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

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

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(72) Inventors: **Jui-Yi TSAI**, Newtown, PA (US);
Jerald FELDMAN, Cherry Hill, NJ (US);
Alexey Borisovich DYATKIN, Ambler, PA (US);
Zhiqiang Ji, Chalfont, PA (US);
Pierre-Luc T. BOUDREAU, Pennington, NJ (US)

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(73) Assignee: **Universal Display Corporation**,
Ewing, NJ (US)

(57) **ABSTRACT**

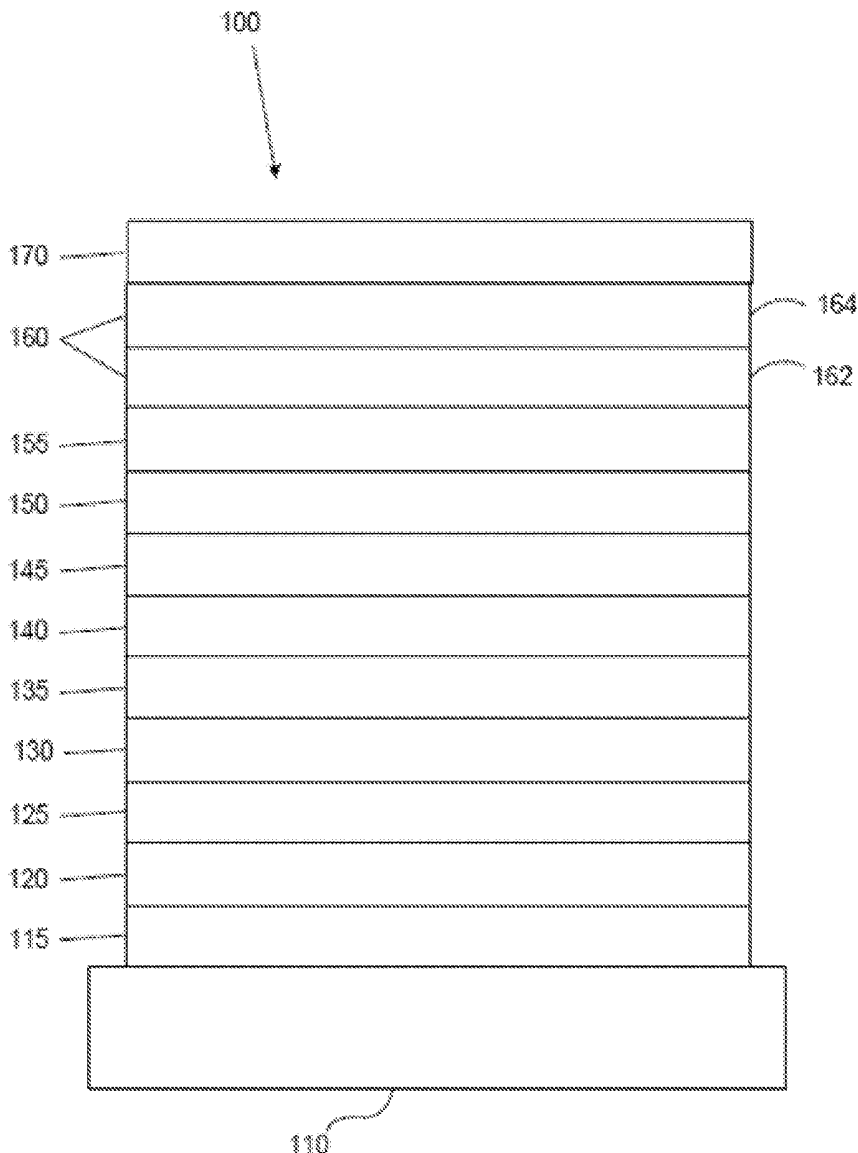
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The present disclosure is directed to cyclometalated metal compounds containing novel ligands having unique fused rings. The inventive compounds are expected to exhibit unique photophysical and electronic properties and are useful in an organic electroluminescence device to improve the performance.

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(60) Provisional application No. 62/727,721, filed on Sep. 6, 2018.



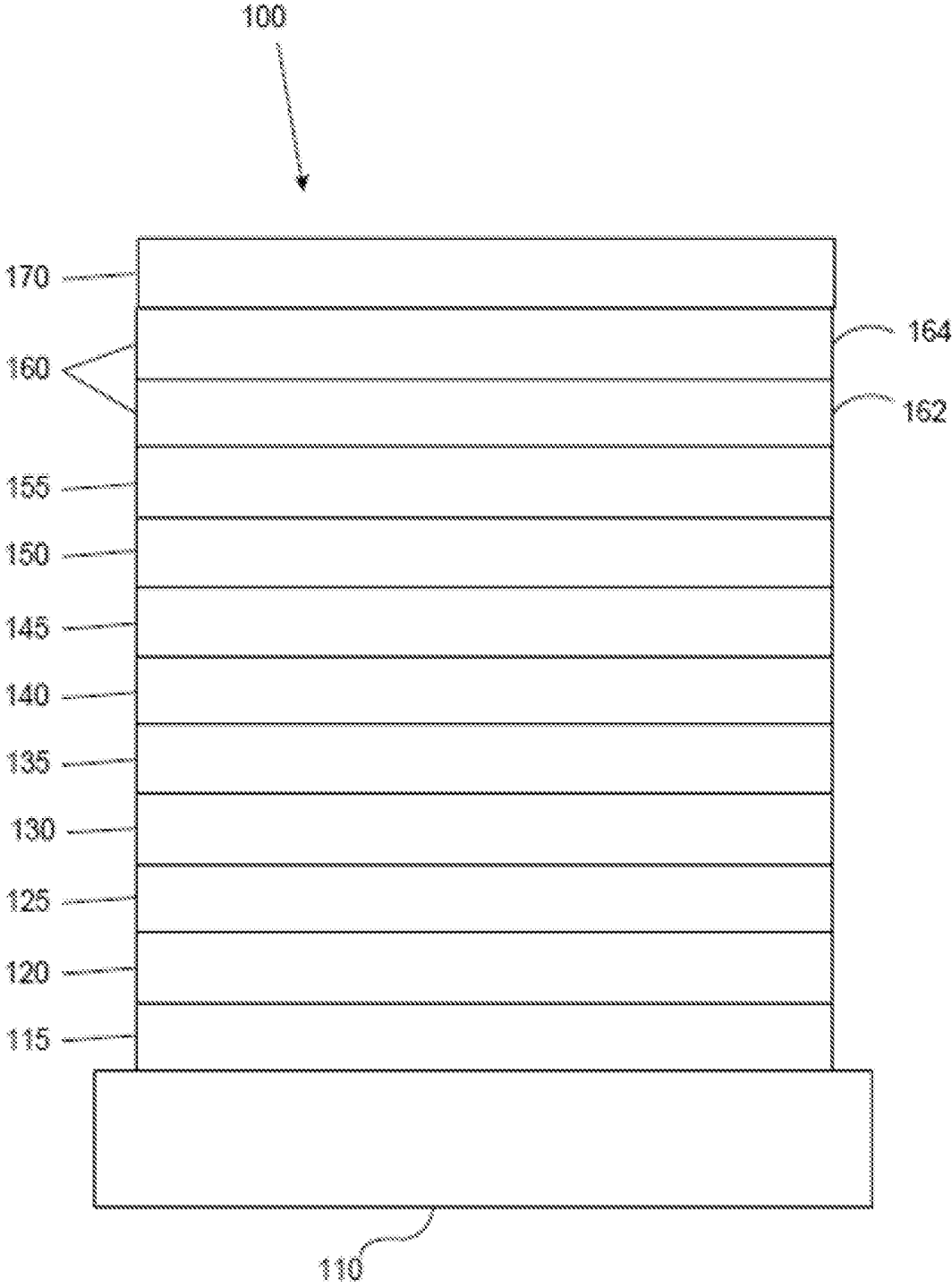


FIG. 1

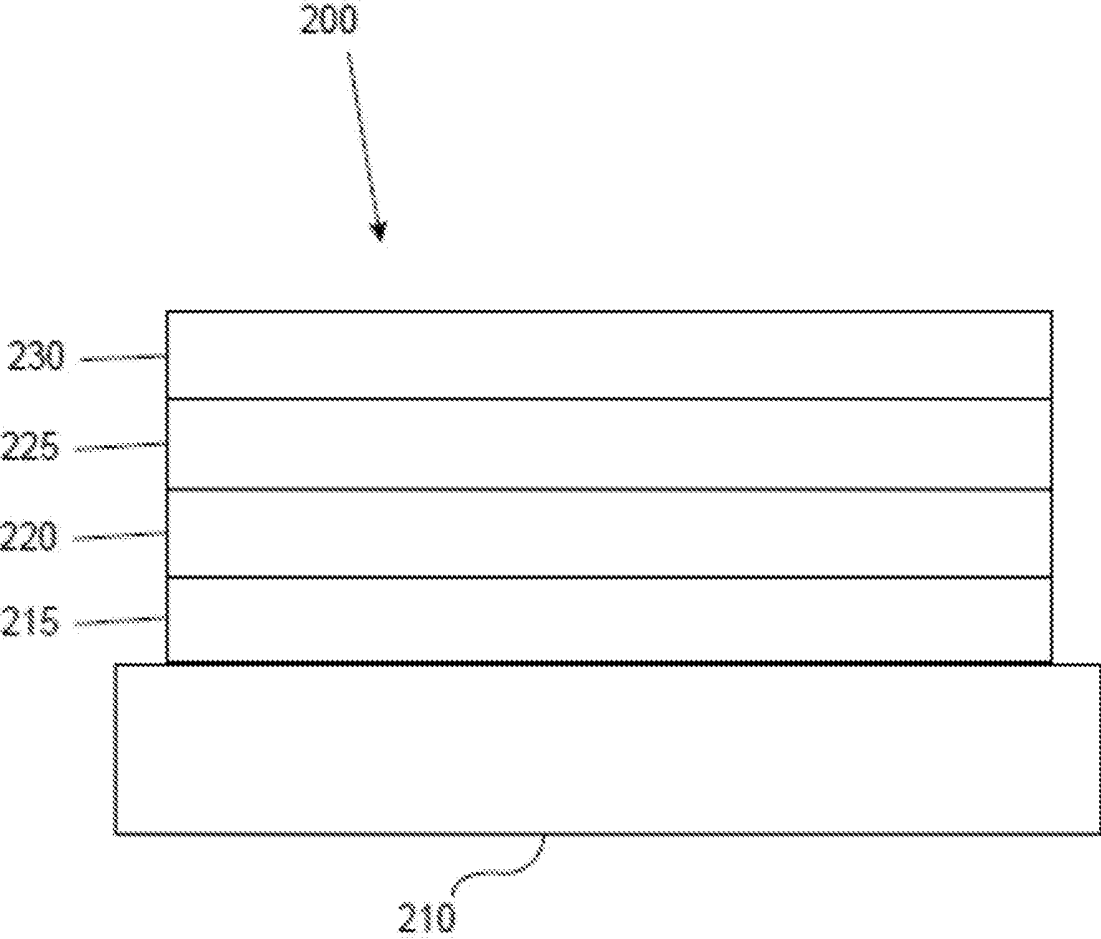


FIG. 2

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application claims priority under 35 U.S.C. § 119(e) to U.S. Provisional Application No. 62/727,721, filed Sep. 6, 2018, the entire contents of which are incorporated herein by reference.

FIELD

[0002] The present disclosure relates to cyclometalated metal compounds containing a novel ligand. The materials are useful in organic electroluminescence devices.

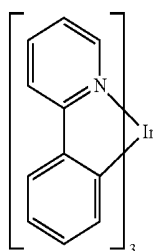
BACKGROUND

[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 pendant 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.

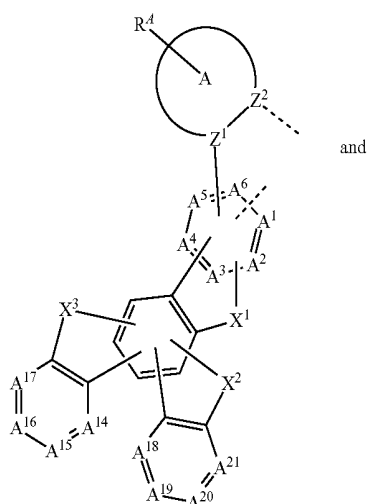
[0014] More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

SUMMARY

[0015] The present disclosure is directed to cyclometalated metal compounds containing novel ligands comprising unique fused rings. The enhanced conjugation of the ligand will drastically modify the lowest triplet excited state. The inventive compounds are expected to exhibit unique photo-physical and electronic properties and are useful in an organic electroluminescence device to improve the performance.

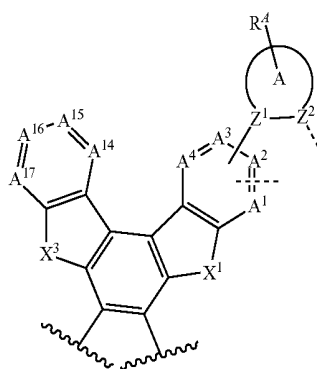
[0016] A compound comprising a first ligand L_A selected from the group consisting of

is disclosed, where, L_A is complexed to a metal M to form a 5-membered chelate ring; A is a 5-membered or 6-membered aryl or heteroaryl ring; Z^1 and Z^2 are each independently C or N ; R^4 represents mono to the maximum allowable substitutions, or no substitution; each A^1 to A^{13} is independently C , CR , or N ; each A^{14} to A^{21} is independently CR or N ; any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ; any of A^1 to A^{13} are C when they are adjacent and fused to a ring; any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring; X^1 , X^2 , and X^3 are each independently selected from the group consisting of O , S , Se , NR^1 , CR^1R^2 , and SiR^1R^2 ; each R , R^1 , R^2 , and R^4 is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined above, and combinations thereof; M is optionally coordinated to other ligands; the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand; any two substituents may be joined or fused together to form a ring; if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ; if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ; where Formulas III through VIII are defined as follows:

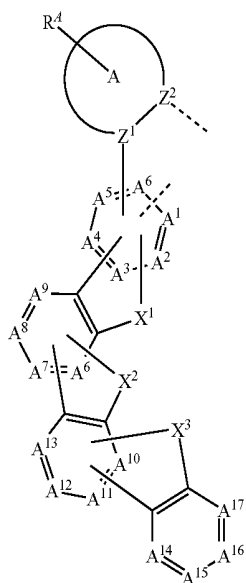


Formula I

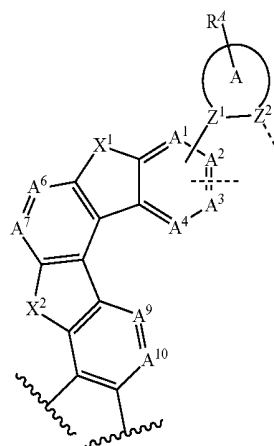
and



Formula III

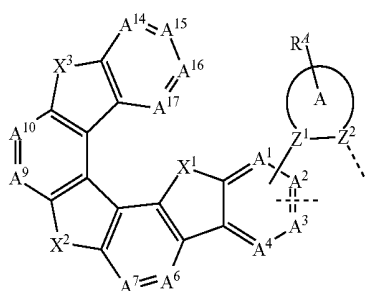


Formula II

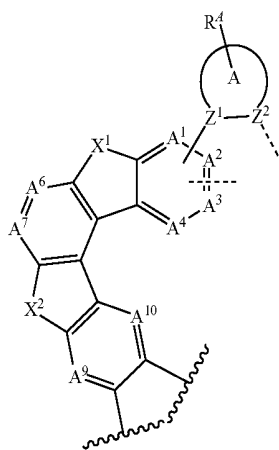


Formula IV

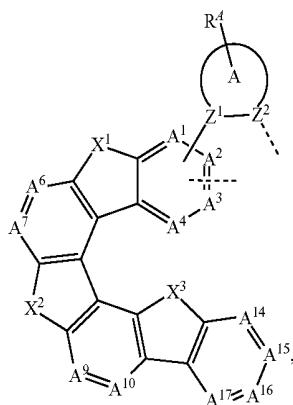
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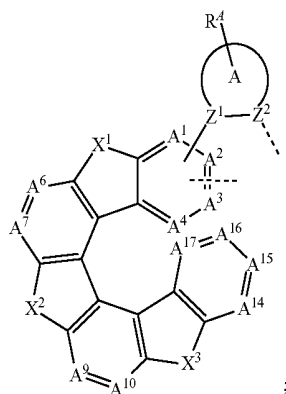
Formula V



Formula VI



Formula VII



Formula VIII

and the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X² or V.

[0017] An OLED comprising the compound of the present disclosure in an organic layer therein is also disclosed.

[0018] A consumer product comprising the OLED is also disclosed.

BRIEF DESCRIPTION OF THE DRAWINGS

[0019] FIG. 1 shows an organic light emitting device.

[0020] FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

DETAILED DESCRIPTION

[0021] 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.

[0022] 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.

[0023] 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.

[0024] 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.

[0025] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F₄-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incor-

porated 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.

[0026] 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**.

[0027] 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.

[0028] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single

organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

[0029] 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 (OVDP), 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.

[0030] 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 entire-

ties. 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.

[0031] 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.

[0032] 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.

[0033] The terms “halo,” “halogen,” and “halide” are used interchangeably and refer to fluorine, chlorine, bromine, and iodine.

[0034] The term “acyl” refers to a substituted carbonyl radical ($C(O)-R_s$).

[0035] The term “ester” refers to a substituted oxycarbonyl ($-O-C(O)-R_s$ or $-C(O)-O-R_s$) radical.

[0036] The term “ether” refers to an $-OR_s$ radical.

[0037] The terms “sulfanyl” or “thio-ether” are used interchangeably and refer to a $-SR_s$ radical.

[0038] The term “sulfinyl” refers to a $-S(O)-R_s$ radical.

[0039] The term “sulfonyl” refers to a $-SO_2-R_s$ radical.

[0040] The term “phosphino” refers to a $-P(R_s)_3$ radical, wherein each R_s can be same or different.

[0041] The term “silyl” refers to a $-Si(R_s)_3$ radical, wherein each 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 is 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 is 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 is optionally substituted.

[0051] The term “heteroaryl” refers to and includes both single-ring 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, benzofurpyridine, 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 is 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 independently 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, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, 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.

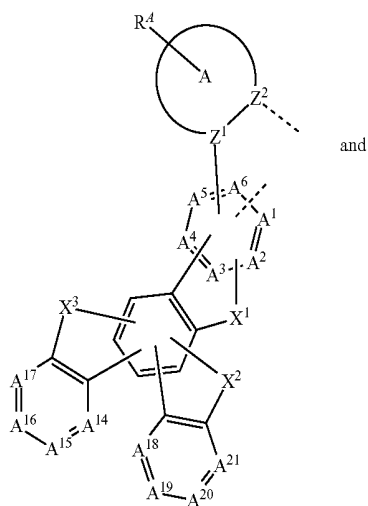
[0060] The “aza” designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzothiophene, etc. means that one or more of the C—H groups in the respective aromatic ring can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[f,h]quinoxaline 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.

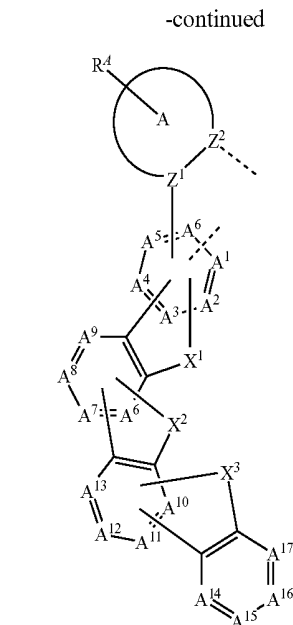
[0063] In some instance, a pair of adjacent substituents can be optionally joined or fused into a ring. The preferred ring is a five, six, or seven-membered carbocyclic or heterocyclic ring, includes both instances where the portion of the ring formed by the pair of substituents is saturated and where 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.

[0064] A compound comprising a first ligand L_A selected from the group consisting of



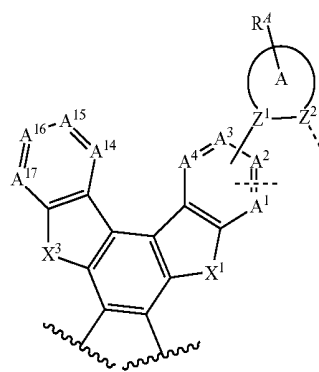
Formula I

and



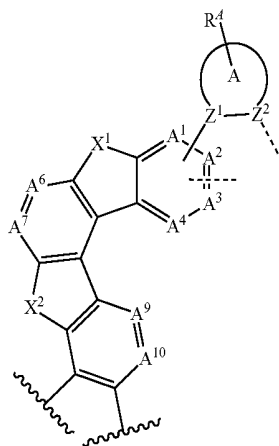
Formula II

is disclosed, where, L_A is complexed to a metal M to form a 5-membered chelate ring; A is a 5-membered or 6-membered aryl or heteroaryl ring; Z^1 and Z^2 are each independently C or N; R^4 represents mono to the maximum allowable substitutions, or no substitution; each A^1 to A^{13} is independently C, CR, or N; each A^{14} to A^{21} is independently CR or N; maximum number of N atoms that can connect to each other within a ring is two; any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ; any of A^1 to A^{13} are C when they are adjacent and fused to a ring; any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring; X^1 , X^2 , and X^3 are each independently selected from the group consisting of O, S, Se, NR^1 , CRR^2 , and SiR^3R^4 ; each R, R^1 , R^2 , and R^4 is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined above, and combinations thereof; M is optionally coordinated to other ligands; the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand; any two substituents may be joined or fused together to form a ring; if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ; if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ; where Formulas III through VIII are defined as follows:



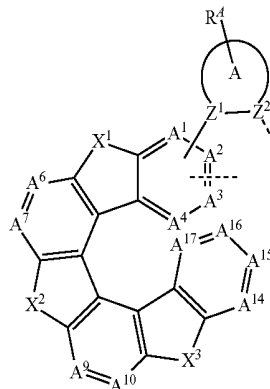
Formula III

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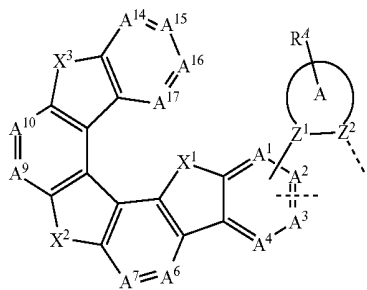


Formula IV

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Formula VIII

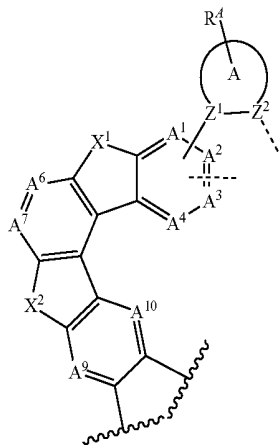


Formula V

and the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X² or V.

[0065] In some embodiments of the compound, each R, R', R'', and R⁴ is independently hydrogen or a substituent selected from the group consisting of the preferred general substituents.

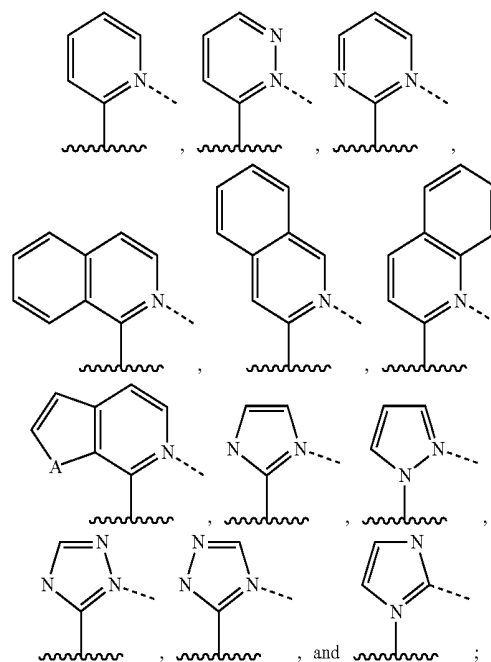
[0066] In some embodiments of the compound, M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pd, Pt, Au, and Cu. In some embodiments, M is Ir or Pt. In some embodiments, the compound is homoleptic. In some embodiments, the compound is heteroleptic.



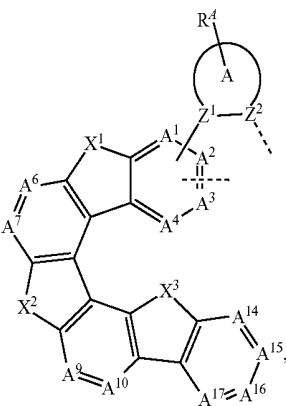
Formula VI

[0067] In some embodiments of the compound, ring A is selected from the group consisting of pyridine, pyrimidine, pyrazine, triazine, imidazole, pyrazole, triazole, and N-heterocyclic carbene. In some embodiments, at least two of the R⁴ in such ring A are alkyl groups.

[0068] In some embodiments of the compound, ring A is selected from the group consisting of



Formula VII



wherein A is O or S; the dashed line indicates a direct bond to M; and the wavy line indicates a bond to A¹, A², A³, or A⁴.

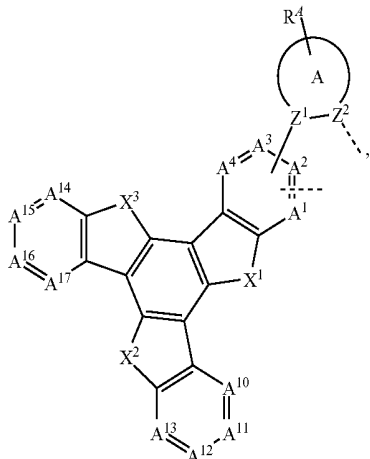
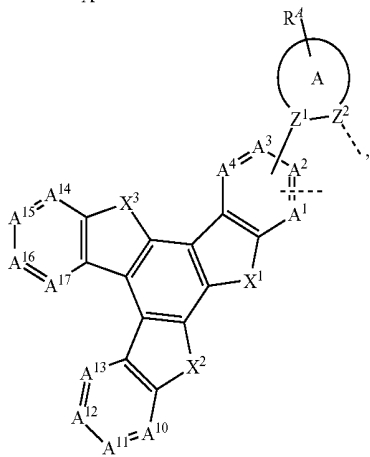
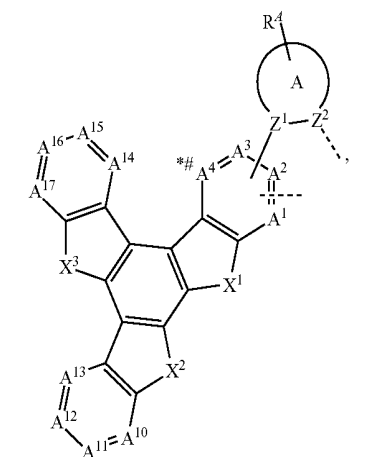
[0069] In some embodiments, each X¹, X², and X³ is O.

[0070] In some embodiments, the compound further comprises two substituted or unsubstituted phenyl-pyridine ligands, wherein the two ligands can be the same or different

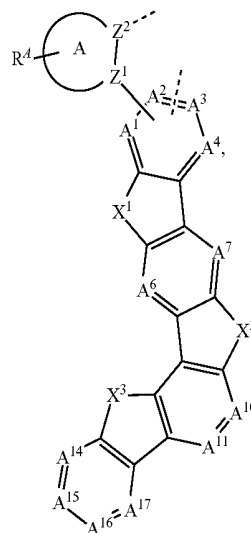
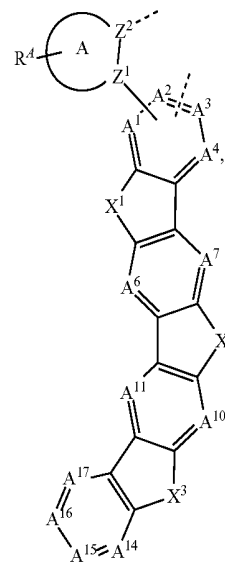
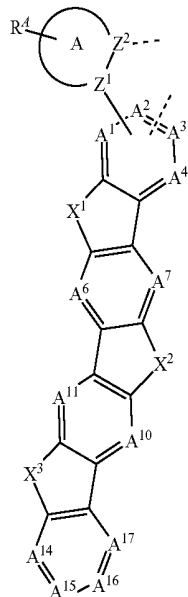
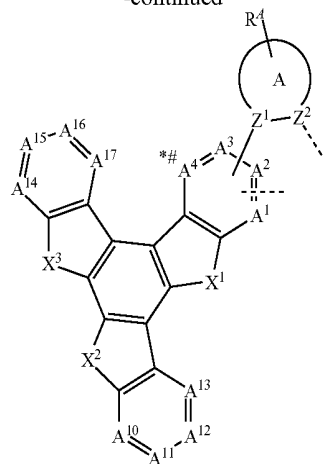
[0071] In some embodiments, each A¹ to A¹³ is C or CR. In some embodiments, at least one of A¹ to A²¹ is N.

[0072] In some embodiments, each R is H. In some embodiments, Z¹ is C, and Z² is N. In some embodiments, Z¹ is N, and Z² is C.

