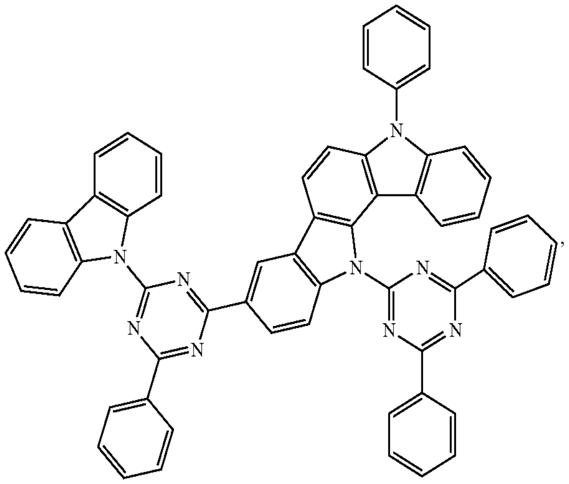
Compound A41



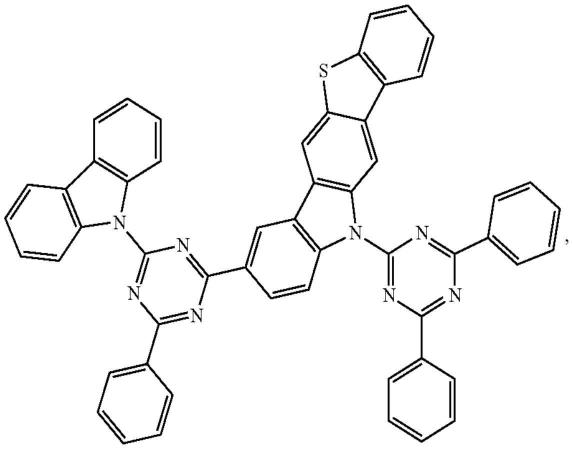
Compound A42



Compound A43



Compound A44



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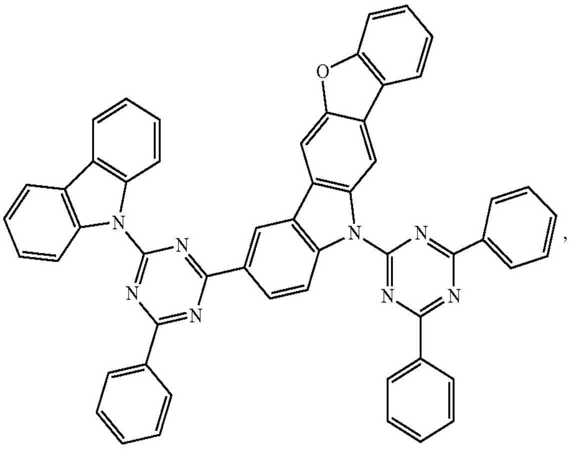
Compound A45



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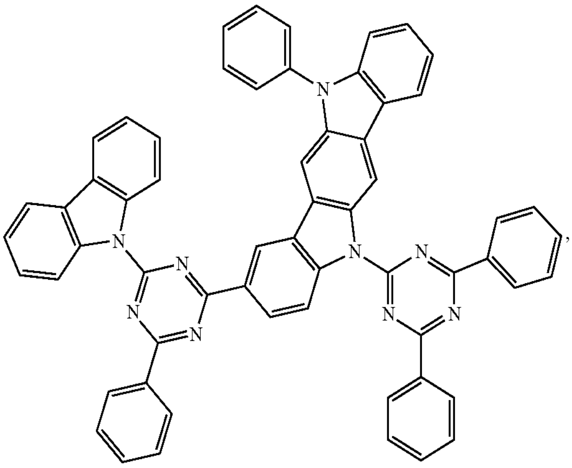
Compound A46



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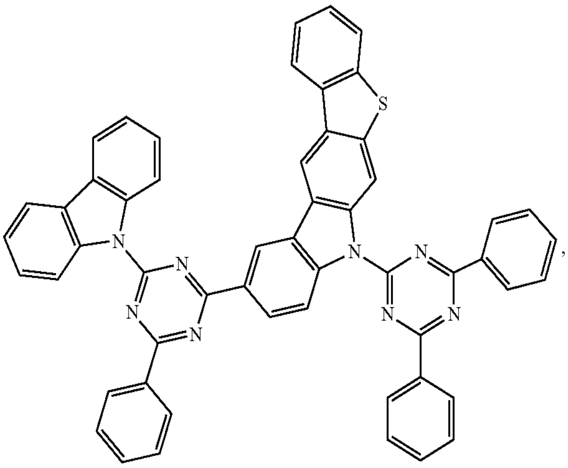
Compound A47



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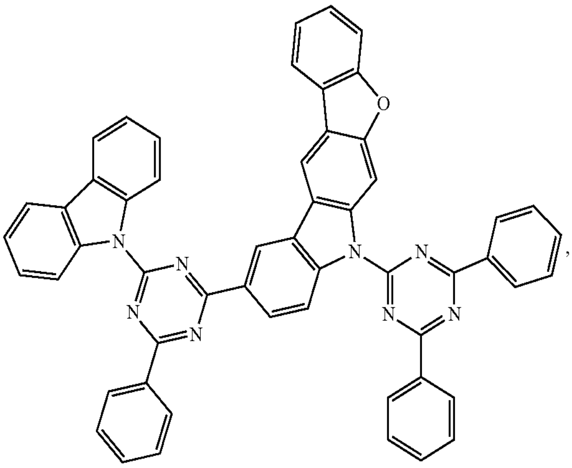
Compound A48



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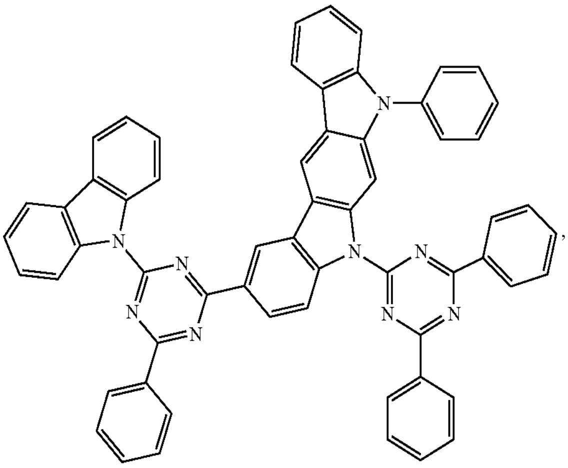

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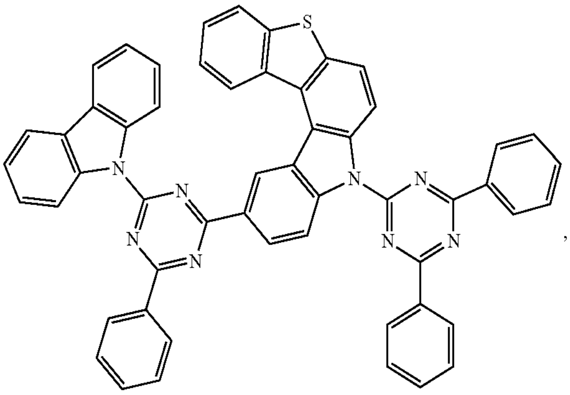
Compound A50



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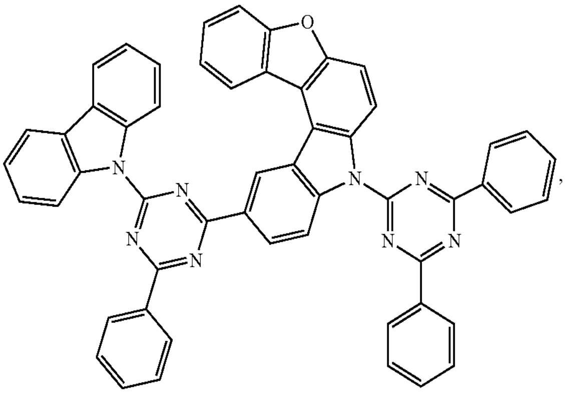
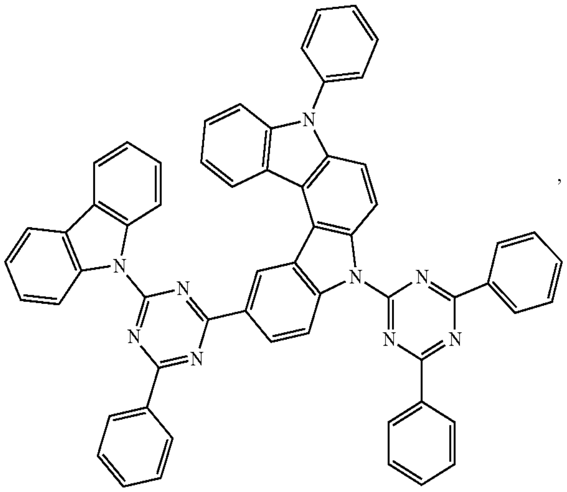


Compound A52



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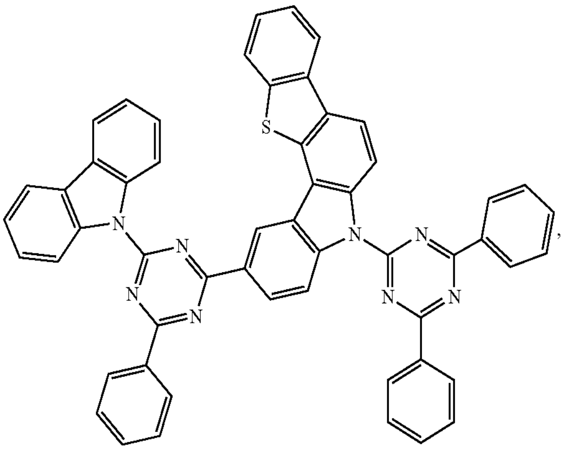

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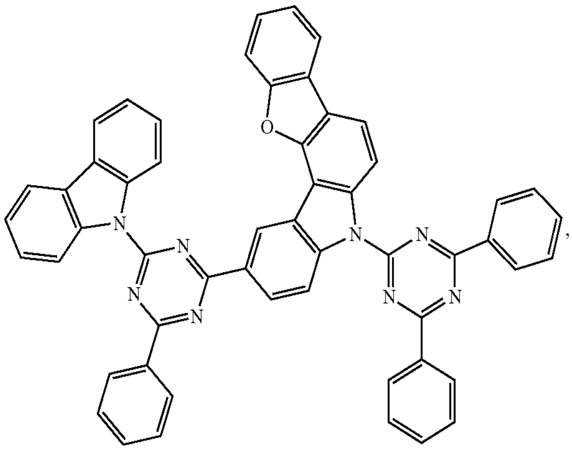
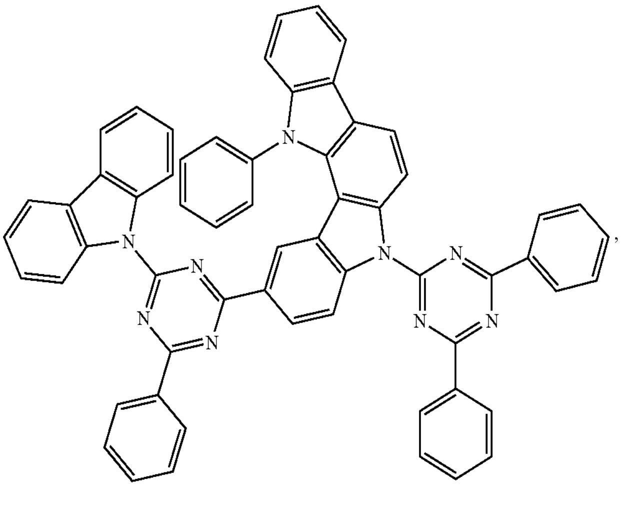


Compound 55



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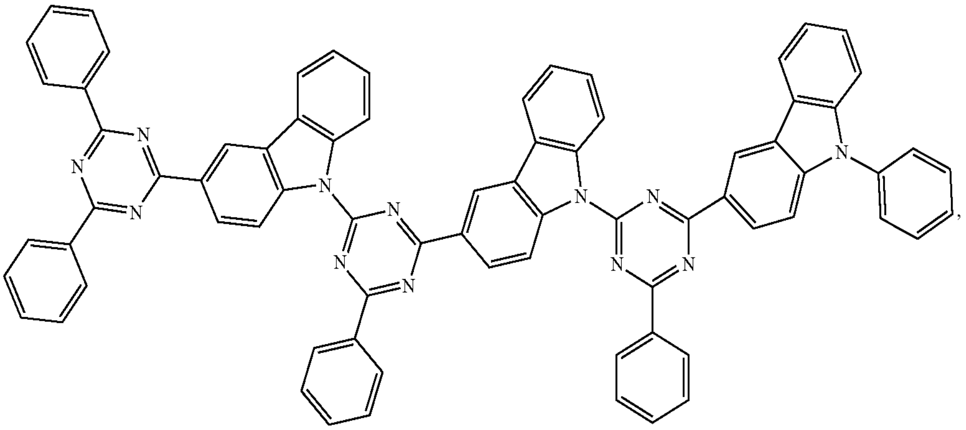
Compound A56



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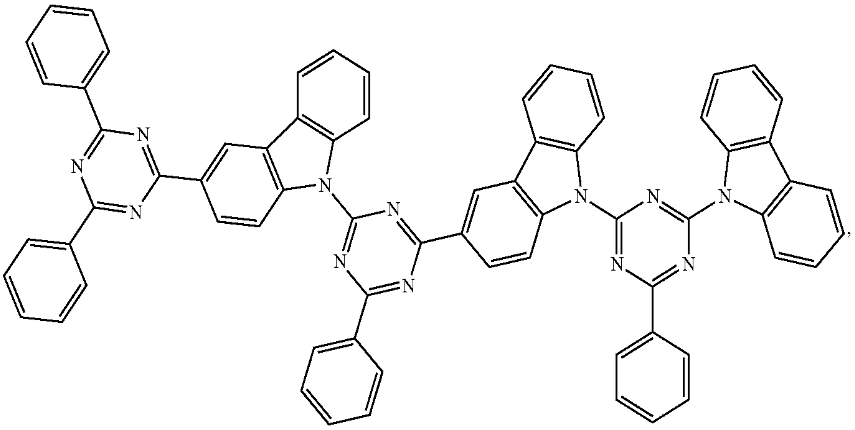

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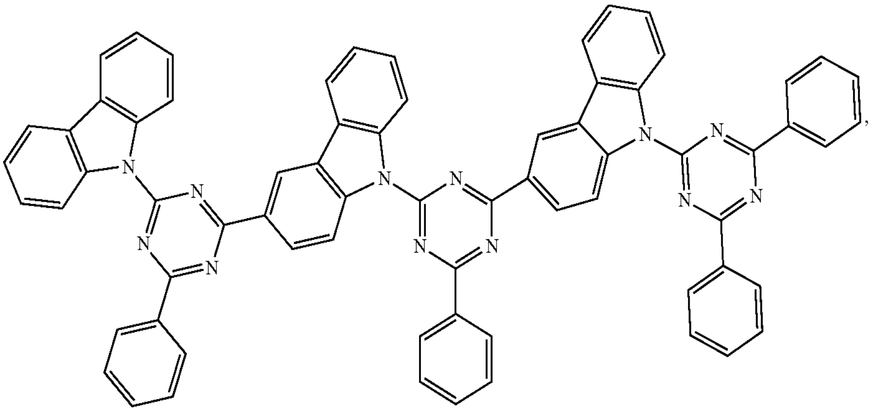

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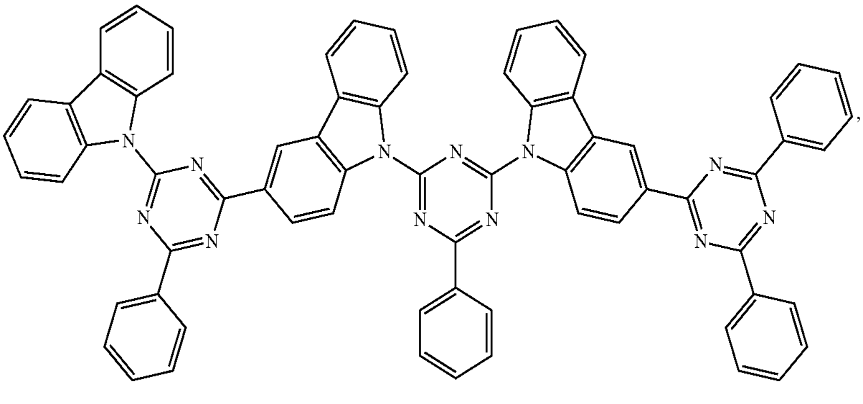

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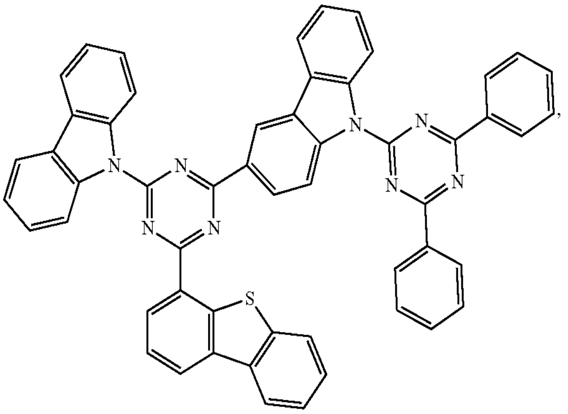

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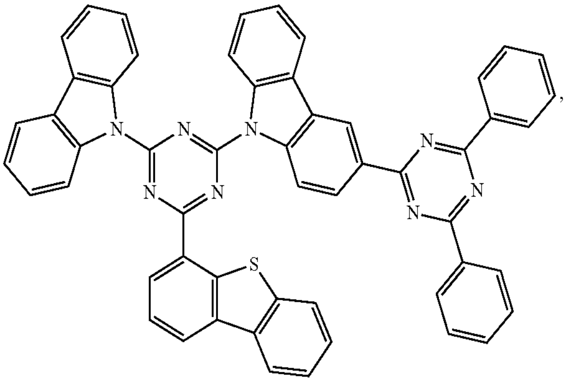

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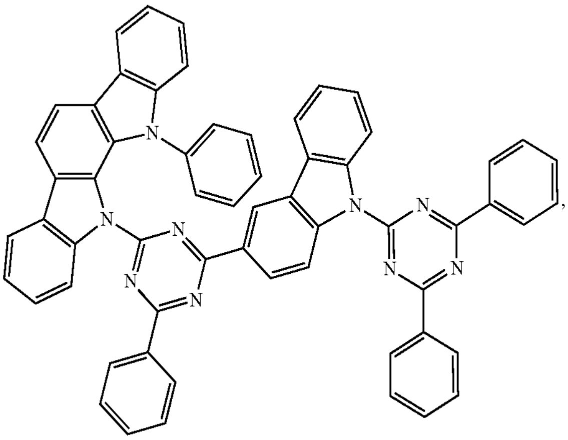

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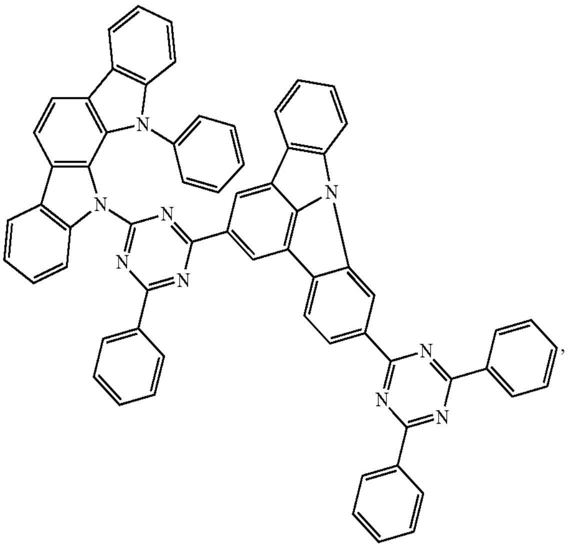

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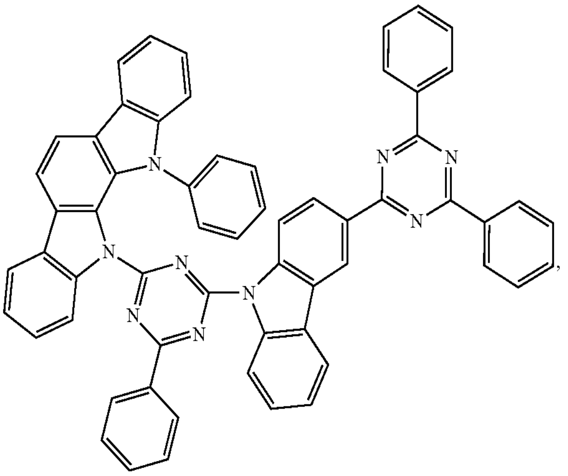

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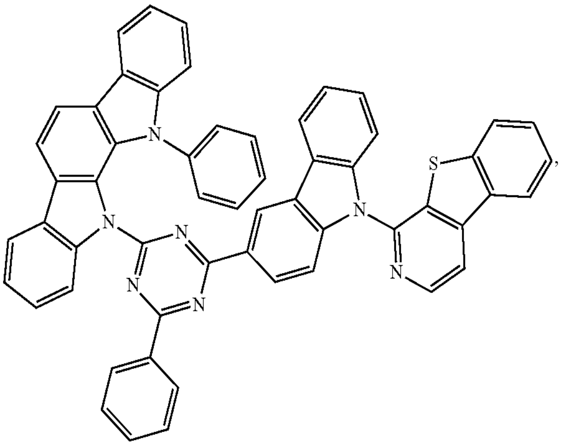

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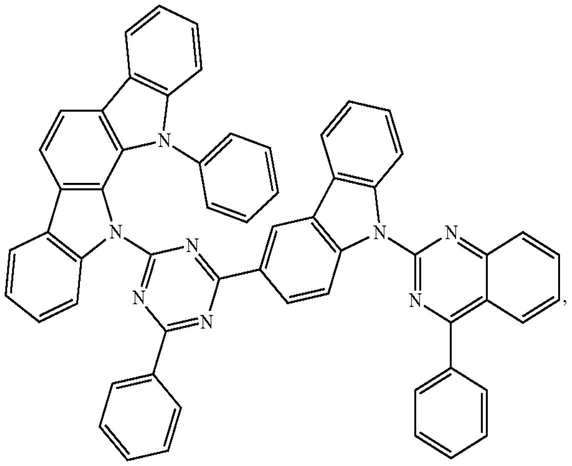
Compound A66



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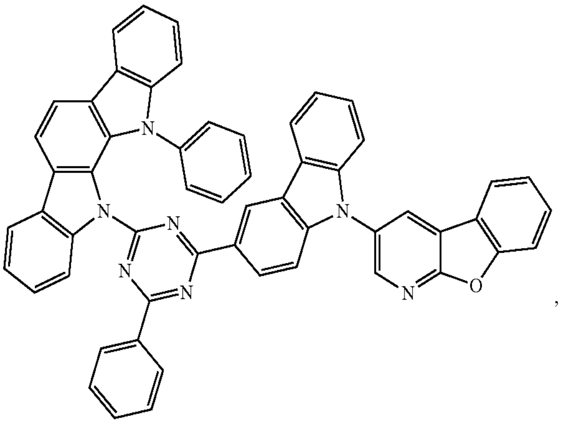

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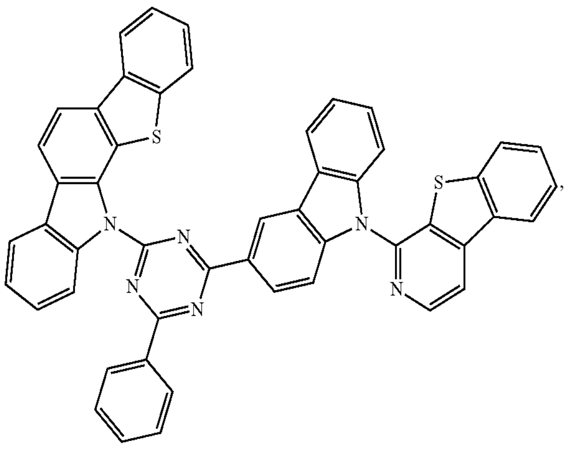

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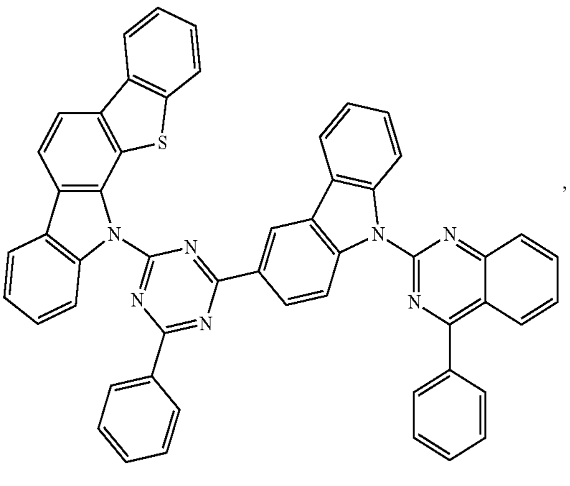

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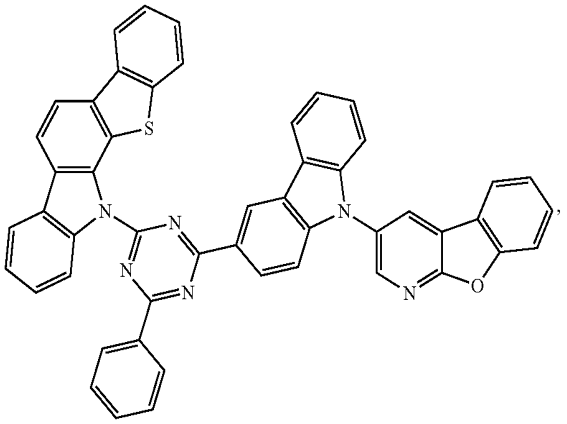

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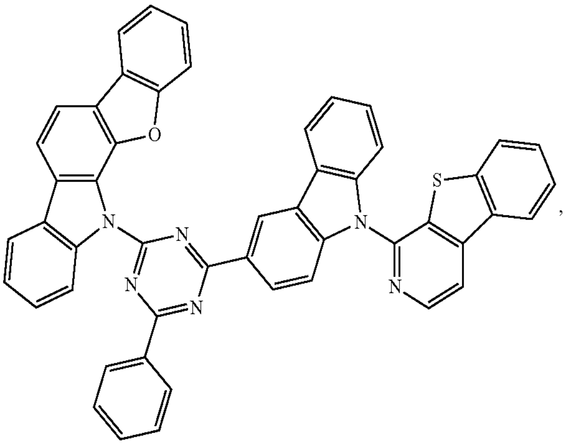

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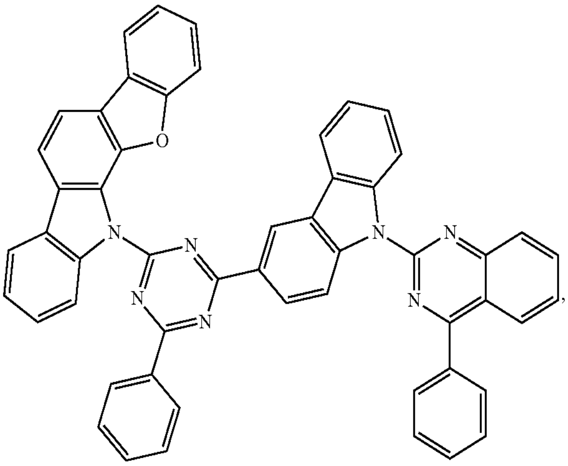
Compound A72



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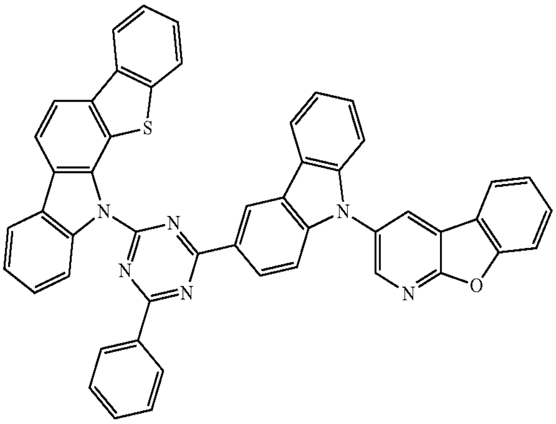
Compound A73



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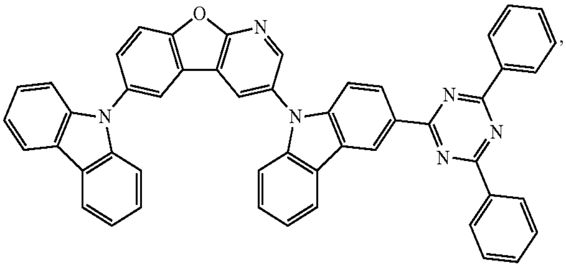
Compound A74



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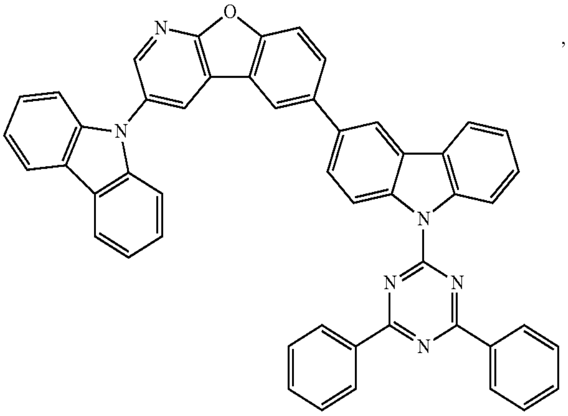

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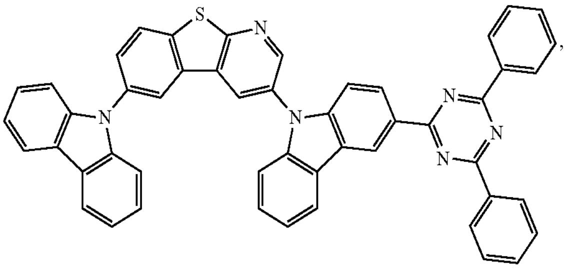

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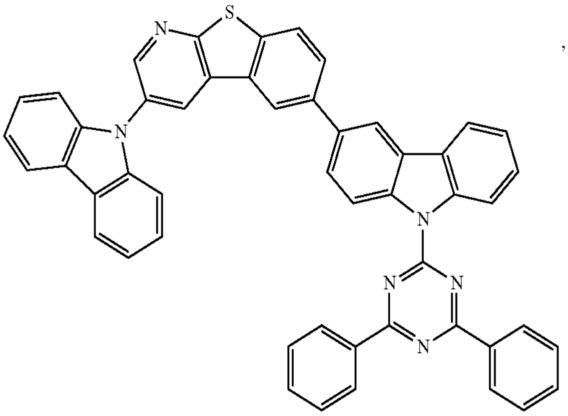

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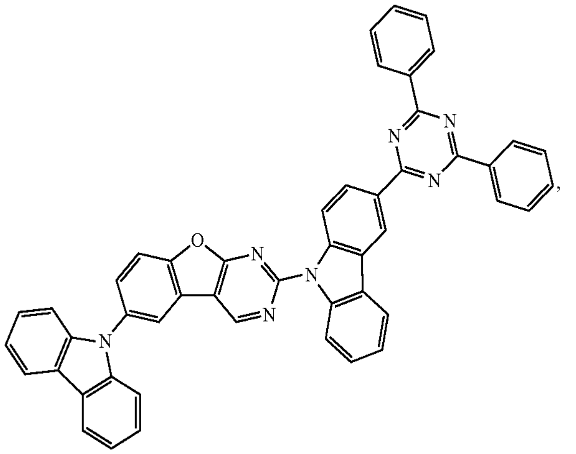

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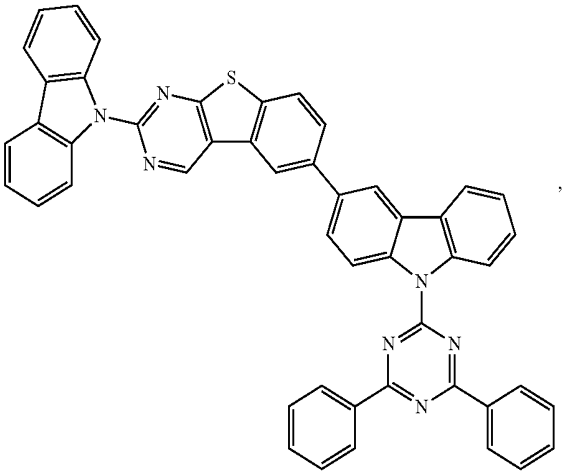

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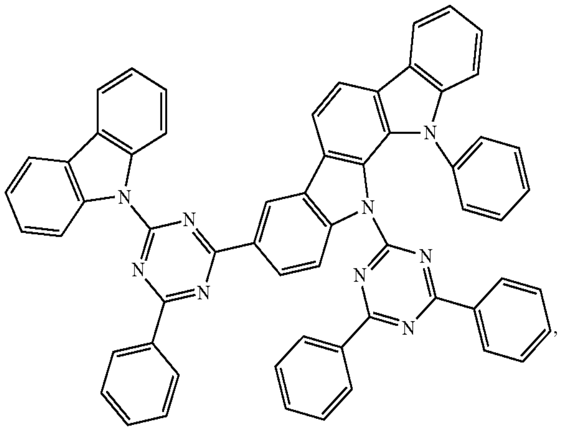

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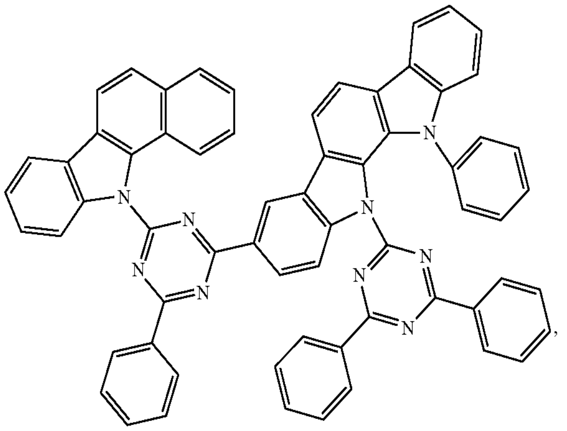

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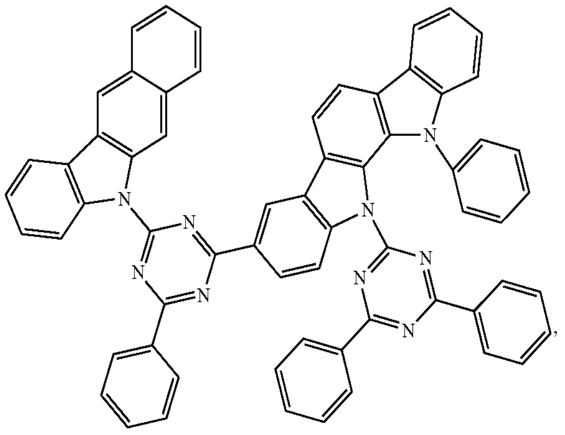

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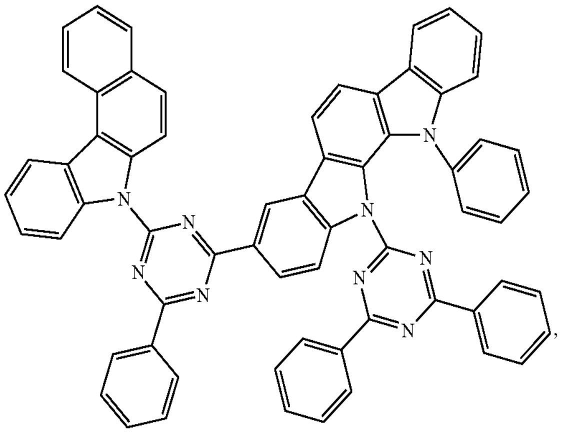

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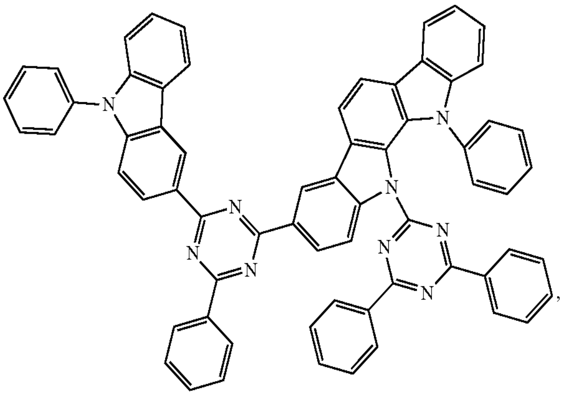

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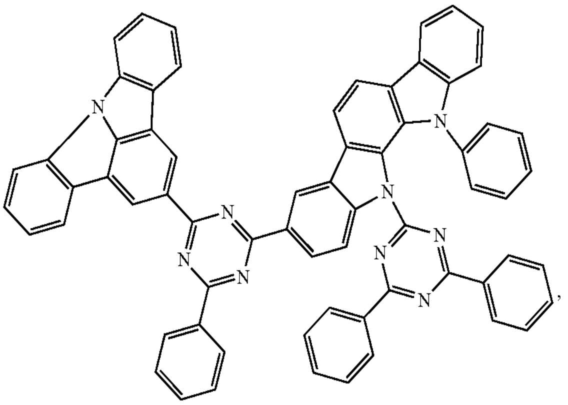

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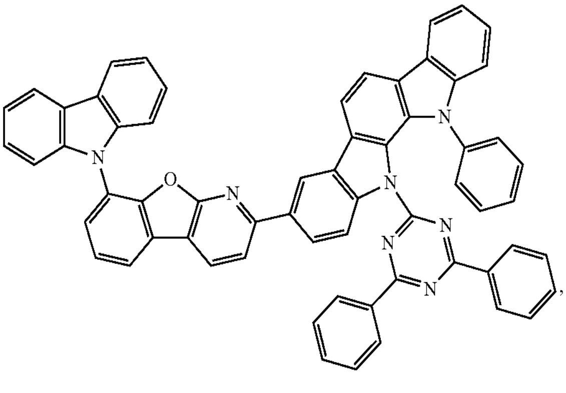

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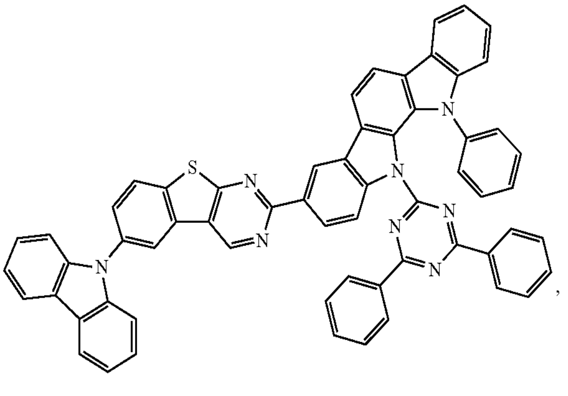

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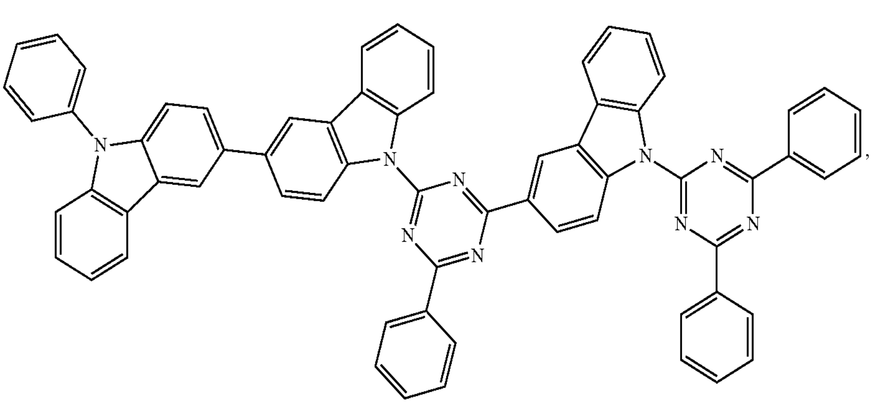

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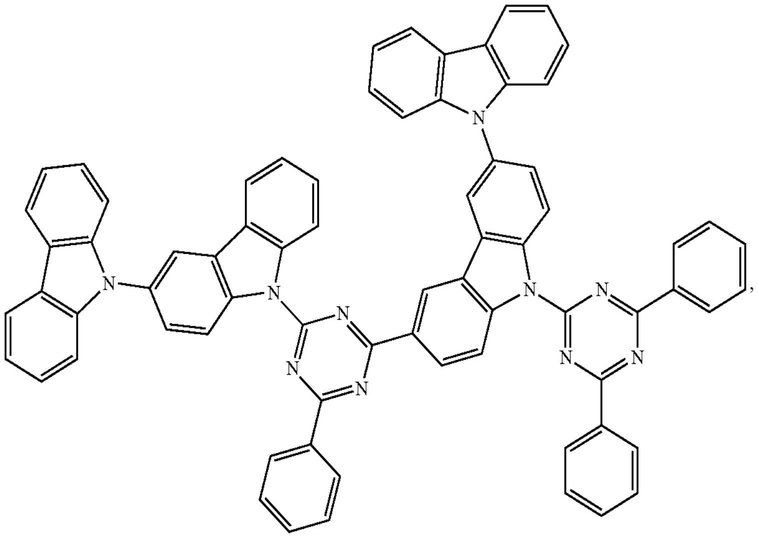

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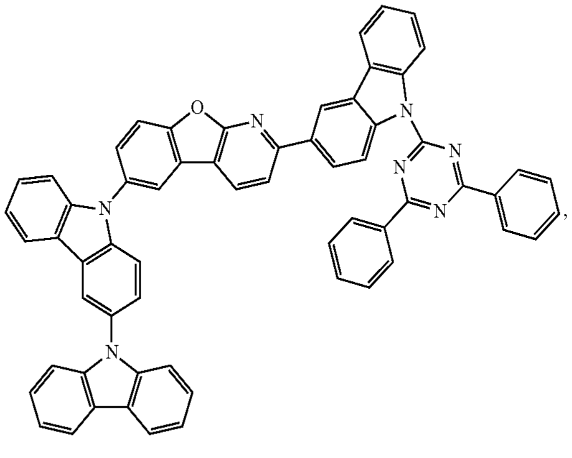

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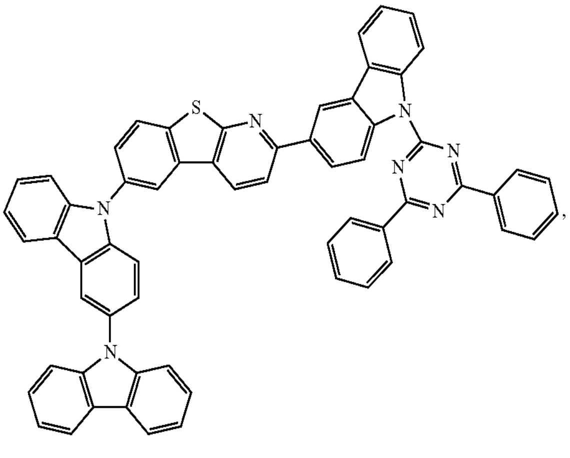

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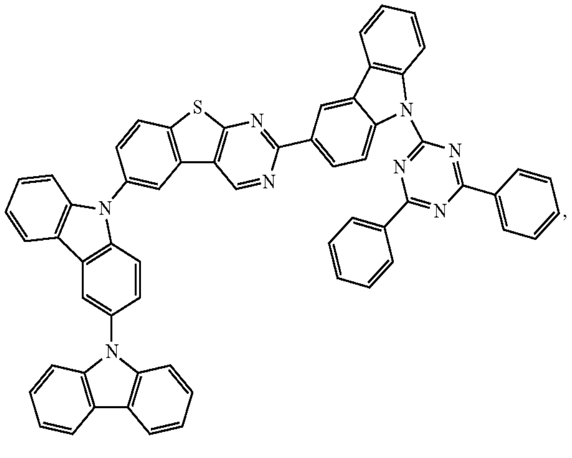

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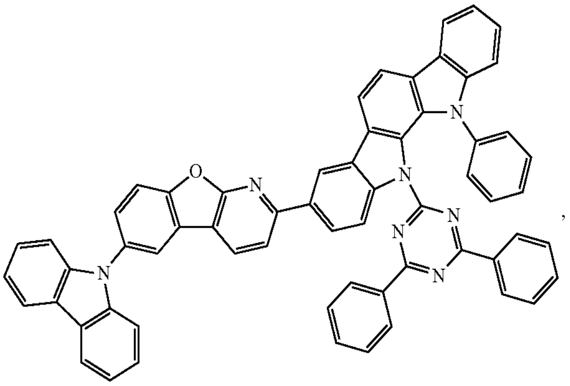

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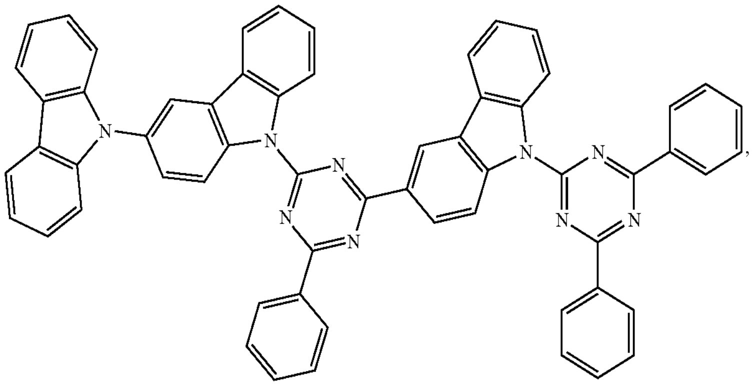

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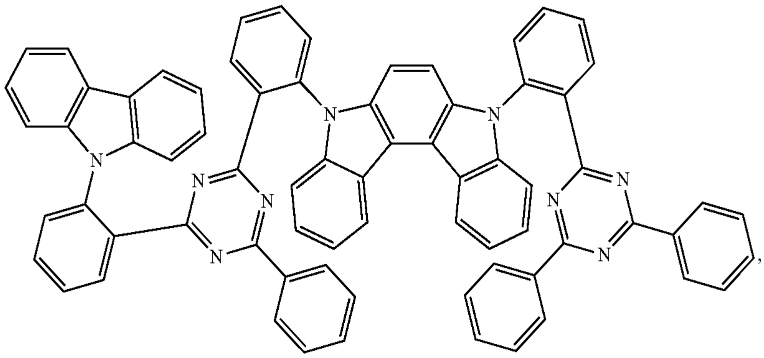

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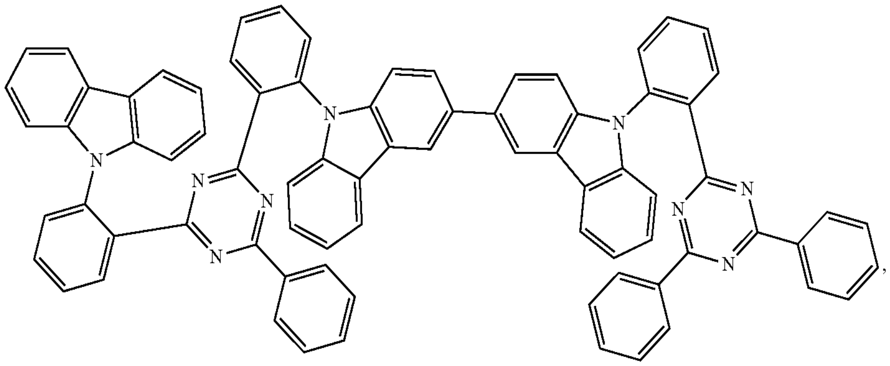

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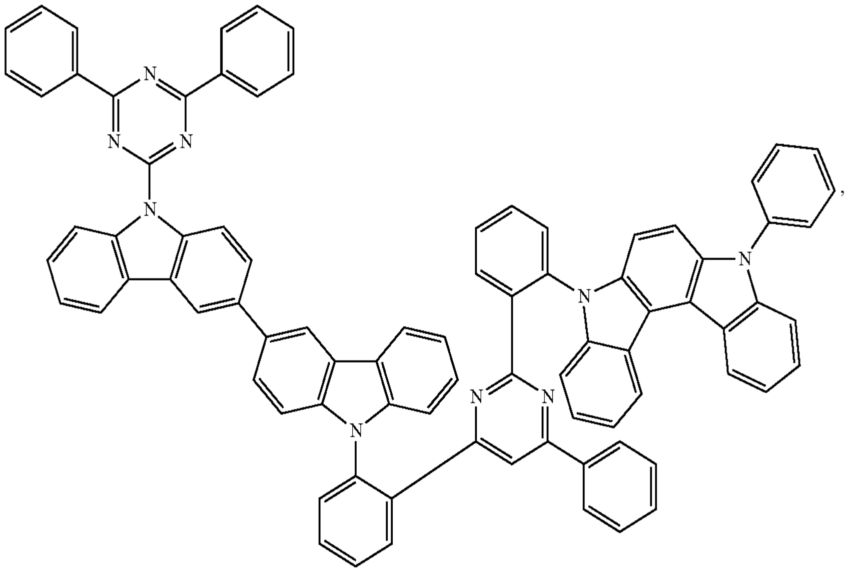

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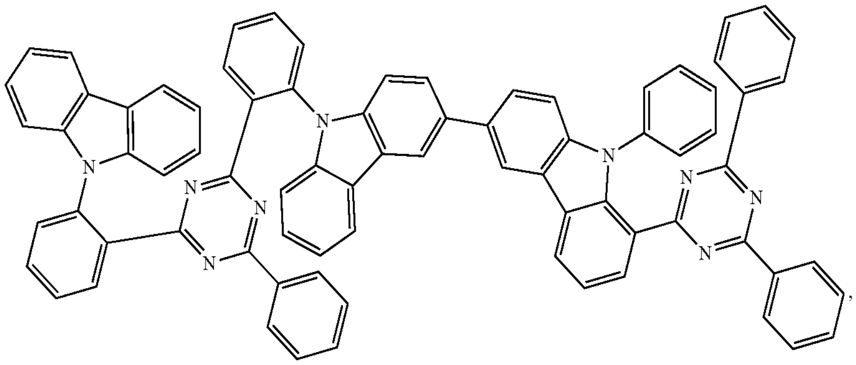
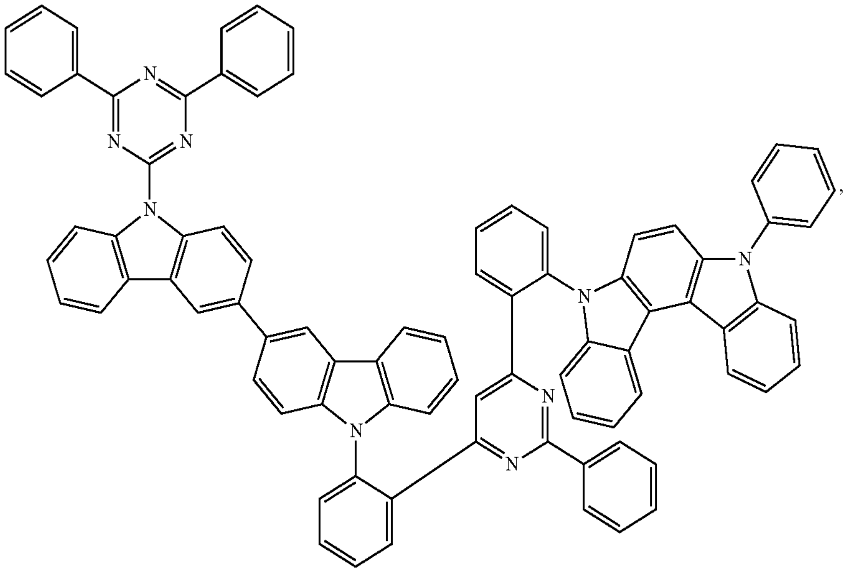


Compound A99



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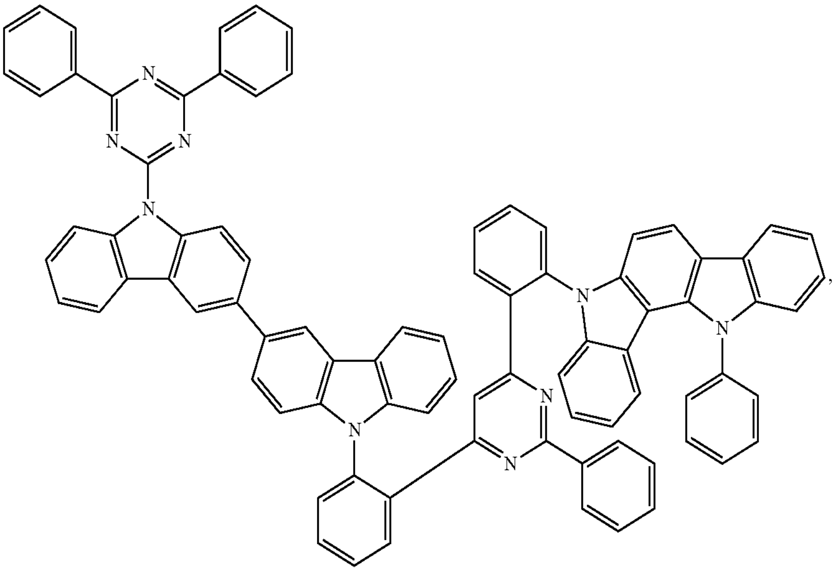
Compound A100



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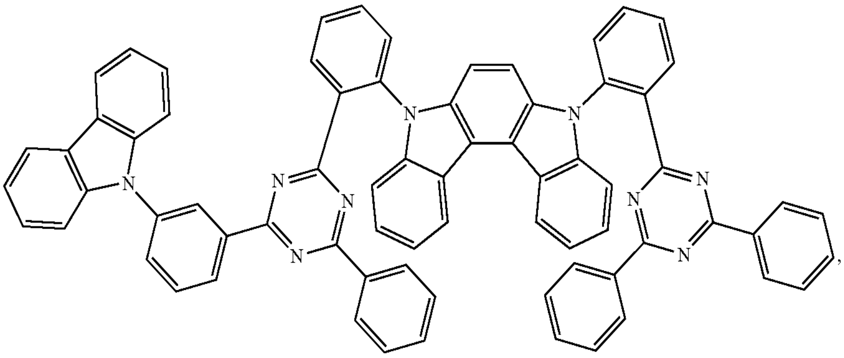

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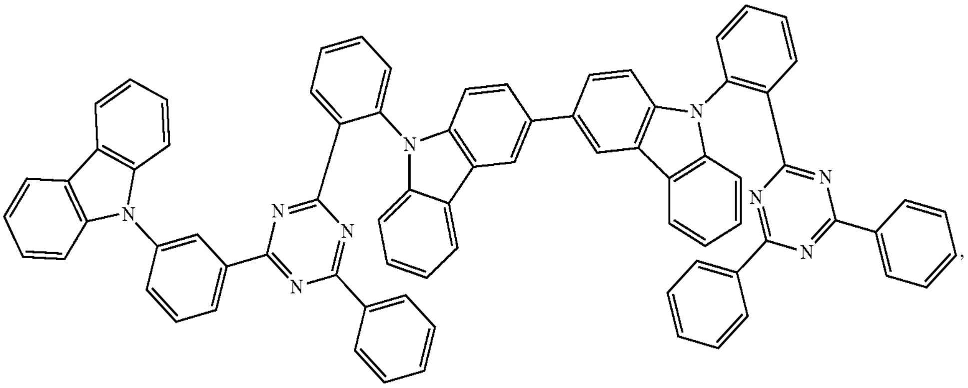

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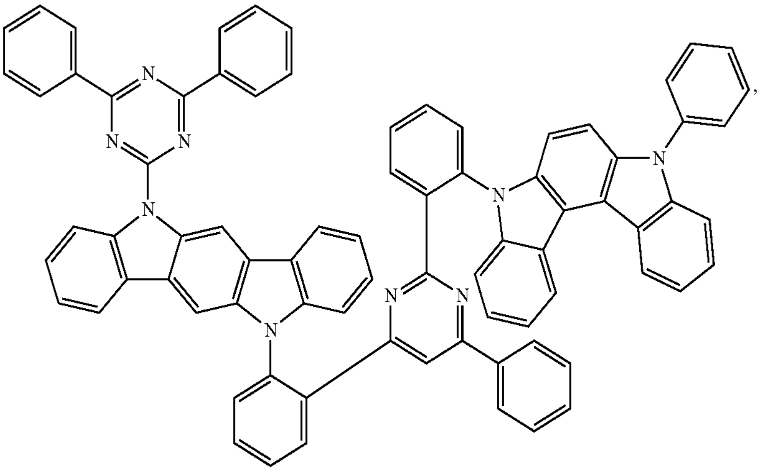

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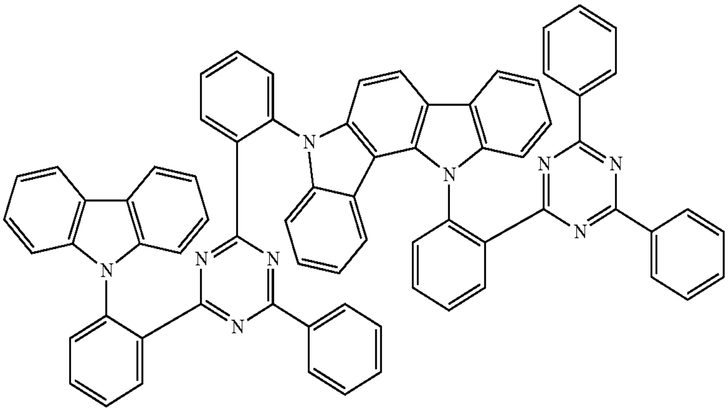

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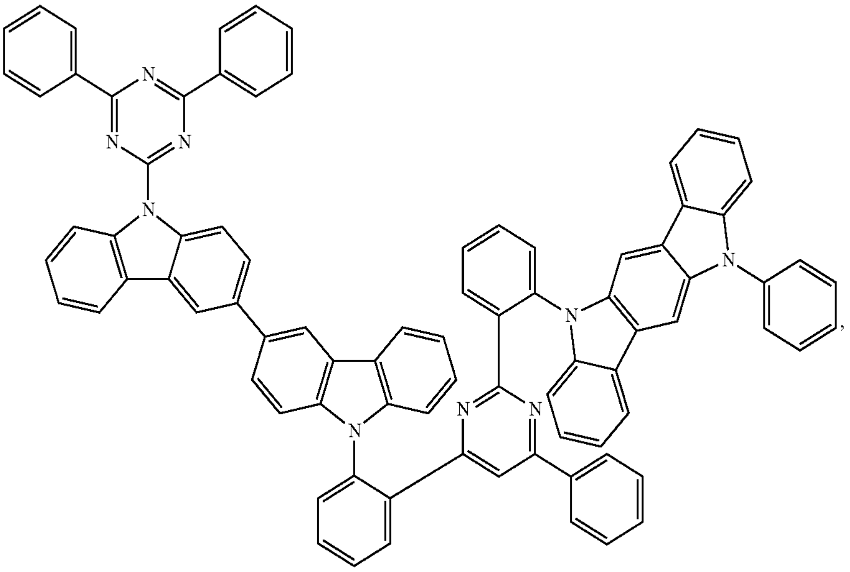

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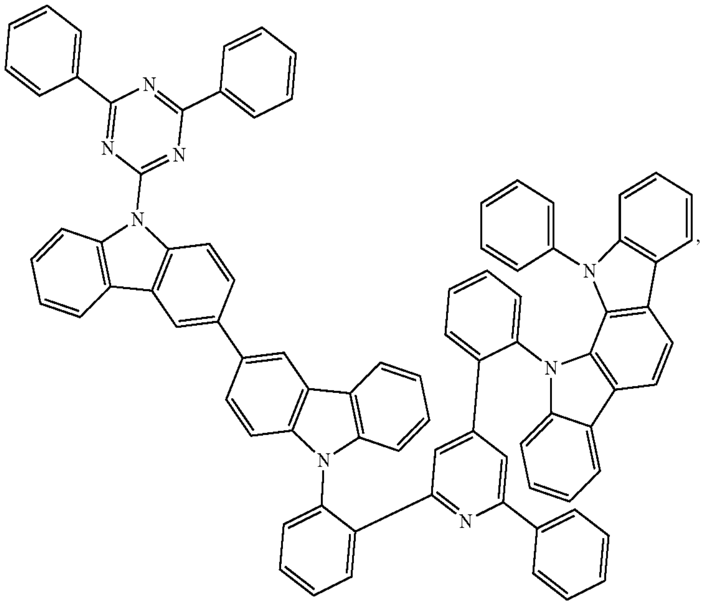
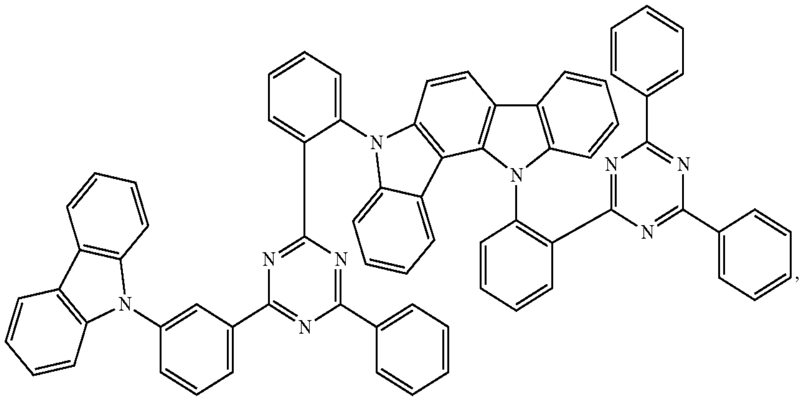


Compound A107



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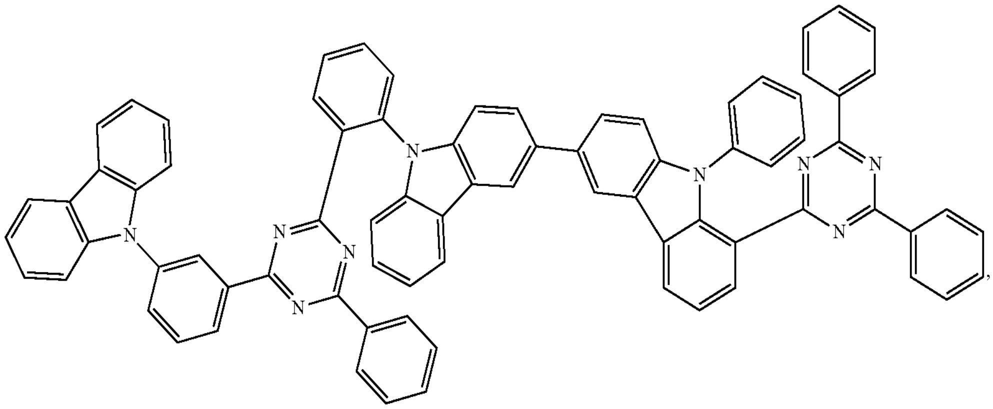

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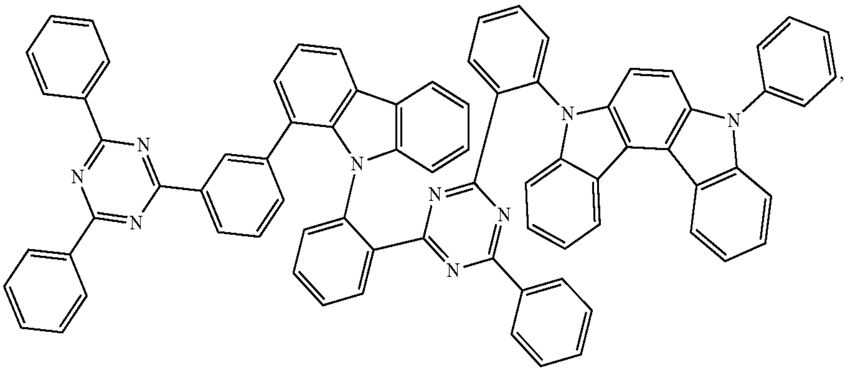
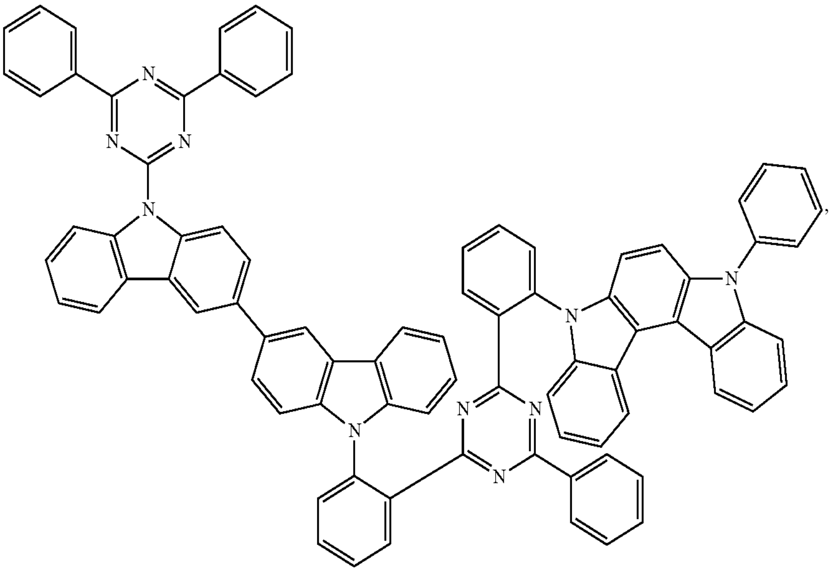
Compound A109



Compound A110



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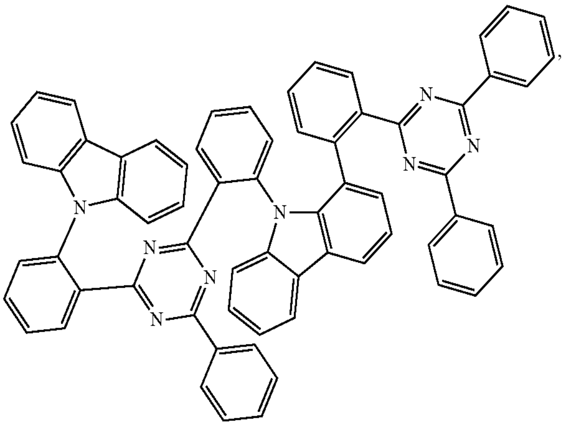
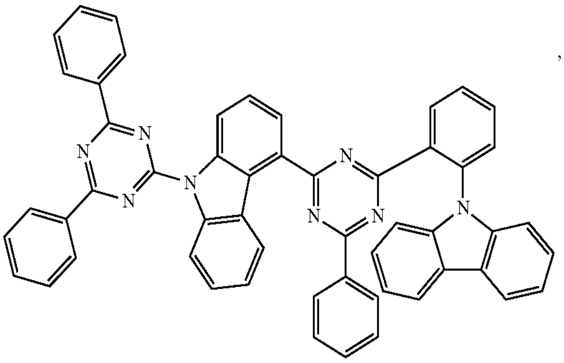


Compound A112



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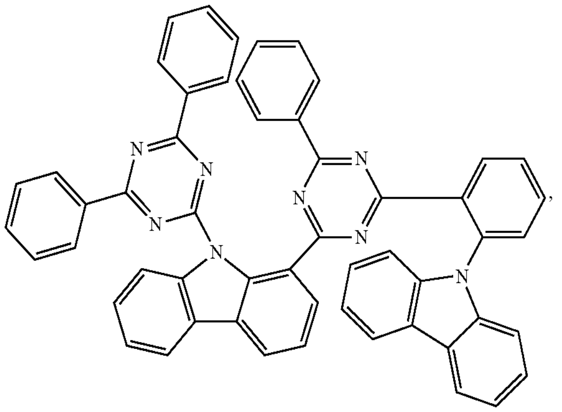
Compound A113



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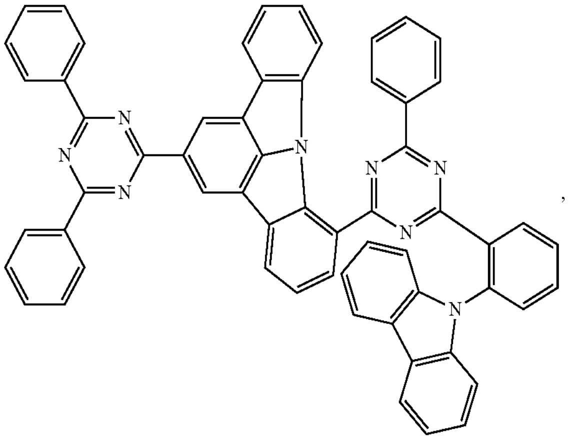
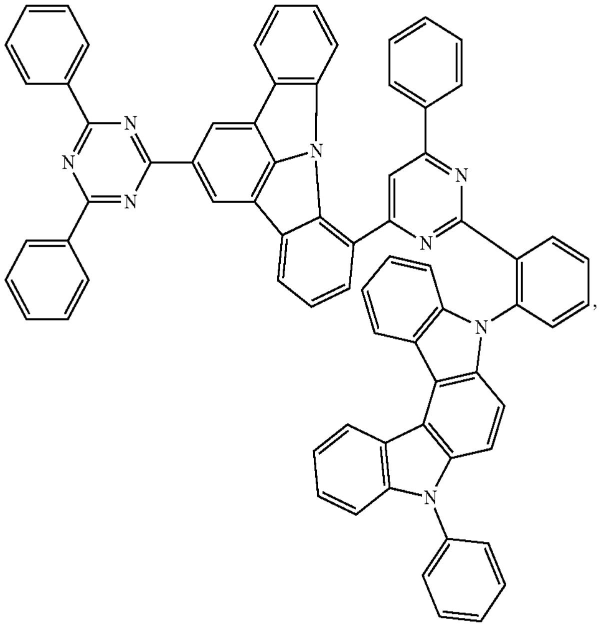


Compound A115



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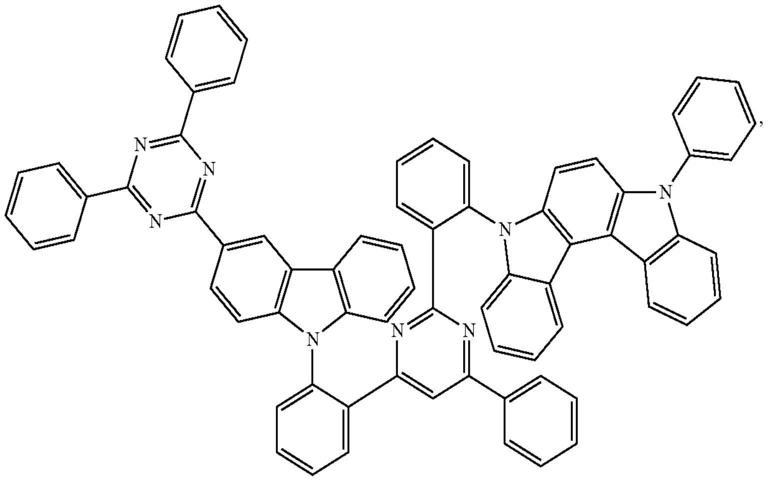

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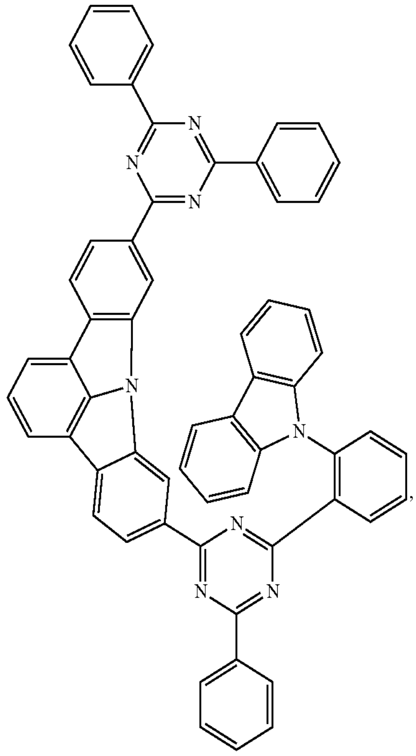
Compound A117



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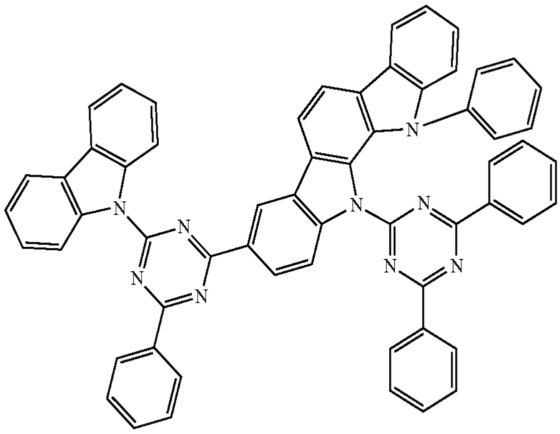
Compound A118



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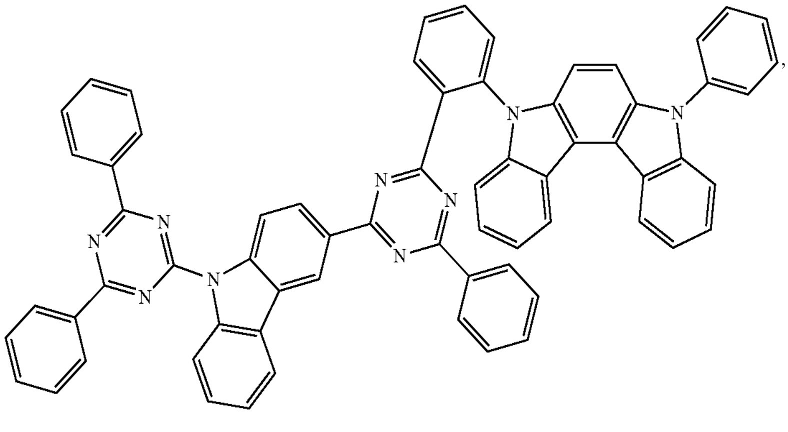
Compound A119



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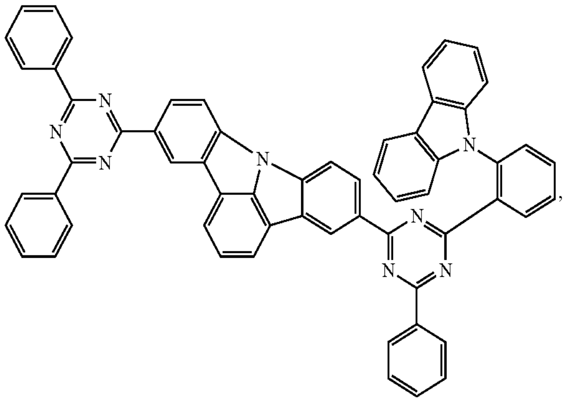
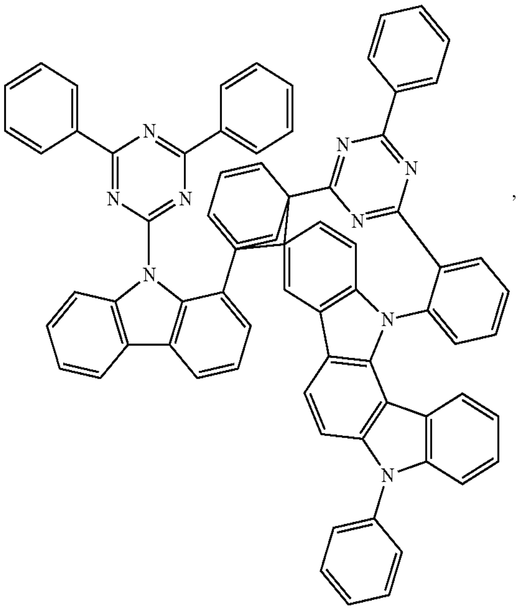
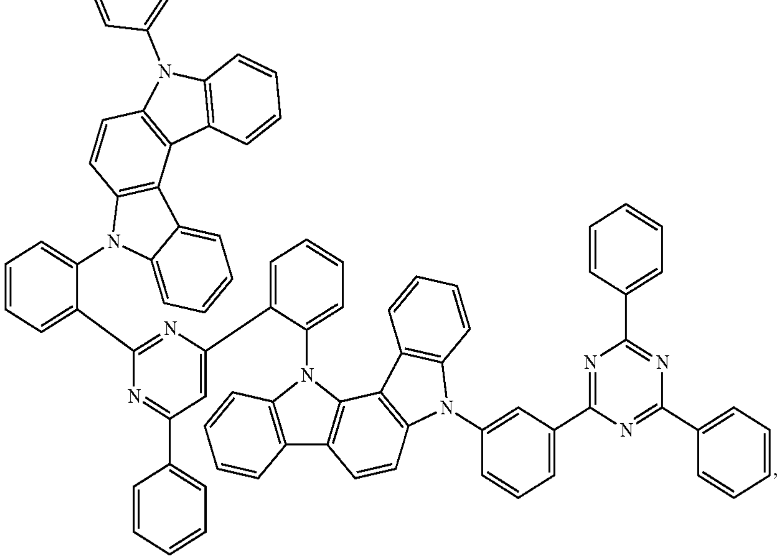
Compound A120



Compound A121



Compound A122



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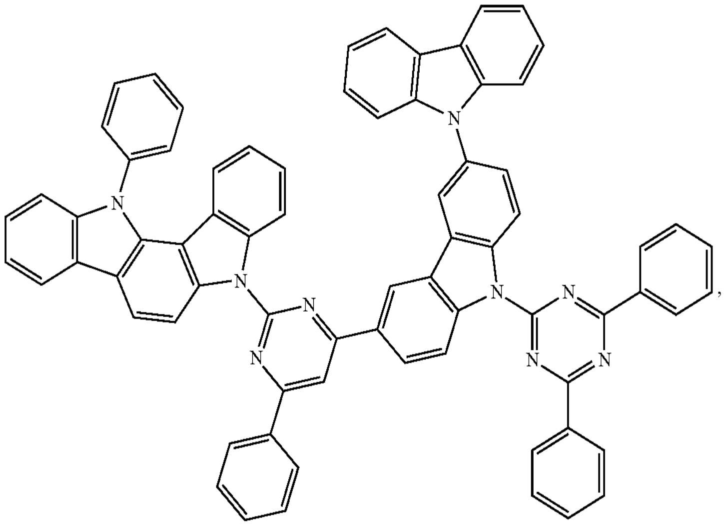
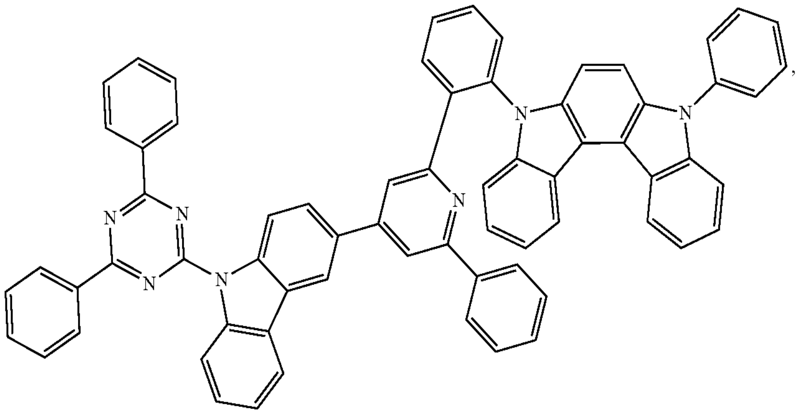
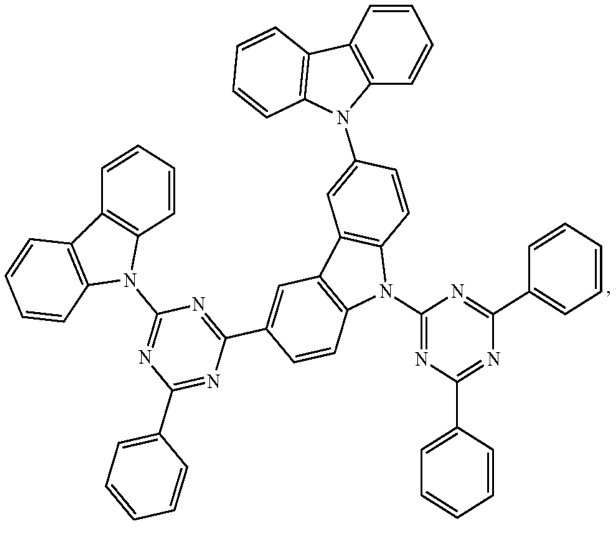
Compound A123



Compound A124



Compound A125



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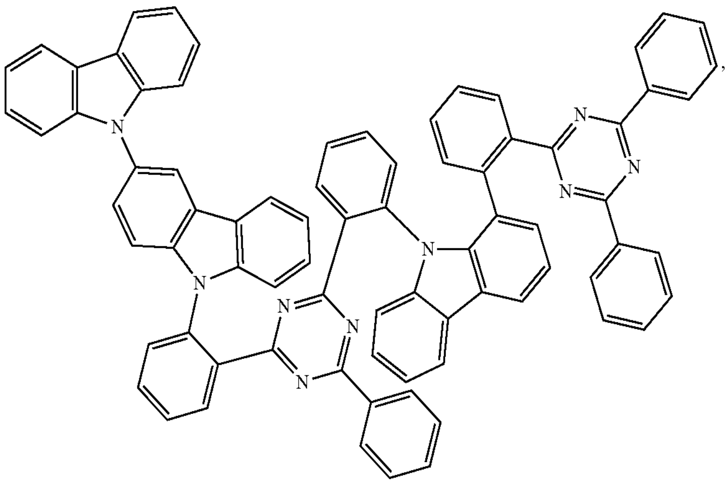
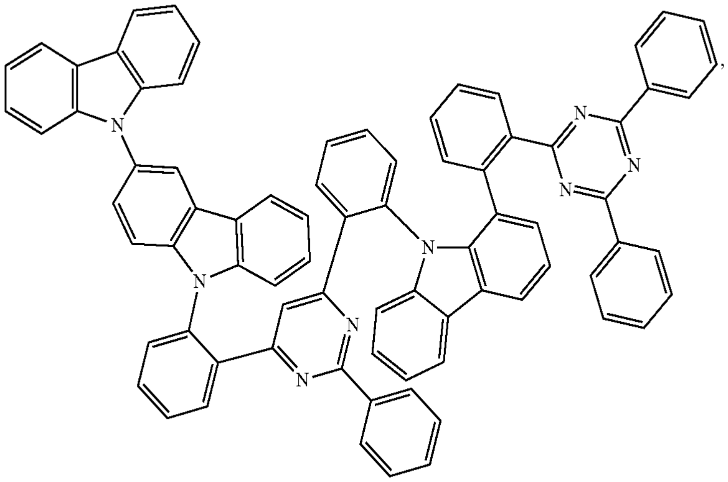
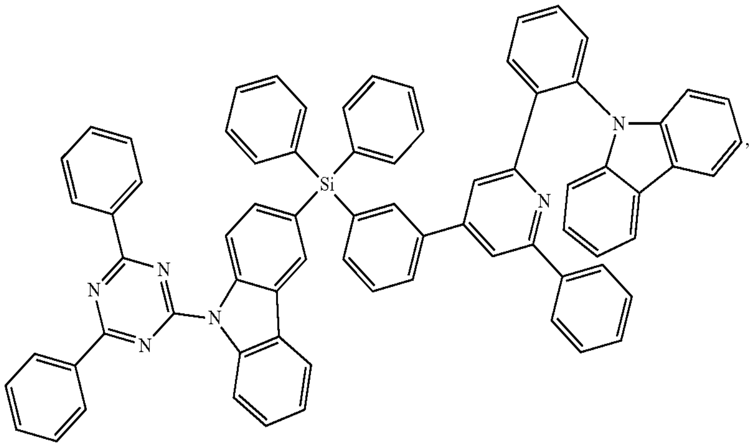
Compound A126



Compound A127



Compound A128



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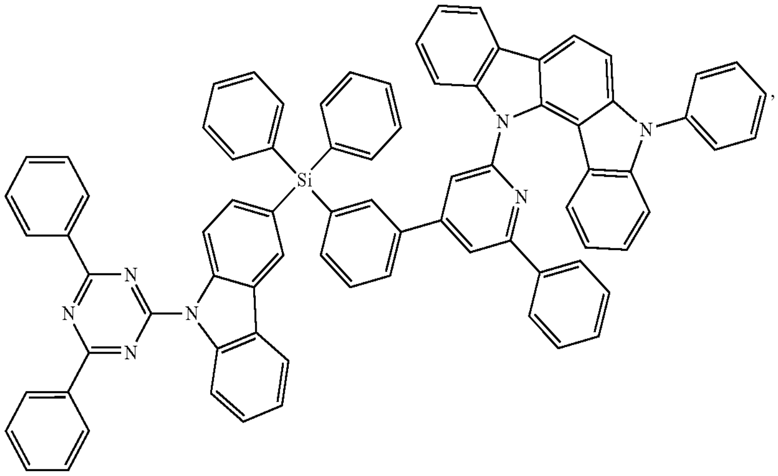
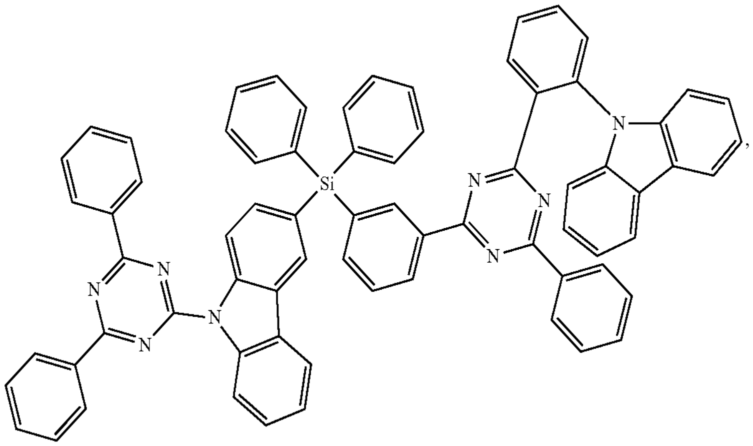
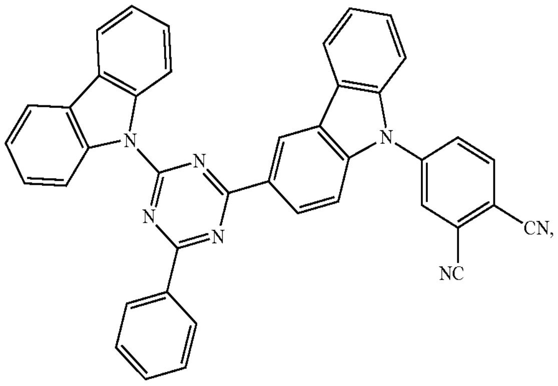
Compound A129



Compound A130



Compound B1



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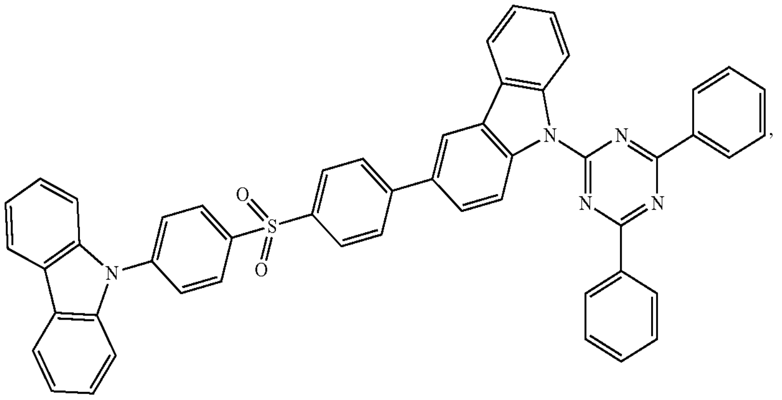
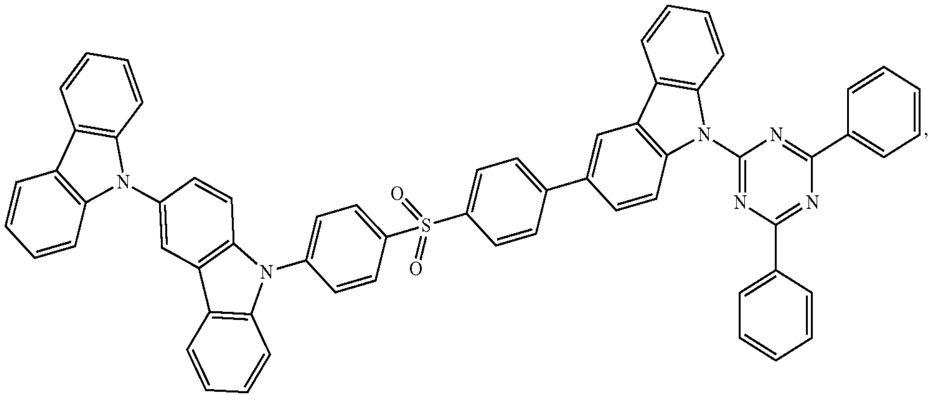
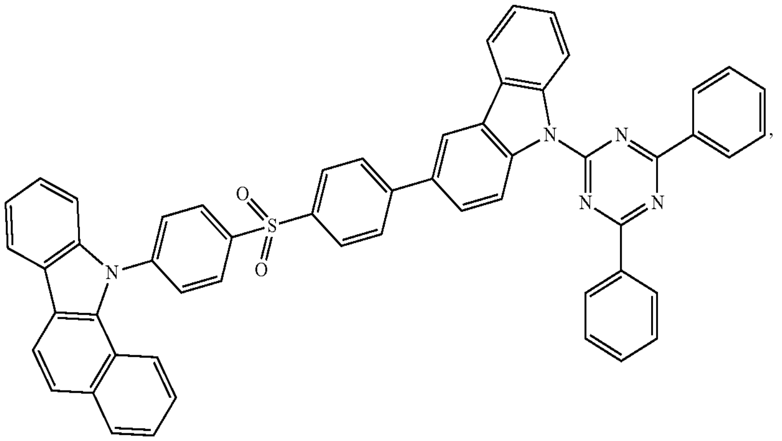
Compound B2



Compound B3



Compound B4



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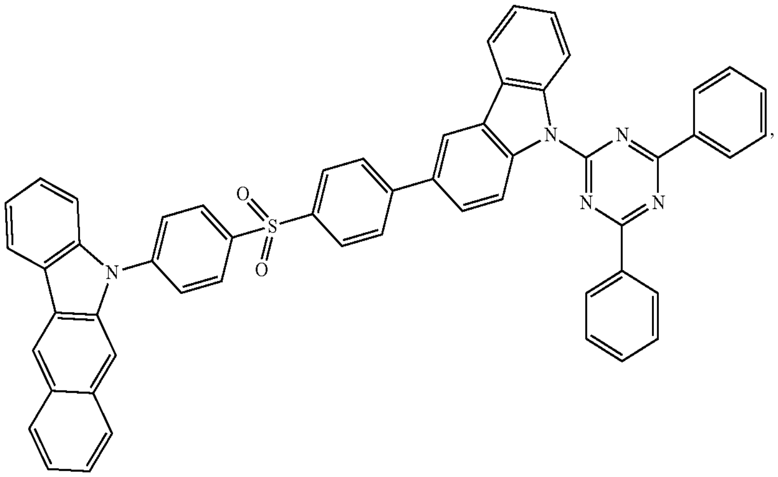
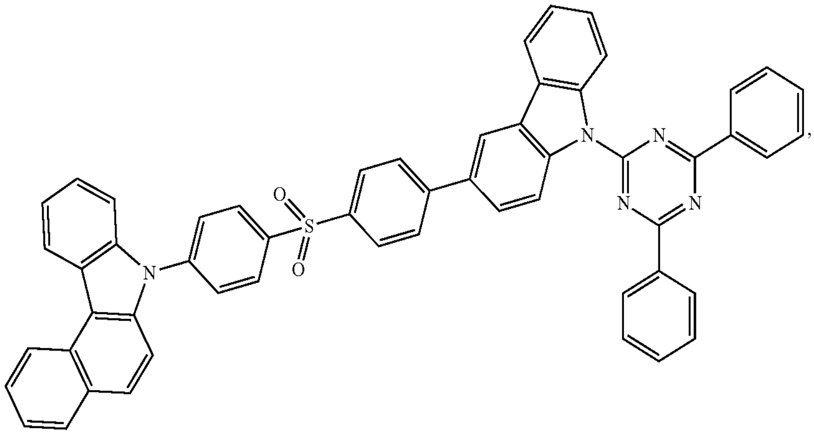
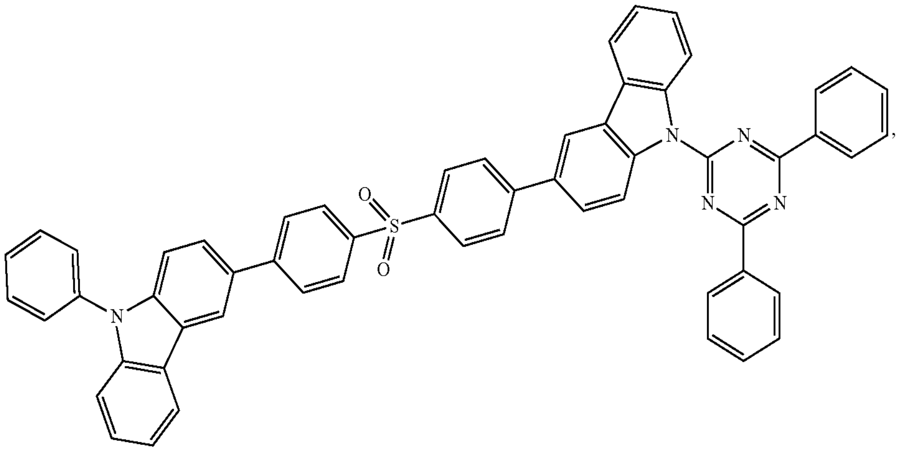
Compound B5



Compound B6



Compound B7



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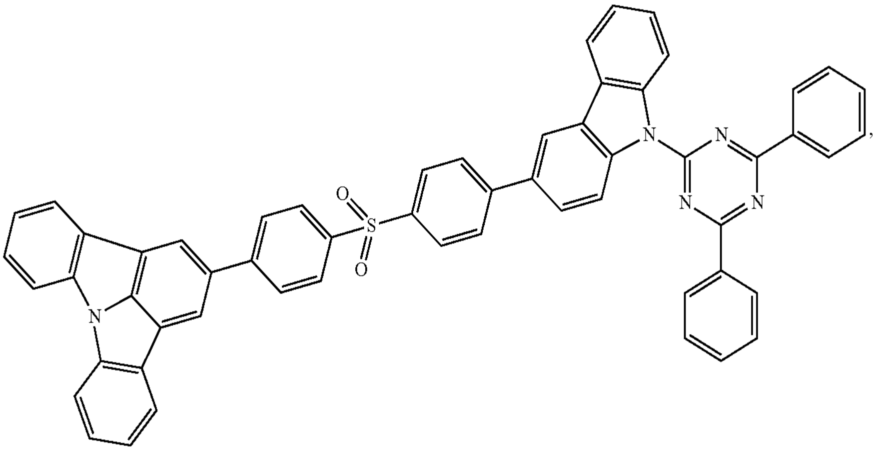
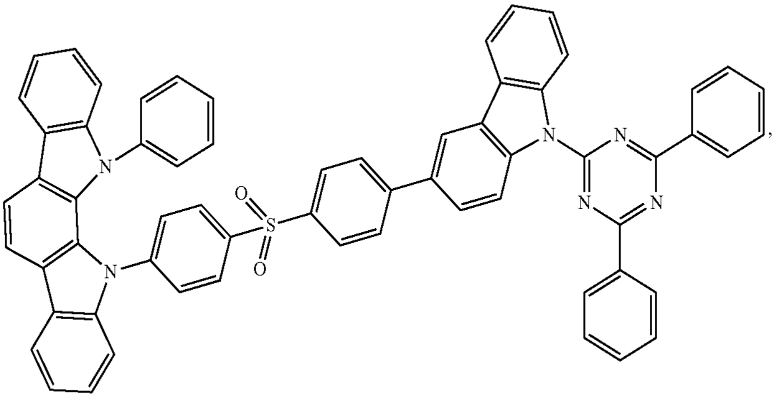
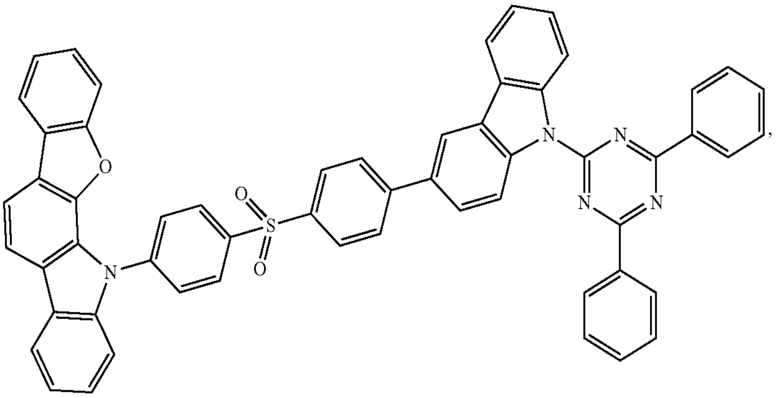
Compound B8



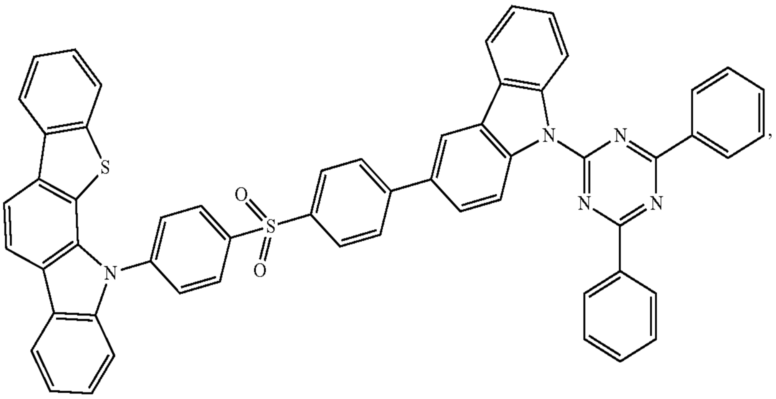
Compound B9



Compound B10



Compound B11



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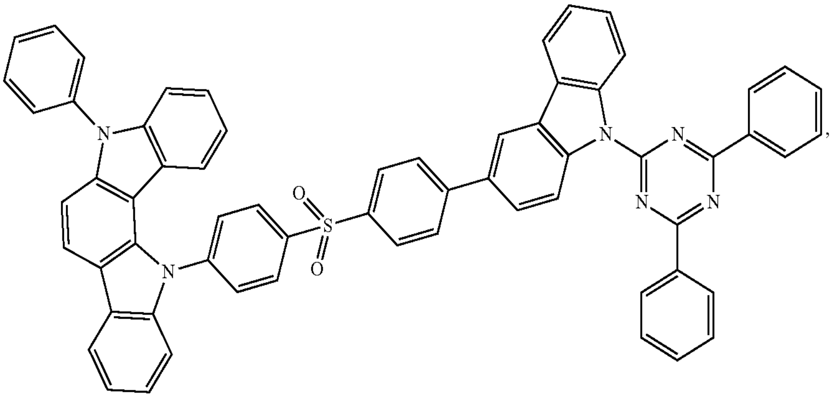
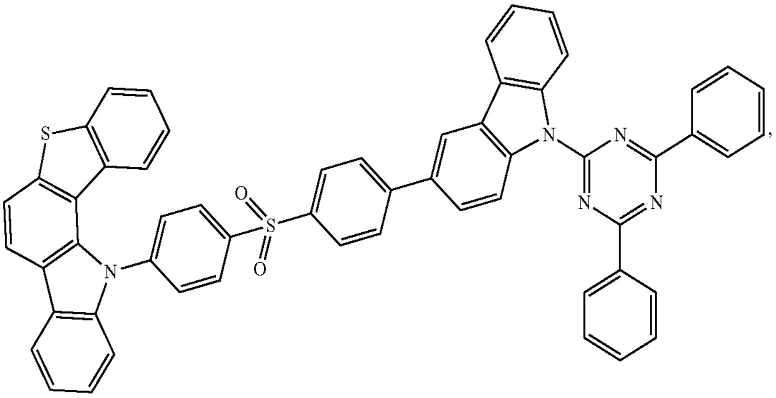
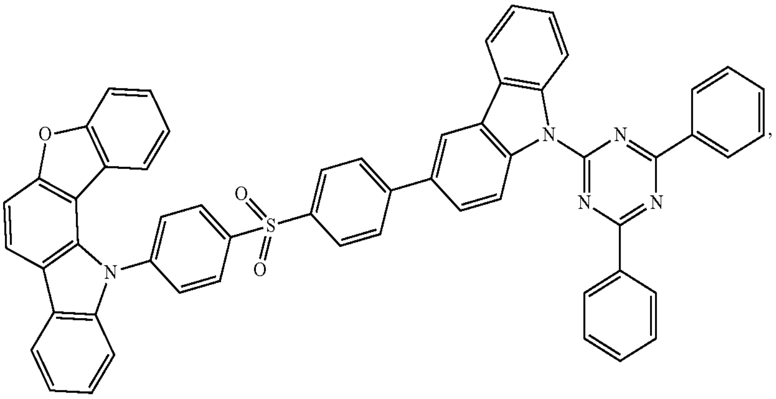
Compound B12



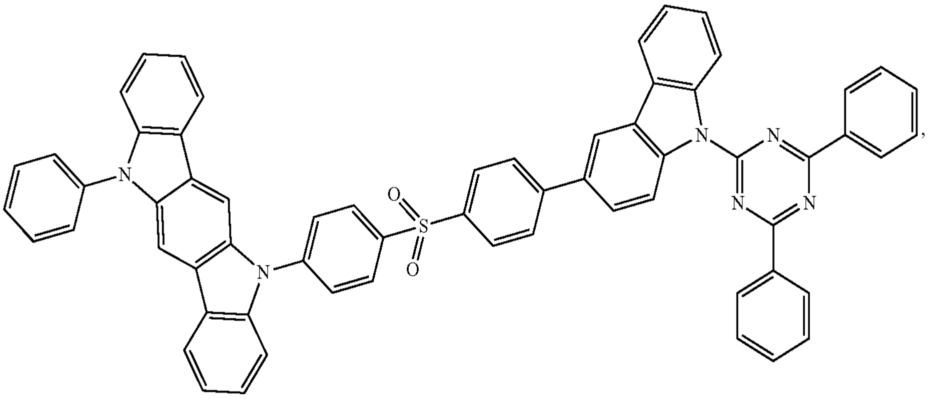
Compound B13



Compound B14



Compound B15



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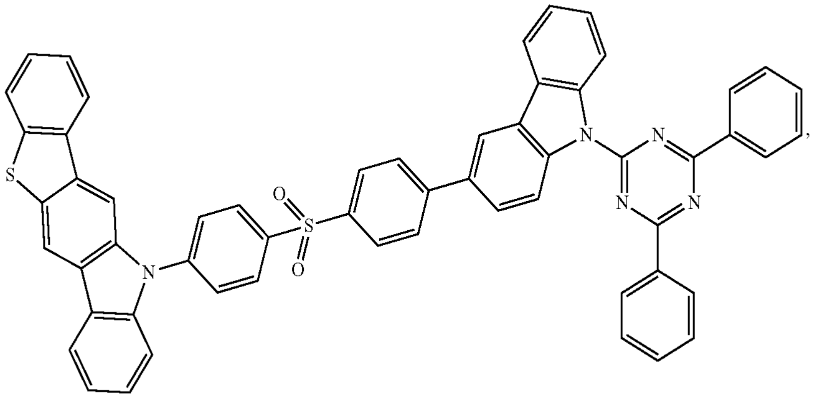
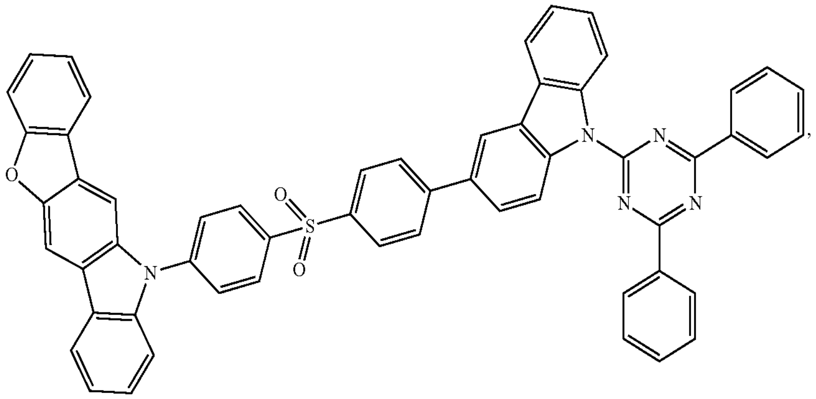
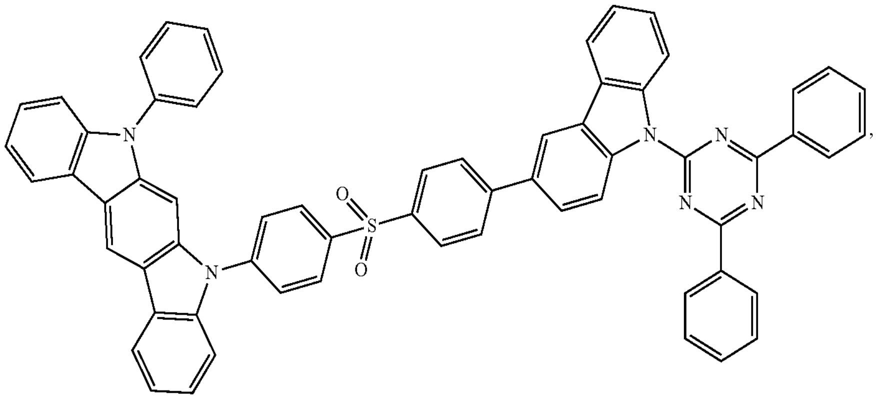
Compound B16



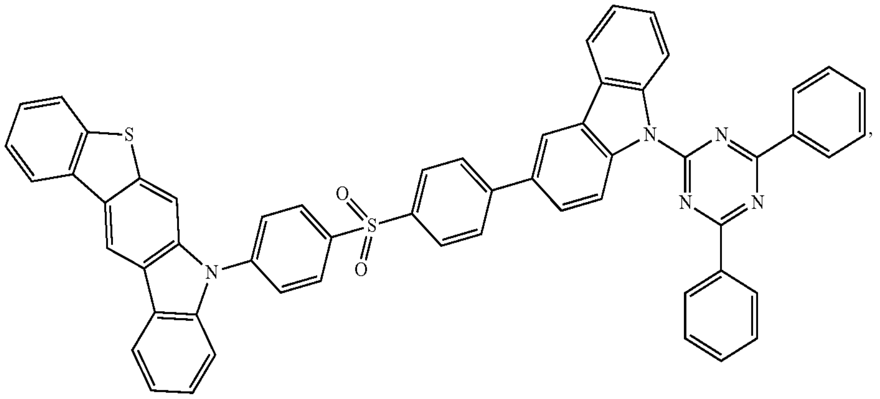
Compound B17



Compound B18



Compound B19



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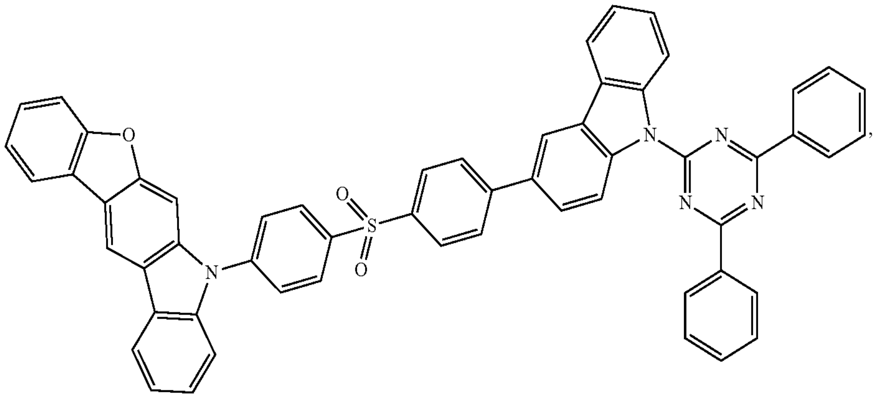
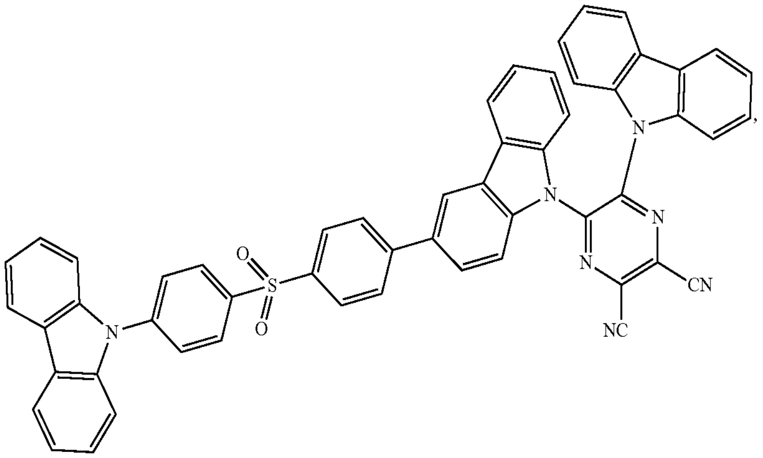
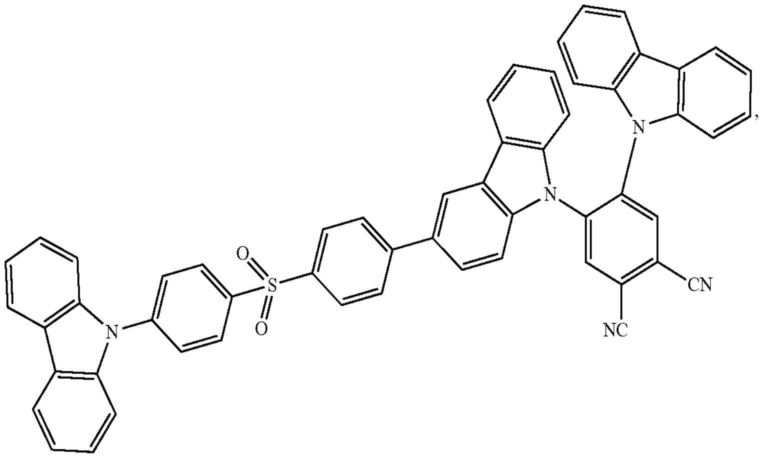
Compound B20



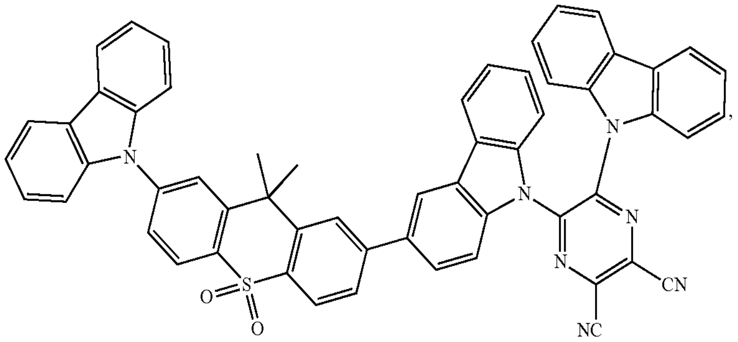
Compound B21



Compound B22



Compound B23



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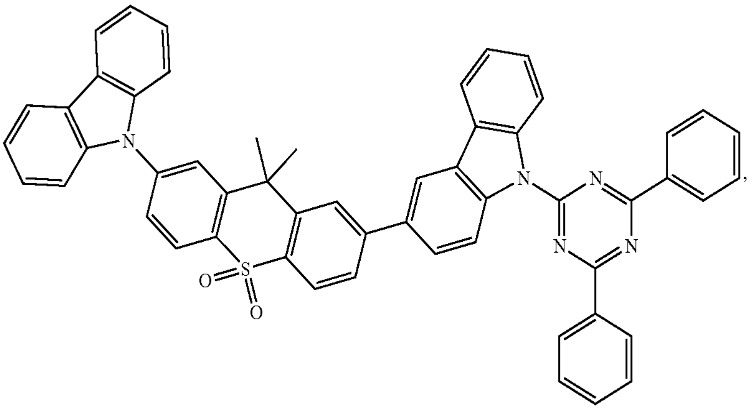
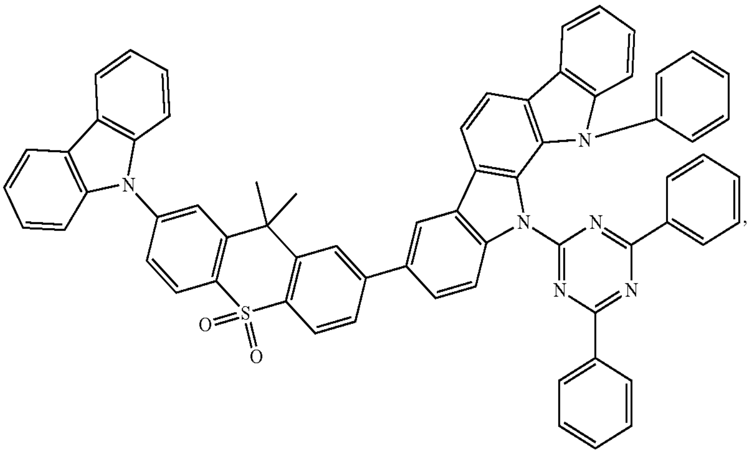
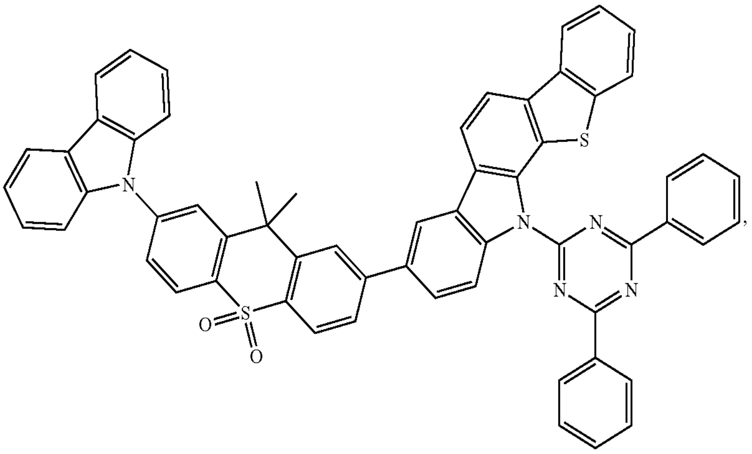
Compound B24



Compound B25



Compound B26



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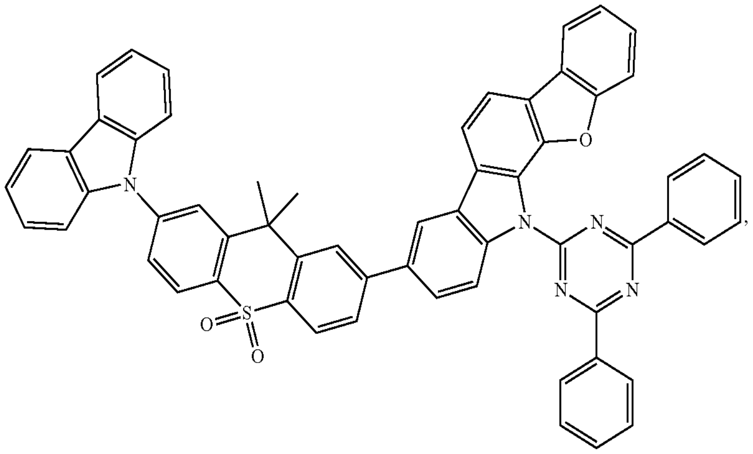
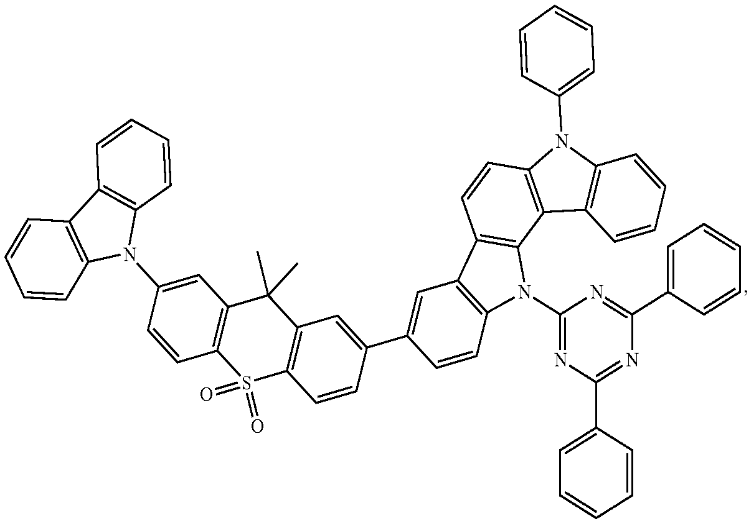
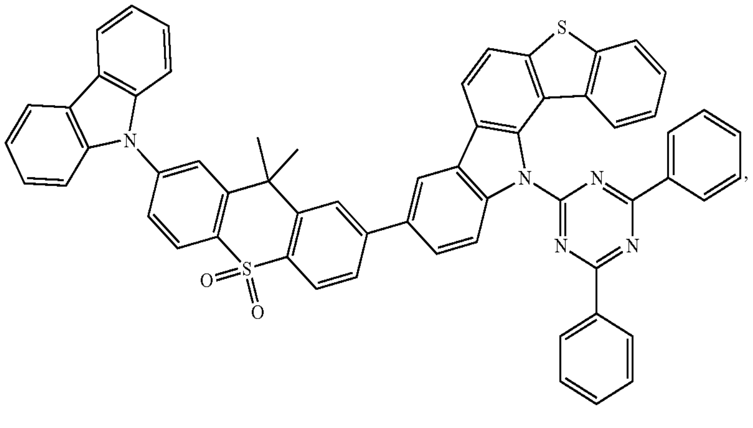
Compound B27



Compound B28



Compound B29



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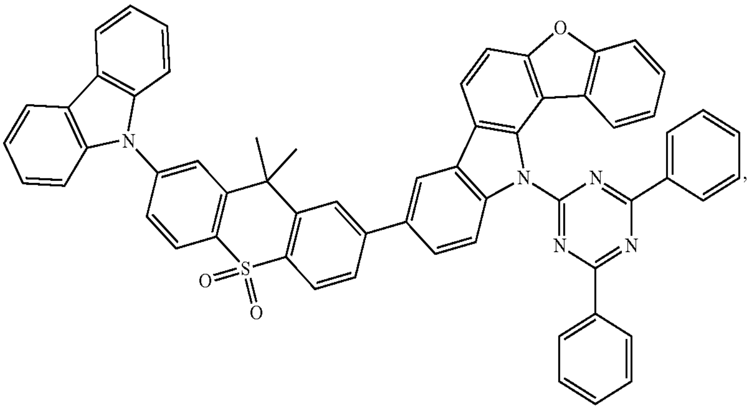
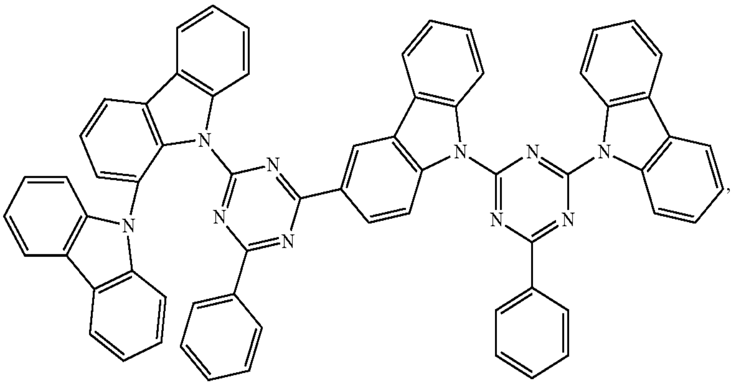
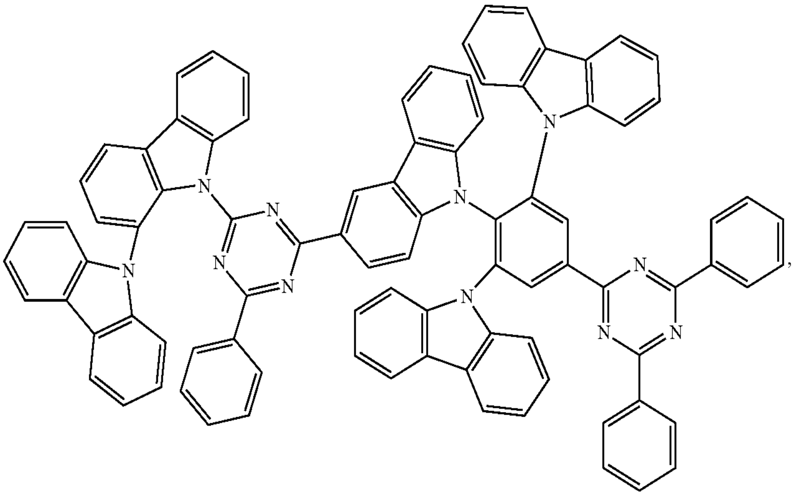
Compound B30



Compound B31



Compound B32



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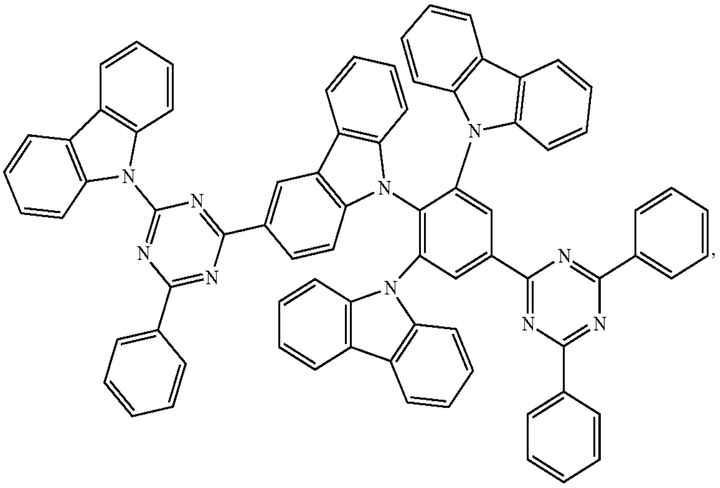
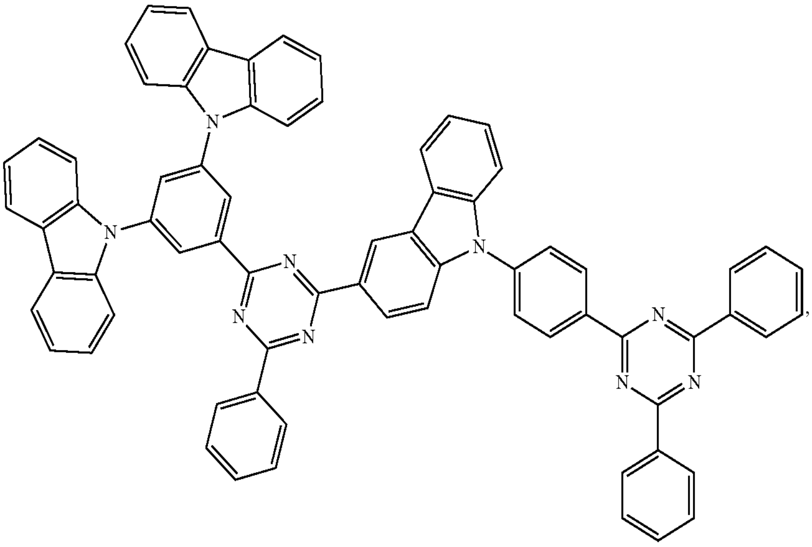
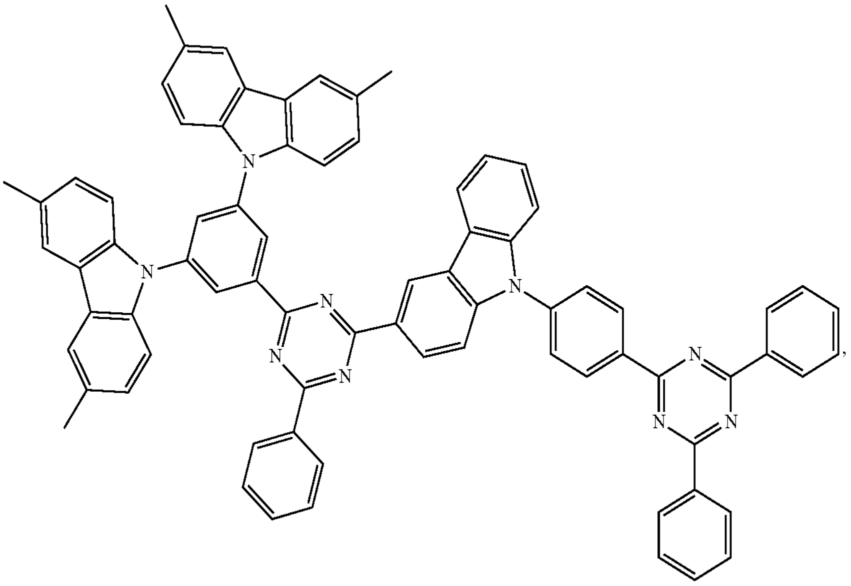
Compound B33



Compound B34



Compound B35



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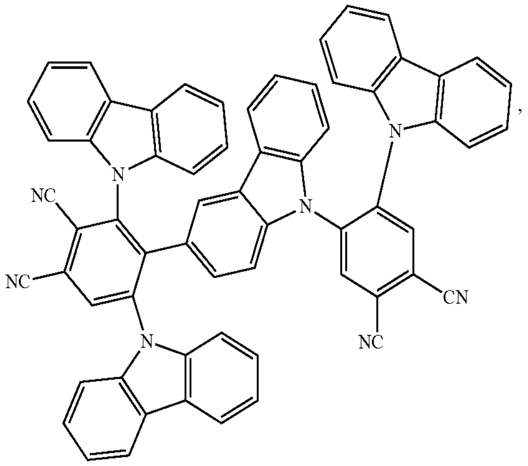
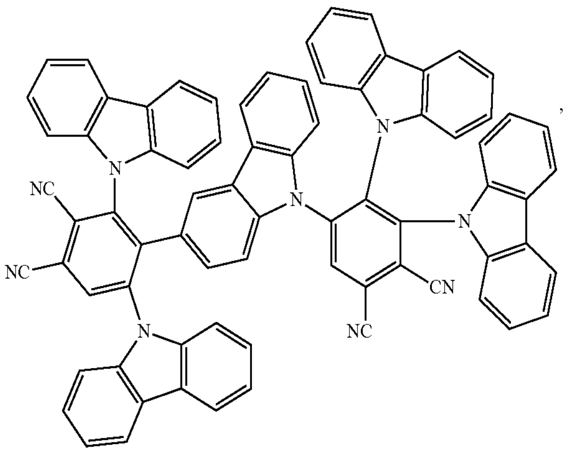
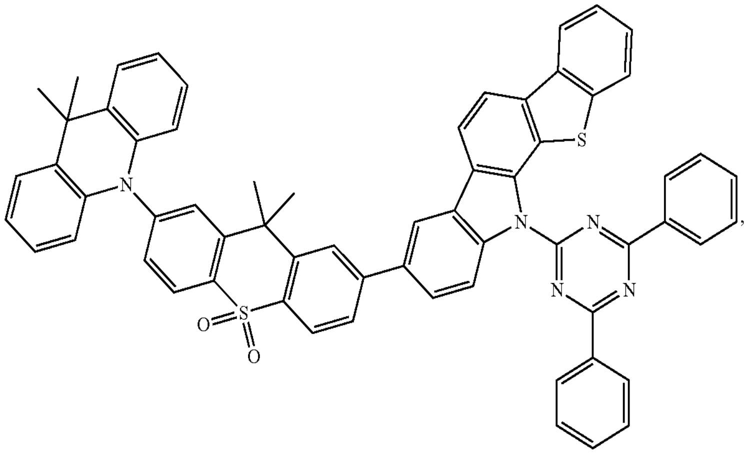
Compound B36



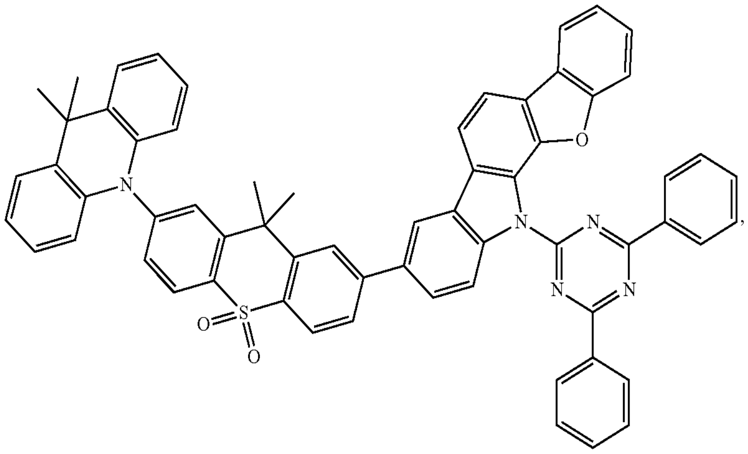
Compound B37



Compound B38



Compound B38



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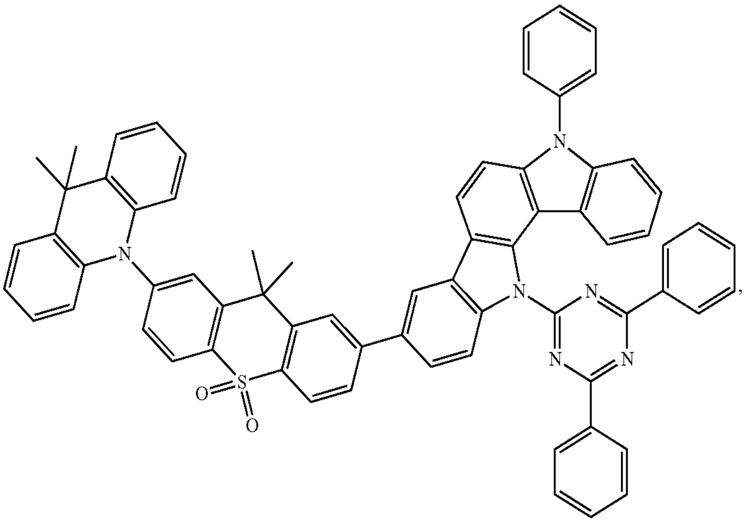
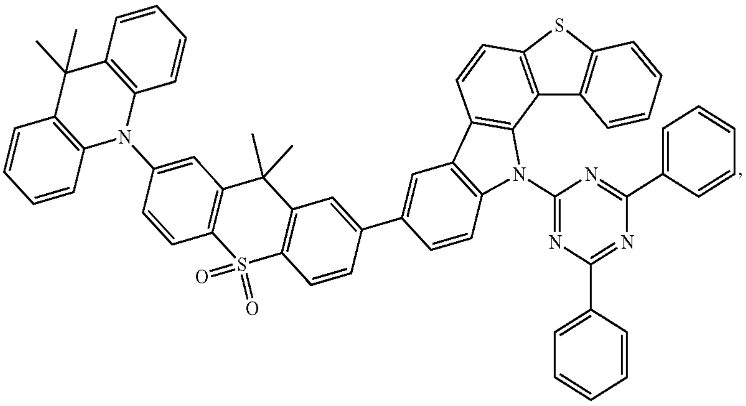
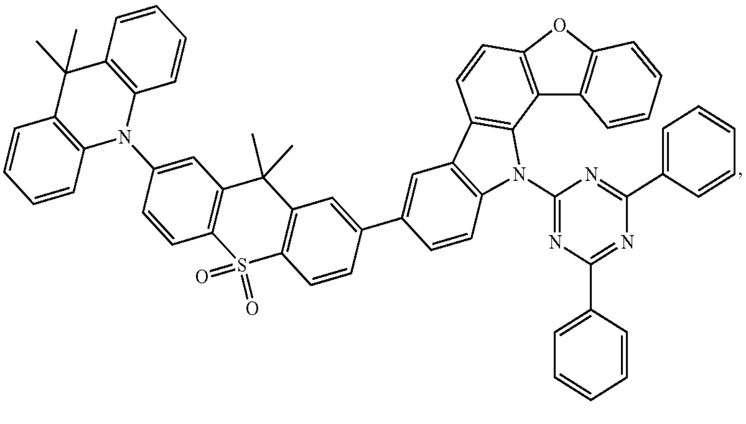
Compound B39



Compound B40



Compound B41



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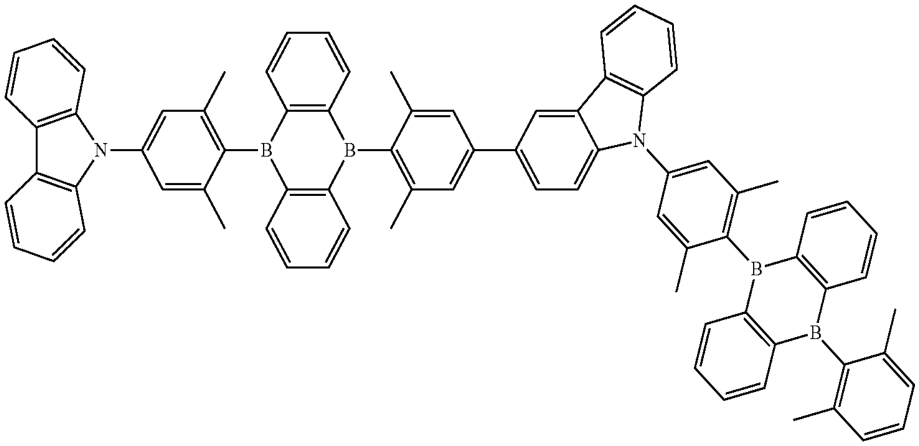
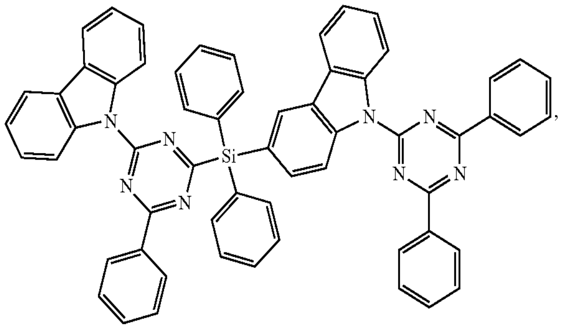
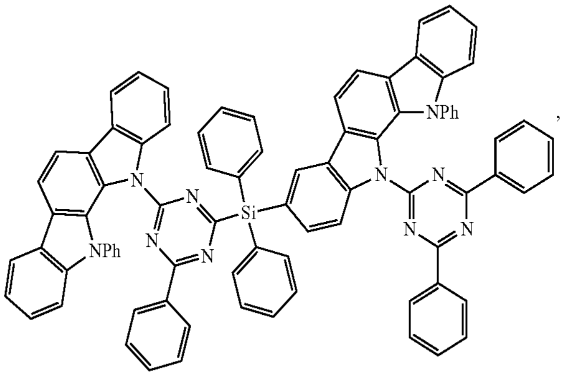
Compound B42



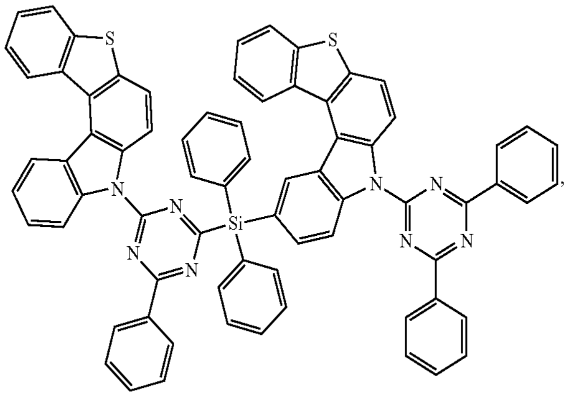
Compound B43



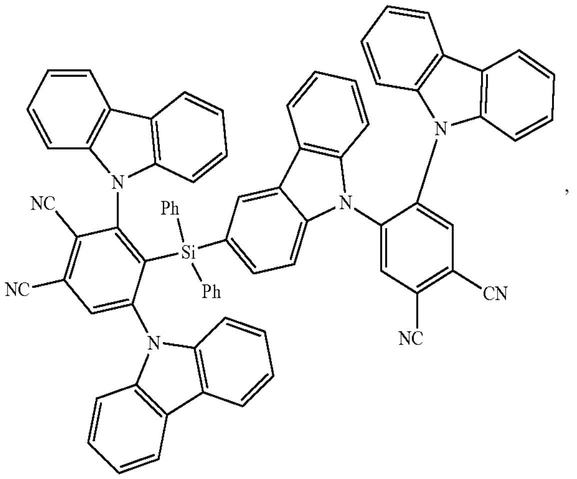
Compound B44



Compound B45



Compound B46



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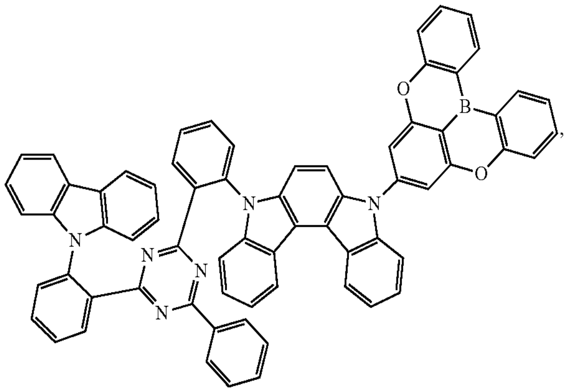
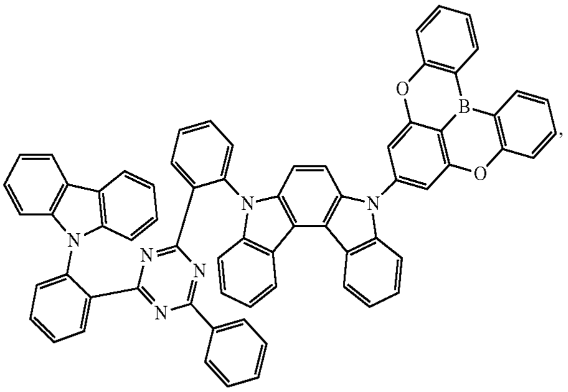
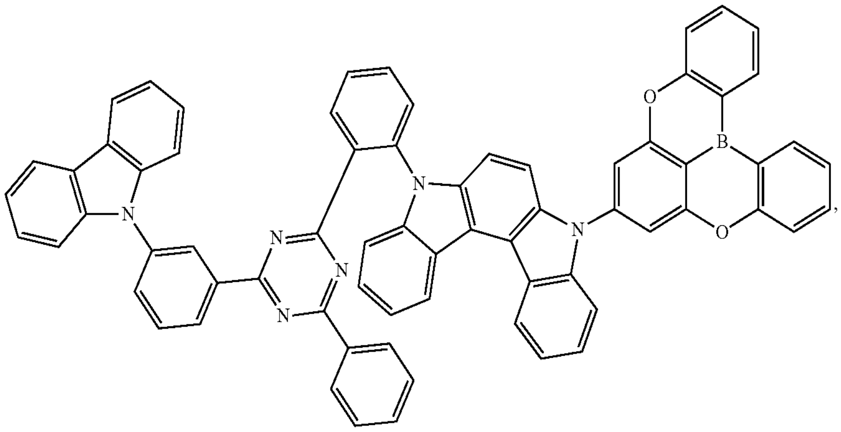
Compound B47



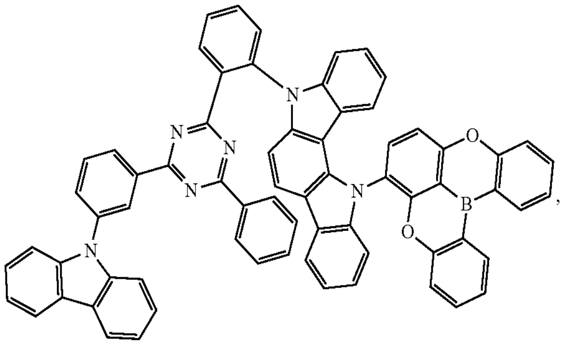
Compound B47



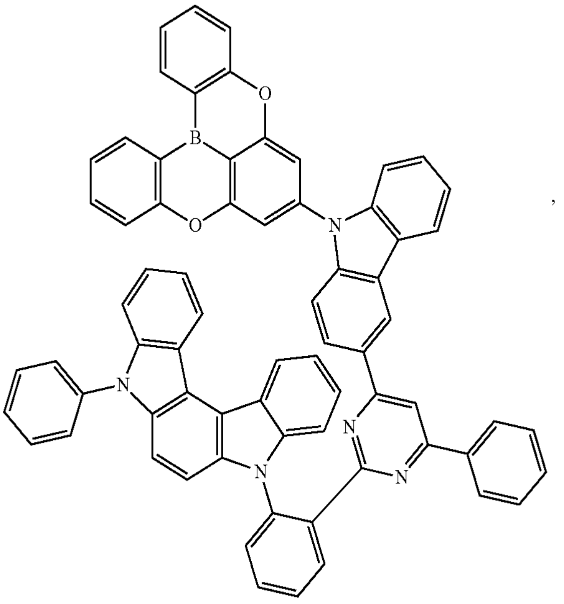
Compound B48



Compound B49



Compound B50



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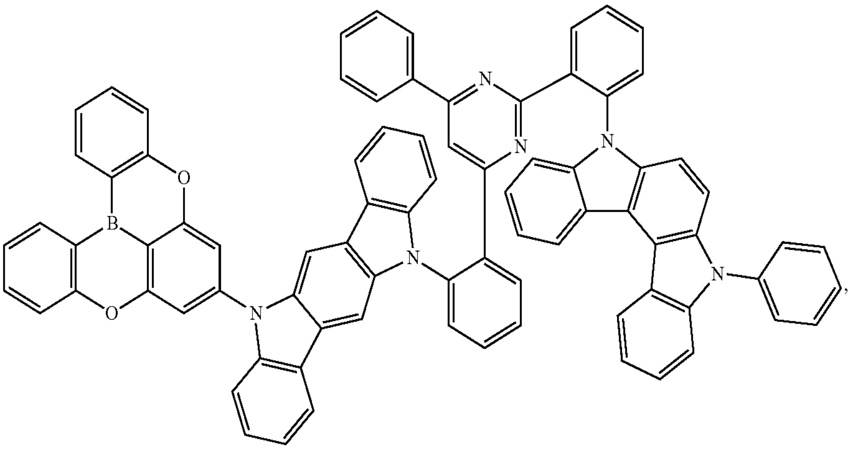
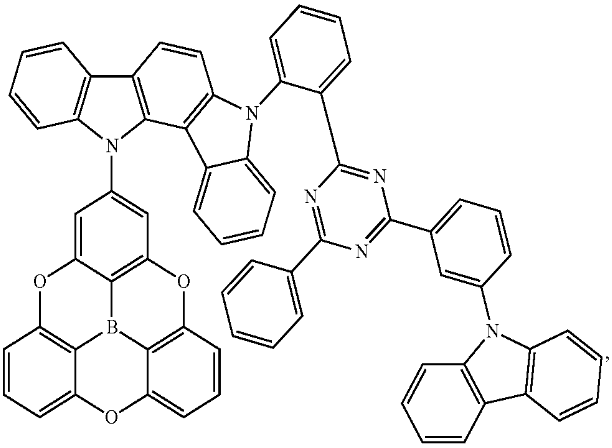
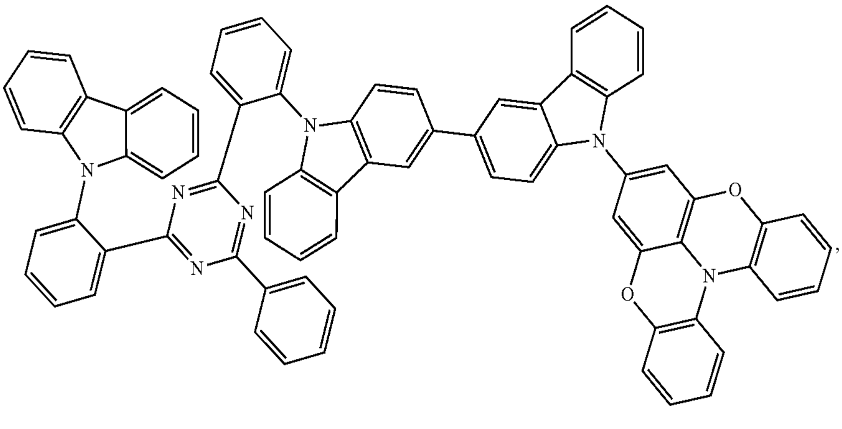
Compound B51



Compound B52



Compound B53



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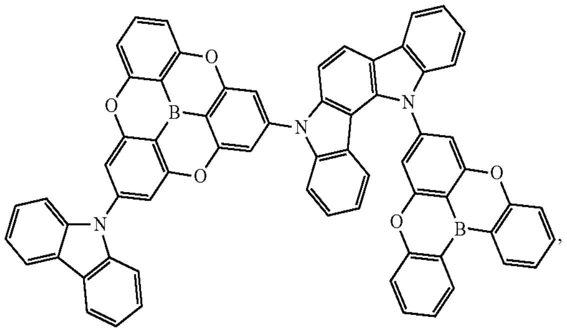
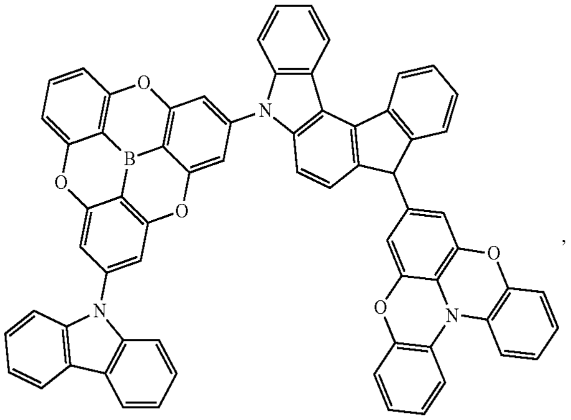
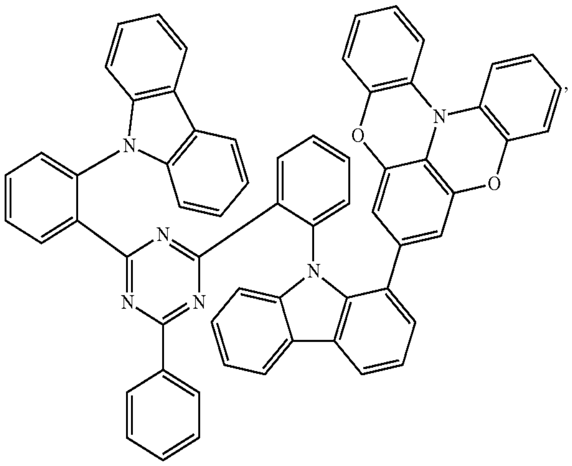
Compound B54



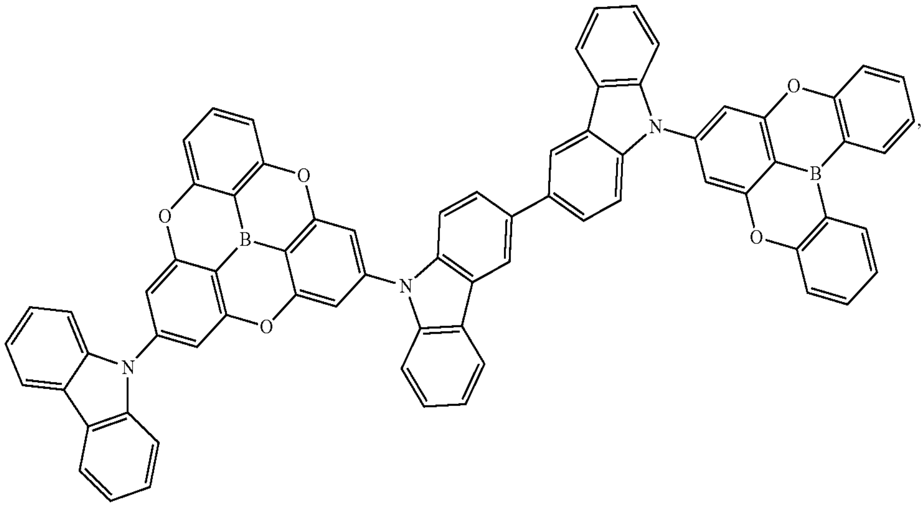
Compound B55



Compound B56



Compound B57



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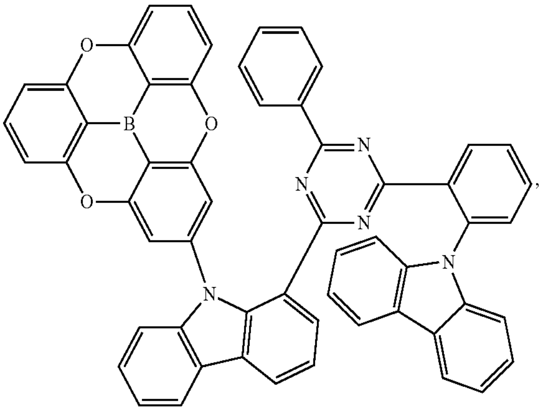
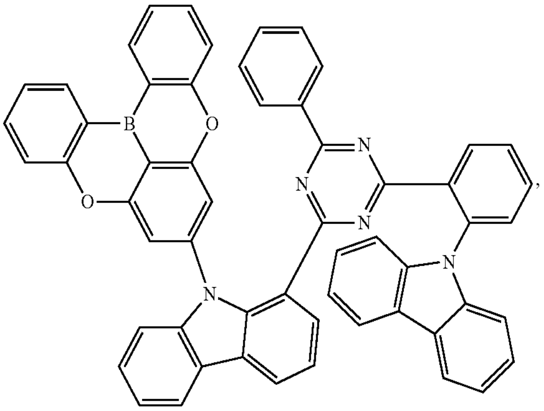
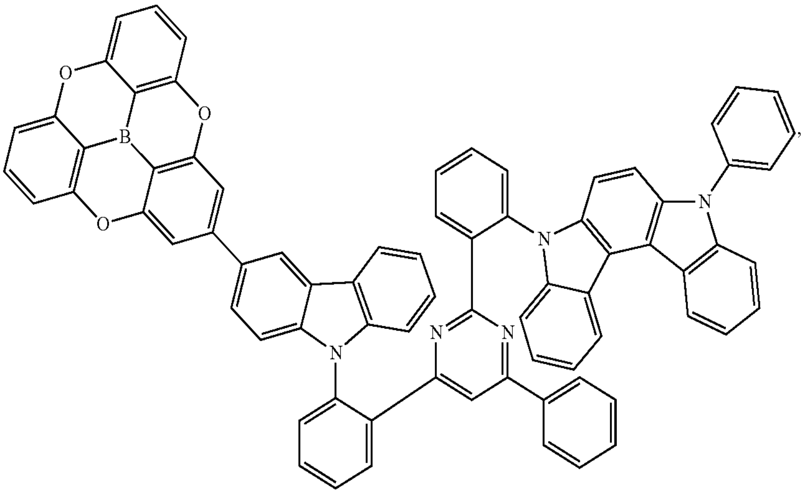
Compound B58



Compound B59



Compound B60



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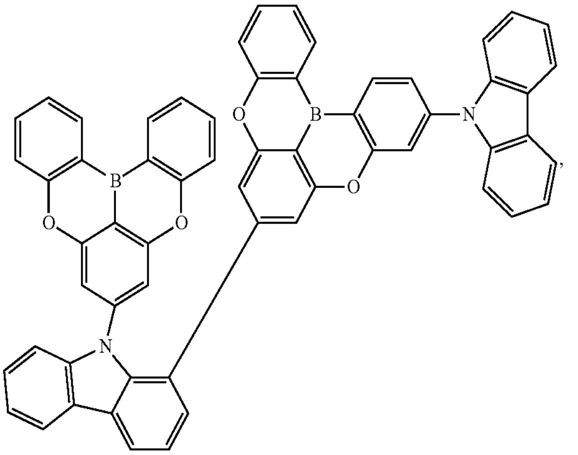

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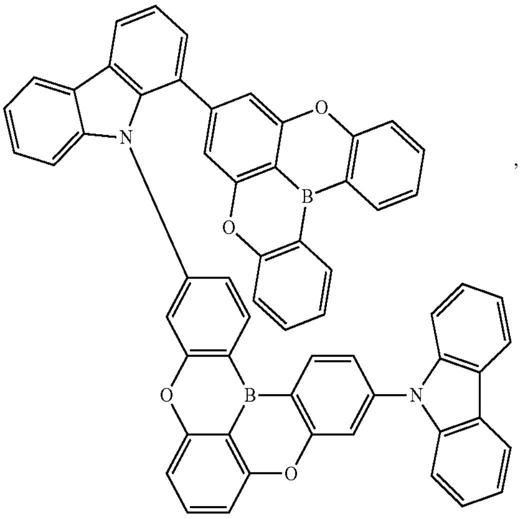

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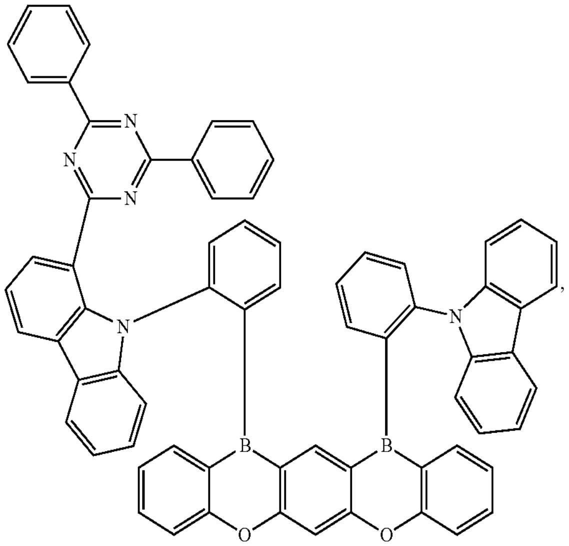
Compound B63



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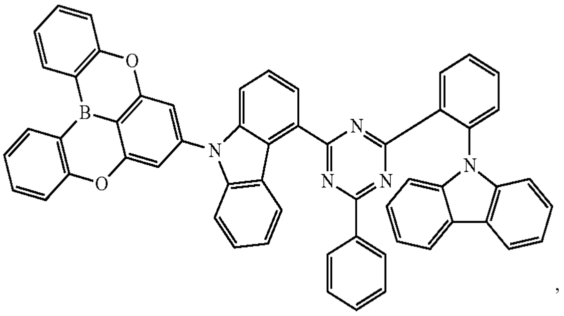

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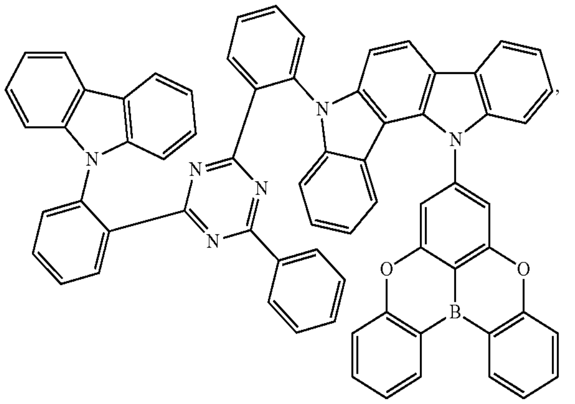
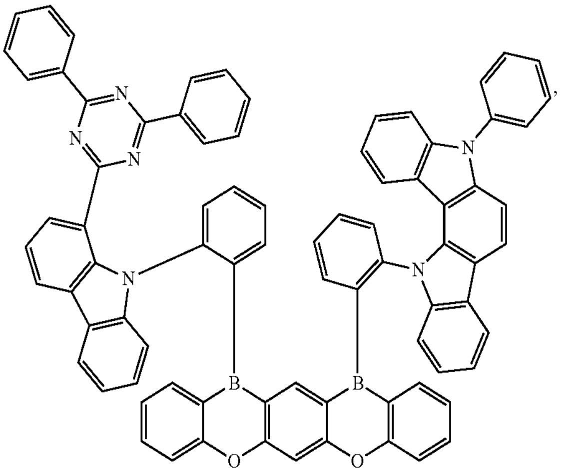
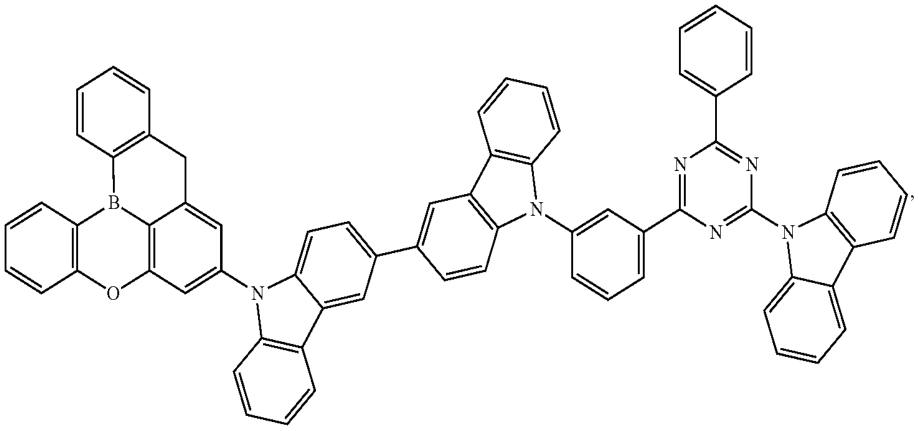


Compound 66



Compound B67



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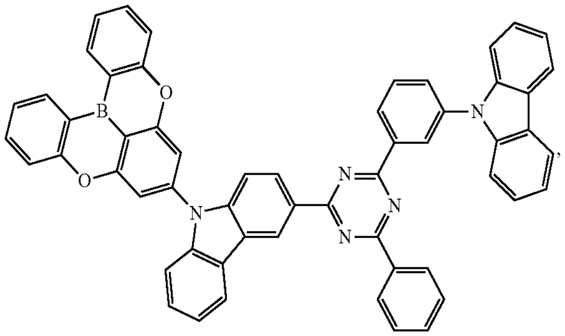
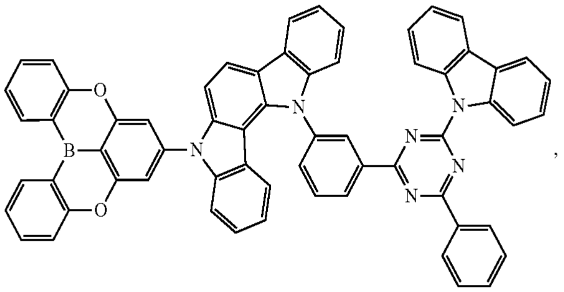
Compound B68



Compound B69



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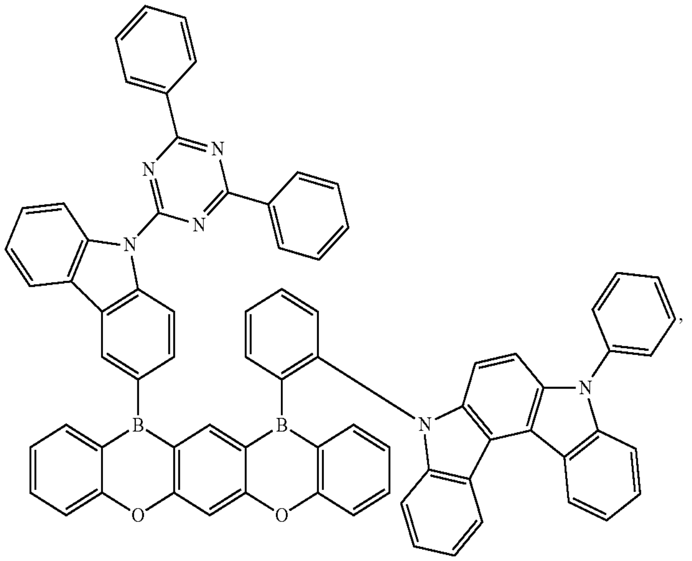
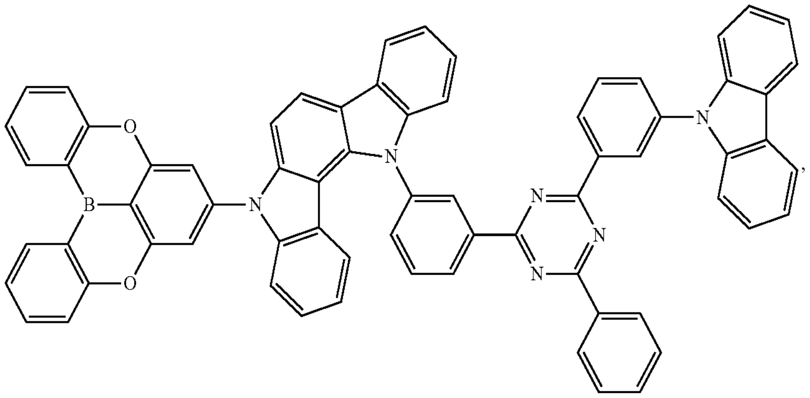


Compound B71



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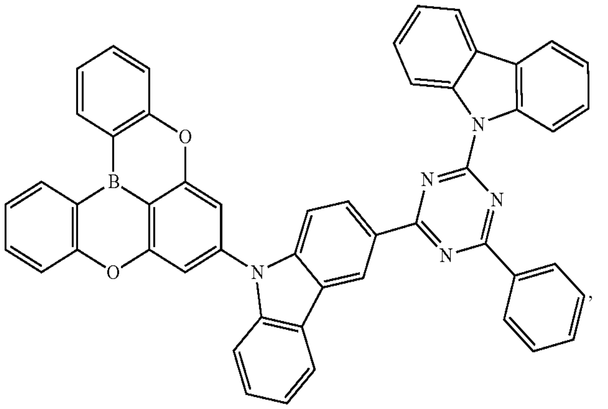
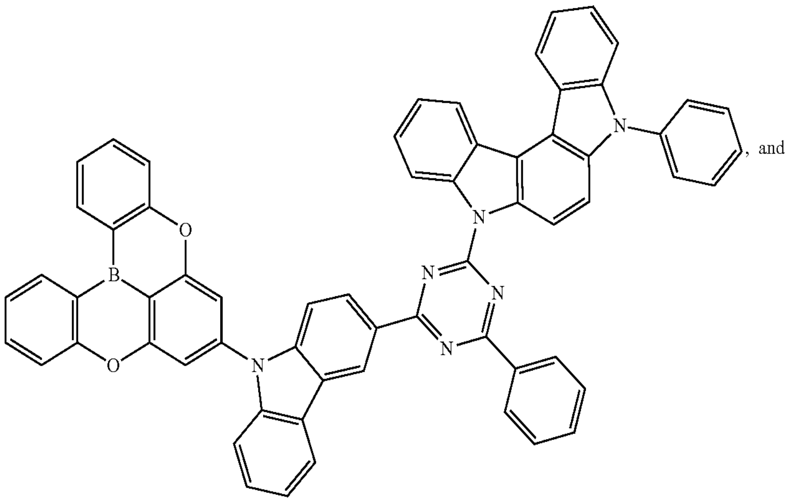
Compound B72



Compound B73



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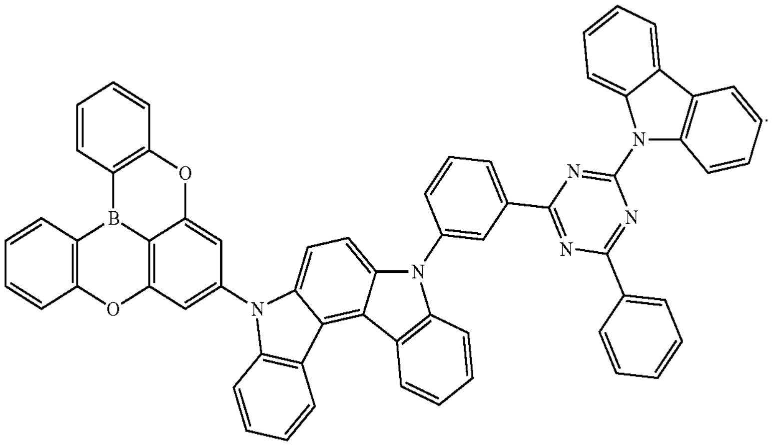
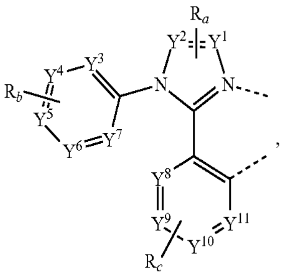
Compound B74

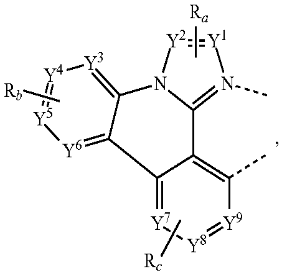


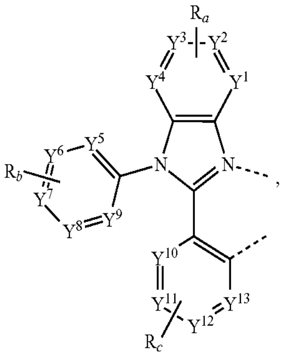
[0082] In some embodiments, the donor group having primary HOMO localization and the acceptor group having primary LUMO localization are not next to each other. That is to say that the GD where the HOMO primarily resides and the GA where the LUMO primarily resides are not adjacent to each other. The HOMO and LUMO are calculated by DFT. Calculations were performed using the B3LYP functional with a 6-31G* basis set. Geometry optimizations were performed in vacuum. Excitation energies were obtained at these optimized geometries using time-dependent density functional theory (TDDFT). A continuum solvent model was applied in the TDDFT calculation to simulate tetrahydrofuran solvent. All calculations were carried out using the program Gaussian.