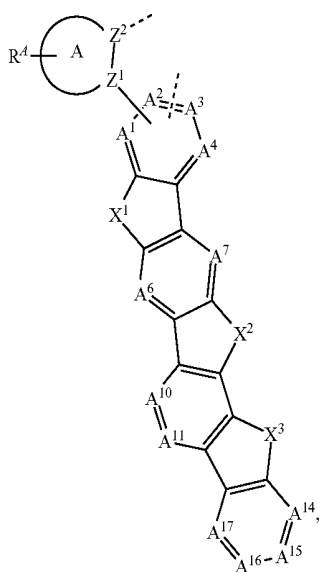
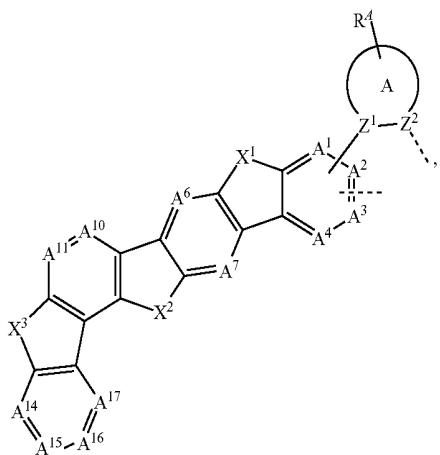
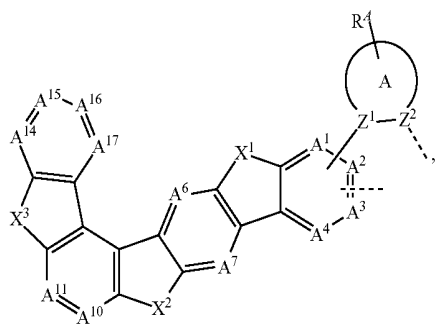
[0073] In some embodiments, the first ligand L_A is selected from the group consisting of:



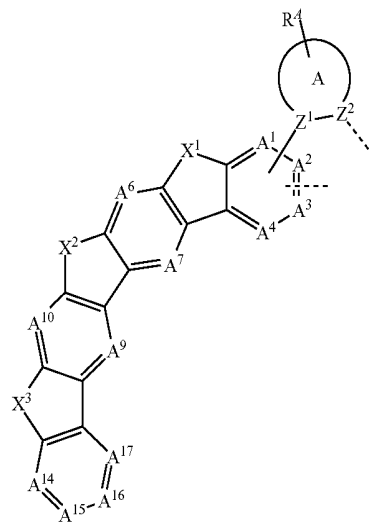
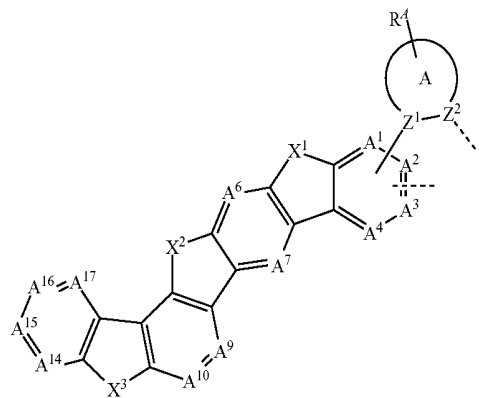
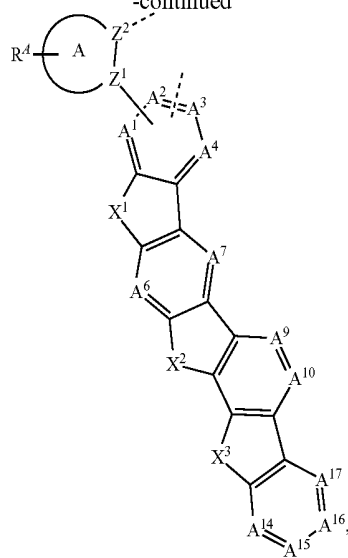
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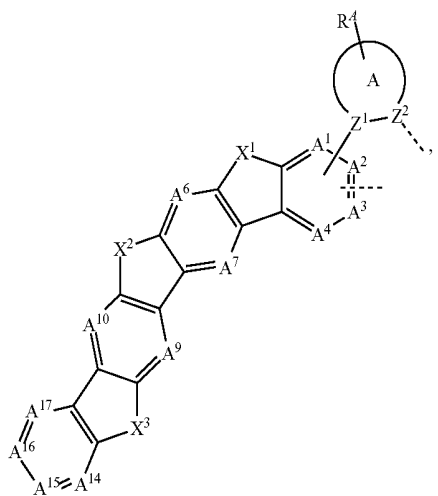
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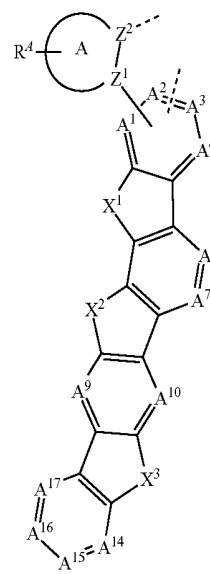
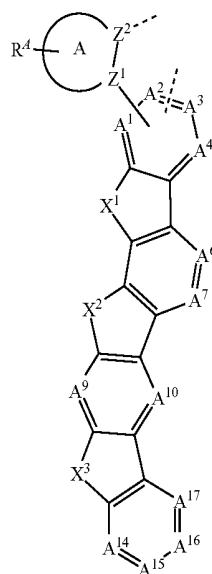
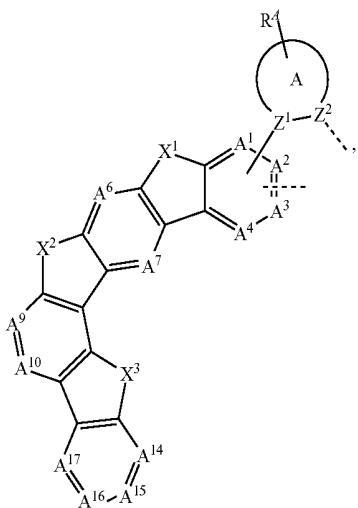
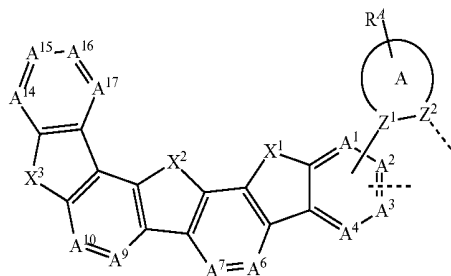
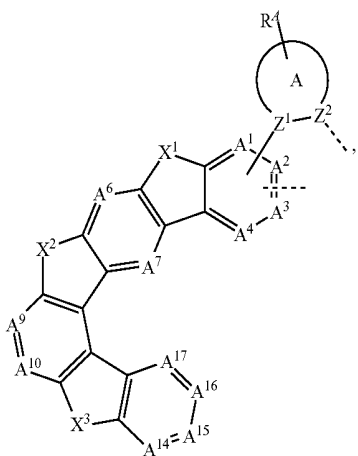
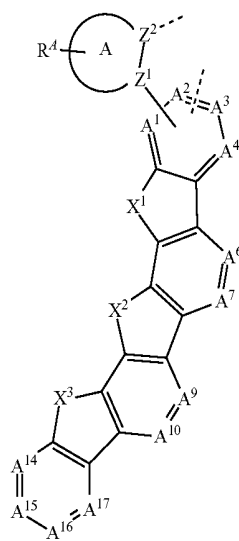
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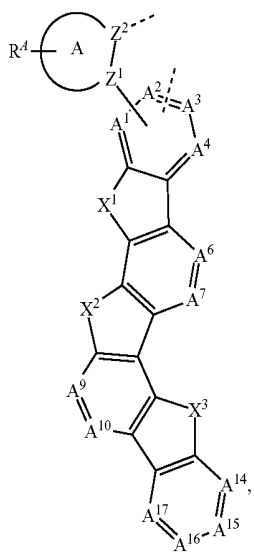
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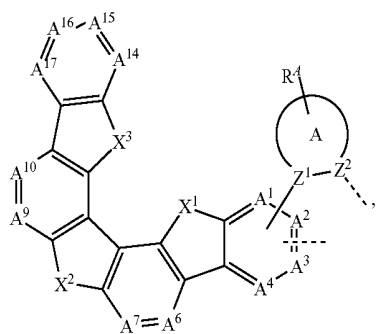
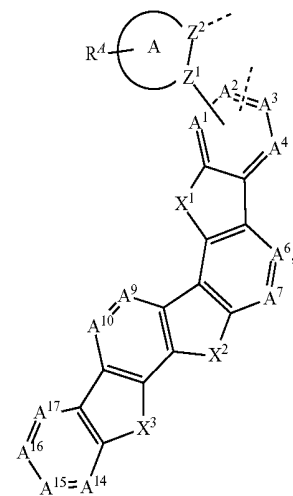
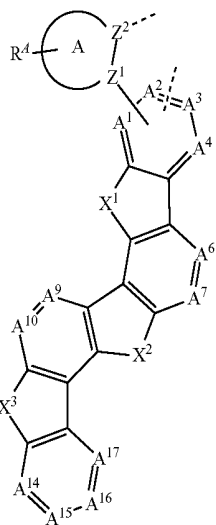
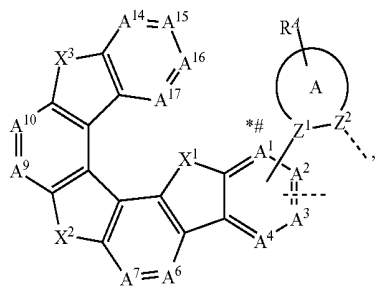
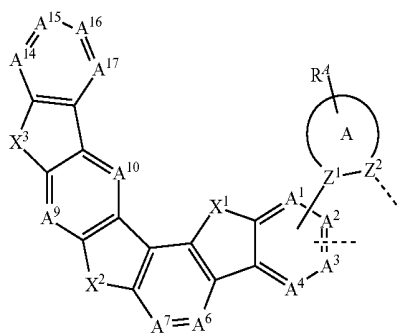
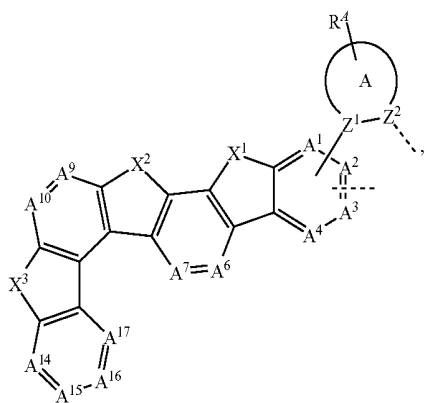
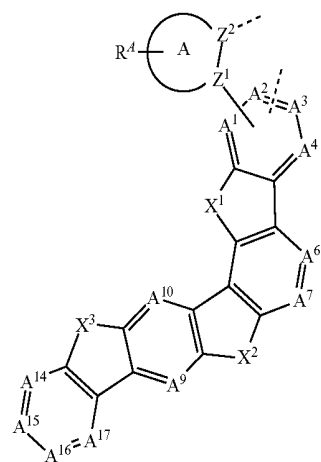
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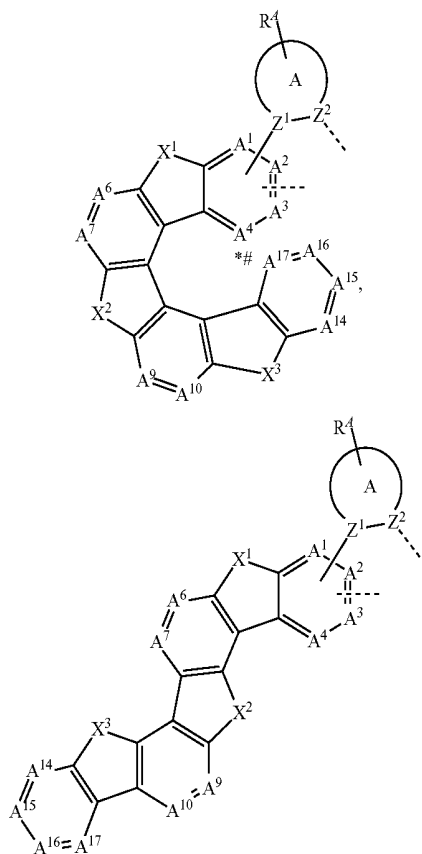
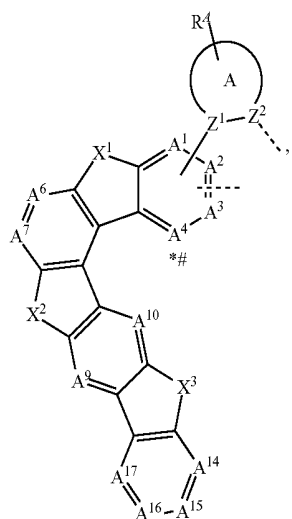
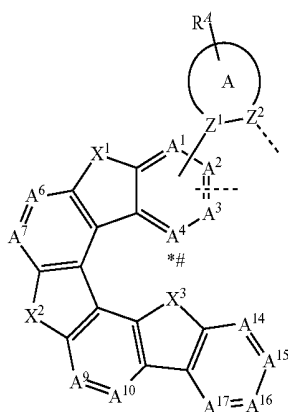
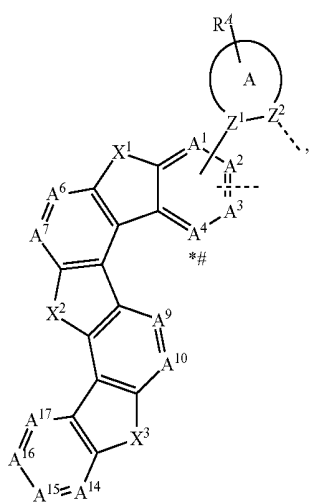
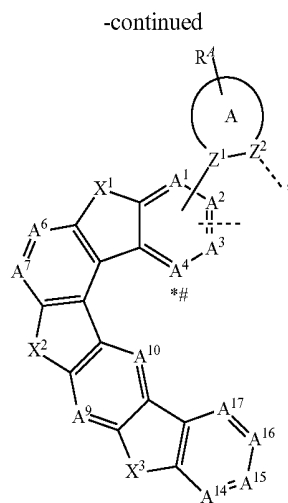
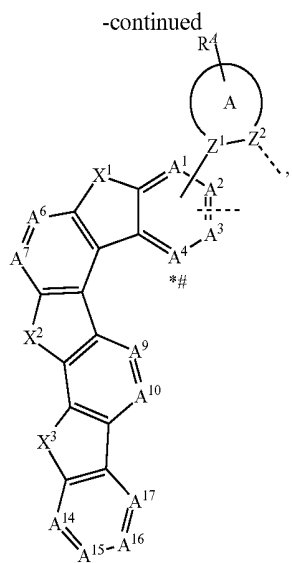


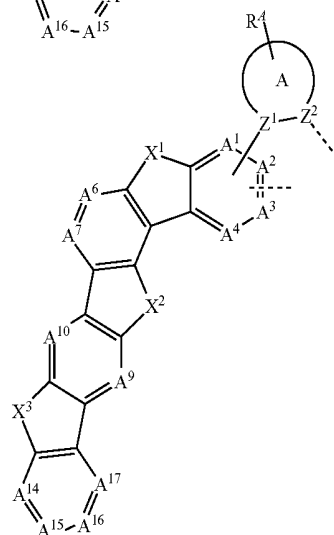
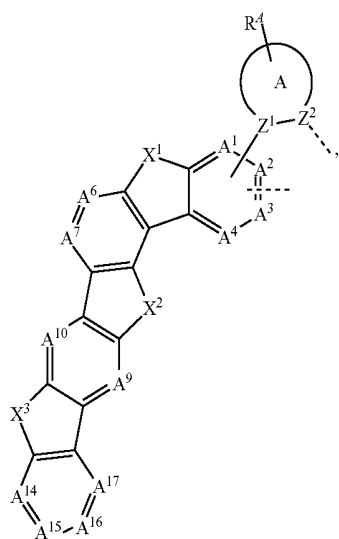
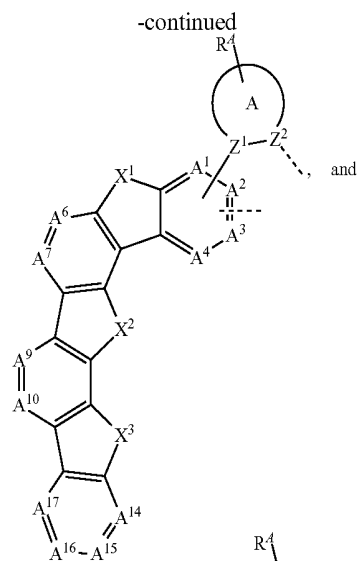
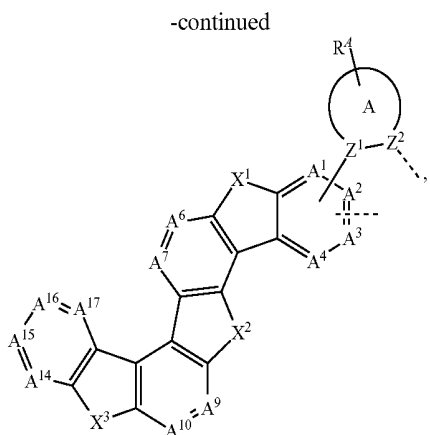
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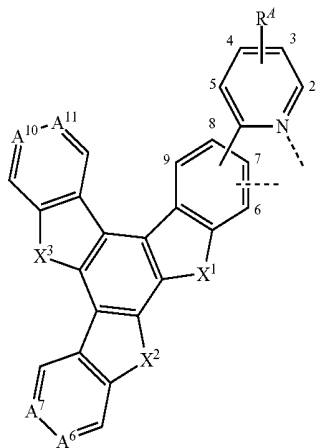
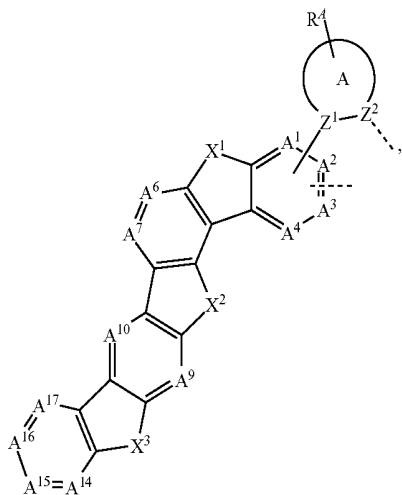




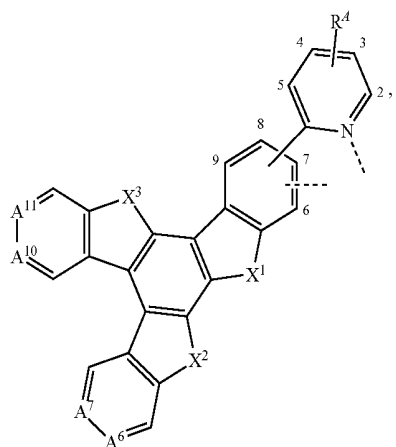
where M does not form a direct bond to A³ or A⁴ if it is marked with an asterisk (*), and where Z¹ does not form a direct bond to A³ or A⁴ if it is marked with a hashtag (#).

[0074] In some embodiments of the compound, the first ligand L_A is selected from the group consisting of L_{A1-1-1} to L_{A38-6-67} based on the formula of where n is an integer from 1 to 38 and for each n, the first ligand L_{A_n-m-l} has a structure according to Formula 1-m to Formula 38-m shown below:

Formula 1-m

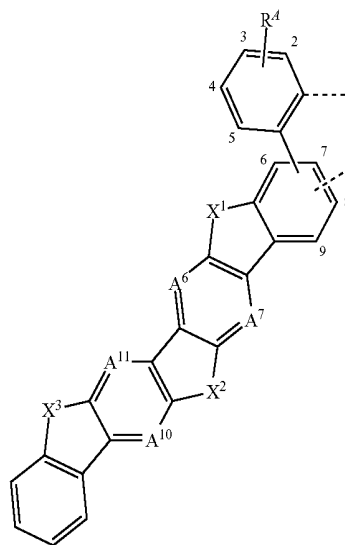


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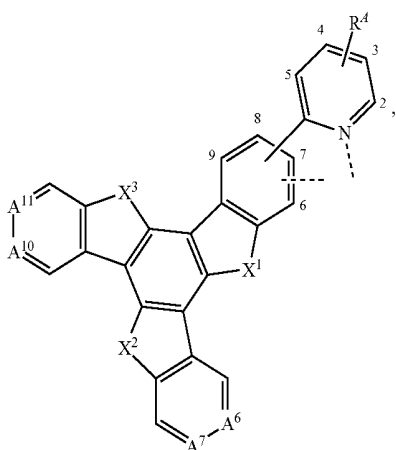
Formula 2-m

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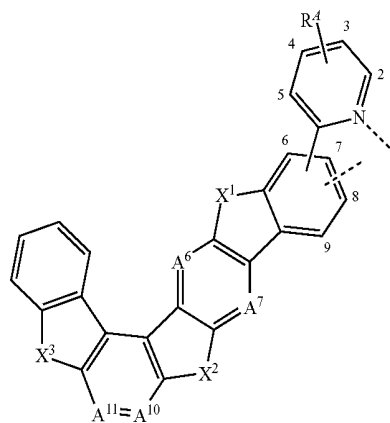


Formula 5-m

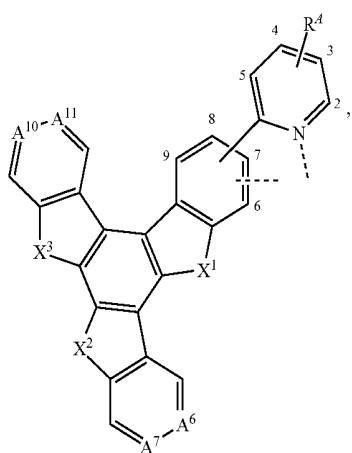
Formula 3-m



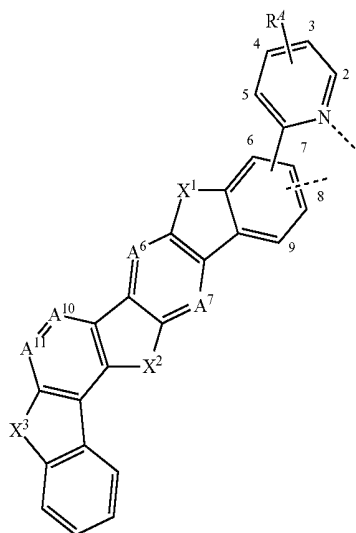
Formula 6-m



Formula 4-m

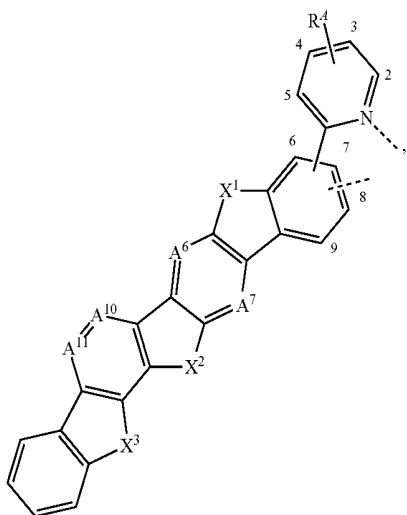


Formula 7-m



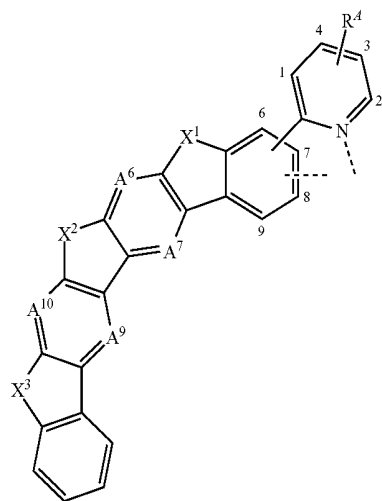
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Formula 8-m

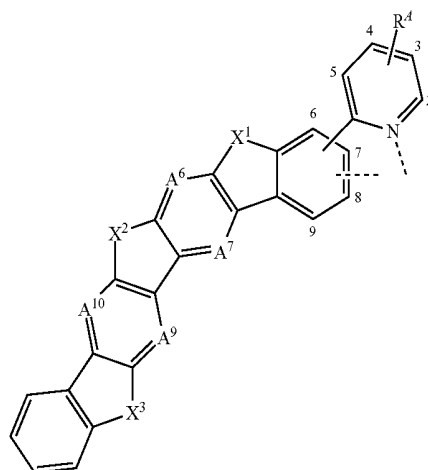
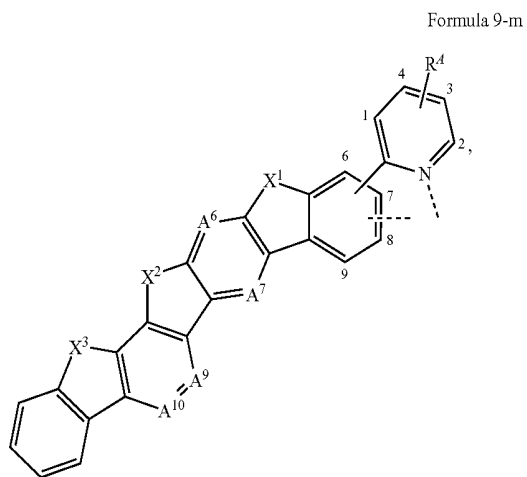


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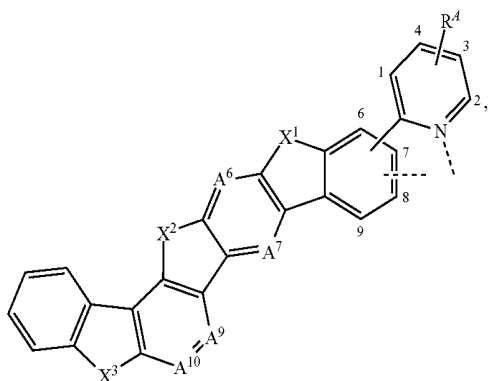
Formula 11-m



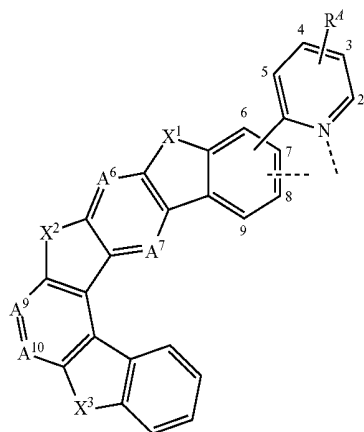
Formula 12-m



Formula 10-m

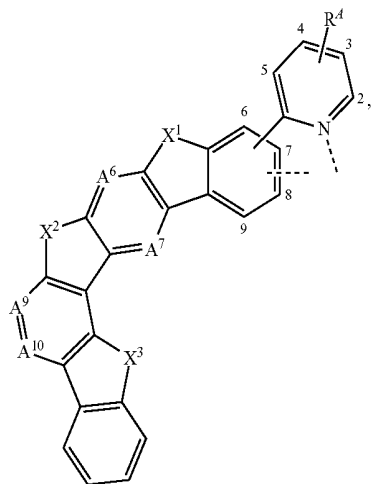


Formula 13-m

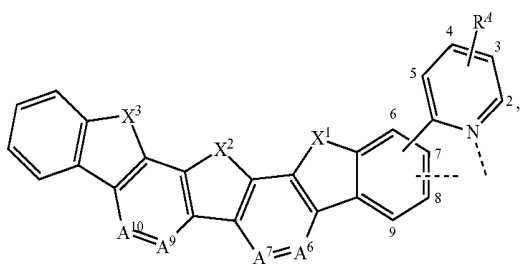


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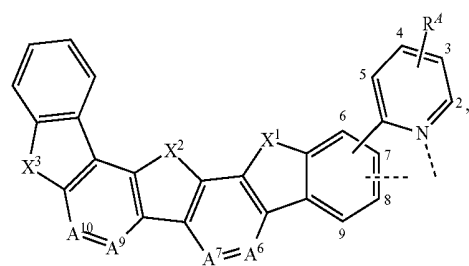
Formula 14-m



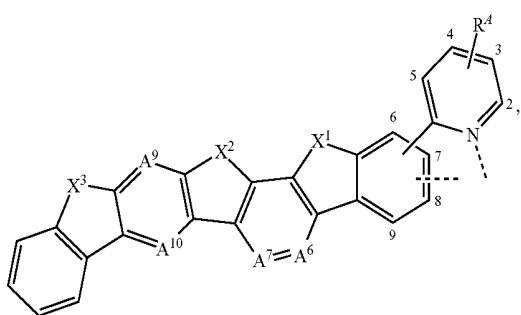
Formula 15-m



Formula 16-m

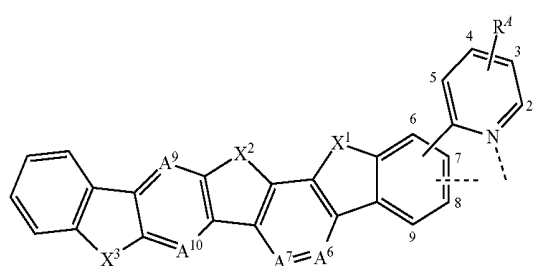


Formula 17-m

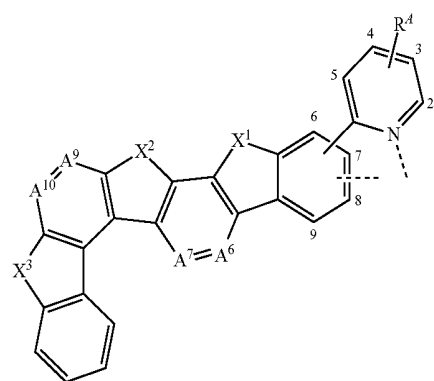


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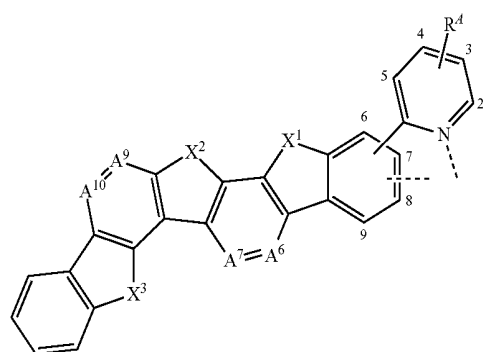
Formula 18-m



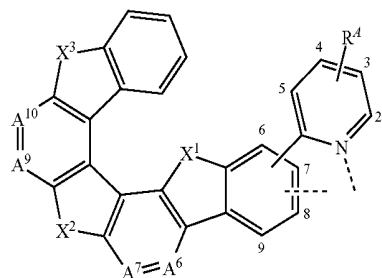
Formula 19-m



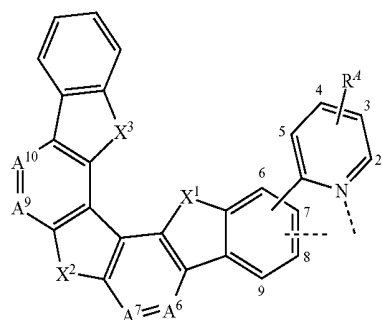
Formula 20-m



Formula 21-m

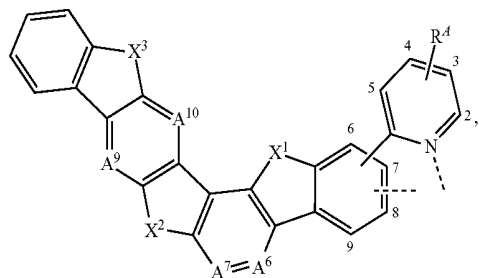


Formula 22-m

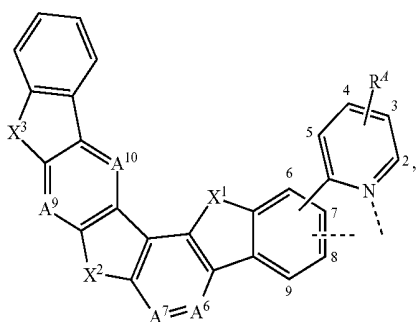


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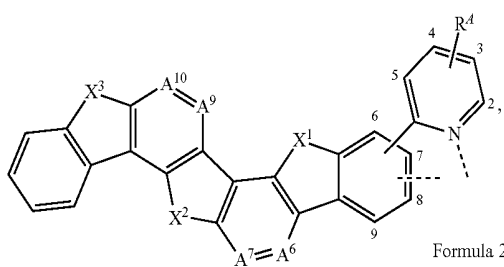
Formula 23-m



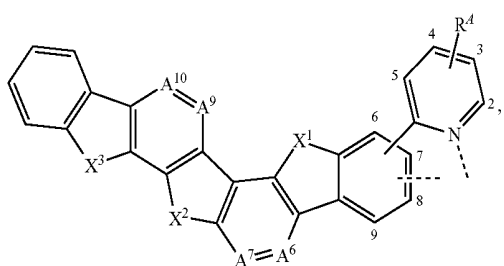
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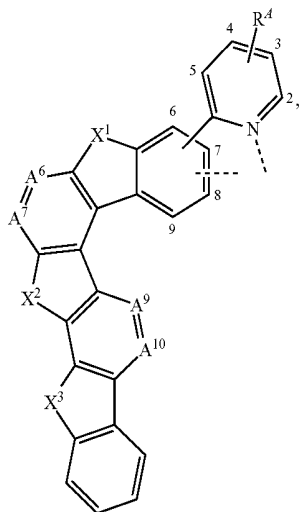
Formula 25-m