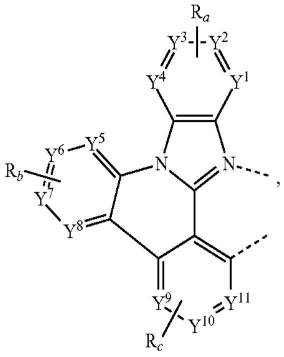
[0083] In some embodiments, an organic light emitting device (OLED) that includes an anode; a cathode; and an organic layer, disposed between the anode and the cathode. The organic layer can include a novel compound as described herein. In some embodiments, the organic layer is an emissive layer and the compound is a host.

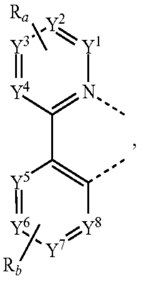
[0084] In some embodiments, the organic layer further comprises a phosphorescent emissive dopant; wherein the emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:

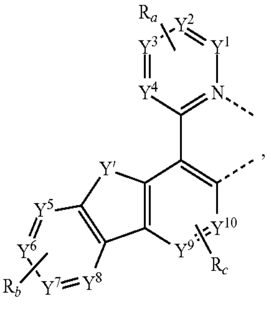


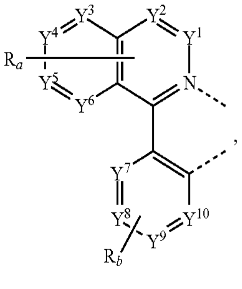












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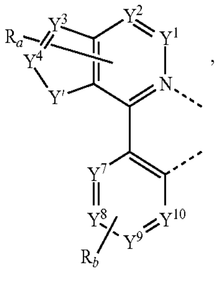

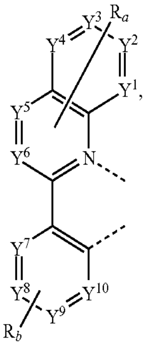

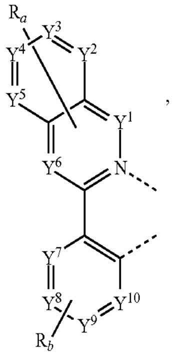

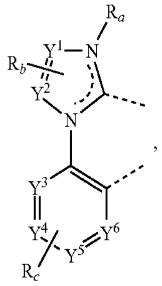

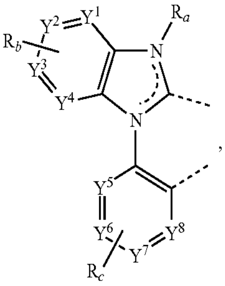

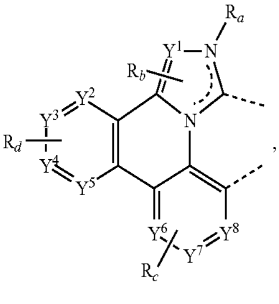

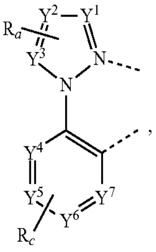

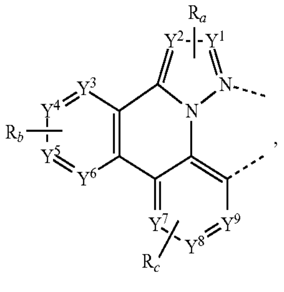

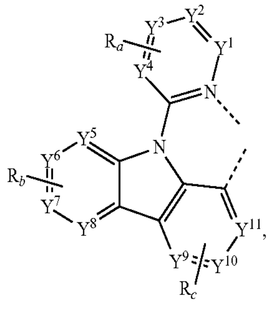

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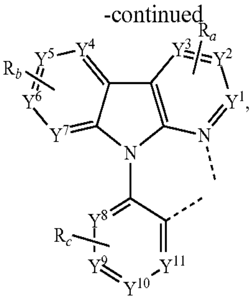

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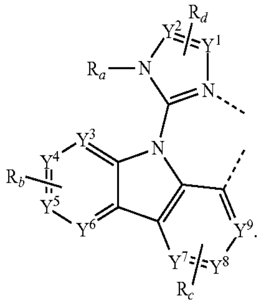


In the ligand structures above:

[0085] each Y^1 to Y^{13} are independently selected from the group consisting of carbon and nitrogen; Y' is selected from the group consisting of BR_e, NR_e, PR_e, O, S, Se, C═C, S═O, SO_2, CR_eR_f, SiR_eR_f, and GeR_eR_f; R_e and R_f are optionally fused or joined to form a ring;

[0086] each R_a, R_b, R_c, and R_d may independently represent from mono substitution to the maximum possible number of substitution, or no substitution;

[0087] each R_a, R_b, R_c, R_d, R_e, and R_f is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof; and

[0088] any two adjacent substituents of R_a, R_b, R_c, and R_d are optionally fused or joined to form a ring or form a multidentate ligand.

[0089] In some embodiments, the organic layer is a blocking layer and the compound is a blocking material in the organic layer. In some embodiments, the organic layer is a transporting layer and the compound is a transporting material in the organic layer.

[0090] In some embodiments, the organic layer is an emissive layer and the compound is an emitter. In some embodiments, the OLED emits a luminescent radiation at room temperature when a voltage is applied across the first organic light emitting device, and the luminescent radiation comprises a delayed fluorescent process. In some embodiments, the emissive layer further comprises a first phosphorescent emitting material. In some embodiments, the emissive layer further comprises a second phosphorescent emitting material. In some embodiments, the emissive layer further comprises a host material.

[0091] In some embodiments, the OLED emits a white light at room temperature when a voltage is applied across the organic light emitting device. In some embodiments, the compound emits a blue light having a peak wavelength between about 400 nm to about 500 nm. In some embodiments, the compound emits a yellow light having a peak wavelength between about 530 nm to about 580 nm.

[0092] In some embodiments, the OLED has one or more characteristics selected from the group consisting of being flexible, being rollable, being foldable, being stretchable, and being curved. In some embodiments, the OLED is transparent or semi-transparent. In some embodiments, the OLED further comprises a layer comprising carbon nanotubes.

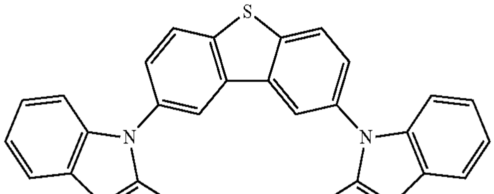
[0093] In some embodiments, the OLED further comprises a layer comprising a delayed fluorescent emitter. In some embodiments, the OLED comprises a RGB pixel arrangement or white plus color filter pixel arrangement. In some embodiments, the OLED is a mobile device, a hand held device, or a wearable device. In some embodiments, the OLED is a display panel having less than 10 inch diagonal or 50 square inch area. In some embodiments, the OLED is a display panel having at least 10 inch diagonal or 50 square inch area. In some embodiments, the OLED is a lighting panel.

[0094] The emissive dopants can be phosphorescent dopants and/or fluorescent dopants. The organic layer can include a novel compound as described herein, and its variations as described herein as a host.

[0095] In some embodiments, a consumer product including a first device that includes an OLED as described herein is provided.

[0096] In some aspects of the invention, an emissive region in an organic light emitting device is described. The emissive region includes a novel compound as described herein. In some emissive region embodiments, the compound is an emissive dopant or a non-emissive dopant.

[0097] In some embodiments, the emissive region further comprises a host, wherein the host contains at least one group selected from the group consisting of metal complex, triphenylene, carbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, aza-triphenylene, aza-carbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene. In some embodiments, the emissive region further comprises a host, wherein the host is selected from the group consisting of:



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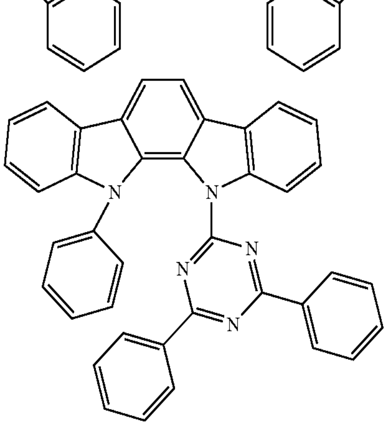

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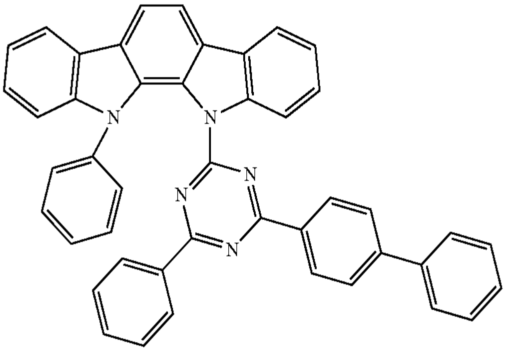

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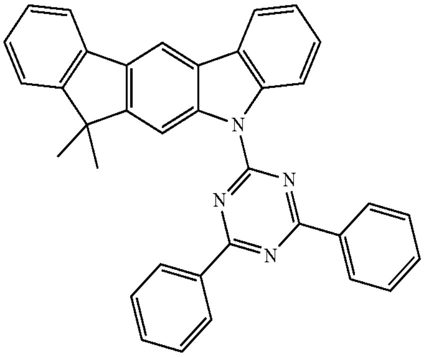

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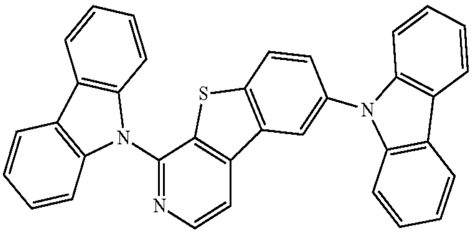

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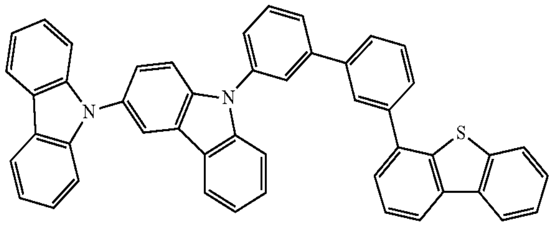

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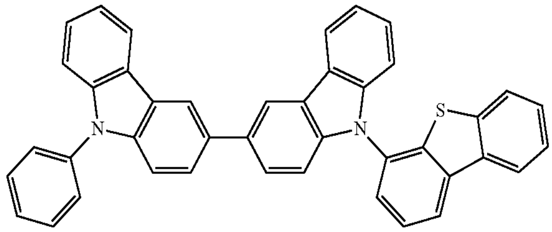

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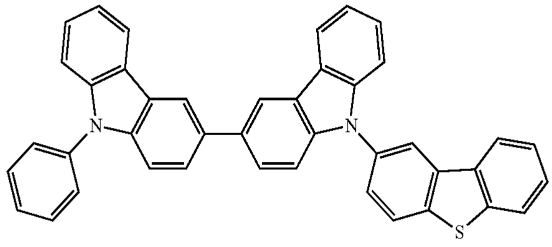

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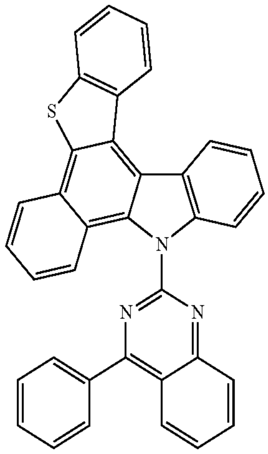

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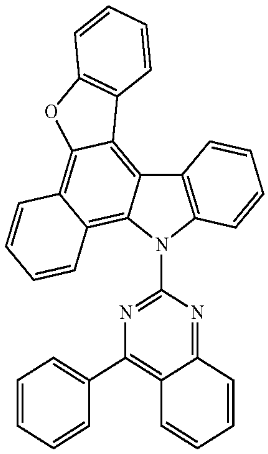

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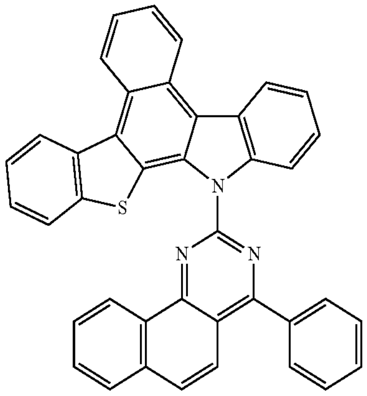

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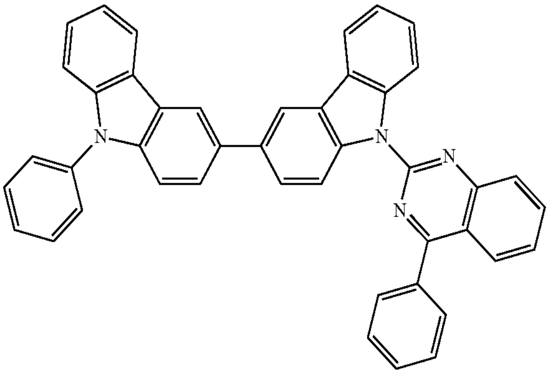

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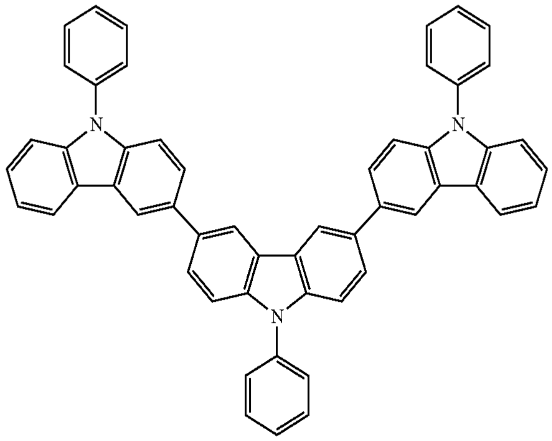

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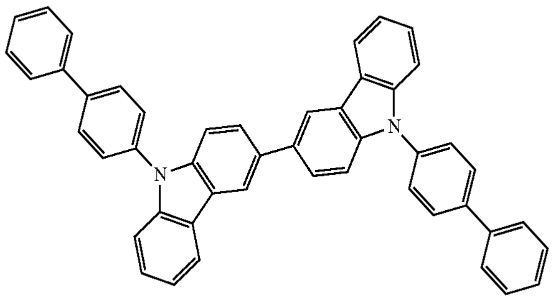

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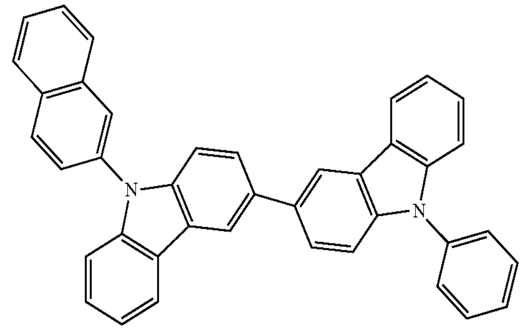

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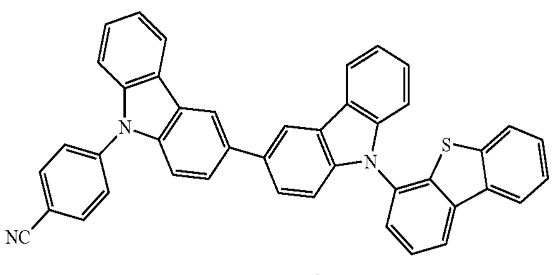

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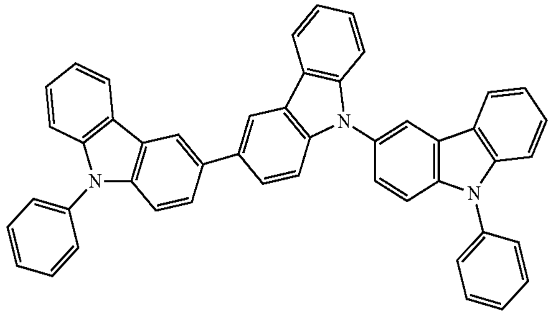

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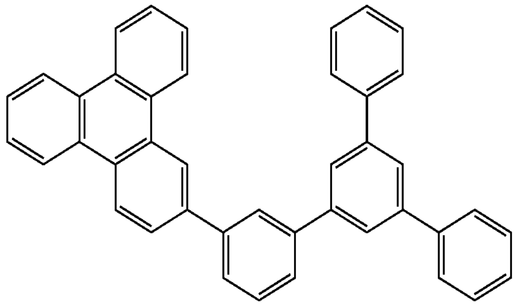
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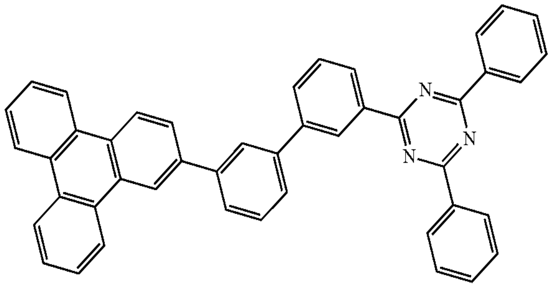

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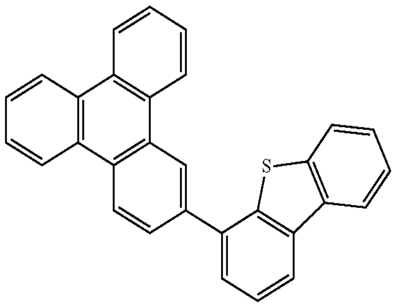

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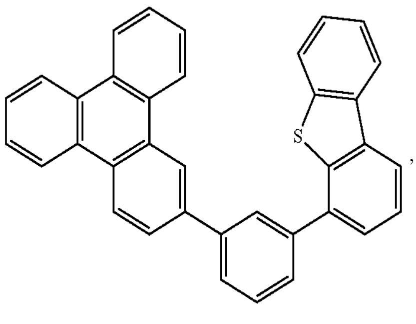

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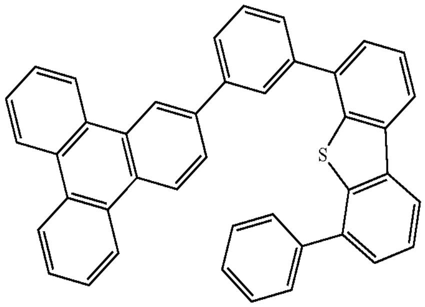

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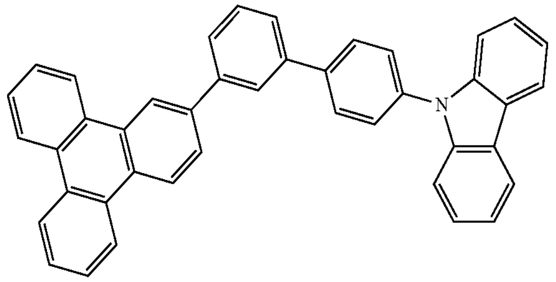
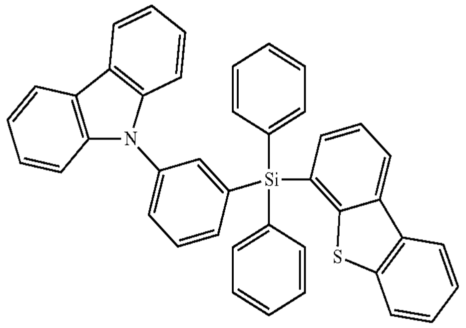
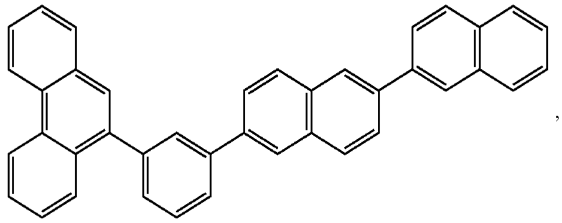
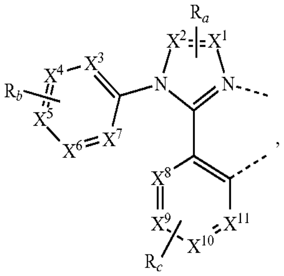


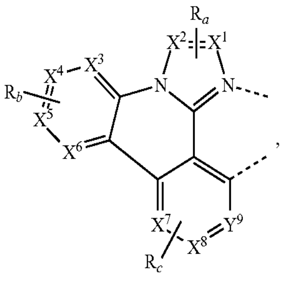




and combinations thereof.

[0098] In some emissive region embodiments, the compound is a host. In some embodiments, the emissive region further comprises a phosphorescent emissive dopant; wherein the emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:





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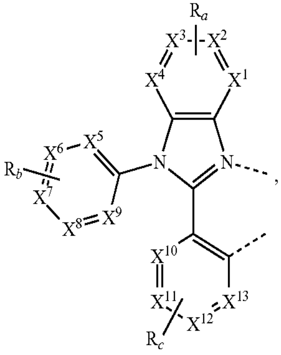

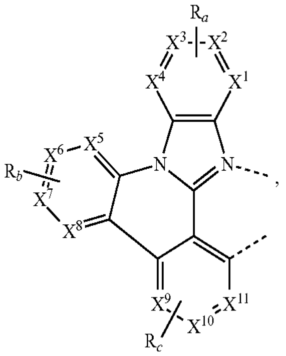

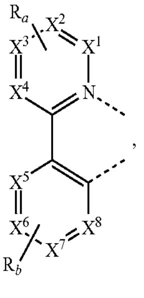

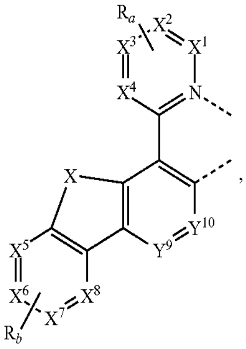

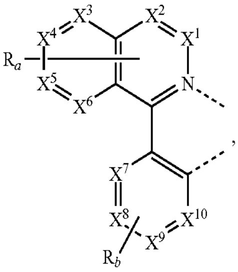

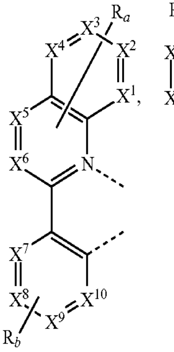

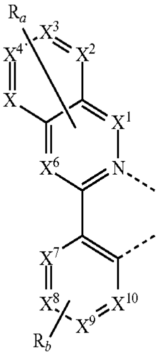

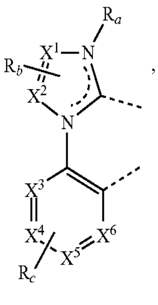

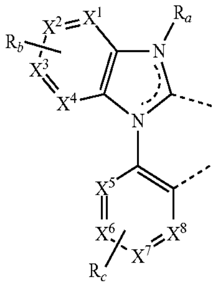

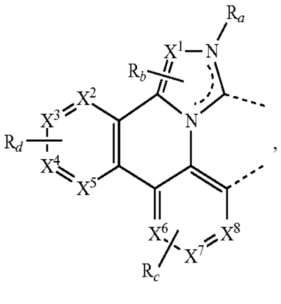

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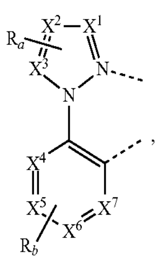

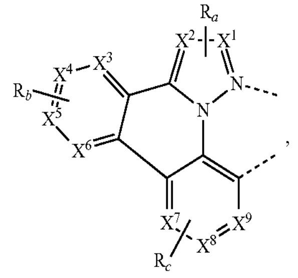

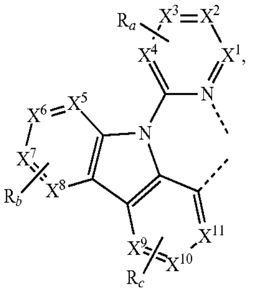

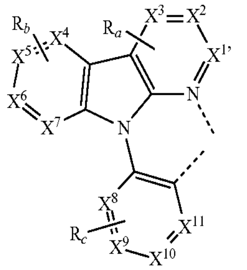

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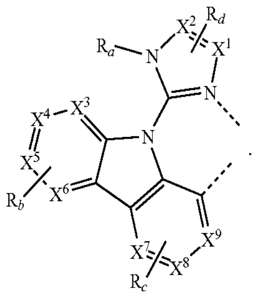


In the ligands above:

[0099] each X^1 to X^{13} are independently selected from the group consisting of carbon and nitrogen;

[0100] X is selected from the group consisting of BR', NR', PR', O, S, Se, C═O, S═O, SO_2, CR'R", SiR'R", and GeR'R";

[0101] R' and R" are optionally fused or joined to form a ring;

[0102] R' and R" are each independently selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

[0103] each R_a, R_b, R_c, and R_d may represent from mono substitution to the possible maximum number of substitution, or no substitution;

[0104] R_a, R_b, R_c, and R_d are each independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

[0105] any two substituents of R_a, R_b, R_c, and R_d are optionally fused or joined to form a ring or form a multidentate ligand.

[0106] According to another aspect, a formulation comprising the compound described herein is also disclosed.

[0107] The OLED disclosed herein can be incorporated into one or more of a consumer product, an electronic component module, and a lighting panel.

[0108] In yet another aspect of the present disclosure, a formulation that comprises the novel compound disclosed herein is described. The formulation can include one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, electron blocking material, hole blocking material, and an electron transport layer material, disclosed herein.

[0109] The present disclosure encompasses any chemical structure comprising the novel compound of the present disclosure, or a monovalent or polyvalent variant thereof. In other words, the inventive compound, or a monovalent or polyvalent variant thereof, can be a part of a larger chemical structure. Such chemical structure can be selected from the group consisting of a monomer, a polymer, a macromolecule, and a supramolecule (also known as supermolecule). As used herein, a "monovalent variant of a compound" refers to a moiety that is identical to the compound except that one hydrogen has been removed and replaced with a bond to the rest of the chemical structure. As used herein, a "polyvalent variant of a compound" refers to a moiety that is identical to the compound except that more than one hydrogen has been removed and replaced with a bond or bonds to the rest of the chemical structure. In the instance of a supramolecule, the inventive compound can also be incorporated into the supramolecule complex without covalent bonds.

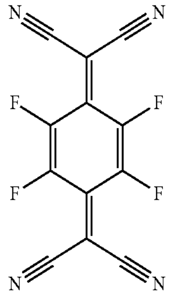
Combination with Other Materials

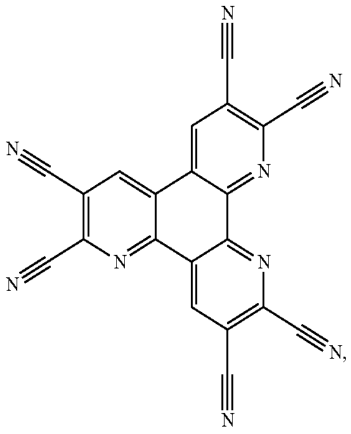
[0110] The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport 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.

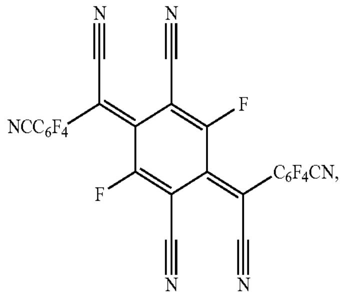
Conductivity Dopants:

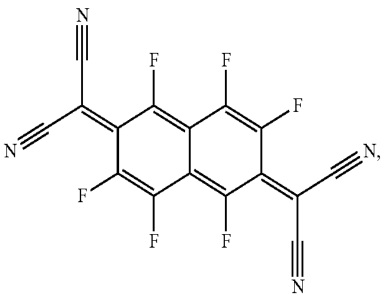
[0111] A charge transport layer can be doped with conductivity dopants to substantially alter its density of charge carriers, which will in turn alter its conductivity. The conductivity is increased by generating charge carriers in the matrix material, and depending on the type of dopant, a change in the Fermi level of the semiconductor may also be achieved. Hole-transporting layer can be doped by p-type conductivity dopants and n-type conductivity dopants are used in the electron-transporting layer.

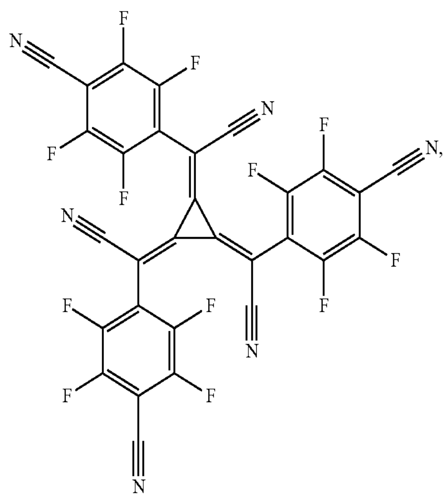
[0112] Non-limiting examples of the conductivity dopants that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: EP01617493, EP01968131, EP2020694, EP2684932, US20050139810, US20070160905, US20090167167, US2010288362, WO06081780, WO2009003455, WO2009008277, WO2009011327, WO2014009310, US2007252140, US2015060804, US20150123047, and US2012146012.











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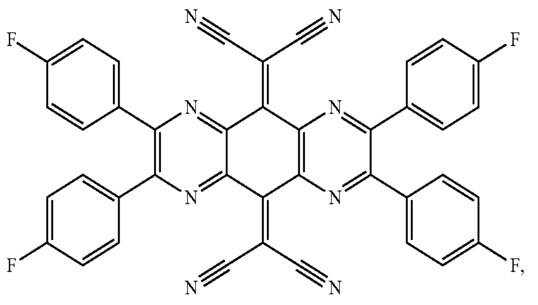

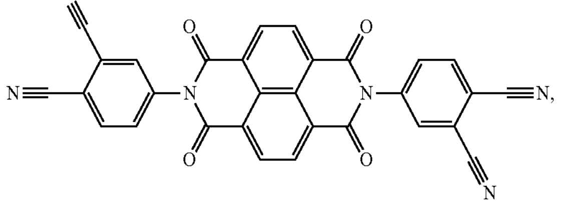

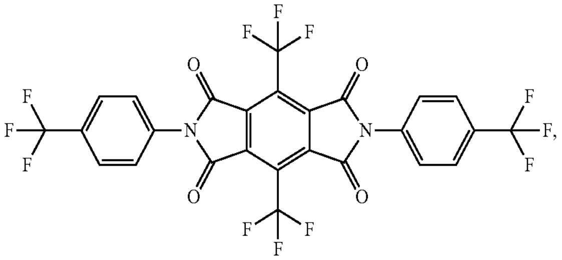

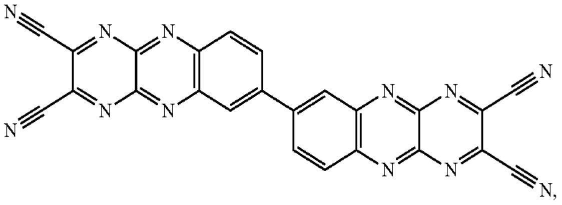

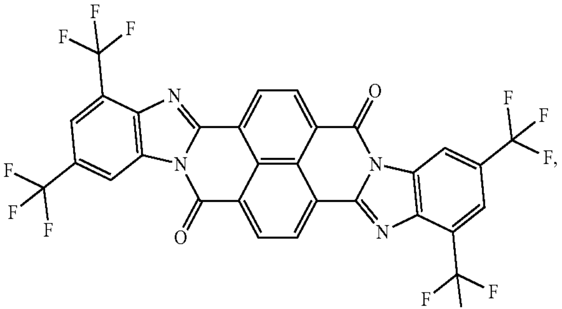

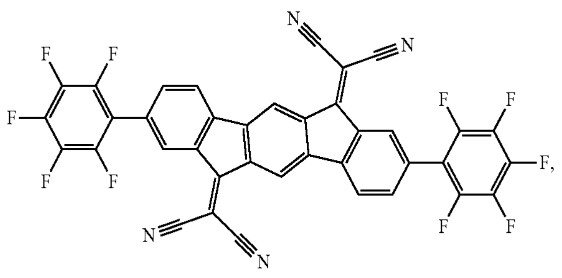

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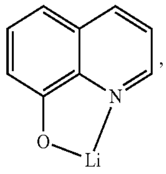

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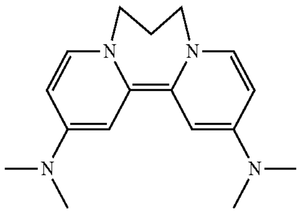
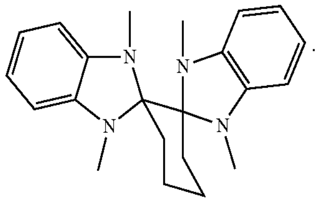
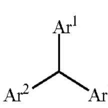


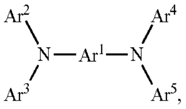


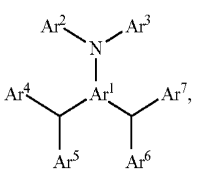
HIL/HTL:

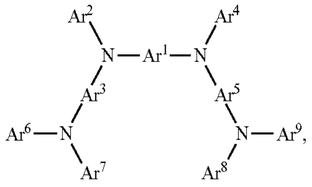
[0113] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but are not limited to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as MoO_x; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

[0114] Examples of aromatic amine derivatives used in HIL or HTL include, but are not limited to the following general structures:









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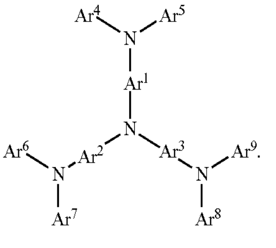
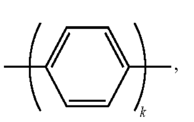
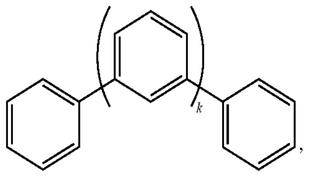
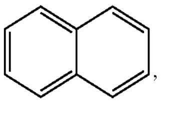


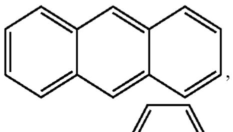
[0115] Each of Ar^1 to Ar^9 is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and the group consisting of 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Each Ar may be unsubstituted or may be substituted by a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

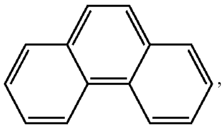
[0116] In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:

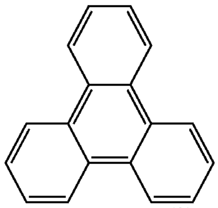


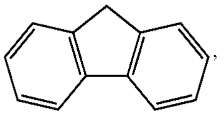












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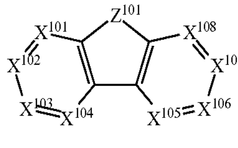
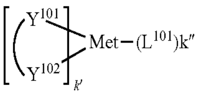


wherein k is an integer from 1 to 20; X^{101} to X^{108} is C (including CH) or N; Z^{101} is NAr^1, O, or S; Ar^1 has the same group defined above.

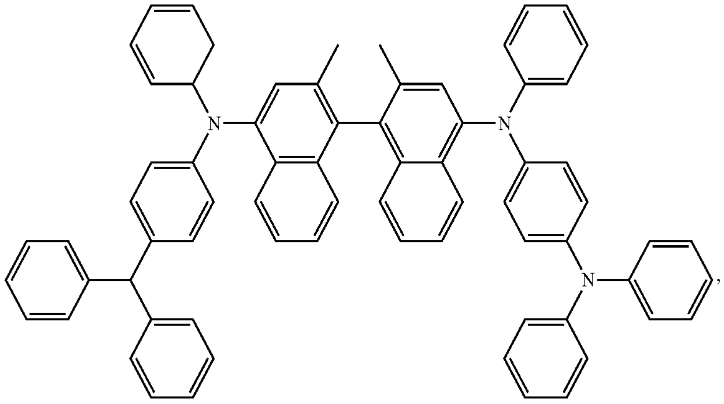
[0117] Examples of metal complexes used in HIL or HTL include, but are not limited to the following general formula:

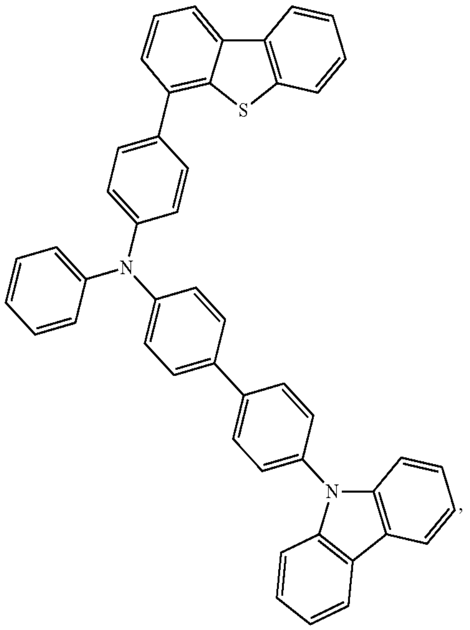


wherein Met is a metal, which can have an atomic weight greater than 40; (Y^{101}-Y^{102}) is a bidentate ligand, Y^{101} and Y^{102} are independently selected from C, N, O, P, and S; L^{101} is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached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

[0118] In one aspect, (Y^{101}-Y^{102}) is a 2-phenylpyridine derivative. In another aspect, (Y^{101}-Y^{102}) is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

[0119] Non-limiting examples of the HIL and HTL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN102702075, DE102012005215, EP01624500, EP01698613, EP01806334, EP01930964, EP01972613, EP01997799, EP02011790, EP02055700, EP02055701, EP1725079, EP2085382, EP2660300, EP650955, JP07-073529, JP2005112765, JP2007091719, JP2008021687, JP2014-009196, KR20110088898, KR20130077473, TW201139402, U.S. Ser. No. 06/517,957, US20020158242, US20030162053, US20050123751, US20060182993, US20060240279, US20070145888, US20070181874, US20070278938, US20080014464, US20080091025, US20080106190, US20080124572, US20080145707, US20080220265, US20080233434, US20080303417, US2008107919, US20090115320, US20090167161, US2009066235, US2011007385, US20110163302, US2011240968, US2011278551, US2012205642, US2013241401, US20140117329, US2014183517, U.S. Pat. Nos. 5,061,569, 5,639,914, WO05075451, WO07125714, WO08023550, WO08023759, WO2009145016, WO2010061824, WO2011075644, WO2012177006, WO2013018530, WO2013039073, WO2013087142, WO2013118812, WO2013120577, WO2013157367, WO2013175747, WO2014002873, WO2014015935, WO2014015937, WO2014030872, WO2014030921, WO2014034791, WO2014104514, WO2014157018,





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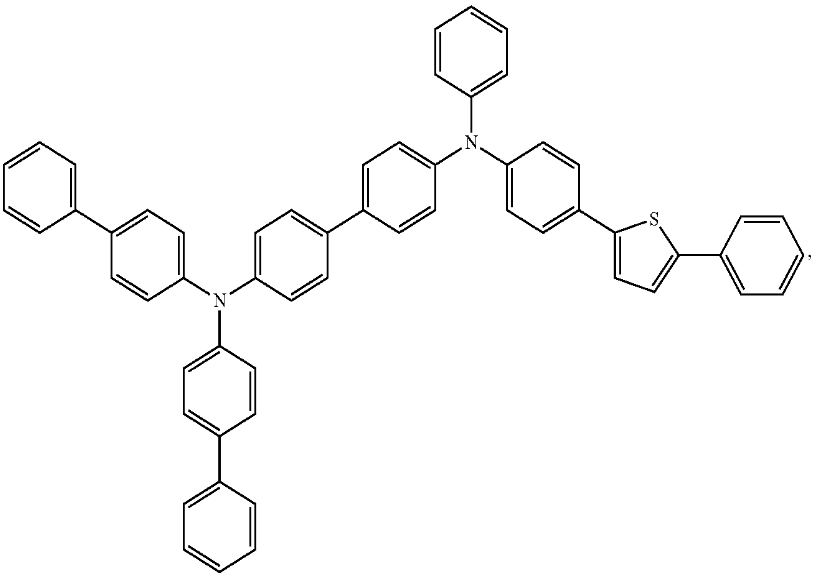

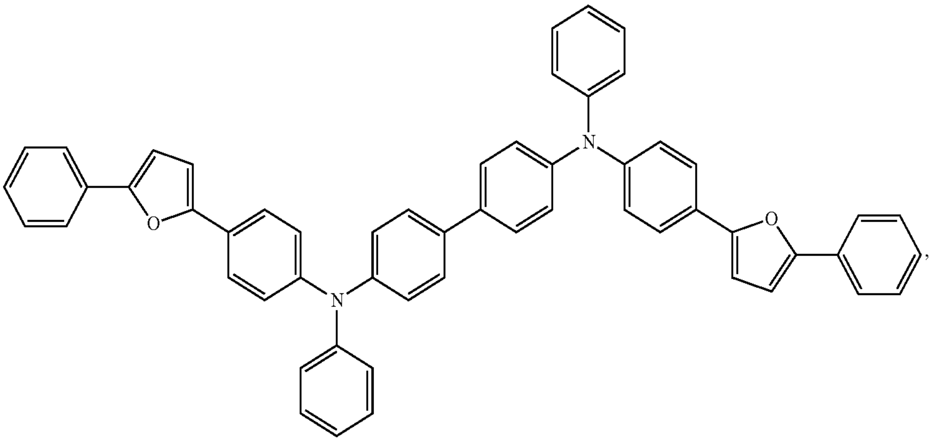

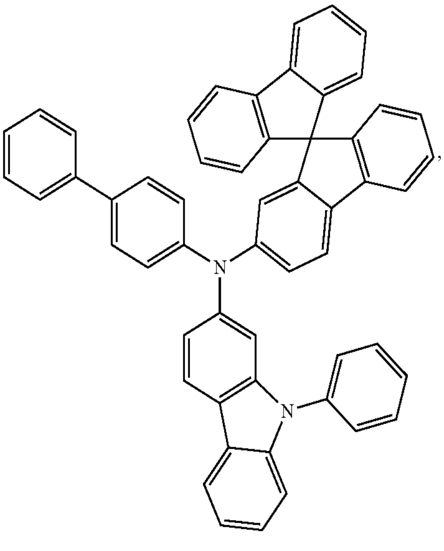

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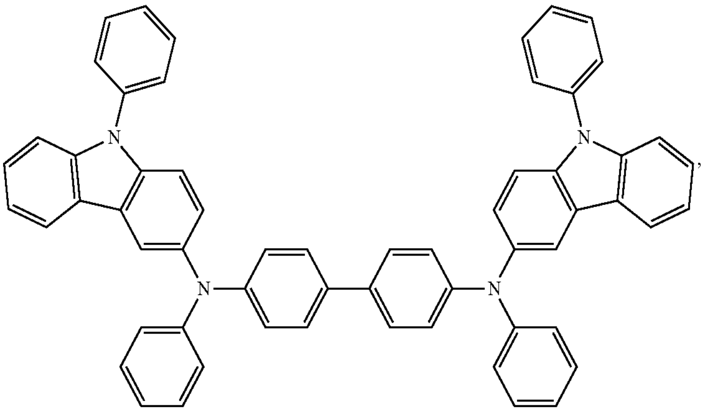

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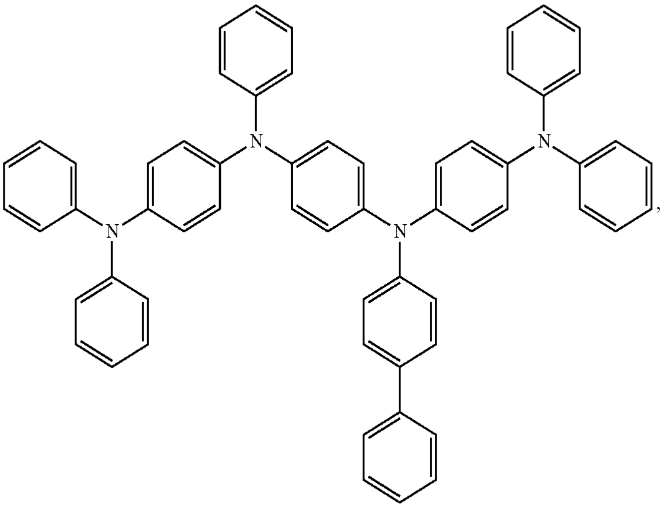

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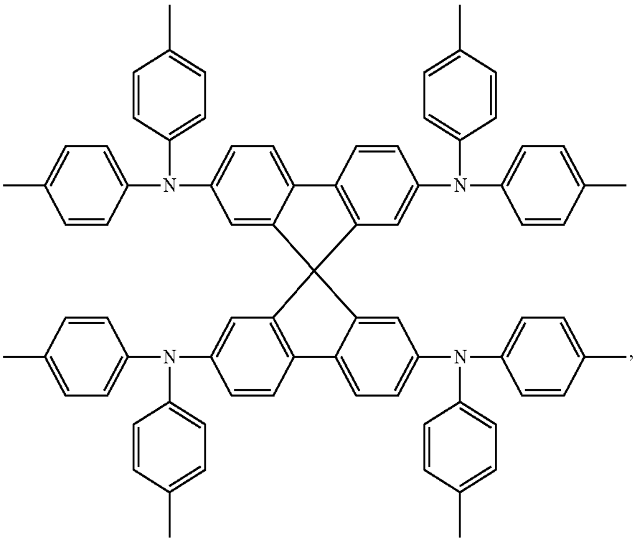

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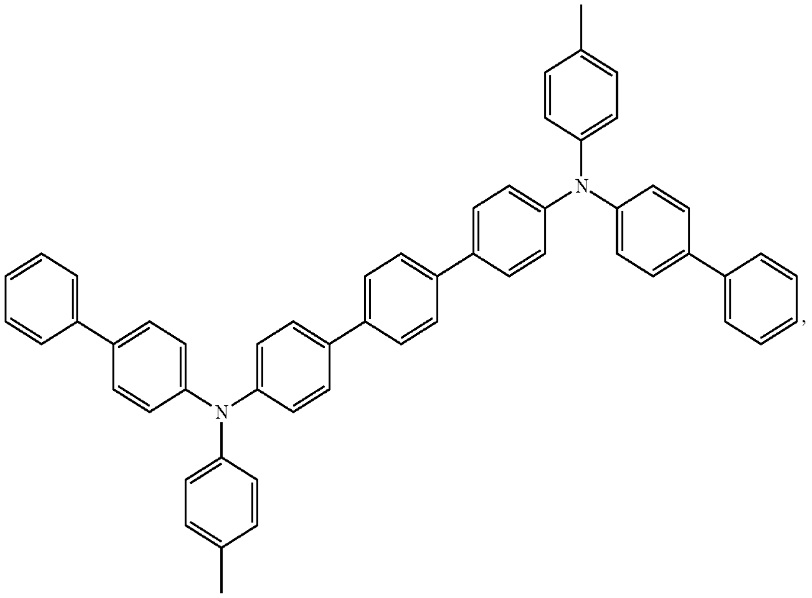

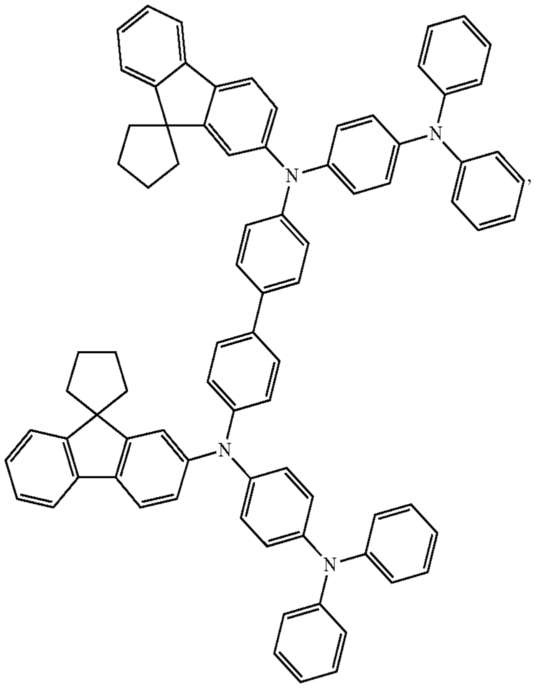

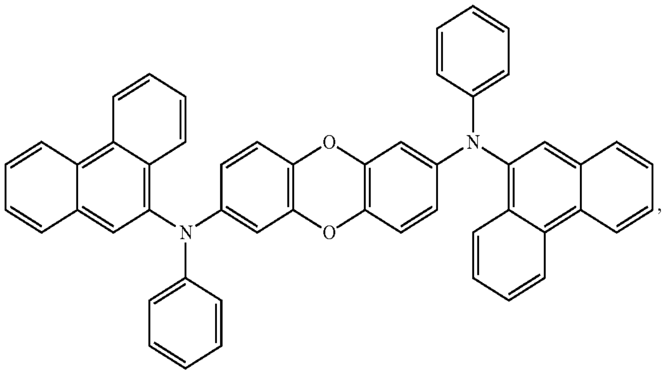

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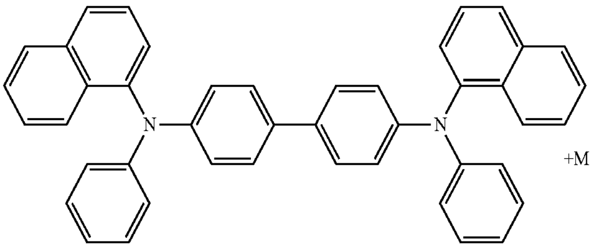

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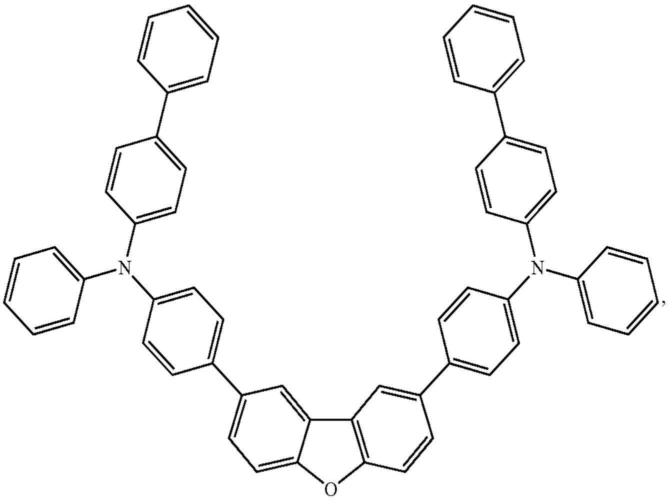

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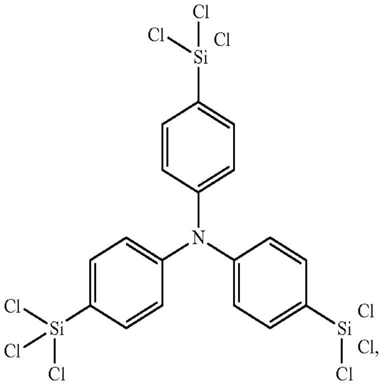

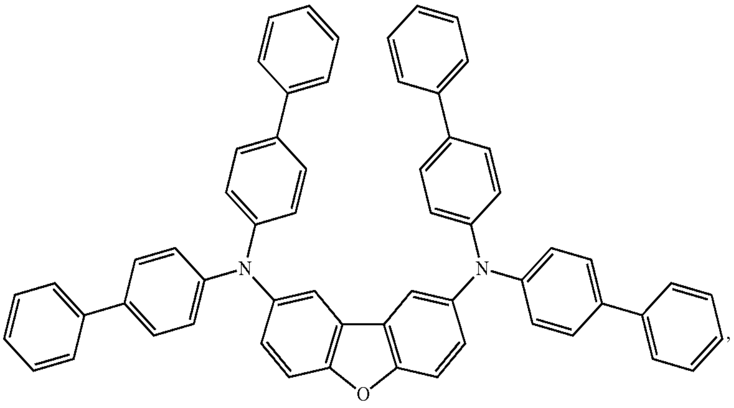

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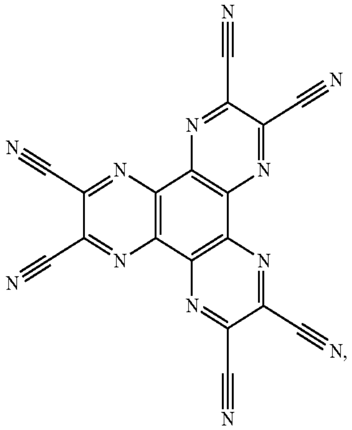

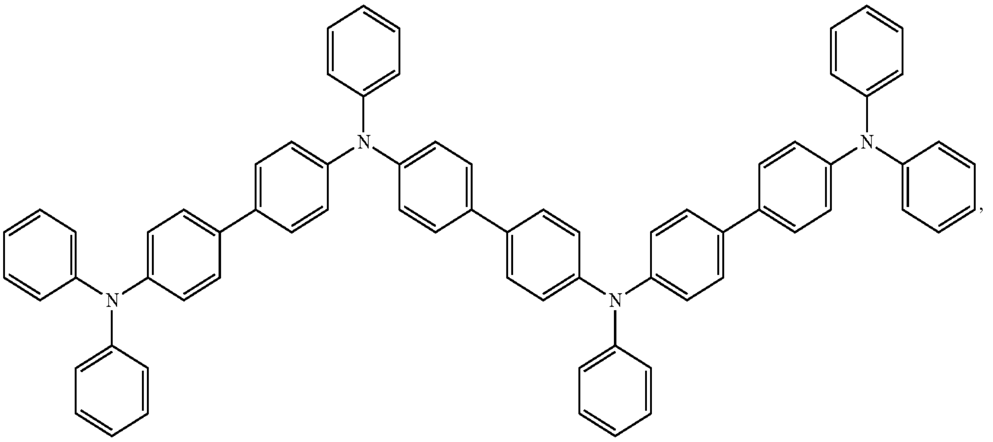

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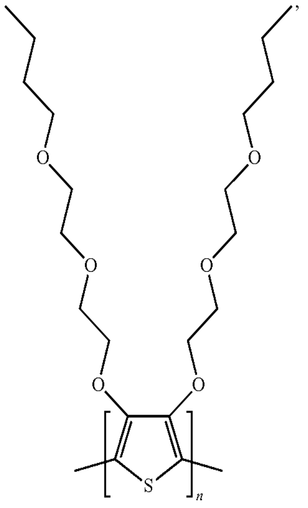

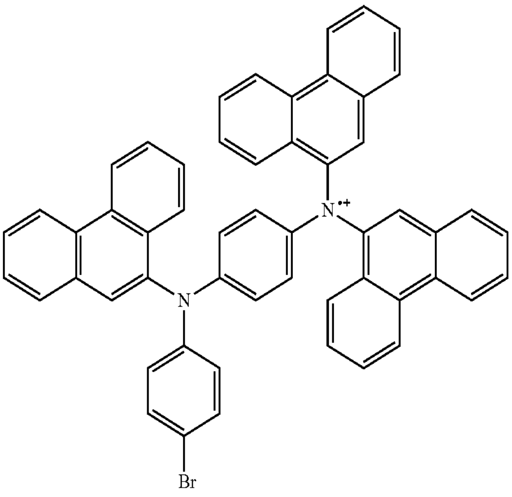

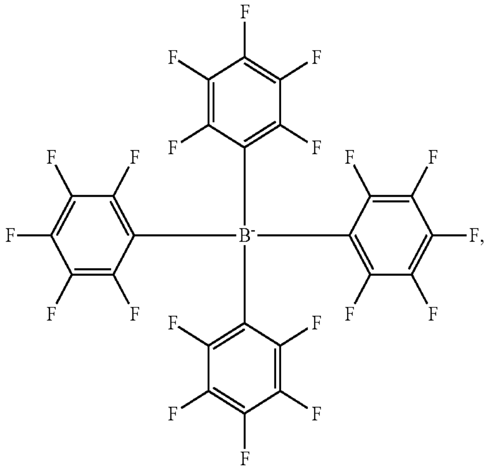

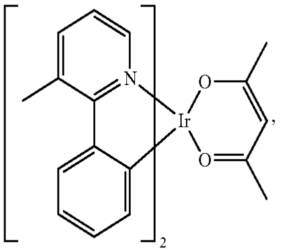

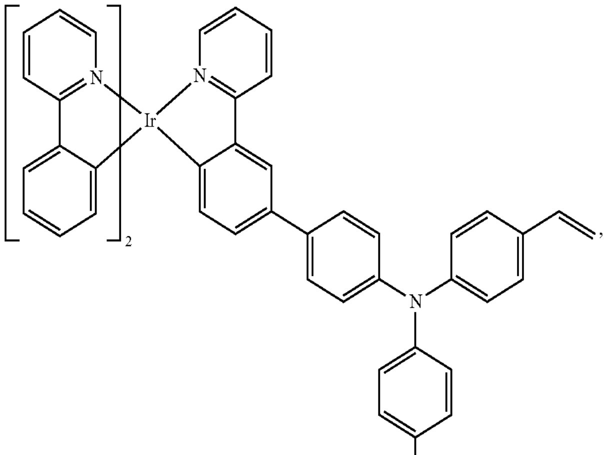

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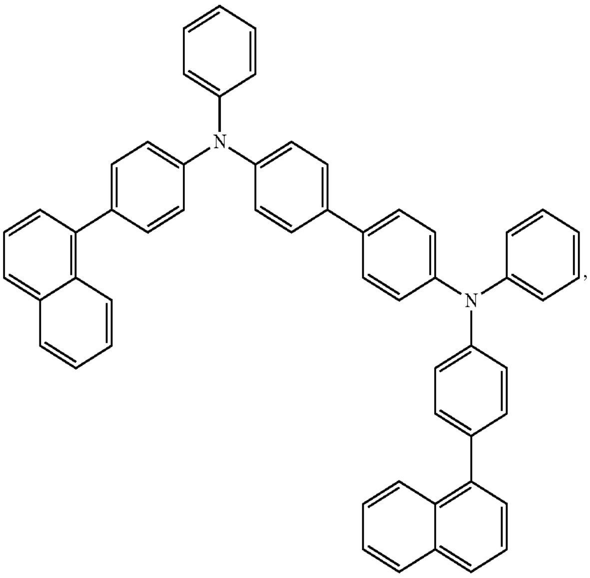

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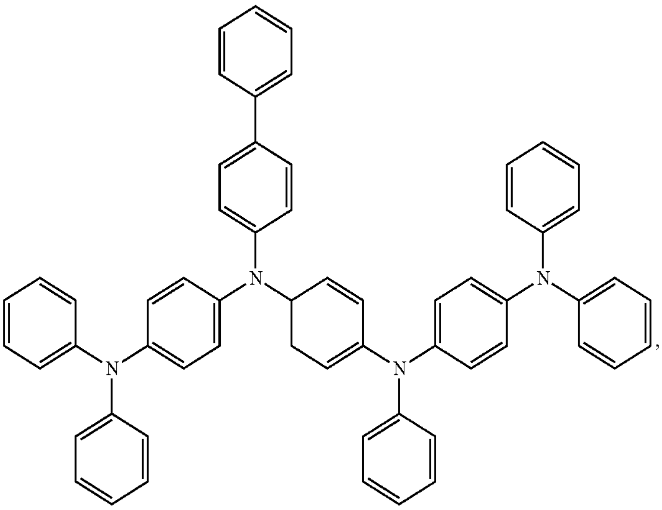

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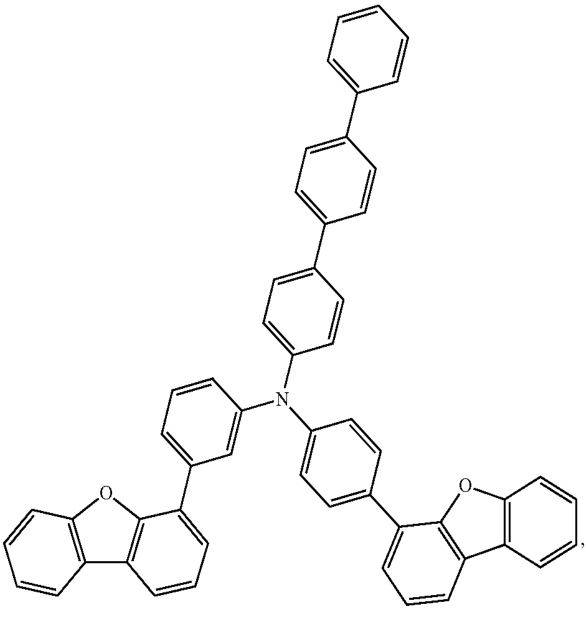

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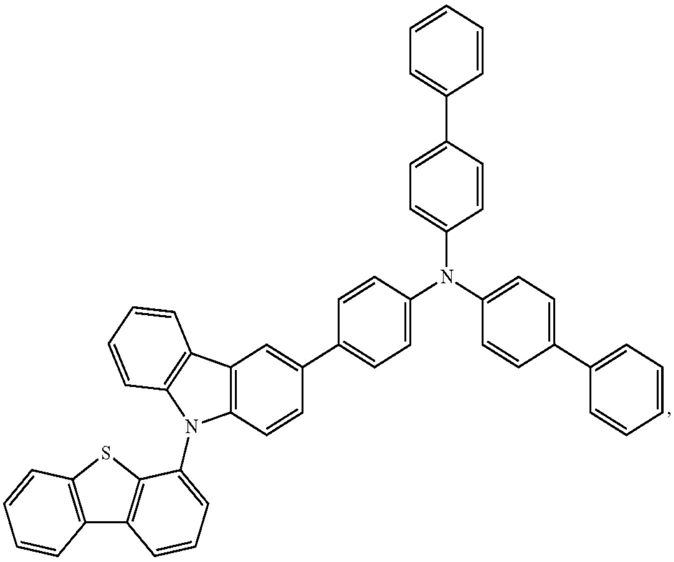

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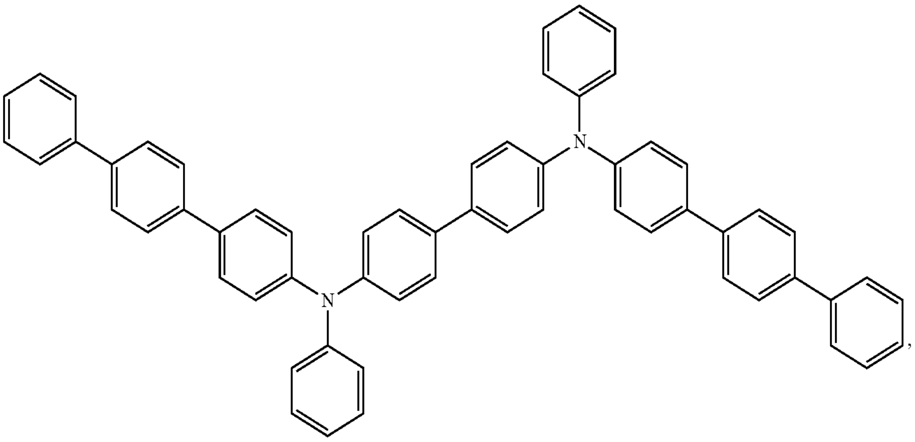

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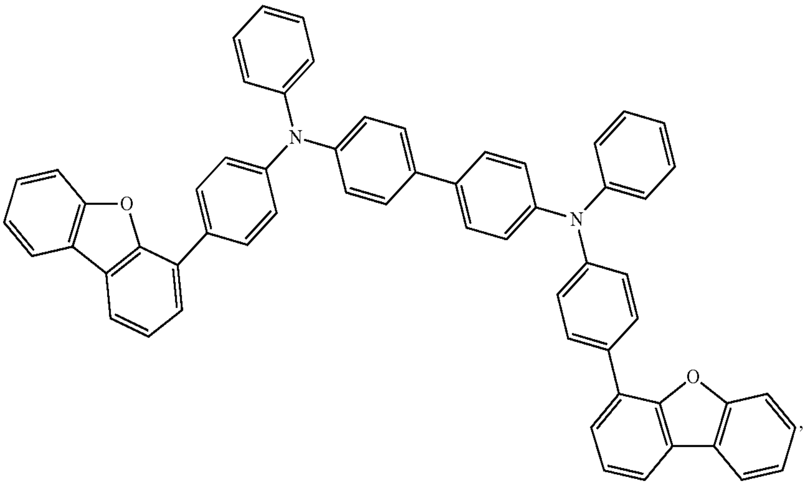

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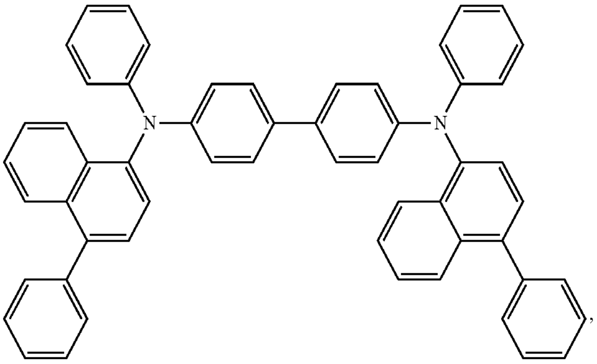

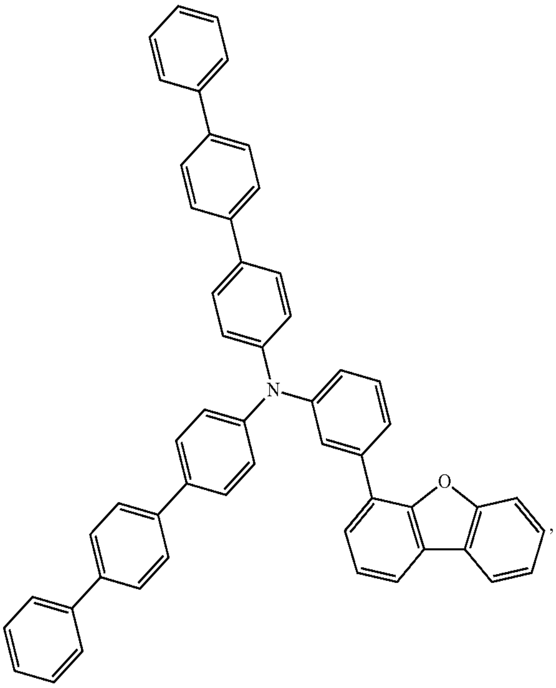

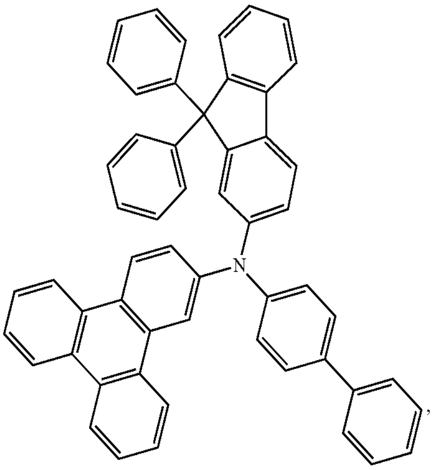

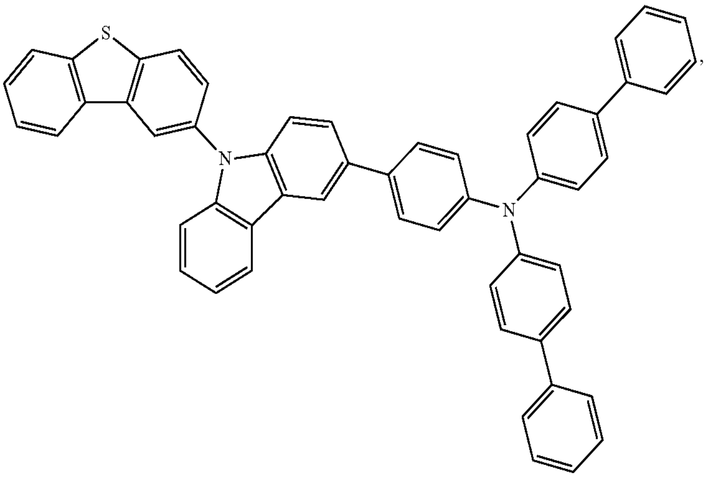

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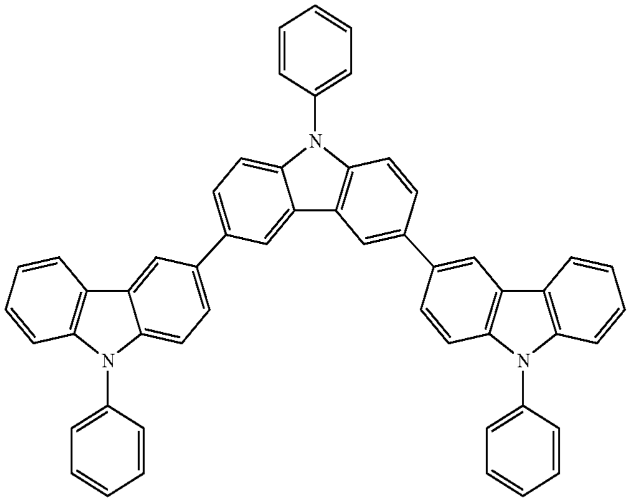

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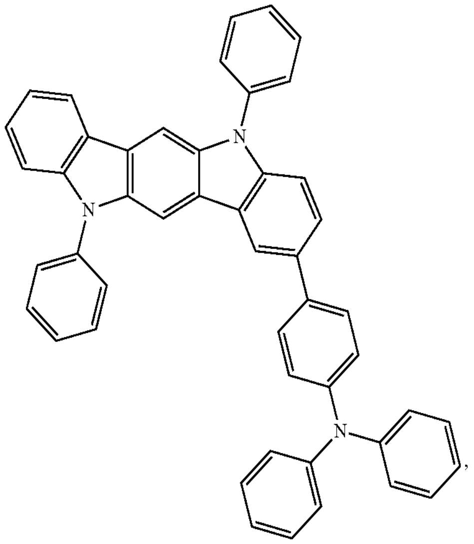

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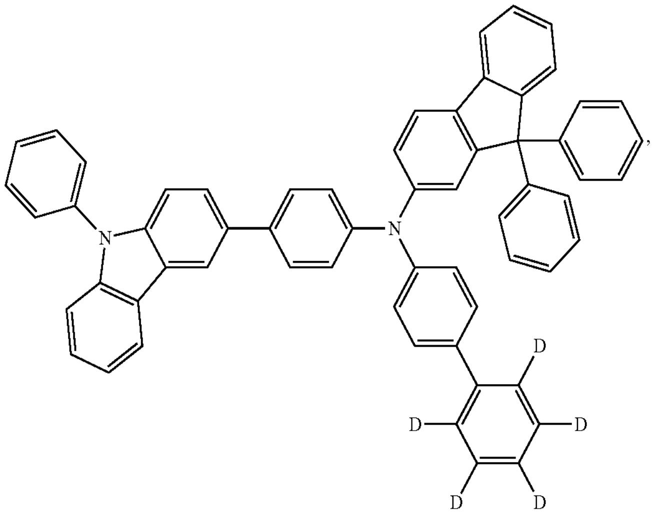

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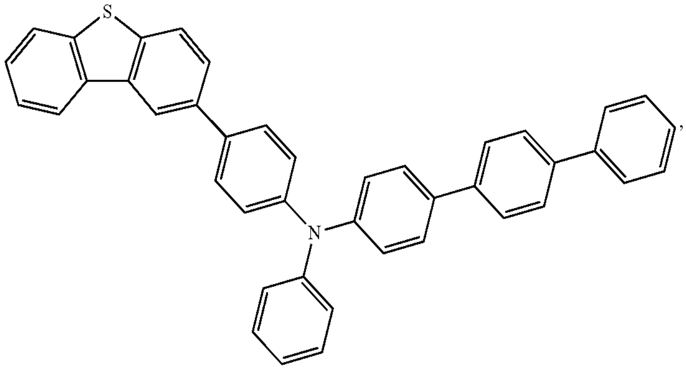

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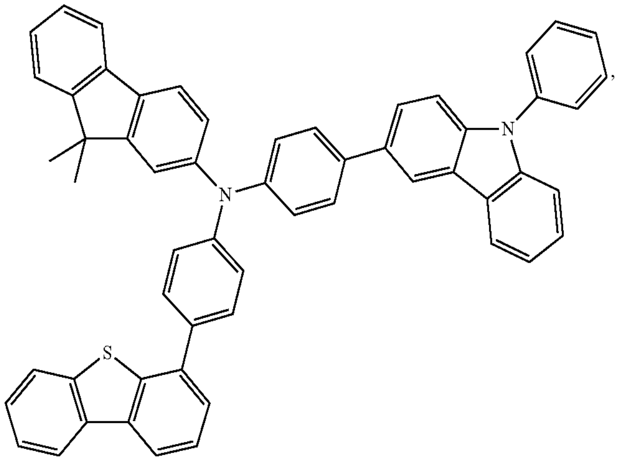

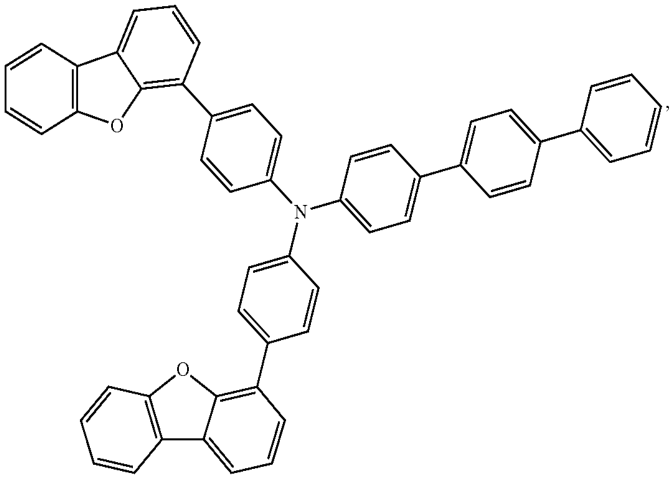

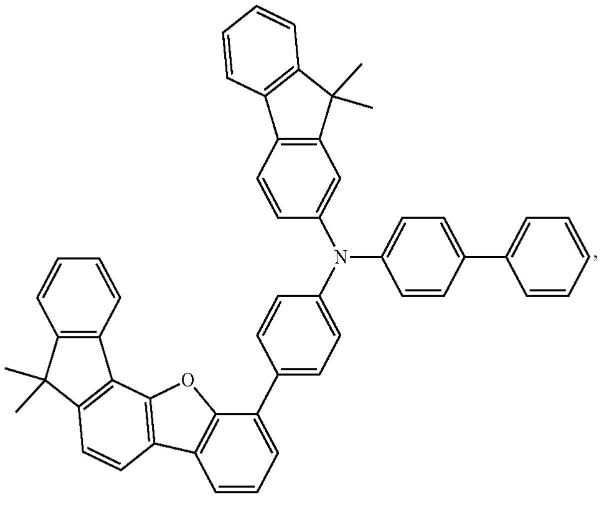

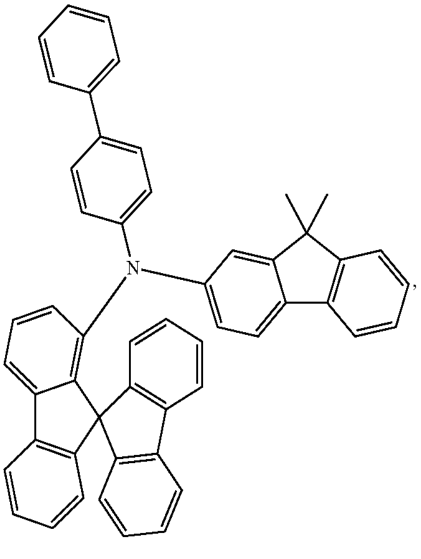

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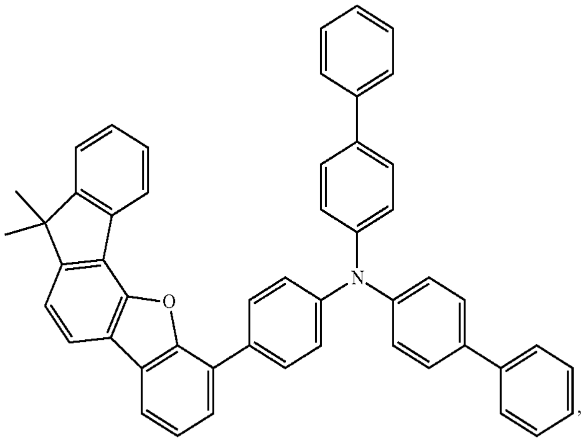

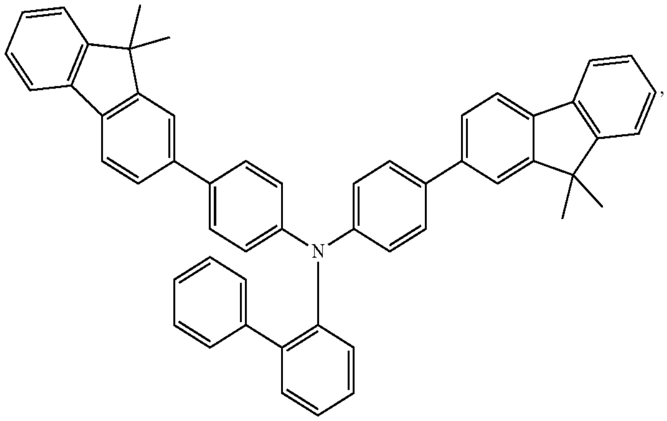

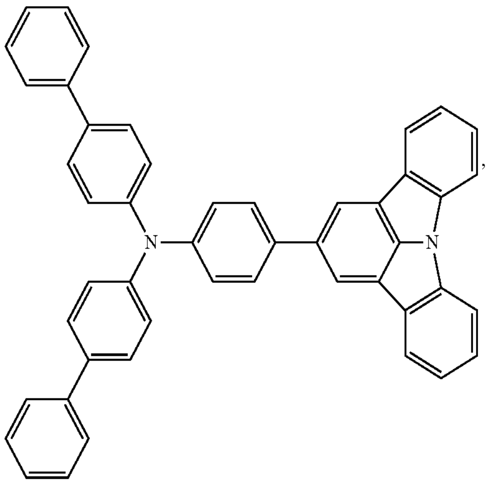

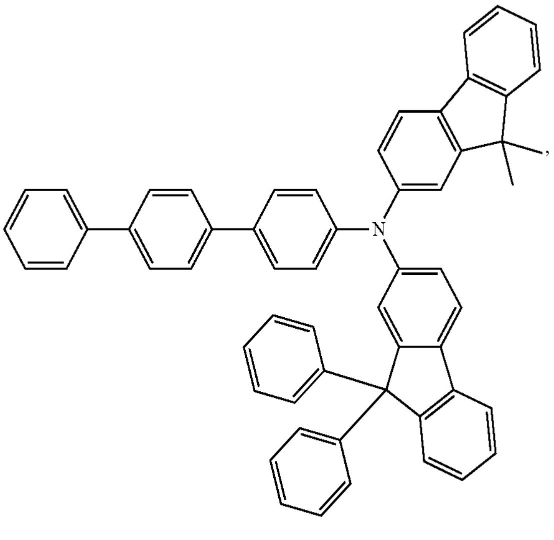

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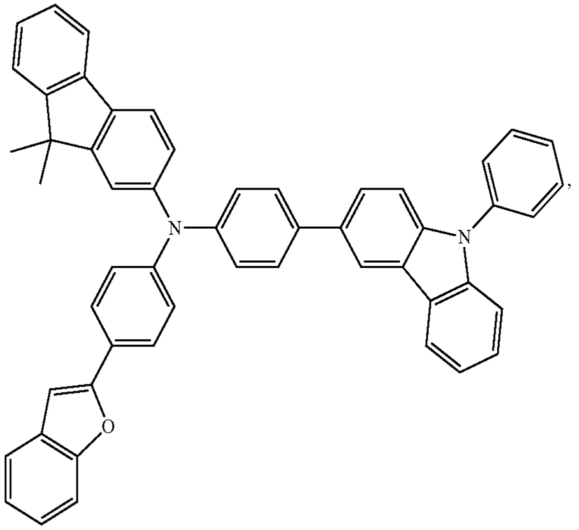