Formula 26-m

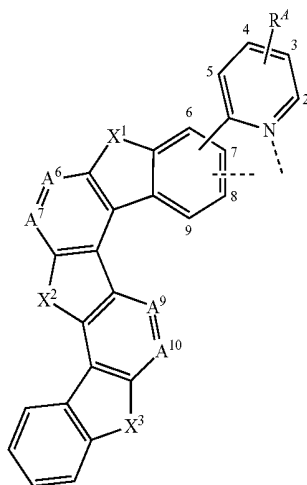


Formula 27-m

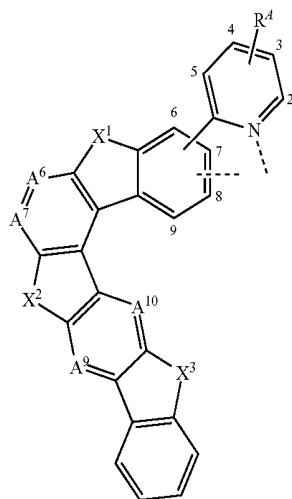


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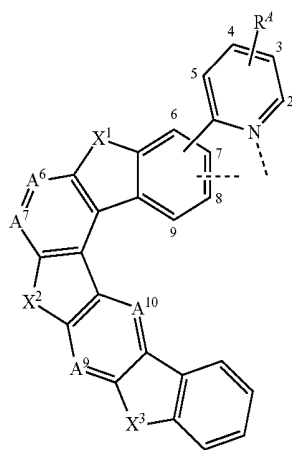
Formula 28-m



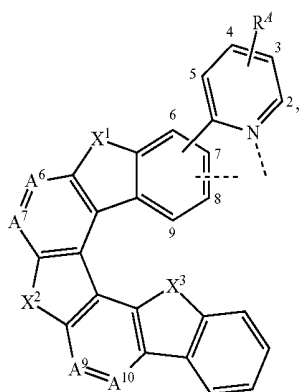
Formula 29-m



Formula 30-m

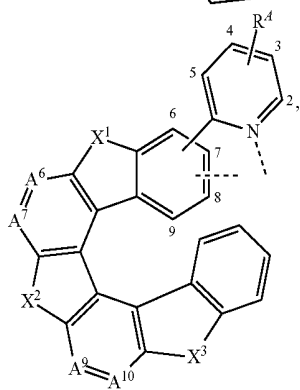


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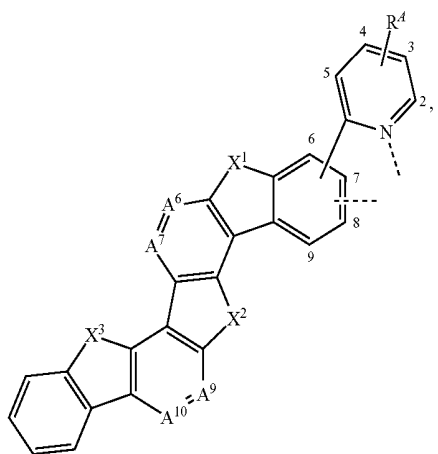


Formula 31-m

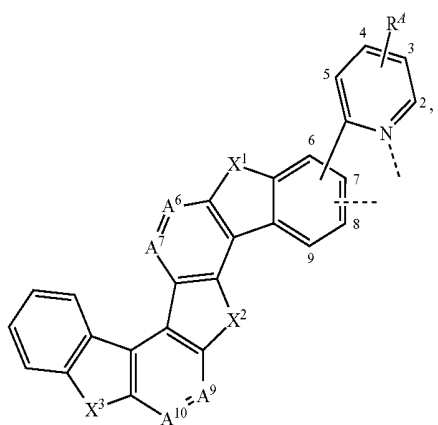
Formula 32-m



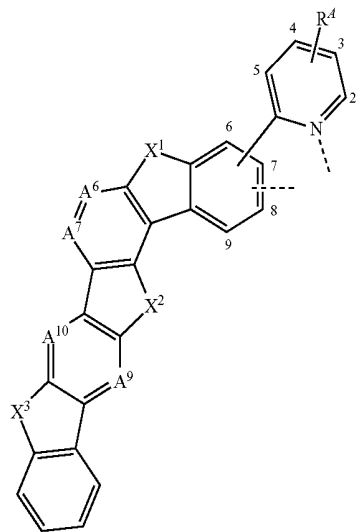
Formula 33-m



Formula 34-m

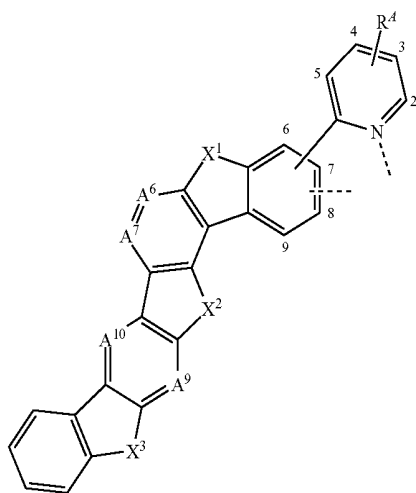


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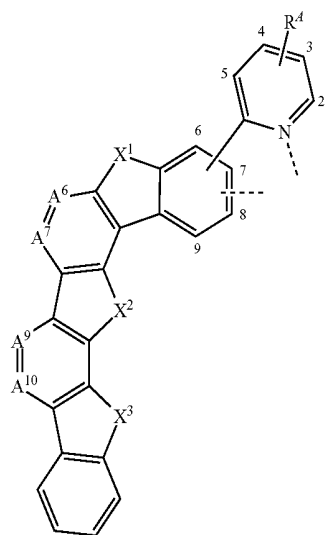


Formula 35-m

Formula 36-m

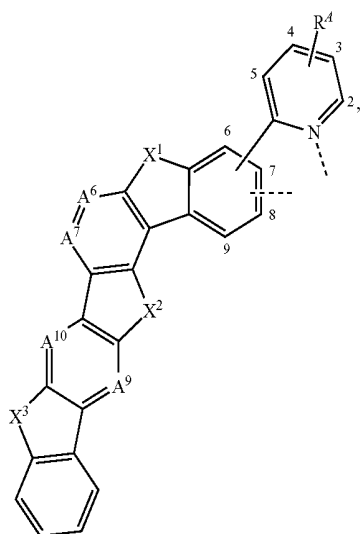


Formula 37-m



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Formula 38-m



where in each Formula n-m, X^1 , X^2 , and X^3 are defined as follows identified by m, an integer from 1 to 6:

| m | X^1 | X^2 | X^3 |
|---|-------|------------------|------------------|
| 1 | O | O | O |
| 2 | O | CMe ₂ | O |
| 3 | O | O | CMe ₂ |
| 4 | O | CMe ₂ | CMe ₂ |
| 5 | O | S | O |
| 6 | O | O | S |

where for each n-m, there are 67 types of substitution patterns identified by the variable l, wherein l is an integer from 1 to 67, and for each l, the substitution variables in Formula n-m are defined as provided below:

| l # | R ⁴ | ** | *** | A ⁶ | A ⁷ | A ¹⁰ | A ¹¹ |
|-----|--|----|-----|----------------|----------------|-----------------|-----------------|
| 1. | 3-Me | 6 | 7 | CH | CH | CH | CH |
| 2. | 3-Me | 6 | 7 | CMe | CH | CH | CH |
| 3. | 3-Me | 6 | 7 | CH | CMe | CH | CH |
| 4. | 3-Me | 6 | 7 | CH | CH | CMe | CH |
| 5. | 3-Me | 6 | 7 | CH | CH | CH | CMe |
| 6. | 3-Me | 6 | 7 | N | CH | CH | CH |
| 7. | 3-Me | 6 | 7 | CH | N | CH | CH |
| 8. | 3-Me | 6 | 7 | CH | CH | N | CH |
| 9. | 3-Me | 6 | 7 | CH | CH | CH | N |
| 10. | 3-i-Pr | 6 | 7 | CH | CH | CH | CH |
| 11. | 3-i-Pr | 6 | 7 | N | CH | CH | CH |
| 12. | 3-i-Pr | 6 | 7 | CH | N | CH | CH |
| 13. | 3-i-Pr | 6 | 7 | CH | CH | N | CH |
| 14. | 3-i-Pr | 6 | 7 | CH | CH | CH | N |
| 15. | 3-t-Bu | 6 | 7 | CH | CH | CH | N |
| 16. | 4-Me | 6 | 7 | CH | CH | CH | CH |
| 17. | 4-t-Bu | 6 | 7 | CH | CH | CH | CH |
| 18. | 3-CH ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 19. | 3,4-Me | 6 | 7 | CH | CH | CH | CH |
| 20. | 3-CH ₂ CMe ₃ ,4-CH ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 21. | 4-CH ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 22. | 3-CH ₂ CMe ₃ ,4-Me | 6 | 7 | CH | CH | CH | CH |
| 23. | 4-CH ₂ CMe ₃ ,3-Me | 6 | 7 | CH | CH | CH | CH |
| 24. | H | 6 | 7 | CH | CH | CH | CH |
| 25. | 3-CH ₂ CMe ₃ | 7 | 8 | CH | CH | CH | CH |

-continued

| l # | R ⁴ | ** | *** | A ⁶ | A ⁷ | A ¹⁰ | A ¹¹ |
|-----|--|----|-----|------------------|------------------|------------------|------------------|
| 26. | 3,4-Me | 7 | 8 | CH | CH | CH | CH |
| 27. | 3-CH ₂ CMe ₃ | 8 | 7 | CH | CH | CH | CH |
| 28. | 3,4-Me | 8 | 7 | CH | CH | CH | CH |
| 29. | 3,4-Me | 6 | 7 | N | CH | CH | CH |
| 30. | 3,4-Me | 6 | 7 | CH | N | CH | CH |
| 31. | 3,4-Me | 6 | 7 | CH | CH | N | CH |
| 32. | 3,4-Me | 6 | 7 | CH | CH | CH | N |
| 33. | 3-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 34. | 3-CD ₃ | 6 | 7 | N | CH | CH | CH |
| 35. | 3-CD ₃ | 6 | 7 | CH | N | CH | CH |
| 36. | 3-CD ₃ | 6 | 7 | CH | CH | N | CH |
| 37. | 3-CD ₃ | 6 | 7 | CH | CH | CH | N |
| 38. | 3-CD(CMe) ₂ | 6 | 7 | CH | CH | CH | CH |
| 39. | 3-CD(CMe) ₂ | 6 | 7 | N | CH | CH | CH |
| 40. | 3-CD(CMe) ₂ | 6 | 7 | CH | N | CH | CH |
| 41. | 3-CD(CMe) ₂ | 6 | 7 | CH | CH | N | CH |
| 42. | 3-CD(CMe) ₂ | 6 | 7 | CH | CH | CH | N |
| 43. | 4-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 44. | 3-CD ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 45. | 3,4-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 46. | 3-CD ₂ CMe ₃ ,4-CD ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 47. | 4-CD ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 48. | 3-CD ₂ CMe ₃ ,4-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 49. | 4-CD ₂ CMe ₃ ,3-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 50. | H | 6 | 7 | CH | CH | CH | CH |
| 51. | 3-CD ₂ CMe ₃ | 7 | 8 | CH | CH | CH | CH |
| 52. | 3,4-CD ₃ | 7 | 8 | CH | CH | CH | CH |
| 53. | 3-CD ₂ CMe ₃ | 8 | 7 | CH | CH | CH | CH |
| 54. | 3,4-CD ₃ | 8 | 7 | CH | CH | CH | CH |
| 55. | 3,4-CD ₃ | 6 | 7 | N | CH | CH | CH |
| 56. | 3,4-CD ₃ | 6 | 7 | CH | N | CH | CH |
| 57. | 3,4-CD ₃ | 6 | 7 | CH | CH | N | CH |
| 58. | 3,4-CD ₃ | 6 | 7 | CH | CH | CH | N |
| 59. | 3-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 60. | 3,4-CD ₃ | 6 | 7 | CCD ₃ | CH | CH | CH |
| 61. | 3,4-CD ₃ | 6 | 7 | CH | CCD ₃ | N | CH |
| 62. | 3,4-CD ₃ | 6 | 7 | CH | CH | CCD ₃ | CH |
| 63. | 3-CD ₃ | 6 | 7 | CH | CH | CH | CCD ₃ |
| 64. | 3-CD ₃ | 6 | 7 | N | CH | CH | CH |
| 65. | 3-CD ₃ | 6 | 7 | CH | N | CH | CH |
| 66. | 3-CD ₃ | 6 | 7 | CH | CH | N | CH |
| 67. | 3-CD ₃ | 6 | 7 | CH | CH | CH | N |

where ** represents pyridine ring attachment position, and *** represents ligation position.

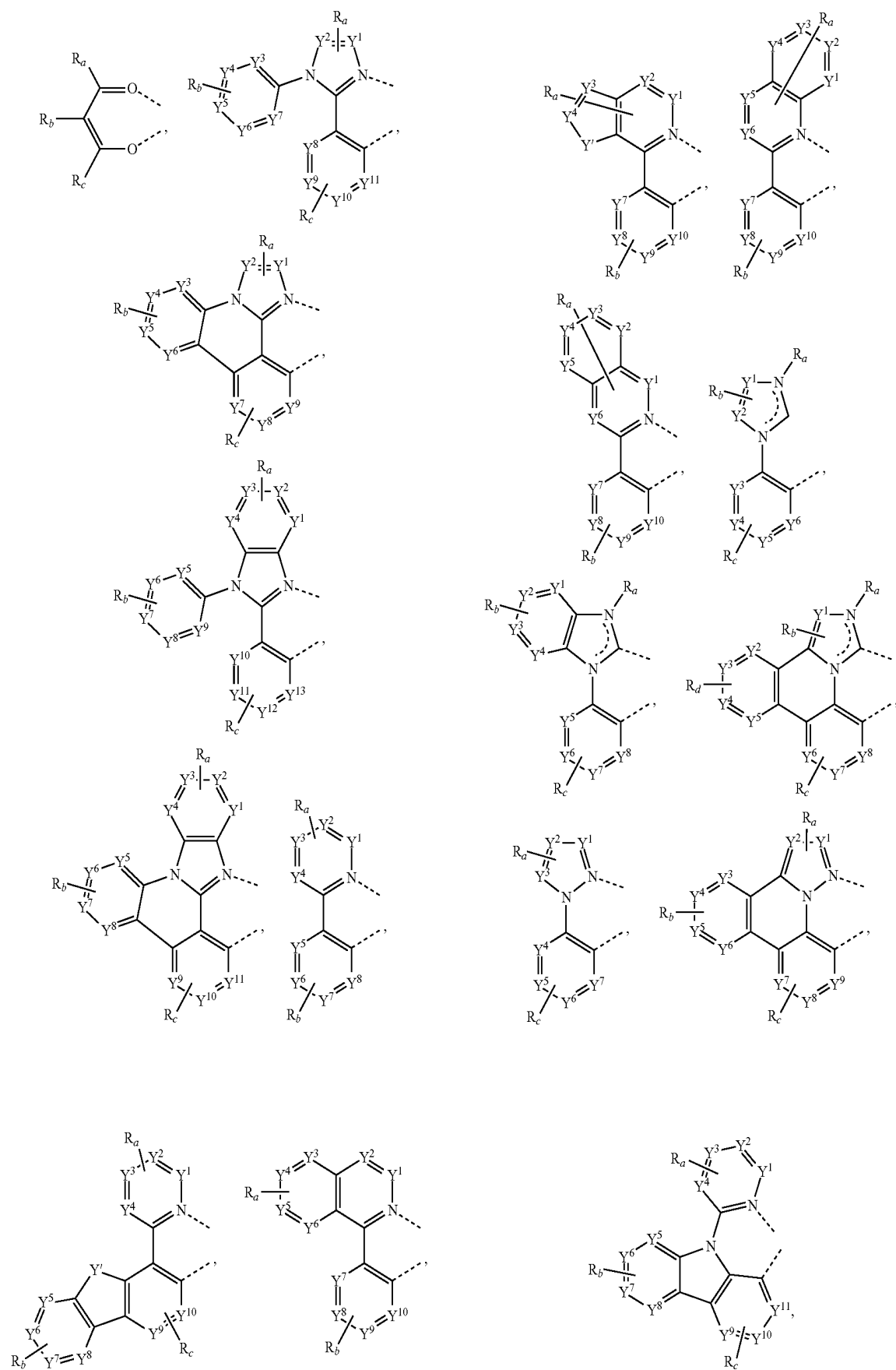
[0075] In some embodiments of the compound, the compound has a formula of $M(L_A)_x(L_B)_y(L_C)_z$, where L_B and L_C are each a bidentate ligand; x is 1, 2, or 3; y is 0, 1, or 2; z is 0, 1, or 2; and $x+y+z$ is the oxidation state of the metal M.

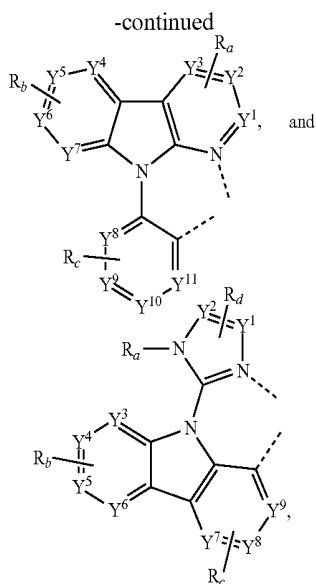
[0076] In some embodiments where the compound has the formula of $M(L_A)_x(L_B)_y(L_C)_z$, the compound has a formula selected from the group consisting of $Ir(L_A)_3$, $Ir(L_A)(L_B)_2$, $Ir(L_A)_2(L_B)$, $Ir(L_A)_2(L_C)$, and $Ir(L_A)(L_B)(L_C)$; where L_A , L_B , and L_C are different from each other.

[0077] In some embodiments where the compound has the formula of $M(L_A)_x(L_B)_y(L_C)_z$, the compound has a formula of $Pt(L_A)(L_B)$, where L_A and L_B can be the same or different. In some embodiments, L_A and L_B are connected to form a tetradentate ligand. In some embodiments, L_A and L_B are connected at two places to form a macrocyclic tetradentate ligand.

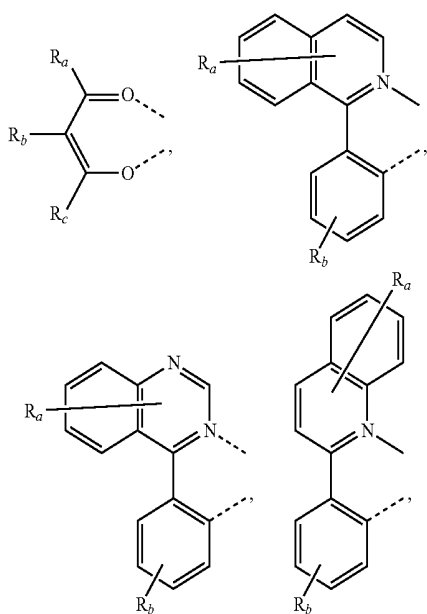
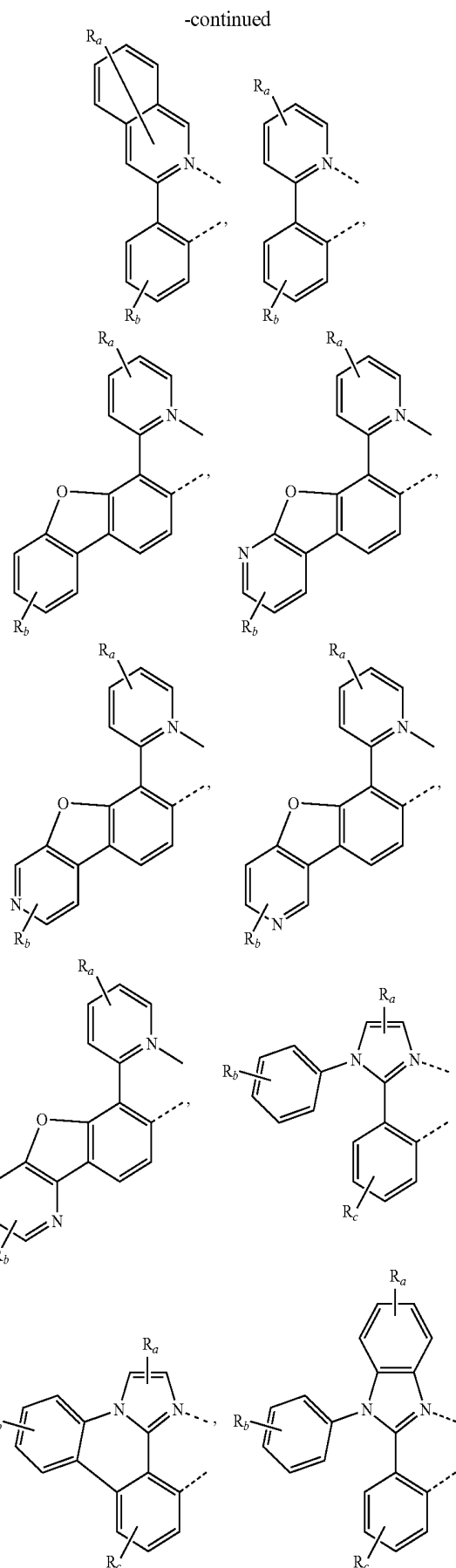
[0078] In some embodiments where the compound has the formula of $M(L_A)_x(L_B)_y(L_C)_z$, L_B and L_C are each independently selected from the group consisting of:

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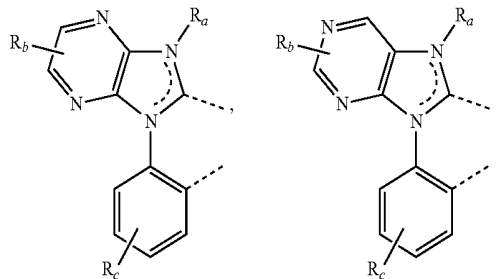
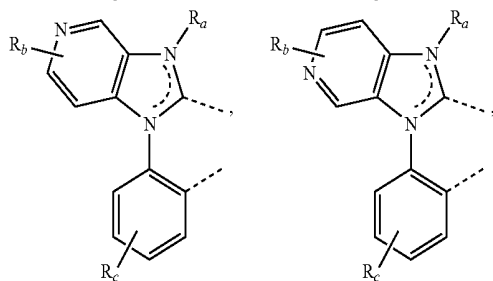
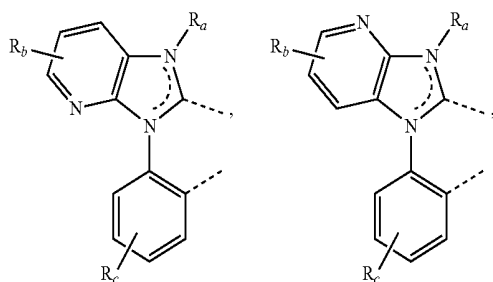
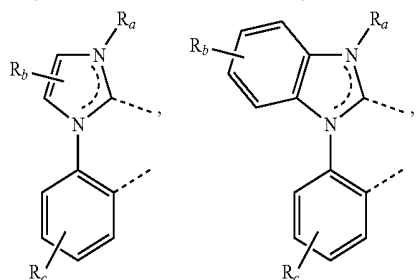
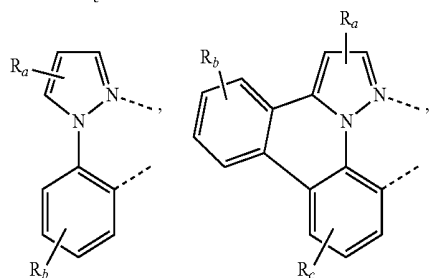
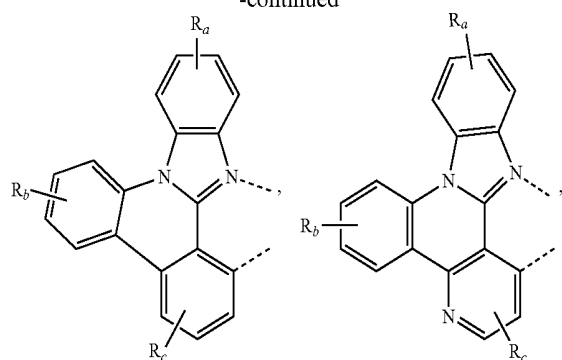




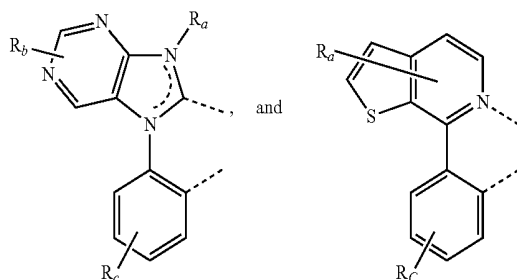
where each Y^1 to Y^{13} is independently selected from the group consisting of C and N; Y^1 is selected from the group consisting of B R_e , N R_e , P R_e , O, S, Se, C=O, S=O, SO₂, CR_eR_f, SiR_eR_f, and GeR_eR_f; R_e and R_f are optionally fused or joined to form a ring; each R_a, R_b, R_c, and R_d independently represents from mono substitution to the maximum possible number of substitutions; each R_a, R_b, R_c, R_d, R_e, and R_f is independently hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and where 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. In some embodiments, L_B and L_C are each independently selected from the group consisting of:



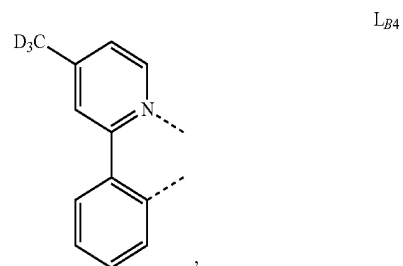
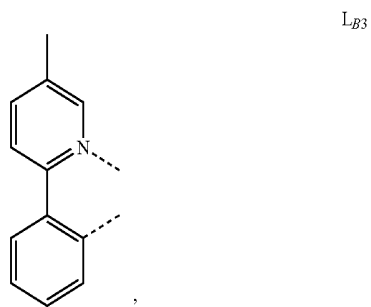
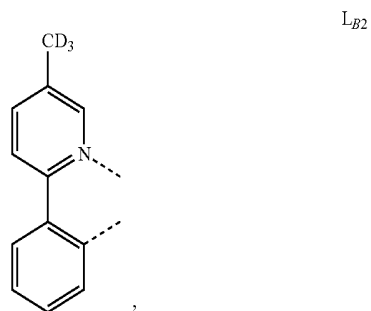
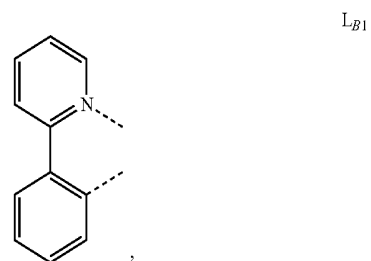
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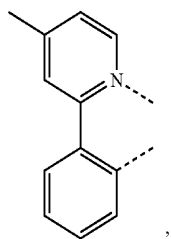
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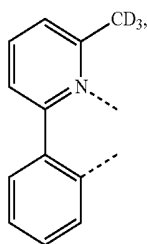
[0079] In some embodiments, L_B is selected from the group consisting of L_{B1} through L_{B263} with general numbering formula L_{Bk} , where k is an integer from 1 to 263:



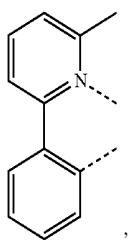
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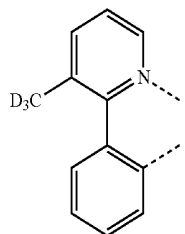
L_{B5}



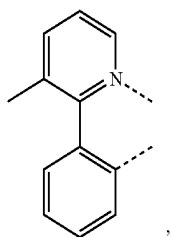
L_{B6}



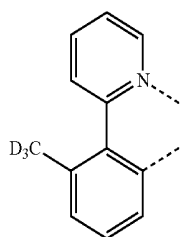
L_{B7}



L_{B8}

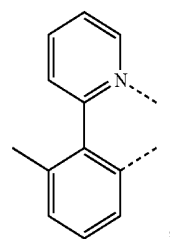


L_{B9}

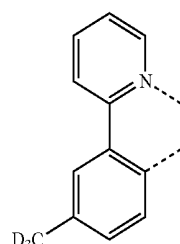


L_{B10}

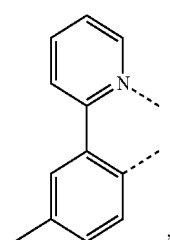
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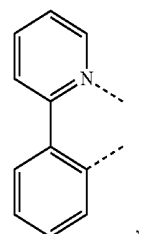
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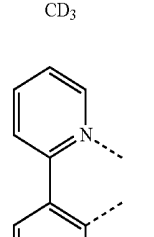
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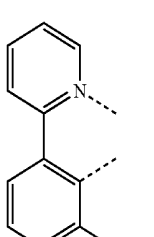
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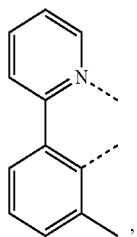


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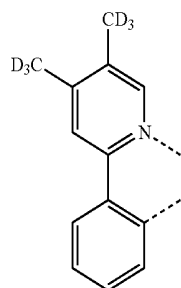


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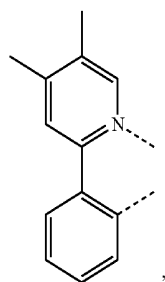
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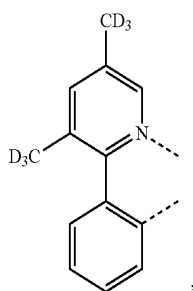
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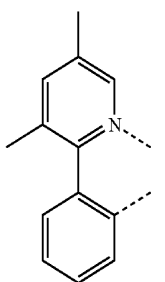
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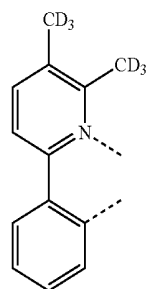


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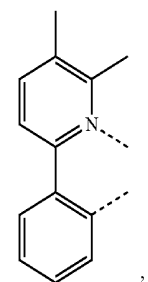


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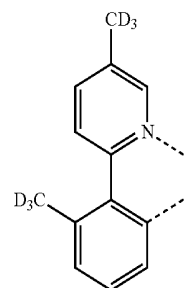
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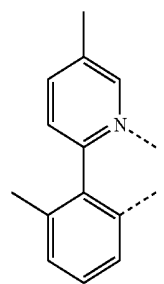
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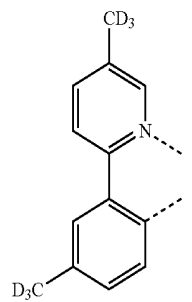
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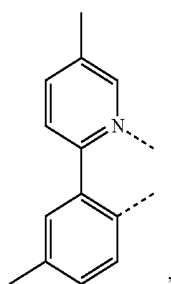


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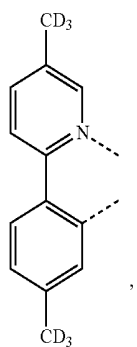


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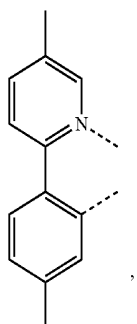
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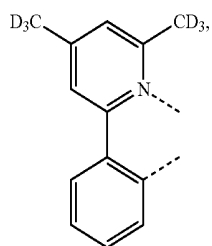
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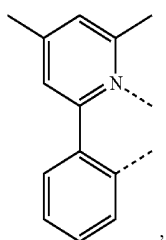
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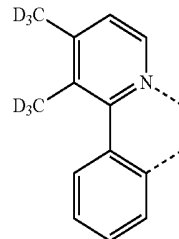


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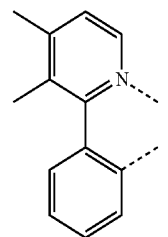


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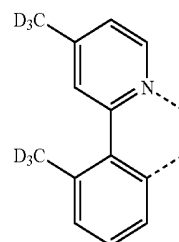
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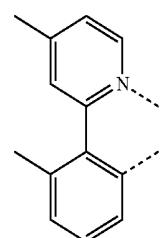
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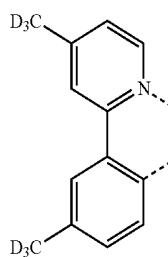
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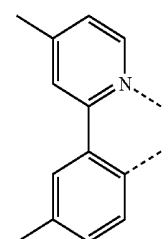
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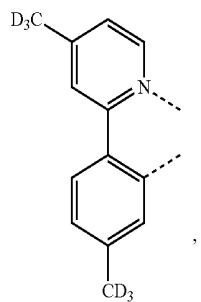


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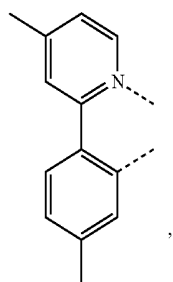


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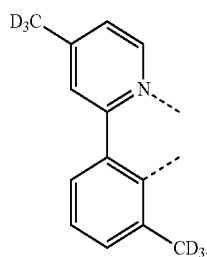
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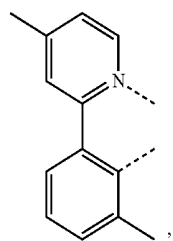
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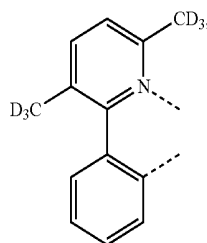
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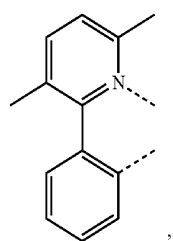
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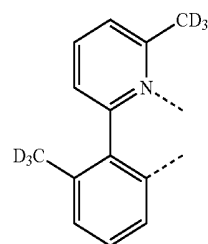


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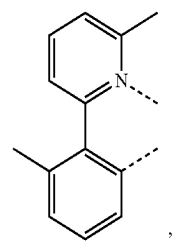


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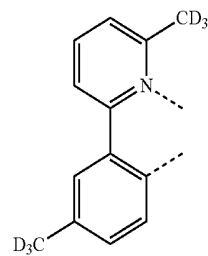
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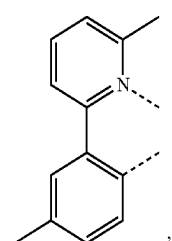
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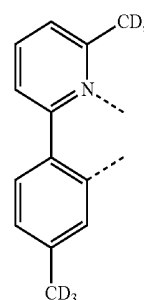
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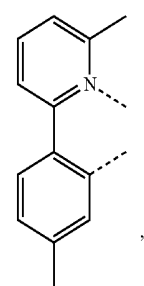
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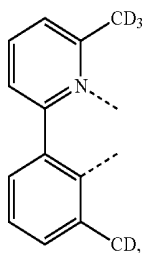


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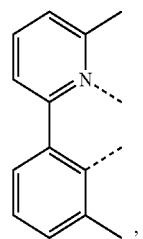


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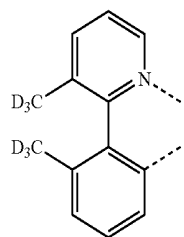
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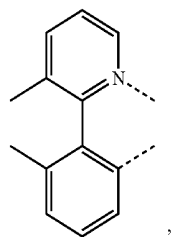
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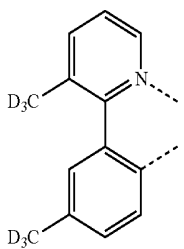
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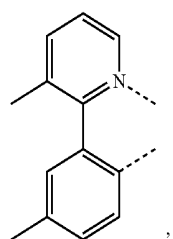
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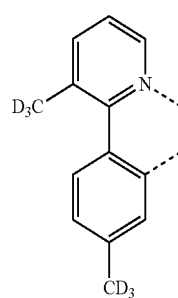


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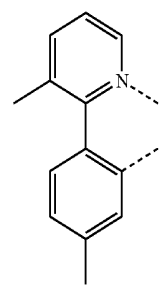


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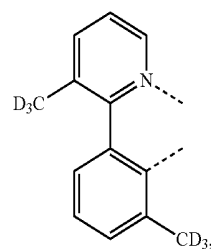
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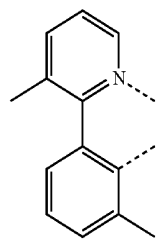
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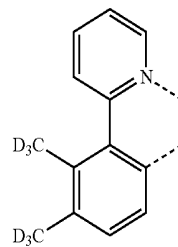
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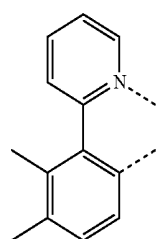
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L_{B59}

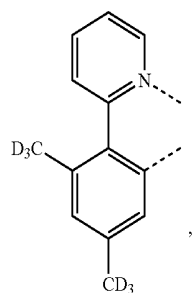


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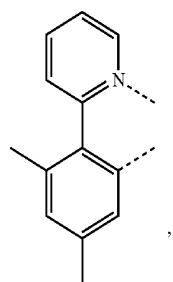


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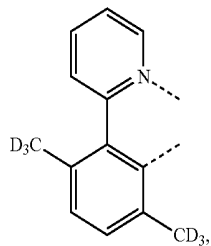
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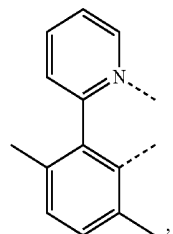
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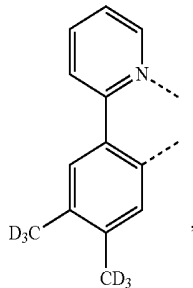
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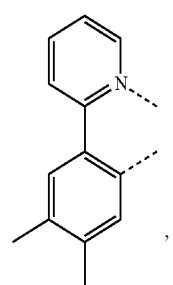
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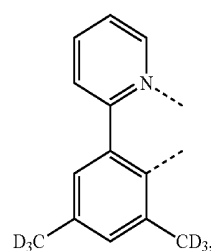


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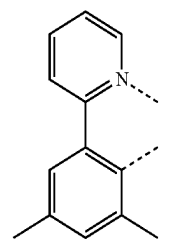


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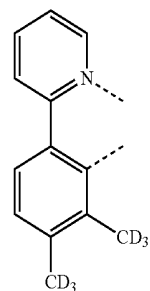
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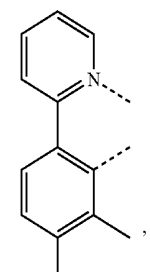
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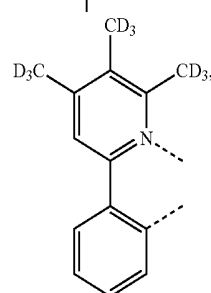
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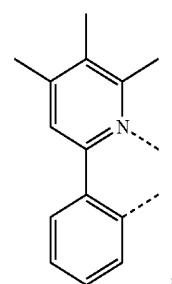
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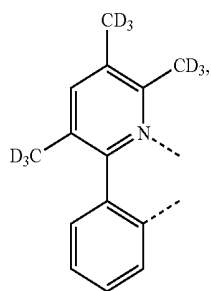


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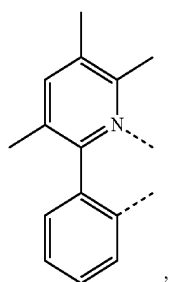


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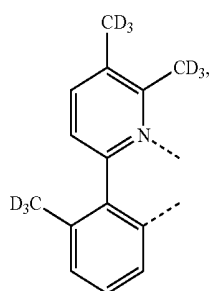
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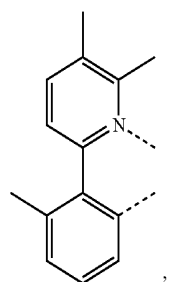
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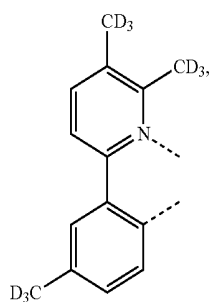
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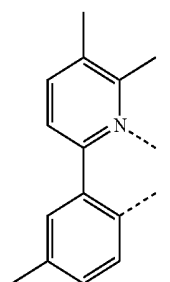


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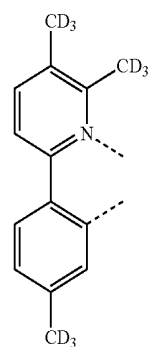


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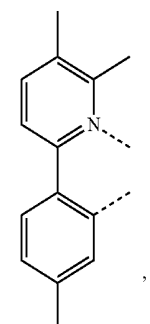
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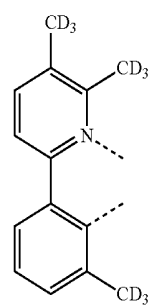
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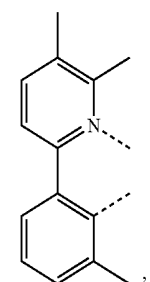
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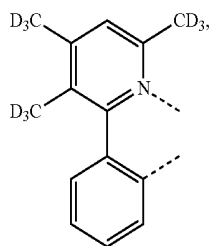


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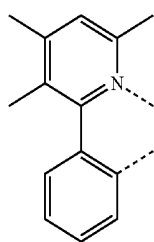


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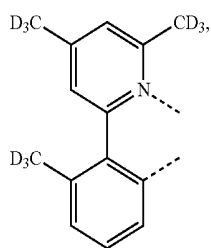
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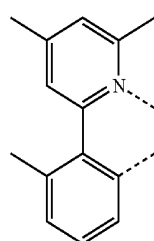
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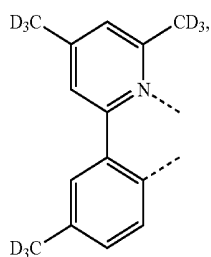
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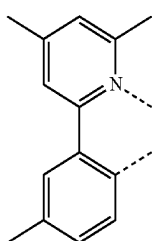
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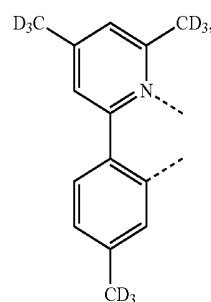


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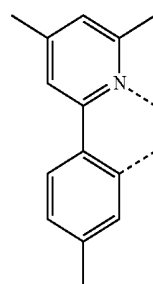


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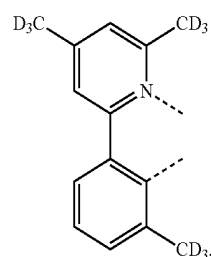
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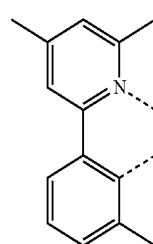
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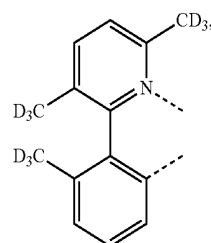
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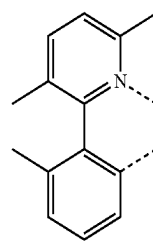
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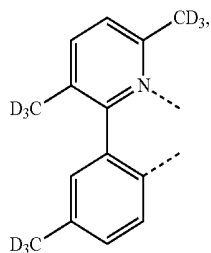


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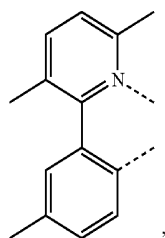


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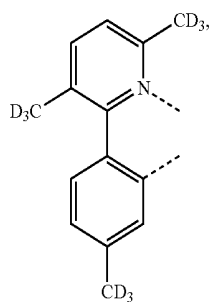
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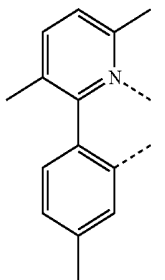
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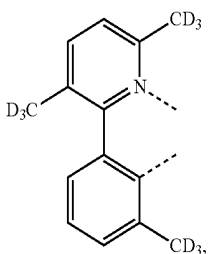
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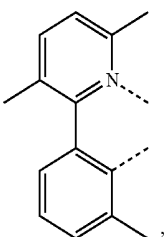
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L_{B99}

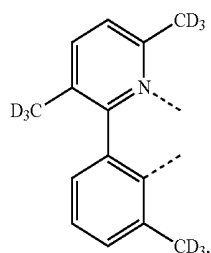


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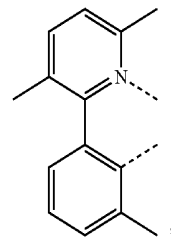


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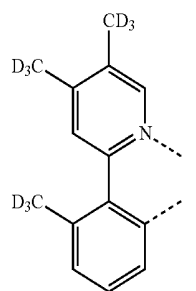
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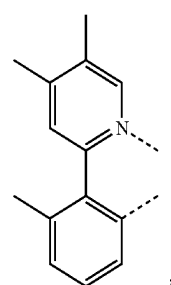
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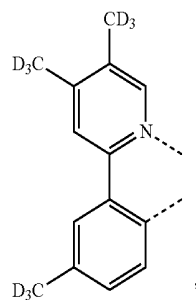
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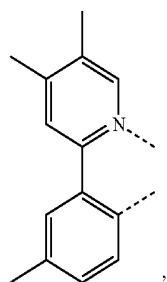


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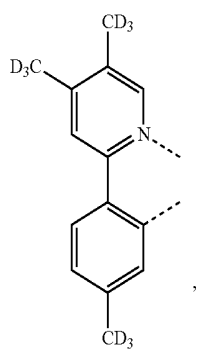


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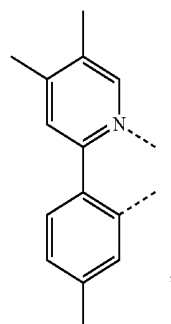
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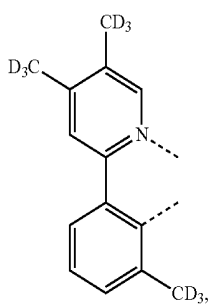
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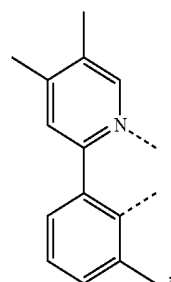
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LB109

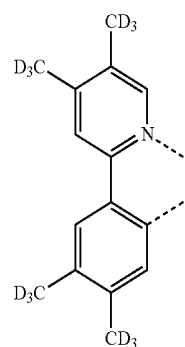


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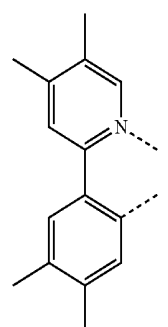


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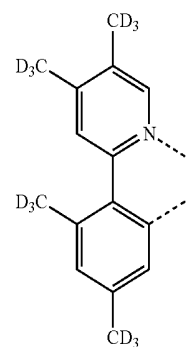
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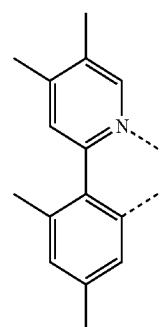
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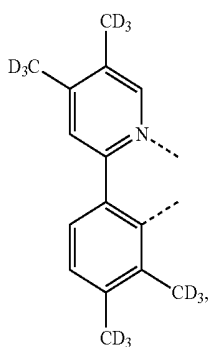


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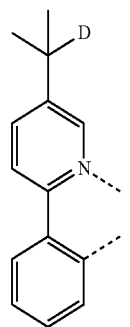
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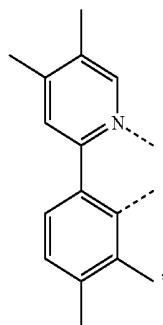
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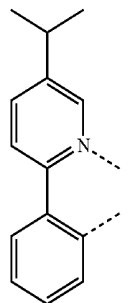


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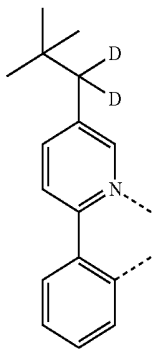
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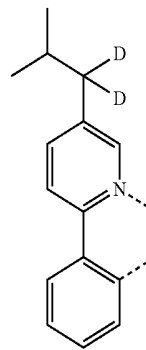
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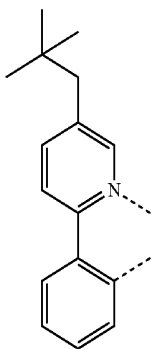
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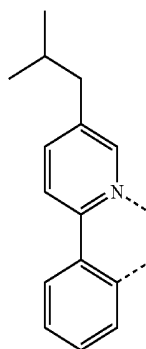
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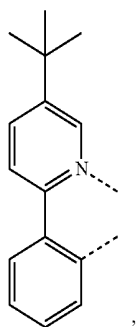
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LB123

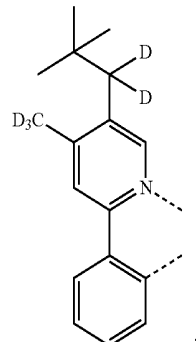


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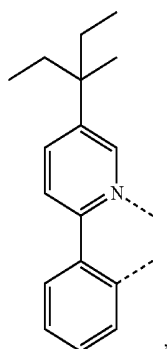


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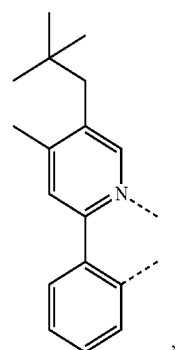
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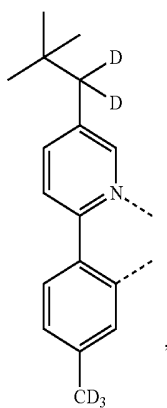
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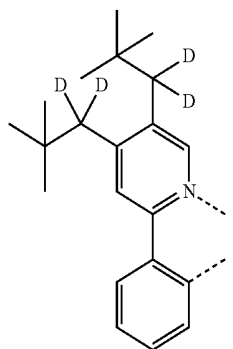
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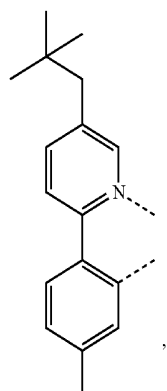
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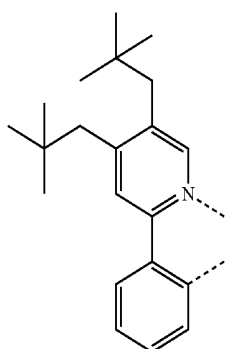
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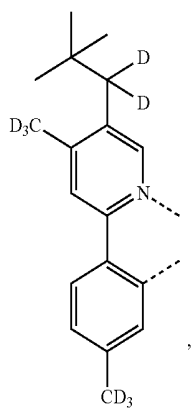


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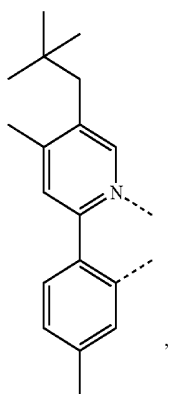


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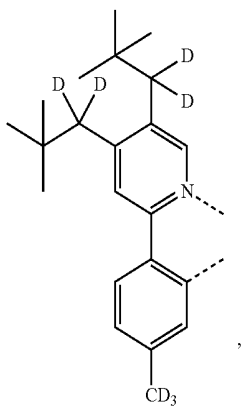
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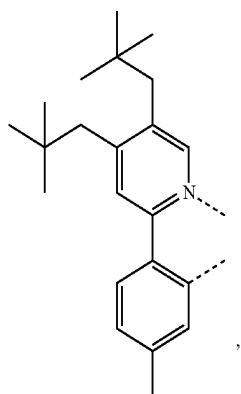
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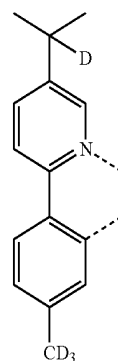


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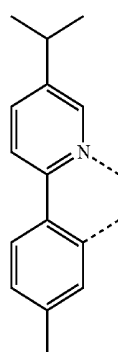


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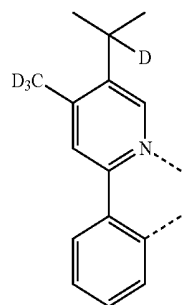
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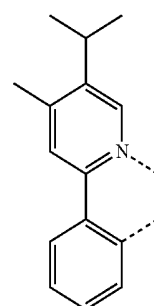
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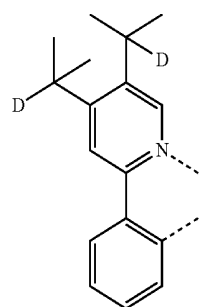
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L_{B138}

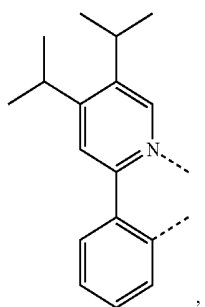


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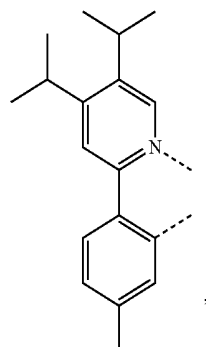
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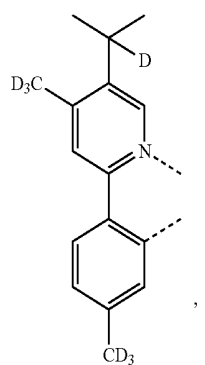


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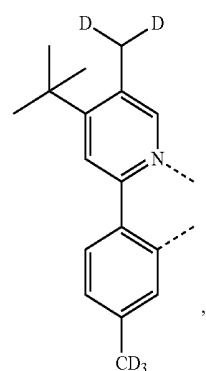
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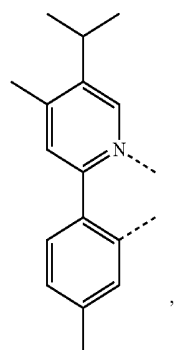
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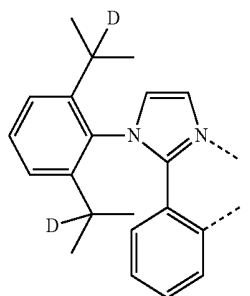
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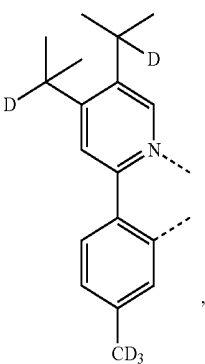
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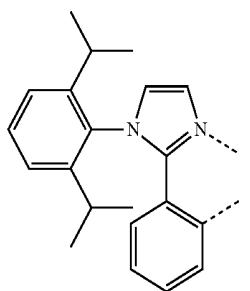
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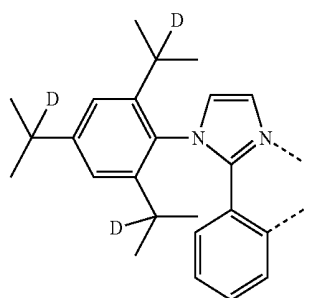
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LB144

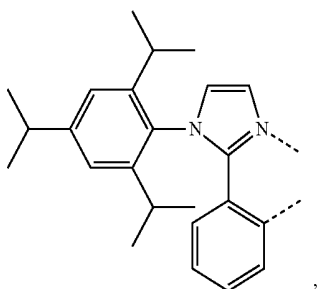


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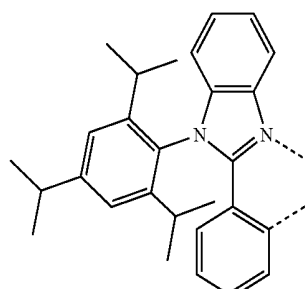
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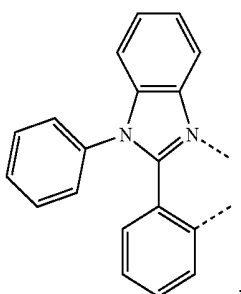


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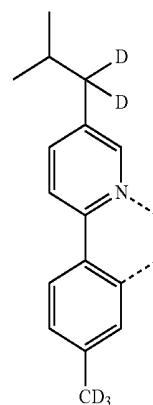
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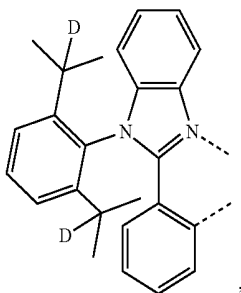
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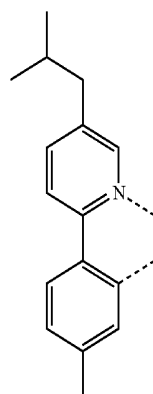
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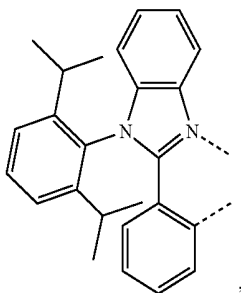
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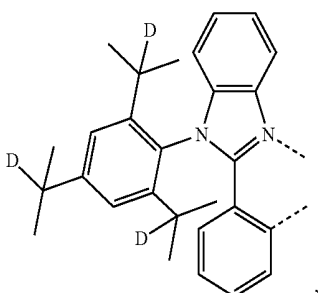
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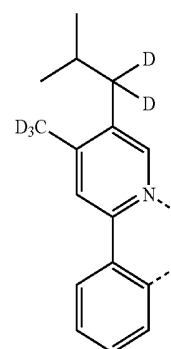
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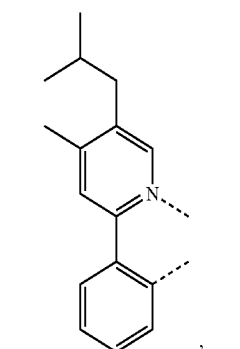


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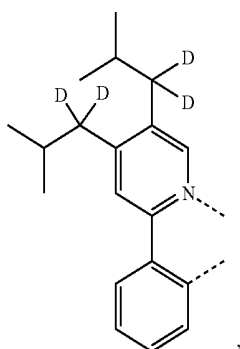


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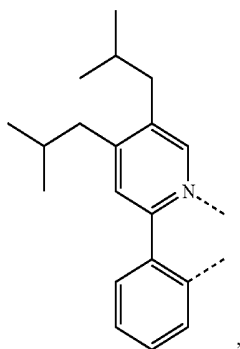
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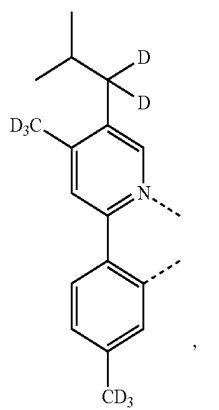
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LB160

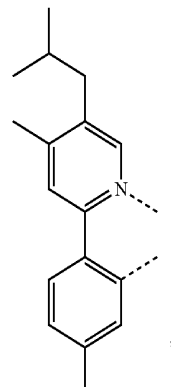


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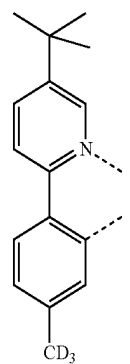


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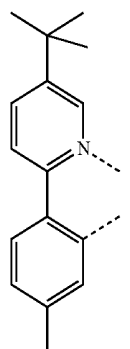
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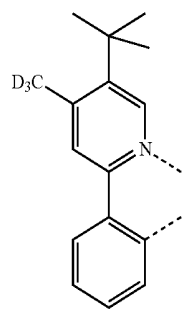
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LB164

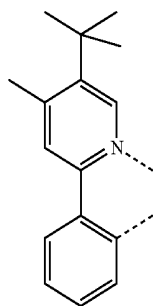


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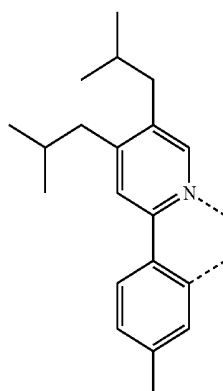
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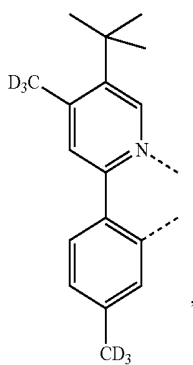


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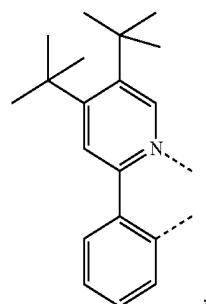
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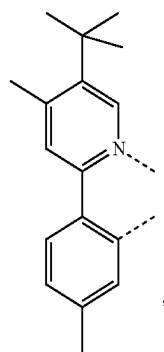
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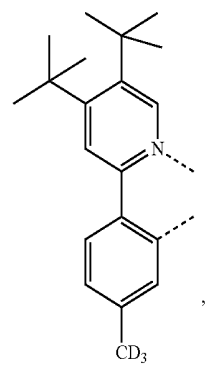
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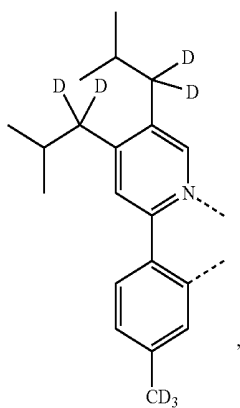
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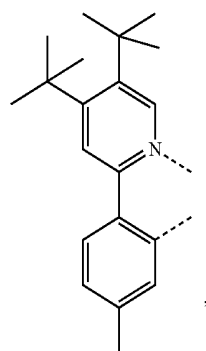
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LB173

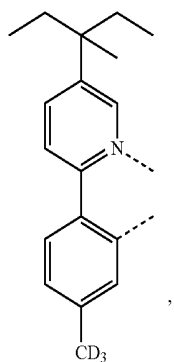


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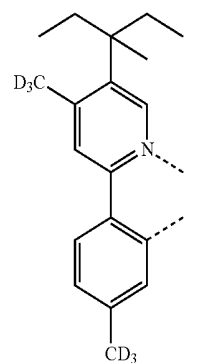
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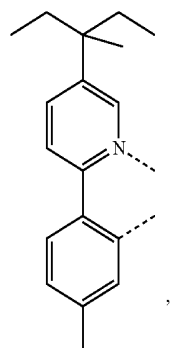
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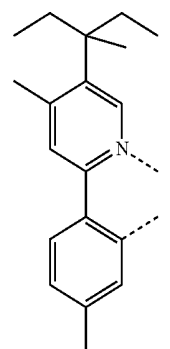


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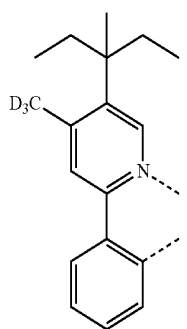
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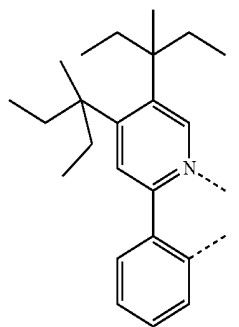
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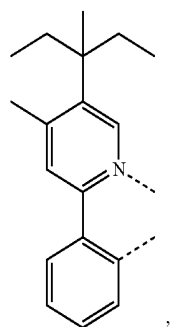
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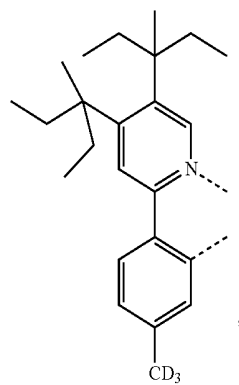
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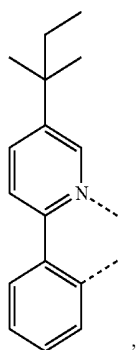
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LB182