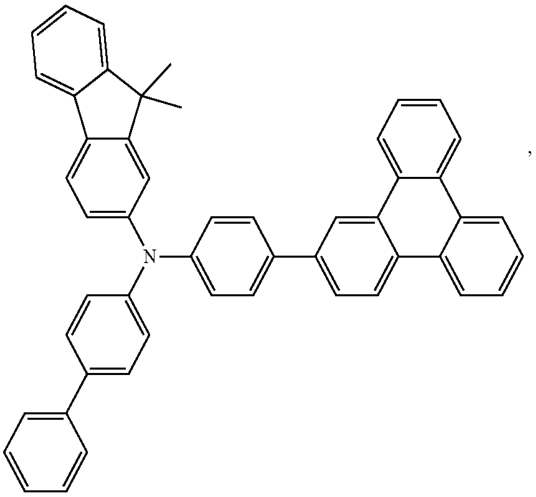

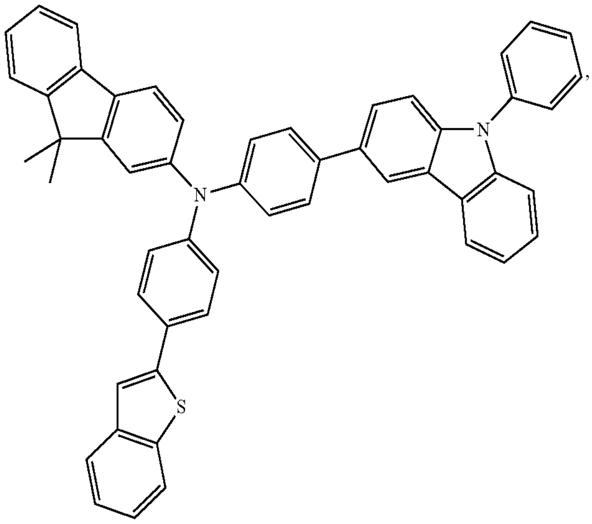

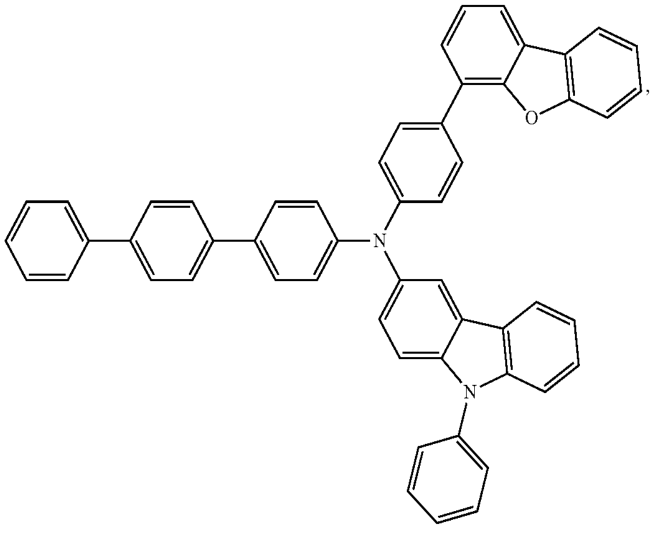

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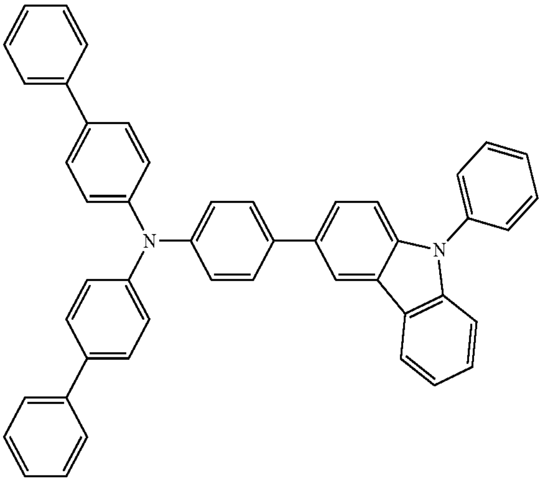
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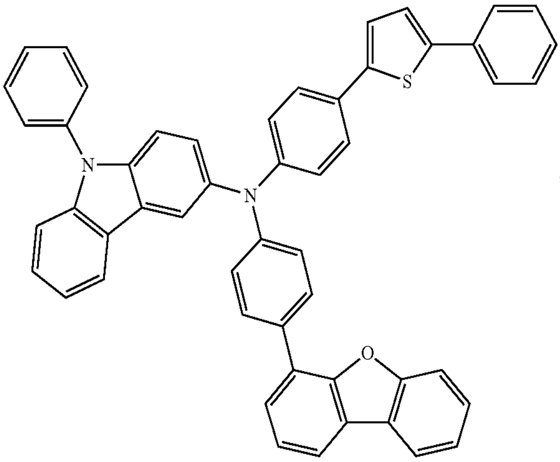
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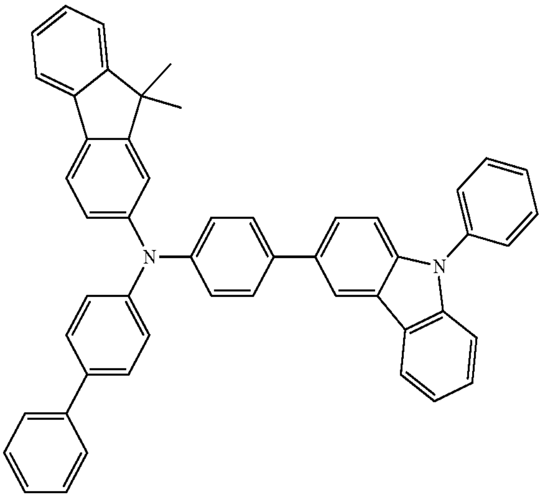
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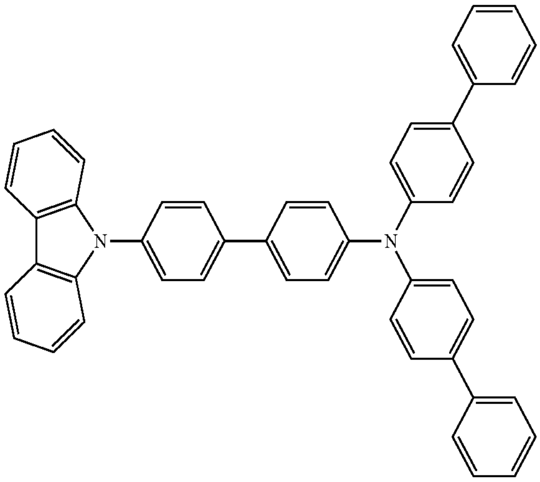
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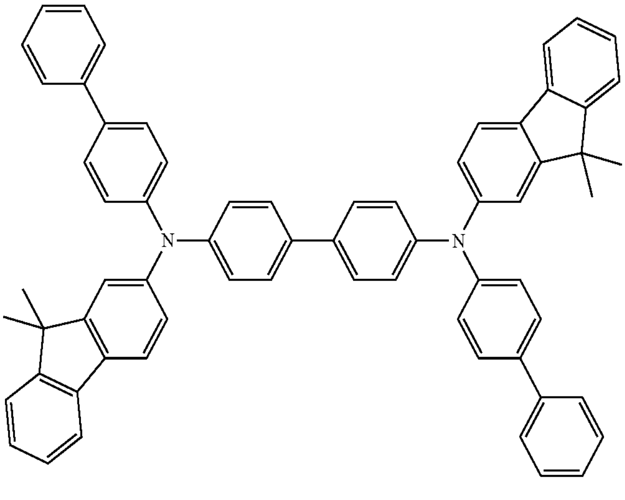
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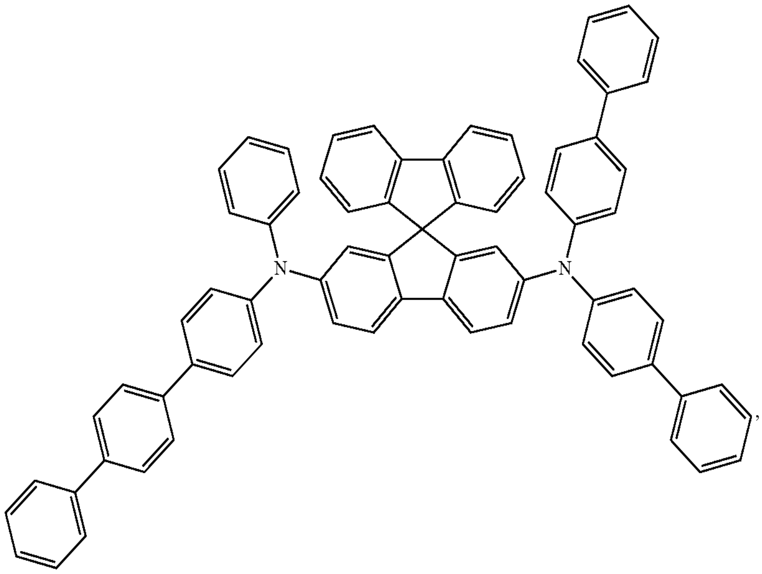

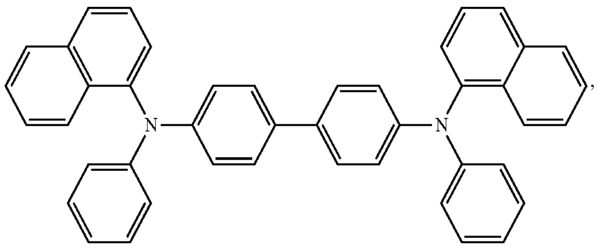

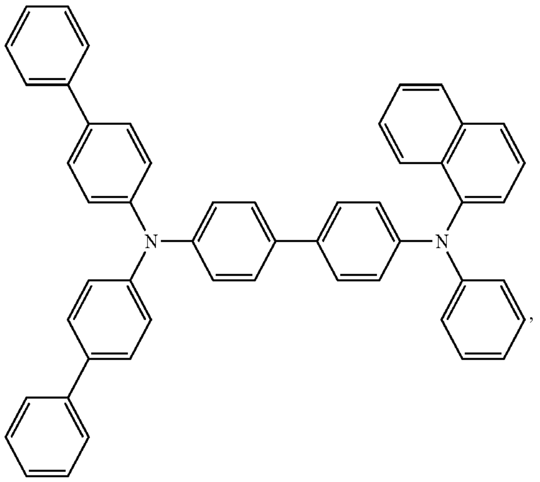

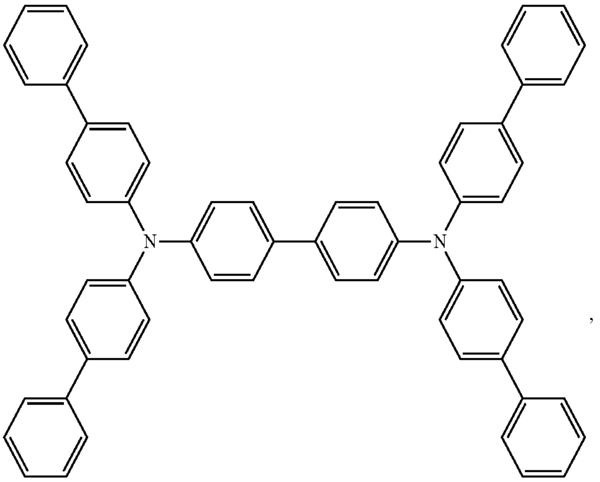

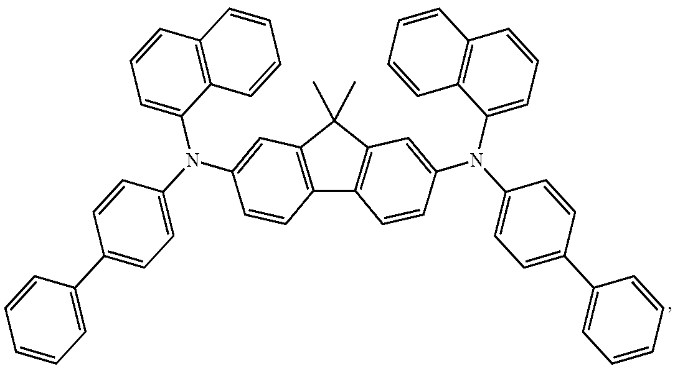

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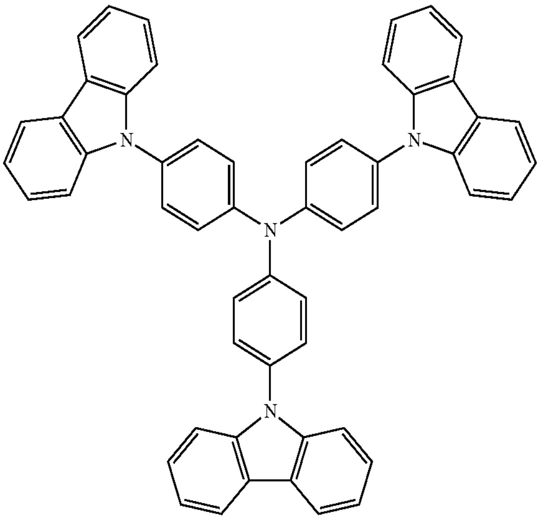

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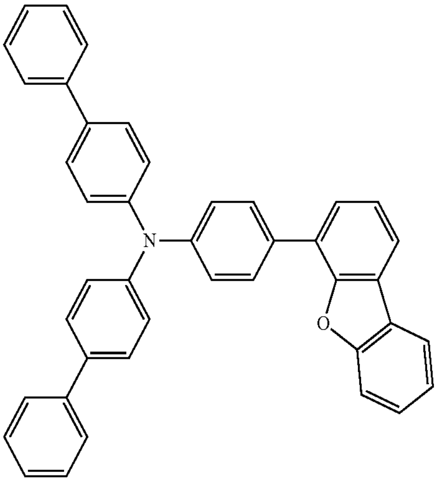

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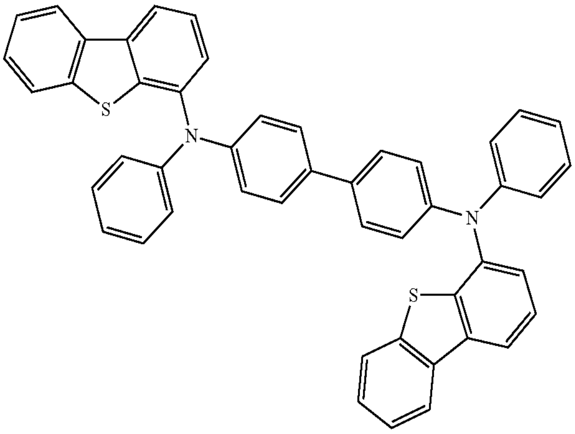

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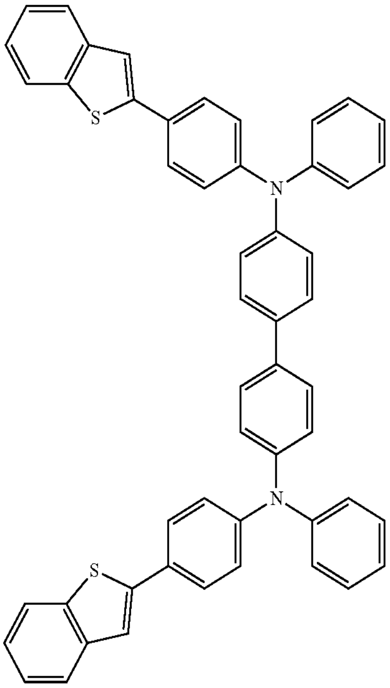

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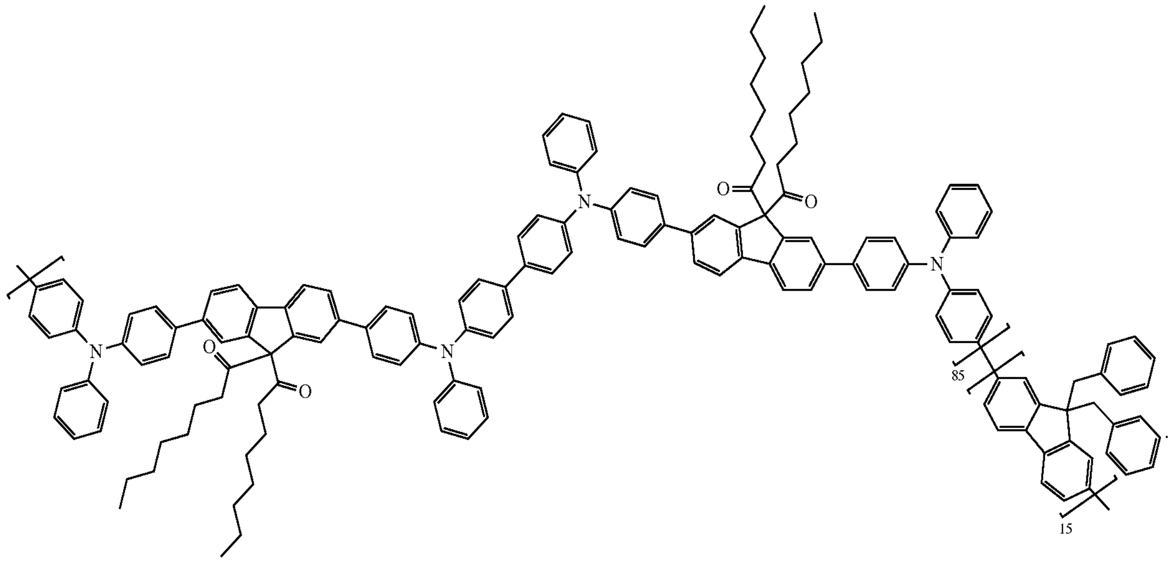


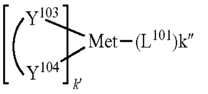
EBL:

[0120] An electron blocking layer (EBL) may be used to reduce the number of electrons and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies, and/or longer lifetime, as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and/or higher triplet energy than the emitter closest to the EBL interface. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and/or higher triplet energy than one or more of the hosts closest to the EBL interface. In one aspect, the compound used in EBL contains the same molecule or the same functional groups used as one of the hosts described below.

Additional Hosts:

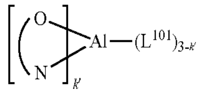
[0121] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting dopant material, and may contain one or more additional host materials using the metal complex as a dopant material. Examples of the host material are not particularly 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. Any host material may be used with any dopant so long as the triplet criteria is satisfied.

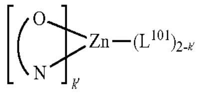
[0122] Examples of metal complexes used as host are preferred to have the following general formula:



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

[0123] In one aspect, the metal complexes are:



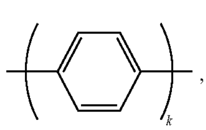


wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

[0124] In another aspect, Met is selected from Ir and Pt. In a further aspect, (Y^{103}-Y^{104}) is a carbene ligand.

[0125] In one aspect, the host compound contains at least one of the following groups selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0126] In one aspect, host compound contains at least one of the following groups in the molecule:



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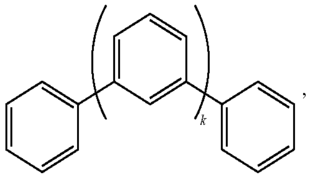

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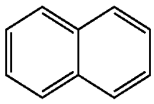

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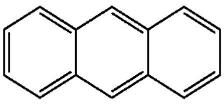

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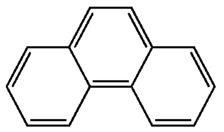

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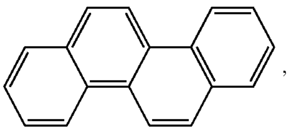

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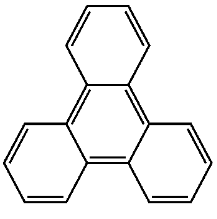

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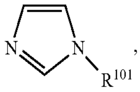

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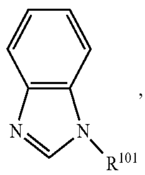

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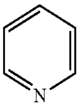

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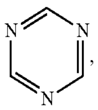

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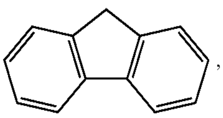

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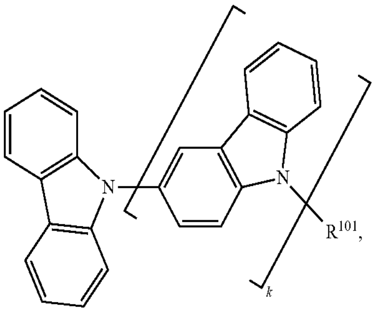

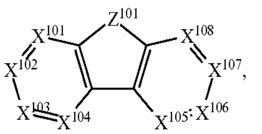

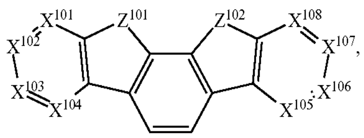

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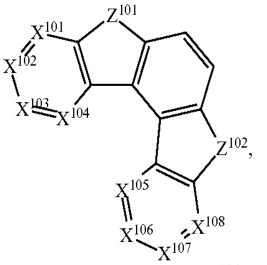

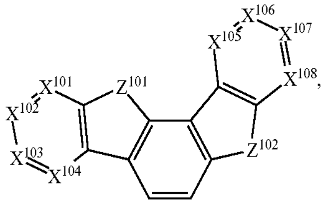

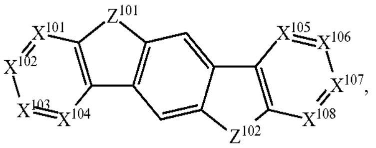

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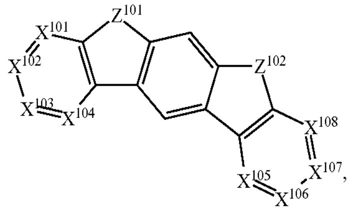
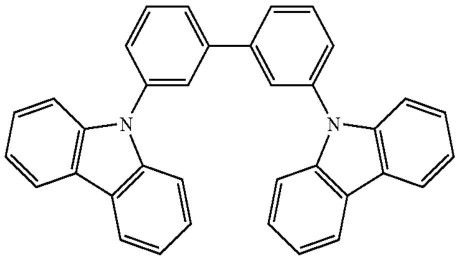


wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, 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. X^{101} to X^{108} are independently selected from C (including CH) or N. Z^{101} and Z^{102} are independently selected from NR^{101}, O, or S.

[0127] Non-limiting examples of the additional host materials that may be used in an OLED in combination with the host compound disclosed herein are exemplified below together with references that disclose those materials: EP2034538, EP2034538A, EP2757608, JP2007254297, KR20100079458, KR20120088644, KR20120129733, KR20130115564, TW201329200, US20030175553, US20050238919, US20060280965, US20090017330, US20090030202, US20090167162, US20090302743, US20090309488, US20100012931, US20100084966, US20100187984, US2010187984, US2012075273, US2012126221, US2013009543, US2013105787, US2013175519, US2014001446, US20140183503, US20140225088, US2014034914, U.S. Pat. No. 7,154,114, WO2001039234, WO2004093207, WO2005014551, WO2005089025, WO2006072002, WO2006114966, WO2007063754, WO2008056746, WO2009003898, WO2009021126, WO2009063833, WO2009066778, WO2009066779, WO2009086028, WO2010056066, WO2010107244, WO2011081423, WO2011081431, WO2011086863, WO2012128298, WO2012133644, WO2012133649, WO2013024872, WO2013035275, WO2013081315, WO2013191404, WO2014142472, US20170263869, US20160163995, U.S. Pat. No. 9,466,803.



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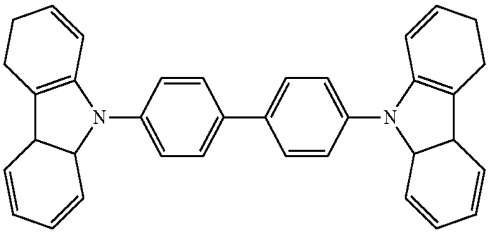

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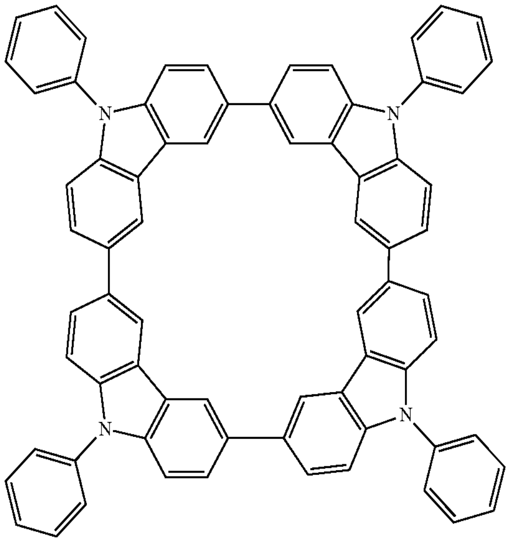

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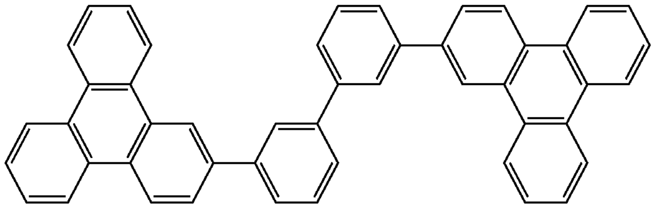

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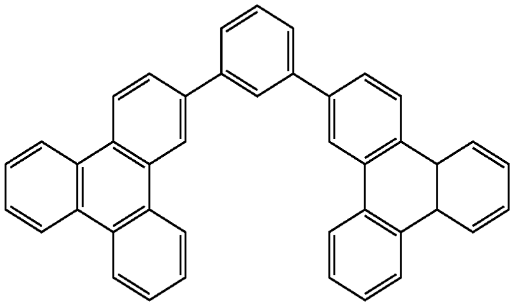

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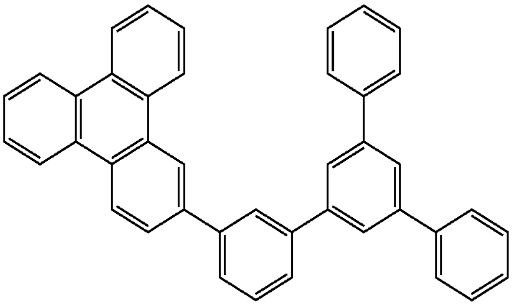

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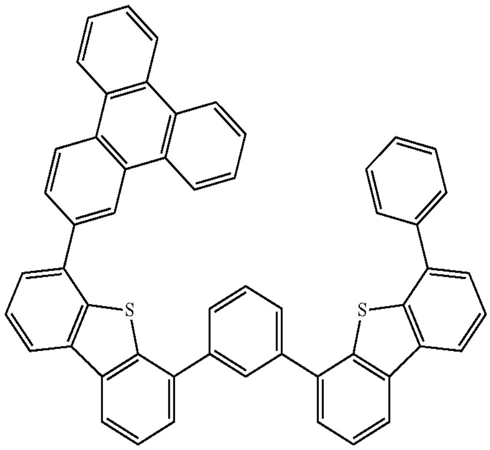

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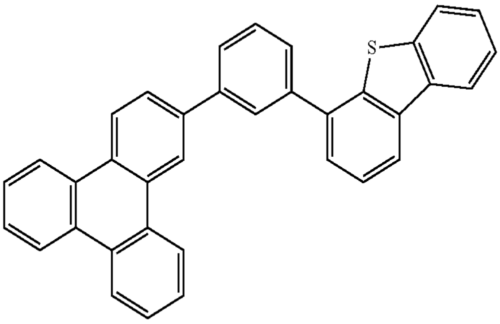

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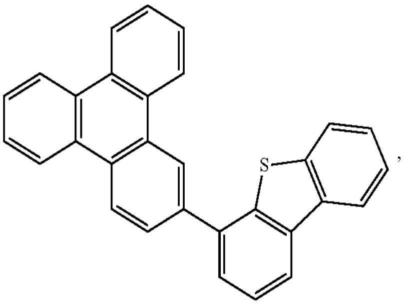

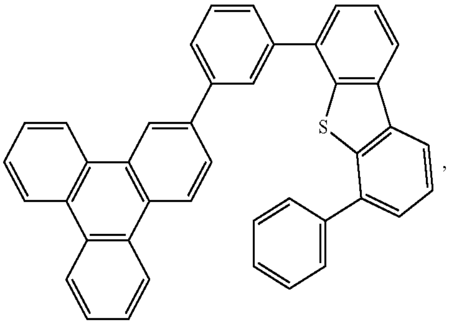

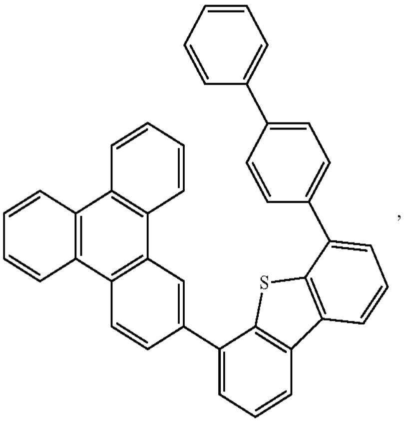

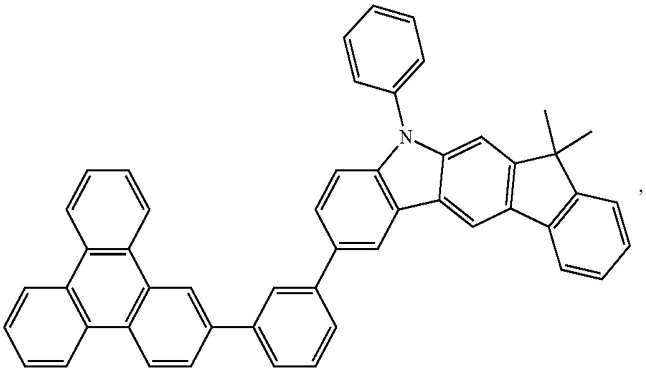

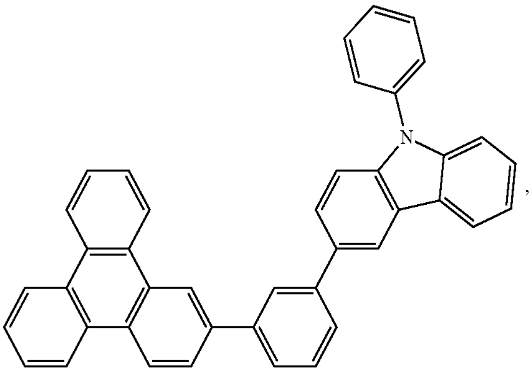

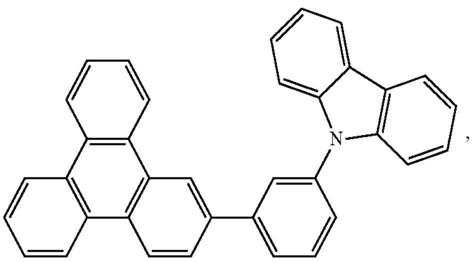

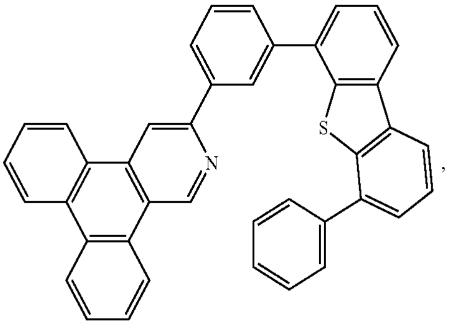

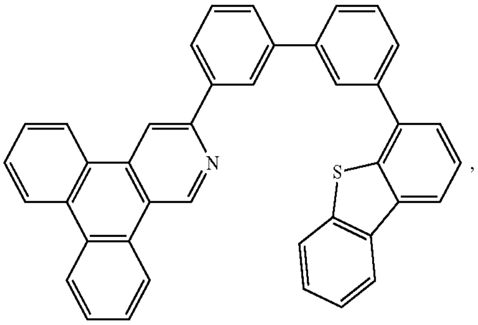

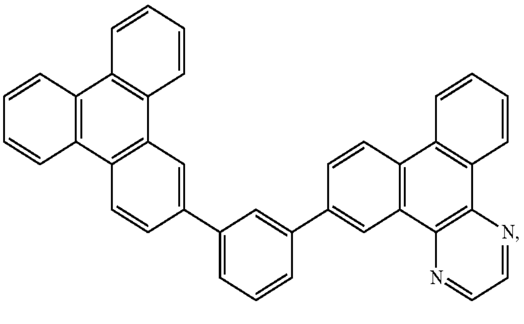

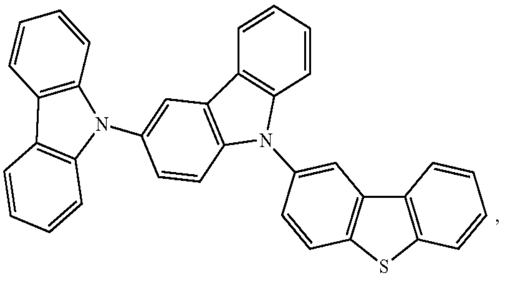

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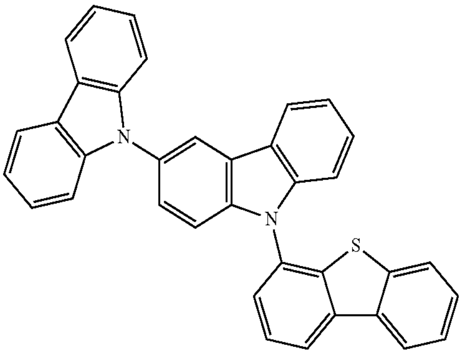

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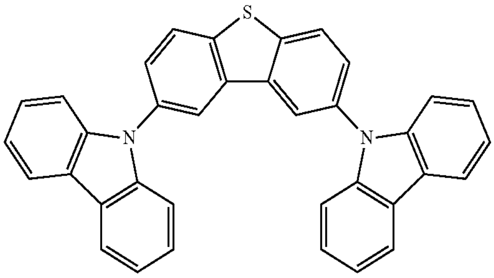

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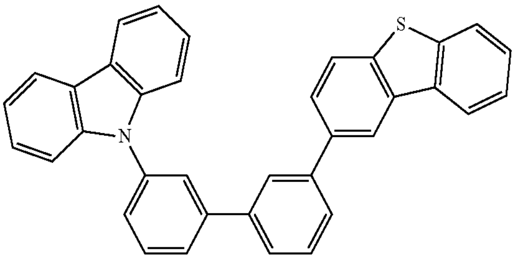

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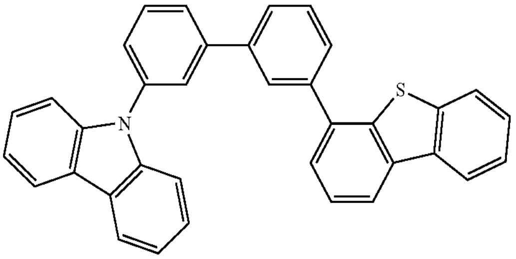

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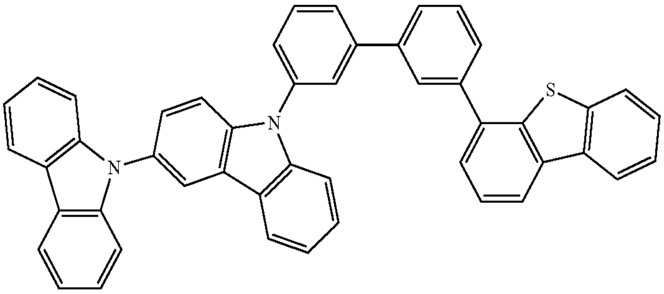

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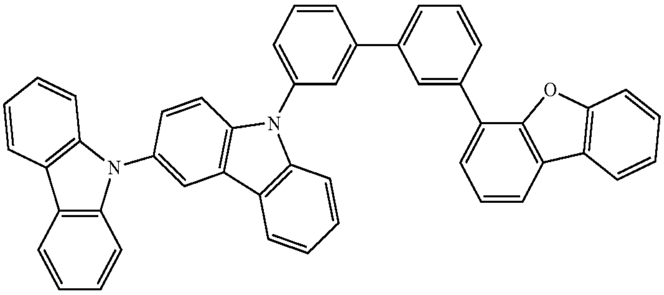

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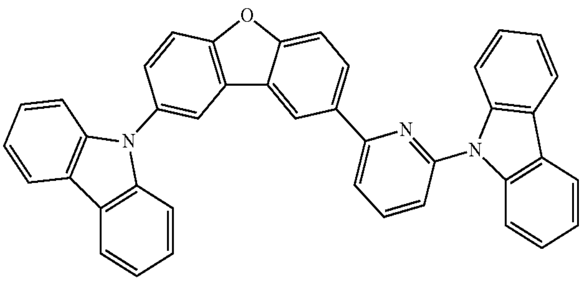

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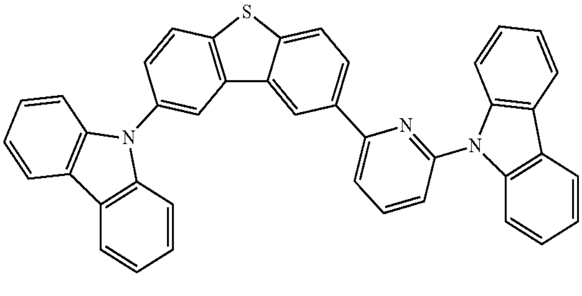

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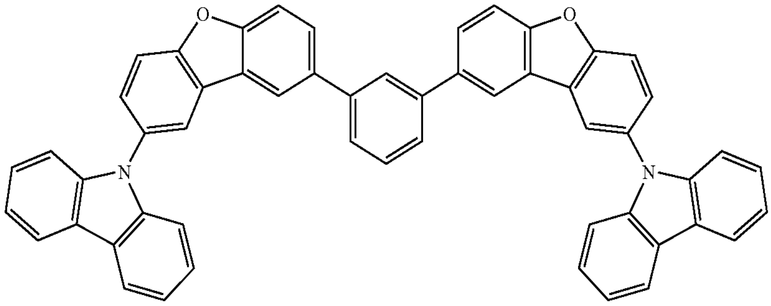

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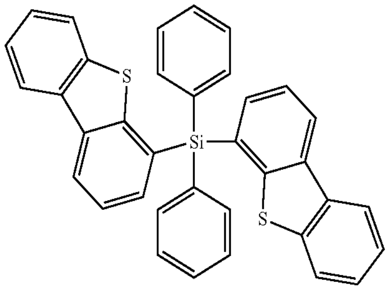

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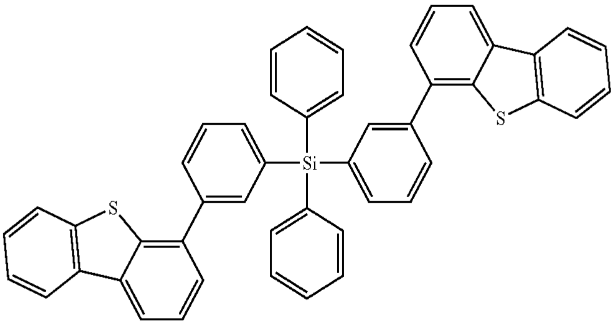

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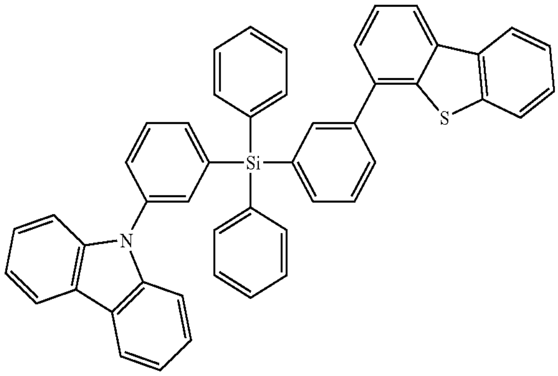

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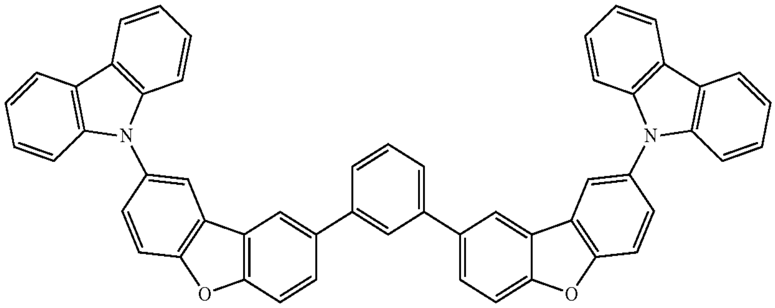

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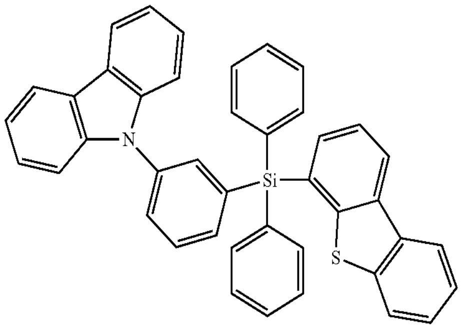

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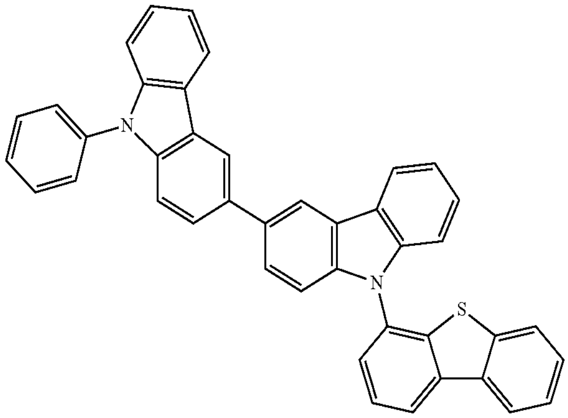

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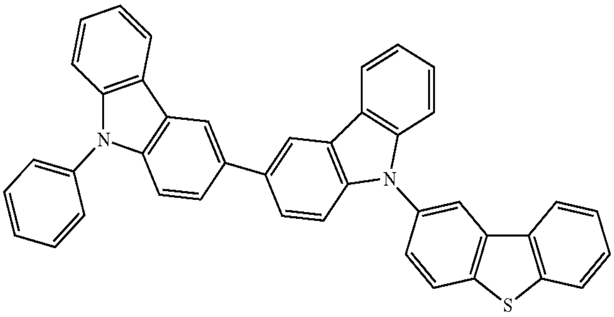

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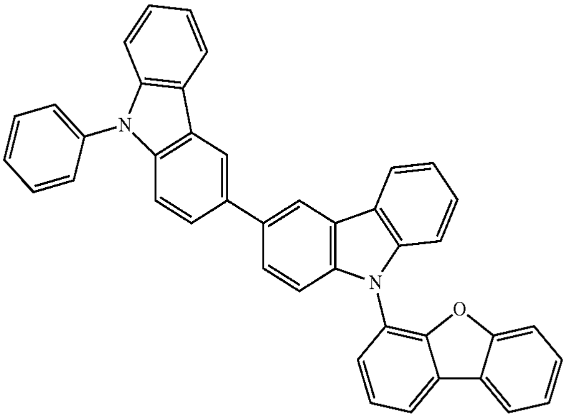

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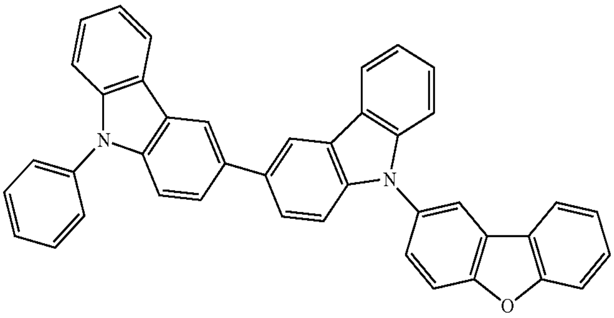

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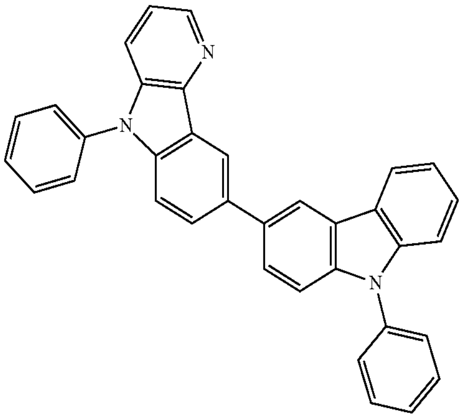

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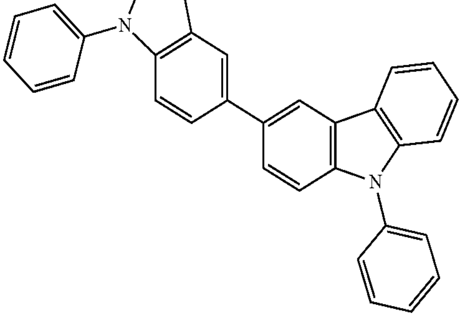

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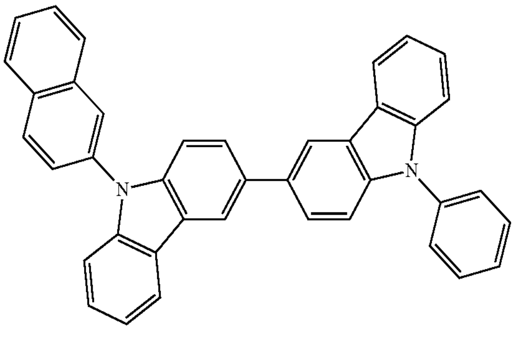

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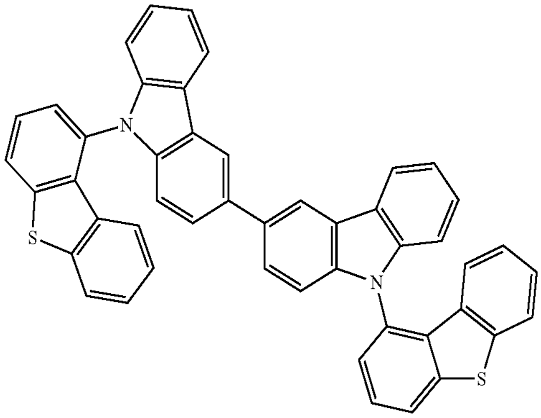

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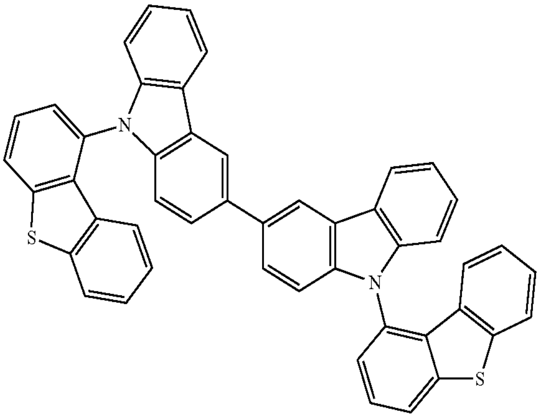

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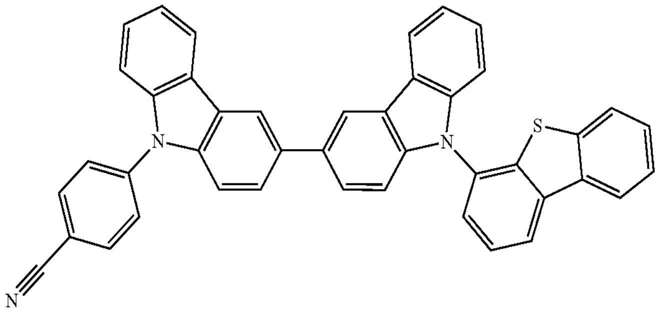

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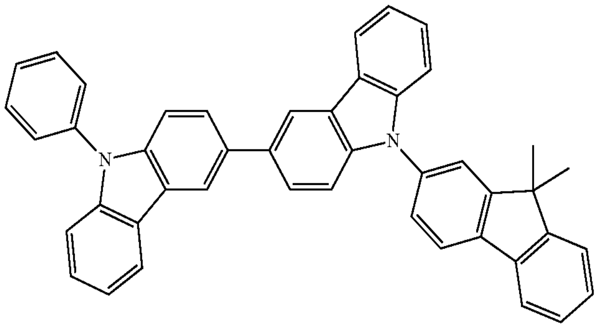

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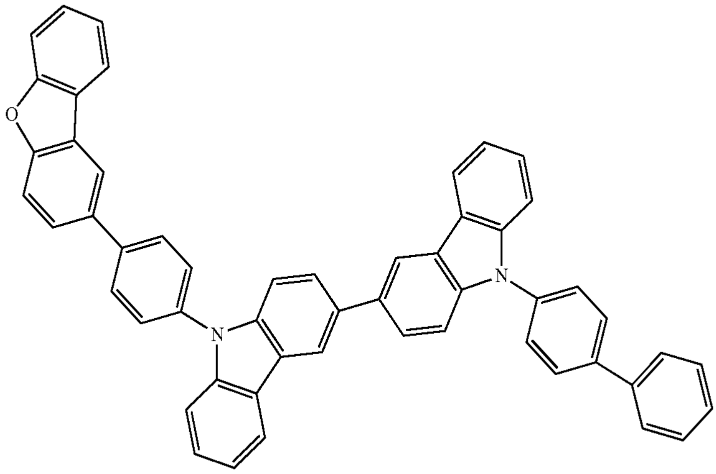

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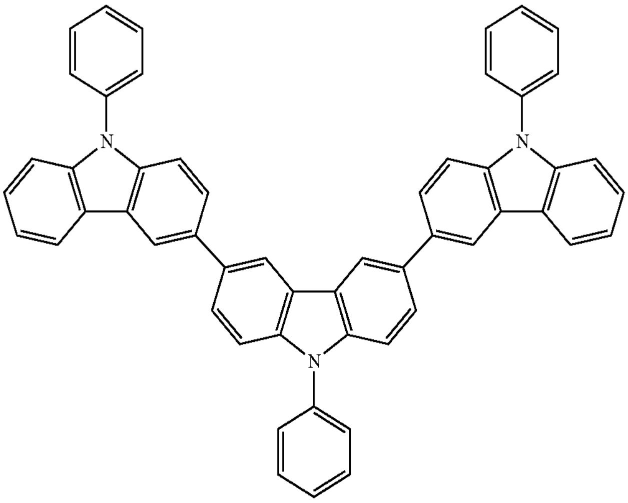

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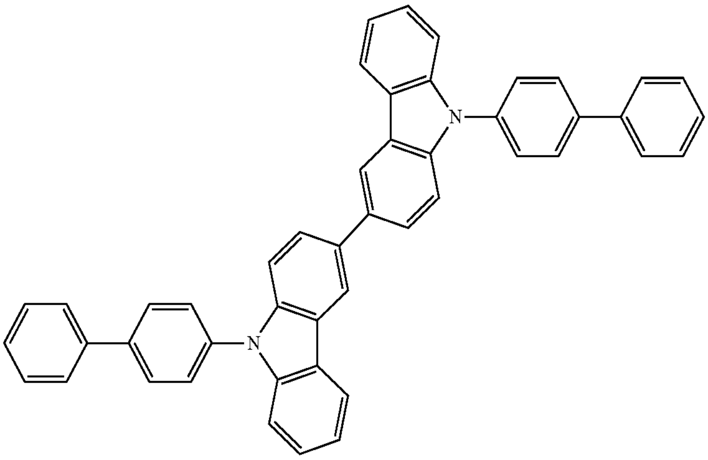

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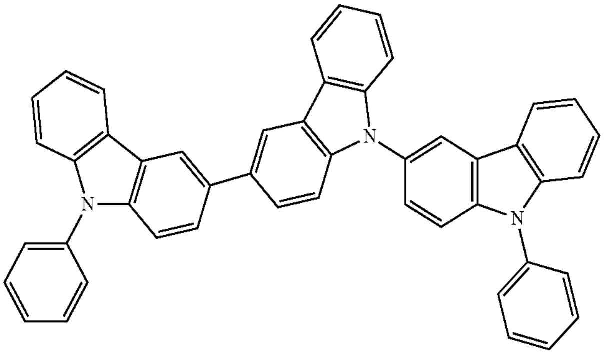

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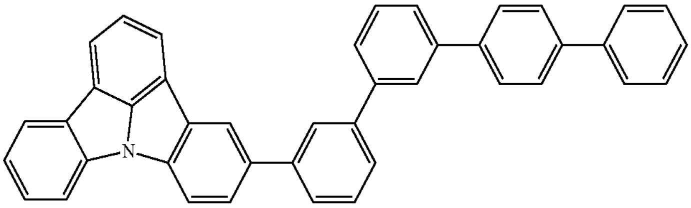

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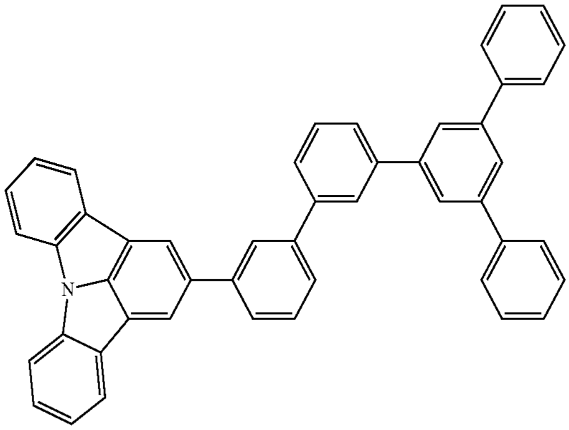

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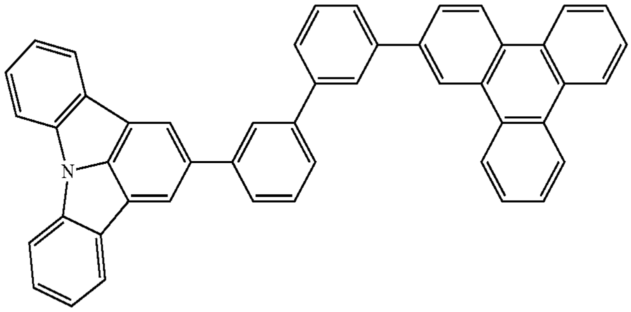

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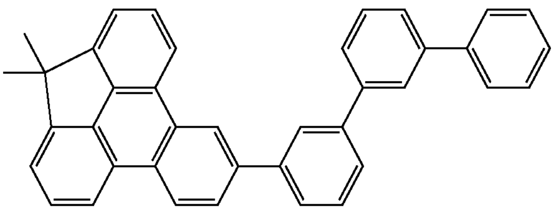

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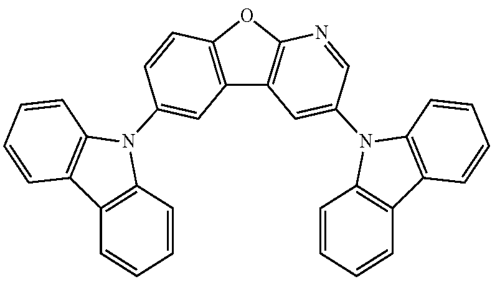

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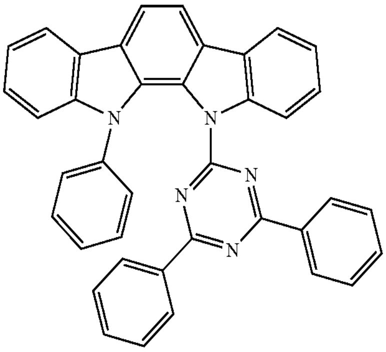

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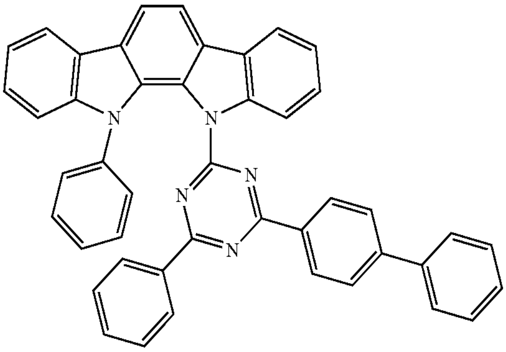

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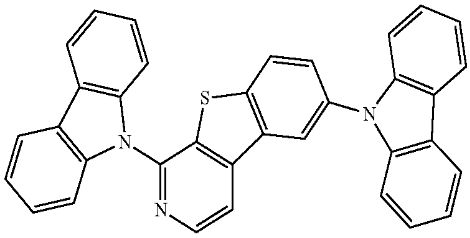

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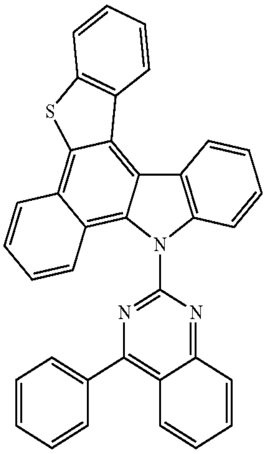

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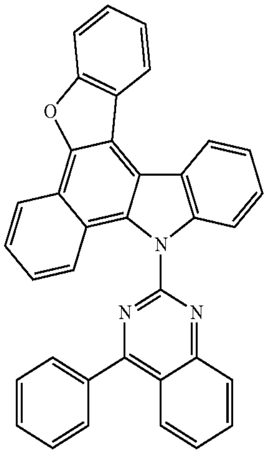

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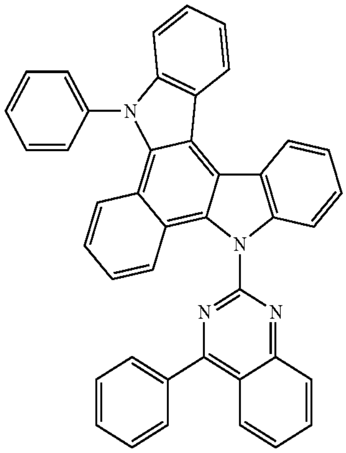

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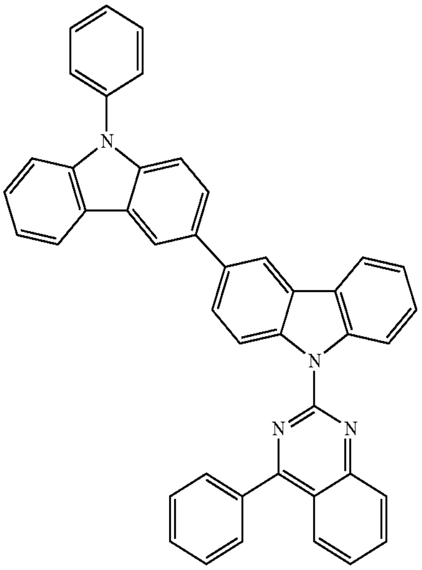

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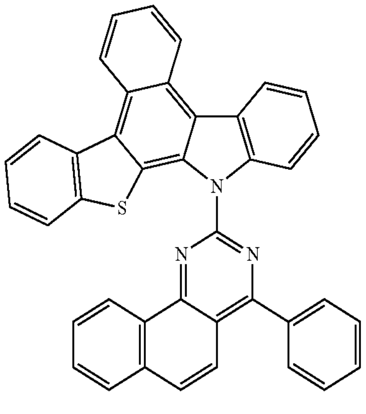

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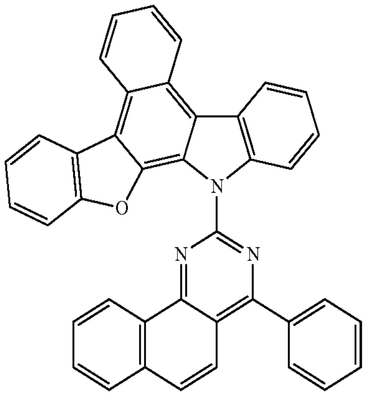

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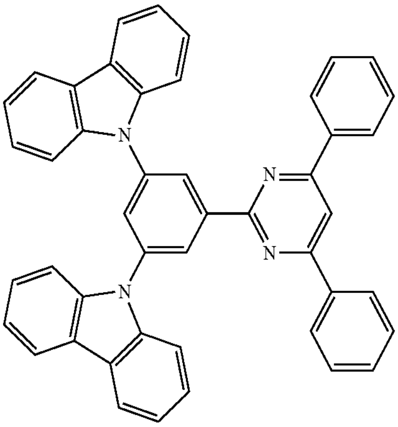

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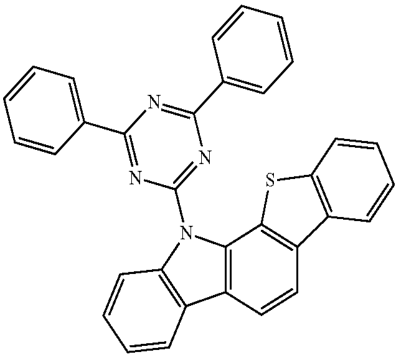

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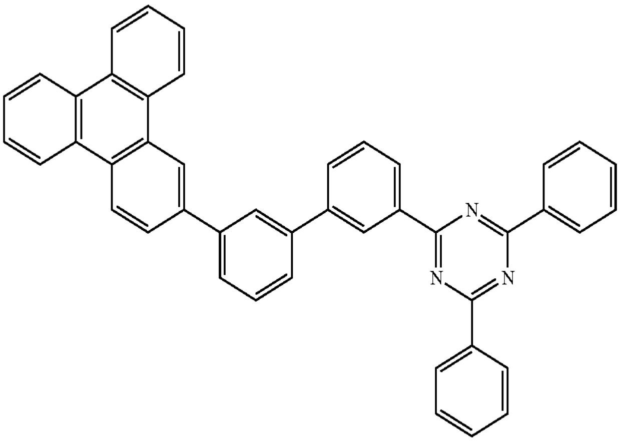

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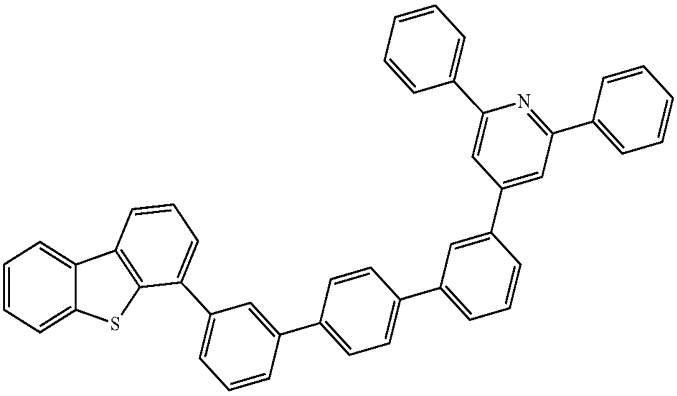

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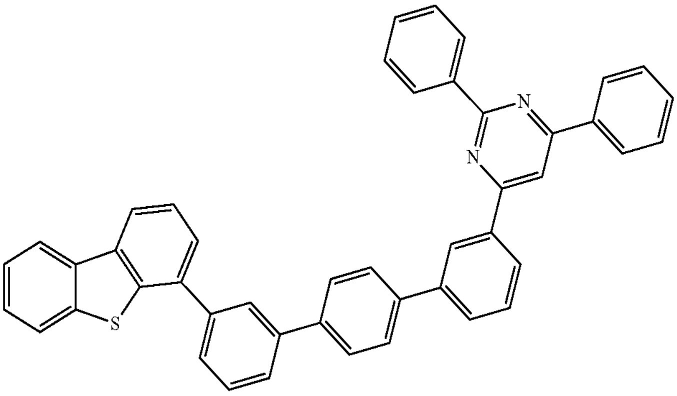

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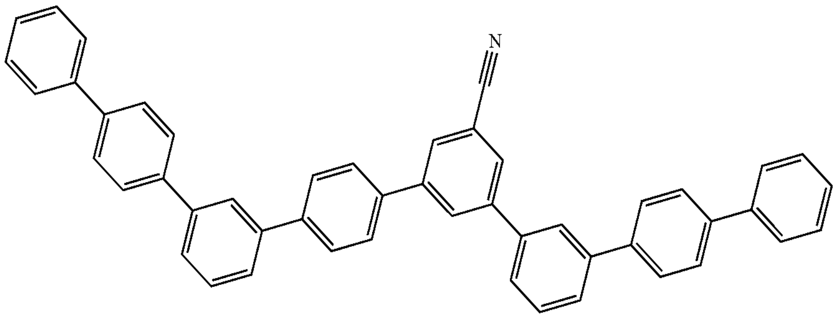

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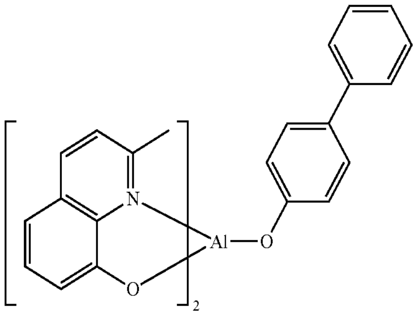

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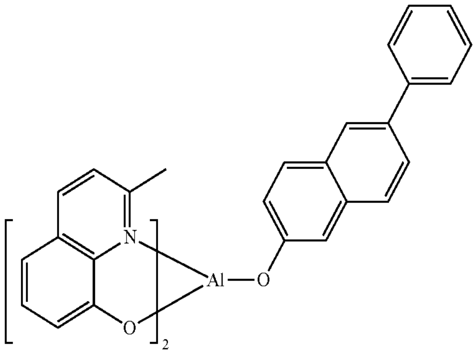

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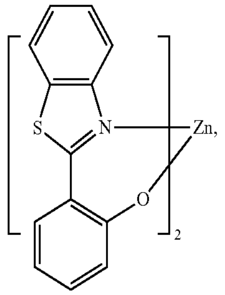

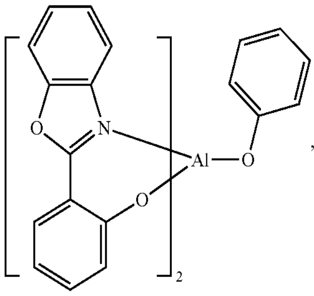

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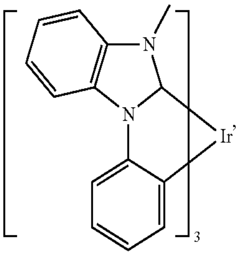

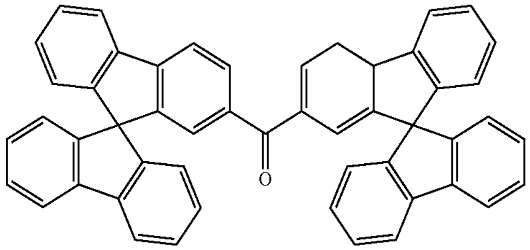

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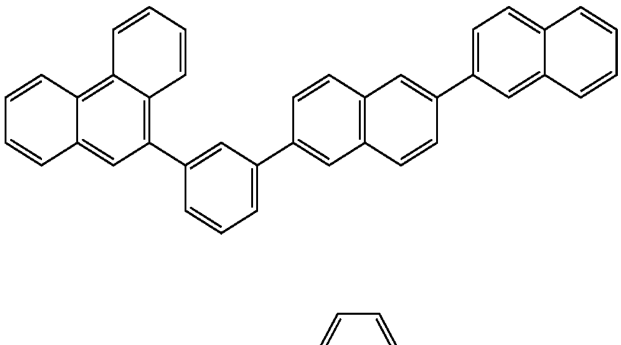

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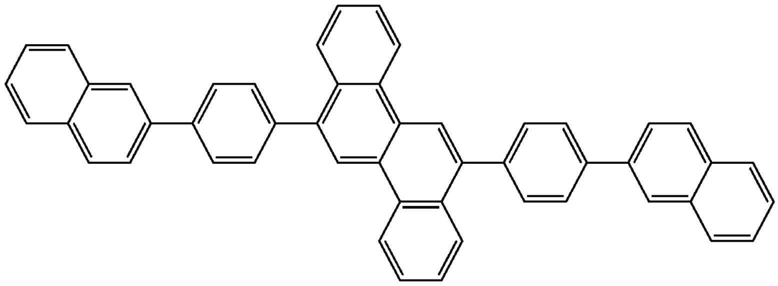

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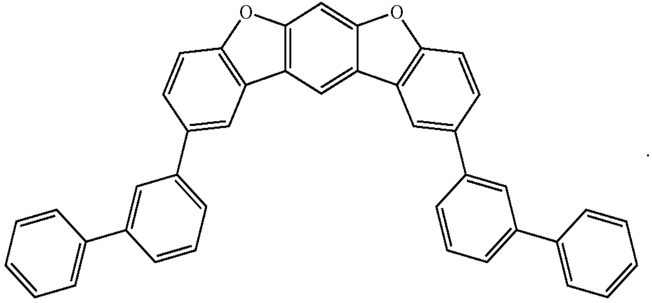
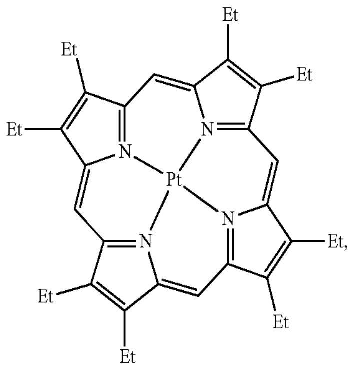
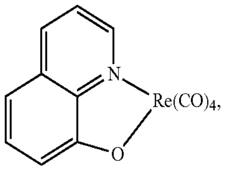


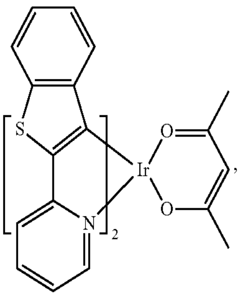
Emitter:

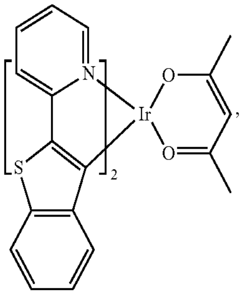
[0128] An emitter example is not particularly limited, and any compound may be used as long as the compound is typically used as an emitter material. Examples of suitable emitter materials include, but are not limited to, compounds which can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, i.e., TADF (also referred to as E-type delayed fluorescence; see, e.g., U.S. application Ser. No. 15/700,352, which is hereby incorporated by reference in its entirety), triplet-triplet annihilation, or combinations of these processes. In some embodiments, the emissive dopant can be a racemic mixture, or can be enriched in one enantiomer.