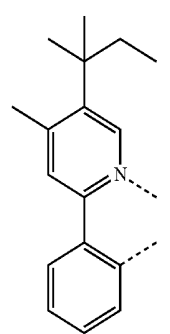


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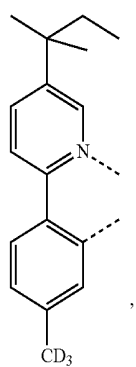


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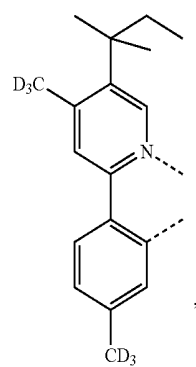
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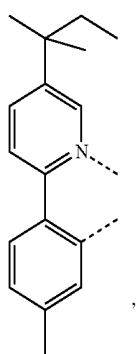
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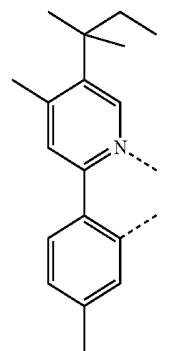
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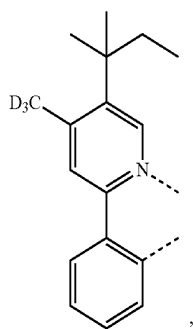
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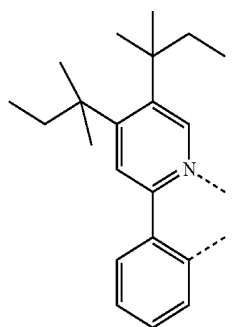
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LB189

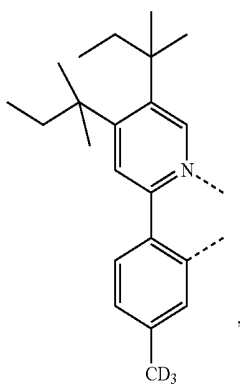


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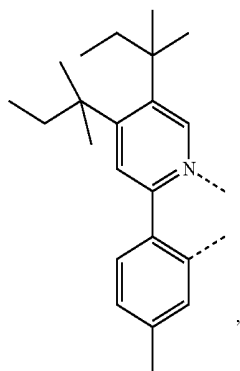


LB190

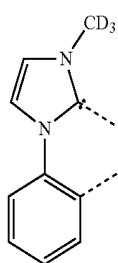
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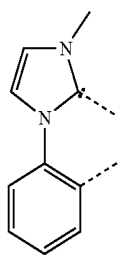
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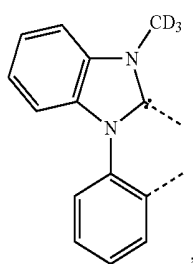
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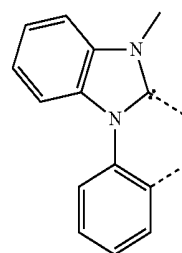


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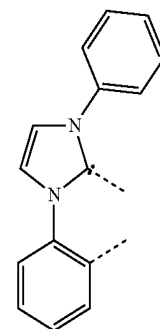


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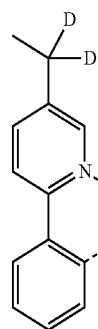
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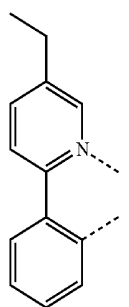
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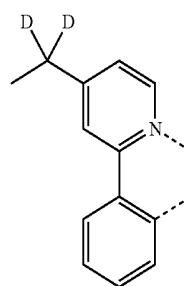
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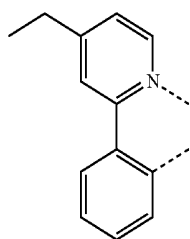


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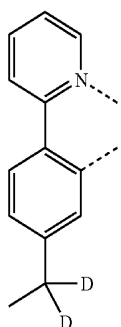


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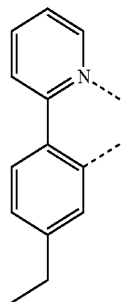
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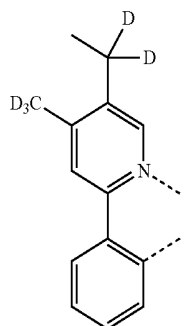
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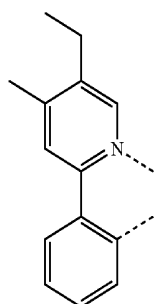
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L_{B203}

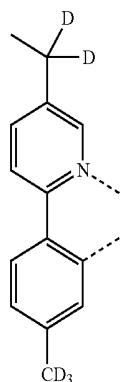


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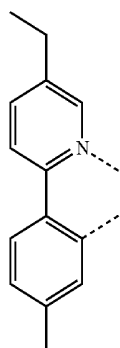


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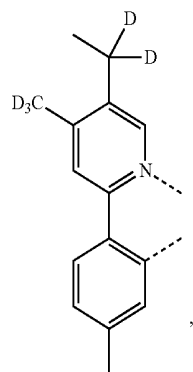
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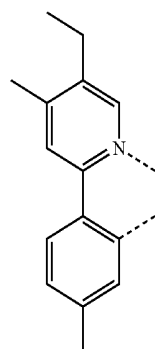
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L_{B207}

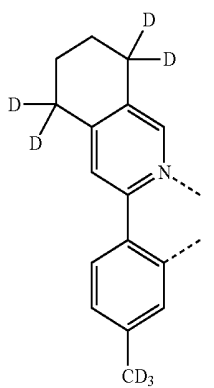


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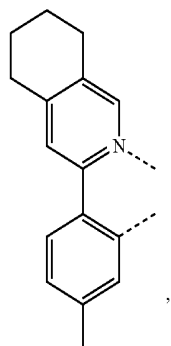


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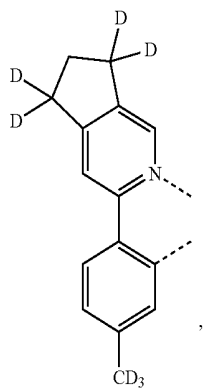
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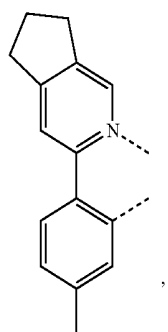
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L_{B211}

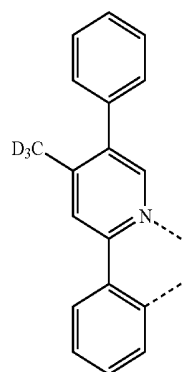


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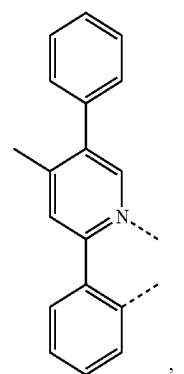


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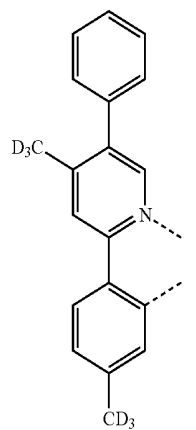
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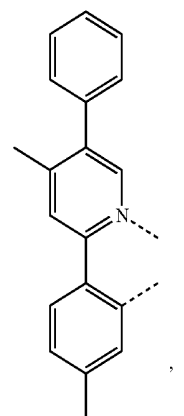
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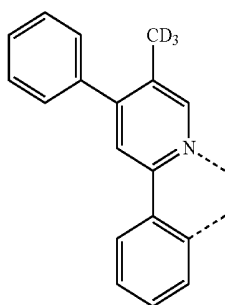


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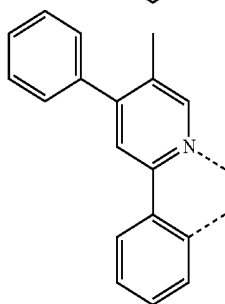


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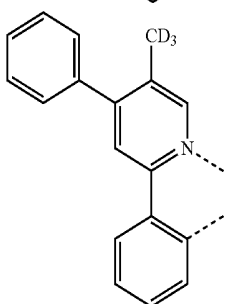
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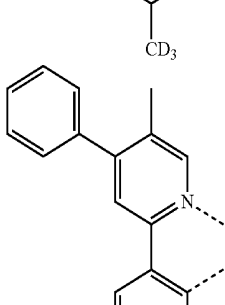
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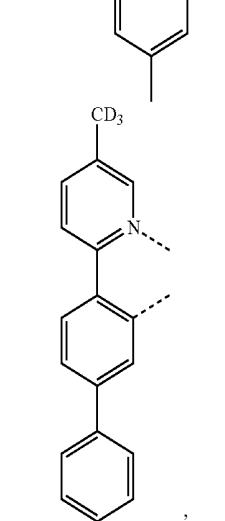
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L_{B220}

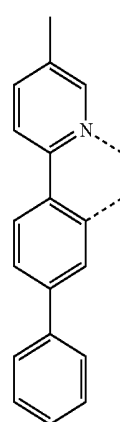


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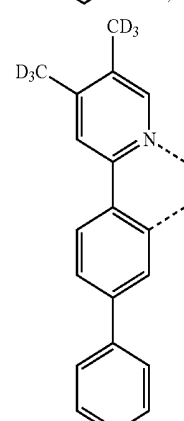


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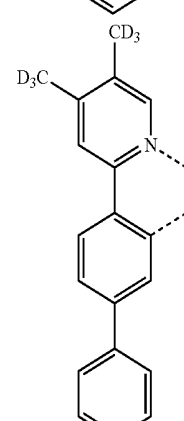
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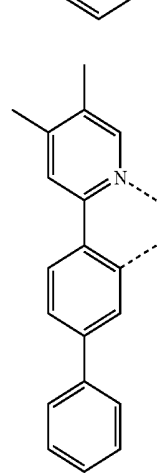
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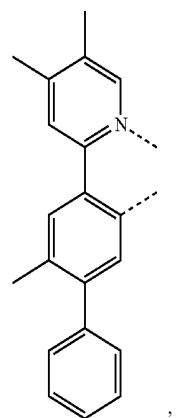
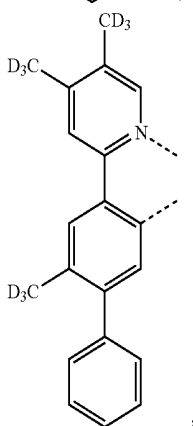
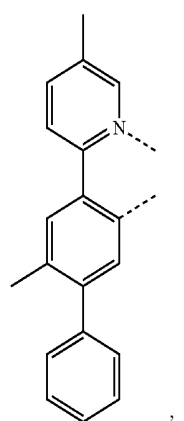
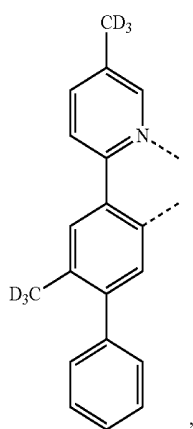


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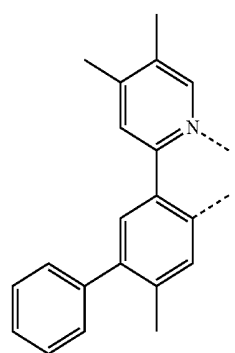
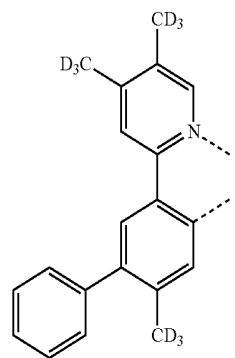
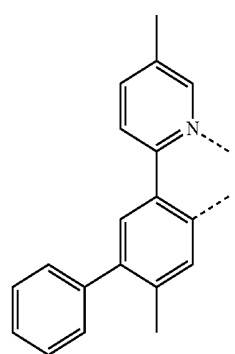
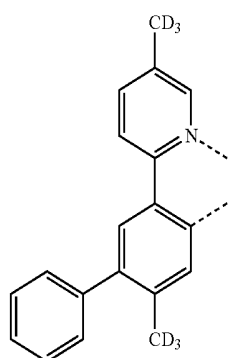


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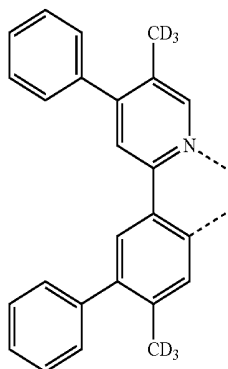
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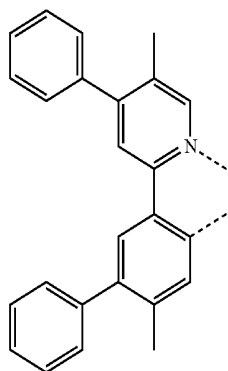
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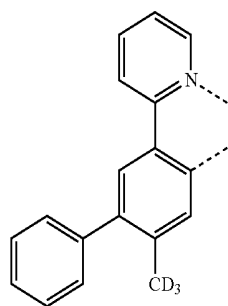
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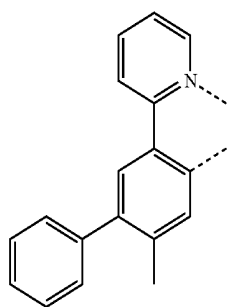
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L_{B236}

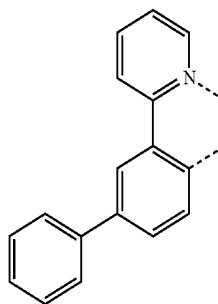


L_{B237}

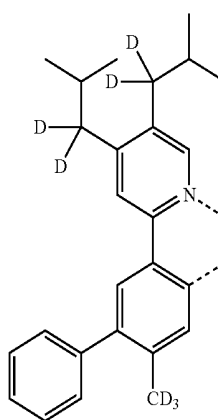


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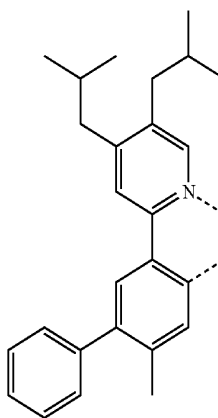
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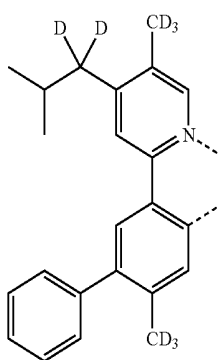
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L_{B240}

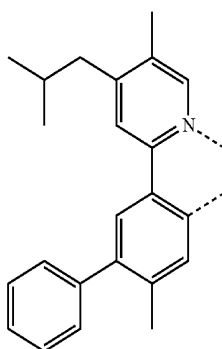


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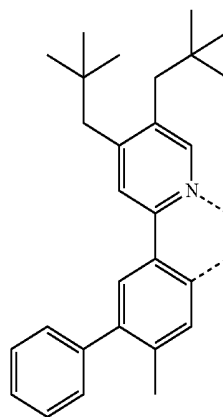
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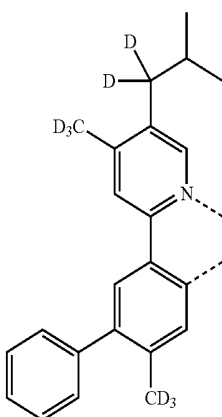


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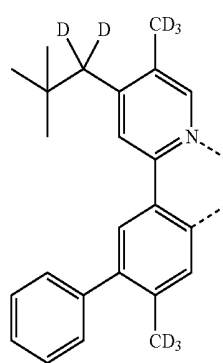
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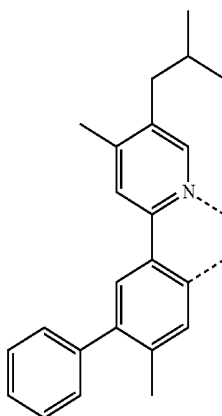
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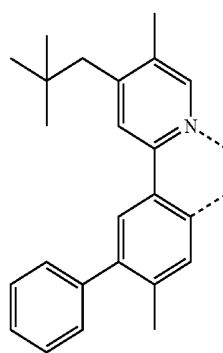
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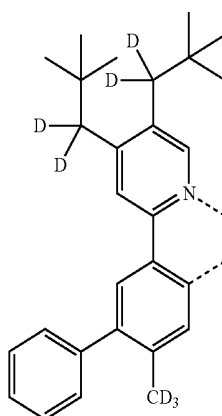
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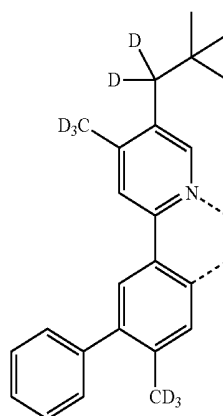
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L_{B249}

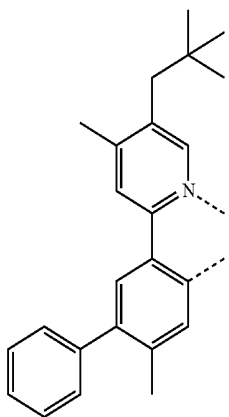


L_{B246}



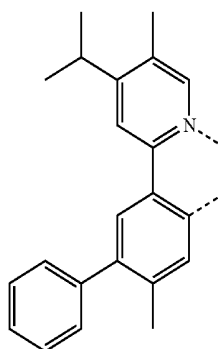
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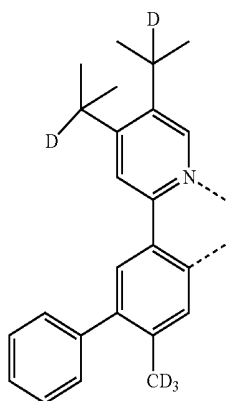


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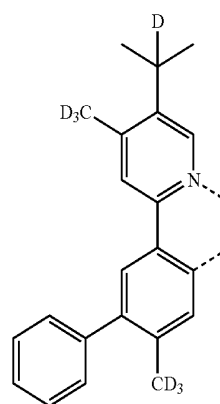
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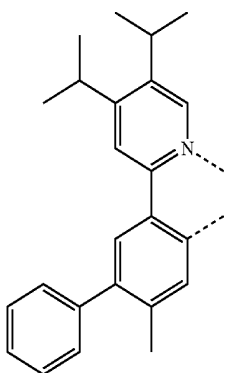
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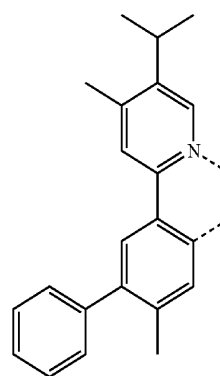
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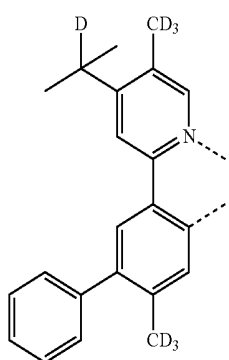
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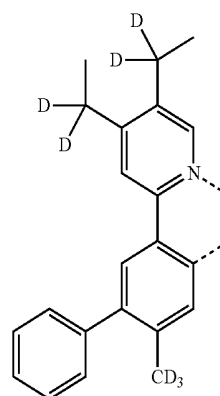
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L_{B257}

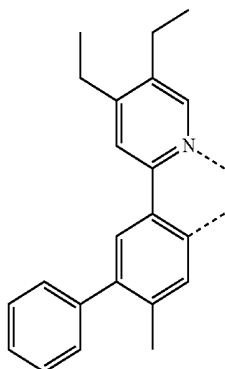


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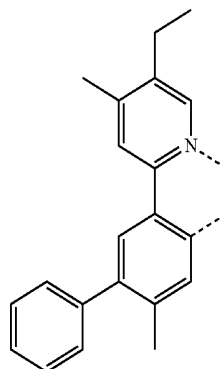
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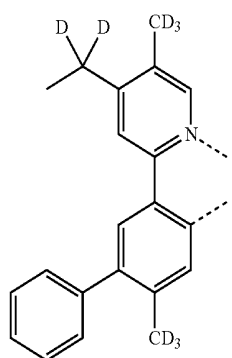


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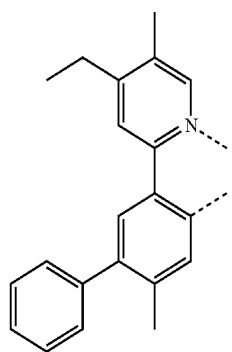


L_{B263}

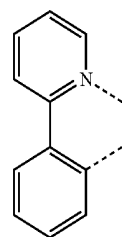


L_{B260}

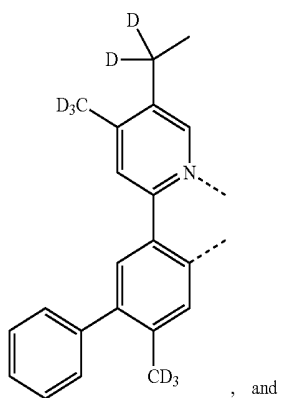
[0080] In some embodiments, L_B is selected from the group consisting of:



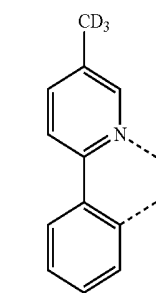
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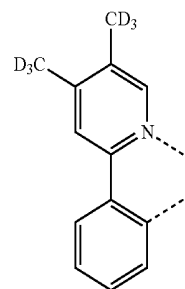
L_{B1}



L_{B262}

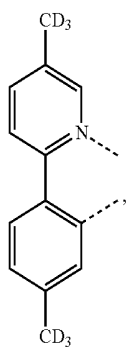


L_{B2}

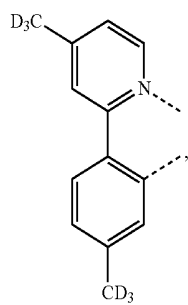


L_{B18}

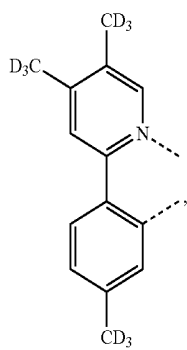
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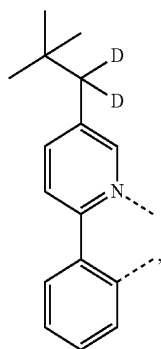
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L_{B38}

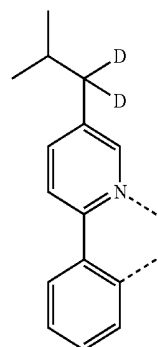


L_{B108}

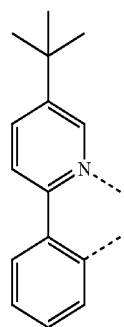


L_{B118}

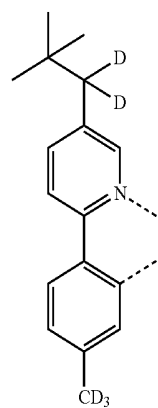
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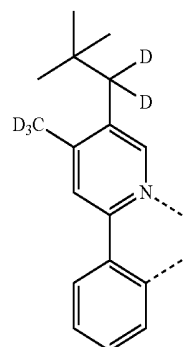
L_{B122}



L_{B124}

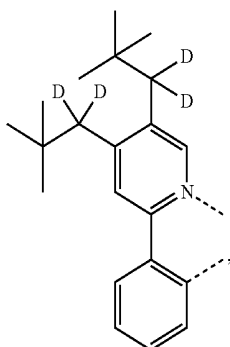


L_{B126}



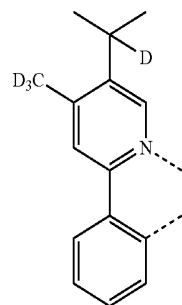
L_{B128}

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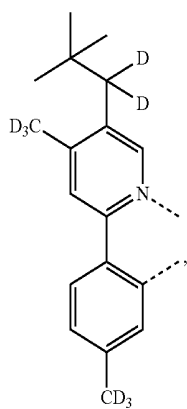


L_{B130}

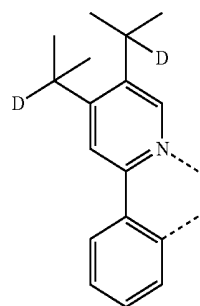
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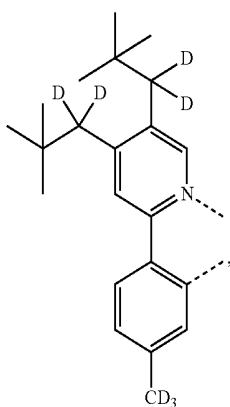
L_{B138}



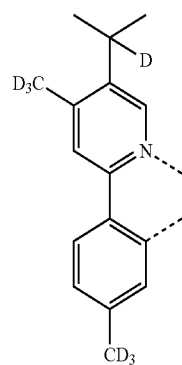
L_{B132}



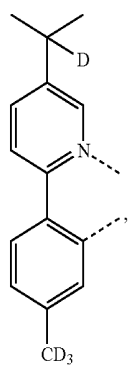
L_{B140}



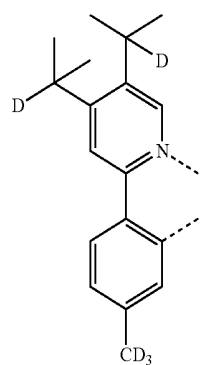
L_{B134}



L_{B142}

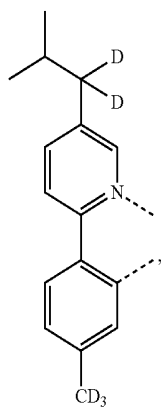


L_{B136}



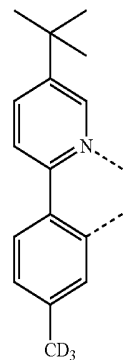
L_{B144}

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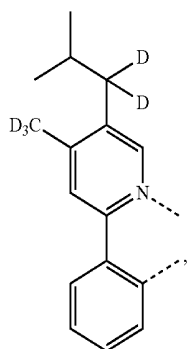


LB156

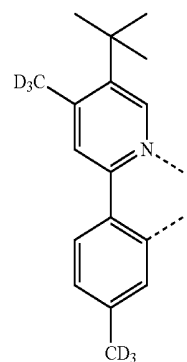
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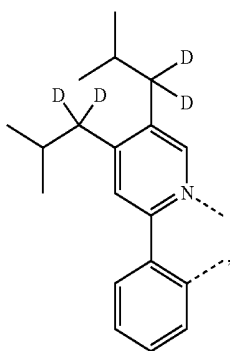
LB164



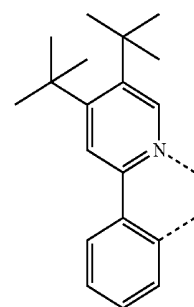
LB158



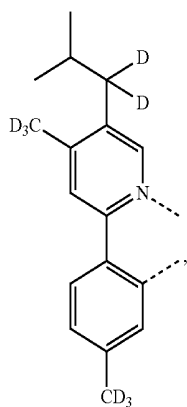
LB168



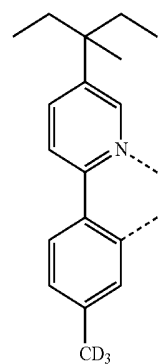
LB160



LB172

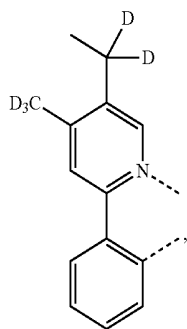


LB162



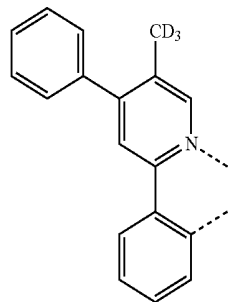
LB175

-continued

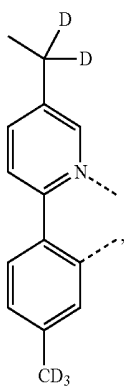


L_{B204}

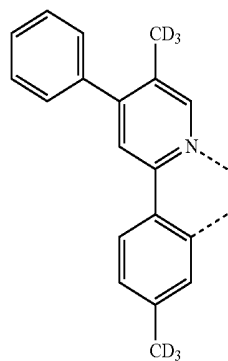
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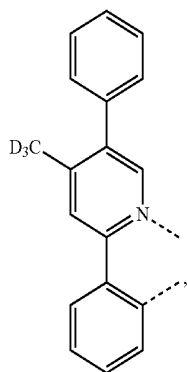
L_{B218}



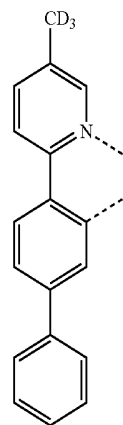
L_{B206}



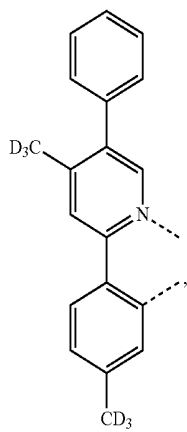
L_{B220}



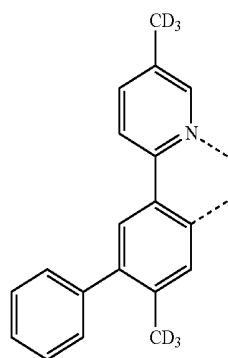
L_{B214}



L_{B222}

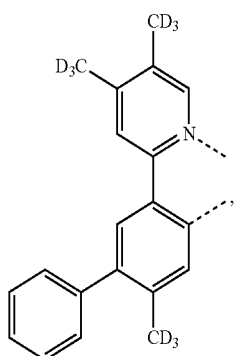


L_{B216}

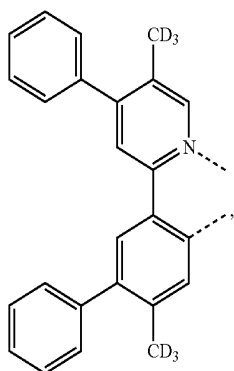


L_{B231}

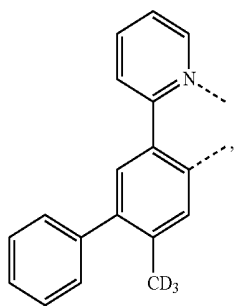
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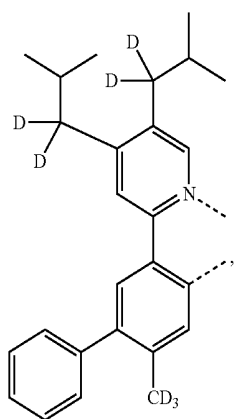
L_{B233}



L_{B235}

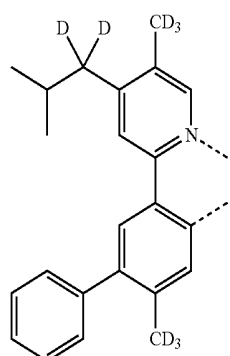


L_{B237}

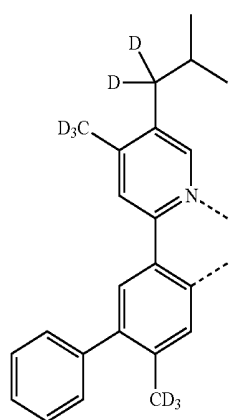


L_{B240}

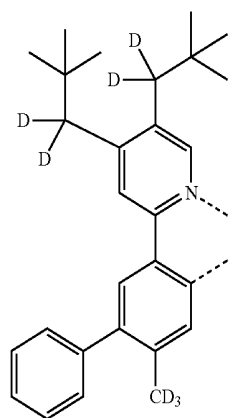
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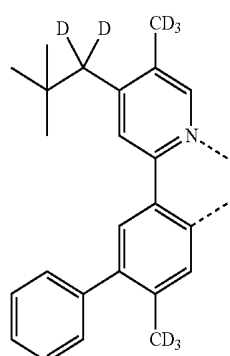
L_{B242}