[0129] Non-limiting examples of the emitter materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103694277, CN1696137, EB01238981, EP01239526, EP01961743, EP1239526, EP1244155, EP1642951, EP1647554, EP1841834, EP1841834B, EP2062907, EP2730583, JP2012074444, JP2013110263, JP4478555, KR1020090133652, KR20120032054, KR20130043460, TW201332980, U.S. Ser. No. 06/699,599, U.S. Ser. No. 06/916,554, US20010019782, US20020034656, US20030068526, US20030072964, US20030138657, US20050123788, US20050244673, US2005123791, US2005260449, US20060008670, US20060065890, US20060127696, US20060134459, US20060134462, US20060202194, US20060251923, US20070034863, US20070087321, US20070103060, US20070111026, US20070190359, US20070231600, US2007034863, US2007104979, US2007104980, US2007138437, US2007224450, US2007278936, US20080020237, US20080233410, US20080261076, US20080297033, US200805851, US2008161567, US2008210930, US20090039776, US20090108737, US20090115322, US20090179555, US2009085476, US2009104472, US20100090591, US20100148663, US20100244004, US20100295032, US2010102716, US2010105902, US2010244004, US2010270916, US20110057559, US20110108822, US20110204333, US2011215710, US2011227049, US2011285275, US2012292601, US20130146848, US2013033172, US2013165653, US2013181190, US2013334521, US20140246656, US2014103305, U.S. Pat. Nos. 6,303,238, 6,413,656, 6,653,654, 6,670,645, 6,687,266, 6,835,469, 6,921,915, 7,279,704, 7,332,232, 7,378,162, 7,534,505, 7,675,228, 7,728,137, 7,740,957, 7,759,489, 7,951,947, 8,067,099, 8,592,586, 8,871,361, WO06081973, WO06121811, WO07018067, WO07108362, WO07115970, WO07115981, WO08035571, WO2002015645, WO2003040257, WO2005019373, WO2006056418, WO2008054584, WO2008078800, WO2008096609, WO2008101842, WO2009000673, WO2009050281, WO2009100991, WO2010028151, WO2010054731, WO2010086089, WO2010118029, WO2011044988, WO2011051404, WO2011107491, WO2012020327, WO2012163471, WO2013094620, WO2013107487, WO2013174471, WO2014007565, WO2014008982, WO2014023377, WO2014024131, WO2014031977, WO2014038456, WO2014112450,









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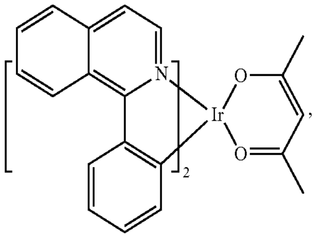

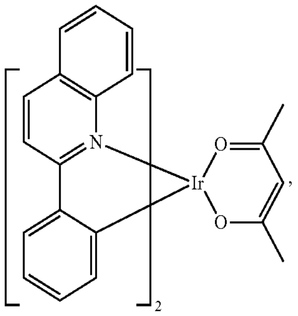

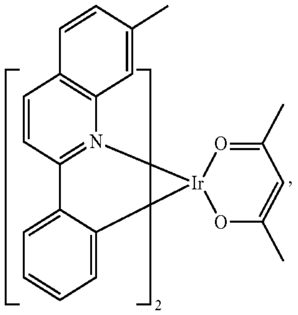

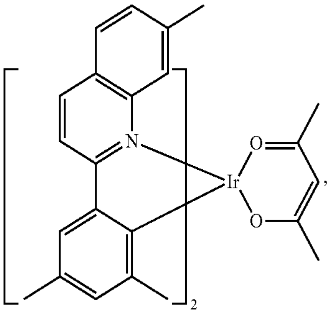

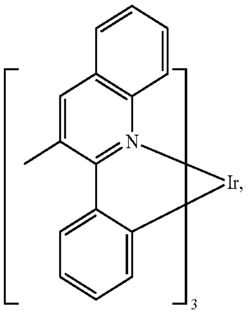

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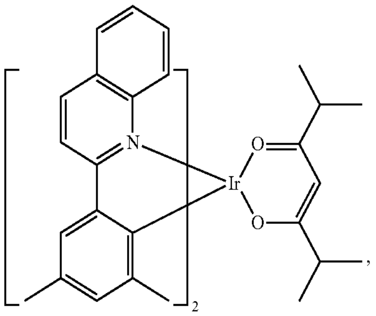

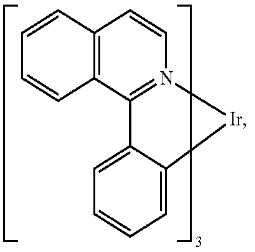

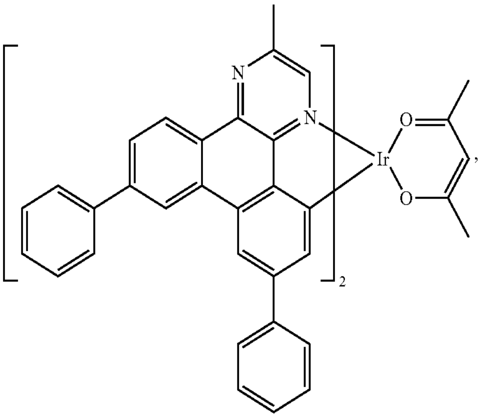

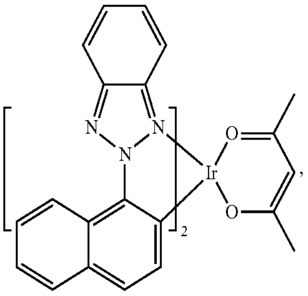

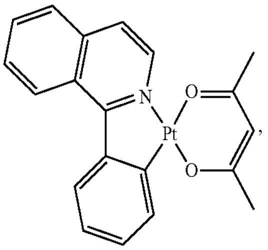

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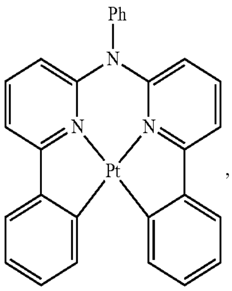

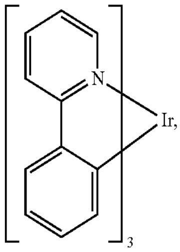

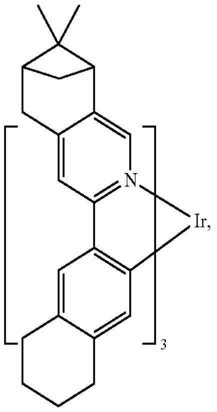

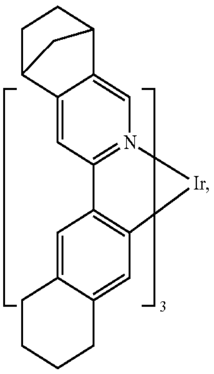

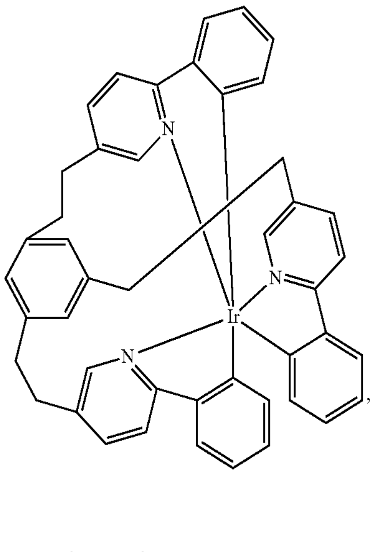

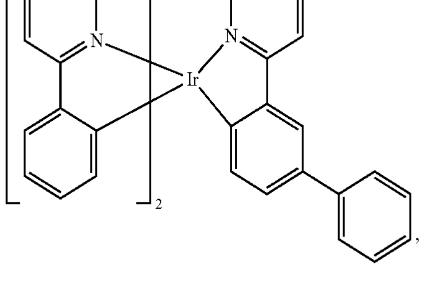

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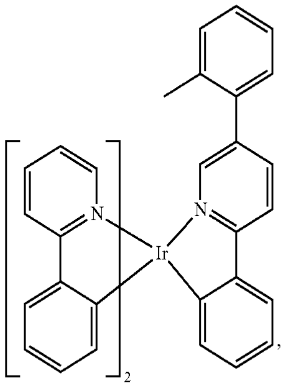

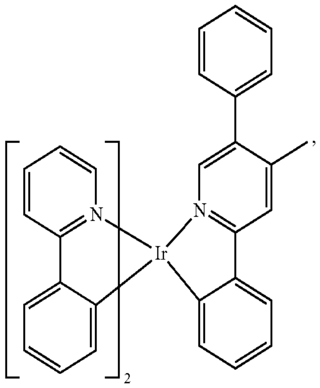

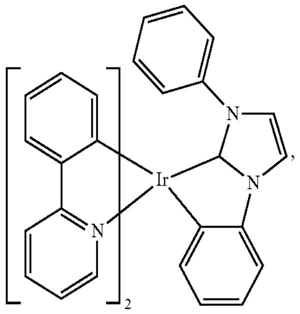

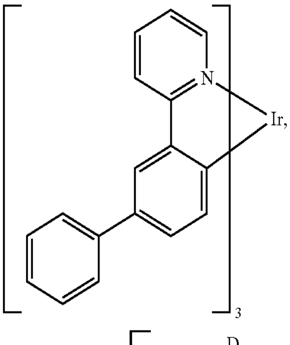

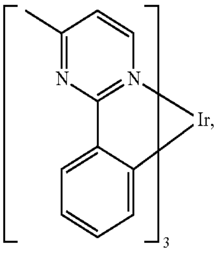

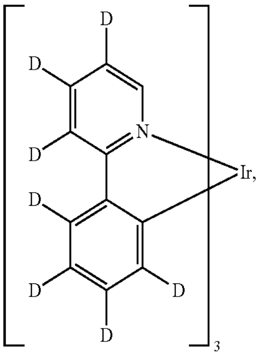

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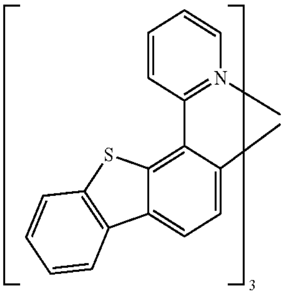

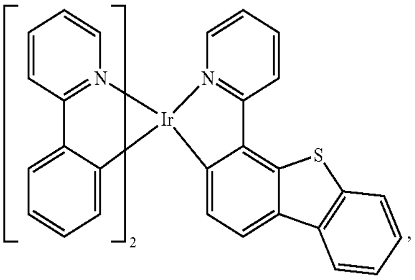

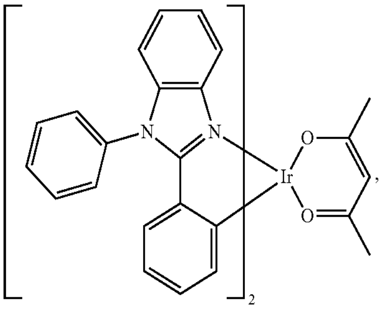

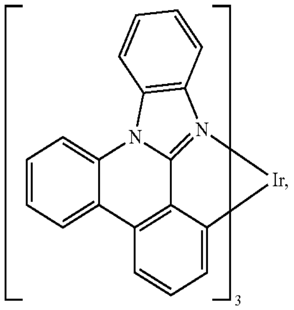

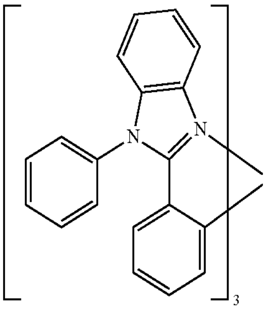

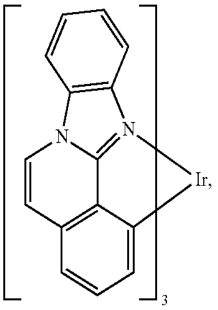

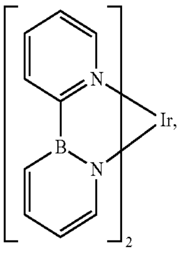

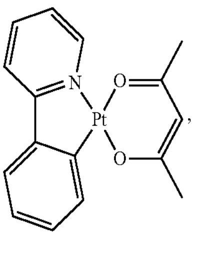

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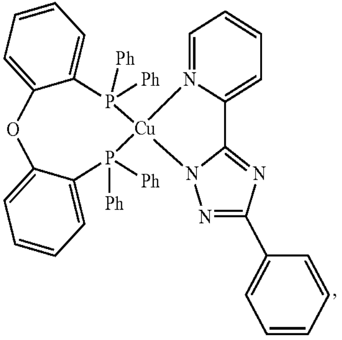

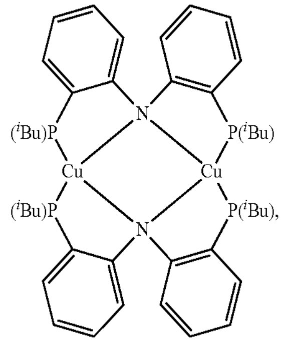

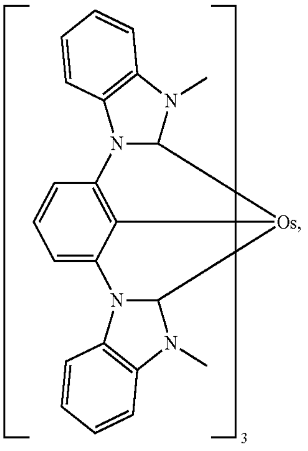

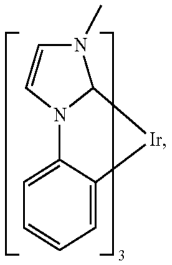

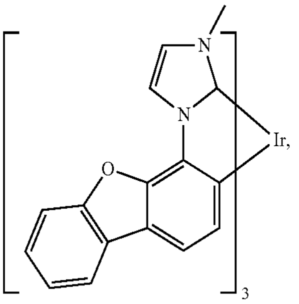

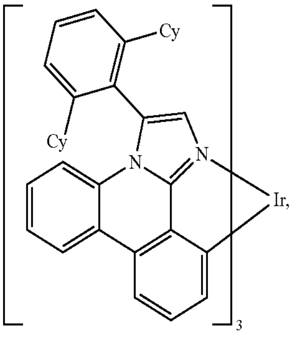

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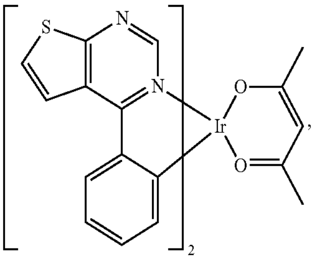

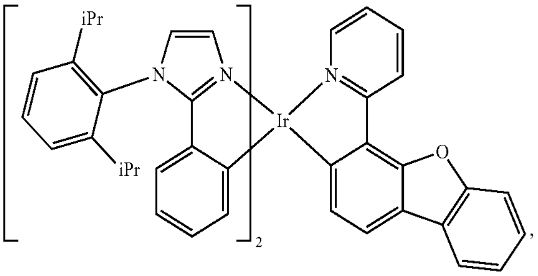

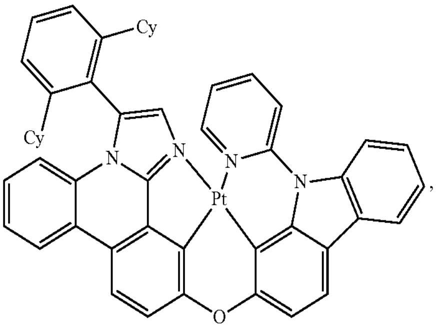

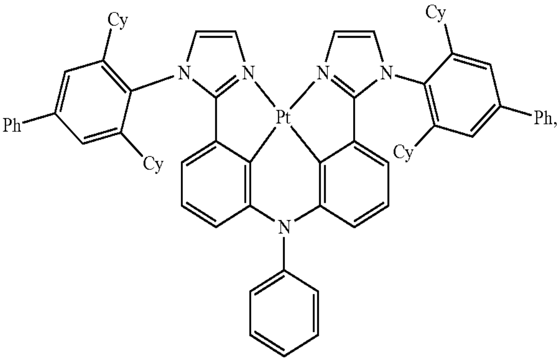

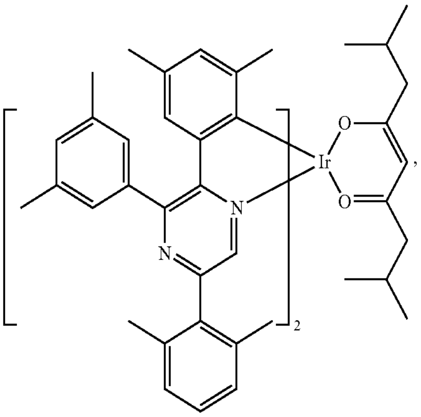

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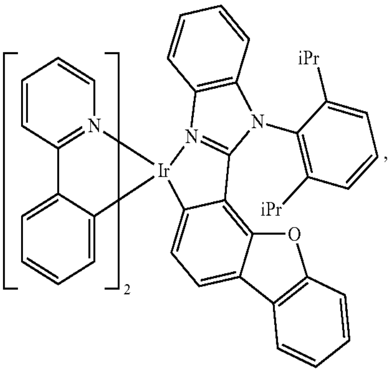

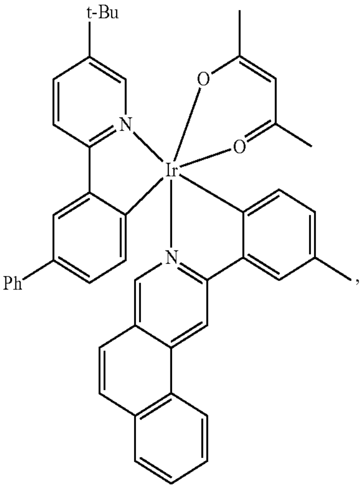

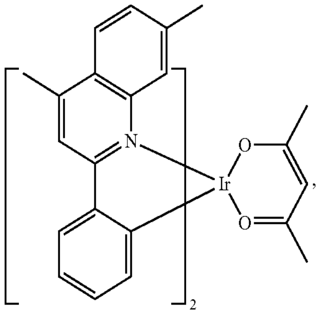

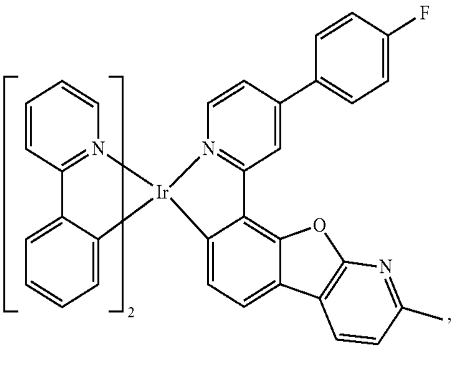

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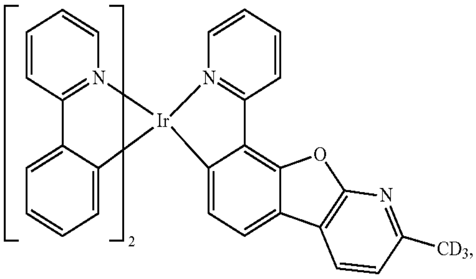

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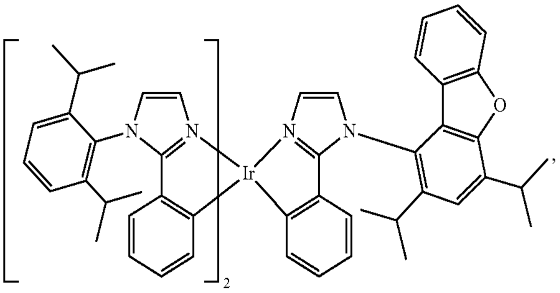

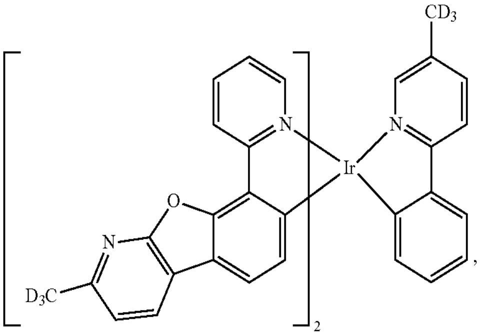

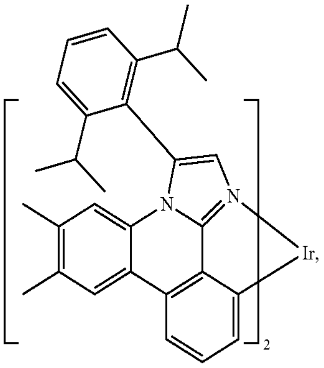

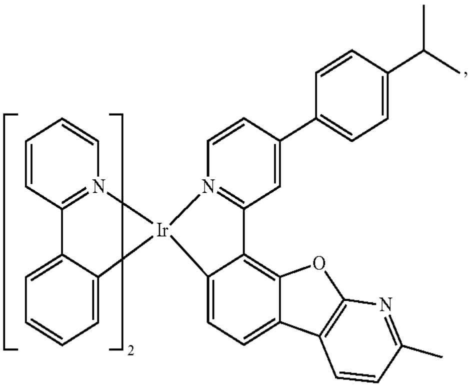

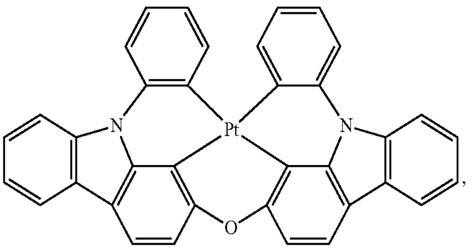

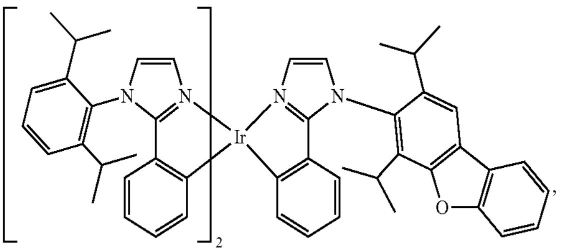

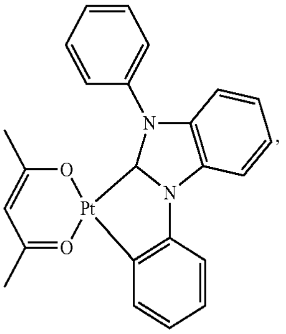

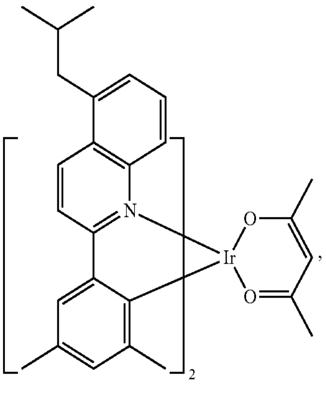

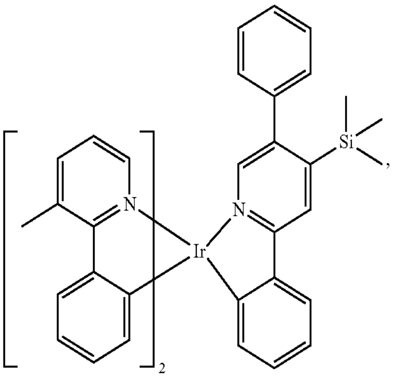

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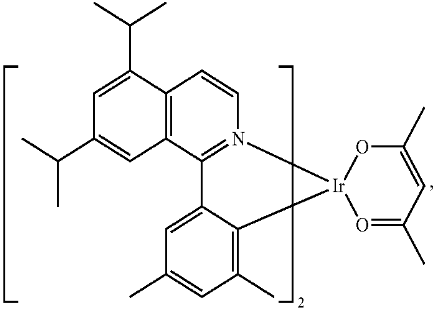

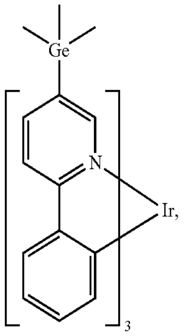

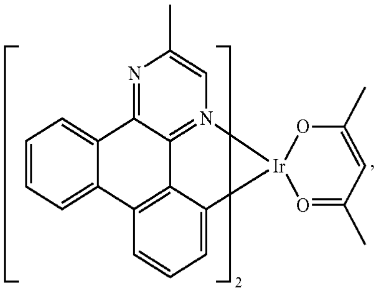

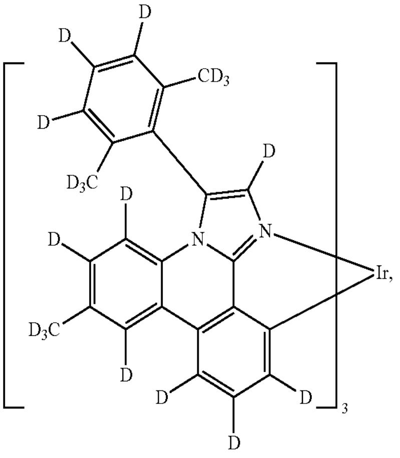

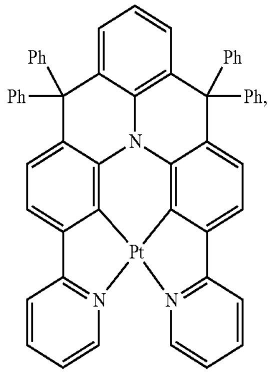

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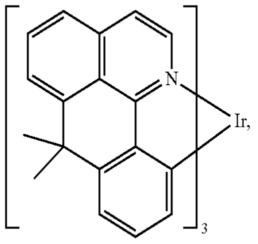

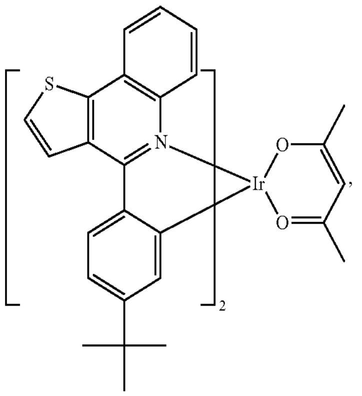

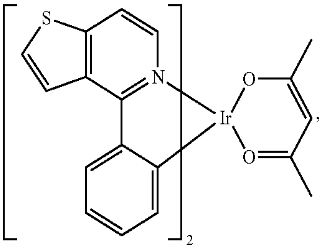

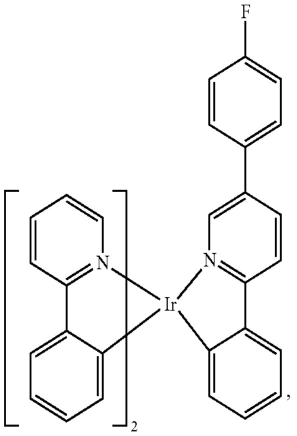

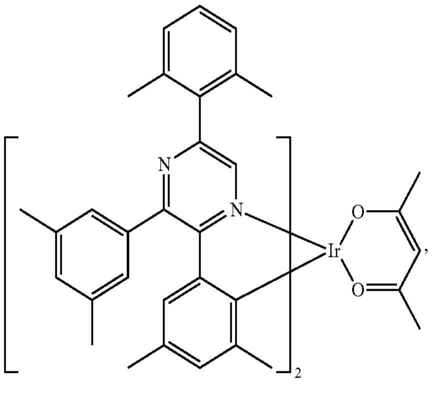

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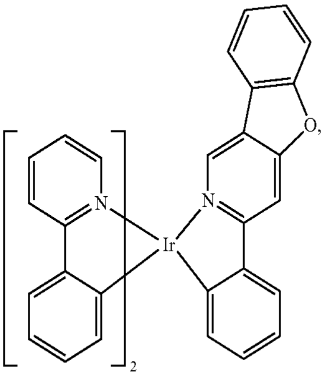

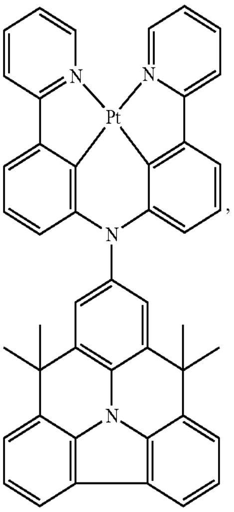

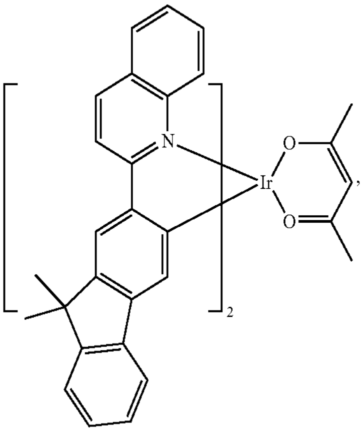

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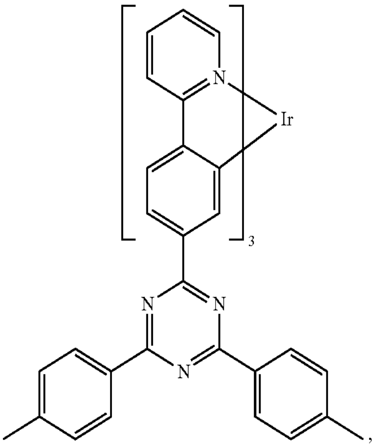

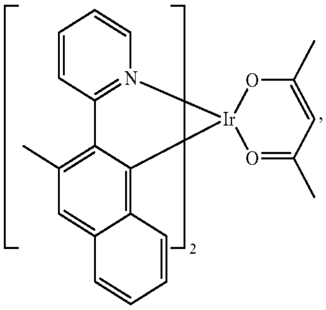

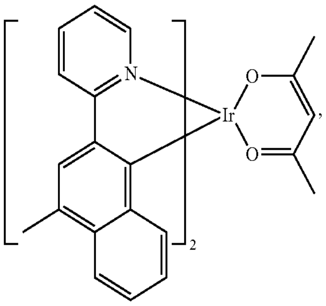

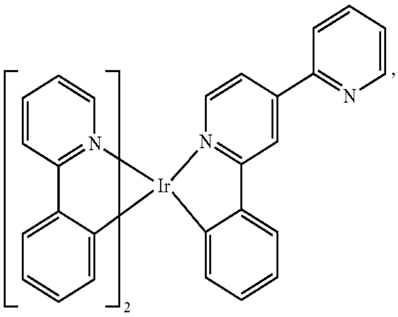

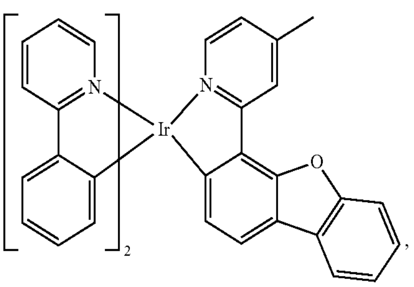

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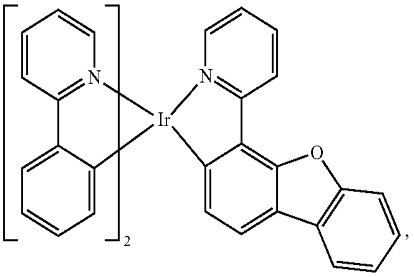

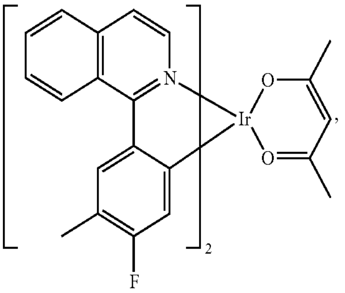

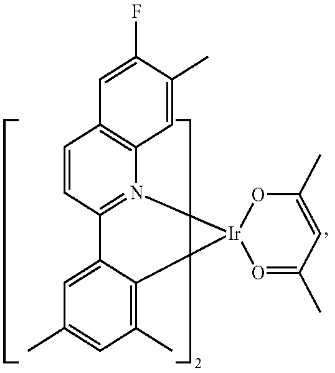

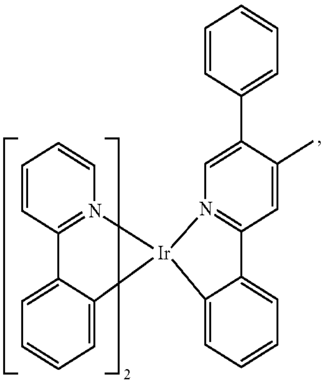

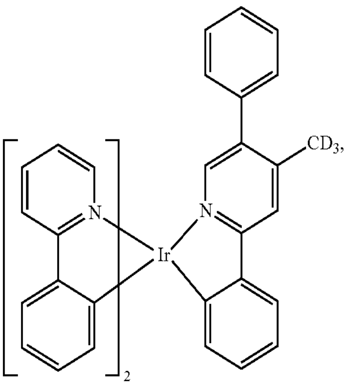

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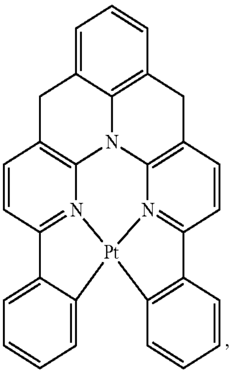

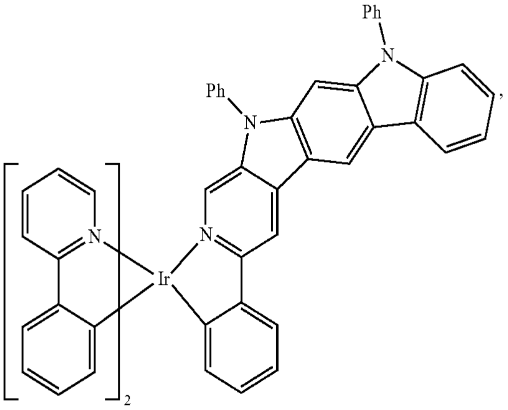

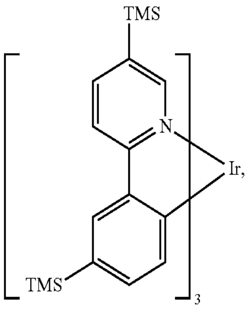

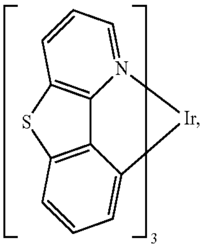

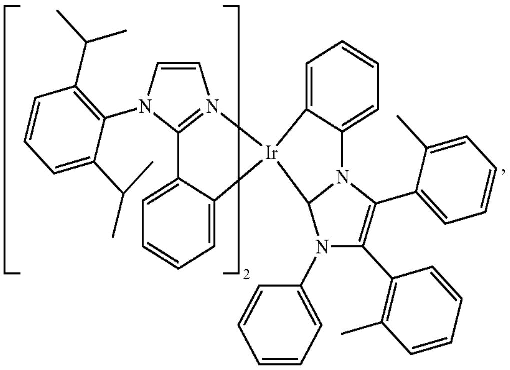

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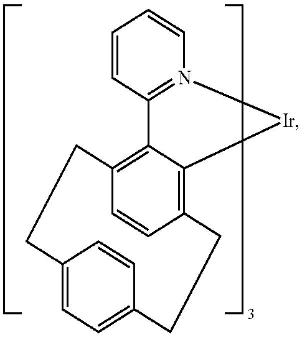

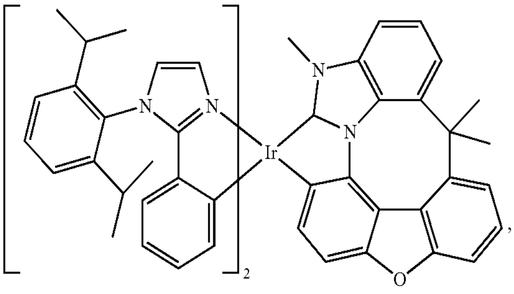

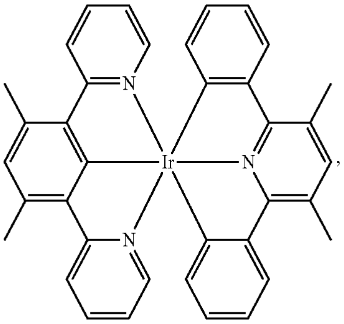

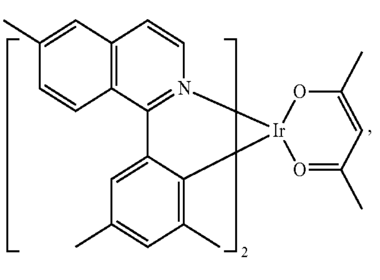

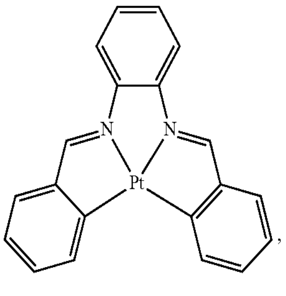

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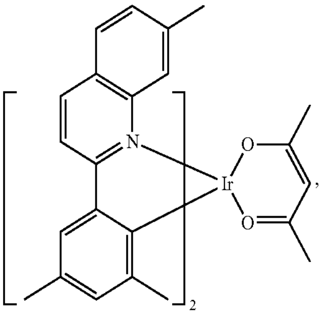

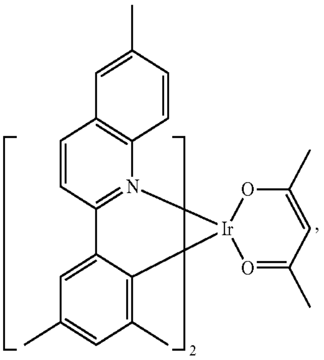

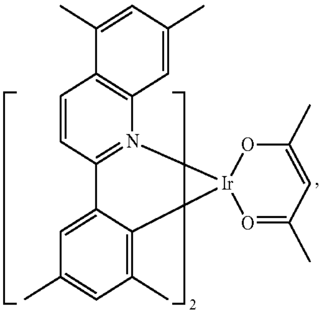

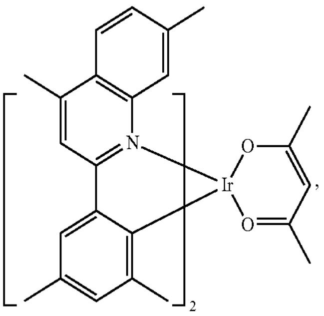

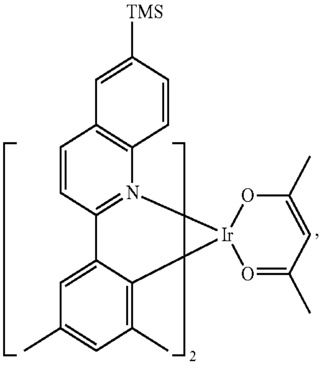

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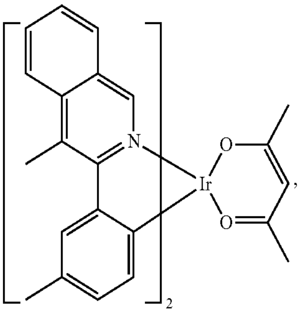

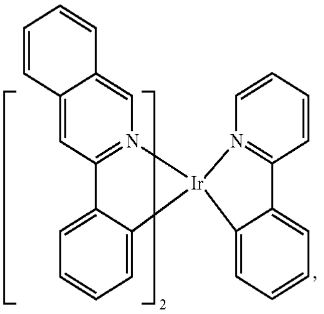

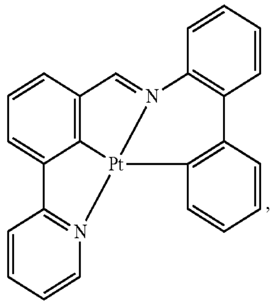

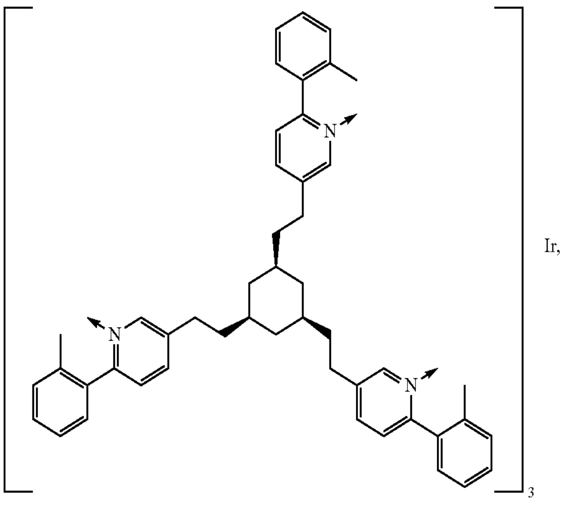

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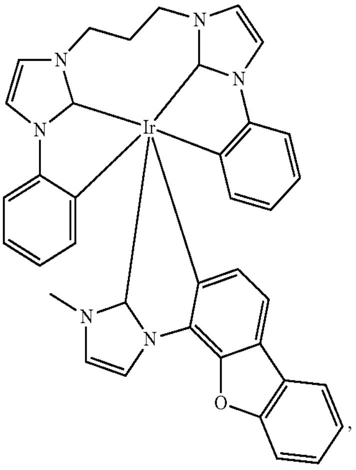

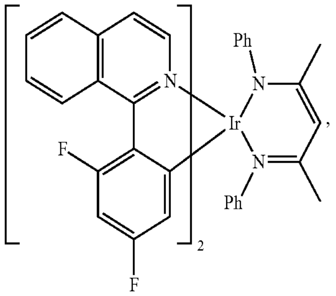

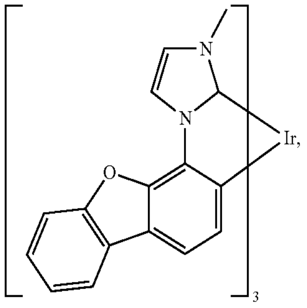

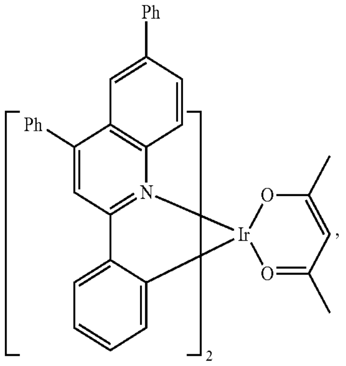

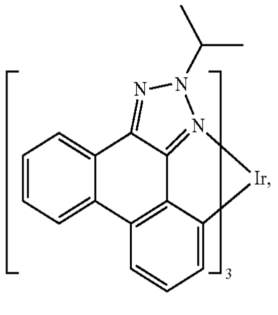

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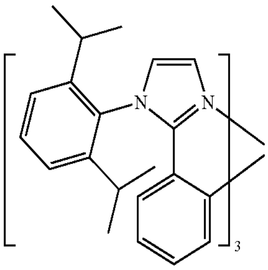

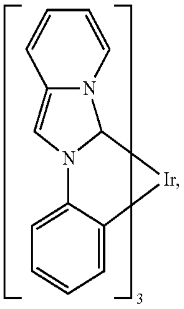

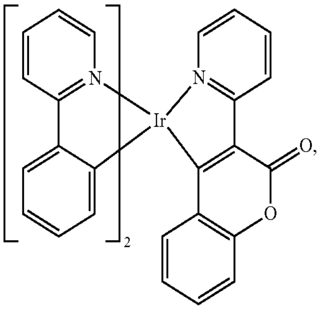

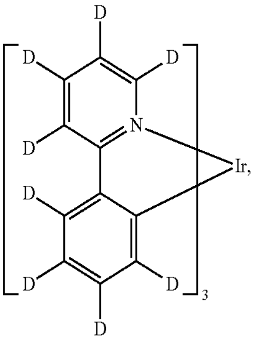

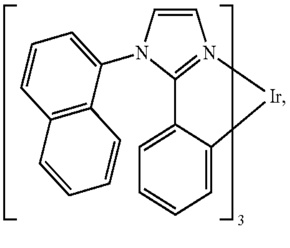

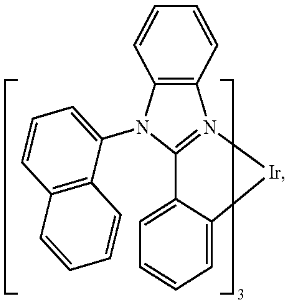

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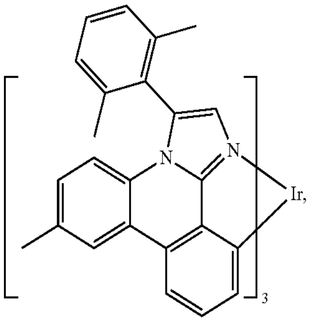

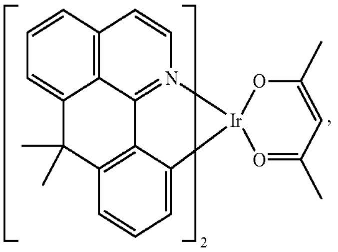

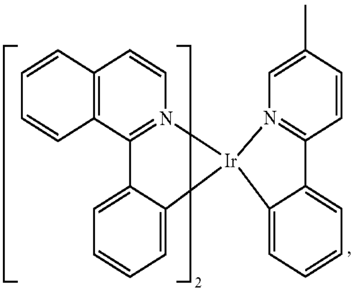

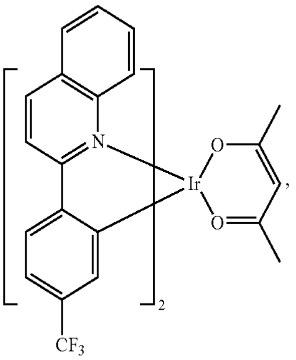

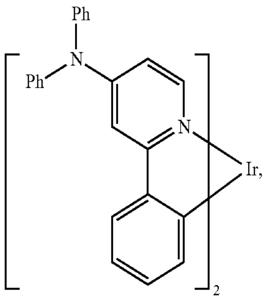

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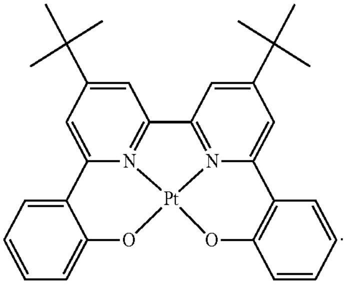
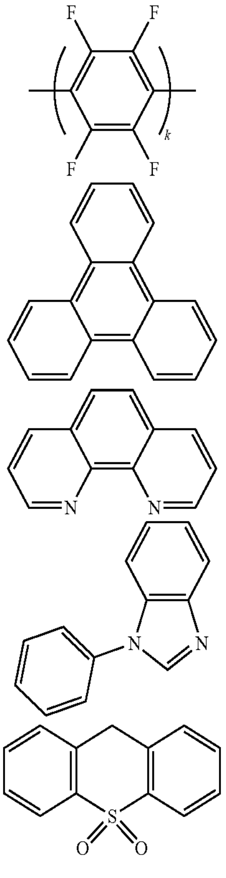


[0130] A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies and/or longer lifetime as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the HBL material has a lower HOMO (further from the vacuum level) and or higher triplet energy than the emitter closest to the HBL interface. In some embodiments, the HBL material has a lower HOMO (further from the vacuum level) and or higher triplet energy than one or more of the hosts closest to the HBL interface.

[0131] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

[0132] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:



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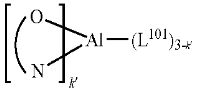
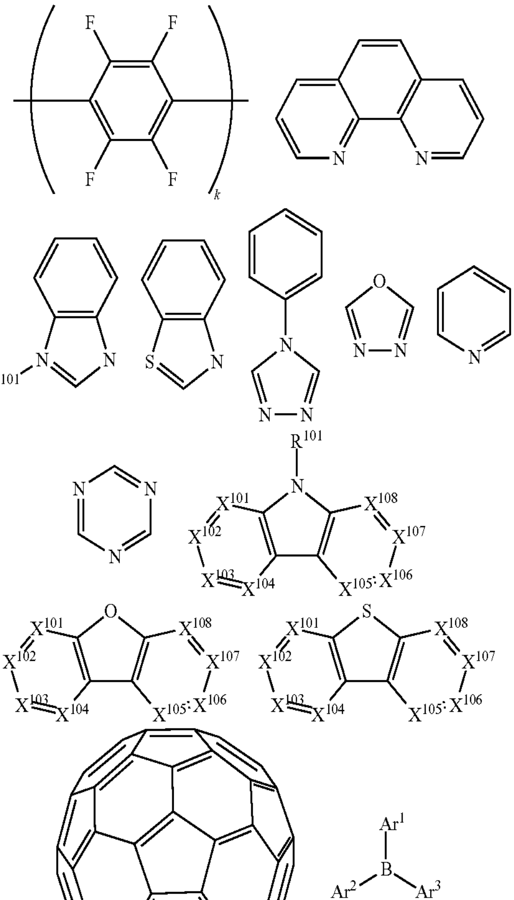


wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

ETL:

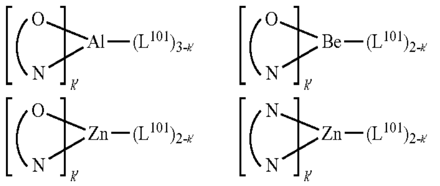
[0133] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

[0134] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:



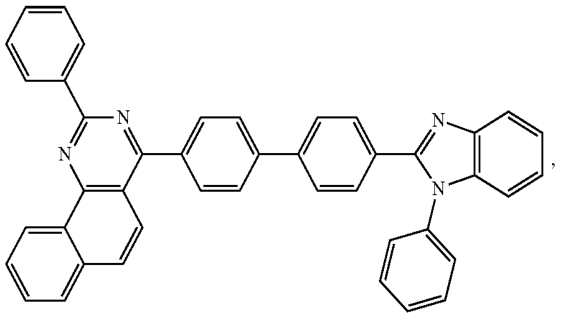
wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile,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

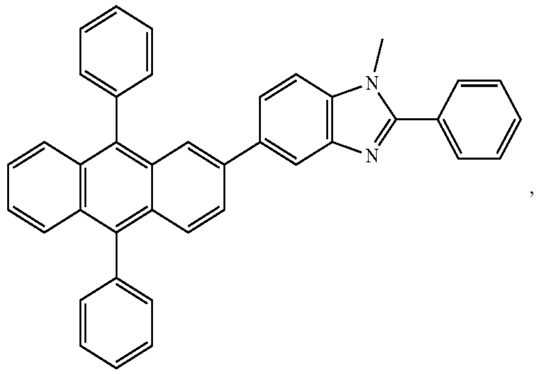
[0135] In another aspect, the metal complexes used in ETL include, but are not limited to the following general formula:



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

[0136] Non-limiting examples of the ETL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103508940, EP01602648, EP01734038, EP01956007, JP2004-022334, JP2005149918, JP2005-268199, KR0117693, KR20130108183, US20040036077, US20070104977, US2007018155, US20090101870, US20090115316, US20090140637, US20090179554, US2009218940, US2010108990, US2011156017, US2011210320, US2012193612, US2012214993, US2014014925, US2014014927, US20140284580, U.S. Pat. Nos. 6,656,612, 8,415,031, WO2003060956, WO2007111263, WO2009148269, WO2010067894, WO2010072300, WO2011074770, WO2011105373, WO2013079217, WO2013145667 WO2013180376, WO2014104499, WO2014104535





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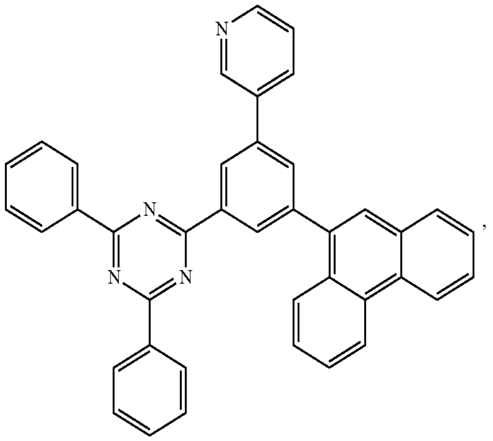

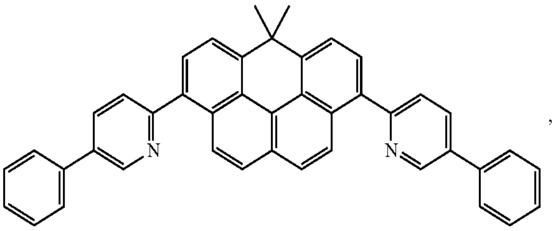

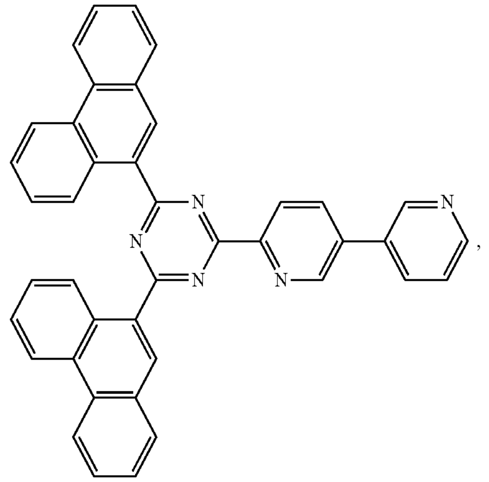

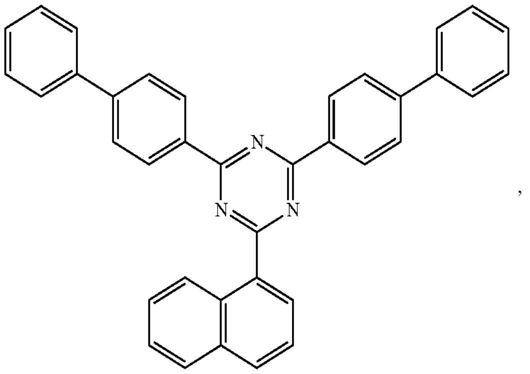

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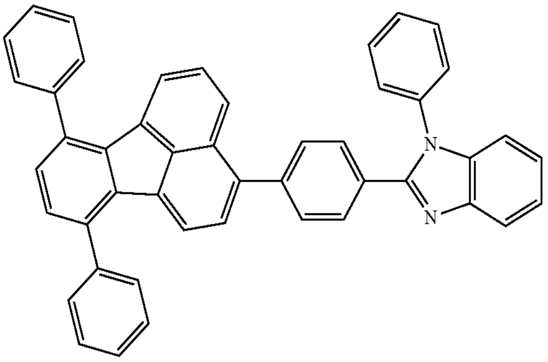

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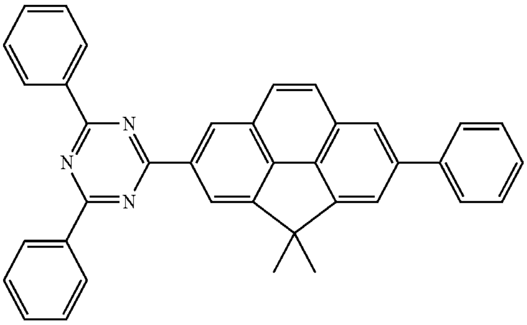

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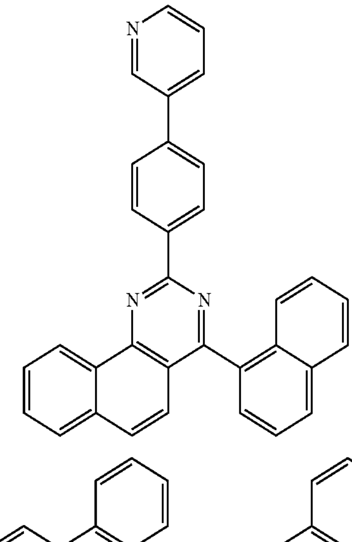

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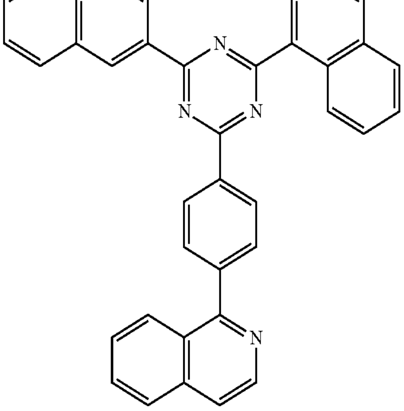

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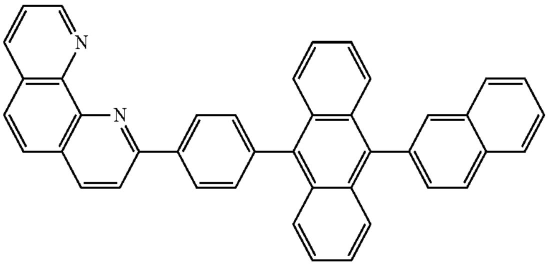

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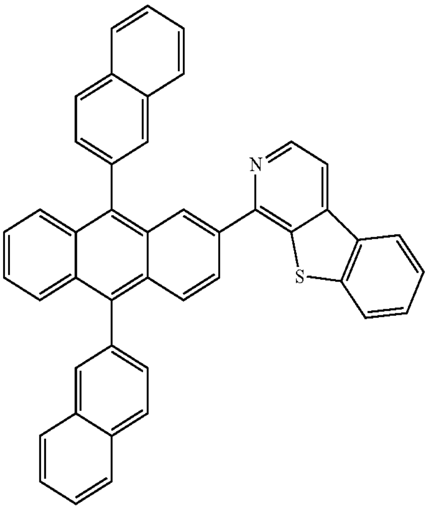

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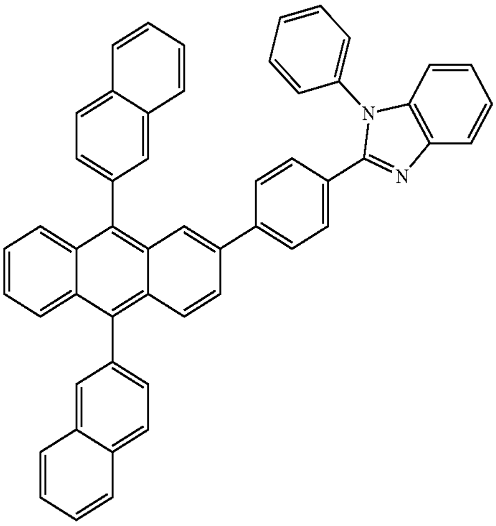

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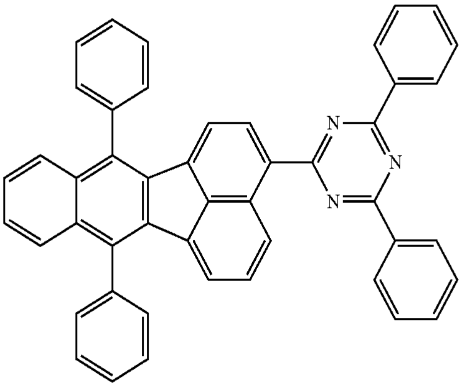

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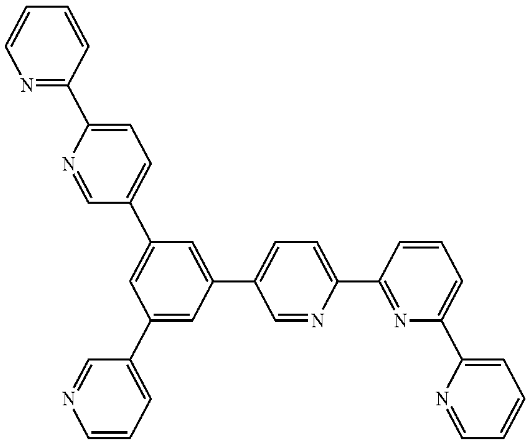

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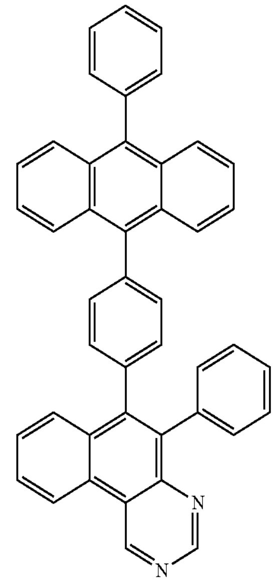

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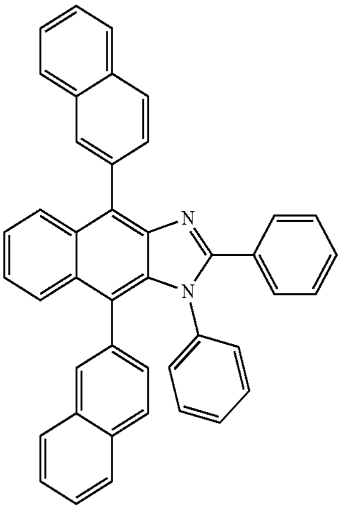

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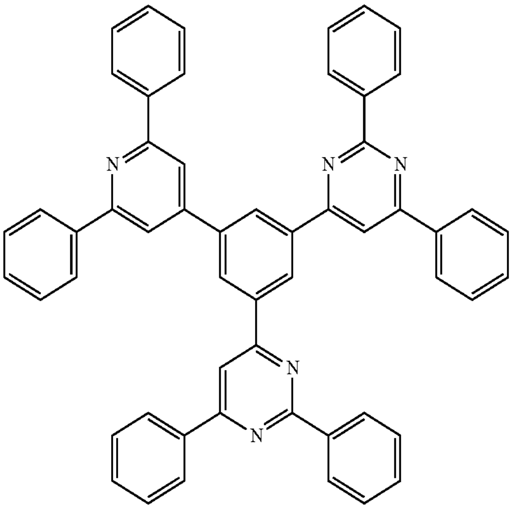

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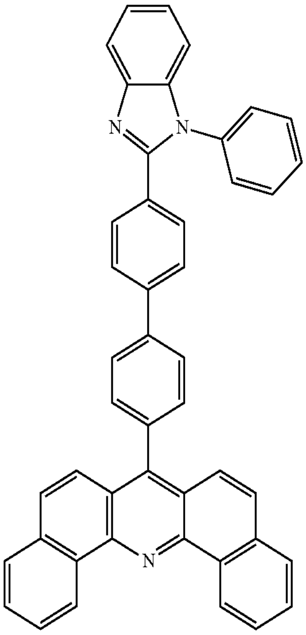

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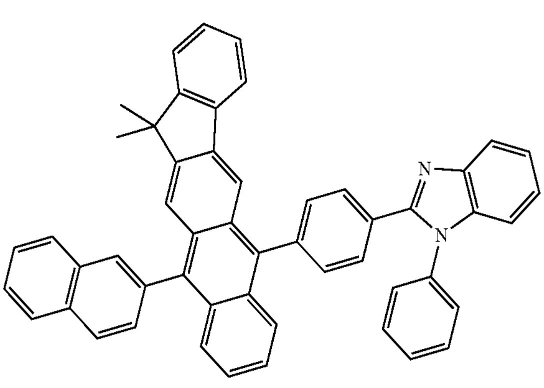

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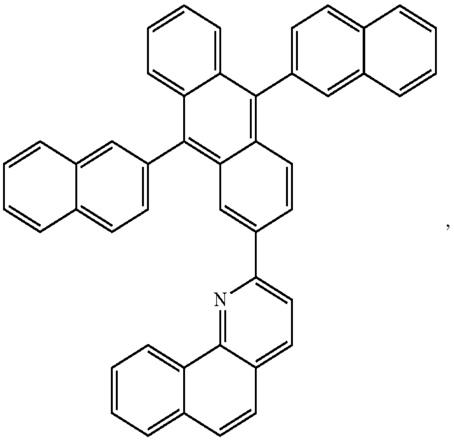

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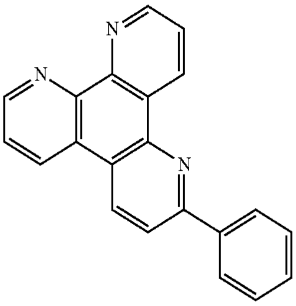

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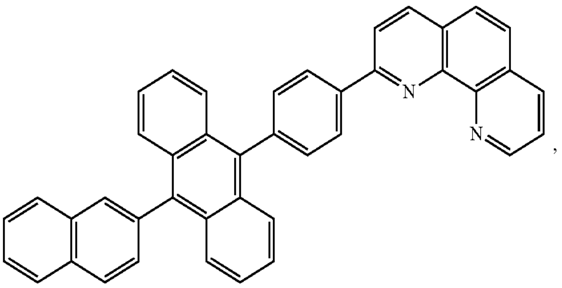

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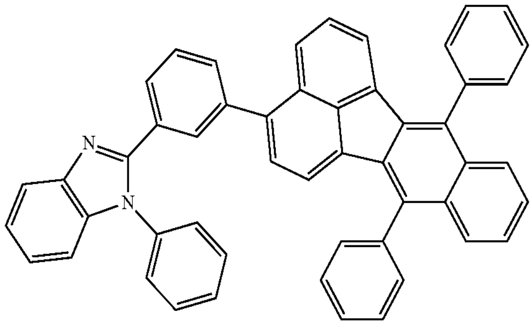

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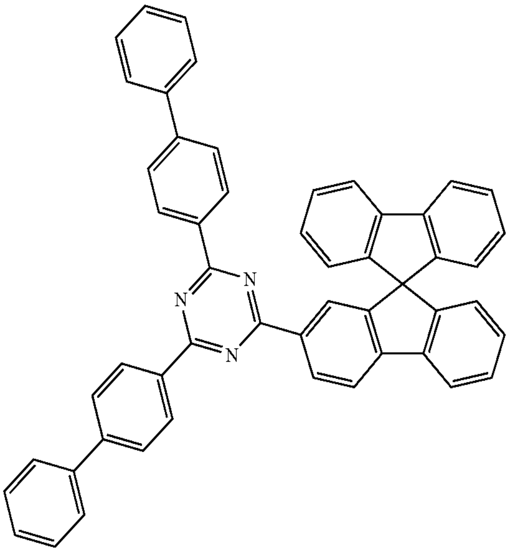

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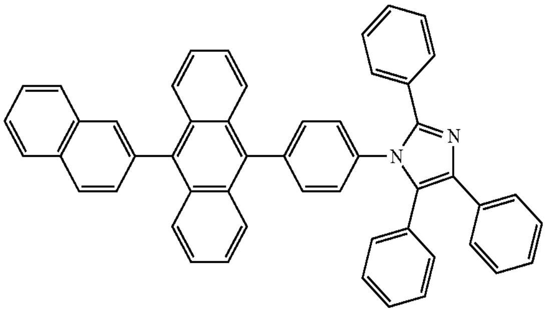

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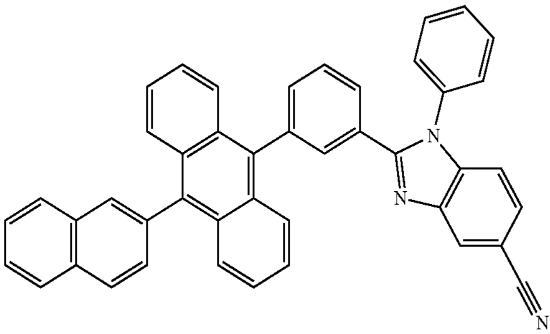

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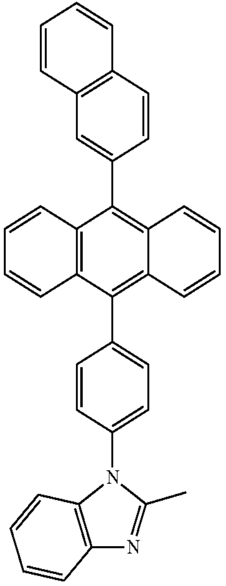

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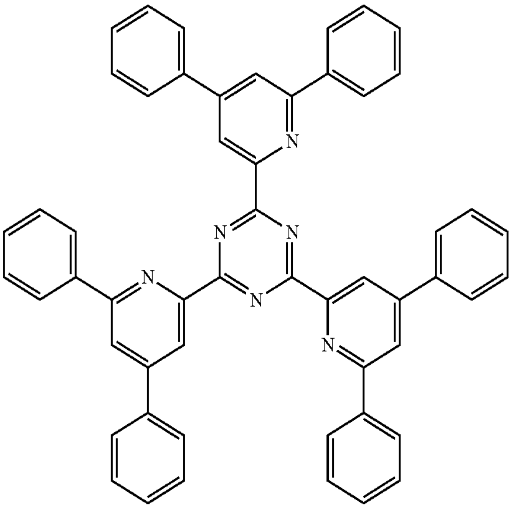

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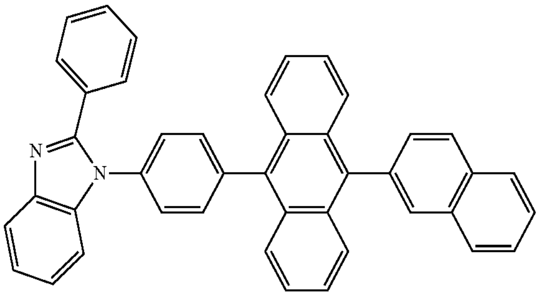

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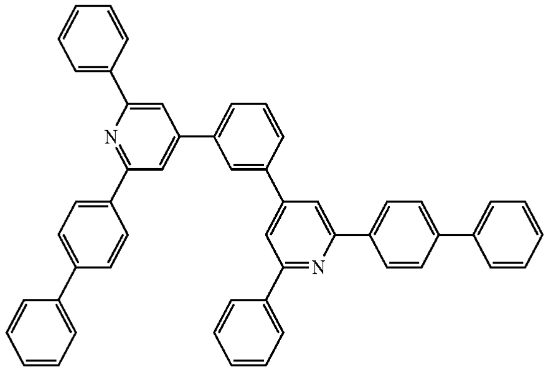

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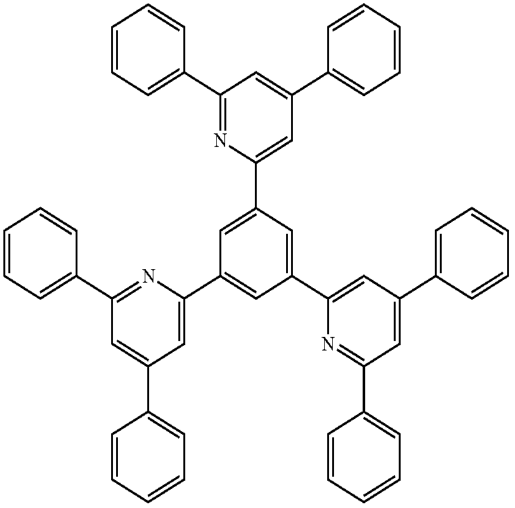

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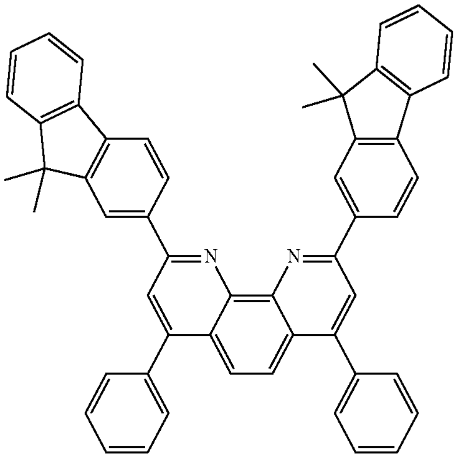

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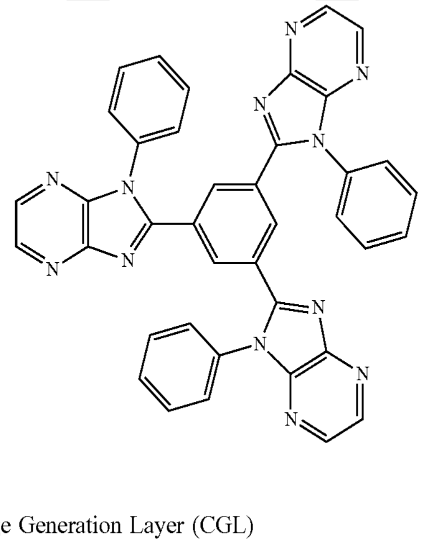

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Charge Generation Layer (CGL)

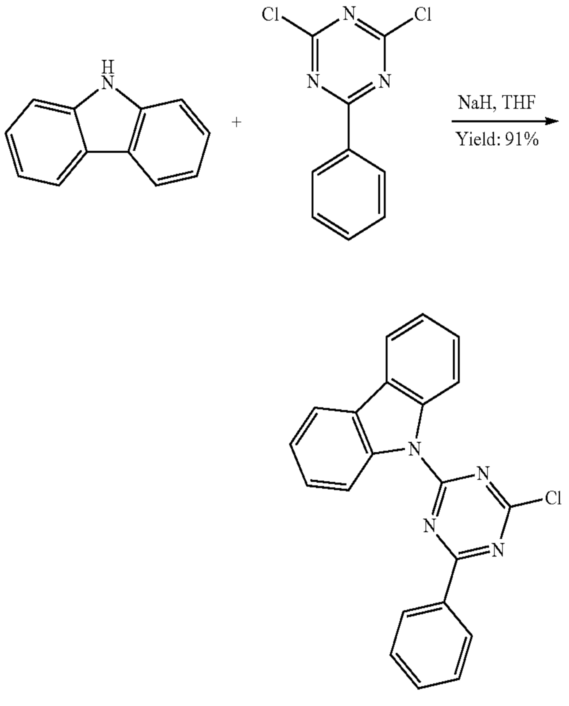
[0137] In tandem or stacked OLEDs, the CGL plays an essential role in the performance, which is composed of an n-doped layer and a p-doped layer for injection of electrons and holes, respectively. Electrons and holes are supplied from the CGL and electrodes. The consumed electrons and holes in the CGL are refilled by the electrons and holes injected from the cathode and anode, respectively; then, the bipolar currents reach a steady state gradually. Typical CGL materials include n and p conductivity dopants used in the transport layers.

[0138] 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.

EXPERIMENTAL

Synthesis of 9-(4-chloro-6-phenyl-1,3,5-triazin-2-yl)-9H-carbazole

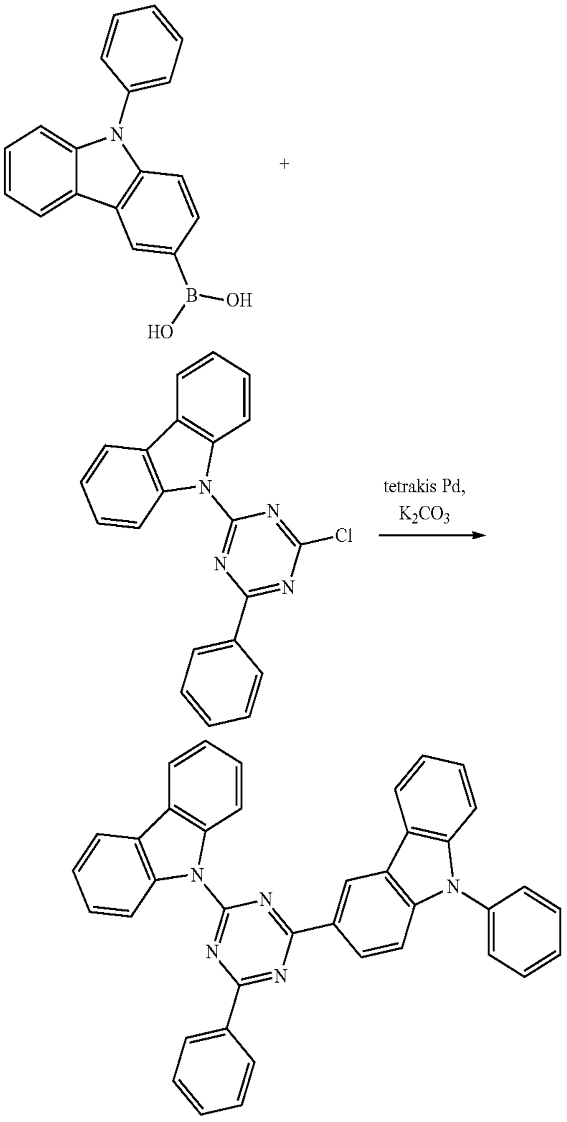
[0139]



[0140] H-carbazole (5.0 g, 22.1 mmol) was added to a dry 500 mL round bottom flask (RBF) under argon atmosphere in tetrahydrofuran (THF)(120 mL) and stirred for 5 minutes to obtain a slurry. Sodium hydride (1.359 g, 22.1 mmol) was added portion wise. The reaction mixture turned a light orange color, then a solution of 2,4-dichloro-6-phenyl-1,3,5-triazine (6.75 g, 22.1 mmol) in THF (10 mL) was added slowly over 2 minutes. The resulting reaction mixture was stirred at 25° C. for 2 hours. The reaction mixture was cooled to 0° C. and treated with water (20 ml), the aqueous layer was separated, and the organic layer was treated with deionized-water (50 mL). Upon stirring, an off-white precipitate was observed. The stirring was continued for 30 minute and solids were filtered using a filter funnel under vacuum to obtain a dry cake. The solids were washed several times with water and dried using lyophilizer for 24 hours to give 9-(4-chloro-6-phenyl-1,3,5-triazin-2-yl)-9H-carbazole (7.2 g, 91% yield).

Synthesis of 3-(4-(9H-carbazol-9-yl)-6-phenyl-1,3,5-triazin-2-yl)-9-phenyl-9H-carbazole

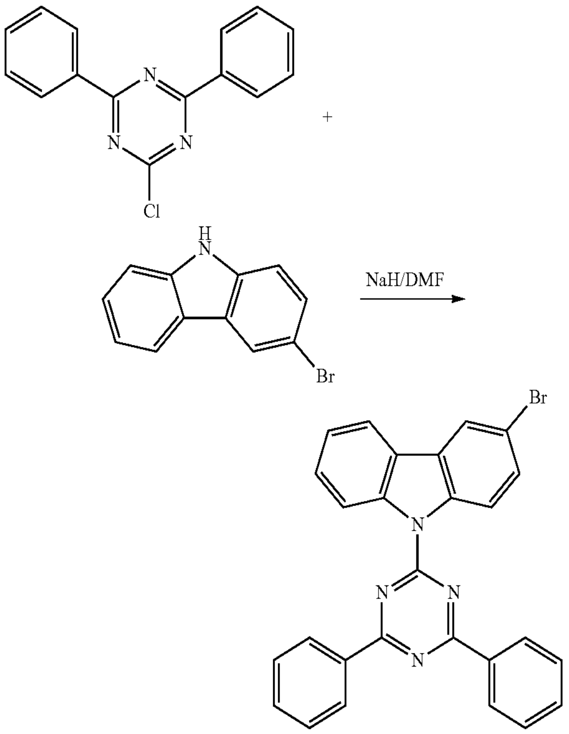
[0141]



[0142] A solution of 9-(4-chloro-6-phenyl-1,3,5-triazin-2-yl)-9H-carbazole (5.0 g, 14.09 mmol), (9-phenyl-9H-carbazol-3-yl) boronic acid (4.83 g, 16.82 mmol), potassium carbonate (5.81 g, 42.02 mmol), in THF (120 ml) and water (14 ml) was prepared and placed under argon atmosphere with a reflux condenser. The reaction mixture was bubbled with argon for 10 minutes, then tetrakis(triphenylphosphine) palladium(0) (Tetrakis Pd) (0.81, 0.701 mmol) was added and argon bubbling continued for 5 more minutes. The reaction mixture was heated to reflux 82° C. for 12 hours. The reaction mixture was cooled to room temperature (~22° C.) and water (50 mL) was added. The solid product was then filtered off and washed with water (50 mL) and dried in lyophilizer to give 3-(4-(9H-carbazol-9-yl)-6-phenyl-1,3,5-triazin-2-yl)-9-phenyl-9H-carbazole as a pale-yellow solid (6.4 g, 81% yield).

Synthesis of 3-bromo-9-(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole

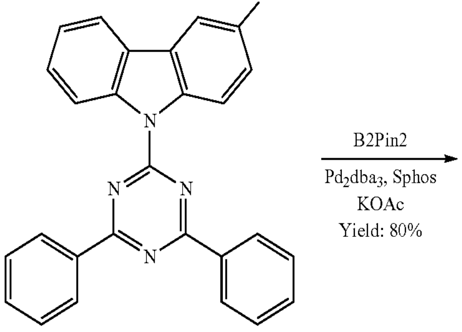
[0143]



[0144] 3-bromo-9H-carbazole (10.0 g, 40.6 mmol) was added to a dry 100 mL RBF under argon atmosphere in THF (200 mL) and stirred for 5 minutes to obtain a slurry. Sodium hydride (1.79 g, 44.7 mmol) was added portion wise, which caused the reaction mixture to turn into a light orange solution. As solution of 2-chloro-4,6-diphenyl-1,3,5-triazine (10.88 g, 40.6 mmol) in THF (20 mL) was added slowly over 2 minutes and the resulting reaction mixture was stirred at 25° C. for 2 hours. The reaction mixture was cooled to 0° C. and treated with water (20 ml). The aqueous layer was separated, and the organic layer was treated with deionized water (50 mL). Upon stirring for 30 minutes, an off-white precipitate was observed and the solids were filtered on filter funnel under vacuum to obtain a dry cake. The solids were washed several times with water and dried under lyophilizer for 24 hours to give 3-bromo-9-(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole (16.5 g, 85% yield).

Synthesis of 9-(4,6-diphenyl-1,3,5-triazin-2-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole

[0145]



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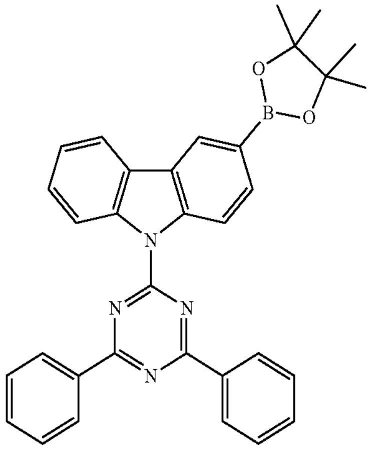
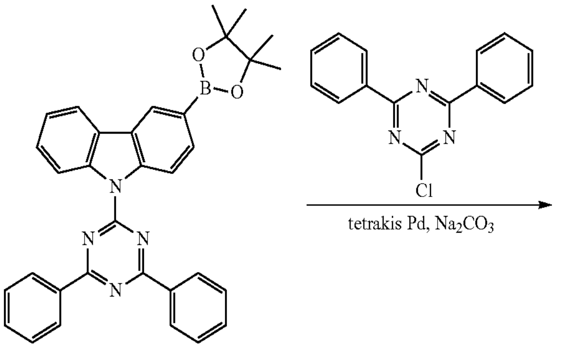


[0146] A dried RBF was charged with 3-bromo-9-(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole (10 g, 20.95 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane (6.38 g, 25.10 mmol) and potassium acetate (4.11 g, 41.90 mmol) in Dioxane (75 mL) was degassed and filled with argon, followed by addition of $Pd(OAc)_2$ (0.094 g, 0.42 mmol) and 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (SPhos) (0.039 g, 0.84 mmol). The resulting mixture was heated at 100° C. for 18 hours. After cooling to room temperature (~22° C.), the solids were precipitated out and the reaction was quenched by water then stirred vigorously for 2 hours. The solids were filtered using a filter funnel under vacuum to obtain a dry cake. The solids were washed several times with water and methanol, then dried under a lyophilizer for 24 hours to give the product 9-(4,6-diphenyl-1,3,5-triazin-2-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (8.85 g, 80%) as an off-white solid.

Synthesis of 3,9-bis(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole

[0147]



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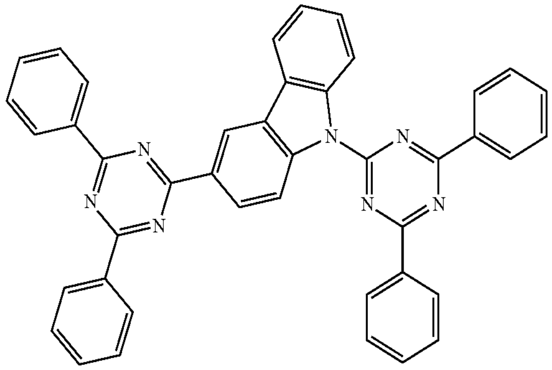
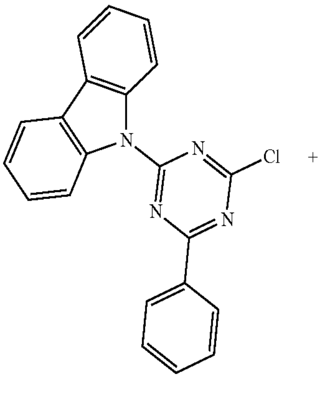


[0148] A solution of 2-chloro-4,6-diphenyl-1,3,5-triazine (4.0 g, 14.94 mmol), 9-(4,6-diphenyl-1,3,5-triazin-2-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (7.84 g, 14.94 mmol), potassium carbonate (5.16 g, 37.40 mmol), in dimethoxyethane (DME):Toluene (240 mL: 240 mL) and water (20 ml) under argon atmosphere with a reflux condenser. The reaction mixture was bubbled with argon for 10 minutes, then Tetrakis Pd (1.73 g, 1.494 mmol) was added and argon bubbling continued for 5 more minutes. The reaction mixture was heated to reflux (82° C.) for 12 hours, then cooled to room temperature (~22° C.) and water (50 mL) was added. The solid product was then filtered off, washed with water (50 mL) and dried in lyophilizer to give a crude product. The crude product was subjected to trituration with hot THF, trituration with hot methanol to remove some polar impurities to yield 3,9-bis(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole (T18-231) as a pale-yellow solid, (6.2 g, 66% yield).

Synthesis of 3-(4-(9H-carbazol-9-yl)-6-phenyl-1,3,5-triazin-2-yl)-9-(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole

[0149]



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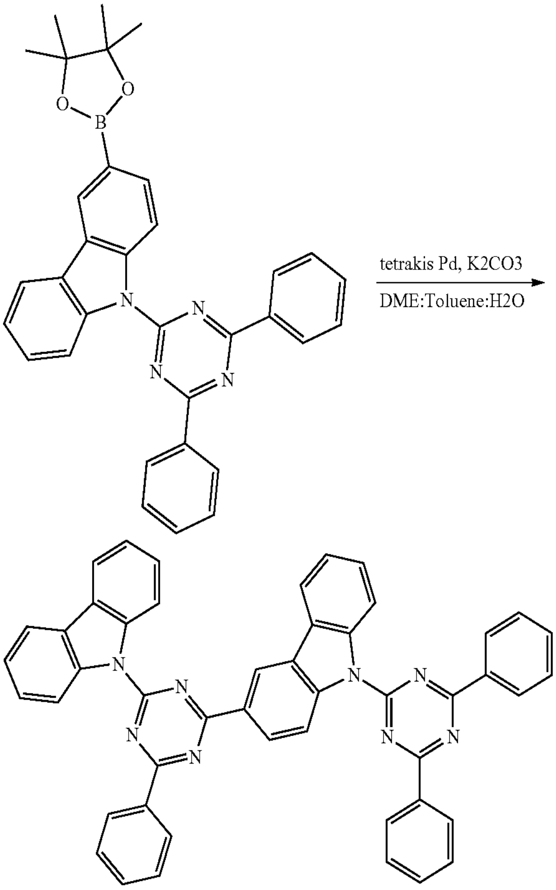


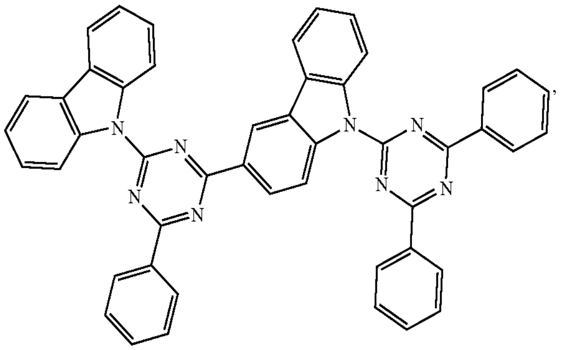
[0150] A solution of 9-(4-chloro-6-phenyl-1,3,5-triazin-2-yl)-9H-carbazole (2.90 g, 10.09 mmol), 9-(4,6-diphenyl-1,3,5-triazin-2-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (2.90 g, 10.09 mmol), potassium carbonate (2.228 g, 21.02 mmol), in DME:Toluene (40 mL: 40 mL) and water (10 ml) under argon atmosphere with a reflux condenser. The reaction mixture was bubbled with argon for 10 minutes, then Tetrakis Pd (0.486, 0.420 mmol) was added and argon bubbling continued for 5 more minutes. The reaction mixture was heated to reflux (82° C.) for 12 hours, then the reaction mixture was cooled to room temperature and water (50 mL) was added. The solid product was filtered off, washed with water (50 mL), and dried in lyophilizer to give 3-(4-(9H-carbazol-9-yl)-6-phenyl-1,3,5-triazin-2-yl)-9-(4,6-diphenyl-1,3,5-triazin-2-yl)-9H-carbazole (T18-232) as an off-white solid (3.85 g, 81% yield).

Device Examples

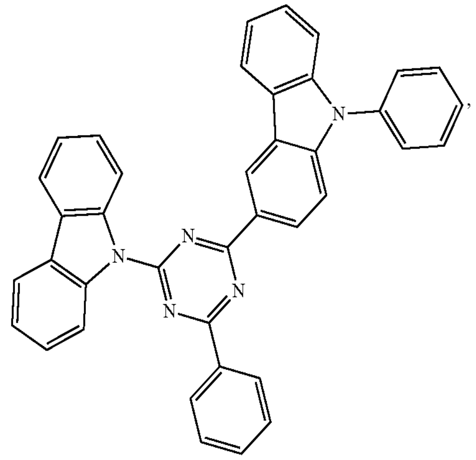
[0151] All devices were fabricated by high vacuum (~10-7 Torr) thermal evaporation. The anode electrode was 80 nm of indium tin oxide (ITO). The cathode electrode consisted of 1 nm of LiF followed by 100 nm of A1. All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H_2O and O_2) immediately after fabrication, and a moisture getter was incorporated inside the package.

[0152] A set of device examples having organic stacks consisting of, sequentially from the ITO surface, 10 nm of LG101 (from LG Chem) as the hole injection layer (HIL), 45 nm of PPh-TPD as the hole-transport layer (HTL), 40 nm of emissive layer (EML), followed by 35 nm of aDBT-ADN with 35 wt % LiQ as the electron-transport layer (ETL). The EML has three components: 10 wt % of the EML being dopant (D1) as the emitter, and 90 wt % of the EML being a mixture of hosts (60 wt % Compound A as disclosed herein or comparative host 1 or comparative host 2 and 40 wt % H-2). The chemical structures of the compounds used are shown below.