L_{B244}

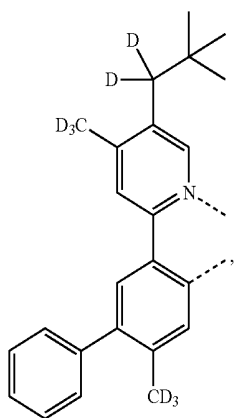


L_{B246}

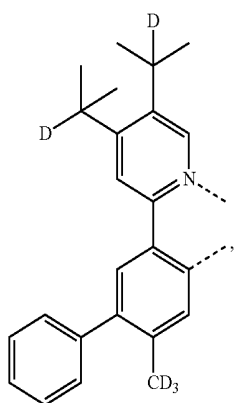


L_{B248}

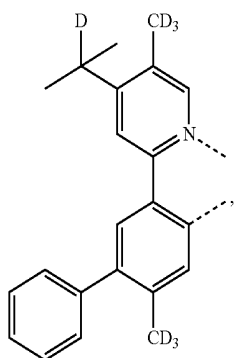
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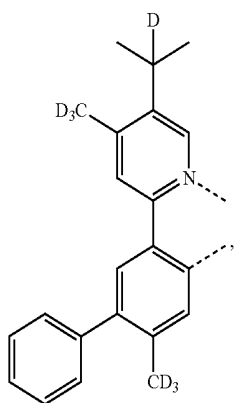
L_{B250}



L_{B252}

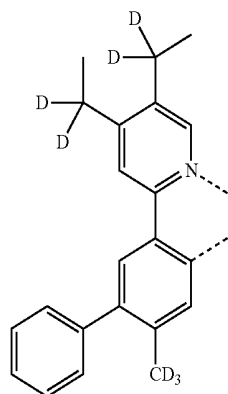


L_{B254}

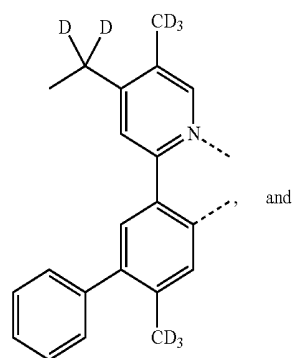


L_{B256}

-continued

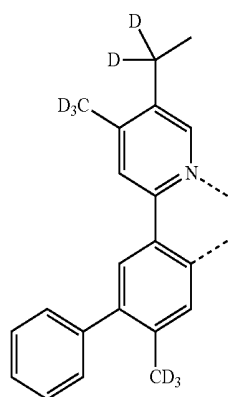


L_{B258}



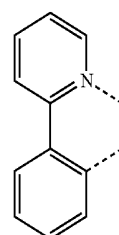
L_{B260}

and



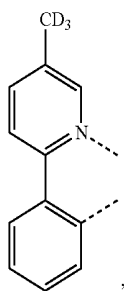
L_{B262}

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

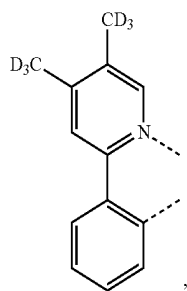


L_{B1}

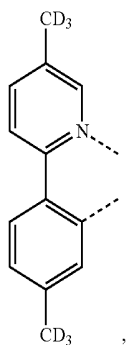
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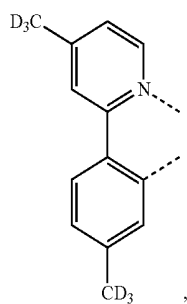
L_{B2}



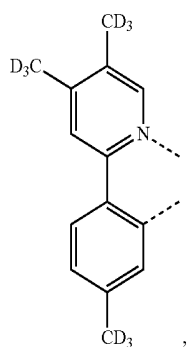
L_{B18}



L_{B28}

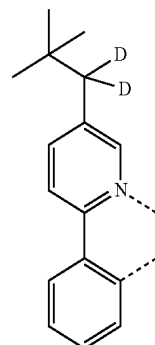


L_{B38}

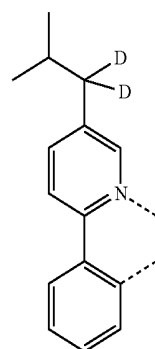


L_{B108}

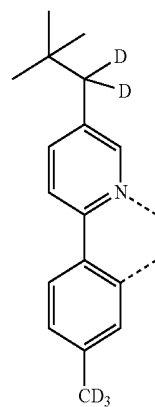
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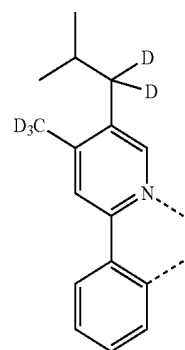
L_{B118}



L_{B122}

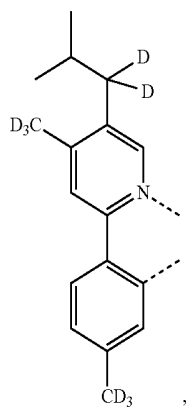


L_{B126}

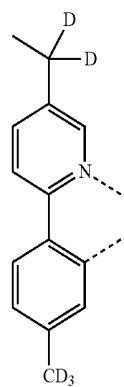
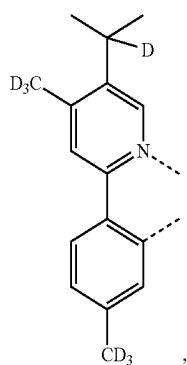
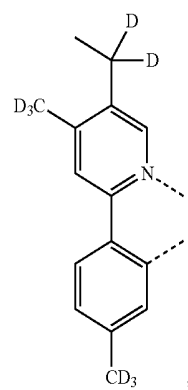
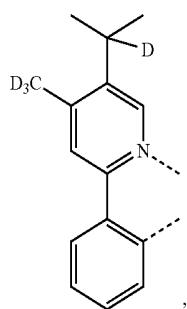
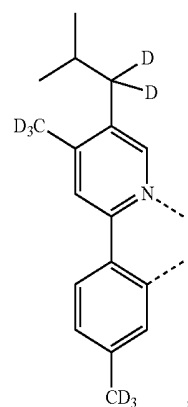
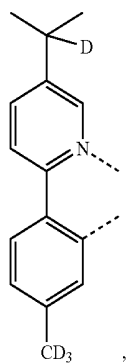
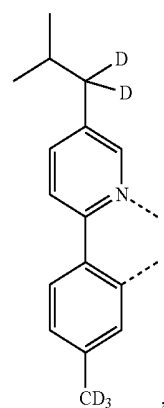


L_{B128}

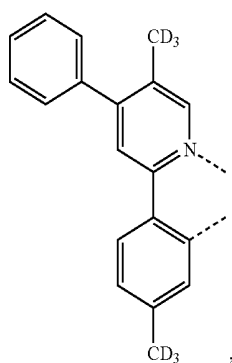
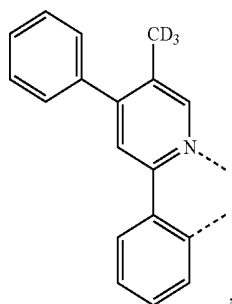
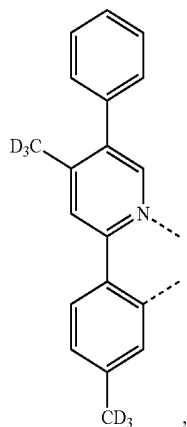
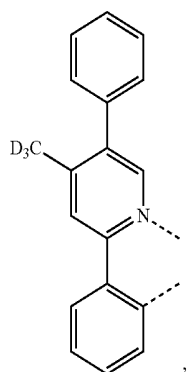
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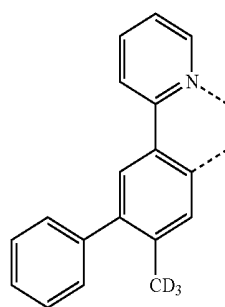
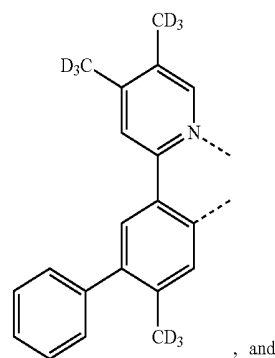
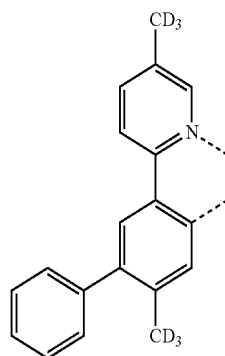
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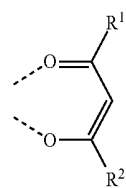
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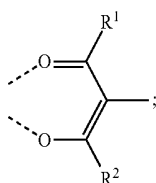
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[0082] In some embodiments, L_C is selected from the group consisting of L_{C1-I} through L_{C768-I} with general numbering formula L_{Cj-I} (j is an integer of 1 to 768) based on a structure of



L_{C1-II} through $L_{C768-II}$ with general numbering formula L_{Cj-II} based on a structure of



wherein for each L_{Cj} , R^1 and R^2 are defined as:

| Ligand | R^1 | R^2 |
|-----------|-----------|-----------|
| L_{C1} | R^{D1} | R^{D1} |
| L_{C2} | R^{D2} | R^{D2} |
| L_{C3} | R^{D3} | R^{D3} |
| L_{C4} | R^{D4} | R^{D4} |
| L_{C5} | R^{D5} | R^{D5} |
| L_{C6} | R^{D6} | R^{D6} |
| L_{C7} | R^{D7} | R^{D7} |
| L_{C8} | R^{D8} | R^{D8} |
| L_{C9} | R^{D9} | R^{D9} |
| L_{C10} | R^{D10} | R^{D10} |
| L_{C11} | R^{D11} | R^{D11} |
| L_{C12} | R^{D12} | R^{D12} |
| L_{C13} | R^{D13} | R^{D13} |
| L_{C14} | R^{D14} | R^{D14} |
| L_{C15} | R^{D15} | R^{D15} |
| L_{C16} | R^{D16} | R^{D16} |
| L_{C17} | R^{D17} | R^{D17} |
| L_{C18} | R^{D18} | R^{D18} |
| L_{C19} | R^{D19} | R^{D19} |
| L_{C20} | R^{D20} | R^{D20} |
| L_{C21} | R^{D21} | R^{D21} |
| L_{C22} | R^{D22} | R^{D22} |
| L_{C23} | R^{D23} | R^{D23} |
| L_{C24} | R^{D24} | R^{D24} |
| L_{C25} | R^{D25} | R^{D25} |
| L_{C26} | R^{D26} | R^{D26} |
| L_{C27} | R^{D27} | R^{D27} |
| L_{C28} | R^{D28} | R^{D28} |
| L_{C29} | R^{D29} | R^{D29} |
| L_{C30} | R^{D30} | R^{D30} |
| L_{C31} | R^{D31} | R^{D31} |
| L_{C32} | R^{D32} | R^{D32} |
| L_{C33} | R^{D33} | R^{D33} |
| L_{C34} | R^{D34} | R^{D34} |
| L_{C35} | R^{D35} | R^{D35} |
| L_{C36} | R^{D36} | R^{D36} |
| L_{C37} | R^{D37} | R^{D37} |
| L_{C38} | R^{D38} | R^{D38} |
| L_{C39} | R^{D39} | R^{D39} |
| L_{C40} | R^{D40} | R^{D40} |
| L_{C41} | R^{D41} | R^{D41} |
| L_{C42} | R^{D42} | R^{D42} |
| L_{C43} | R^{D43} | R^{D43} |
| L_{C44} | R^{D44} | R^{D44} |
| L_{C45} | R^{D45} | R^{D45} |
| L_{C46} | R^{D46} | R^{D46} |
| L_{C47} | R^{D47} | R^{D47} |
| L_{C48} | R^{D48} | R^{D48} |
| L_{C49} | R^{D49} | R^{D49} |
| L_{C50} | R^{D50} | R^{D50} |
| L_{C51} | R^{D51} | R^{D51} |
| L_{C52} | R^{D52} | R^{D52} |
| L_{C53} | R^{D53} | R^{D53} |
| L_{C54} | R^{D54} | R^{D54} |
| L_{C55} | R^{D55} | R^{D55} |
| L_{C56} | R^{D56} | R^{D56} |
| L_{C57} | R^{D57} | R^{D57} |
| L_{C58} | R^{D58} | R^{D58} |
| L_{C59} | R^{D59} | R^{D59} |
| L_{C60} | R^{D60} | R^{D60} |
| L_{C61} | R^{D61} | R^{D61} |
| L_{C62} | R^{D62} | R^{D62} |

-continued

| Ligand | R^1 | R^2 |
|------------|------------|------------|
| L_{C63} | R^{D63} | R^{D63} |
| L_{C64} | R^{D64} | R^{D64} |
| L_{C65} | R^{D65} | R^{D65} |
| L_{C66} | R^{D66} | R^{D66} |
| L_{C67} | R^{D67} | R^{D67} |
| L_{C68} | R^{D68} | R^{D68} |
| L_{C69} | R^{D69} | R^{D69} |
| L_{C70} | R^{D70} | R^{D70} |
| L_{C71} | R^{D71} | R^{D71} |
| L_{C72} | R^{D72} | R^{D72} |
| L_{C73} | R^{D73} | R^{D73} |
| L_{C74} | R^{D74} | R^{D74} |
| L_{C75} | R^{D75} | R^{D75} |
| L_{C76} | R^{D76} | R^{D76} |
| L_{C77} | R^{D77} | R^{D77} |
| L_{C78} | R^{D78} | R^{D78} |
| L_{C79} | R^{D79} | R^{D79} |
| L_{C80} | R^{D80} | R^{D80} |
| L_{C81} | R^{D81} | R^{D81} |
| L_{C82} | R^{D82} | R^{D82} |
| L_{C83} | R^{D83} | R^{D83} |
| L_{C84} | R^{D84} | R^{D84} |
| L_{C85} | R^{D85} | R^{D85} |
| L_{C86} | R^{D86} | R^{D86} |
| L_{C87} | R^{D87} | R^{D87} |
| L_{C88} | R^{D88} | R^{D88} |
| L_{C89} | R^{D89} | R^{D89} |
| L_{C90} | R^{D90} | R^{D90} |
| L_{C91} | R^{D91} | R^{D91} |
| L_{C92} | R^{D92} | R^{D92} |
| L_{C93} | R^{D93} | R^{D93} |
| L_{C94} | R^{D94} | R^{D94} |
| L_{C95} | R^{D95} | R^{D95} |
| L_{C96} | R^{D96} | R^{D96} |
| L_{C97} | R^{D97} | R^{D97} |
| L_{C98} | R^{D98} | R^{D98} |
| L_{C99} | R^{D99} | R^{D99} |
| L_{C100} | R^{D100} | R^{D100} |
| L_{C101} | R^{D101} | R^{D101} |
| L_{C102} | R^{D102} | R^{D102} |
| L_{C103} | R^{D103} | R^{D103} |
| L_{C104} | R^{D104} | R^{D104} |
| L_{C105} | R^{D105} | R^{D105} |
| L_{C106} | R^{D106} | R^{D106} |
| L_{C107} | R^{D107} | R^{D107} |
| L_{C108} | R^{D108} | R^{D108} |
| L_{C109} | R^{D109} | R^{D109} |
| L_{C110} | R^{D110} | R^{D110} |
| L_{C111} | R^{D111} | R^{D111} |
| L_{C112} | R^{D112} | R^{D112} |
| L_{C113} | R^{D113} | R^{D113} |
| L_{C114} | R^{D114} | R^{D114} |
| L_{C115} | R^{D115} | R^{D115} |
| L_{C116} | R^{D116} | R^{D116} |
| L_{C117} | R^{D117} | R^{D117} |
| L_{C118} | R^{D118} | R^{D118} |
| L_{C119} | R^{D119} | R^{D119} |
| L_{C120} | R^{D120} | R^{D120} |
| L_{C121} | R^{D121} | R^{D121} |
| L_{C122} | R^{D122} | R^{D122} |
| L_{C123} | R^{D123} | R^{D123} |
| L_{C124} | R^{D124} | R^{D124} |
| L_{C125} | R^{D125} | R^{D125} |
| L_{C126} | R^{D126} | R^{D126} |
| L_{C127} | R^{D127} | R^{D127} |
| L_{C128} | R^{D128} | R^{D128} |
| L_{C129} | R^{D129} | R^{D129} |
| L_{C130} | R^{D130} | R^{D130} |
| L_{C131} | R^{D131} | R^{D131} |
| L_{C132} | R^{D132} | R^{D132} |
| L_{C133} | R^{D133} | R^{D133} |
| L_{C134} | R^{D134} | R^{D134} |
| L_{C135} | R^{D135} | R^{D135} |
| L_{C136} | R^{D136} | R^{D136} |

-continued

| Ligand | R ¹ | R ² |
|--------|-------------------|-------------------|
| LC137 | R ^{D137} | R ^{D137} |
| LC138 | R ^{D138} | R ^{D138} |
| LC139 | R ^{D139} | R ^{D139} |
| LC140 | R ^{D140} | R ^{D140} |
| LC141 | R ^{D141} | R ^{D141} |
| LC142 | R ^{D142} | R ^{D142} |
| LC143 | R ^{D143} | R ^{D143} |
| LC144 | R ^{D144} | R ^{D144} |
| LC145 | R ^{D145} | R ^{D145} |
| LC146 | R ^{D146} | R ^{D146} |
| LC147 | R ^{D147} | R ^{D147} |
| LC148 | R ^{D148} | R ^{D148} |
| LC149 | R ^{D149} | R ^{D149} |
| LC150 | R ^{D150} | R ^{D150} |
| LC151 | R ^{D151} | R ^{D151} |
| LC152 | R ^{D152} | R ^{D152} |
| LC153 | R ^{D153} | R ^{D153} |
| LC154 | R ^{D154} | R ^{D154} |
| LC155 | R ^{D155} | R ^{D155} |
| LC156 | R ^{D156} | R ^{D156} |
| LC157 | R ^{D157} | R ^{D157} |
| LC158 | R ^{D158} | R ^{D158} |
| LC159 | R ^{D159} | R ^{D159} |
| LC160 | R ^{D160} | R ^{D160} |
| LC161 | R ^{D161} | R ^{D161} |
| LC162 | R ^{D162} | R ^{D162} |
| LC163 | R ^{D163} | R ^{D163} |
| LC164 | R ^{D164} | R ^{D164} |
| LC165 | R ^{D165} | R ^{D165} |
| LC166 | R ^{D166} | R ^{D166} |
| LC167 | R ^{D167} | R ^{D167} |
| LC168 | R ^{D168} | R ^{D168} |
| LC169 | R ^{D169} | R ^{D169} |
| LC170 | R ^{D170} | R ^{D170} |
| LC171 | R ^{D171} | R ^{D171} |
| LC172 | R ^{D172} | R ^{D172} |
| LC173 | R ^{D173} | R ^{D173} |
| LC174 | R ^{D174} | R ^{D174} |
| LC175 | R ^{D175} | R ^{D175} |
| LC176 | R ^{D176} | R ^{D176} |
| LC177 | R ^{D177} | R ^{D177} |
| LC178 | R ^{D178} | R ^{D178} |
| LC179 | R ^{D179} | R ^{D179} |
| LC180 | R ^{D180} | R ^{D180} |
| LC181 | R ^{D181} | R ^{D181} |
| LC182 | R ^{D182} | R ^{D182} |
| LC183 | R ^{D183} | R ^{D183} |
| LC184 | R ^{D184} | R ^{D184} |
| LC185 | R ^{D185} | R ^{D185} |
| LC186 | R ^{D186} | R ^{D186} |
| LC187 | R ^{D187} | R ^{D187} |
| LC188 | R ^{D188} | R ^{D188} |
| LC189 | R ^{D189} | R ^{D189} |
| LC180 | R ^{D180} | R ^{D180} |
| LC191 | R ^{D191} | R ^{D191} |
| LC192 | R ^{D192} | R ^{D192} |
| LC193 | R ^{D1} | R ^{D3} |
| LC194 | R ^{D1} | R ^{D4} |
| LC195 | R ^{D1} | R ^{D5} |
| LC196 | R ^{D1} | R ^{D9} |
| LC197 | R ^{D1} | R ^{D10} |
| LC198 | R ^{D1} | R ^{D17} |
| LC199 | R ^{D1} | R ^{D18} |
| LC200 | R ^{D1} | R ^{D20} |
| LC201 | R ^{D1} | R ^{D22} |
| LC202 | R ^{D1} | R ^{D37} |
| LC203 | R ^{D1} | R ^{D40} |
| LC204 | R ^{D1} | R ^{D41} |
| LC205 | R ^{D1} | R ^{D42} |
| LC206 | R ^{D1} | R ^{D43} |
| LC207 | R ^{D1} | R ^{D48} |
| LC208 | R ^{D1} | R ^{D49} |
| LC209 | R ^{D1} | R ^{D50} |
| LC210 | R ^{D1} | R ^{D54} |