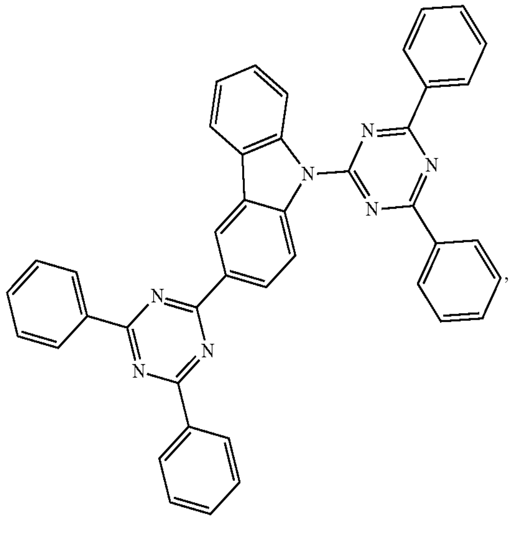
Compound A



Comparative 1



Comparative 2



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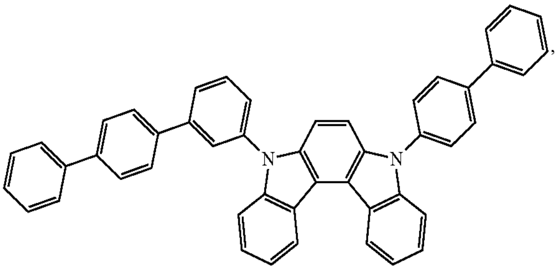
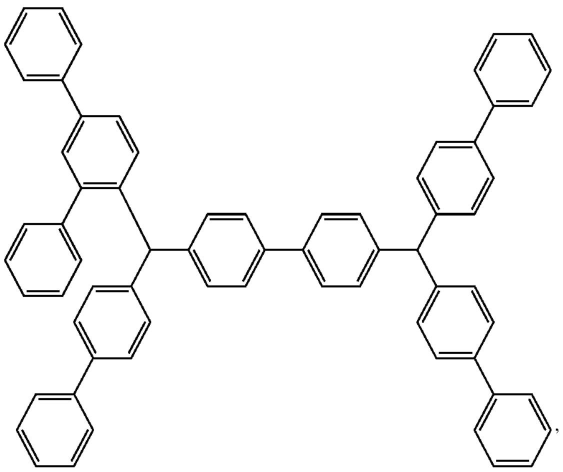
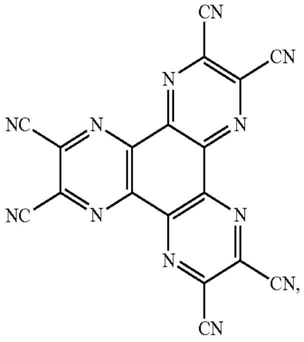
H-2



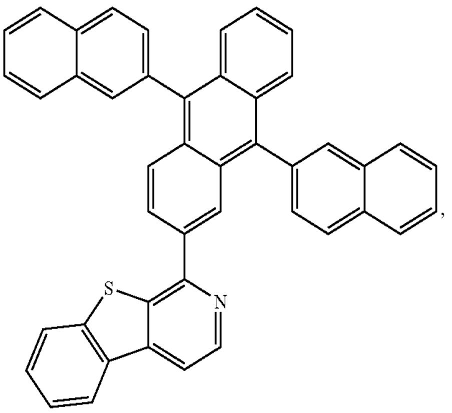
PPh,TPD



HATCN



aDBT-ADN



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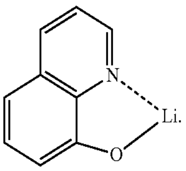
Liq



[0153] Provided in Table 1 below is a summary of the device data recorded at 10 mA/cm^2 for the device examples. The device lifetime (LT95) is reported at 80 mA/cm^2. All results are normalized to device C-2.

TABLE 1

Device ID	Host	λ max (nm)	Voltage [a.u.]	LE [a.u.]	PE [a.u.]	EQE (a.u.)	LT 95 (a.u.)
Device 1	Compound A	527	1.05	1.12	1.06	1.11	1.16
Device C-1	Comparative compound 1	527	1.16	1.22	1.03	1.21	1.11
Device C-2	Comparative compound 2	527	1.00	1.00	1.00	1.00	1.00

[0154] The data in Table 1 show that the device including compound A exhibits a lower voltage and better device lifetime when compared with compartive device 1 having two donor and one acceptor groups, and have better efficiencies and lifetime when comparison with comparative device 2 having one donor and two acceptor groups. The results indicate that only when the novel compounds disclosed herein, having two donor and two acceptor groups, are used as host material in device, the optimal device performance can be achieved in all aspects of parameters.

[0155] It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

We claim:

1. A compound comprising:

at least two donor groups G^D; and

at least two acceptor groups G^A;

wherein each donor group G^D and acceptor group G^A can be the same or different;

wherein any pair of donor groups G^D is separated by at least one acceptor group G^A;

wherein any pair of acceptor groups G^A is separated by at least one donor group G^D; and

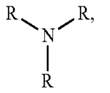
wherein the total number of the donor groups G^D is equal to the total number of the acceptor groups G^A.

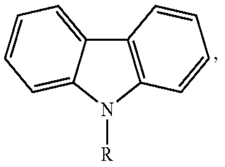
2. The compound of claim **1**, wherein the compound has exactly two donor groups G^D and exactly two acceptor groups G^A.

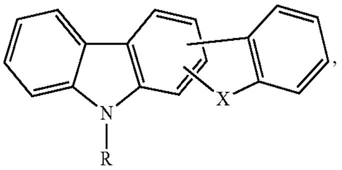
3. The compound of claim **1**, wherein each donor group G^D independently comprises at least one moiety selected from the group consisting of amino, indole, carbazole, benzothiophene, benzofuran, benzoselenophene, dibenzothiophene, dibenzofuran, and dibenzoselenophene.

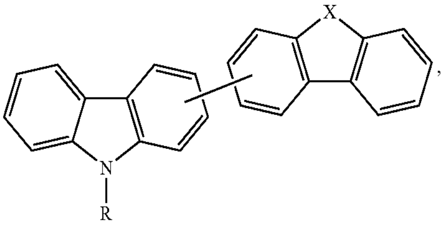
4. The compound of claim **1**, wherein each acceptor group G^A independently comprises at least one moiety selected from the group consisting of nitrile, isonitrile, fluoride, borane, a six-membered aromatic ring having at least one nitrogen, and a 5-membered aromatic ring having at least two heteroatoms.

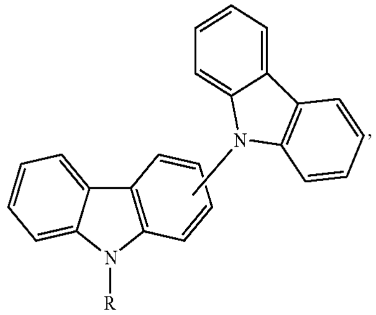
5. The compound of claim **1**, wherein each donor group G^D independently comprises at least one moiety selected from the group consisting of:

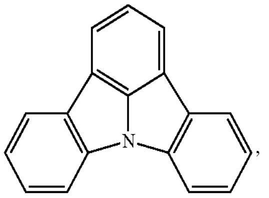


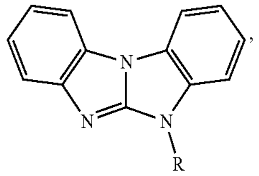


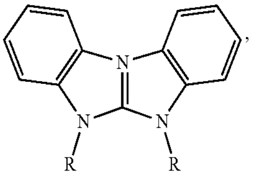












wherein X is selected from the group consisting of O, S, Se, and NR; and wherein each R is independently selected from (i) G^A, (ii) an organic linker bonded to G^A, and (iii) a terminal group selected from the group consisting of alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, aryl, heteroaryl, and combinations thereof.

6. The compound of claim **1**, wherein each acceptor group G^A independently comprises at least one moiety selected from the group consisting of nitrile, isonitrile, borane, fluoride, pyridine, pyrimidine, pyrazine, triazine, aza-carbazole, aza-dibenzothiophene, aza-dibenzofuran, aza-dibenzoselenophene, aza-triphenylene, imidazole, pyrazole, oxazole, thiazole, isoxazole, isothiazole, triazole, thiadiazole, and oxadiazole.

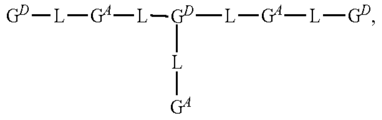
7. The compound of claim **1**, wherein the compound is capable of functioning as an E-type delayed fluorescent emitter at room temperature.

8. The compound of claim **1**, wherein donor group G^D having primary HOMO localization and the acceptor group G^A having primary LUMO localization are not next to each other.

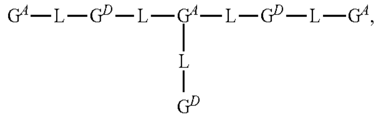
9. The compound of claim **1**, wherein the compound has a structure selected from the group consisting of:

$$G^D-L-G^A-L-G^D-L-G^A,$$

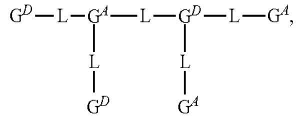
$$G^D-L-G^A-L-G^D-L-G^A-L-G^D-L-G^A,$$



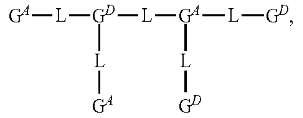
$$G^D-L-G^A-L-\underset{\substack{|\\ L\\ |\\ G^A}}{G^D}-L-G^A-L-G^D,$$



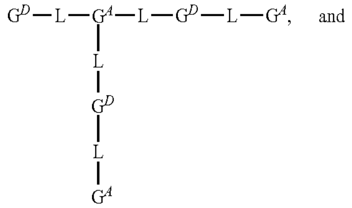
$$G^A-L-G^D-L-\underset{\substack{|\\ L\\ |\\ G^D}}{G^A}-L-G^D-L-G^A,$$



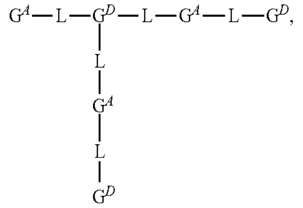
$$G^D-L-\underset{\substack{|\\ L\\ |\\ G^D}}{G^A}-L-\underset{\substack{|\\ L\\ |\\ G^A}}{G^D}-L-G^A,$$



$$G^A-L-\underset{\substack{|\\ L\\ |\\ G^A}}{G^D}-L-\underset{\substack{|\\ L\\ |\\ G^D}}{G^A}-L-G^D,$$



$$G^D-L-\underset{\substack{|\\ L\\ |\\ G^D\\ |\\ L\\ |\\ G^A}}{G^A}-L-G^D-L-G^A, \text{ and}$$

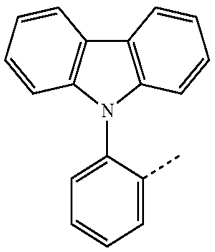


$$G^A-L-\underset{\substack{|\\ L\\ |\\ G^A\\ |\\ L\\ |\\ G^D}}{G^D}-L-G^A-L-G^D,$$

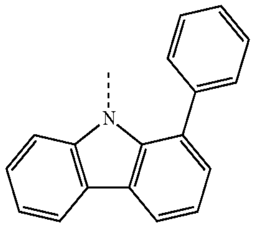
wherein each L is independently a direct bond or an organic linker.

10. The compound of claim **9**, wherein each L is independently selected from the group consisting of a direct bond, aryl, heteroaryl, alkyl, cycloalkyl, silyl, and combination thereof.

11. The compound of claim **1**, wherein at least one donor group G^D comprises a moiety selected from the group consisting of



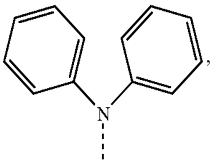
, and



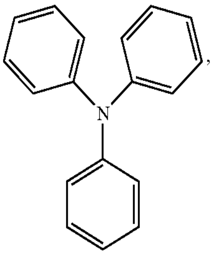
.

12. The compound of claim **1**, wherein each donor group G^D is independently selected from the group consisting of:

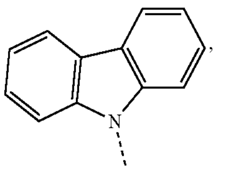
D1



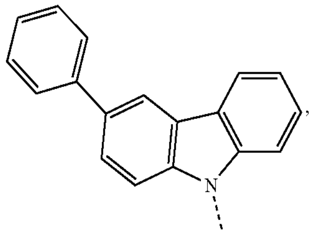
D2



D3



D4



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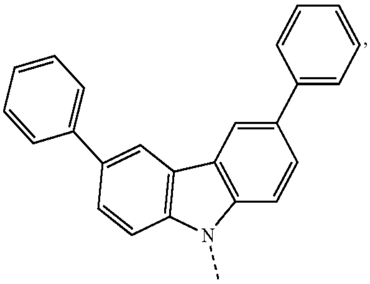
D5



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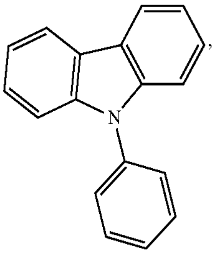

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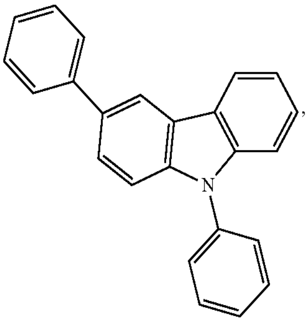

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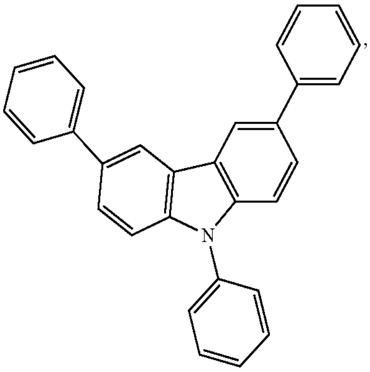

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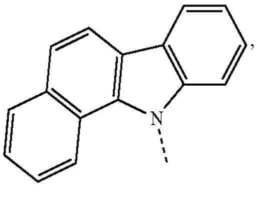

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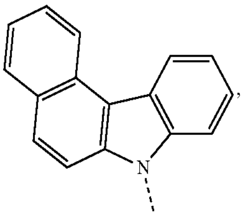

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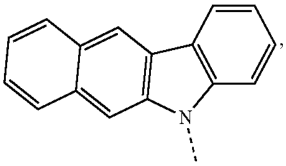

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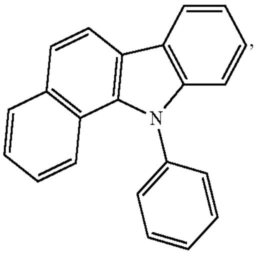

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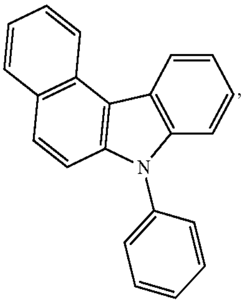

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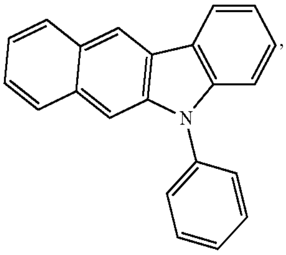

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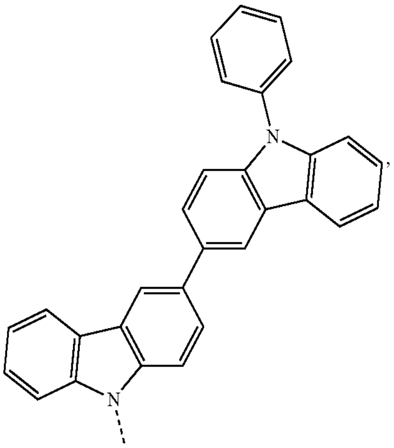

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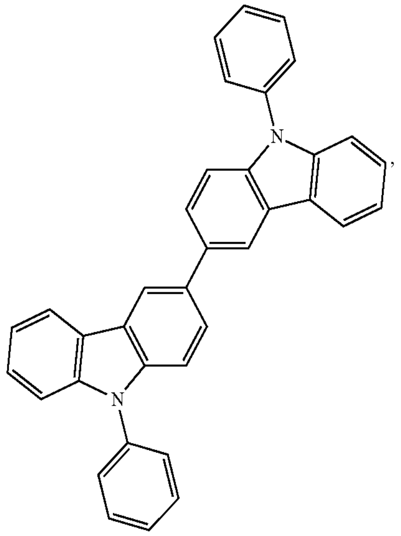

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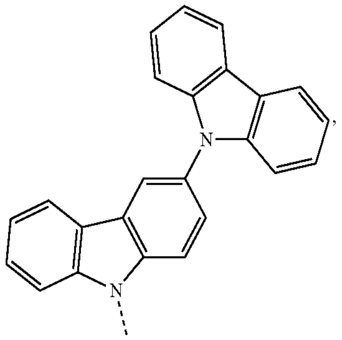

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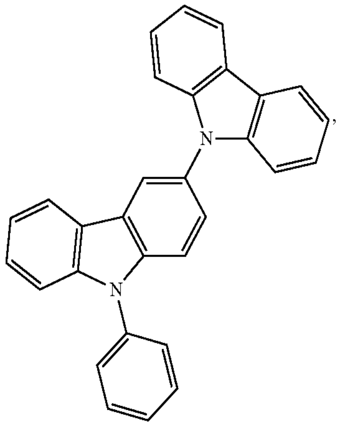

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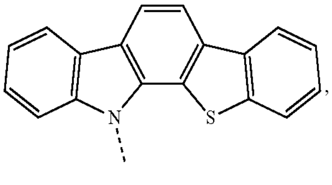

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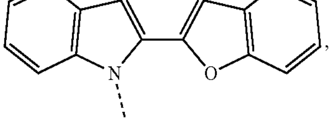

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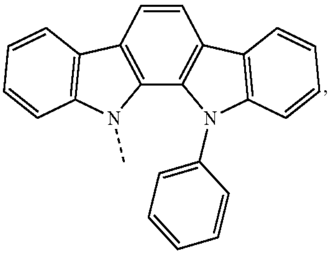

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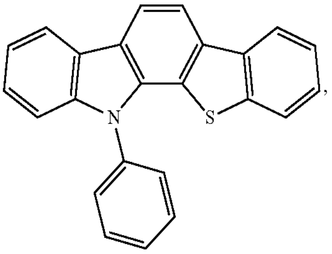

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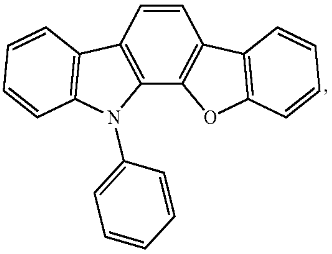

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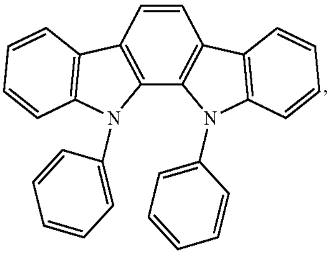

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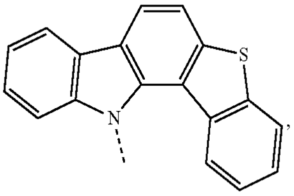

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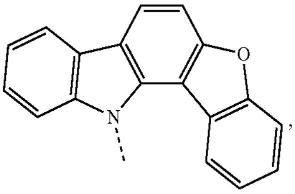

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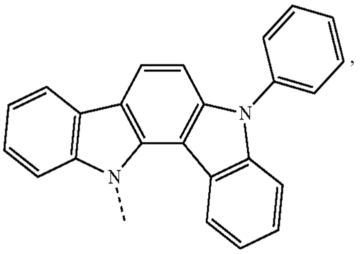
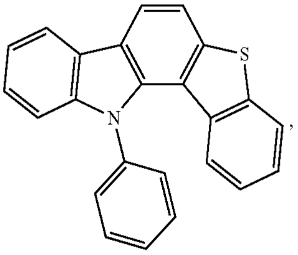
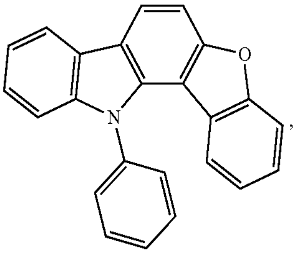
D27



D28



D29



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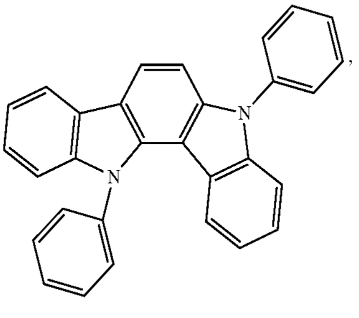

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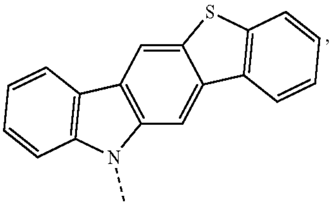

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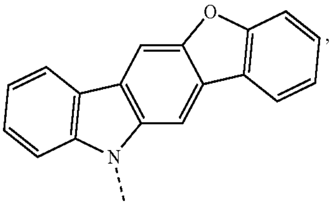

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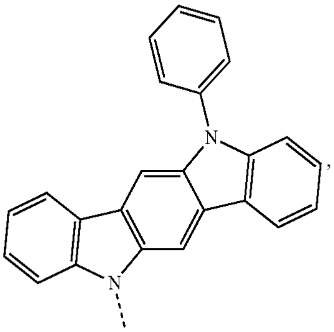

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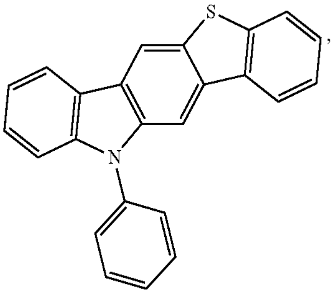

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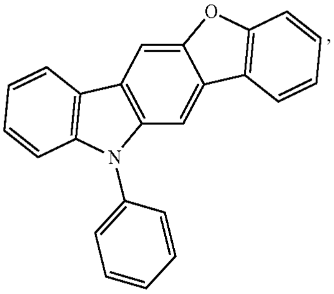

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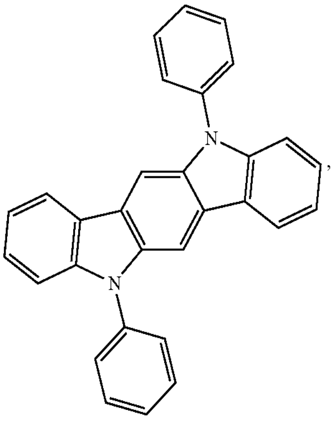

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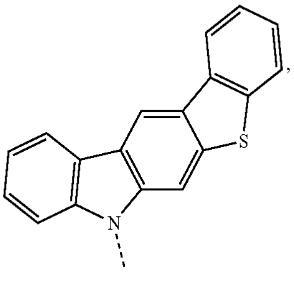

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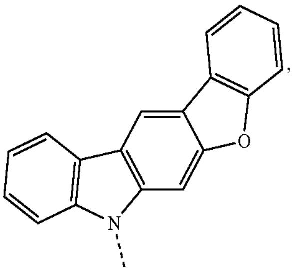

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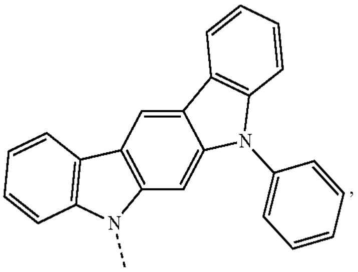

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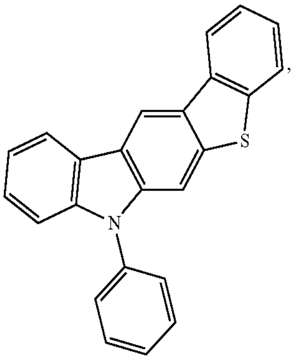

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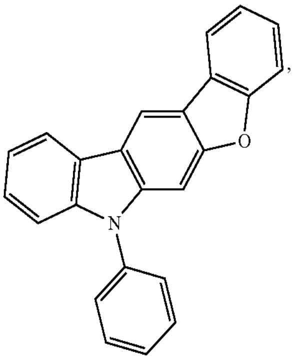

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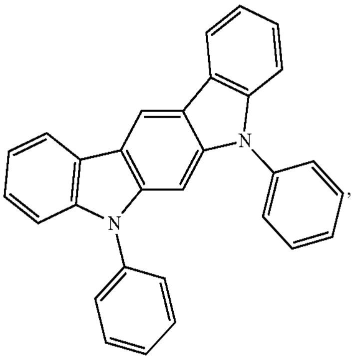

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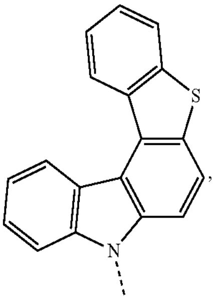

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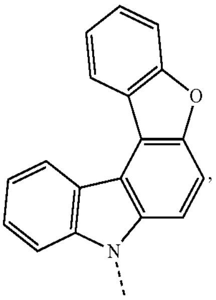

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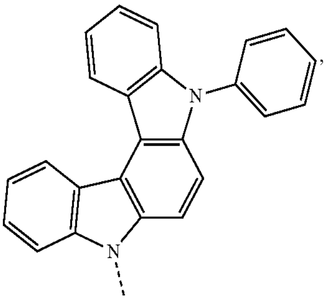

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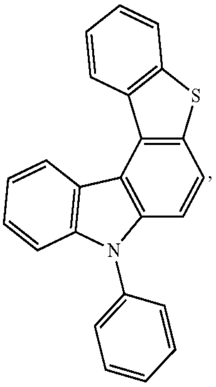

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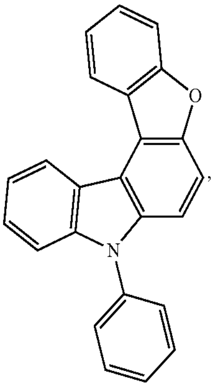

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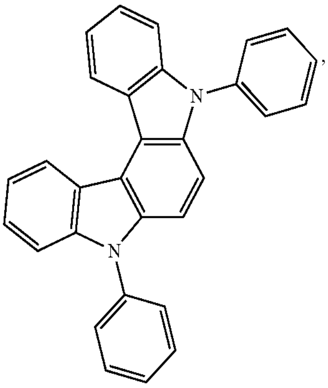

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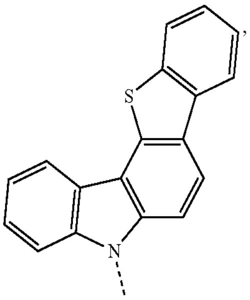

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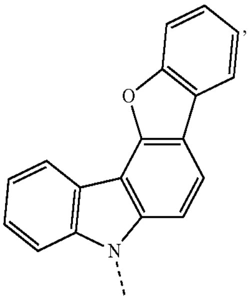

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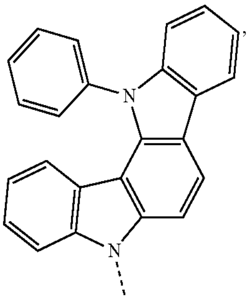

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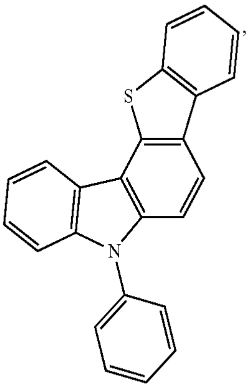

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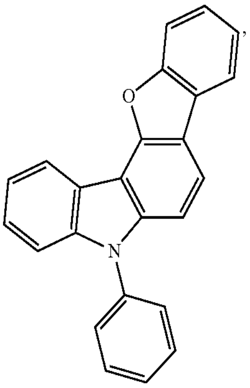

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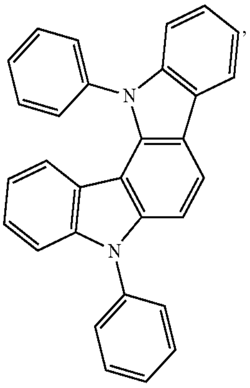

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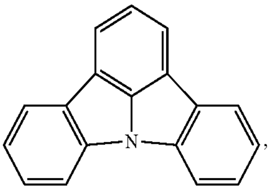

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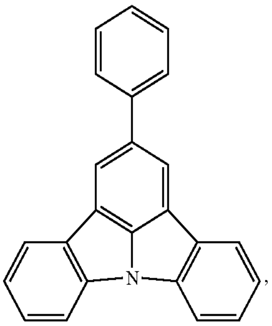

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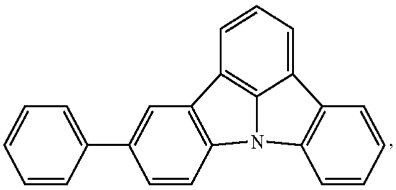

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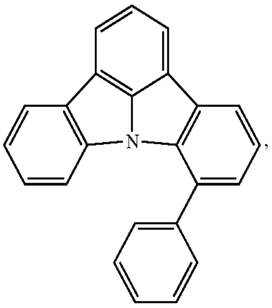

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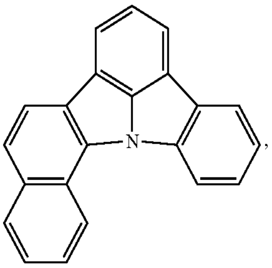

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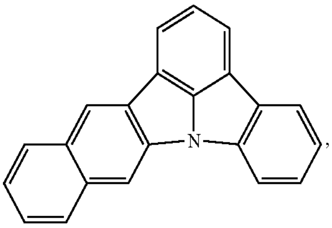

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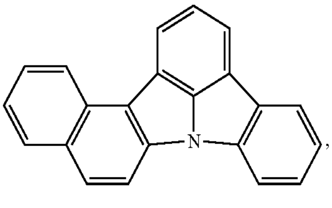

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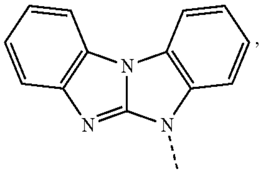

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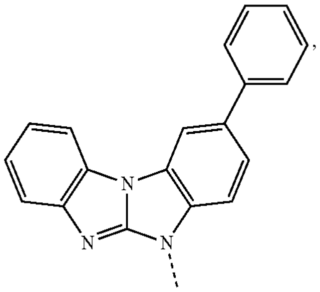

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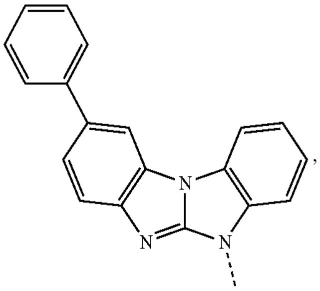

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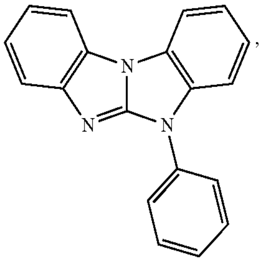

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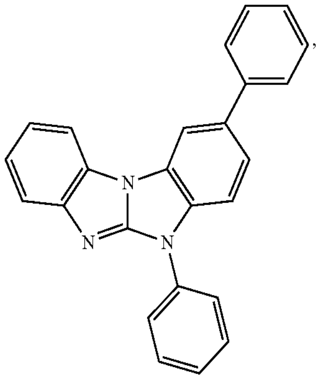

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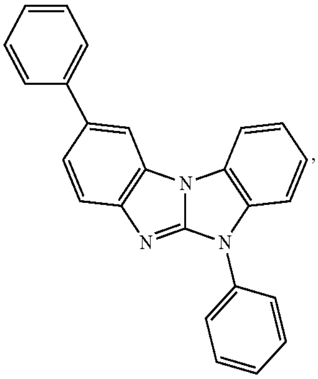
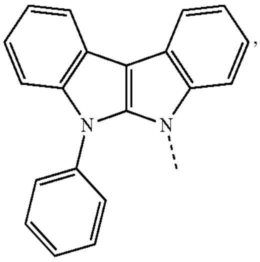
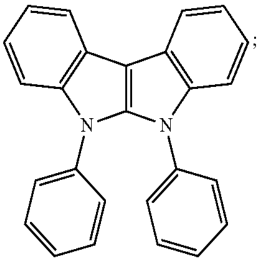


D68



, and

D69

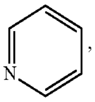


wherein each donor group G^D is at least divalent unless the donor group G^D is a monovalent end group; and

wherein, in structures containing a dashed line, the dashed line represents a bond to a linker or an acceptor group G^A.

13. The compound of claim **1**, wherein each acceptor group G^A is independently selected from the group consisting of:

A1



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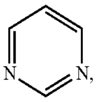
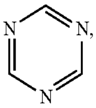


A3



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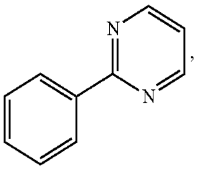
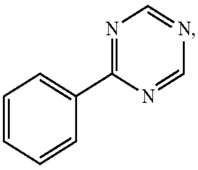
A4



A5



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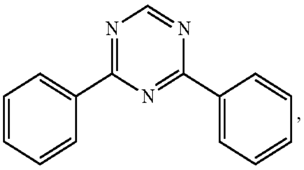

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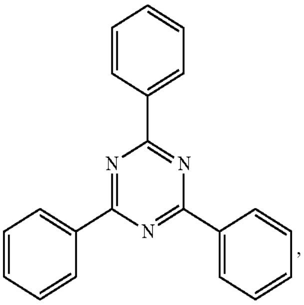

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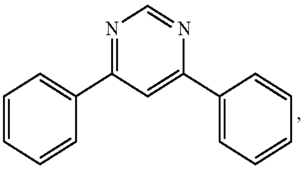

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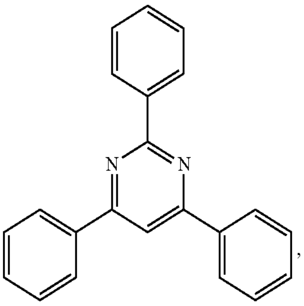

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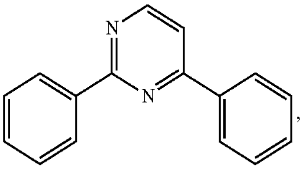

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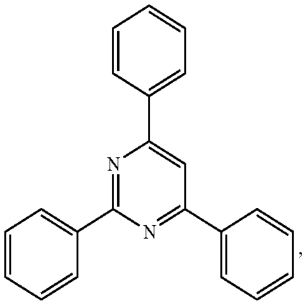

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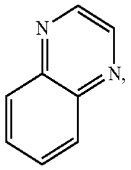

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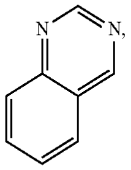

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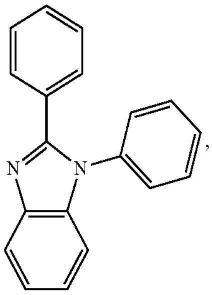

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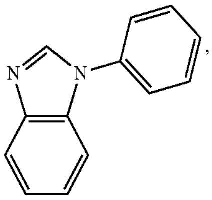

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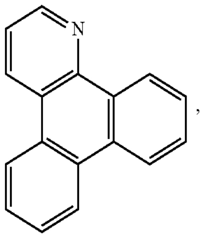

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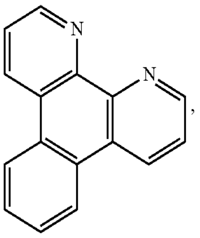

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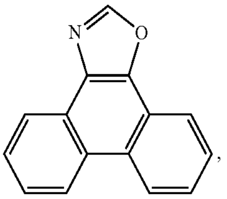

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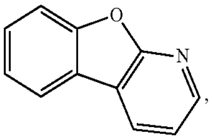

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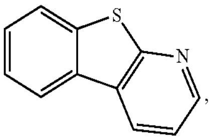

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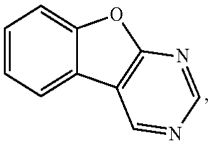

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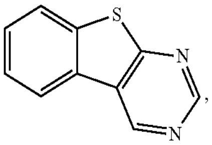

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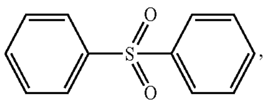

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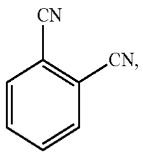

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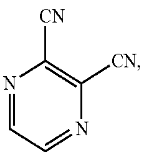

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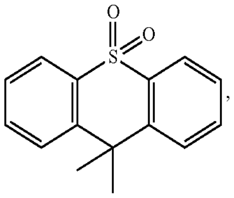

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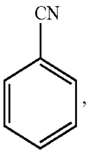

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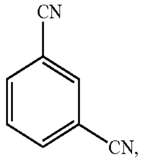

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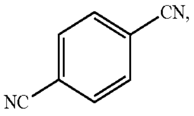

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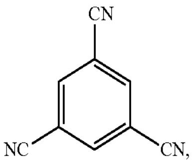

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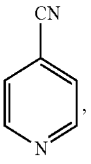
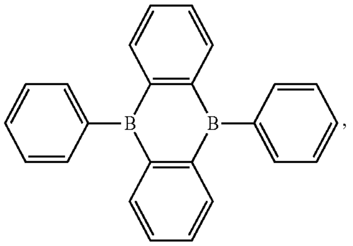


B10



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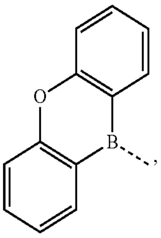

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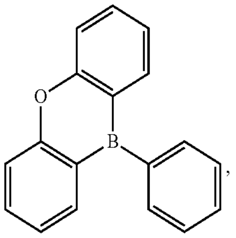
B12



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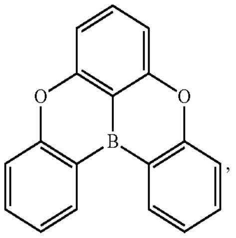
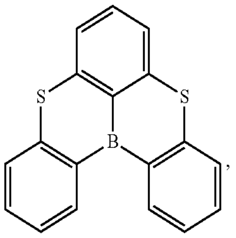


B14



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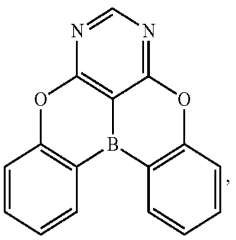

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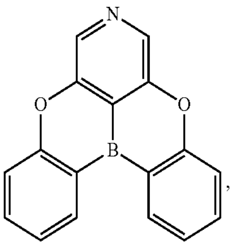

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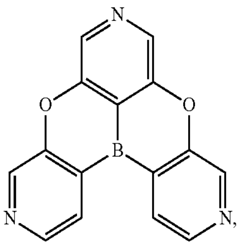

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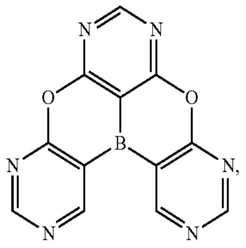
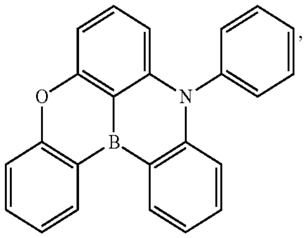


B19



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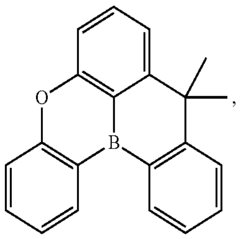

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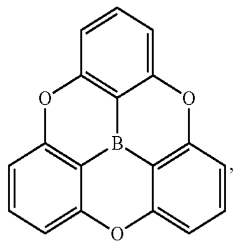

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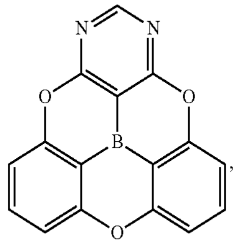

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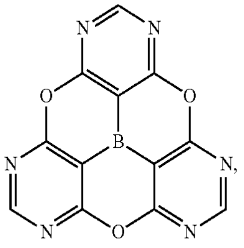

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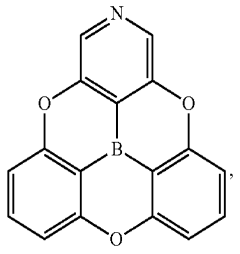
B24



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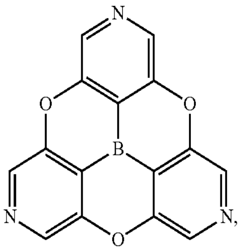

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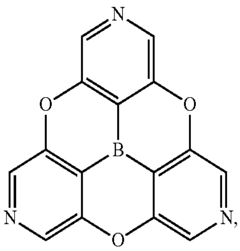

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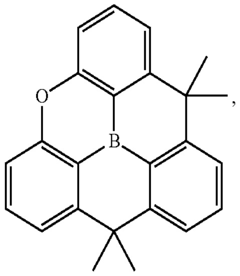

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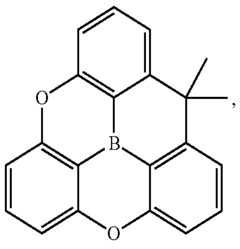

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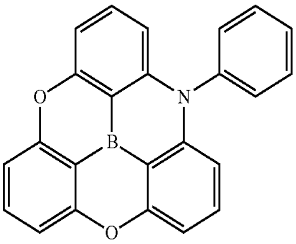
B29



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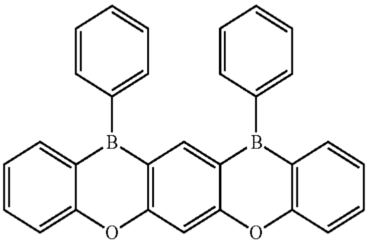
B30

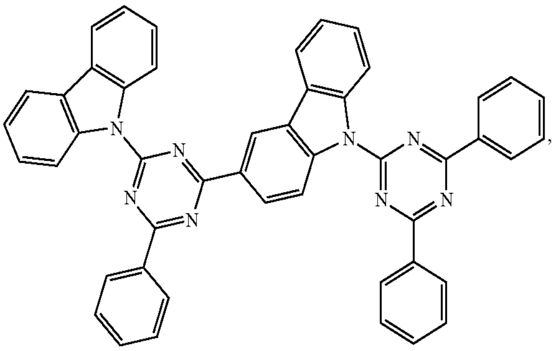


;

wherein each acceptor group G^A is at least divalent unless the acceptor group G^A is a monovalent end group.

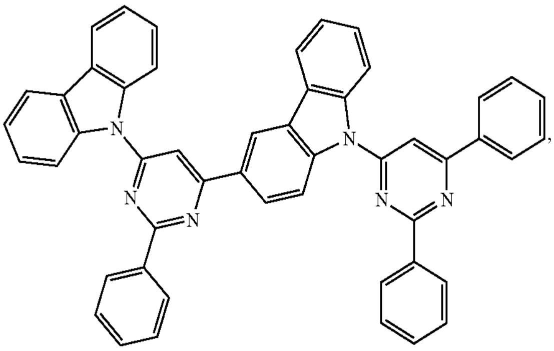
14. The compound of claim **1**, wherein the compound is selected from the group consisting of:

Compound A1



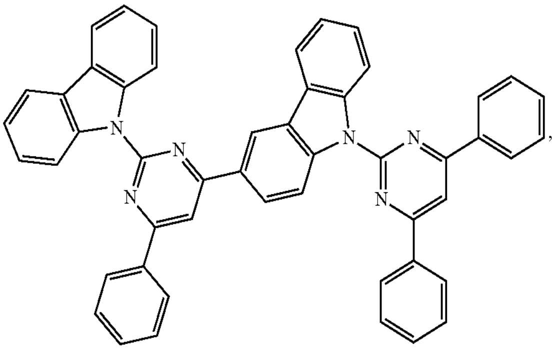
,

Compound A2



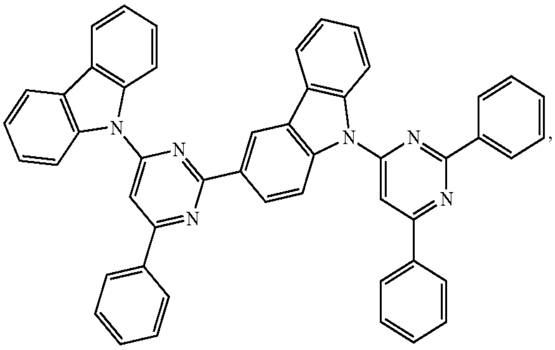
,

Compound A3



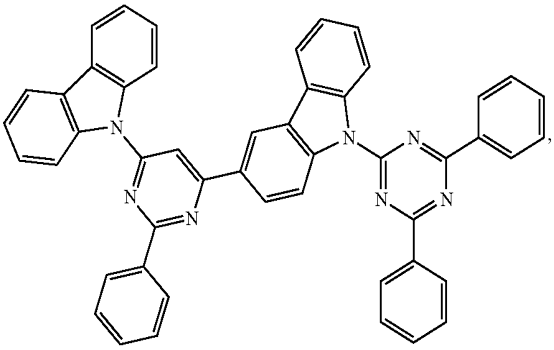
,

Compound A4



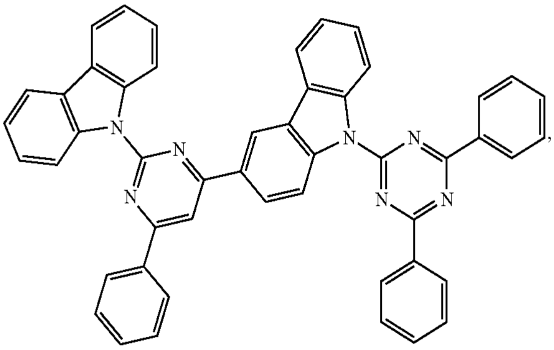
,

Compound A5



,

Compound A6



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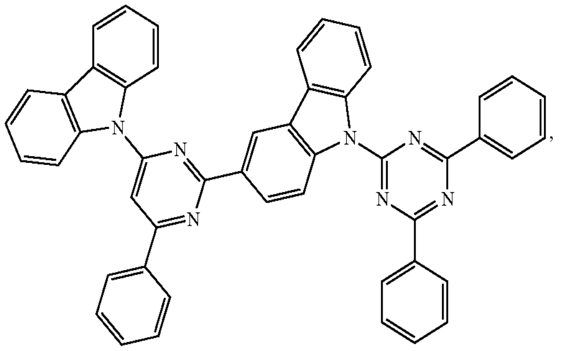
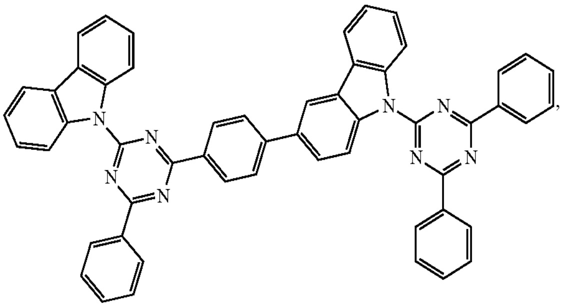
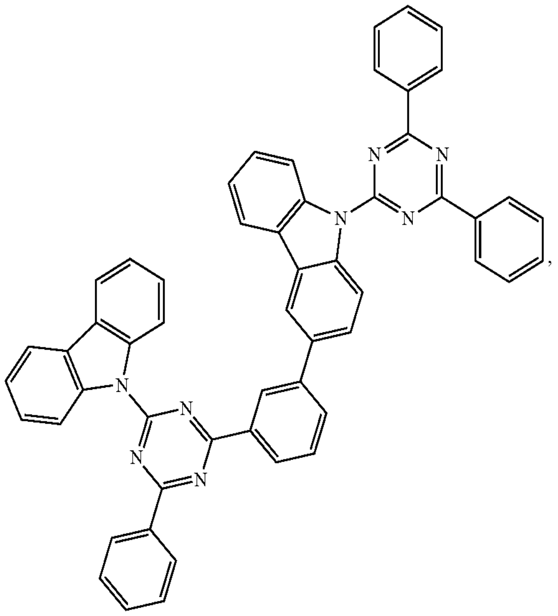
Compound A7



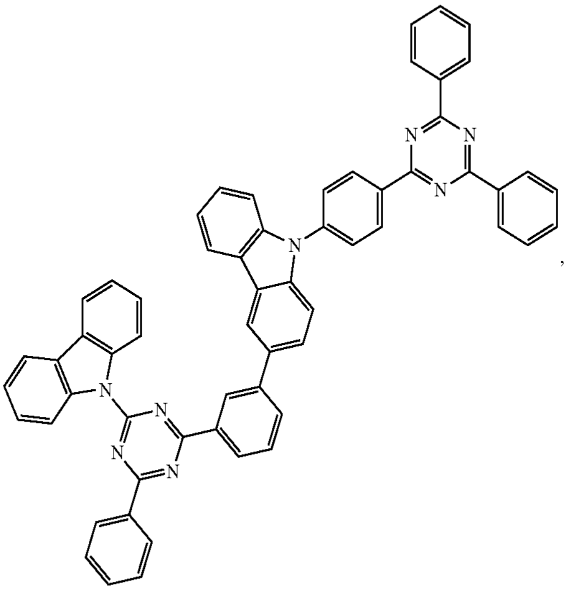
Compound A8



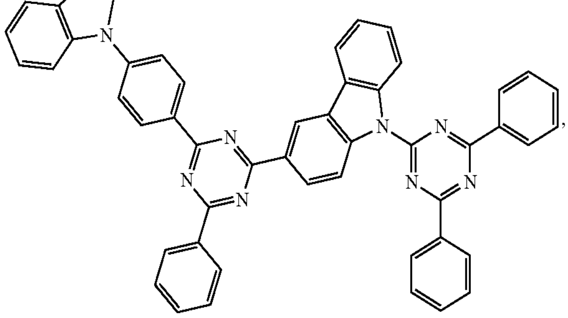
Compound A9



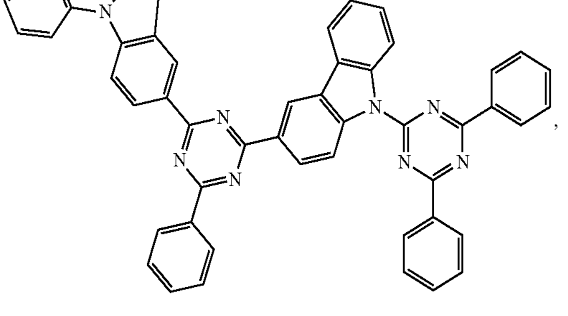
Compound A10



Compound A11



Compound A12



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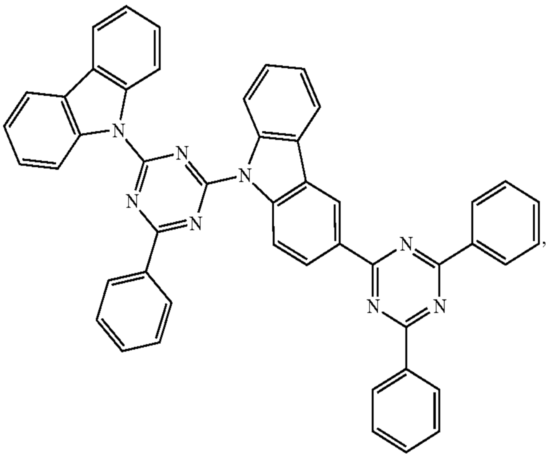
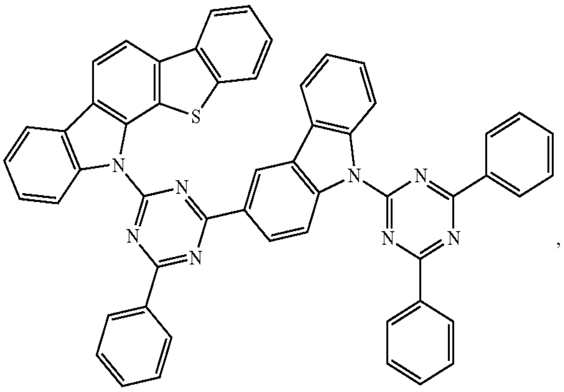
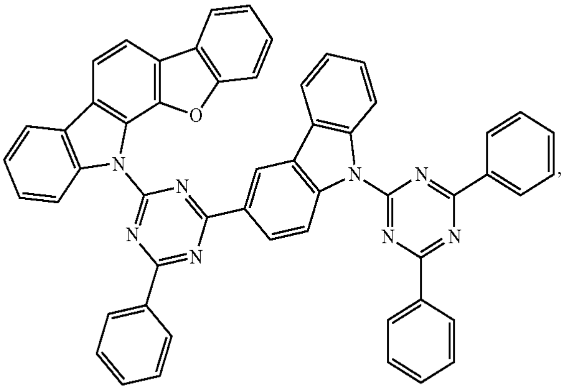
Compound A13



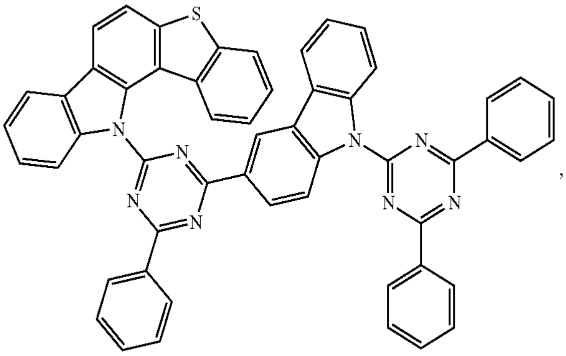
Compound A14



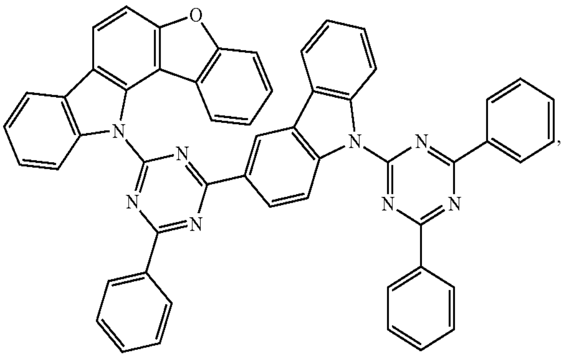
Compound A15



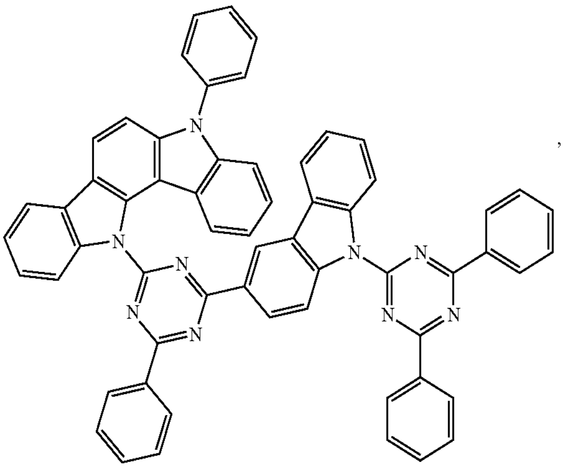
Compound A16



Compound A17



Compound A18



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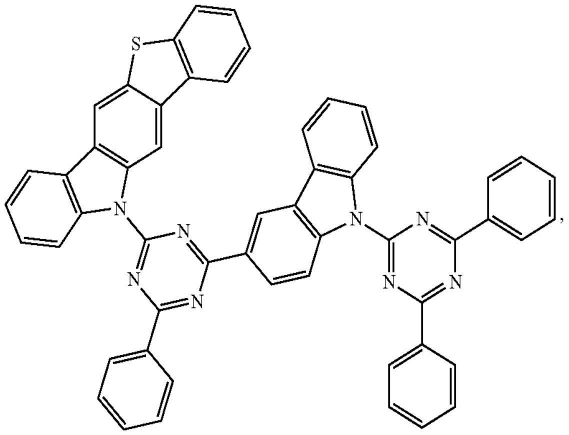
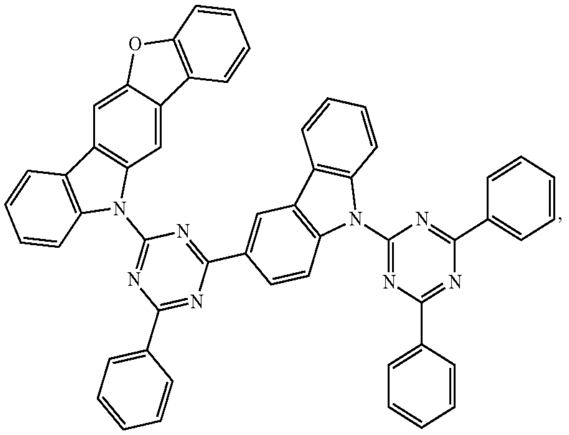
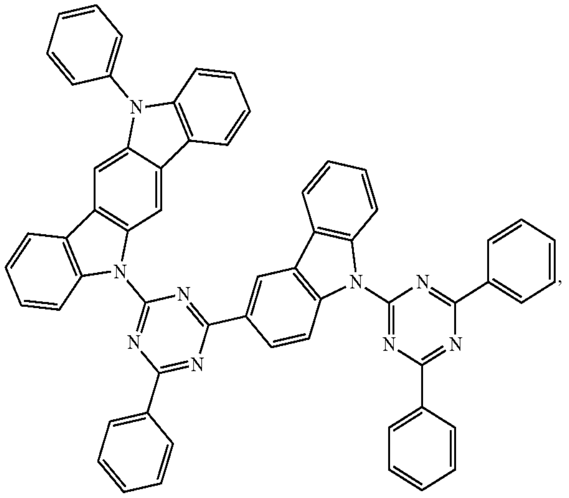
Compound A19



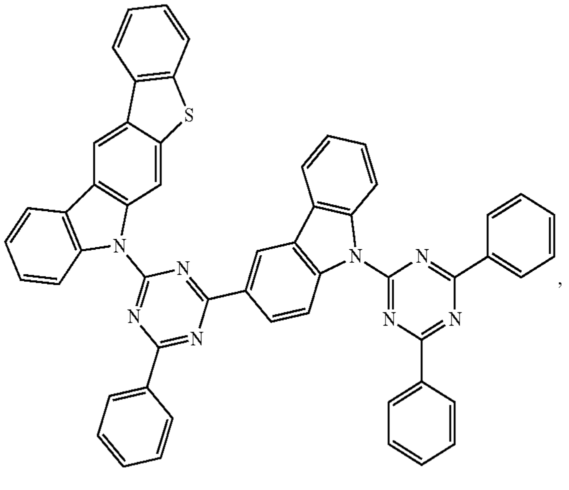
Compound A20



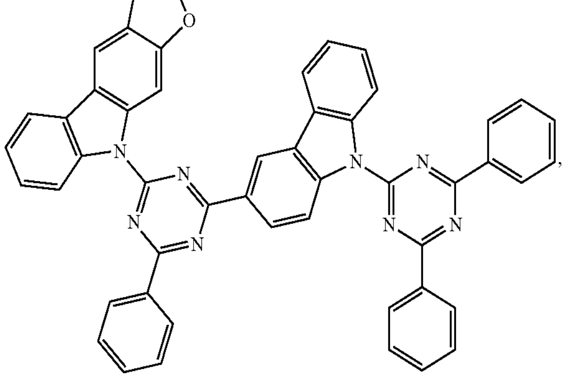
Compound A21



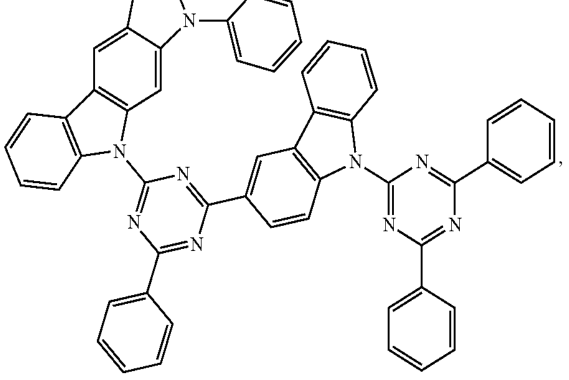
Compound A22



Compound A23



Compound A24



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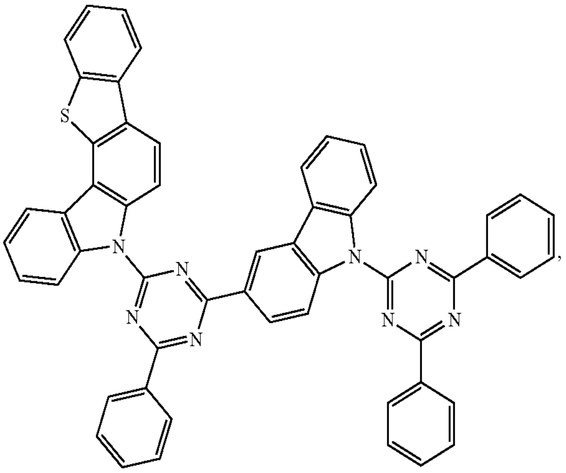
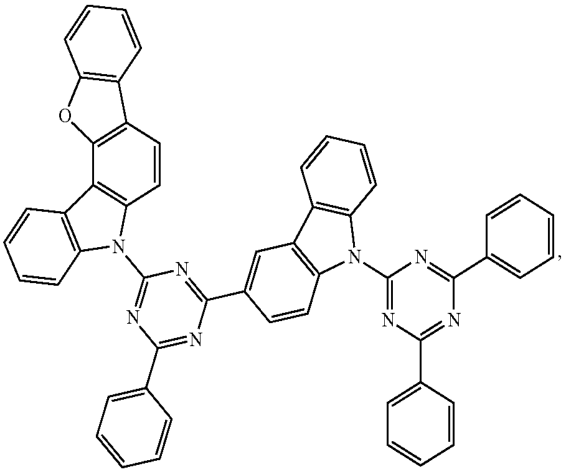
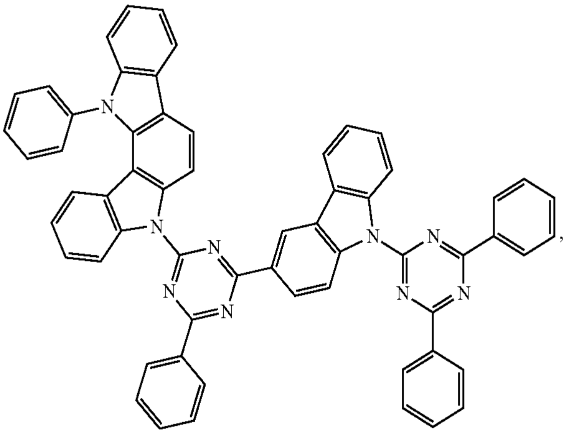
Compound A25



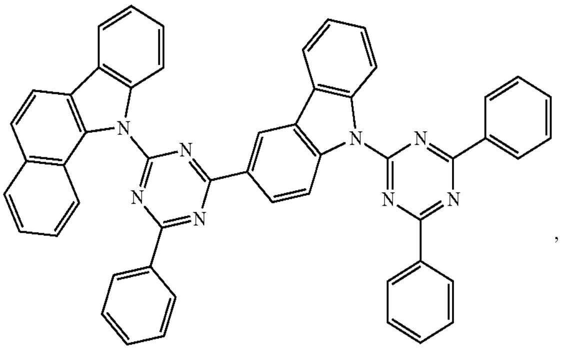
Compound A26



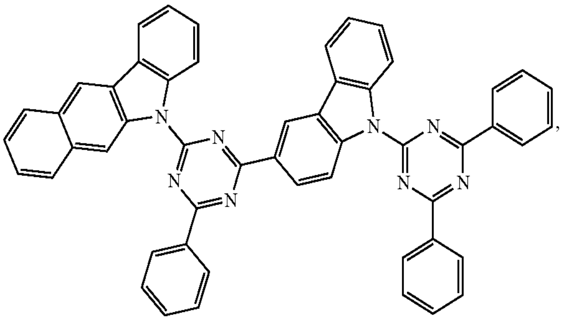
Compound A27



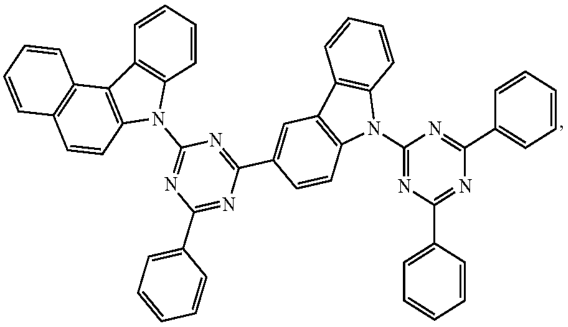
Compound A28



Compound A29



Compound A30



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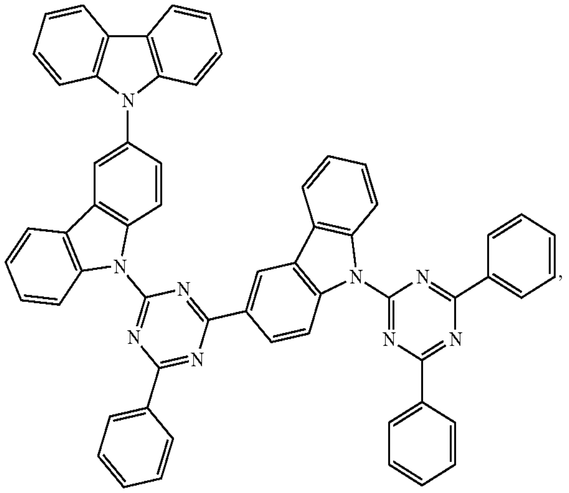
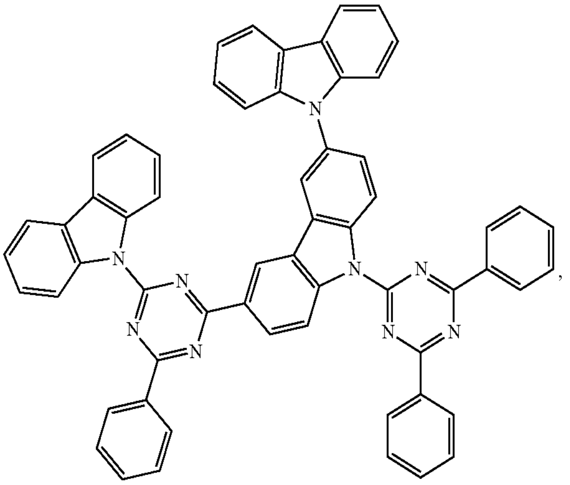
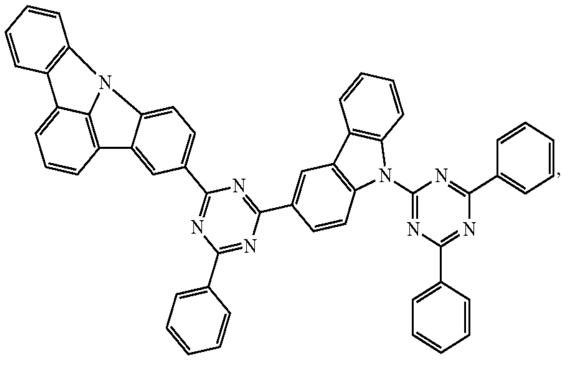
Compound A31



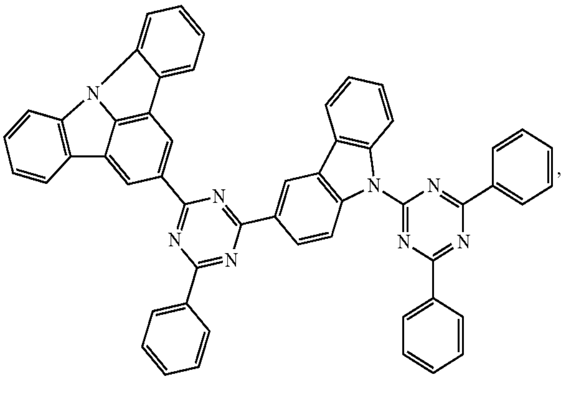
Compound A32



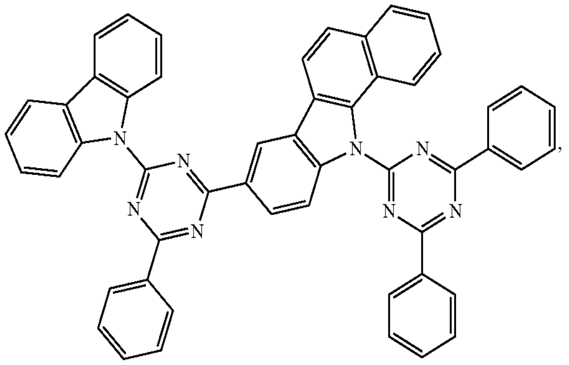
Compound A33



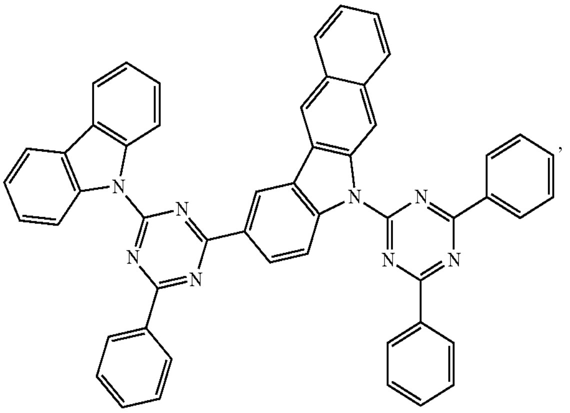
Compound A34



Compound A35



Compound A36



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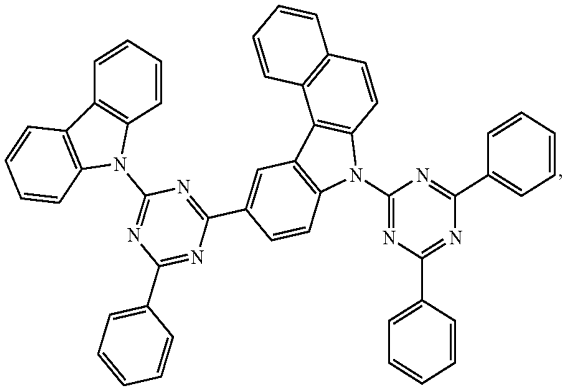
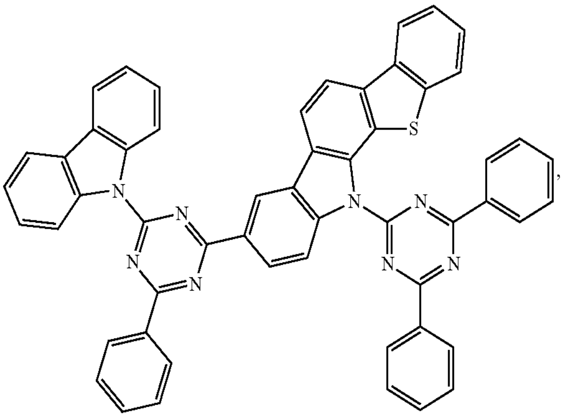
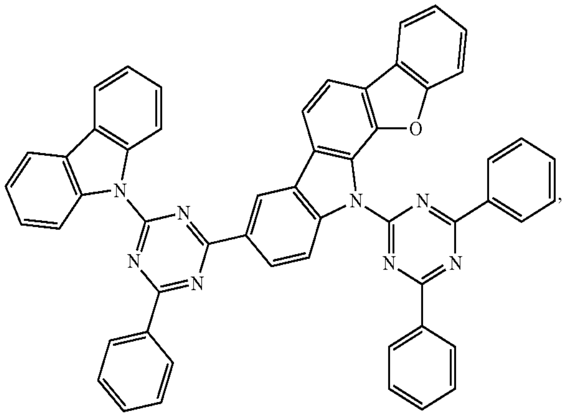
Compound A37



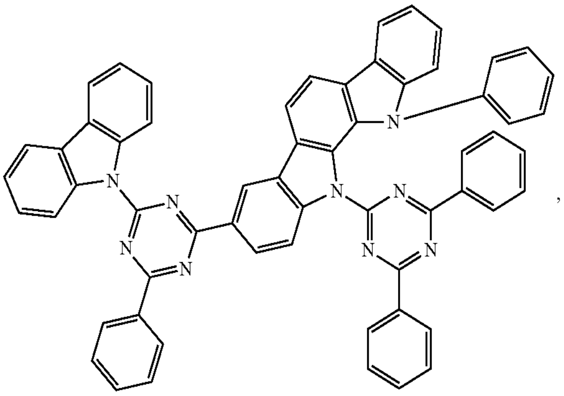
Compound A38



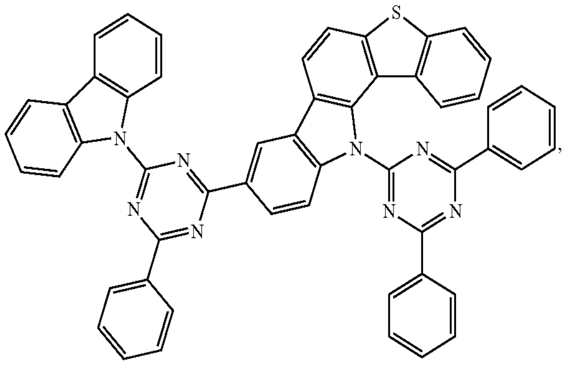
Compound A39



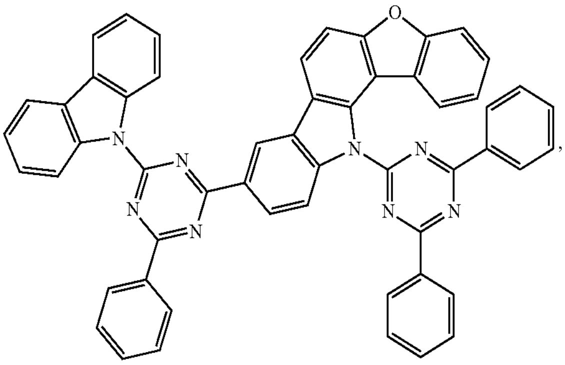
Compound A40



Compound A41



Compound A42



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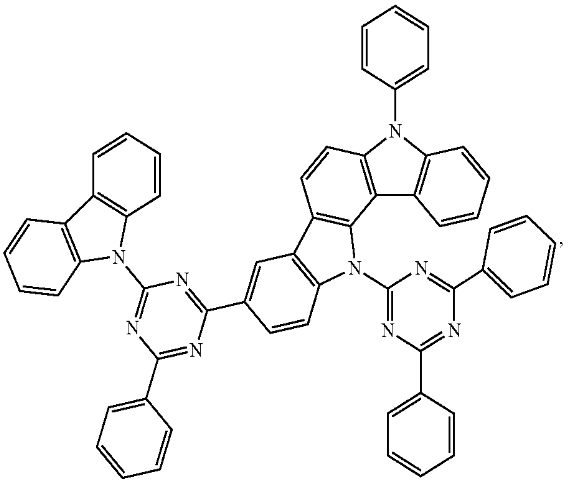
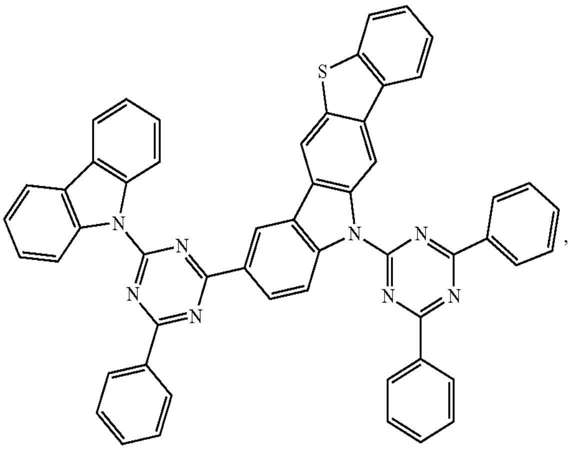
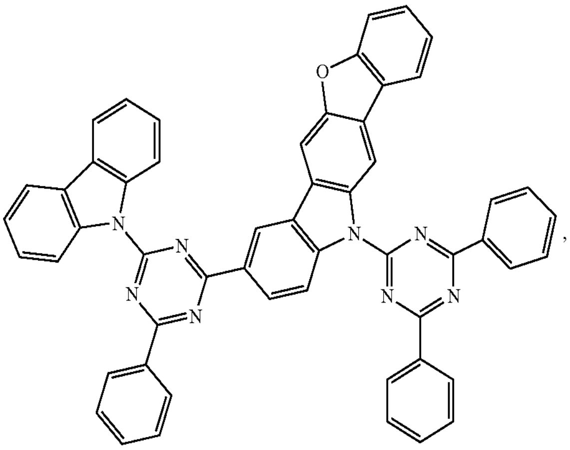
Compound A43



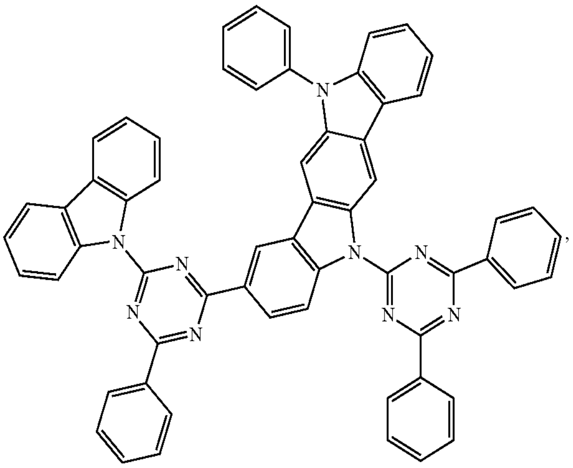
Compound A44



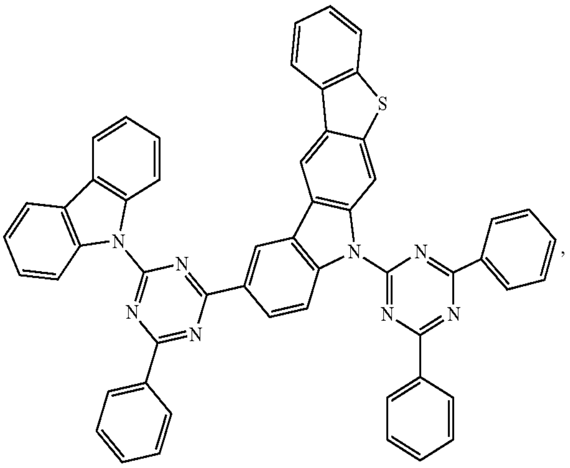
Compound A45



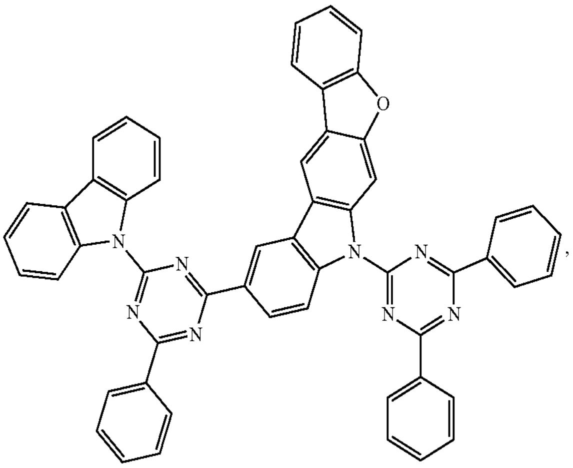
Compound A46



Compound A47



Compound A48



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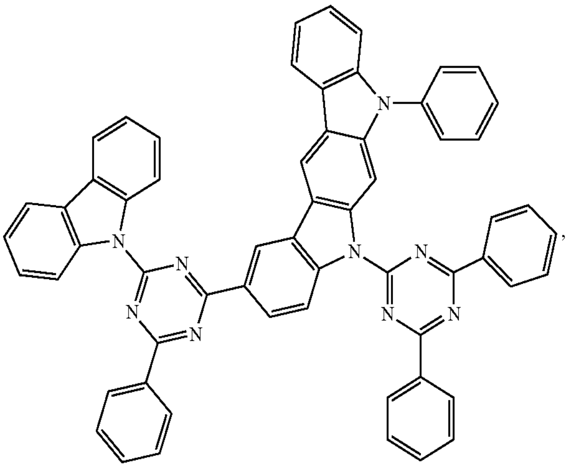
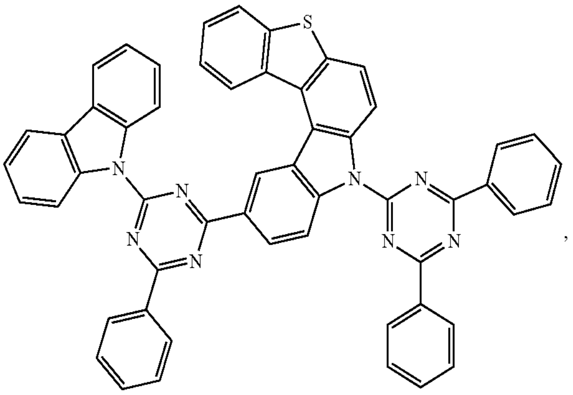
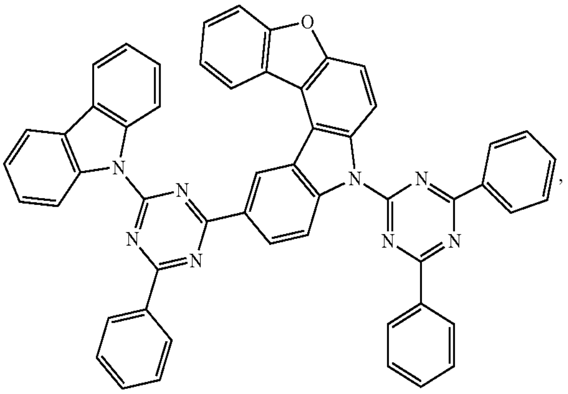
Compound A49



Compound A50



Compound A51



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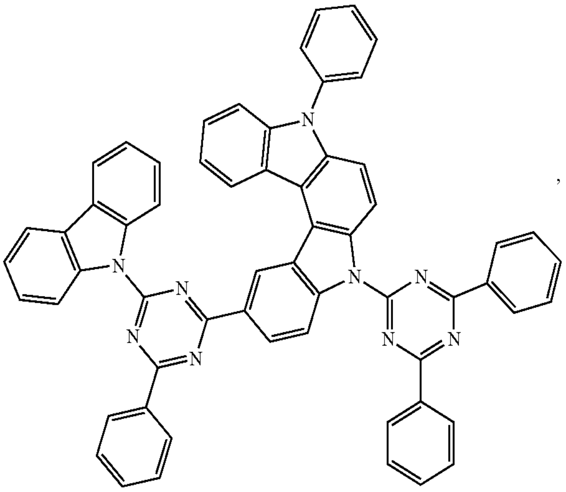