-continued

| Ligand | R ¹ | R ² |
|--------|-----------------|-------------------|
| LC211 | R ^{D1} | R ^{D55} |
| LC212 | R ^{D1} | R ^{D58} |
| LC213 | R ^{D1} | R ^{D59} |
| LC214 | R ^{D1} | R ^{D78} |
| LC215 | R ^{D1} | R ^{D79} |
| LC216 | R ^{D1} | R ^{D81} |
| LC217 | R ^{D1} | R ^{D87} |
| LC218 | R ^{D1} | R ^{D88} |
| LC219 | R ^{D1} | R ^{D89} |
| LC220 | R ^{D1} | R ^{D93} |
| LC221 | R ^{D1} | R ^{D116} |
| LC222 | R ^{D1} | R ^{D117} |
| LC223 | R ^{D1} | R ^{D118} |
| LC224 | R ^{D1} | R ^{D119} |
| LC225 | R ^{D1} | R ^{D120} |
| LC226 | R ^{D1} | R ^{D133} |
| LC227 | R ^{D1} | R ^{D134} |
| LC228 | R ^{D1} | R ^{D135} |
| LC229 | R ^{D1} | R ^{D136} |
| LC230 | R ^{D1} | R ^{D143} |
| LC231 | R ^{D1} | R ^{D144} |
| LC232 | R ^{D1} | R ^{D145} |
| LC233 | R ^{D1} | R ^{D146} |
| LC234 | R ^{D1} | R ^{D147} |
| LC235 | R ^{D1} | R ^{D149} |
| LC236 | R ^{D1} | R ^{D151} |
| LC237 | R ^{D1} | R ^{D154} |
| LC238 | R ^{D1} | R ^{D155} |
| LC239 | R ^{D1} | R ^{D161} |
| LC240 | R ^{D1} | R ^{D175} |
| LC241 | R ^{D4} | R ^{D3} |
| LC242 | R ^{D4} | R ^{D5} |
| LC243 | R ^{D4} | R ^{D9} |
| LC244 | R ^{D4} | R ^{D10} |
| LC245 | R ^{D4} | R ^{D17} |
| LC246 | R ^{D4} | R ^{D18} |
| LC247 | R ^{D4} | R ^{D20} |
| LC248 | R ^{D4} | R ^{D22} |
| LC249 | R ^{D4} | R ^{D37} |
| LC250 | R ^{D4} | R ^{D40} |
| LC251 | R ^{D4} | R ^{D41} |
| LC252 | R ^{D4} | R ^{D42} |
| LC253 | R ^{D4} | R ^{D43} |
| LC254 | R ^{D4} | R ^{D48} |
| LC255 | R ^{D4} | R ^{D49} |
| LC256 | R ^{D4} | R ^{D50} |
| LC257 | R ^{D4} | R ^{D54} |
| LC258 | R ^{D4} | R ^{D55} |
| LC259 | R ^{D4} | R ^{D58} |
| LC260 | R ^{D4} | R ^{D59} |
| LC261 | R ^{D4} | R ^{D78} |
| LC262 | R ^{D4} | R ^{D79} |
| LC263 | R ^{D4} | R ^{D81} |
| LC264 | R ^{D4} | R ^{D87} |
| LC265 | R ^{D4} | R ^{D88} |
| LC266 | R ^{D4} | R ^{D89} |
| LC267 | R ^{D4} | R ^{D93} |
| LC268 | R ^{D4} | R ^{D116} |
| LC269 | R ^{D4} | R ^{D117} |
| LC270 | R ^{D4} | R ^{D118} |
| LC271 | R ^{D4} | R ^{D119} |
| LC272 | R ^{D4} | R ^{D120} |
| LC273 | R ^{D4} | R ^{D133} |
| LC274 | R ^{D4} | R ^{D134} |
| LC275 | R ^{D4} | R ^{D135} |
| LC276 | R ^{D4} | R ^{D136} |
| LC277 | R ^{D4} | R ^{D143} |
| LC278 | R ^{D4} | R ^{D144} |
| LC279 | R ^{D4} | R ^{D145} |
| LC280 | R ^{D4} | R ^{D146} |
| LC281 | R ^{D4} | R ^{D147} |
| LC282 | R ^{D4} | R ^{D149} |
| LC283 | R ^{D4} | R ^{D151} |
| LC284 | R ^{D4} | R ^{D154} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|------------------|-------------------|
| L _{C285} | R ^{D4} | R ^{D155} |
| L _{C286} | R ^{D4} | R ^{D161} |
| L _{C287} | R ^{D4} | R ^{D175} |
| L _{C288} | R ^{D9} | R ^{D3} |
| L _{C289} | R ^{D9} | R ^{D5} |
| L _{C280} | R ^{D9} | R ^{D10} |
| L _{C291} | R ^{D9} | R ^{D17} |
| L _{C292} | R ^{D9} | R ^{D18} |
| L _{C293} | R ^{D9} | R ^{D20} |
| L _{C294} | R ^{D9} | R ^{D22} |
| L _{C295} | R ^{D9} | R ^{D37} |
| L _{C296} | R ^{D9} | R ^{D40} |
| L _{C297} | R ^{D9} | R ^{D41} |
| L _{C298} | R ^{D9} | R ^{D42} |
| L _{C299} | R ^{D9} | R ^{D43} |
| L _{C300} | R ^{D9} | R ^{D48} |
| L _{C301} | R ^{D9} | R ^{D49} |
| L _{C302} | R ^{D9} | R ^{D50} |
| L _{C303} | R ^{D9} | R ^{D54} |
| L _{C304} | R ^{D9} | R ^{D55} |
| L _{C305} | R ^{D9} | R ^{D58} |
| L _{C306} | R ^{D9} | R ^{D59} |
| L _{C307} | R ^{D9} | R ^{D78} |
| L _{C308} | R ^{D9} | R ^{D79} |
| L _{C309} | R ^{D9} | R ^{D81} |
| L _{C310} | R ^{D9} | R ^{D87} |
| L _{C311} | R ^{D9} | R ^{D88} |
| L _{C312} | R ^{D9} | R ^{D89} |
| L _{C313} | R ^{D9} | R ^{D93} |
| L _{C314} | R ^{D9} | R ^{D116} |
| L _{C315} | R ^{D9} | R ^{D117} |
| L _{C316} | R ^{D9} | R ^{D118} |
| L _{C317} | R ^{D9} | R ^{D119} |
| L _{C318} | R ^{D9} | R ^{D120} |
| L _{C319} | R ^{D9} | R ^{D133} |
| L _{C320} | R ^{D9} | R ^{D134} |
| L _{C321} | R ^{D9} | R ^{D135} |
| L _{C322} | R ^{D9} | R ^{D136} |
| L _{C323} | R ^{D9} | R ^{D143} |
| L _{C324} | R ^{D9} | R ^{D144} |
| L _{C325} | R ^{D9} | R ^{D145} |
| L _{C326} | R ^{D9} | R ^{D146} |
| L _{C327} | R ^{D9} | R ^{D147} |
| L _{C328} | R ^{D9} | R ^{D149} |
| L _{C329} | R ^{D9} | R ^{D151} |
| L _{C330} | R ^{D9} | R ^{D154} |
| L _{C331} | R ^{D9} | R ^{D155} |
| L _{C332} | R ^{D9} | R ^{D161} |
| L _{C333} | R ^{D9} | R ^{D175} |
| L _{C334} | R ^{D10} | R ^{D3} |
| L _{C335} | R ^{D10} | R ^{D5} |
| L _{C336} | R ^{D10} | R ^{D17} |
| L _{C337} | R ^{D10} | R ^{D18} |
| L _{C338} | R ^{D10} | R ^{D20} |
| L _{C339} | R ^{D10} | R ^{D22} |
| L _{C340} | R ^{D10} | R ^{D37} |
| L _{C341} | R ^{D10} | R ^{D40} |
| L _{C342} | R ^{D10} | R ^{D41} |
| L _{C343} | R ^{D10} | R ^{D42} |
| L _{C344} | R ^{D10} | R ^{D43} |
| L _{C345} | R ^{D10} | R ^{D48} |
| L _{C346} | R ^{D10} | R ^{D49} |
| L _{C347} | R ^{D10} | R ^{D50} |
| L _{C348} | R ^{D10} | R ^{D54} |
| L _{C349} | R ^{D10} | R ^{D55} |
| L _{C350} | R ^{D10} | R ^{D58} |
| L _{C351} | R ^{D10} | R ^{D59} |
| L _{C352} | R ^{D10} | R ^{D78} |
| L _{C353} | R ^{D10} | R ^{D79} |
| L _{C354} | R ^{D10} | R ^{D81} |
| L _{C355} | R ^{D10} | R ^{D87} |
| L _{C356} | R ^{D10} | R ^{D88} |
| L _{C357} | R ^{D10} | R ^{D89} |
| L _{C358} | R ^{D10} | R ^{D93} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|------------------|-------------------|
| L _{C359} | R ^{D10} | R ^{D116} |
| L _{C360} | R ^{D10} | R ^{D117} |
| L _{C361} | R ^{D10} | R ^{D118} |
| L _{C362} | R ^{D10} | R ^{D119} |
| L _{C363} | R ^{D10} | R ^{D120} |
| L _{C364} | R ^{D10} | R ^{D133} |
| L _{C365} | R ^{D10} | R ^{D134} |
| L _{C366} | R ^{D10} | R ^{D135} |
| L _{C367} | R ^{D10} | R ^{D136} |
| L _{C368} | R ^{D10} | R ^{D143} |
| L _{C369} | R ^{D10} | R ^{D144} |
| L _{C370} | R ^{D10} | R ^{D145} |
| L _{C371} | R ^{D10} | R ^{D146} |
| L _{C372} | R ^{D10} | R ^{D147} |
| L _{C373} | R ^{D10} | R ^{D149} |
| L _{C374} | R ^{D10} | R ^{D151} |
| L _{C375} | R ^{D10} | R ^{D154} |
| L _{C376} | R ^{D10} | R ^{D155} |
| L _{C377} | R ^{D10} | R ^{D161} |
| L _{C378} | R ^{D10} | R ^{D175} |
| L _{C379} | R ^{D17} | R ^{D3} |
| L _{C380} | R ^{D17} | R ^{D5} |
| L _{C381} | R ^{D17} | R ^{D18} |
| L _{C382} | R ^{D17} | R ^{D20} |
| L _{C383} | R ^{D17} | R ^{D22} |
| L _{C384} | R ^{D17} | R ^{D37} |
| L _{C385} | R ^{D17} | R ^{D40} |
| L _{C386} | R ^{D17} | R ^{D41} |
| L _{C387} | R ^{D17} | R ^{D42} |
| L _{C388} | R ^{D17} | R ^{D43} |
| L _{C389} | R ^{D17} | R ^{D48} |
| L _{C390} | R ^{D17} | R ^{D49} |
| L _{C391} | R ^{D17} | R ^{D50} |
| L _{C392} | R ^{D17} | R ^{D54} |
| L _{C393} | R ^{D17} | R ^{D55} |
| L _{C394} | R ^{D17} | R ^{D58} |
| L _{C395} | R ^{D17} | R ^{D59} |
| L _{C396} | R ^{D17} | R ^{D78} |
| L _{C397} | R ^{D17} | R ^{D79} |
| L _{C398} | R ^{D17} | R ^{D81} |
| L _{C399} | R ^{D17} | R ^{D87} |
| L _{C400} | R ^{D17} | R ^{D88} |
| L _{C401} | R ^{D17} | R ^{D89} |
| L _{C402} | R ^{D17} | R ^{D93} |
| L _{C403} | R ^{D17} | R ^{D116} |
| L _{C404} | R ^{D17} | R ^{D117} |
| L _{C405} | R ^{D17} | R ^{D118} |
| L _{C406} | R ^{D17} | R ^{D119} |
| L _{C407} | R ^{D17} | R ^{D120} |
| L _{C408} | R ^{D17} | R ^{D133} |
| L _{C409} | R ^{D17} | R ^{D134} |
| L _{C410} | R ^{D17} | R ^{D135} |
| L _{C411} | R ^{D17} | R ^{D136} |
| L _{C412} | R ^{D17} | R ^{D143} |
| L _{C413} | R ^{D17} | R ^{D144} |
| L _{C414} | R ^{D17} | R ^{D145} |
| L _{C415} | R ^{D17} | R ^{D146} |
| L _{C416} | R ^{D17} | R ^{D147} |
| L _{C417} | R ^{D17} | R ^{D149} |
| L _{C418} | R ^{D17} | R ^{D151} |
| L _{C419} | R ^{D17} | R ^{D154} |
| L _{C420} | R ^{D17} | R ^{D155} |
| L _{C421} | R ^{D17} | R ^{D161} |
| L _{C422} | R ^{D17} | R ^{D175} |
| L _{C423} | R ^{D50} | R ^{D3} |
| L _{C424} | R ^{D50} | R ^{D5} |
| L _{C425} | R ^{D50} | R ^{D18} |
| L _{C426} | R ^{D50} | R ^{D20} |
| L _{C427} | R ^{D50} | R ^{D22} |
| L _{C428} | R ^{D50} | R ^{D37} |
| L _{C429} | R ^{D50} | R ^{D40} |
| L _{C430} | R ^{D50} | R ^{D41} |
| L _{C431} | R ^{D50} | R ^{D42} |
| L _{C432} | R ^{D50} | R ^{D43} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|------------------|-------------------|
| L _{C433} | R ^{D50} | R ^{D48} |
| L _{C434} | R ^{D50} | R ^{D49} |
| L _{C435} | R ^{D50} | R ^{D54} |
| L _{C436} | R ^{D50} | R ^{D55} |
| L _{C437} | R ^{D50} | R ^{D58} |
| L _{C438} | R ^{D50} | R ^{D59} |
| L _{C439} | R ^{D50} | R ^{D78} |
| L _{C440} | R ^{D50} | R ^{D79} |
| L _{C441} | R ^{D50} | R ^{D81} |
| L _{C442} | R ^{D50} | R ^{D87} |
| L _{C443} | R ^{D50} | R ^{D88} |
| L _{C444} | R ^{D50} | R ^{D89} |
| L _{C445} | R ^{D50} | R ^{D93} |
| L _{C446} | R ^{D50} | R ^{D116} |
| L _{C447} | R ^{D50} | R ^{D117} |
| L _{C448} | R ^{D50} | R ^{D118} |
| L _{C449} | R ^{D50} | R ^{D119} |
| L _{C450} | R ^{D50} | R ^{D120} |
| L _{C451} | R ^{D50} | R ^{D133} |
| L _{C452} | R ^{D50} | R ^{D134} |
| L _{C453} | R ^{D50} | R ^{D135} |
| L _{C454} | R ^{D50} | R ^{D136} |
| L _{C455} | R ^{D50} | R ^{D143} |
| L _{C456} | R ^{D50} | R ^{D144} |
| L _{C457} | R ^{D50} | R ^{D145} |
| L _{C458} | R ^{D50} | R ^{D146} |
| L _{C459} | R ^{D50} | R ^{D147} |
| L _{C460} | R ^{D50} | R ^{D149} |
| L _{C461} | R ^{D50} | R ^{D151} |
| L _{C462} | R ^{D50} | R ^{D154} |
| L _{C463} | R ^{D50} | R ^{D155} |
| L _{C464} | R ^{D50} | R ^{D161} |
| L _{C465} | R ^{D50} | R ^{D175} |
| L _{C466} | R ^{D55} | R ^{D3} |
| L _{C467} | R ^{D55} | R ^{D5} |
| L _{C468} | R ^{D55} | R ^{D18} |
| L _{C469} | R ^{D55} | R ^{D20} |
| L _{C470} | R ^{D55} | R ^{D22} |
| L _{C471} | R ^{D55} | R ^{D37} |
| L _{C472} | R ^{D55} | R ^{D40} |
| L _{C473} | R ^{D55} | R ^{D41} |
| L _{C474} | R ^{D55} | R ^{D42} |
| L _{C475} | R ^{D55} | R ^{D43} |
| L _{C476} | R ^{D55} | R ^{D48} |
| L _{C477} | R ^{D55} | R ^{D49} |
| L _{C478} | R ^{D55} | R ^{D54} |
| L _{C479} | R ^{D55} | R ^{D58} |
| L _{C480} | R ^{D55} | R ^{D59} |
| L _{C481} | R ^{D55} | R ^{D78} |
| L _{C482} | R ^{D55} | R ^{D79} |
| L _{C483} | R ^{D55} | R ^{D81} |
| L _{C484} | R ^{D55} | R ^{D87} |
| L _{C485} | R ^{D55} | R ^{D88} |
| L _{C486} | R ^{D55} | R ^{D89} |
| L _{C487} | R ^{D55} | R ^{D93} |
| L _{C488} | R ^{D55} | R ^{D116} |
| L _{C489} | R ^{D55} | R ^{D117} |
| L _{C480} | R ^{D55} | R ^{D118} |
| L _{C491} | R ^{D55} | R ^{D119} |
| L _{C492} | R ^{D55} | R ^{D120} |
| L _{C493} | R ^{D55} | R ^{D133} |
| L _{C494} | R ^{D55} | R ^{D134} |
| L _{C495} | R ^{D55} | R ^{D135} |
| L _{C496} | R ^{D55} | R ^{D136} |
| L _{C497} | R ^{D55} | R ^{D143} |
| L _{C498} | R ^{D55} | R ^{D144} |
| L _{C499} | R ^{D55} | R ^{D145} |
| L _{C500} | R ^{D55} | R ^{D146} |
| L _{C501} | R ^{D55} | R ^{D147} |
| L _{C502} | R ^{D55} | R ^{D149} |
| L _{C503} | R ^{D55} | R ^{D151} |
| L _{C504} | R ^{D55} | R ^{D154} |
| L _{C505} | R ^{D55} | R ^{D155} |
| L _{C506} | R ^{D55} | R ^{D161} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|-------------------|-------------------|
| L _{C507} | R ^{D55} | R ^{D175} |
| L _{C508} | R ^{D116} | R ^{D3} |
| L _{C509} | R ^{D116} | R ^{D5} |
| L _{C510} | R ^{D116} | R ^{D17} |
| L _{C511} | R ^{D116} | R ^{D18} |
| L _{C512} | R ^{D116} | R ^{D20} |
| L _{C513} | R ^{D116} | R ^{D22} |
| L _{C514} | R ^{D116} | R ^{D37} |
| L _{C515} | R ^{D116} | R ^{D40} |
| L _{C516} | R ^{D116} | R ^{D41} |
| L _{C517} | R ^{D116} | R ^{D42} |
| L _{C518} | R ^{D116} | R ^{D43} |
| L _{C519} | R ^{D116} | R ^{D48} |
| L _{C520} | R ^{D116} | R ^{D49} |
| L _{C521} | R ^{D116} | R ^{D54} |
| L _{C522} | R ^{D116} | R ^{D58} |
| L _{C523} | R ^{D116} | R ^{D59} |
| L _{C524} | R ^{D116} | R ^{D78} |
| L _{C525} | R ^{D116} | R ^{D79} |
| L _{C526} | R ^{D116} | R ^{D81} |
| L _{C527} | R ^{D116} | R ^{D87} |
| L _{C528} | R ^{D116} | R ^{D88} |
| L _{C529} | R ^{D116} | R ^{D89} |
| L _{C530} | R ^{D116} | R ^{D93} |
| L _{C531} | R ^{D116} | R ^{D117} |
| L _{C532} | R ^{D116} | R ^{D118} |
| L _{C533} | R ^{D116} | R ^{D119} |
| L _{C534} | R ^{D116} | R ^{D120} |
| L _{C535} | R ^{D116} | R ^{D133} |
| L _{C536} | R ^{D116} | R ^{D134} |
| L _{C537} | R ^{D116} | R ^{D135} |
| L _{C538} | R ^{D116} | R ^{D136} |
| L _{C539} | R ^{D116} | R ^{D143} |
| L _{C540} | R ^{D116} | R ^{D144} |
| L _{C541} | R ^{D116} | R ^{D145} |
| L _{C542} | R ^{D116} | R ^{D146} |
| L _{C543} | R ^{D116} | R ^{D147} |
| L _{C544} | R ^{D116} | R ^{D149} |
| L _{C545} | R ^{D116} | R ^{D151} |
| L _{C546} | R ^{D116} | R ^{D154} |
| L _{C547} | R ^{D116} | R ^{D155} |
| L _{C548} | R ^{D116} | R ^{D161} |
| L _{C549} | R ^{D116} | R ^{D175} |
| L _{C550} | R ^{D143} | R ^{D3} |
| L _{C551} | R ^{D143} | R ^{D5} |
| L _{C552} | R ^{D143} | R ^{D17} |
| L _{C553} | R ^{D143} | R ^{D18} |
| L _{C554} | R ^{D143} | R ^{D20} |
| L _{C555} | R ^{D143} | R ^{D22} |
| L _{C556} | R ^{D143} | R ^{D37} |
| L _{C557} | R ^{D143} | R ^{D40} |
| L _{C558} | R ^{D143} | R ^{D41} |
| L _{C559} | R ^{D143} | R ^{D42} |
| L _{C560} | R ^{D143} | R ^{D43} |
| L _{C561} | R ^{D143} | R ^{D48} |
| L _{C562} | R ^{D143} | R ^{D49} |
| L _{C563} | R ^{D143} | R ^{D54} |
| L _{C564} | R ^{D143} | R ^{D58} |
| L _{C565} | R ^{D143} | R ^{D59} |
| L _{C566} | R ^{D143} | R ^{D78} |
| L _{C567} | R ^{D143} | R ^{D79} |
| L _{C568} | R ^{D143} | R ^{D81} |
| L _{C569} | R ^{D143} | R ^{D87} |
| L _{C570} | R ^{D143} | R ^{D88} |
| L _{C571} | R ^{D143} | R ^{D89} |
| L _{C572} | R ^{D143} | R ^{D93} |
| L _{C573} | R ^{D143} | R ^{D116} |
| L _{C574} | R ^{D143} | R ^{D117} |
| L _{C575} | R ^{D143} | R ^{D118} |
| L _{C576} | R ^{D143} | R ^{D119} |
| L _{C577} | R ^{D143} | R ^{D120} |
| L _{C578} | R ^{D143} | R ^{D133} |
| L _{C579} | R ^{D143} | R ^{D134} |
| L _{C580} | R ^{D143} | R ^{D135} |

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| Ligand | R ¹ | R ² |
|--------|-------------------|-------------------|
| LC581 | R ^{D143} | R ^{D136} |
| LC582 | R ^{D143} | R ^{D144} |
| LC583 | R ^{D143} | R ^{D145} |
| LC584 | R ^{D143} | R ^{D146} |
| LC585 | R ^{D143} | R ^{D147} |
| LC586 | R ^{D143} | R ^{D149} |
| LC587 | R ^{D143} | R ^{D151} |
| LC588 | R ^{D143} | R ^{D154} |
| LC589 | R ^{D143} | R ^{D155} |
| LC580 | R ^{D143} | R ^{D161} |
| LC591 | R ^{D143} | R ^{D175} |
| LC592 | R ^{D144} | R ^{D3} |
| LC593 | R ^{D144} | R ^{D5} |
| LC594 | R ^{D144} | R ^{D17} |
| LC595 | R ^{D144} | R ^{D18} |
| LC596 | R ^{D144} | R ^{D20} |
| LC597 | R ^{D144} | R ^{D22} |
| LC598 | R ^{D144} | R ^{D37} |
| LC599 | R ^{D144} | R ^{D40} |
| LC600 | R ^{D144} | R ^{D41} |
| LC601 | R ^{D144} | R ^{D42} |
| LC602 | R ^{D144} | R ^{D43} |
| LC603 | R ^{D144} | R ^{D48} |
| LC604 | R ^{D144} | R ^{D49} |
| LC605 | R ^{D144} | R ^{D54} |
| LC606 | R ^{D144} | R ^{D58} |
| LC607 | R ^{D144} | R ^{D59} |
| LC608 | R ^{D144} | R ^{D78} |
| LC609 | R ^{D144} | R ^{D79} |
| LC610 | R ^{D144} | R ^{D81} |
| LC611 | R ^{D144} | R ^{D87} |
| LC612 | R ^{D144} | R ^{D88} |
| LC613 | R ^{D144} | R ^{D89} |
| LC614 | R ^{D144} | R ^{D93} |
| LC615 | R ^{D144} | R ^{D116} |
| LC616 | R ^{D144} | R ^{D117} |
| LC617 | R ^{D144} | R ^{D118} |
| LC618 | R ^{D144} | R ^{D119} |
| LC619 | R ^{D144} | R ^{D120} |
| LC620 | R ^{D144} | R ^{D133} |
| LC621 | R ^{D144} | R ^{D134} |
| LC622 | R ^{D144} | R ^{D135} |
| LC623 | R ^{D144} | R ^{D136} |
| LC624 | R ^{D144} | R ^{D145} |
| LC625 | R ^{D144} | R ^{D146} |
| LC626 | R ^{D144} | R ^{D147} |
| LC627 | R ^{D144} | R ^{D149} |
| LC628 | R ^{D144} | R ^{D151} |
| LC629 | R ^{D144} | R ^{D154} |
| LC630 | R ^{D144} | R ^{D155} |
| LC631 | R ^{D144} | R ^{D161} |
| LC632 | R ^{D144} | R ^{D175} |
| LC633 | R ^{D145} | R ^{D3} |
| LC634 | R ^{D145} | R ^{D5} |
| LC635 | R ^{D145} | R ^{D17} |
| LC636 | R ^{D145} | R ^{D18} |
| LC637 | R ^{D145} | R ^{D20} |
| LC638 | R ^{D145} | R ^{D22} |
| LC639 | R ^{D145} | R ^{D37} |
| LC640 | R ^{D145} | R ^{D40} |
| LC641 | R ^{D145} | R ^{D41} |
| LC642 | R ^{D145} | R ^{D42} |
| LC643 | R ^{D145} | R ^{D43} |
| LC644 | R ^{D145} | R ^{D48} |
| LC645 | R ^{D145} | R ^{D49} |
| LC646 | R ^{D145} | R ^{D54} |
| LC647 | R ^{D145} | R ^{D58} |
| LC648 | R ^{D145} | R ^{D59} |
| LC649 | R ^{D145} | R ^{D78} |
| LC650 | R ^{D145} | R ^{D79} |
| LC651 | R ^{D145} | R ^{D81} |
| LC652 | R ^{D145} | R ^{D87} |
| LC653 | R ^{D145} | R ^{D88} |
| LC654 | R ^{D145} | R ^{D89} |

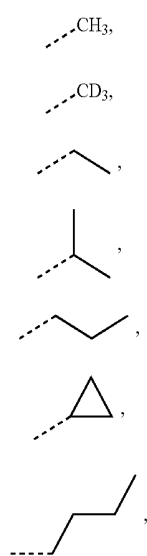
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| Ligand | R ¹ | R ² |
|--------|-------------------|-------------------|
| LC655 | R ^{D145} | R ^{D93} |
| LC656 | R ^{D145} | R ^{D116} |
| LC657 | R ^{D145} | R ^{D117} |
| LC658 | R ^{D145} | R ^{D118} |
| LC659 | R ^{D145} | R ^{D119} |
| LC660 | R ^{D145} | R ^{D120} |
| LC661 | R ^{D145} | R ^{D133} |
| LC662 | R ^{D145} | R ^{D134} |
| LC663 | R ^{D145} | R ^{D135} |
| LC664 | R ^{D145} | R ^{D136} |
| LC665 | R ^{D145} | R ^{D146} |
| LC666 | R ^{D145} | R ^{D147} |
| LC667 | R ^{D145} | R ^{D149} |
| LC668 | R ^{D145} | R ^{D151} |
| LC669 | R ^{D145} | R ^{D154} |
| LC670 | R ^{D145} | R ^{D155} |
| LC671 | R ^{D145} | R ^{D161} |
| LC672 | R ^{D145} | R ^{D175} |
| LC673 | R ^{D146} | R ^{D3} |
| LC674 | R ^{D146} | R ^{D5} |
| LC675 | R ^{D146} | R ^{D17} |
| LC676 | R ^{D146} | R ^{D18} |
| LC677 | R ^{D146} | R ^{D20} |
| LC678 | R ^{D146} | R ^{D22} |
| LC679 | R ^{D146} | R ^{D37} |
| LC680 | R ^{D146} | R ^{D40} |
| LC681 | R ^{D146} | R ^{D41} |
| LC682 | R ^{D146} | R ^{D42} |
| LC683 | R ^{D146} | R ^{D43} |
| LC684 | R ^{D146} | R ^{D48} |
| LC685 | R ^{D146} | R ^{D49} |
| LC686 | R ^{D146} | R ^{D54} |
| LC687 | R ^{D146} | R ^{D58} |
| LC688 | R ^{D146} | R ^{D59} |
| LC689 | R ^{D146} | R ^{D78} |
| LC690 | R ^{D146} | R ^{D79} |
| LC691 | R ^{D146} | R ^{D81} |
| LC692 | R ^{D146} | R ^{D87} |
| LC693 | R ^{D146} | R ^{D88} |
| LC694 | R ^{D146} | R ^{D89} |
| LC695 | R ^{D146} | R ^{D93} |
| LC696 | R ^{D146} | R ^{D117} |
| LC697 | R ^{D146} | R ^{D118} |
| LC698 | R ^{D146} | R ^{D119} |
| LC699 | R ^{D146} | R ^{D120} |
| LC700 | R ^{D146} | R ^{D133} |
| LC701 | R ^{D146} | R ^{D134} |
| LC702 | R ^{D146} | R ^{D135} |
| LC703 | R ^{D146} | R ^{D136} |
| LC704 | R ^{D146} | R ^{D146} |
| LC705 | R ^{D146} | R ^{D147} |
| LC706 | R ^{D146} | R ^{D149} |
| LC707 | R ^{D146} | R ^{D151} |
| LC708 | R ^{D146} | R ^{D154} |
| LC709 | R ^{D146} | R ^{D155} |
| LC710 | R ^{D146} | R ^{D161} |
| LC711 | R ^{D146} | R ^{D175} |
| LC712 | R ^{D133} | R ^{D3} |
| LC713 | R ^{D133} | R ^{D5} |
| LC714 | R ^{D133} | R ^{D3} |
| LC715 | R ^{D133} | R ^{D18} |
| LC716 | R ^{D133} | R ^{D20} |
| LC717 | R ^{D133} | R ^{D22} |
| LC718 | R ^{D133} | R ^{D37} |
| LC719 | R ^{D133} | R ^{D40} |
| LC720 | R ^{D133} | R ^{D41} |
| LC721 | R ^{D133} | R ^{D42} |
| LC722 | R ^{D133} | R ^{D43} |
| LC723 | R ^{D133} | R ^{D48} |
| LC724 | R ^{D133} | R ^{D49} |
| LC725 | R ^{D133} | R ^{D54} |
| LC726 | R ^{D133} | R ^{D58} |
| LC727 | R ^{D133} | R ^{D59} |
| LC728 | R ^{D133} | R ^{D78} |

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| Ligand | R ¹ | R ² |
|-------------------|-------------------|-------------------|
| L _{C729} | R ^{D133} | R ^{D79} |
| L _{C730} | R ^{D133} | R ^{D81} |
| L _{C731} | R ^{D133} | R ^{D87} |
| L _{C732} | R ^{D133} | R ^{D88} |
| L _{C733} | R ^{D133} | R ^{D89} |
| L _{C734} | R ^{D133} | R ^{D93} |
| L _{C735} | R ^{D133} | R ^{D117} |
| L _{C736} | R ^{D133} | R ^{D118} |
| L _{C737} | R ^{D133} | R ^{D119} |
| L _{C738} | R ^{D133} | R ^{D120} |
| L _{C739} | R ^{D133} | R ^{D133} |
| L _{C740} | R ^{D133} | R ^{D134} |
| L _{C741} | R ^{D133} | R ^{D135} |
| L _{C742} | R ^{D133} | R ^{D136} |
| L _{C743} | R ^{D133} | R ^{D146} |
| L _{C744} | R ^{D133} | R ^{D147} |
| L _{C745} | R ^{D133} | R ^{D149} |
| L _{C746} | R ^{D133} | R ^{D151} |
| L _{C747} | R ^{D133} | R ^{D154} |
| L _{C748} | R ^{D133} | R ^{D155} |
| L _{C749} | R ^{D133} | R ^{D161} |
| L _{C750} | R ^{D133} | R ^{D175} |
| L _{C751} | R ^{D175} | R ^{D3} |
| L _{C752} | R ^{D175} | R ^{D5} |
| L _{C753} | R ^{D175} | R ^{D18} |
| L _{C754} | R ^{D175} | R ^{D20} |
| L _{C755} | R ^{D175} | R ^{D22} |
| L _{C756} | R ^{D175} | R ^{D37} |
| L _{C757} | R ^{D175} | R ^{D40} |
| L _{C758} | R ^{D175} | R ^{D41} |
| L _{C759} | R ^{D175} | R ^{D42} |
| L _{C760} | R ^{D175} | R ^{D43} |
| L _{C761} | R ^{D175} | R ^{D48} |
| L _{C762} | R ^{D175} | R ^{D49} |
| L _{C763} | R ^{D175} | R ^{D54} |
| L _{C764} | R ^{D175} | R ^{D58} |
| L _{C765} | R ^{D175} | R ^{D59} |
| L _{C766} | R ^{D175} | R ^{D78} |
| L _{C767} | R ^{D175} | R ^{D79} |
| L _{C768} | R ^{D175} | R ^{D81} |

wherein R^{D1} to R^{D192} have the following structures:



R^{D1}

R^{D2}

R^{D3}

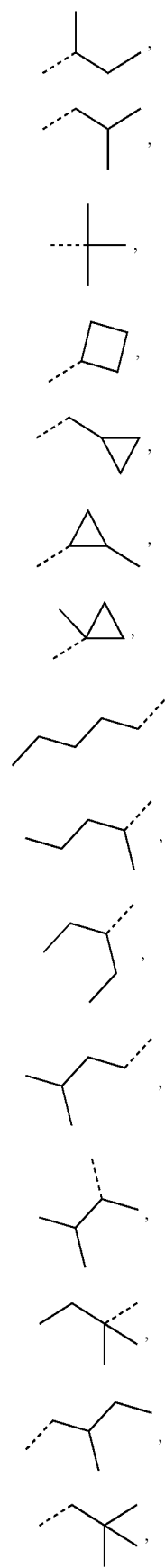
R^{D4}

R^{D5}

R^{D6}

R^{D7}

-continued



R^{D8}

R^{D9}

R^{D10}

R^{D11}

R^{D12}

R^{D13}

R^{D14}

R^{D15}

R^{D16}

R^{D17}

R^{D18}

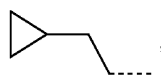
R^{D19}

R^{D20}

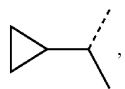
R^{D21}

R^{D22}

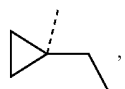
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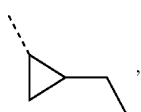
R^{D23}



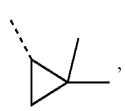
R^{D24}



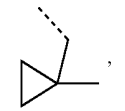
R^{D25}



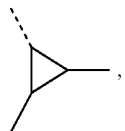
R^{D26}



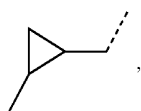
R^{D27}



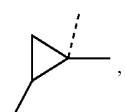
R^{D28}



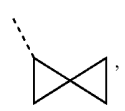
R^{D29}



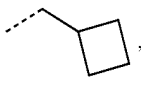
R^{D30}



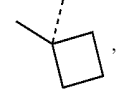
R^{D31}



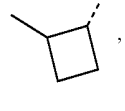
R^{D32}



R^{D33}



R^{D34}

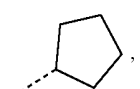


R^{D35}

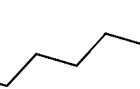
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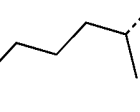
R^{D36}



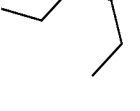
R^{D37}



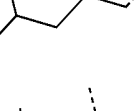
R^{D38}



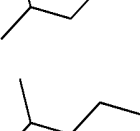
R^{D39}



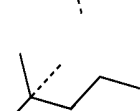
R^{D40}



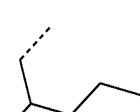
R^{D41}



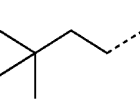
R^{D42}



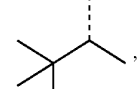
R^{D43}



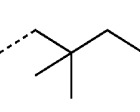
R^{D44}



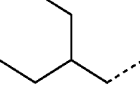
R^{D45}



R^{D46}



R^{D47}

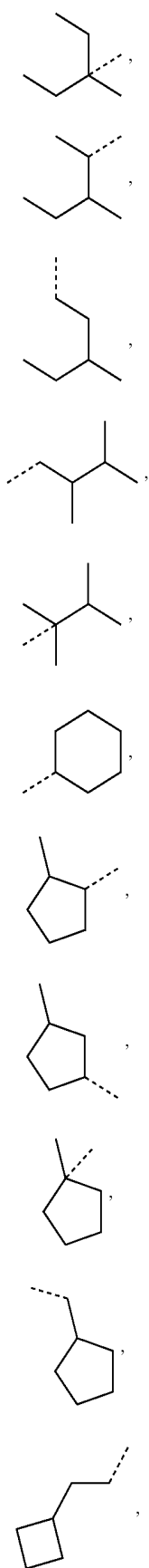


R^{D48}



R^{D49}

-continued



R^{D50}

R^{D51}

R^{D52}

R^{D53}

R^{D54}

R^{D55}

R^{D56}

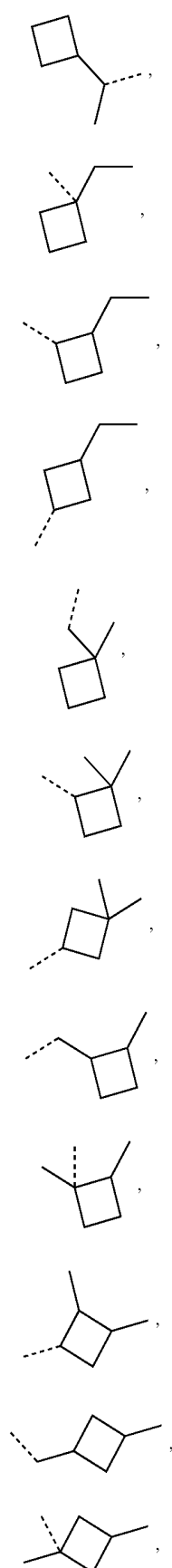
R^{D57}

R^{D58}

R^{D59}

R^{D60}

-continued



R^{D61}

R^{D62}

R^{D63}

R^{D64}

R^{D65}

R^{D66}

R^{D67}

R^{D68}

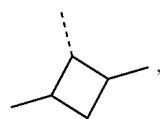
R^{D69}

R^{D70}

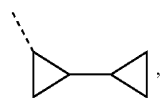
R^{D71}

R^{D72}

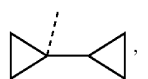
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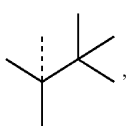
R^{D73}



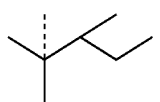
R^{D74}



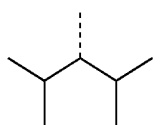
R^{D75}



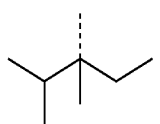
R^{D76}



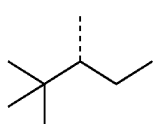
R^{D77}



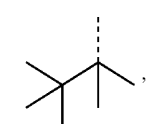
R^{D78}



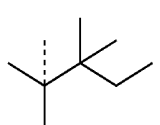
R^{D79}



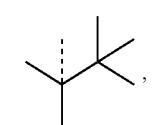
R^{D80}



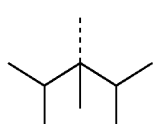
R^{D81}



R^{D82}

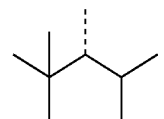


R^{D83}

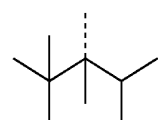


R^{D84}

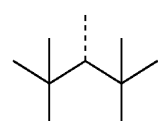
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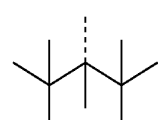
R^{D85}



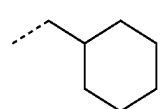
R^{D86}



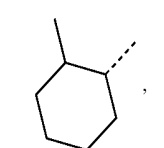
R^{D87}



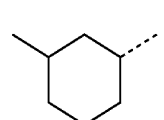
R^{D88}



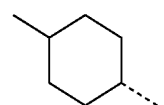
R^{D89}



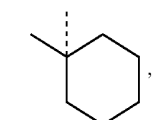
R^{D90}



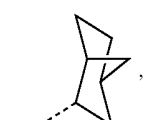
R^{D91}



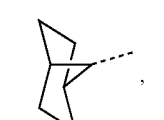
R^{D92}



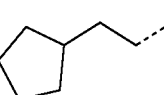
R^{D93}



R^{D94}

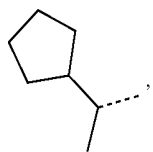


R^{D95}

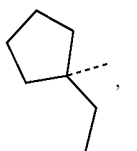


R^{D96}

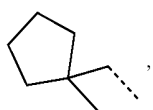
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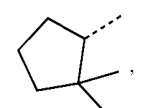
R^{D97}



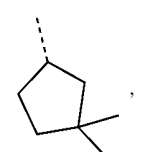
R^{D98}



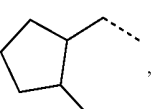
R^{D99}



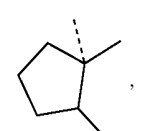
R^{D100}



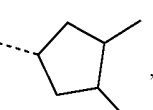
R^{D101}



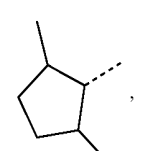
R^{D102}



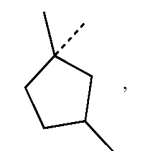
R^{D103}



R^{D104}

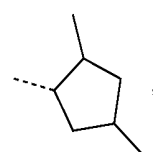


R^{D105}

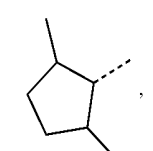


R^{D106}

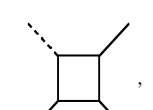
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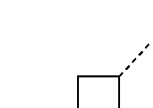
R^{D107}