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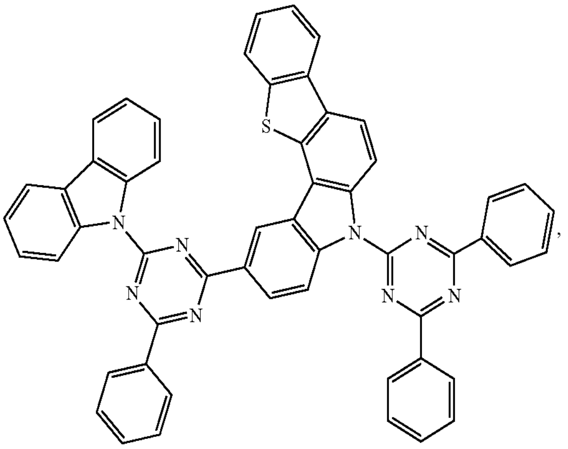

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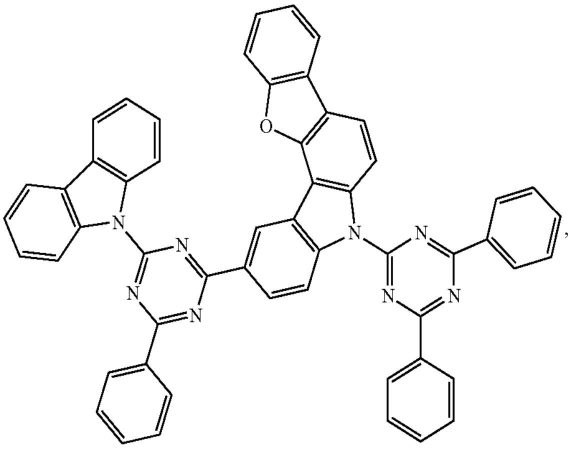

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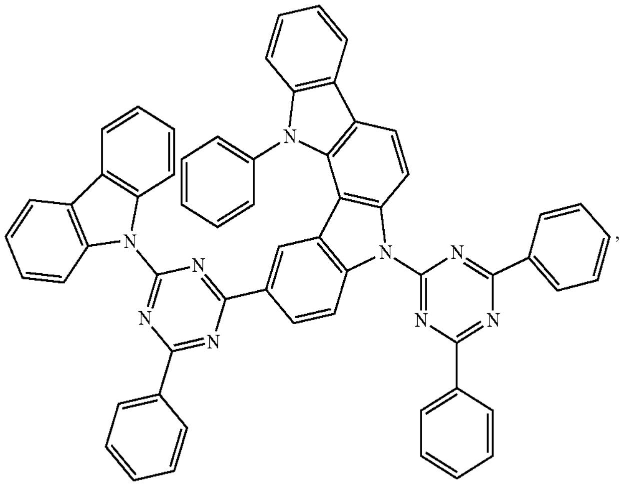
Compound 55



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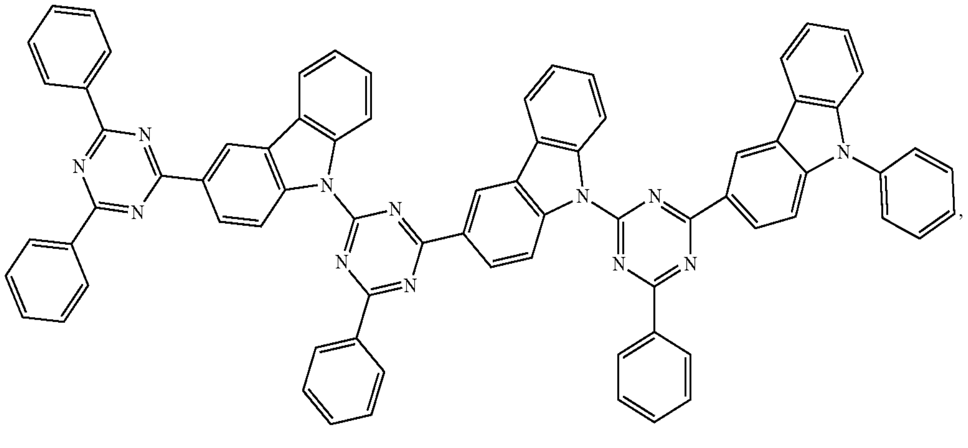

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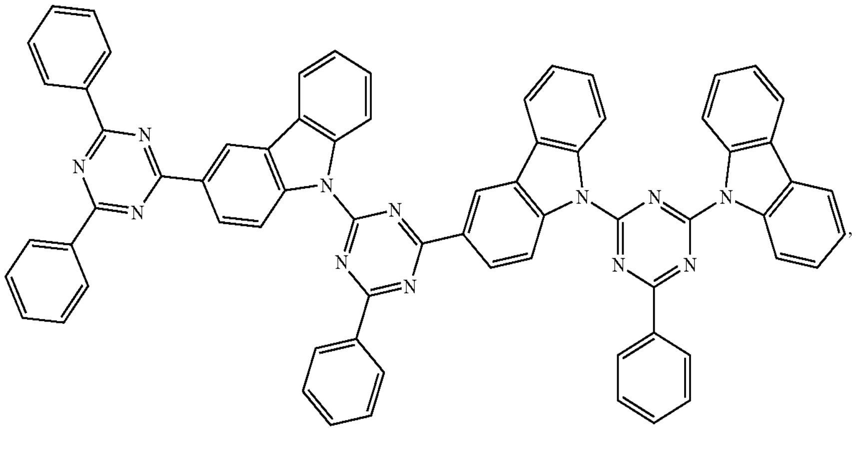

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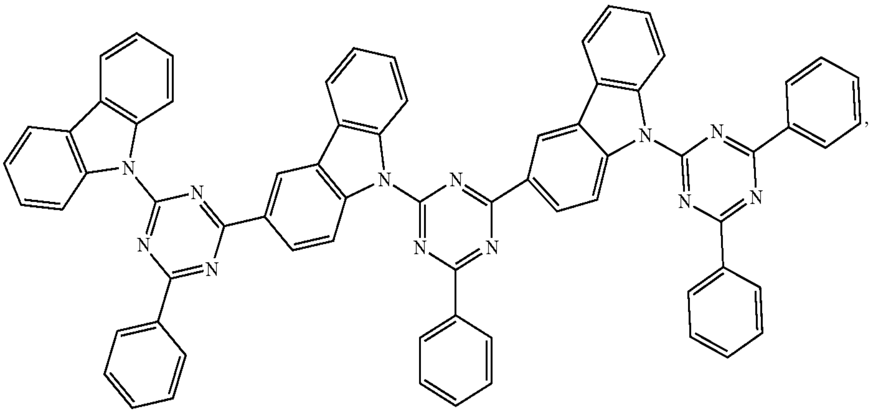

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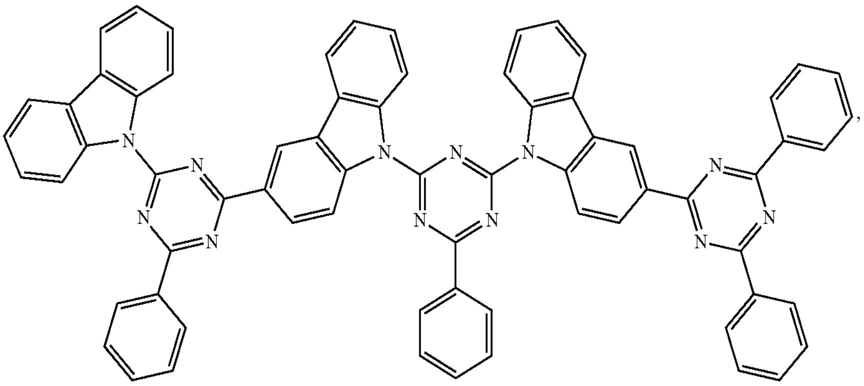

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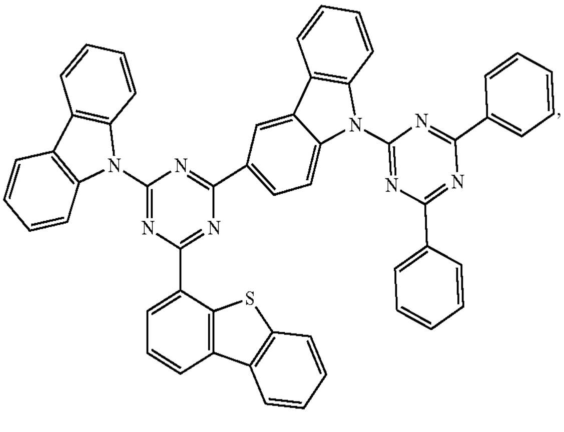

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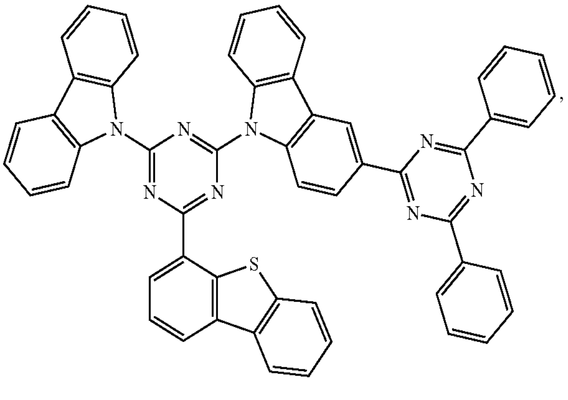

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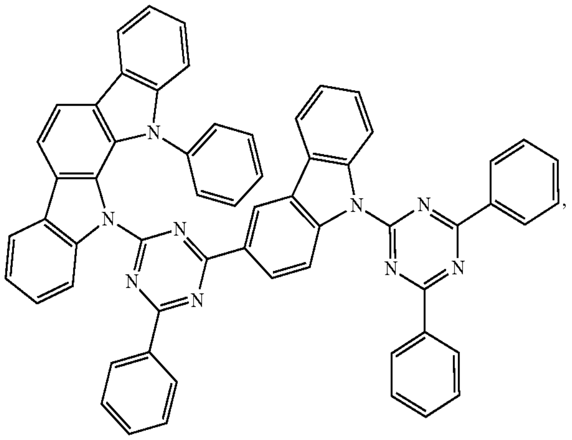

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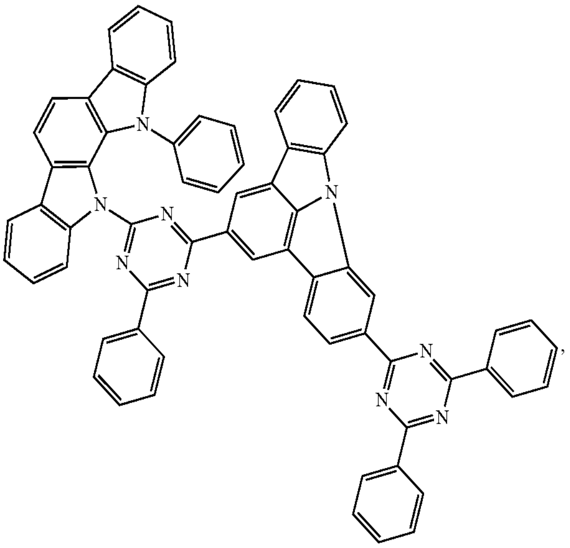

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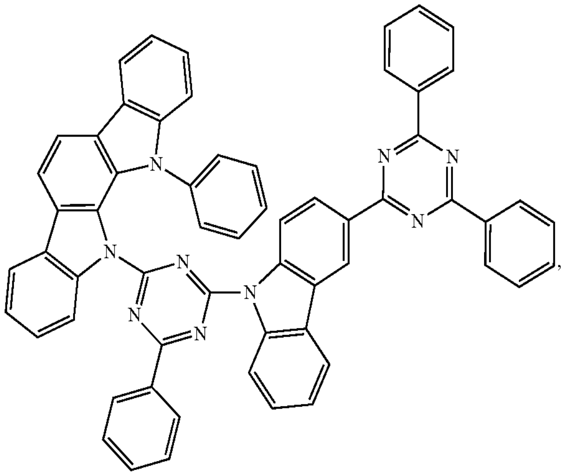

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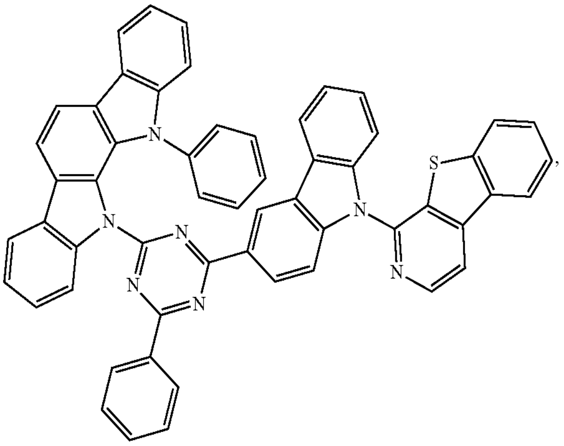

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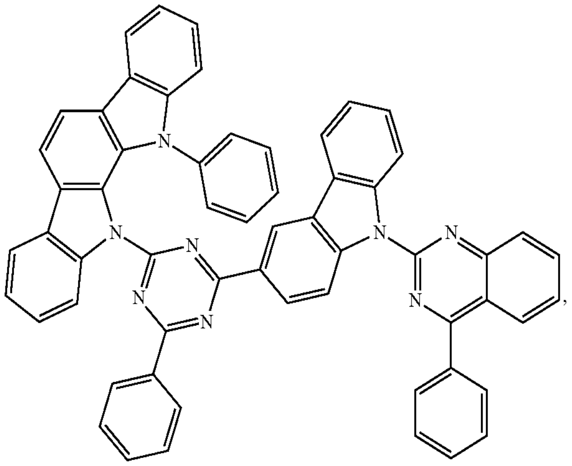

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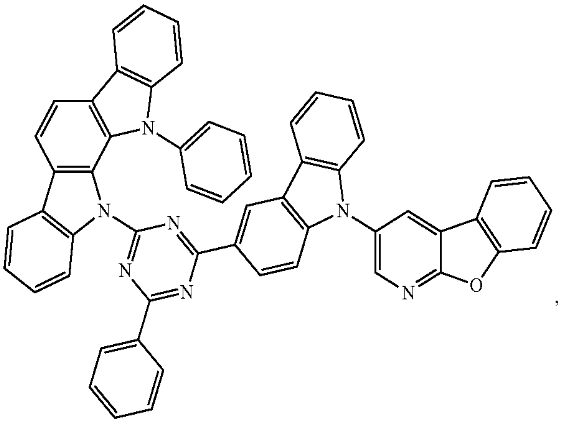

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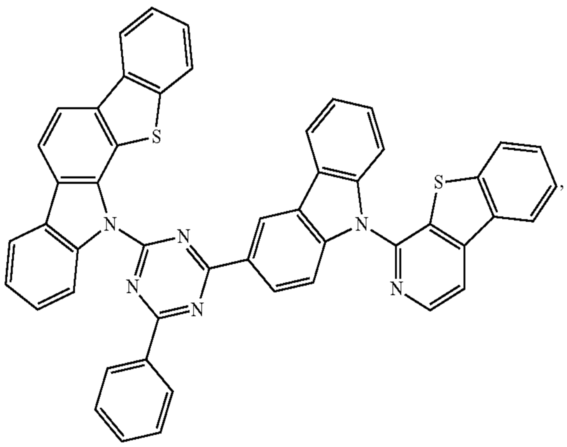

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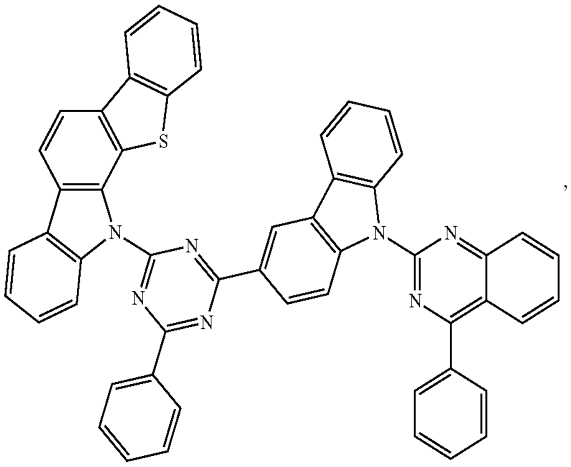

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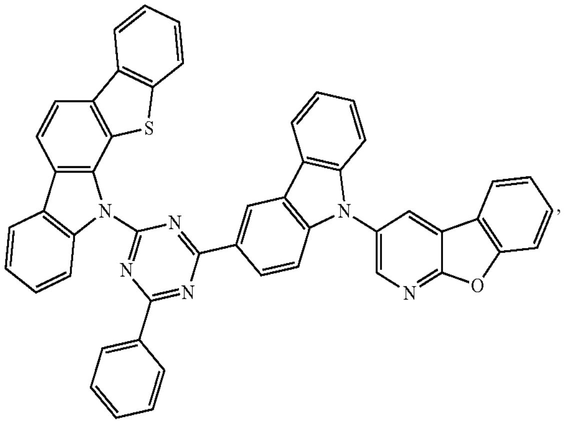

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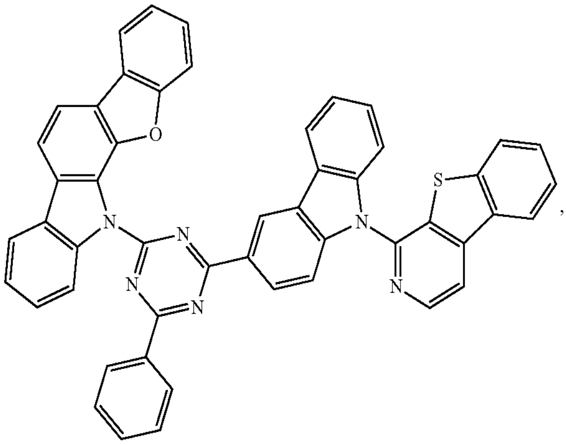

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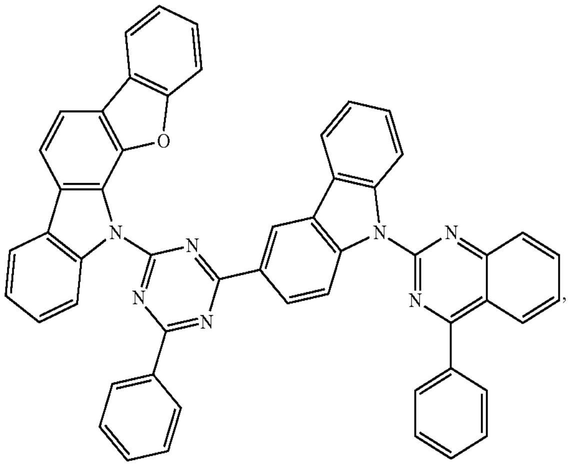

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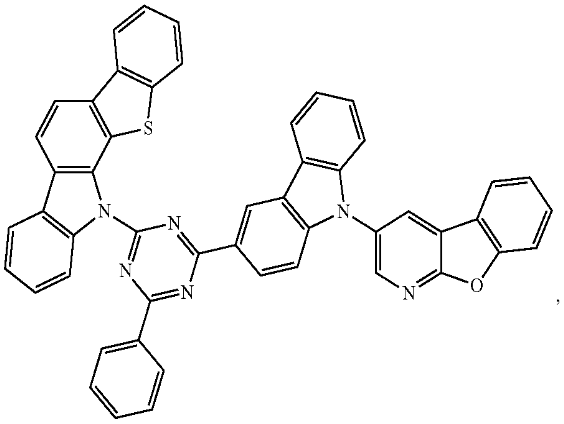

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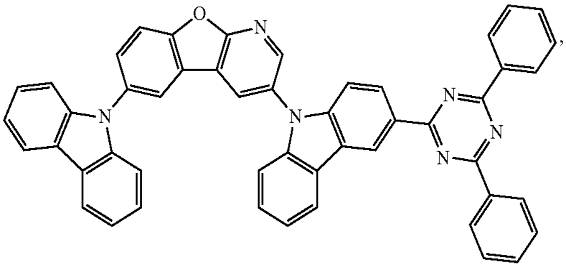

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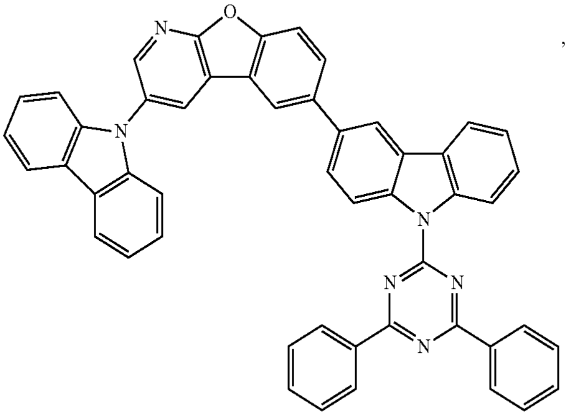

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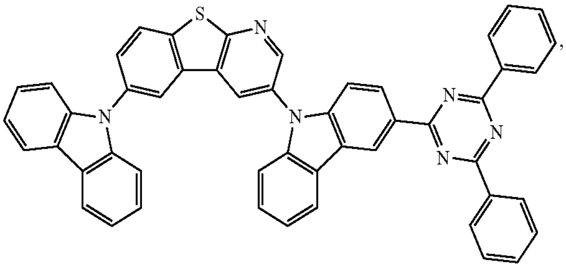

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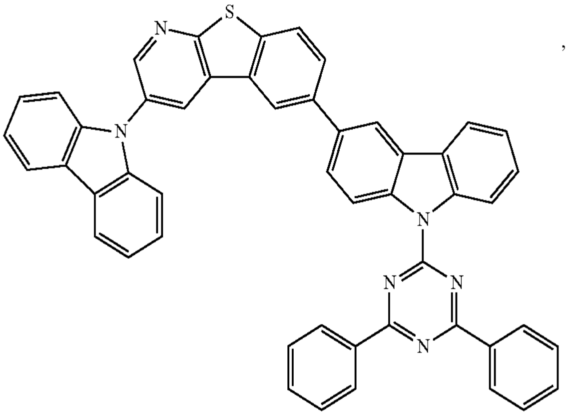

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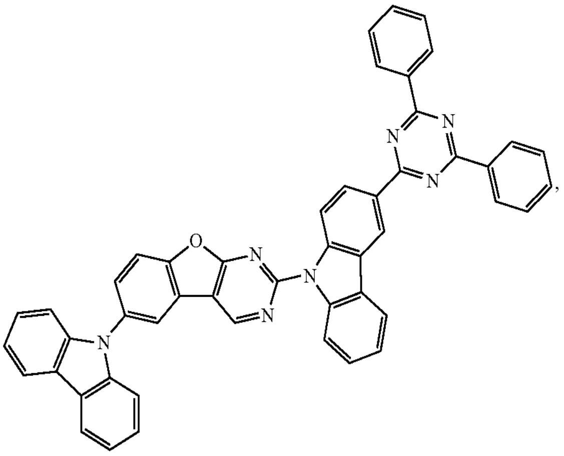

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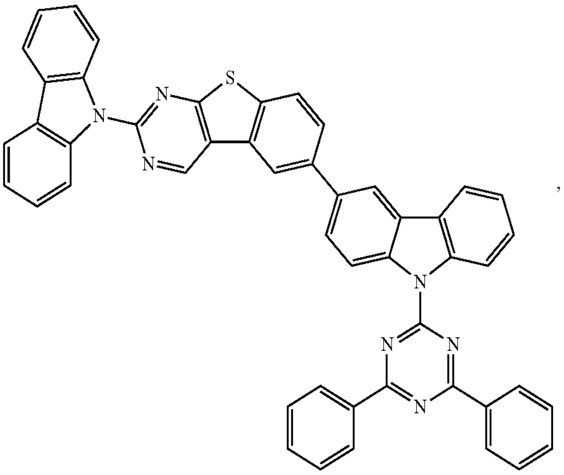

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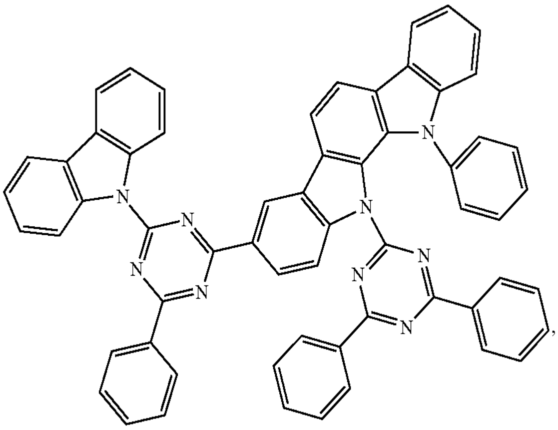

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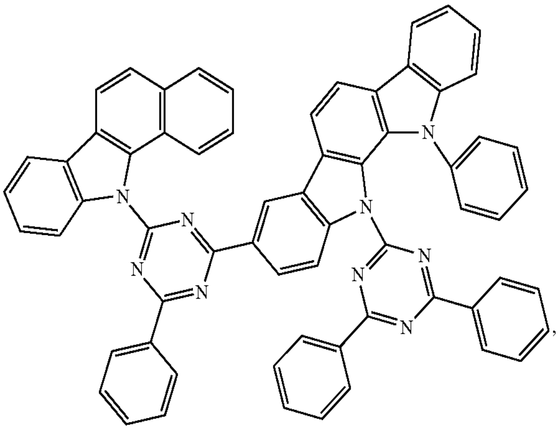

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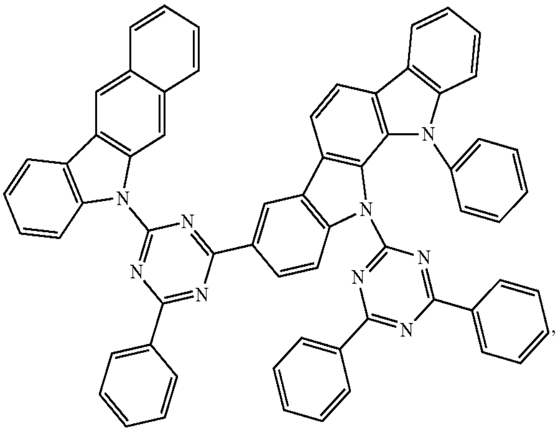

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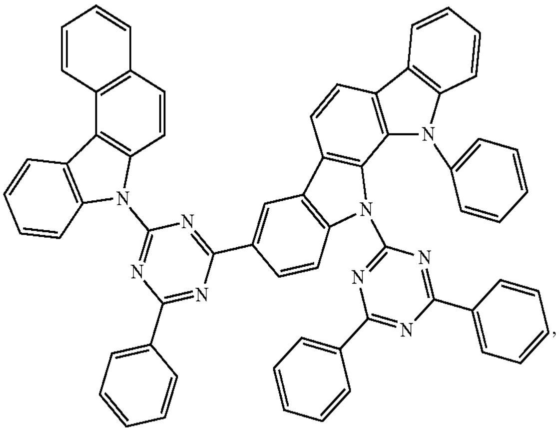

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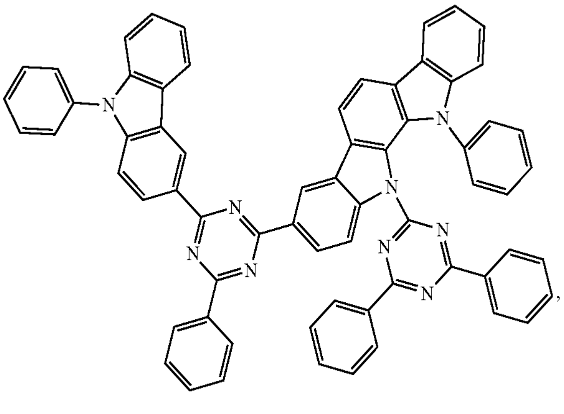

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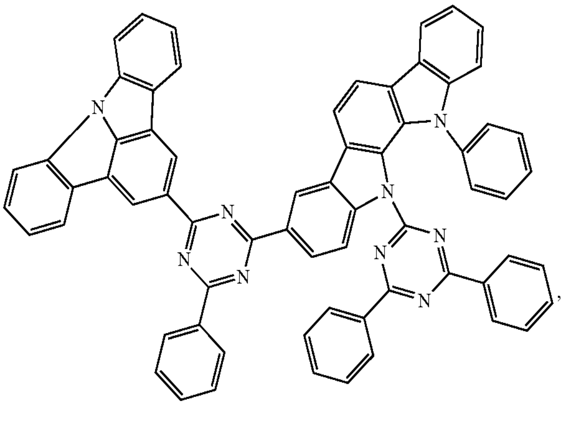

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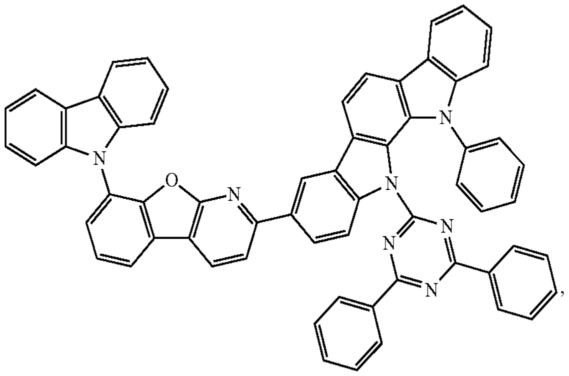

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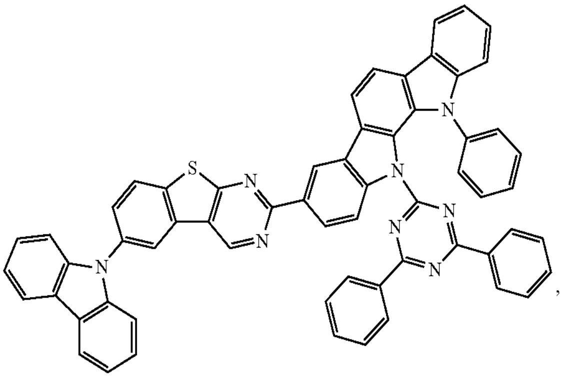

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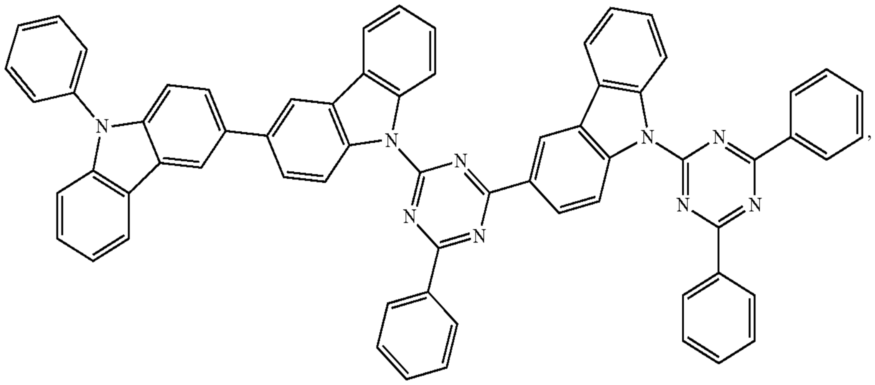

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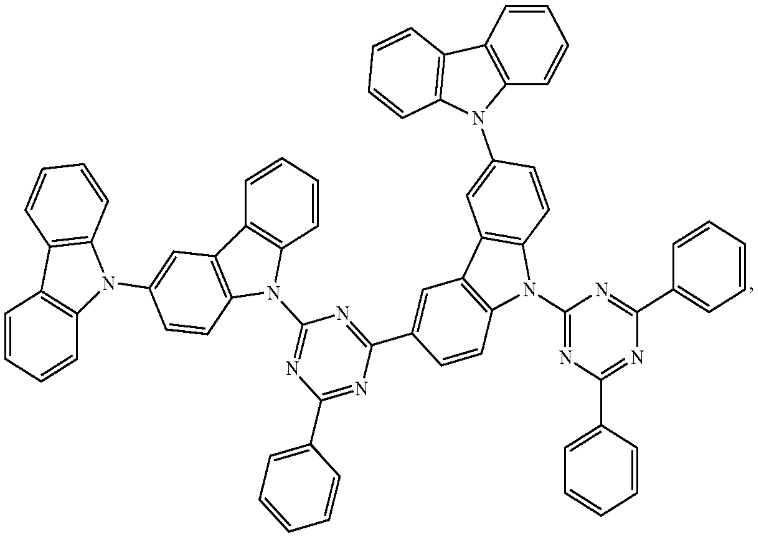

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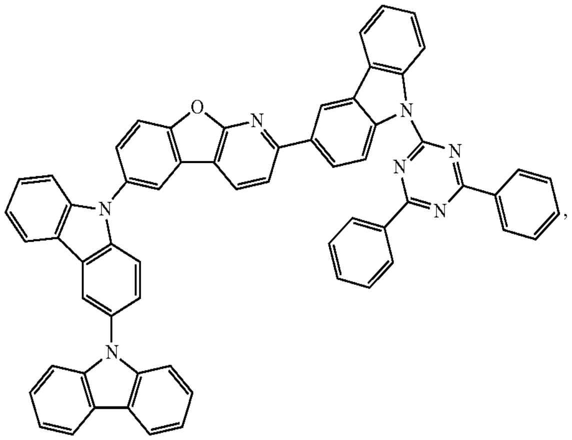

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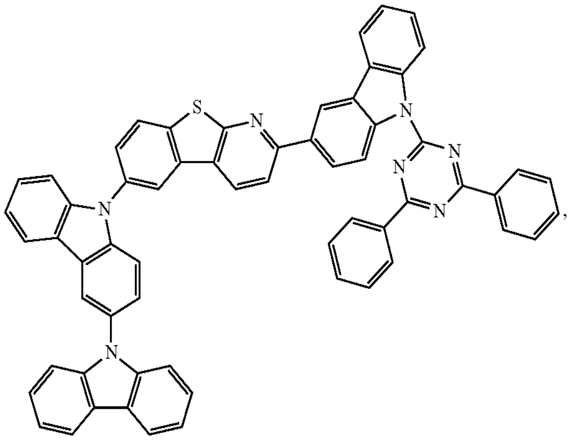

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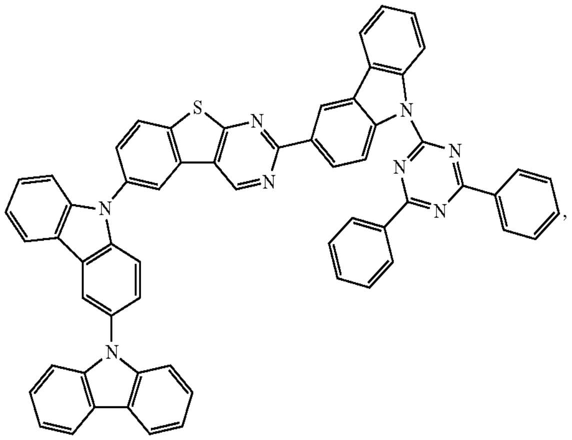

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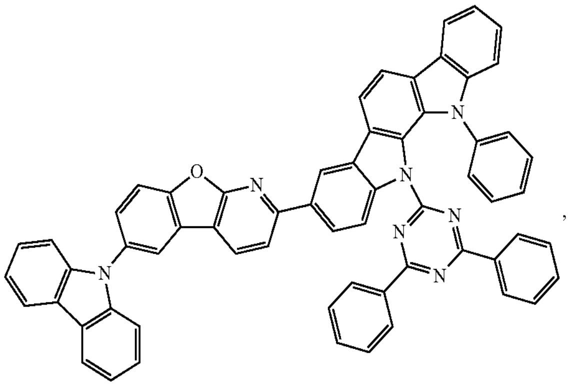

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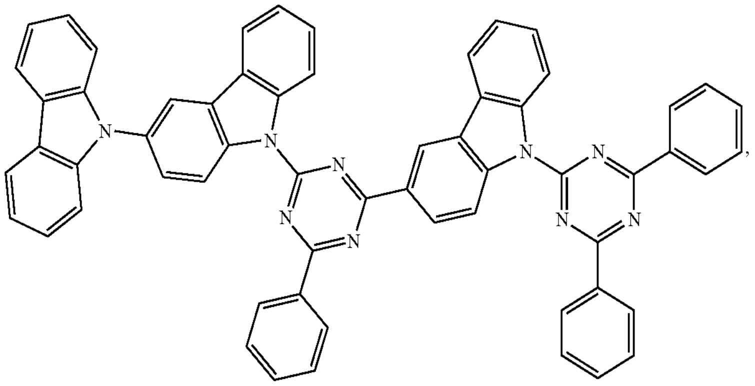

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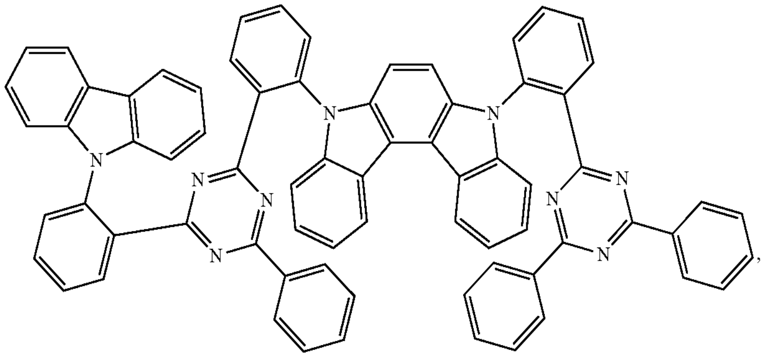

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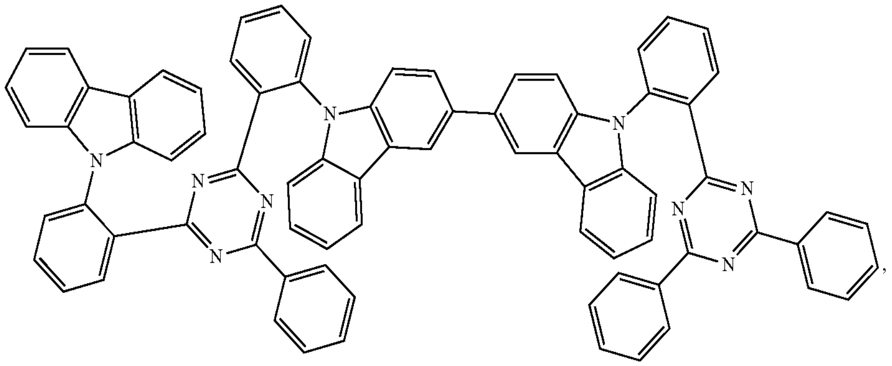

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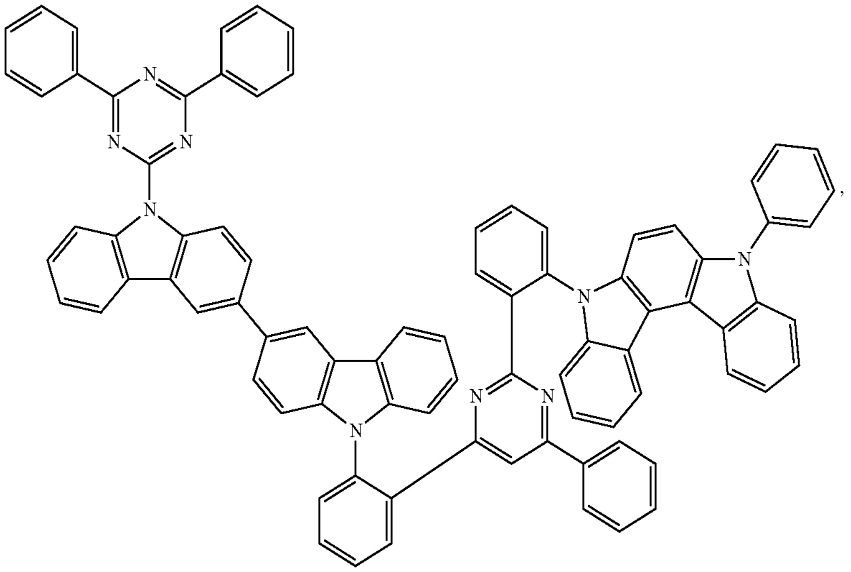

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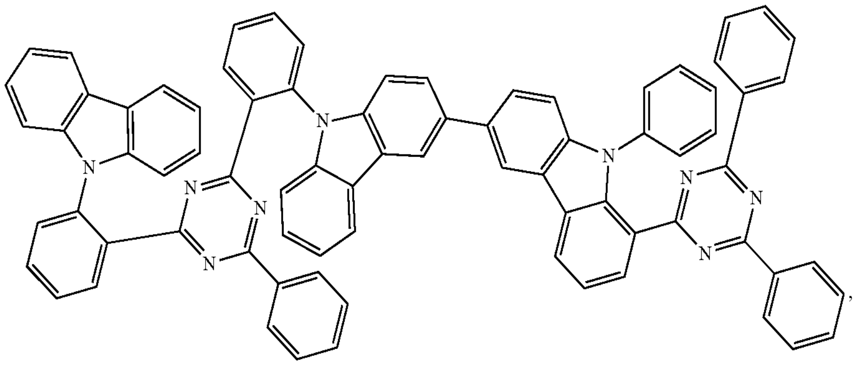

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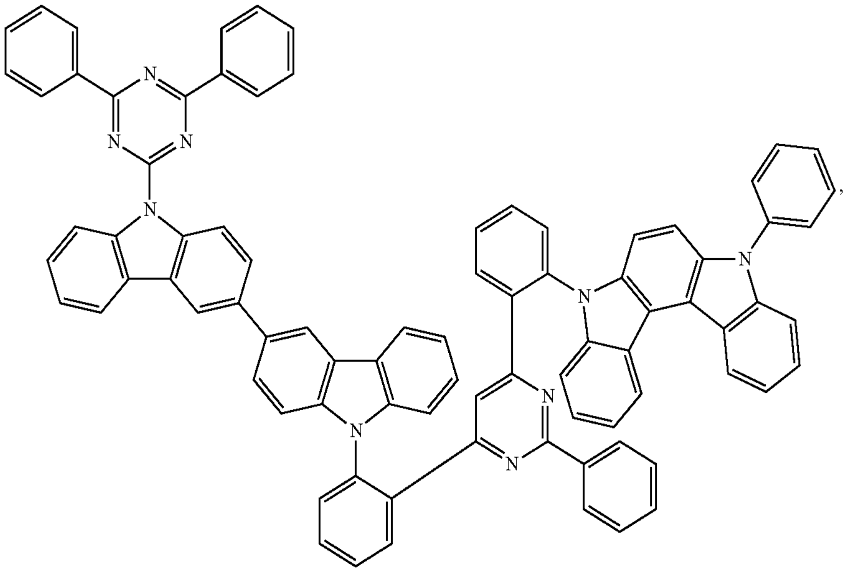

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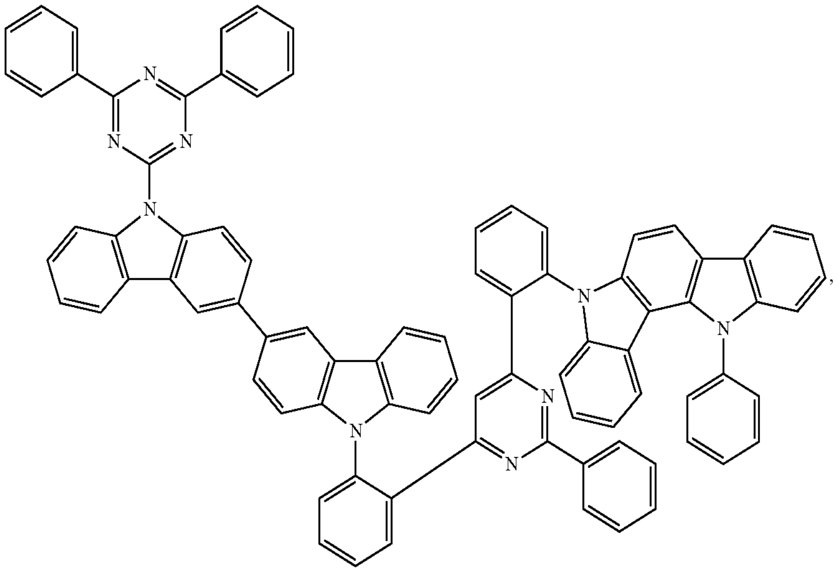

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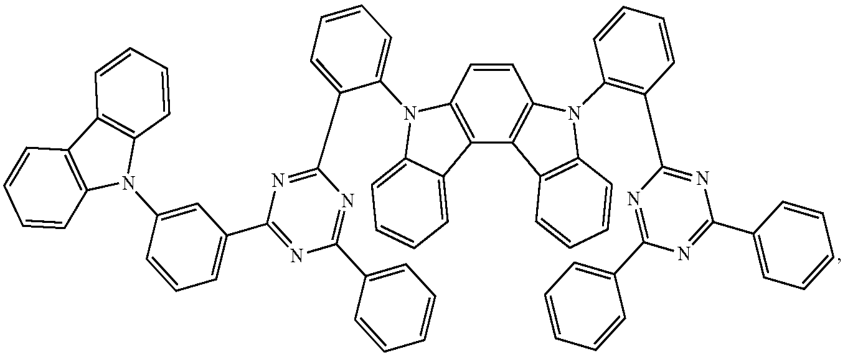

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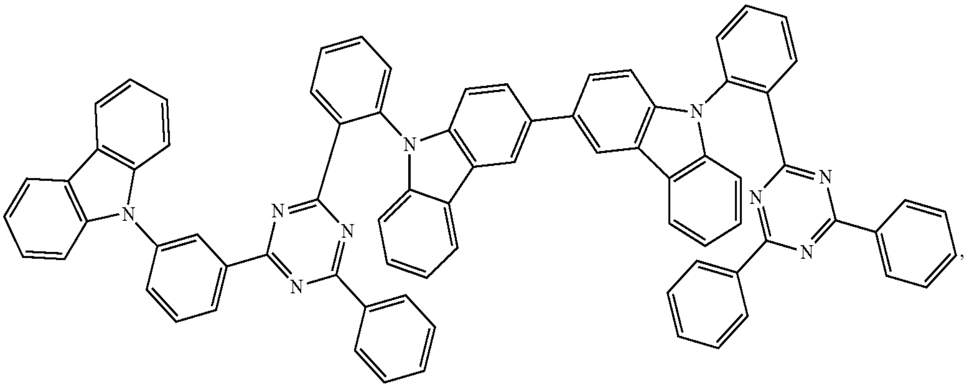

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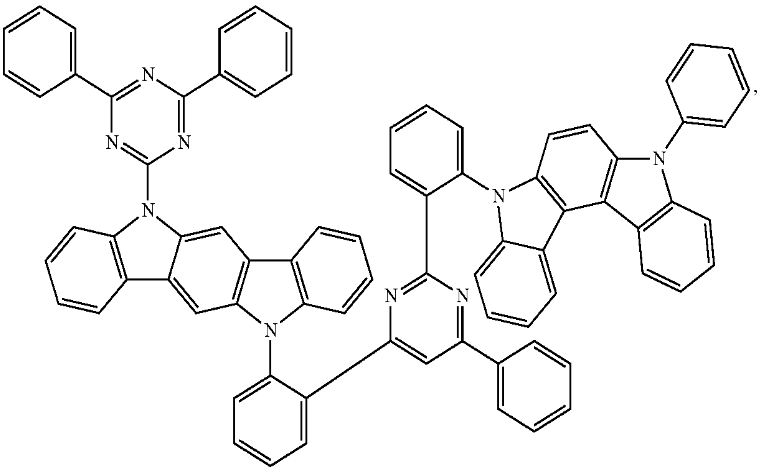

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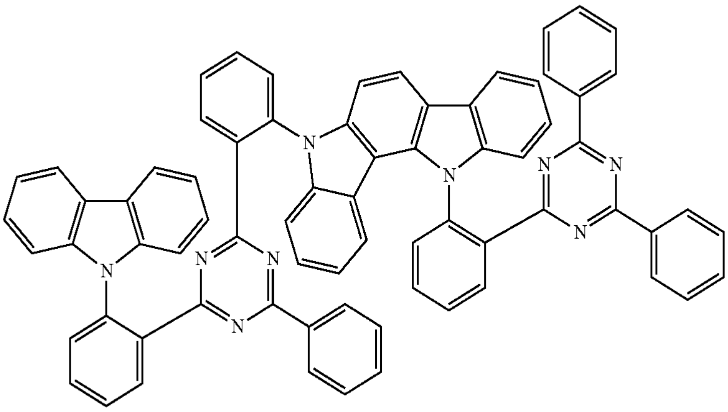

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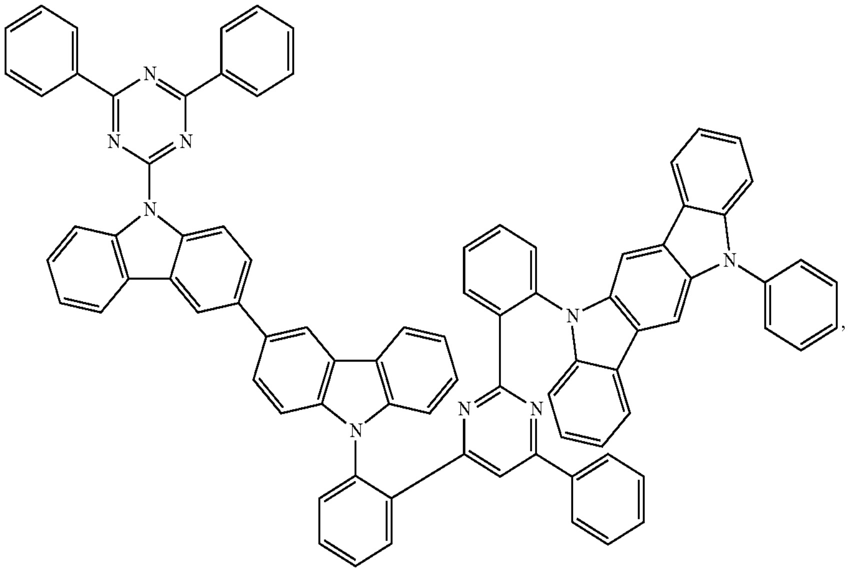

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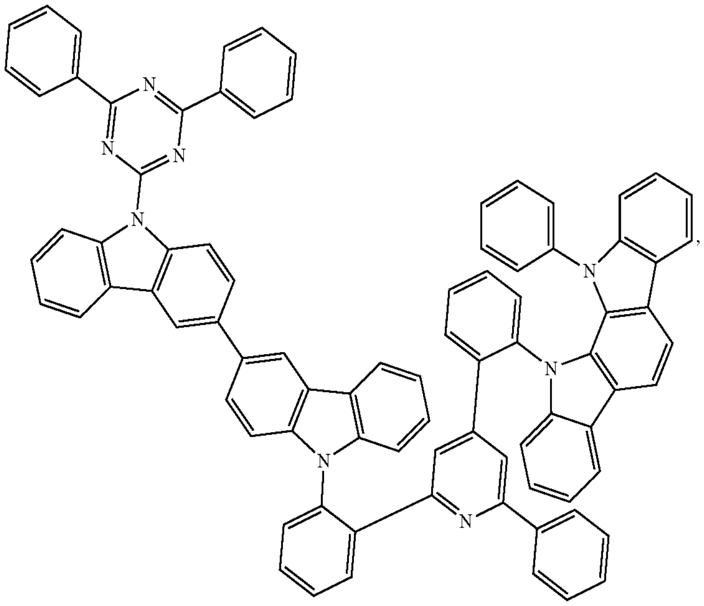

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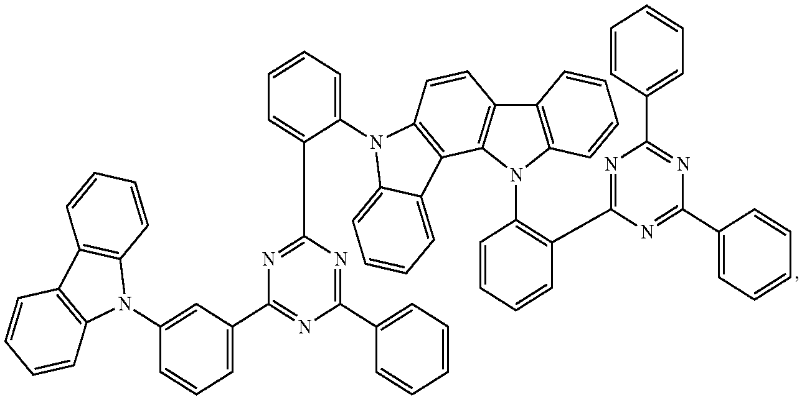

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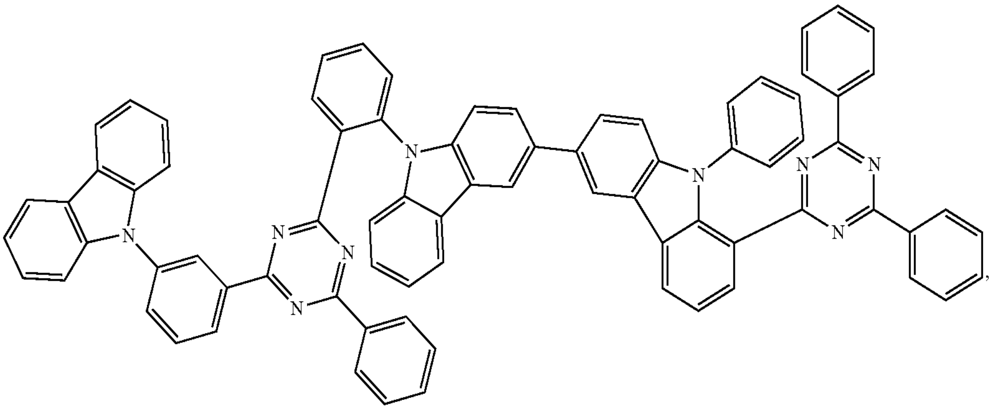
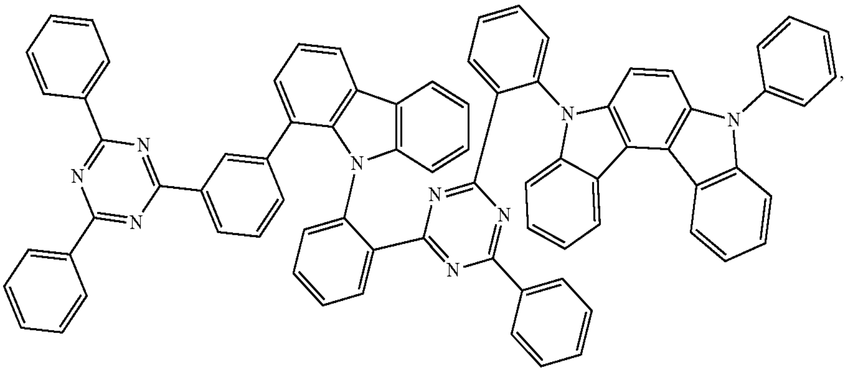


Compound A109



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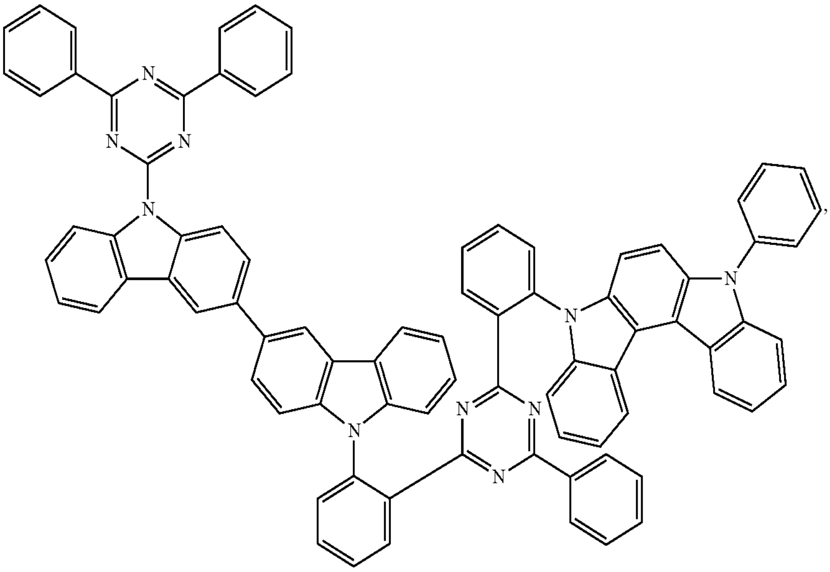

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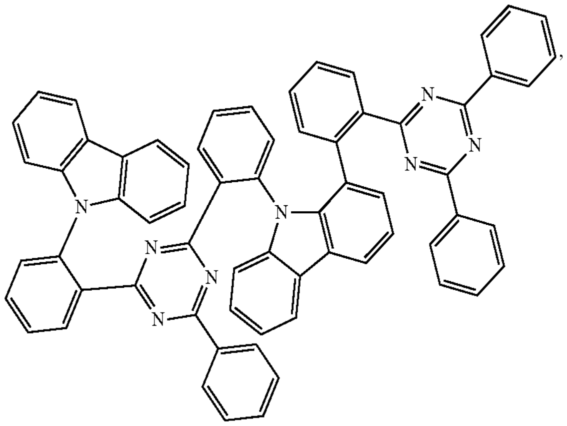

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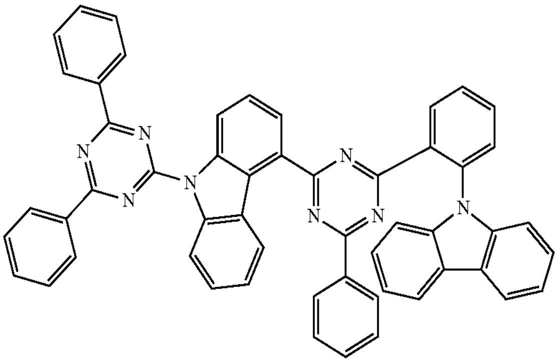

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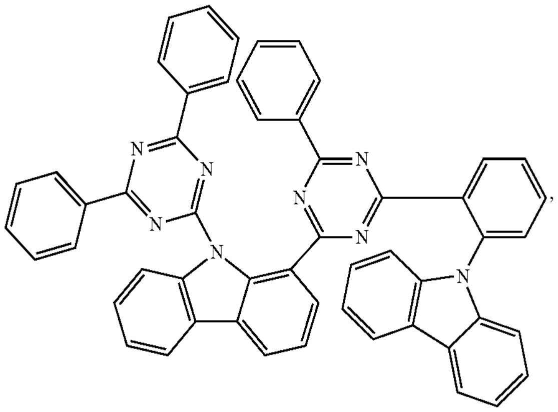

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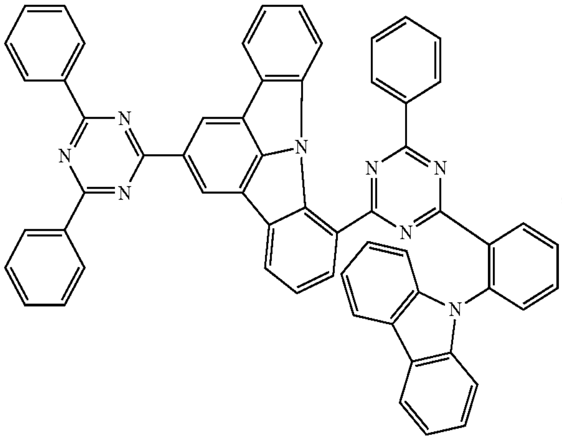

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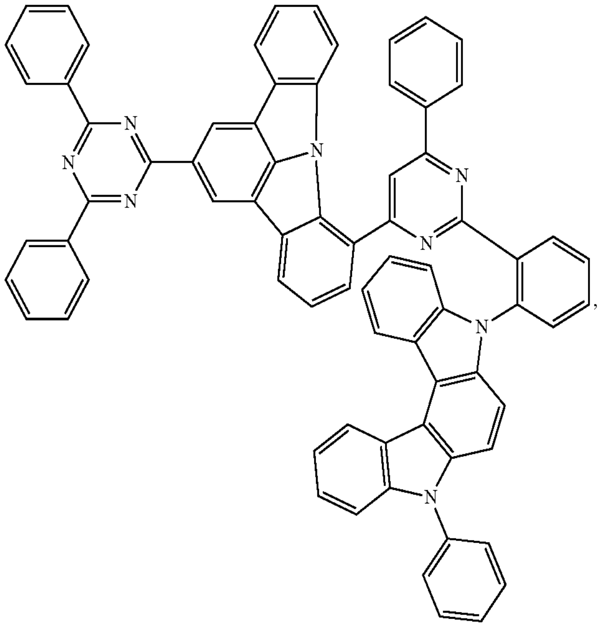

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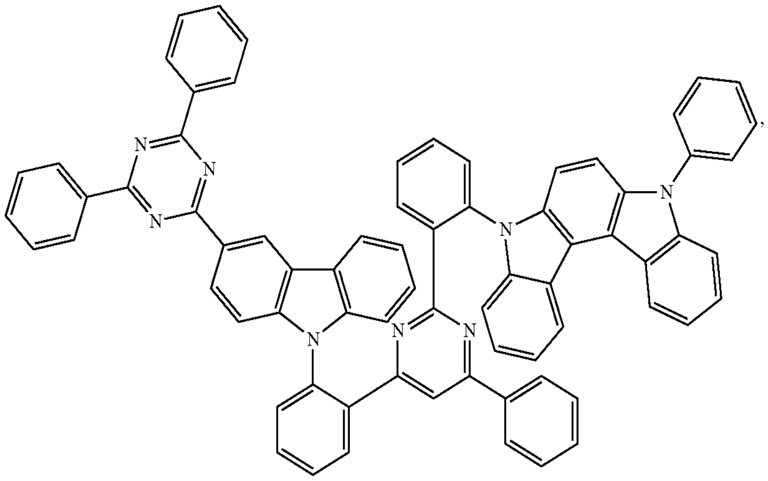

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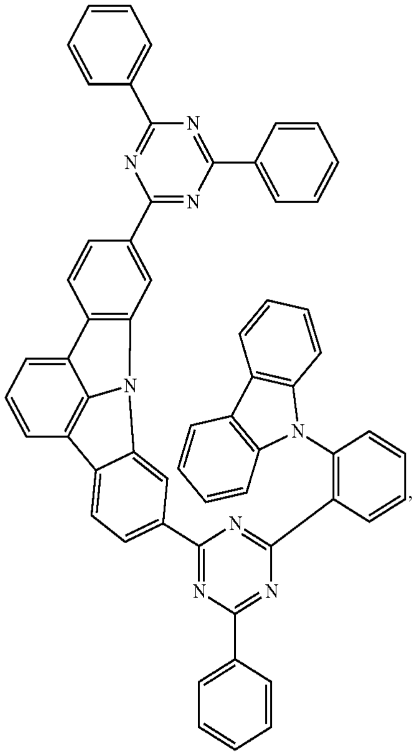

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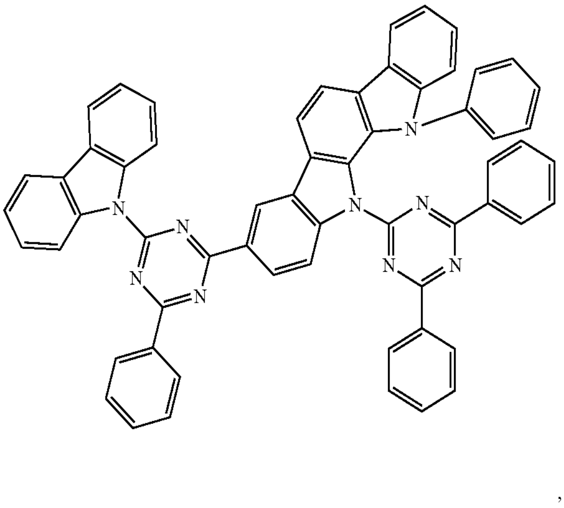

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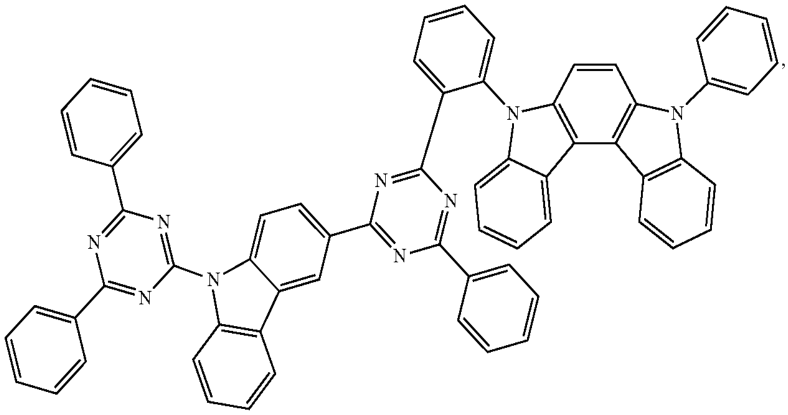

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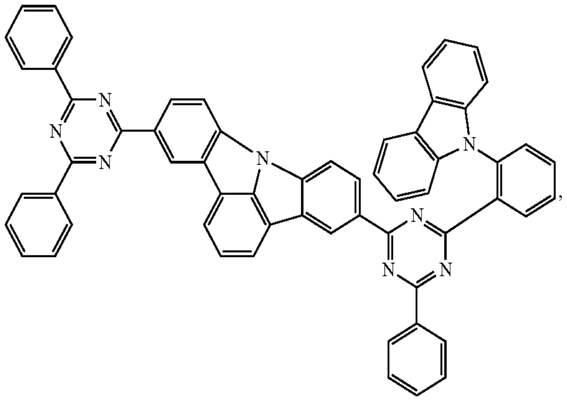

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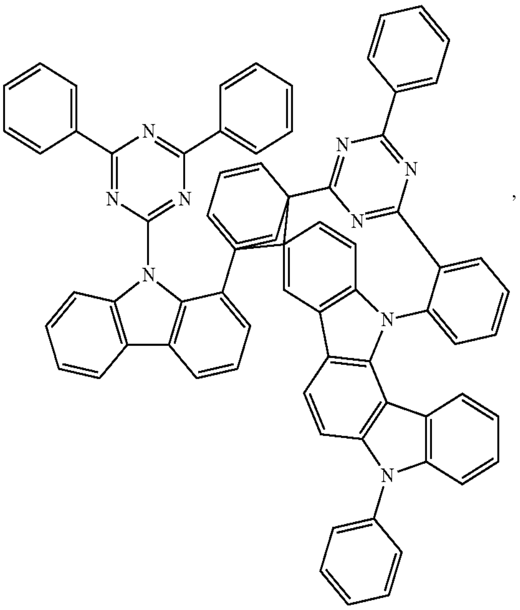
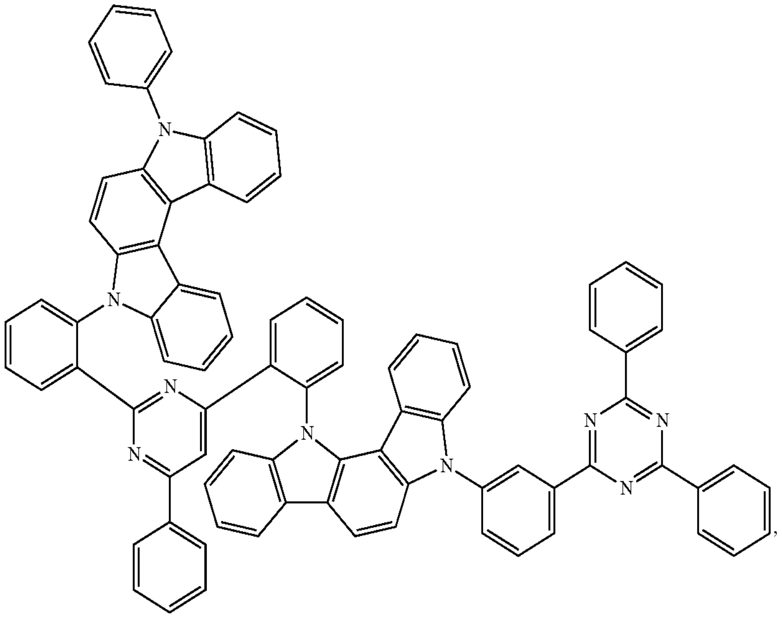


Compound A122



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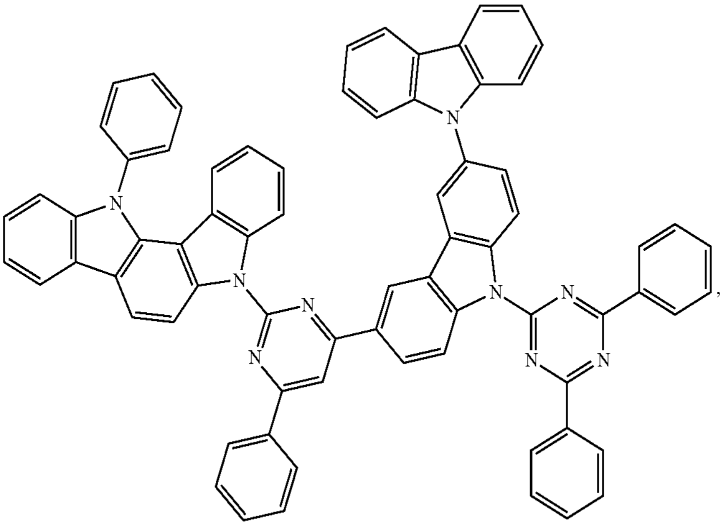
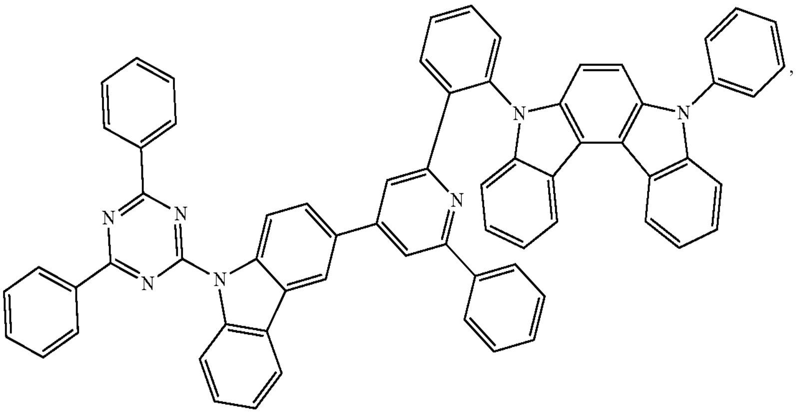
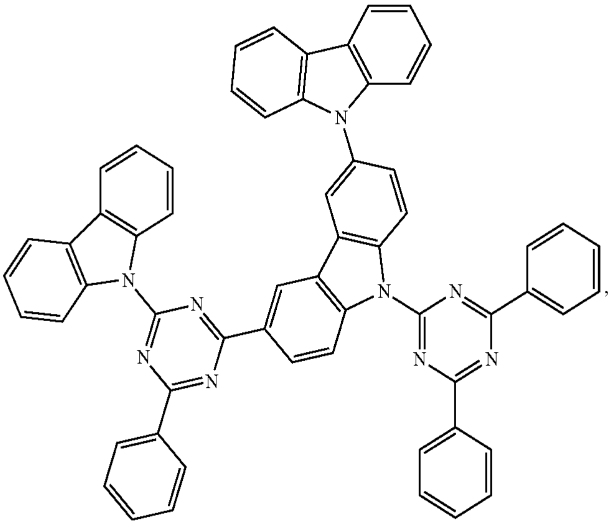
Compound A123



Compound A124



Compound A125



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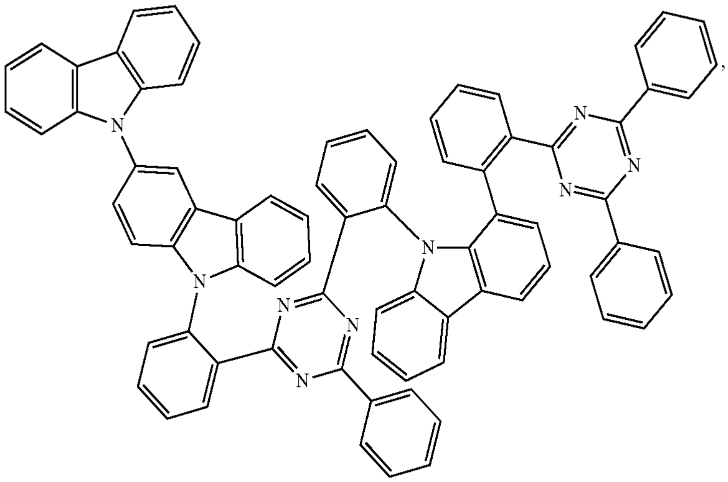
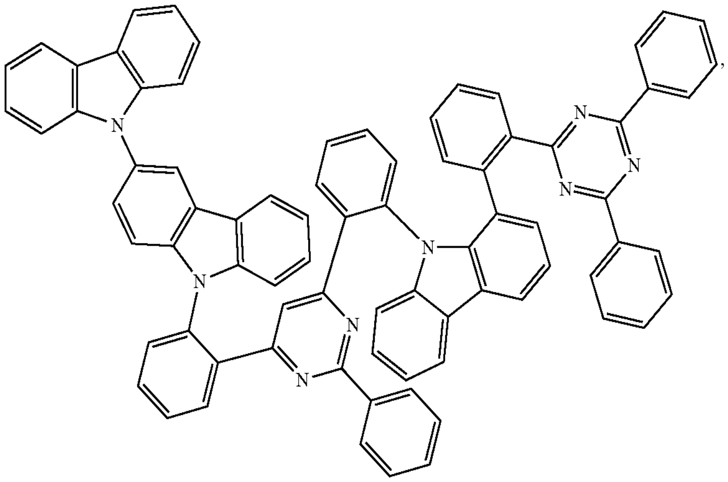
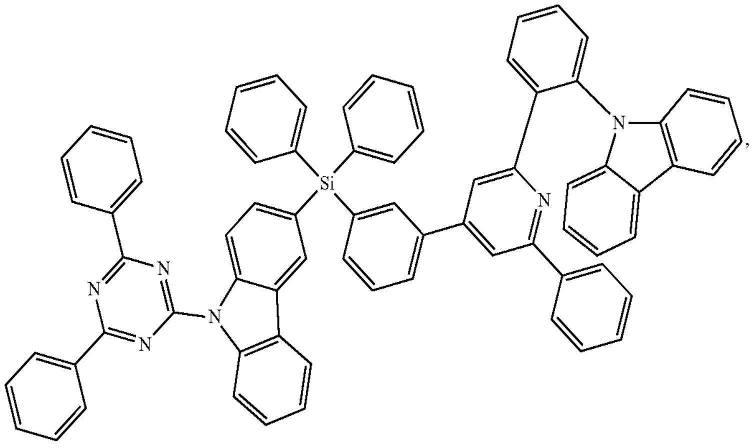


Compound A127



Compound A128



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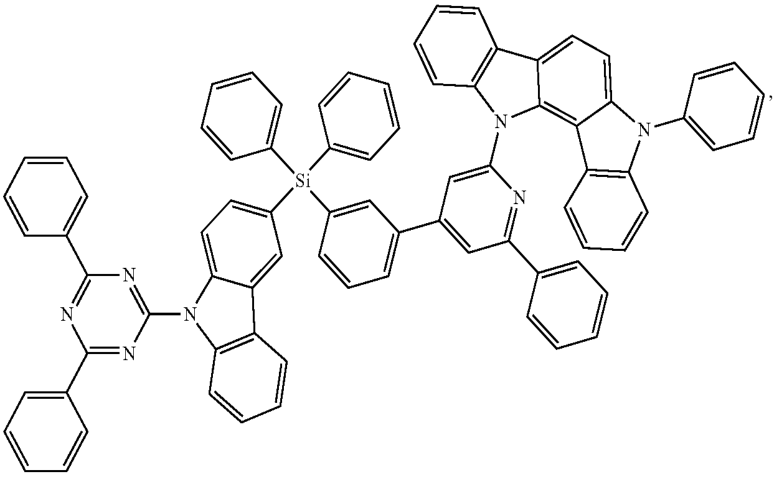

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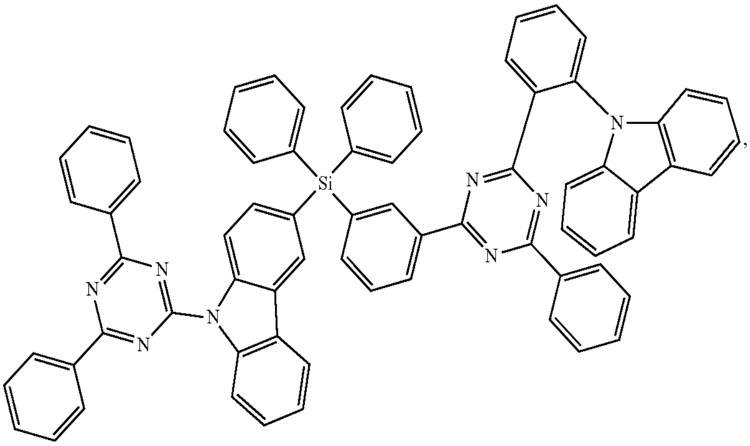
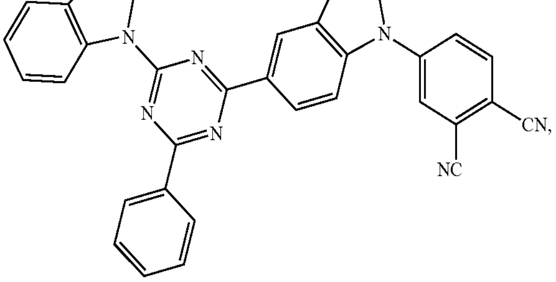


Compound B1



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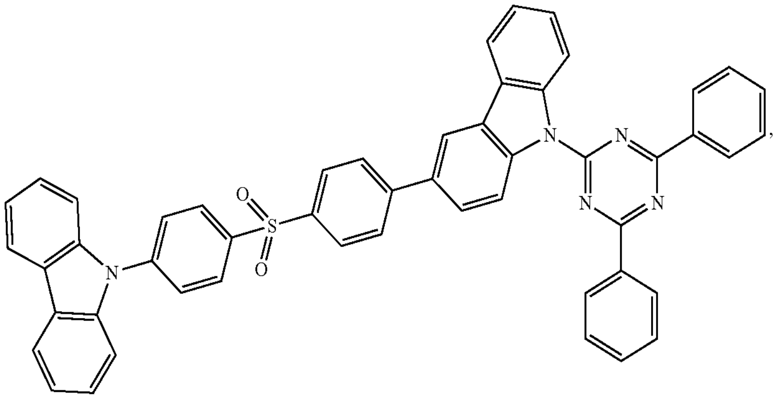
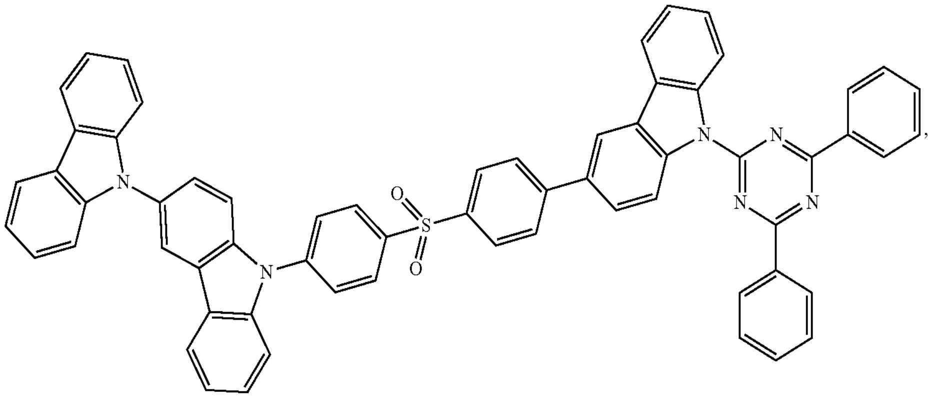
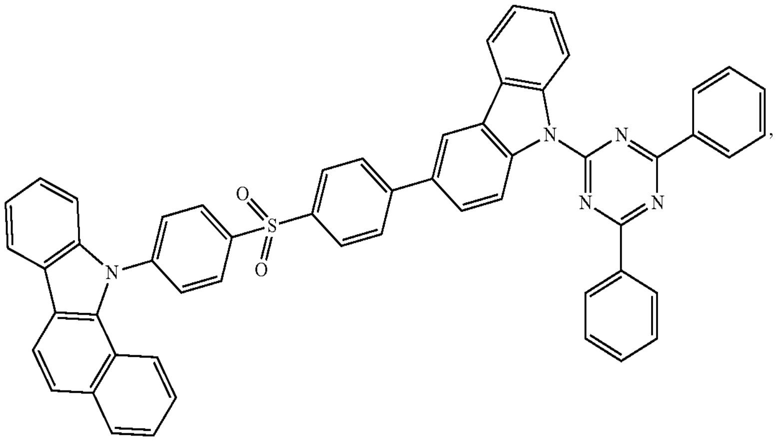
Compound B2



Compound B3



Compound B4



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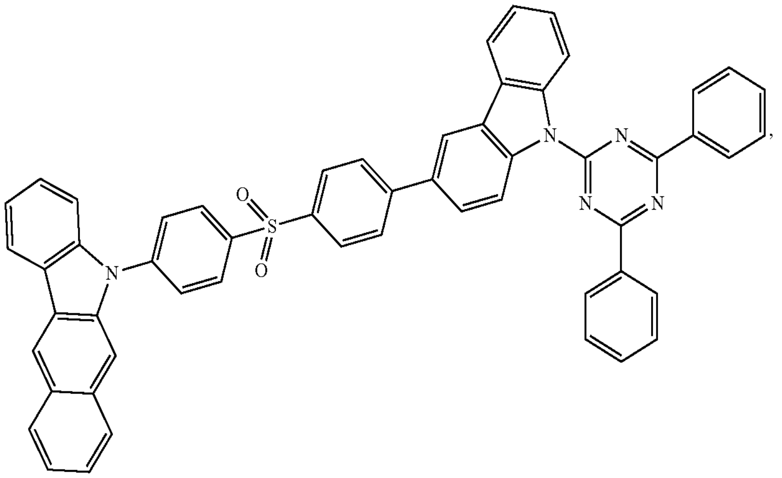
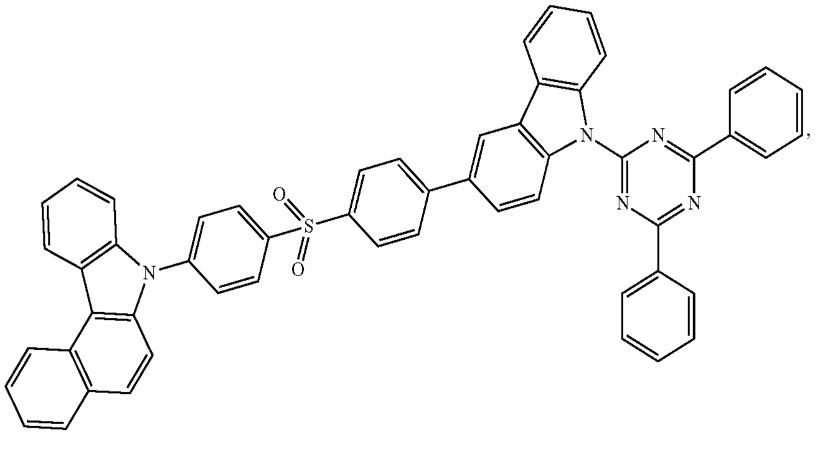
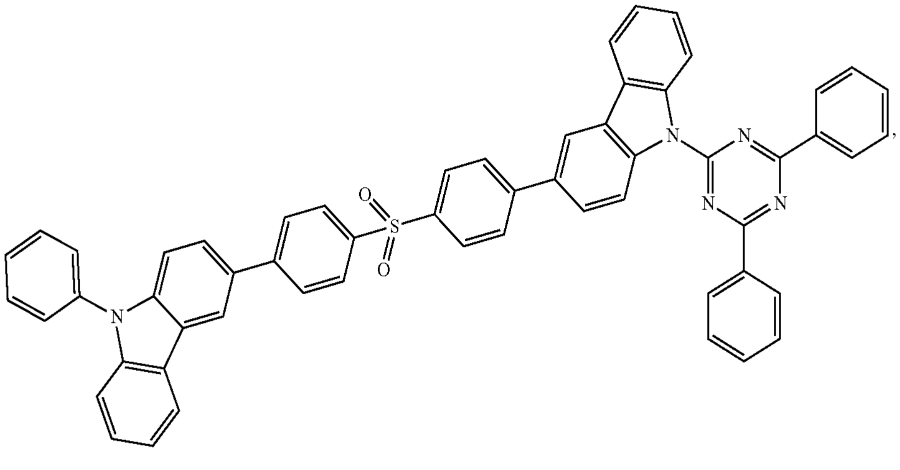
Compound B5



Compound B6



Compound B7



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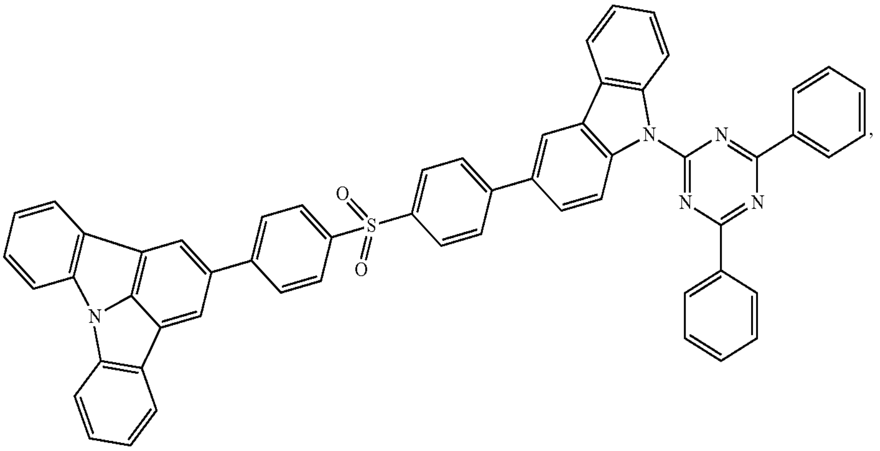
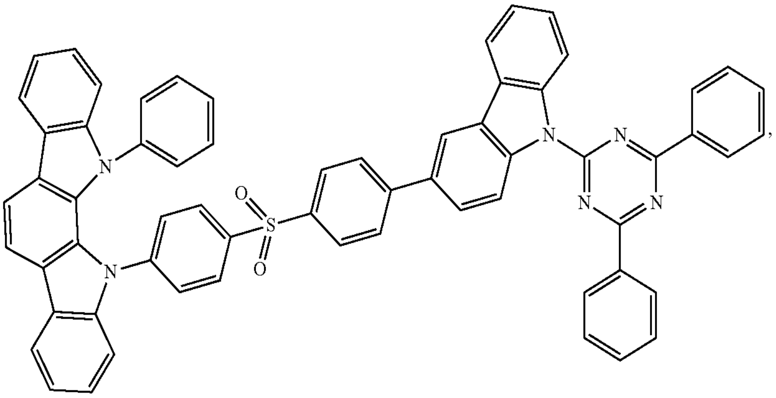
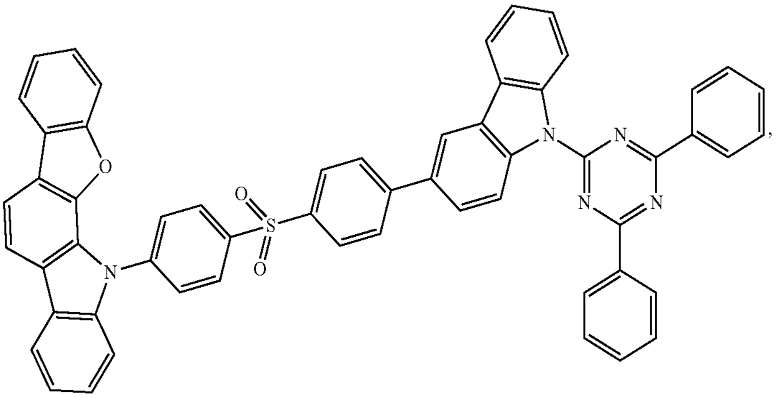
Compound B8



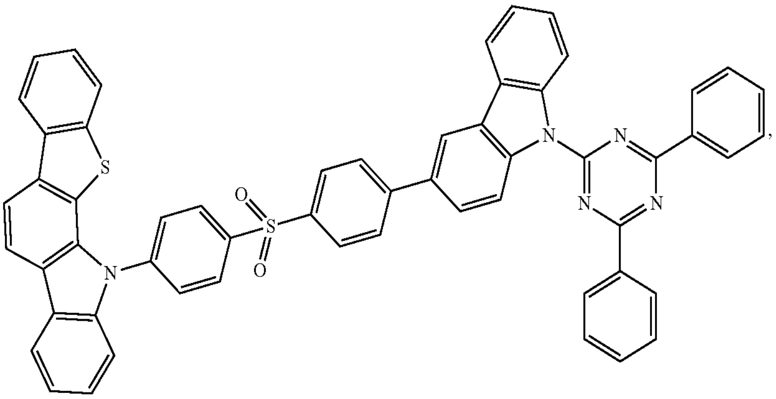
Compound B9



Compound B10



Compound B11



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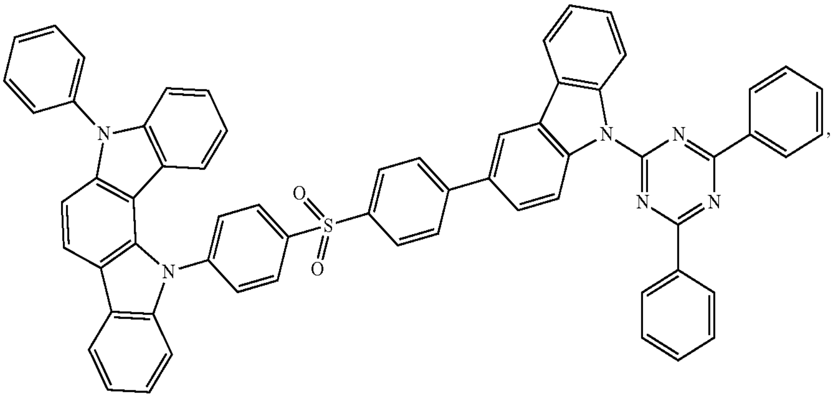
Compound B12



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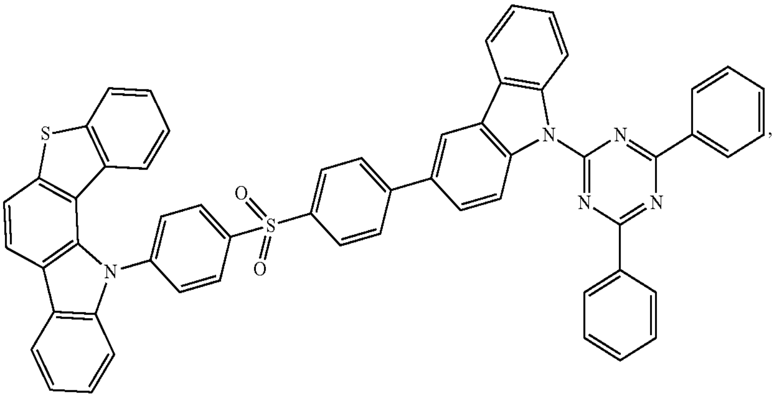
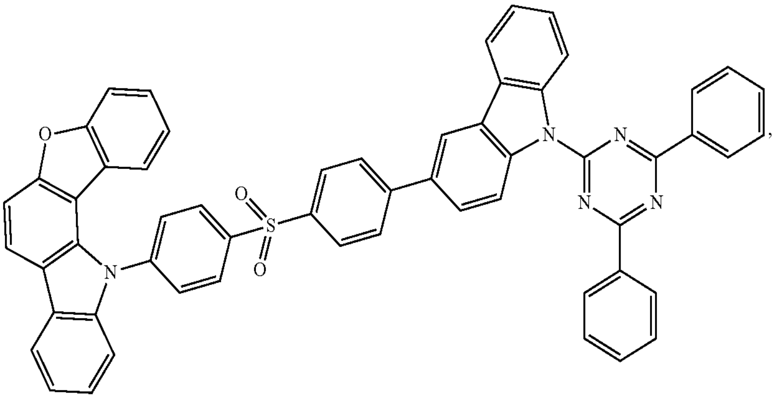
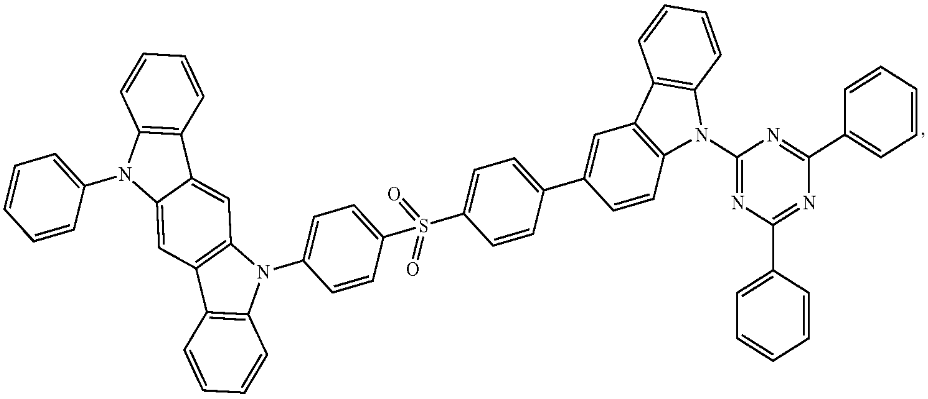


Compound B14



Compound B15



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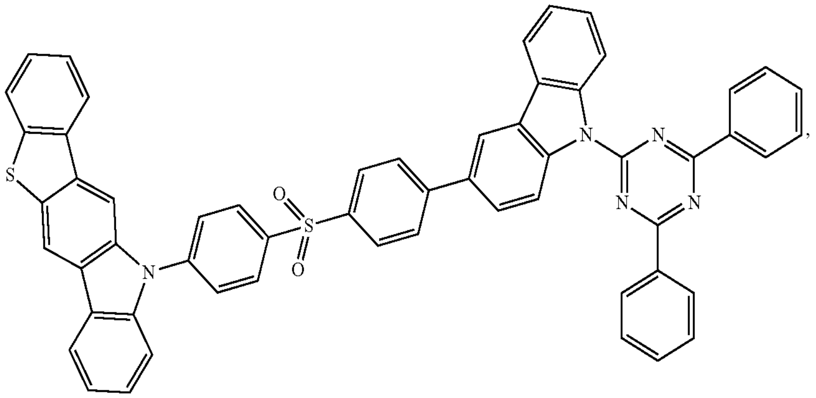
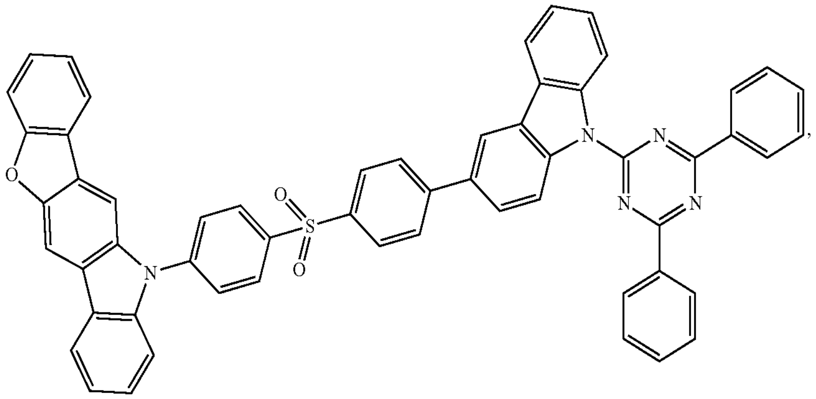
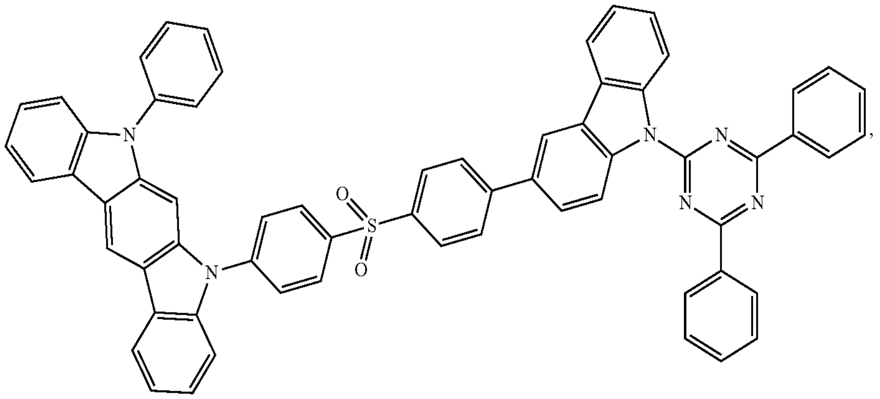
Compound B16



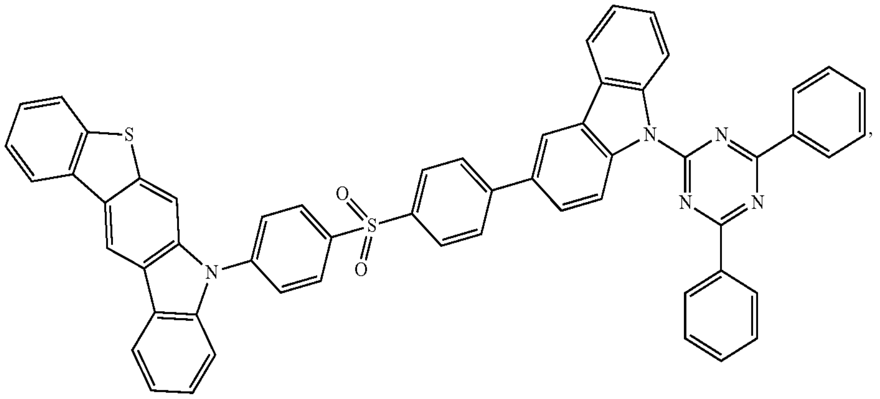
Compound B17



Compound B18



Compound B19



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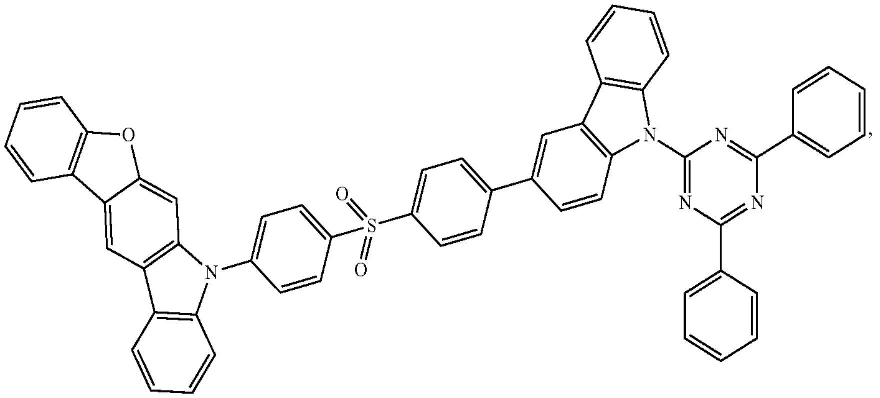
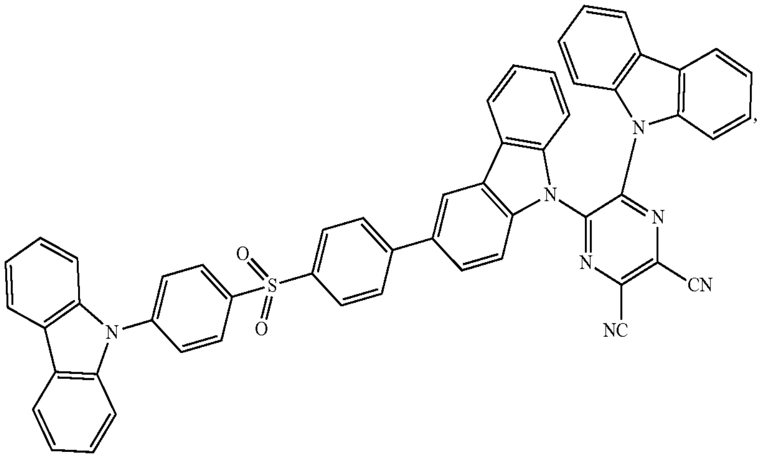
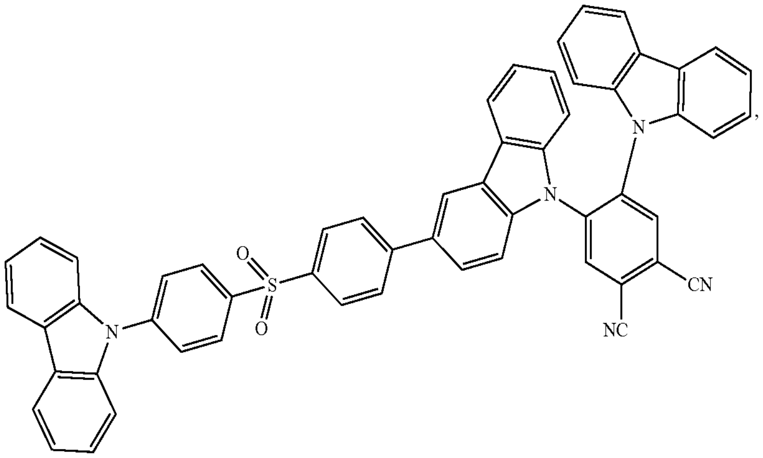
Compound B20



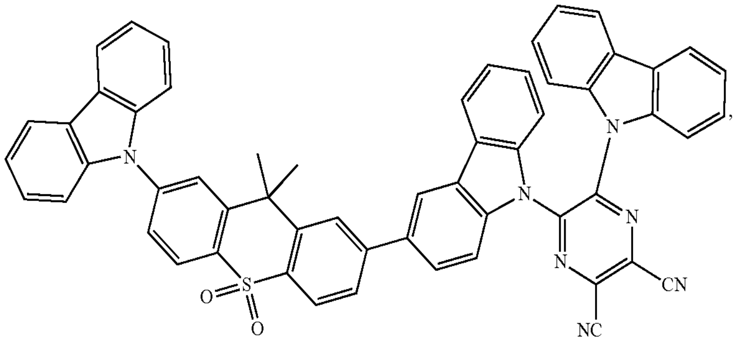
Compound B21



Compound B22



Compound B23



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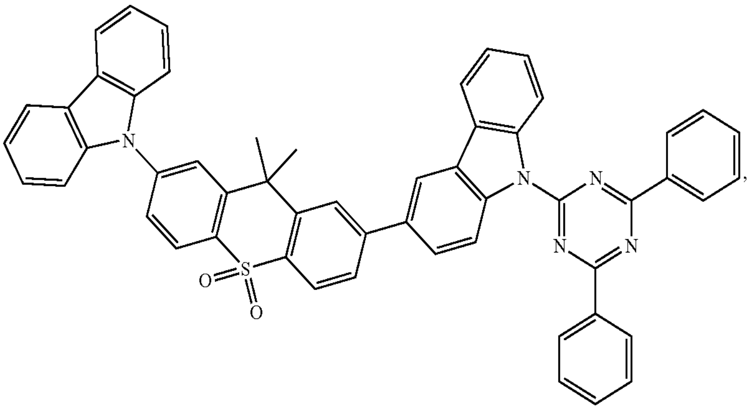
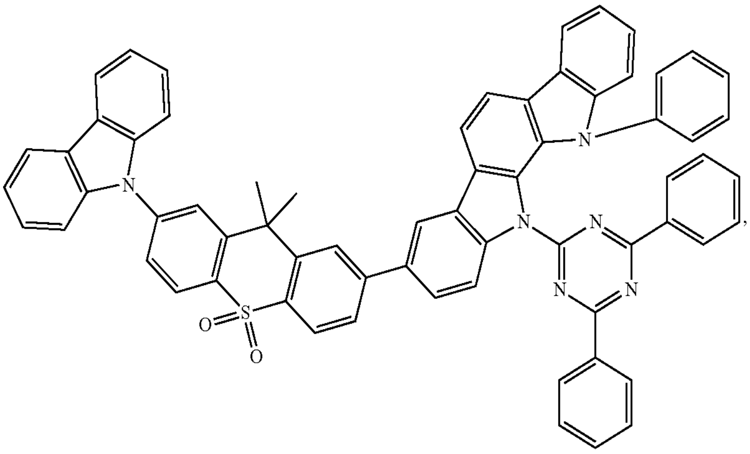
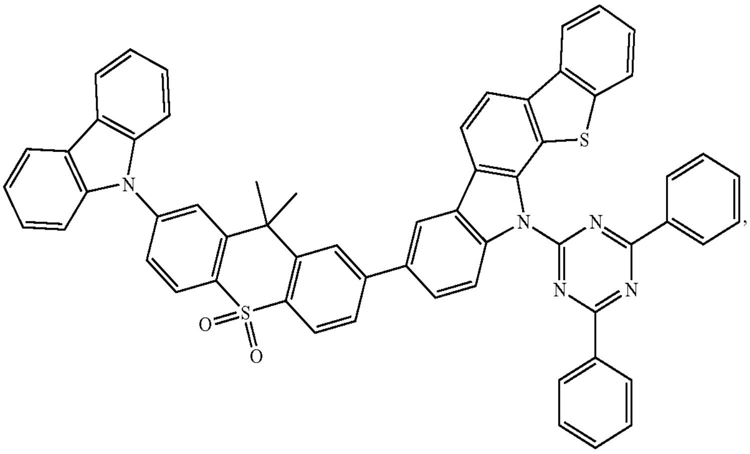
Compound B24



Compound B25



Compound B26



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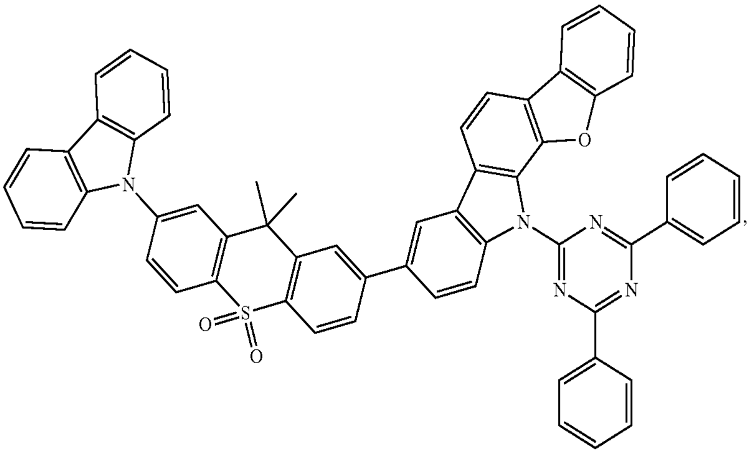
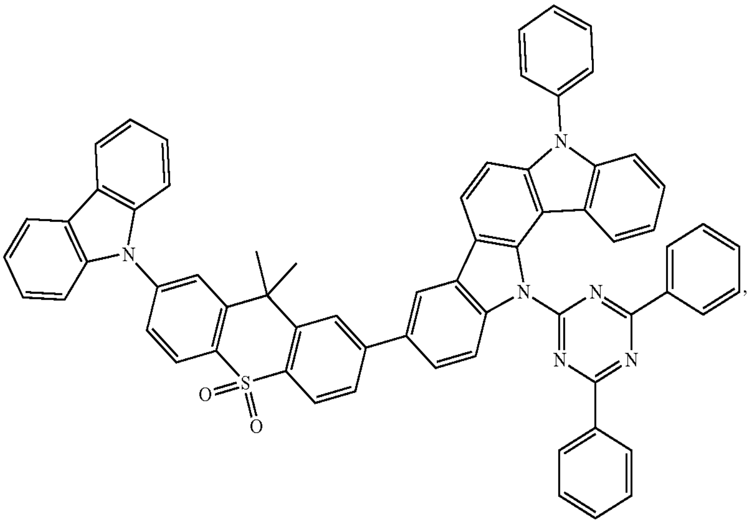
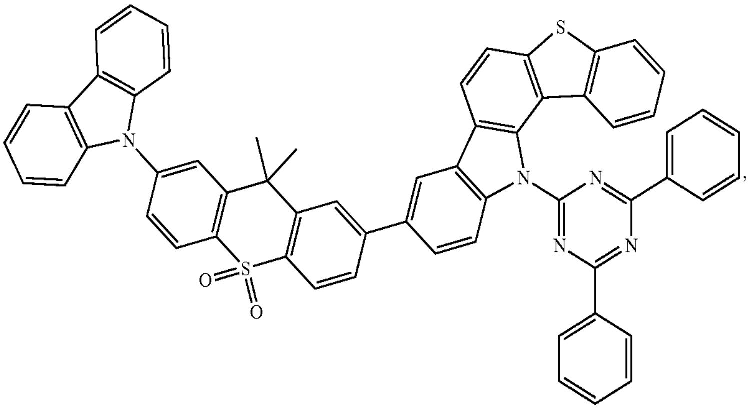
Compound B27



Compound B28



Compound B29



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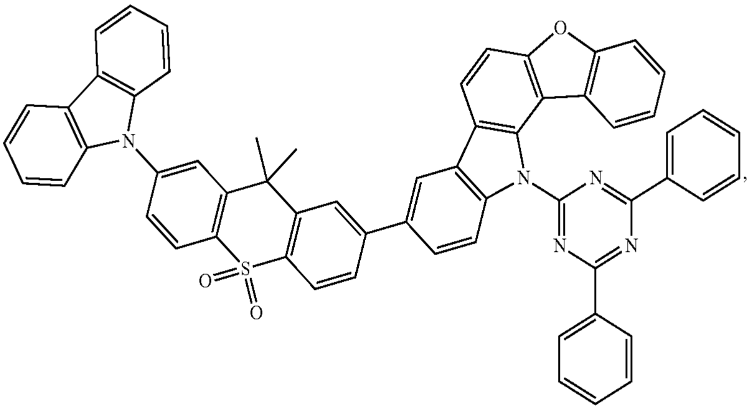
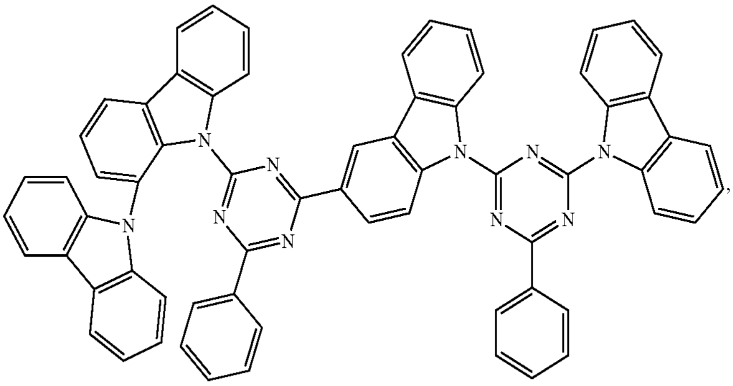
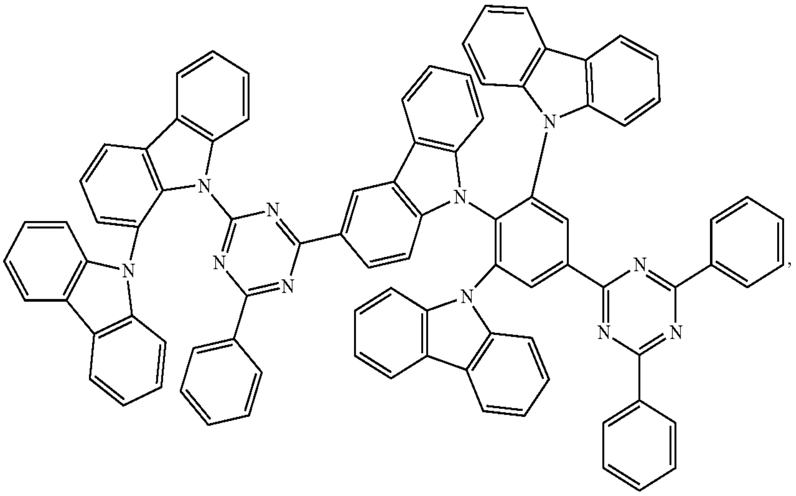
Compound B30



Compound B31



Compound B32



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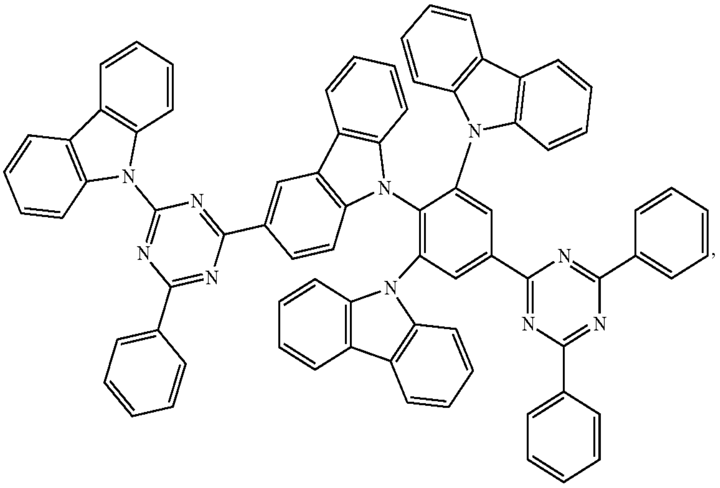
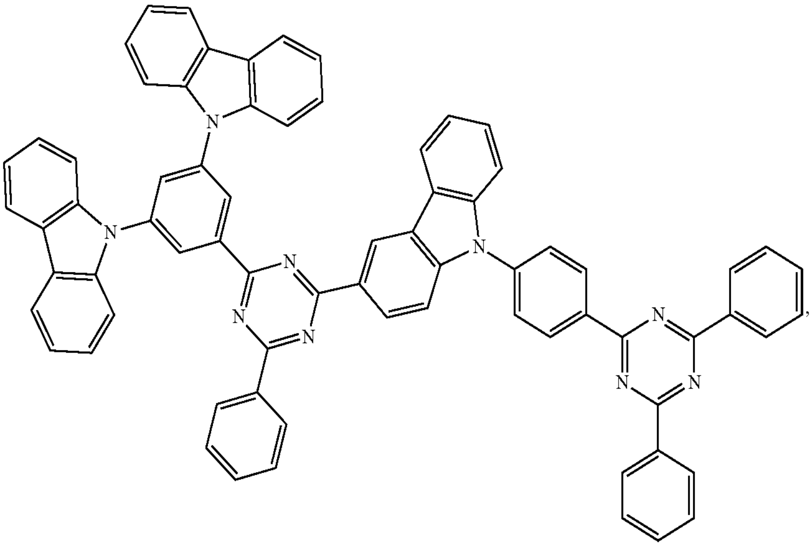
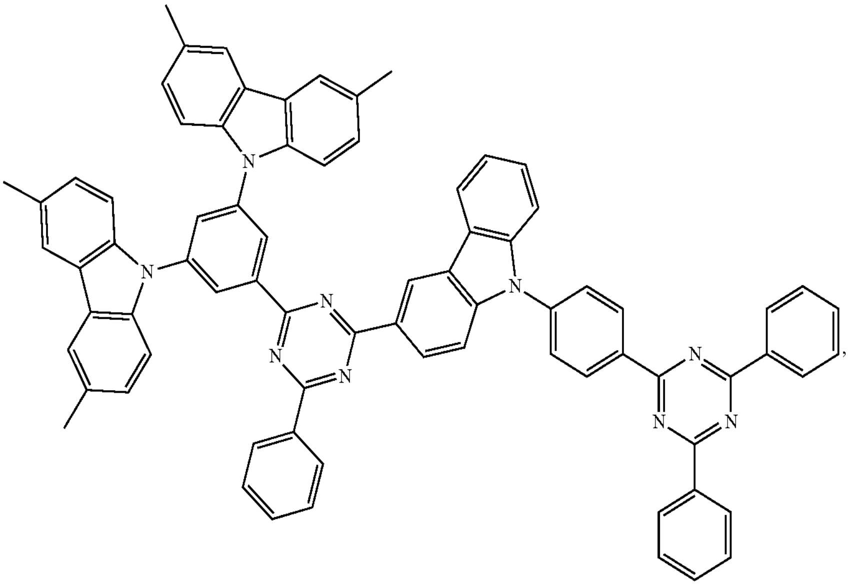
Compound B33



Compound B34



Compound B35



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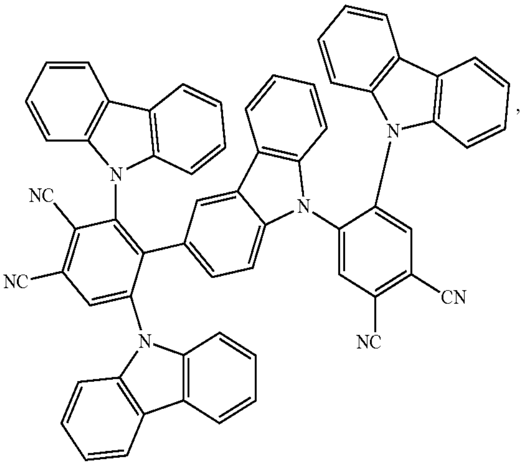
Compound B36



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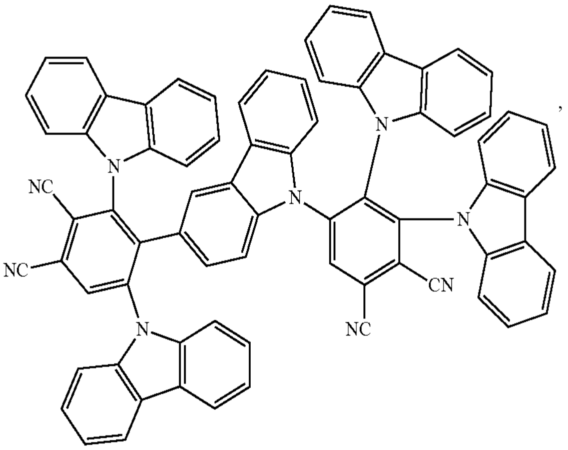
Compound B37



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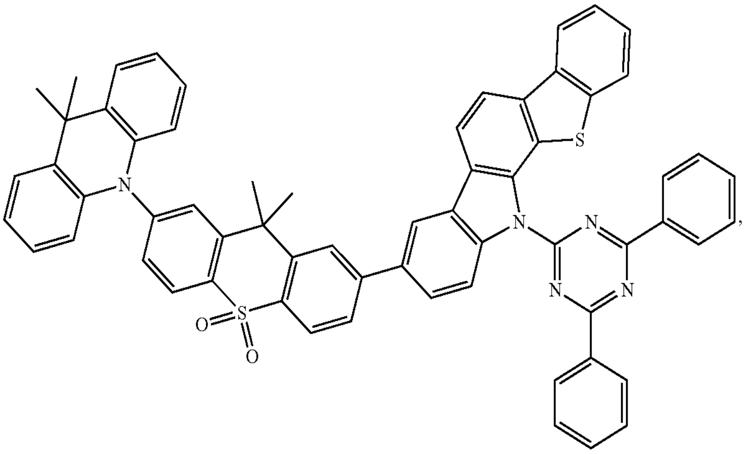
Compound B38



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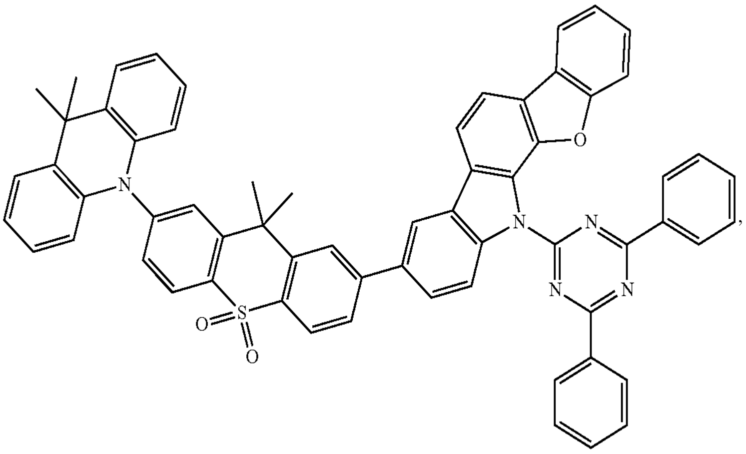
Compound B38



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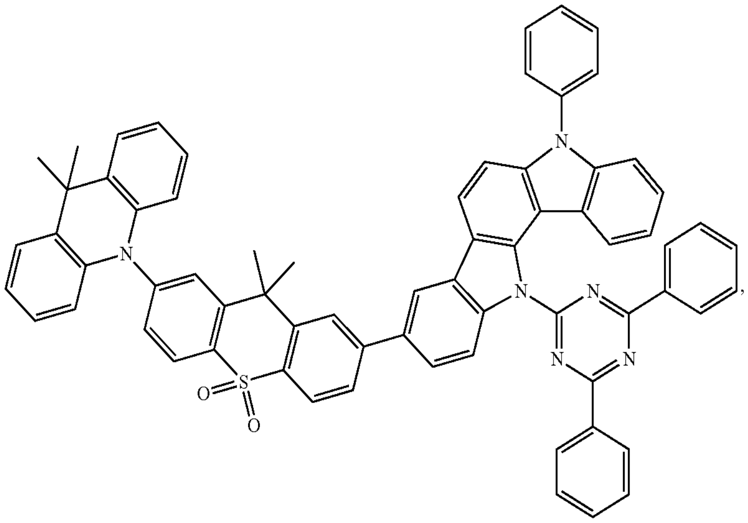
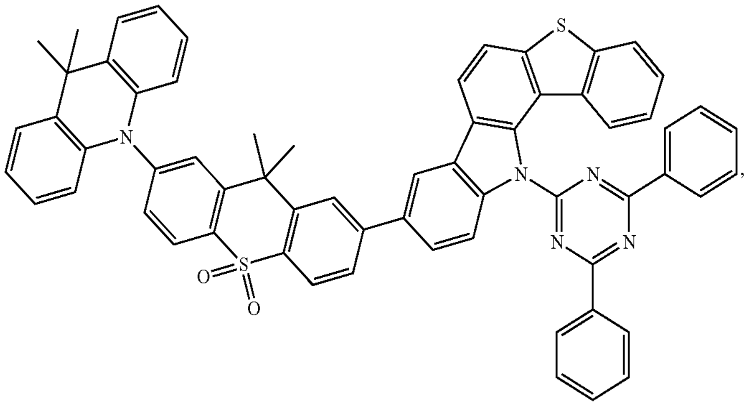
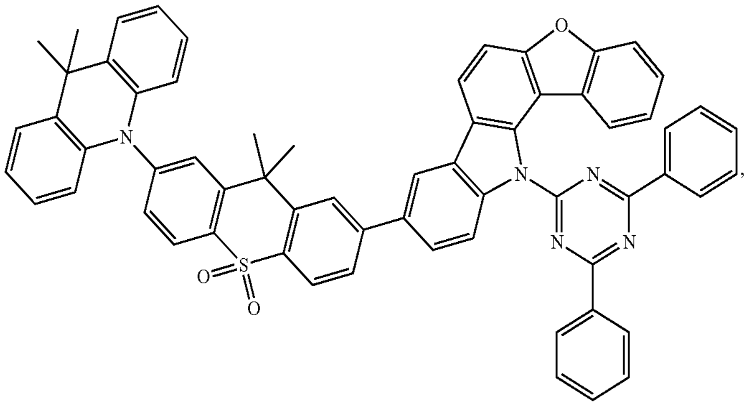
Compound B39



Compound B40



Compound B41



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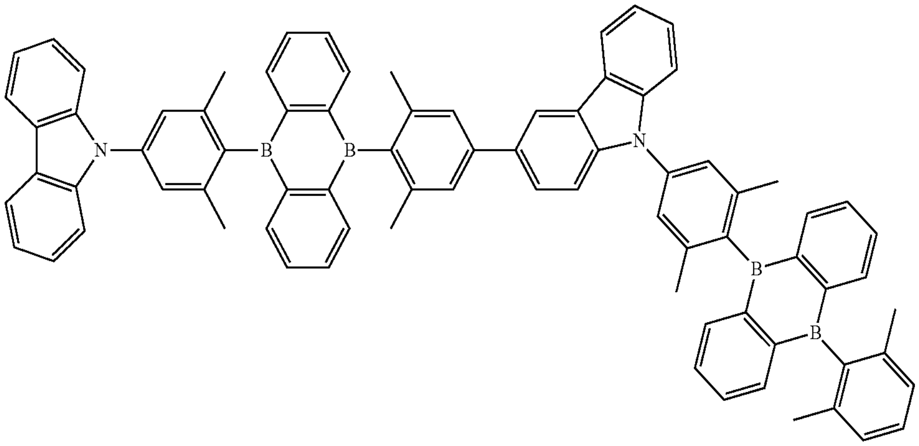
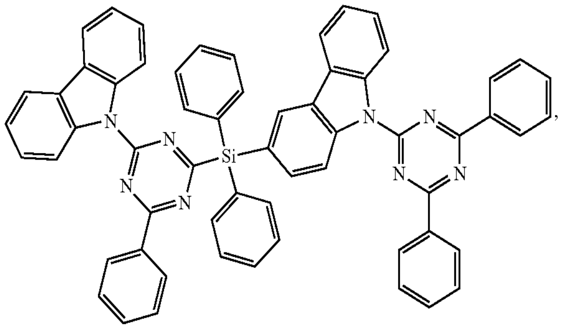
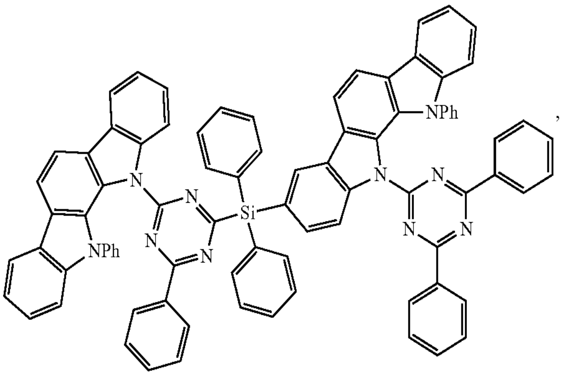
Compound B42



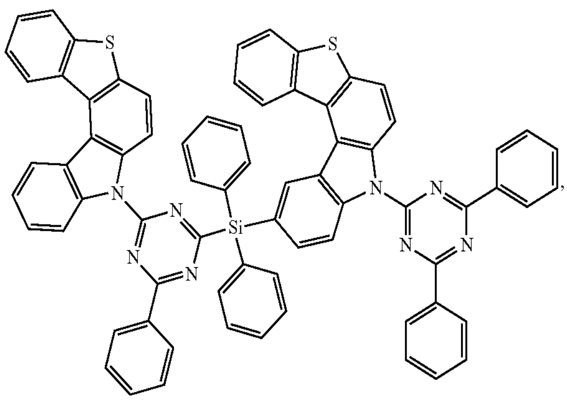
Compound B43



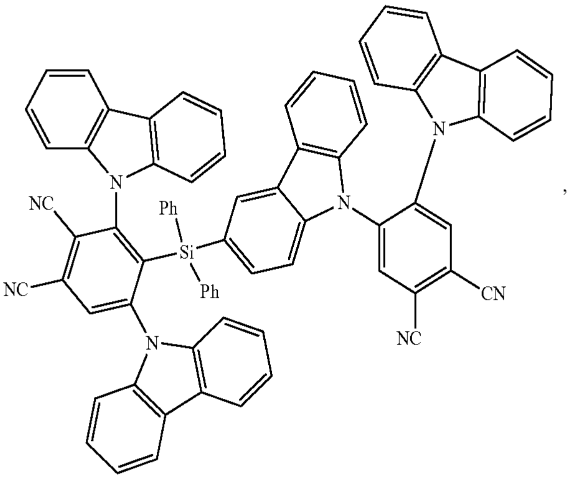
Compound B44



Compound B45



Compound B46



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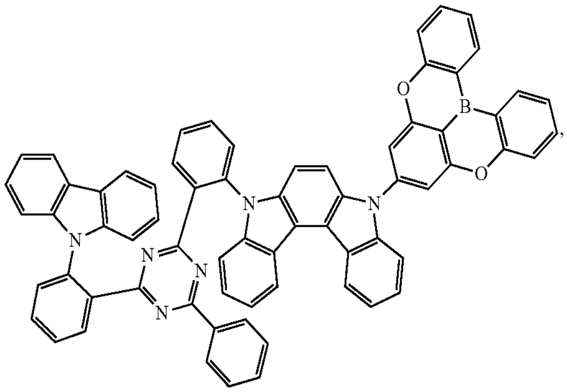
Compound B47



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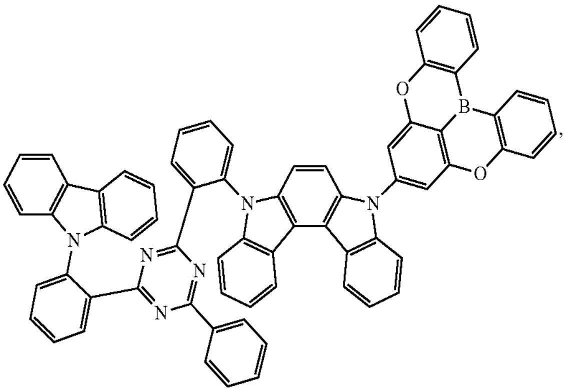
Compound B47



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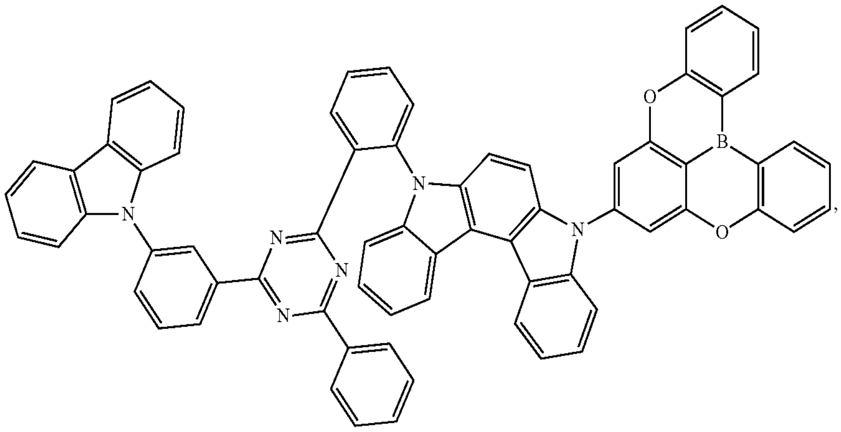
Compound B48



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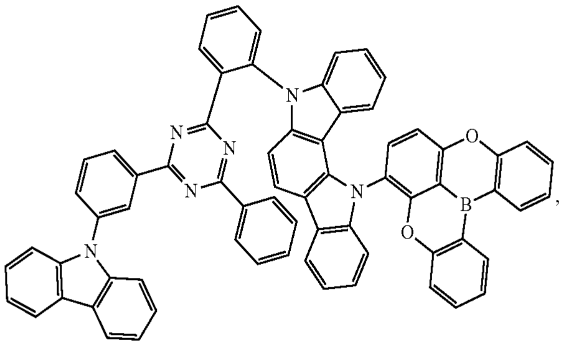
Compound B49



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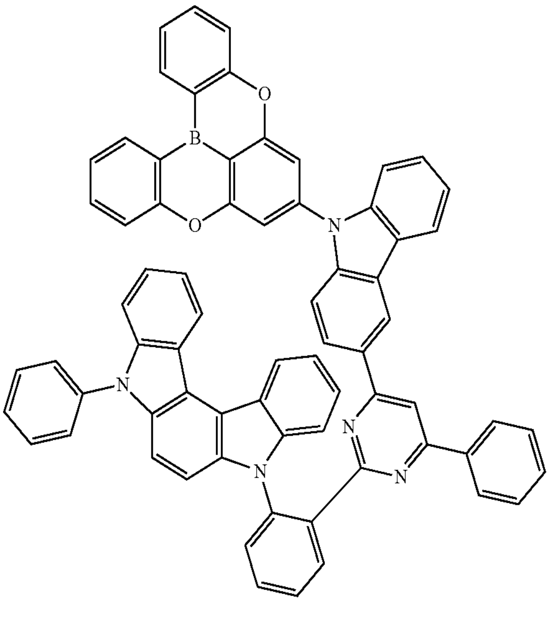
Compound B50



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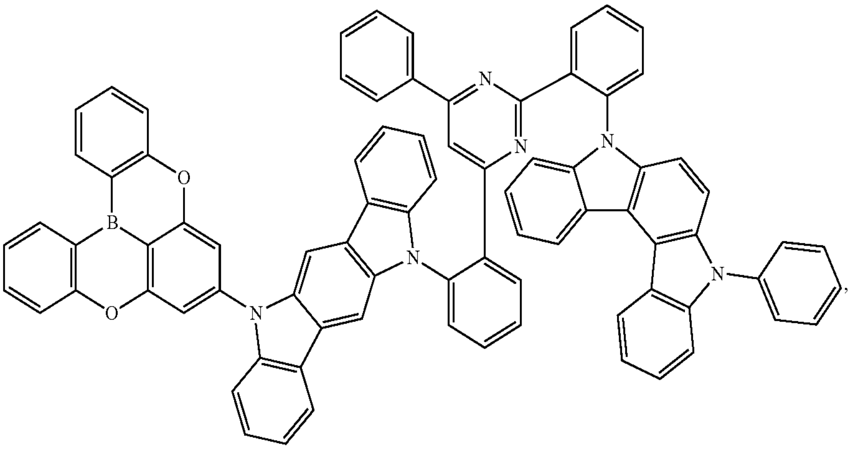
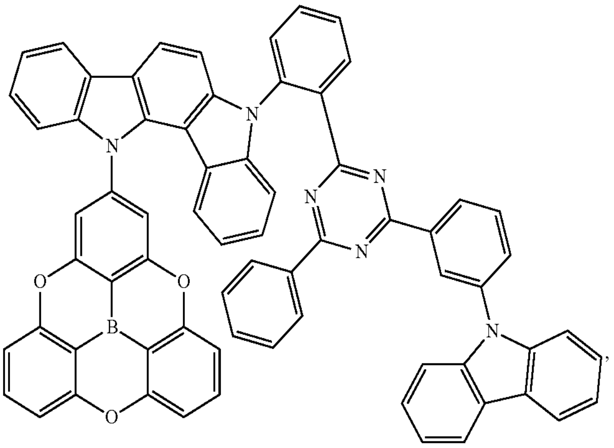
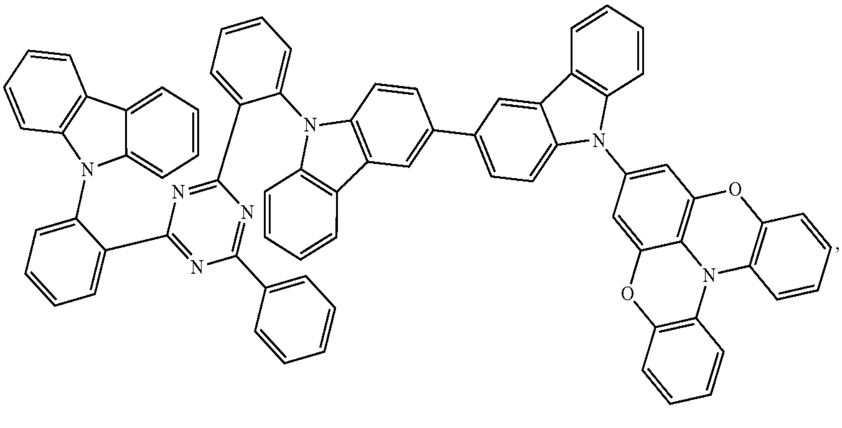
Compound B51



Compound B52



Compound B53



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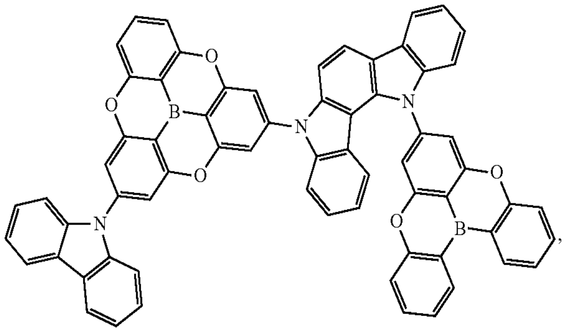
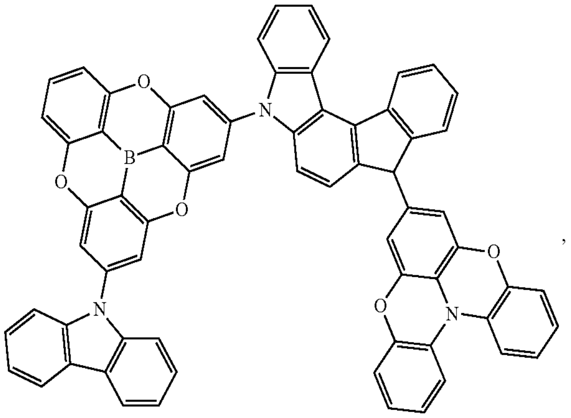
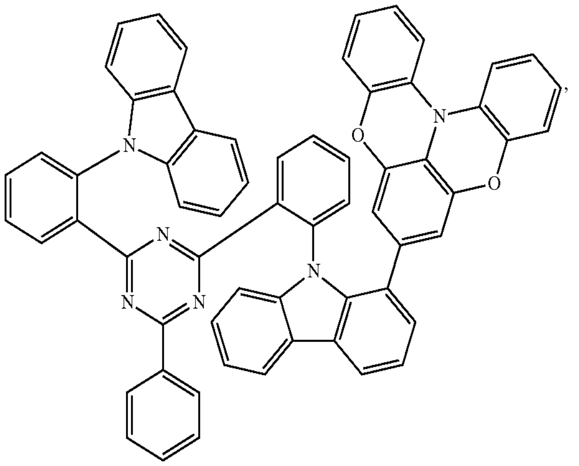
Compound B54



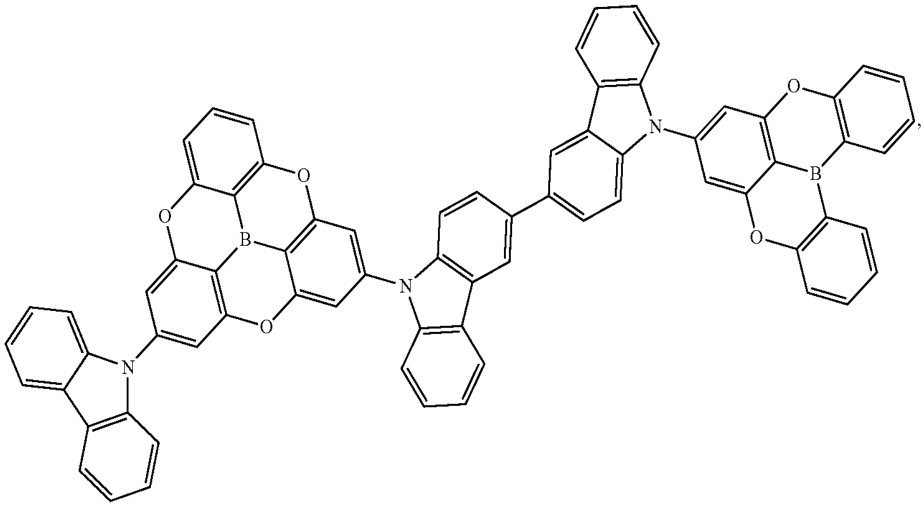
Compound B55



Compound B56



Compound B57



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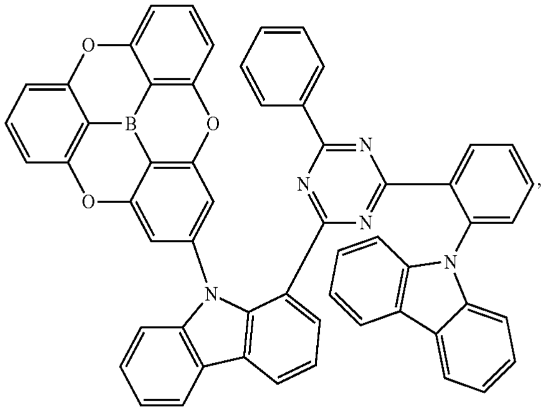
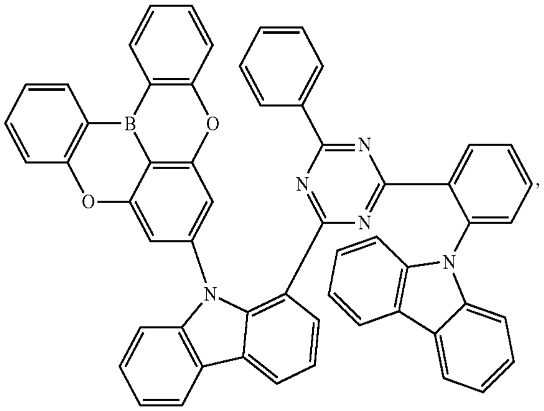
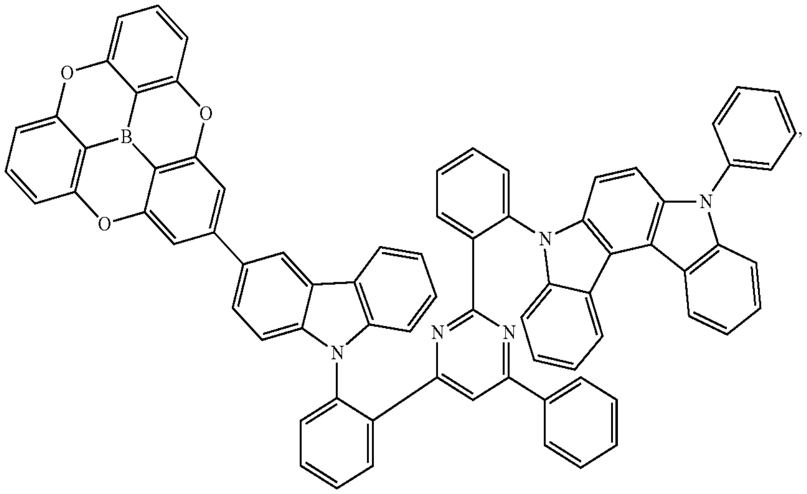
Compound B58



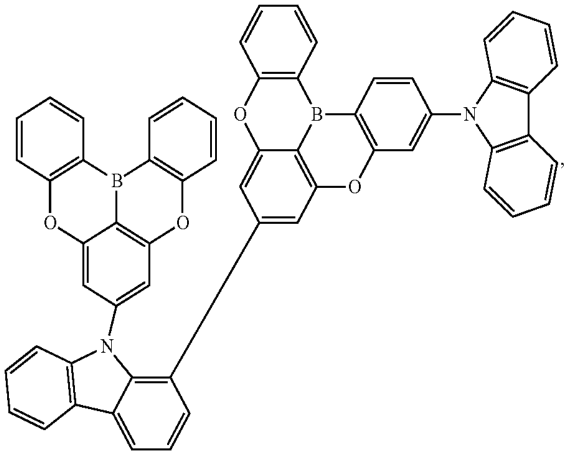
Compound B59



Compound B60



Compound B61



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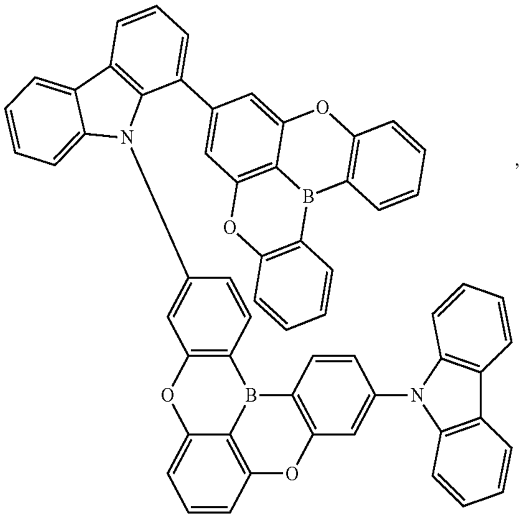

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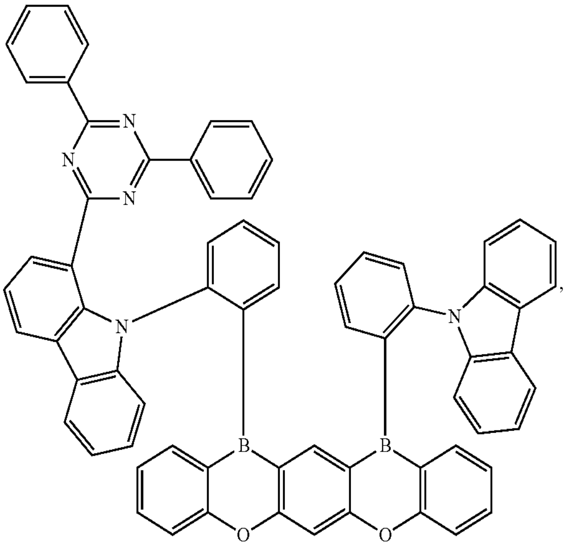

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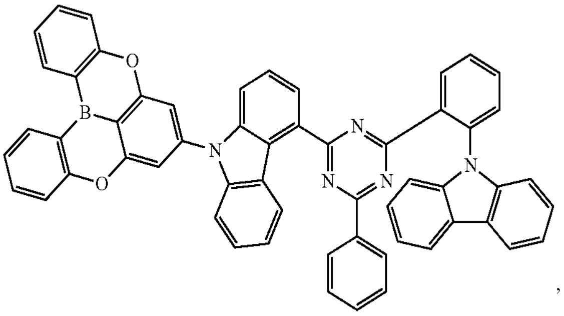

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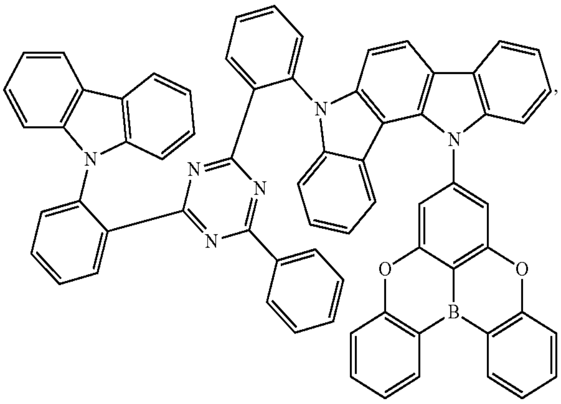
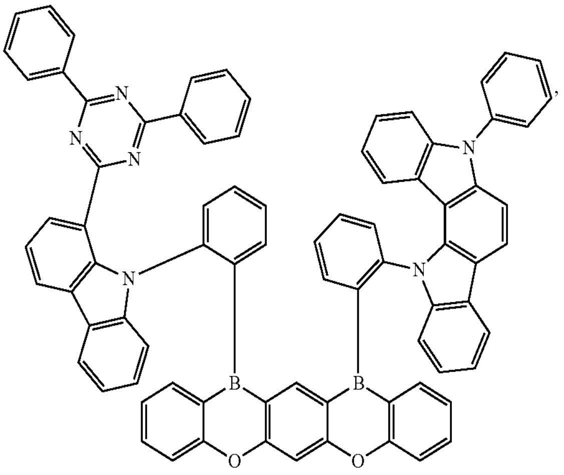
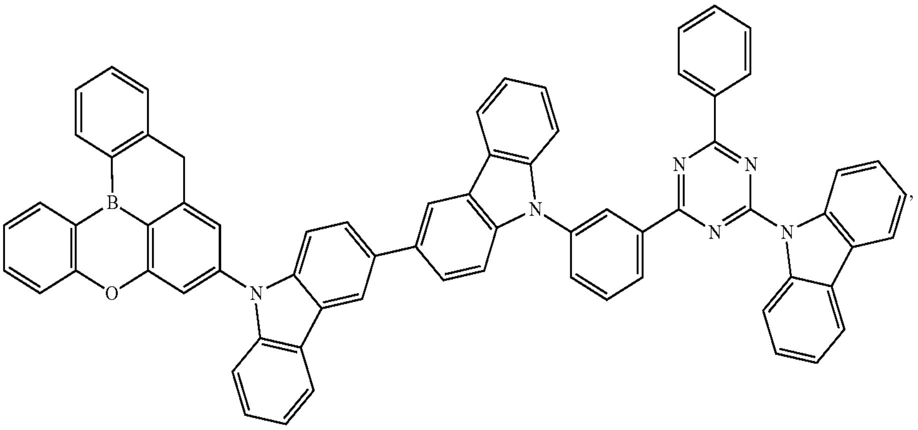


Compound 66



Compound B67



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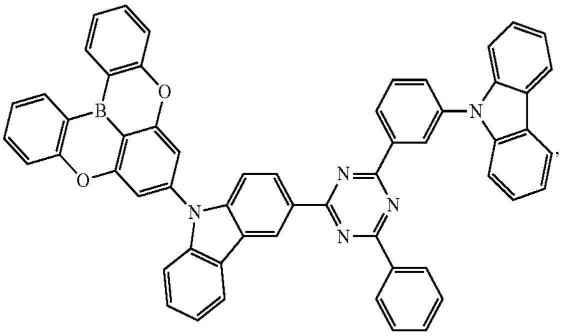

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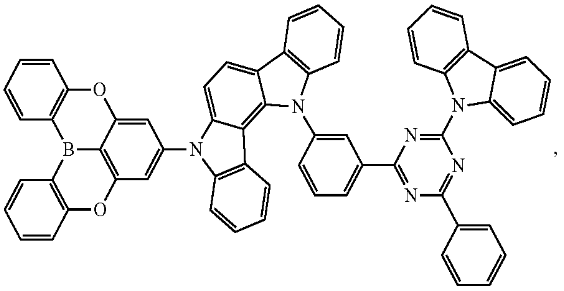
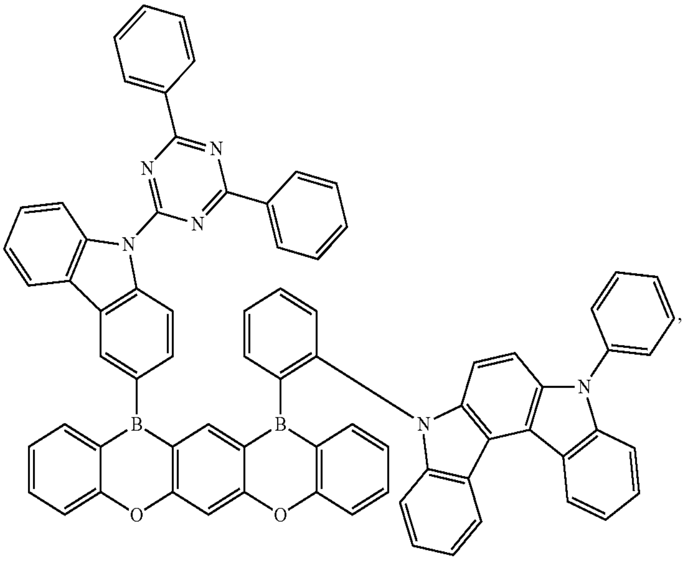


Compound B70



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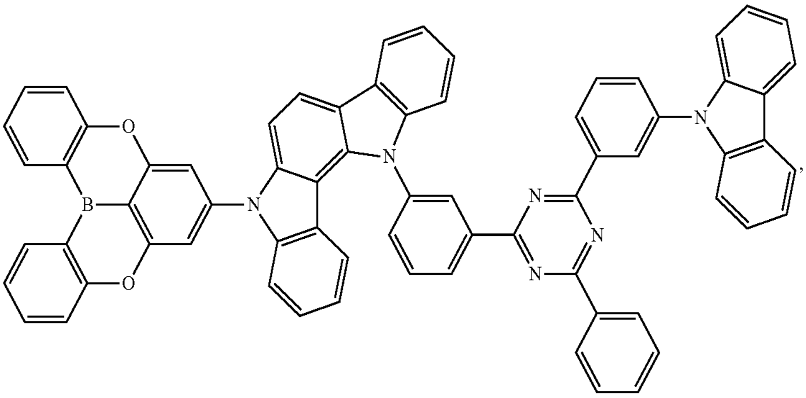

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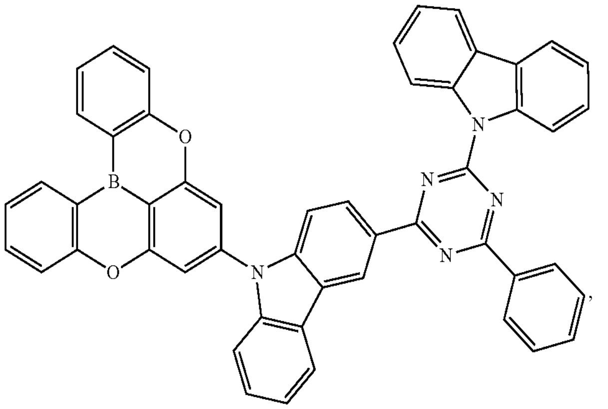
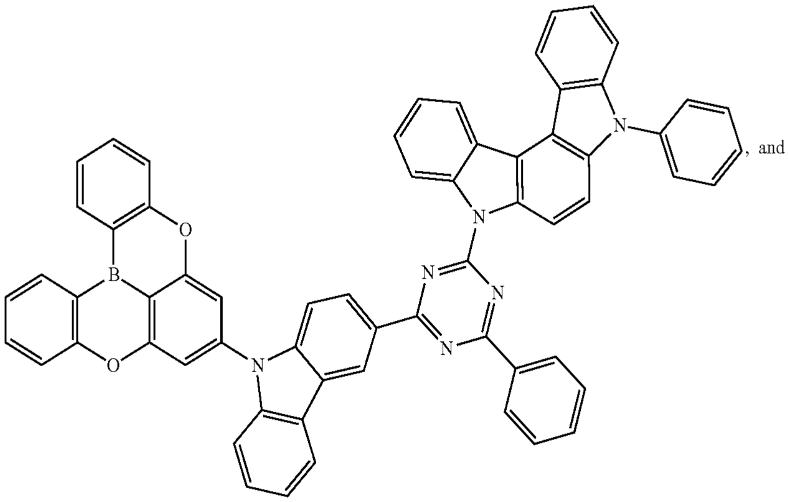
Compound B72

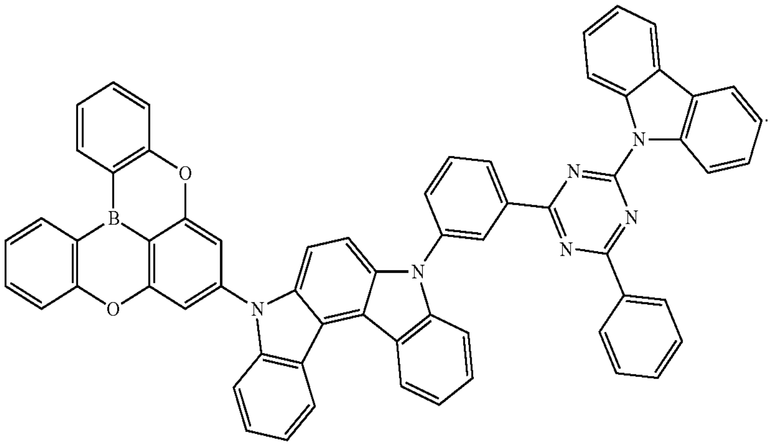


Compound B73



, and

Compound B74



15. An organic light emitting device (OLED) comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, where the organic layer includes a compound comprising:

at least two donor groups G^D; and

at least two acceptor groups G^A;

wherein each donor group G^D and acceptor group G^A can be the same or different;

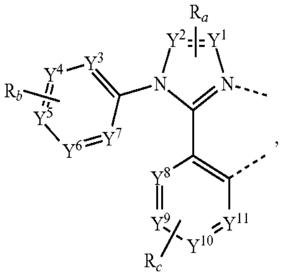
wherein any pair of donor groups G^D is separated by at least one acceptor group G^A;

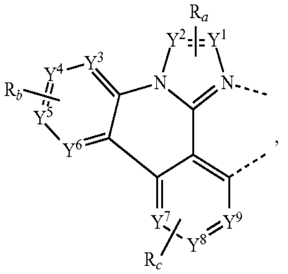
wherein any pair of acceptor groups G^A is separated by at least one donor group G^D; and

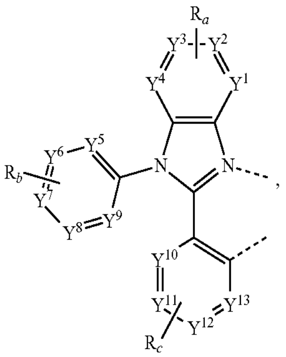
wherein the total number of the donor groups G^D is equal to the total number of the acceptor groups G^A.

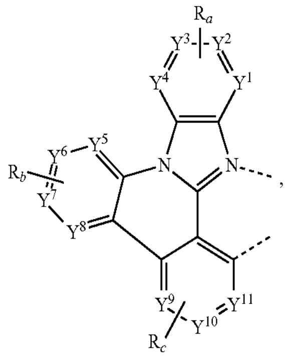
16. The OLED of claim **15**, wherein the organic layer is an emissive layer and the compound is a host.

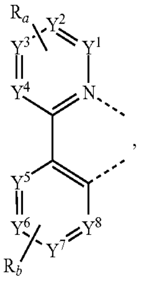
17. The OLED of claim **15**, wherein the organic layer further comprises a phosphorescent emissive dopant; wherein the emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:

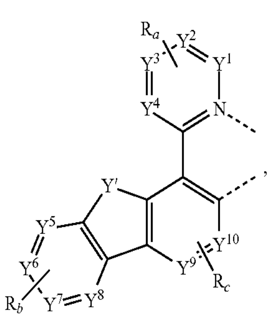


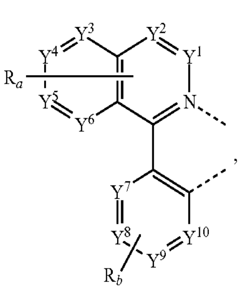












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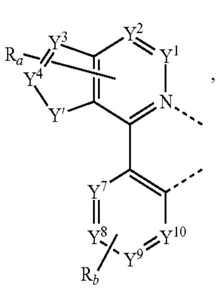

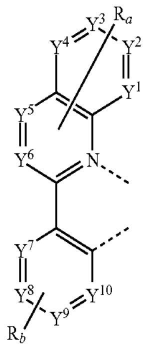

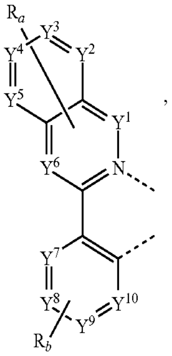

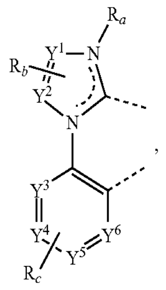

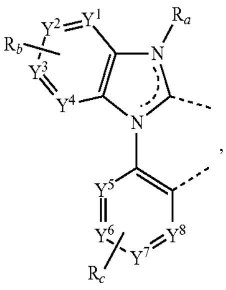

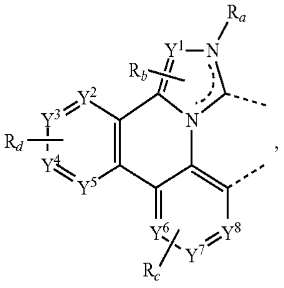

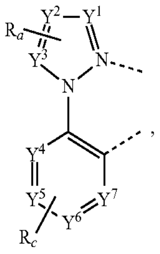

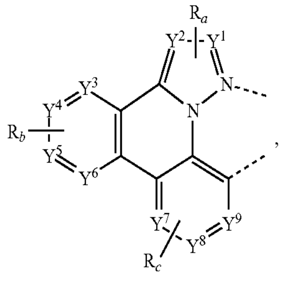

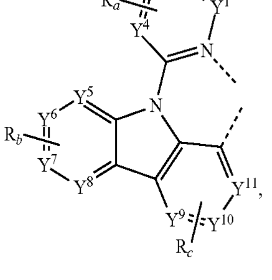

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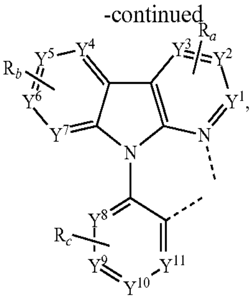

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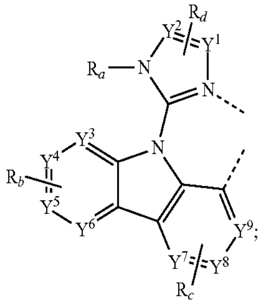

;

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

wherein Y' is selected from the group consisting of BR_e, NR_e, PR_e, O, S, Se, C═O, S═O, SO_2, CR_eR_f, SiR_eR_f, and GeR_eR_f;

wherein R_e and R_f are optionally fused or joined to form a ring;

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

wherein each R_a, R_b, R_c, R_d, R_e, and R_f is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof; and

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

18. The OLED of claim **15**, wherein the organic layer is a blocking layer and the compound is a blocking material in the organic layer, or wherein the organic layer is a transporting layer and the compound is a transporting material in the organic layer.

19. The OLED of claim **15**, wherein the organic layer is an emissive layer and the compound is an emitter.

20. A consumer product comprising a first device comprising a first organic light emitting device comprising:

an anode;

a cathode; and

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

at least two donor groups G^D; and

at least two acceptor groups G^A;

wherein each donor group G^D and acceptor group G^A can be the same or different;

wherein any pair of donor groups G^D is separated by at least one acceptor group G^A;

wherein any pair of acceptor groups G^A is separated by at least one donor group G^D; and

wherein the total number of the donor groups G^D is equal to the total number of the acceptor groups G^A.

* * * * *

专利名称(译)	有机电致发光材料和器件		
公开(公告)号	US20200144512A1	公开(公告)日	2020-05-07
申请号	US16/736961	申请日	2020-01-08
[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	LIN CHUN JI ZHIQIANG FLEETHAM TYLER		
发明人	LIN, CHUN JI, ZHIQIANG FLEETHAM, TYLER		
IPC分类号	H01L51/00 C07D403/14 C09K11/02 C09K11/06		
CPC分类号	H01L51/5096 H01L51/0084 H01L51/5072 C09K11/025 H01L51/5016 C09K2211/18 C07D403/14 C09K11/06 C09K2211/1018 H01L51/5056 H01L51/0072 H01L51/0067 H01L51/5088 H01L2251/5384		
优先权	62/697464 2018-07-13 US		
外部链接	Espacenet USPTO		

摘要(译)

公开了包括至少两个供体基团Gd和至少两个受体基团G 一个的新型化合物。 在这些化合物中，每个供体基团G d和受体基团G 一个可以相同或不同； 任意一对供体基团G d被至少一个受体基团G 一个隔开； 任意一对受体基团G 一个被至少一个供体基团G d隔开； 供体组G的总数 d等于受体组G的总数 一个 。 还公开了包含所述化合物的有机发光器件，消费产品，制剂和化学结构。