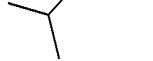
R^{D108}



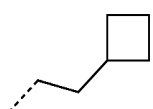
R^{D109}



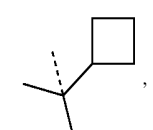
R^{D110}



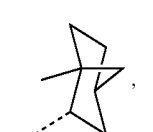
R^{D111}



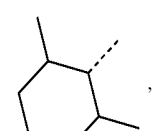
R^{D112}



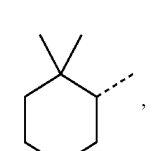
R^{D113}



R^{D114}

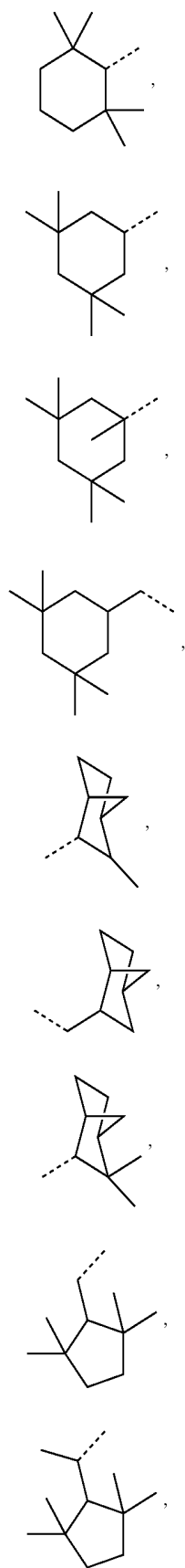


R^{D115}



R^{D116}

-continued



R^{D117}

R^{D118}

R^{D119}

R^{D120}

R^{D121}

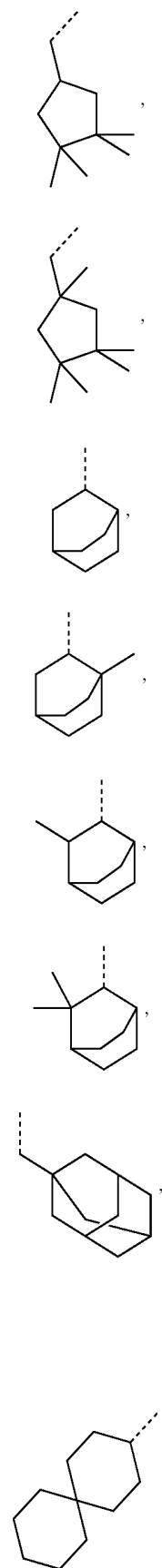
R^{D122}

R^{D123}

R^{D124}

R^{D125}

-continued



R^{D126}

R^{D127}

R^{D128}

R^{D129}

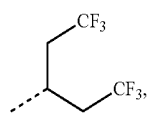
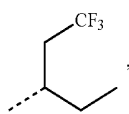
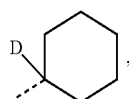
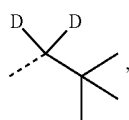
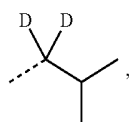
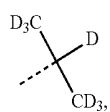
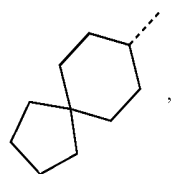
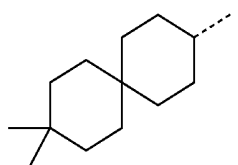
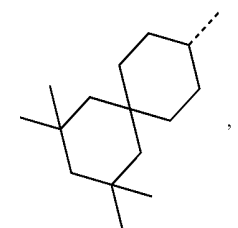
R^{D130}

R^{D131}

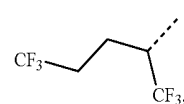
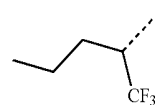
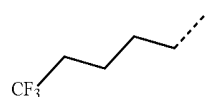
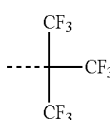
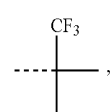
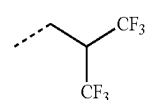
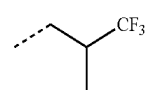
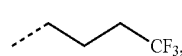
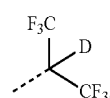
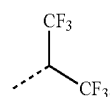
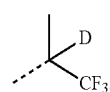
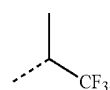
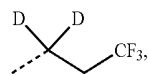
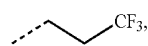
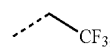
R^{D132}

R^{D133}

-continued



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R^{D134}

R^{D135}

R^{D136}

R^{D137}

R^{D138}

R^{D139}

R^{D140}

R^{D141}

R^{D142}

R^{D143}

R^{D144}

R^{D145}

R^{D146}

R^{D147}

R^{D148}

R^{D149}

R^{D150}

R^{D151}

R^{D152}

R^{D153}

R^{D154}

R^{D155}

R^{D156}

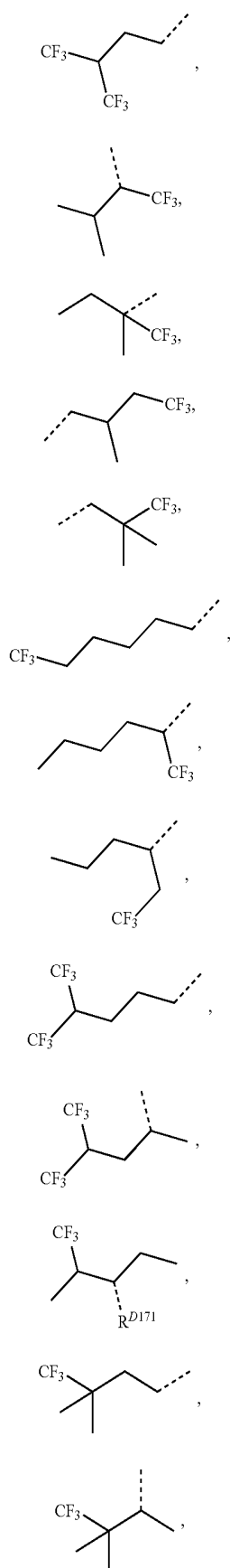
R^{D157}

R^{D158}

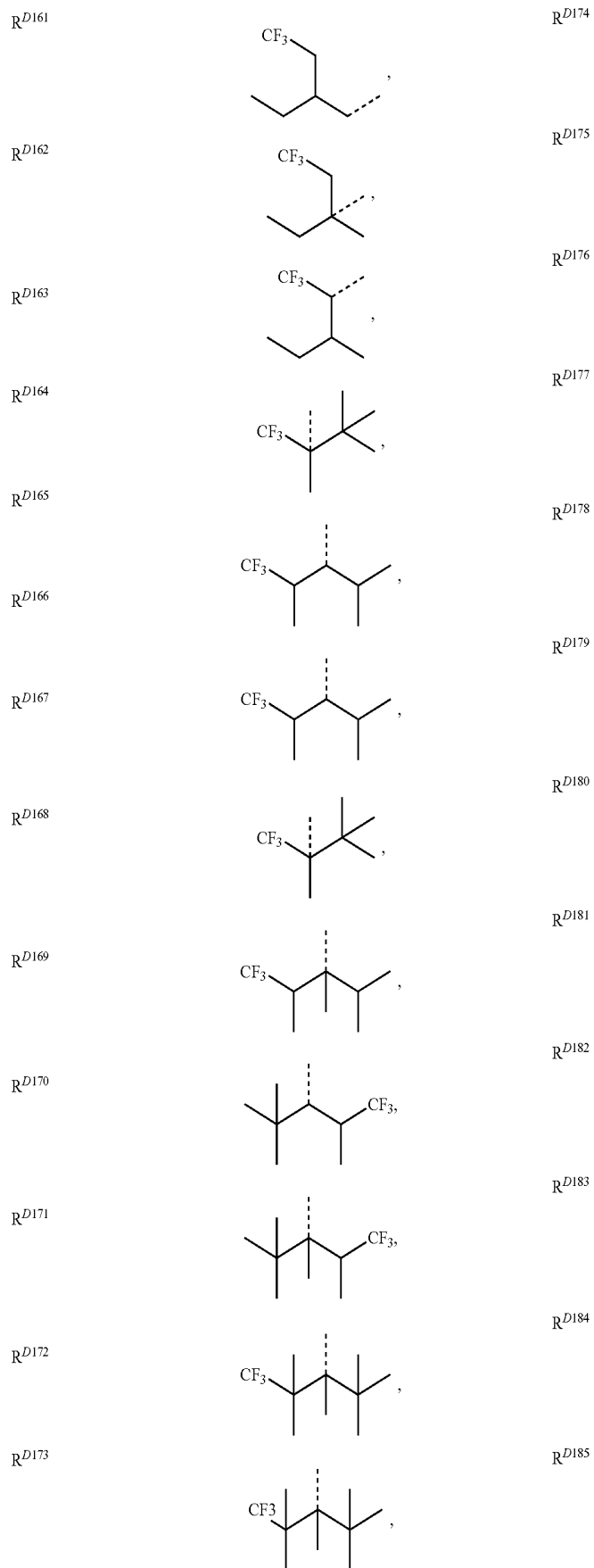
R^{D159}

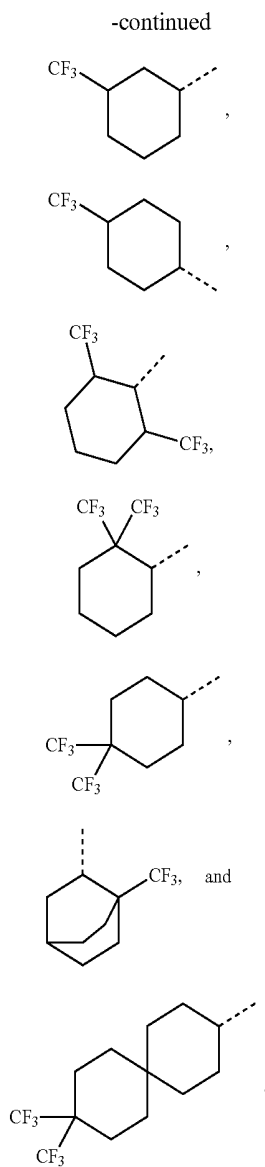
R^{D160}

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R^{D186}

R^{D187}

R^{D188}

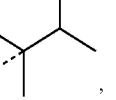
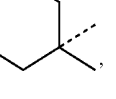
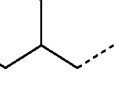
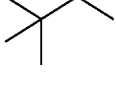
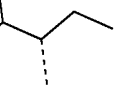
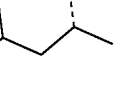
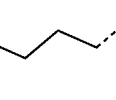
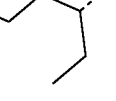
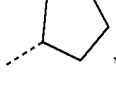
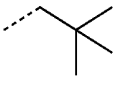
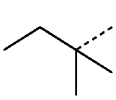
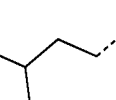
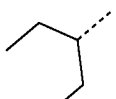
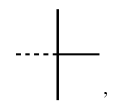
R^{D189}

R^{D190}

R^{D191}

R^{D192}

-continued



R^{D10}

R^{D17}

R^{D18}

R^{D20}

R^{D22}

R^{D37}

R^{D40}

R^{D41}

R^{D42}

R^{D43}

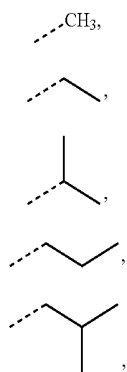
R^{D48}

R^{D49}

R^{D50}

R^{D54}

[0083] In some embodiments, L_{Cj} is selected from the group consisting of the items as defined in the above table when the corresponding R^1 and R^2 are defined to be selected from the following structures:



R^{D1}

R^{D3}

R^{D4}

R^{D5}

R^{D9}

-continued



R^{D55}

R^{D58}

R^{D59}

R^{D78}

R^{D79}

R^{D81}

R^{D87}

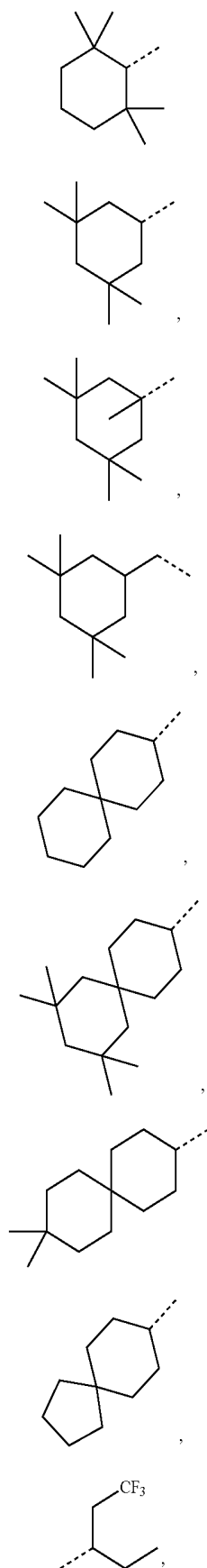
R^{D88}

R^{D89}

R^{D93}

R^{D116}

-continued



R^{D117}

R^{D118}

R^{D119}

R^{D120}

R^{D133}

R^{D134}

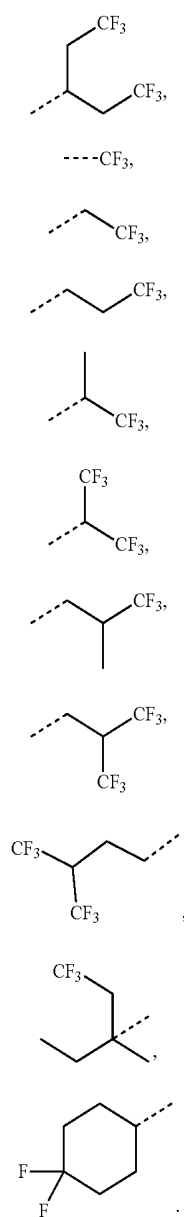
R^{D135}

R^{D136}

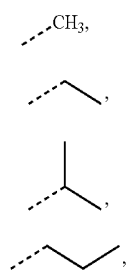
R^{D143}

CF₃

-continued



[0084] In some embodiments, L_{Cj} is selected from the group consisting of the items as defined in the above table when the corresponding R^1 and R^2 are defined to be selected from the following structures:



R^{D144}

R^{D145}

R^{D146}

R^{D147}

R^{D149}

R^{D151}

R^{D154}

R^{D155}

R^{D161}

R^{D175}

R^{D190}

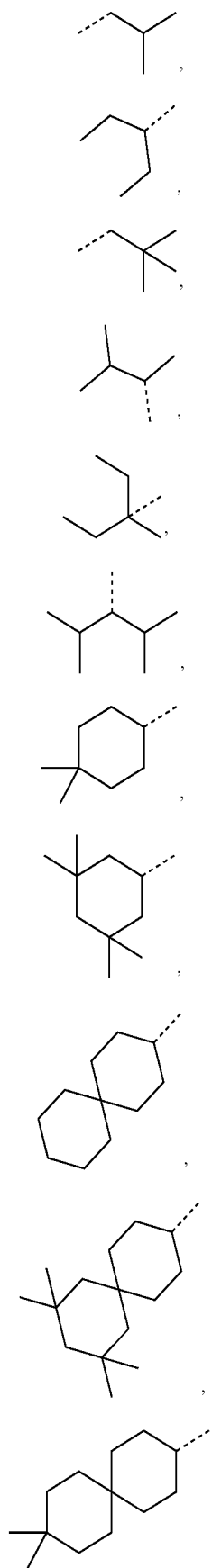
R^{D1}

R^{D3}

R^{D4}

R^{D5}

-continued



R^{D9}

R^{D17}

R^{D22}

R^{D43}

R^{D50}

R^{D78}

R^{D116}

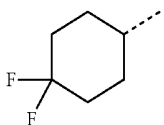
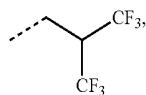
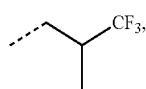
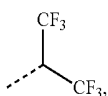
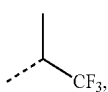
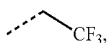
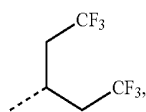
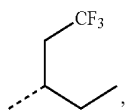
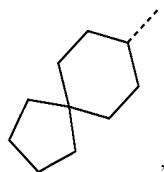
R^{D118}

R^{D133}

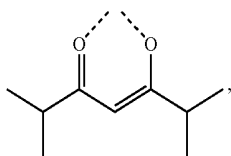
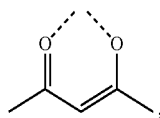
R^{D134}

R^{D135}

-continued

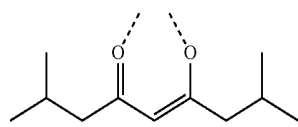


[0085] In some embodiments, L_C is selected from the group consisting of:



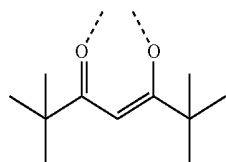
-continued

R^{D136}



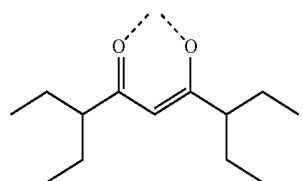
L_{C9-T}

R^{D143}



L_{C10-T}

R^{D144}



L_{C17-T}

R^{D145}

R^{D146}

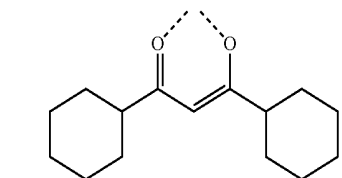
R^{D149}

R^{D151}

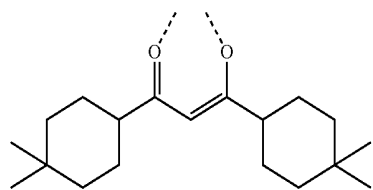
R^{D154}

R^{D155}

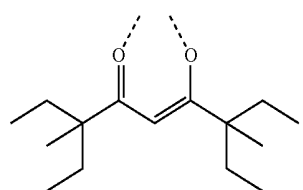
R^{D190}



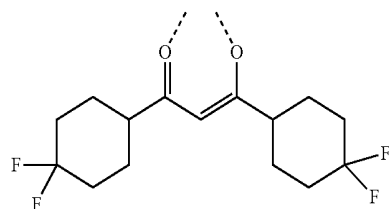
L_{C55-T}



L_{C116-T}



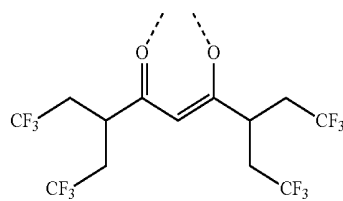
L_{C50-T}



L_{C190-T}

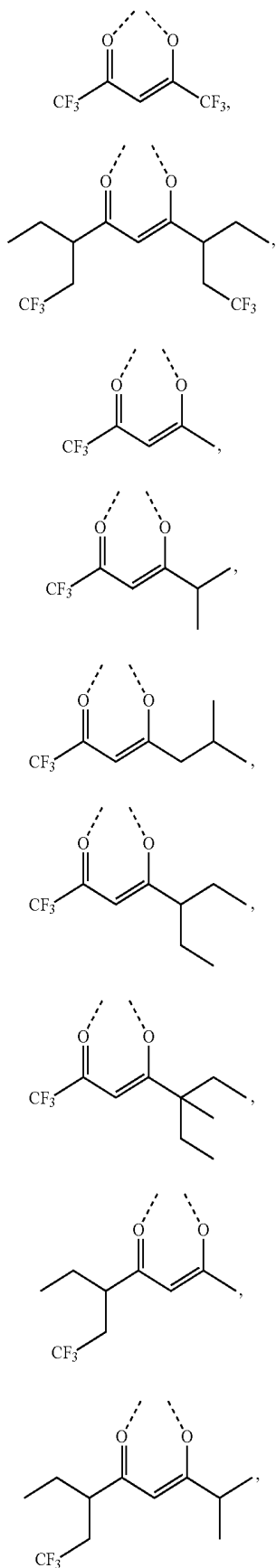
L_{C1-T}

L_{C4-T}

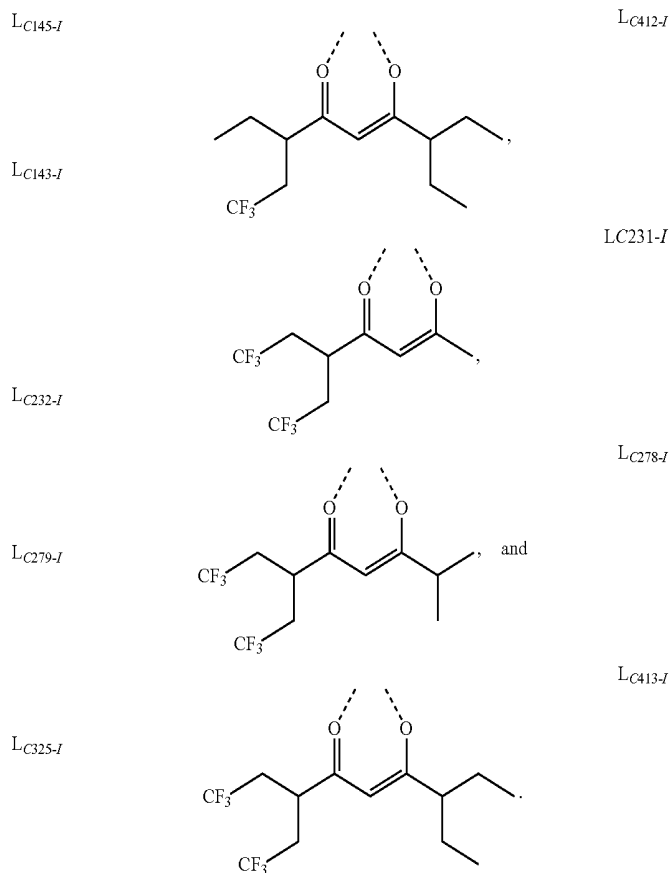


L_{C144-T}

-continued

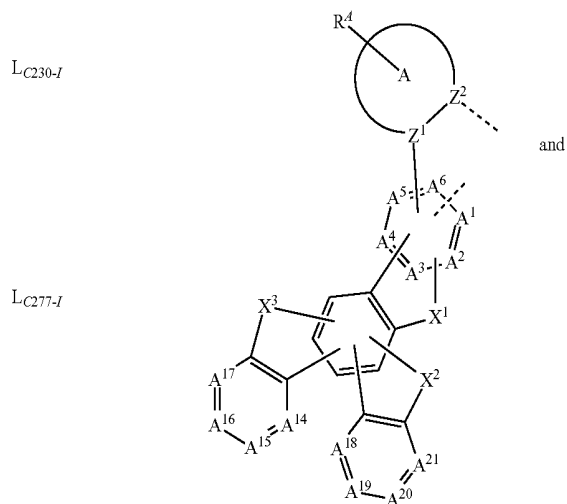


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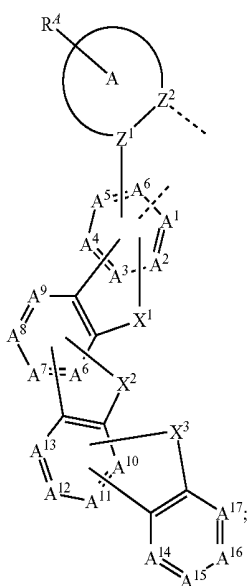


[0086] In some embodiments where the compound has the formula of $M(L_A)_x(L_B)_y(L_C)_z$, the compound is a compound having the formula $Ir(L_{An-m-I})_3$, a compound having the formula $Ir(L_{An-m-I})(L_{Bk})_2$, or a compound having the formula $Ir(L_{An-m-I})_2(L_{Cj-I})$ or $Ir(L_{An-m-I})_2(L_{Cj-II})$; where the variables x, y, z, n, m, l, k and j are as defined above, and each L_{An-m-I} , L_{Bk} , L_{Cj-I} , and L_{Cj-II} has a structure as defined above.

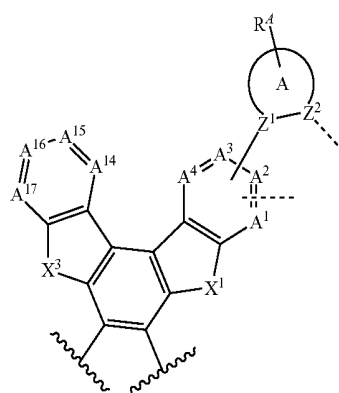
[0087] An organic light emitting device (OLED) is also disclosed, where the OLED comprises: an anode; a cathode; and an organic layer, disposed between the anode and the cathode, comprising a compound comprising a first ligand L_A selected from the group consisting of Formula I



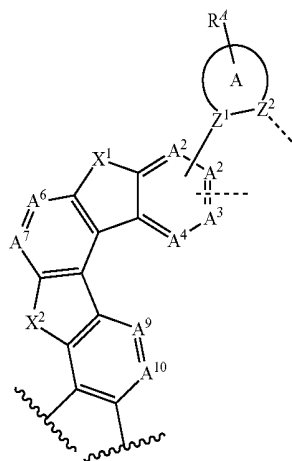
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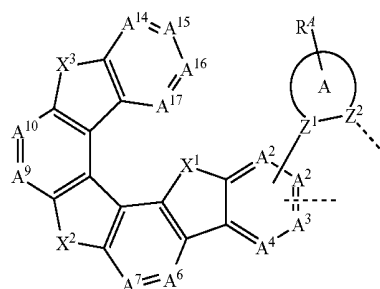
Formula II



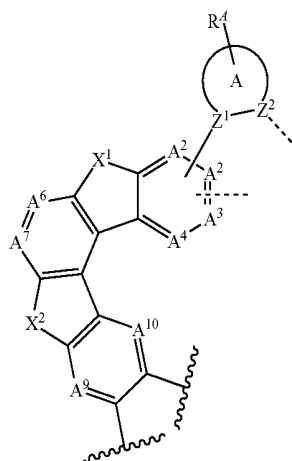
Formula III



Formula IV



Formula V



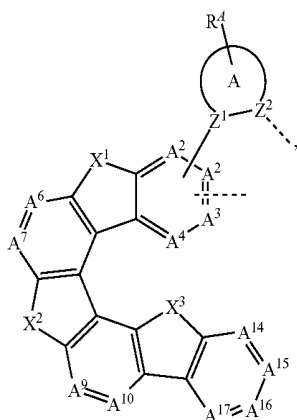
Formula VI

where, L_A is complexed to a metal M to form a 5-membered chelate ring; A is a 5-membered or 6-membered aryl or heteroaryl ring; Z^1 and Z^2 are each independently C or N ; R^4 represents mono to the maximum allowable substitutions, or no substitution; each A^1 to A^{13} is independently C , CR , or N ; each A^{14} to A^{21} is independently CR or N ; any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ; any of A^1 to A^{13} are C when they are adjacent and fused to a ring; any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring; X^1 , X^2 , and X^3 are each independently selected from the group consisting of O , S , NR' , $CR'R''$, and $SiR'R''$; each R , R' , R'' , and R^4 is independently a 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 acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; M is optionally coordinated to other ligands; the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand; any two substituents may be joined or fused together to form a ring;

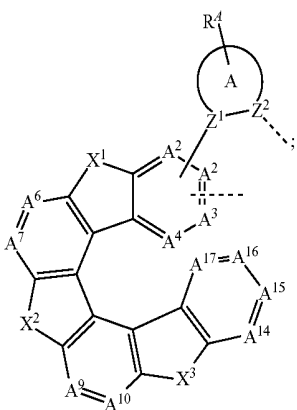
[0088] if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ;

[0089] if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ; Formulas III through VIII are defined as

-continued



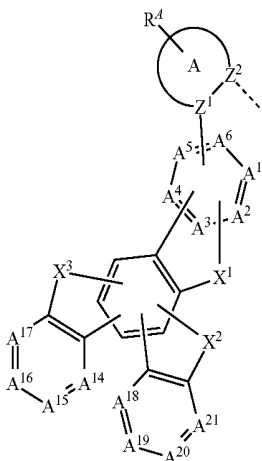
Formula VII



Formula VIII

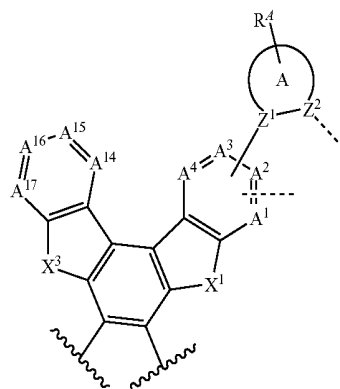
and the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X² or X³.

[0090] A consumer product comprising an OLED is also disclosed, where the OLED comprises: an anode; a cathode; and an organic layer, disposed between the anode and the cathode. The organic layer comprising a compound comprising a first ligand L_A selected from the group consisting of



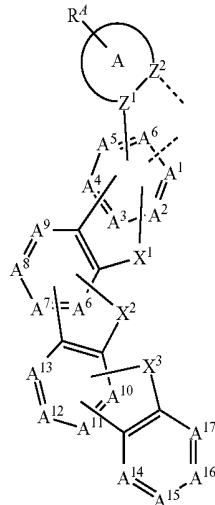
Formula I

and



Formula III

-continued



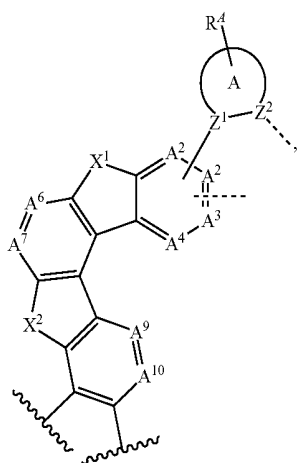
Formula II

where, L_A is complexed to a metal M to form a 5-membered chelate ring; A is a 5-membered or 6-membered aryl or heteroaryl ring; Z¹ and Z² are each independently C or N; R⁴ represents mono to the maximum allowable substitutions, or no substitution; each A¹ to A¹³ is independently C, CR, or N; each A¹ to A²¹ is independently CR or N; any of A¹ to A⁶ is C when it forms a direct bond to M or Z¹; any of A¹ to A¹³ are C when they are adjacent and fused to a ring; any ring comprising X¹, X², and X³ is a 5-membered ring; X¹, X², and X³ are each independently selected from the group consisting of O, S, NR¹, CR¹R², and SiR¹R²R³; each R, R¹, R², and R⁴ is independently a 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 acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; M is optionally coordinated to other ligands; the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand; any two substituents may be joined or fused together to form a ring;

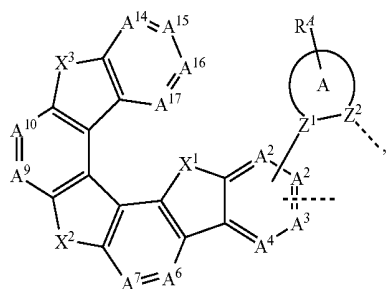
[0091] if the first ligand L_A comprises a structure of Formula III through VII, then neither Z¹ nor M forms a direct bond to A⁴;

[0092] if the first ligand L_A comprises a structure of Formula VIII, then neither Z¹ nor M forms a direct bond to A³ or A⁴; Formulas III through VIII are defined as

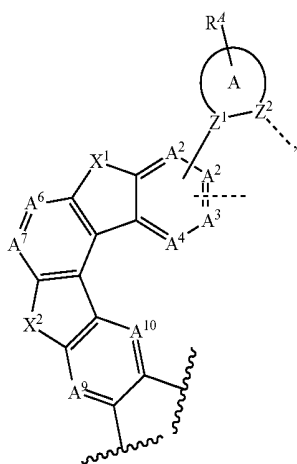
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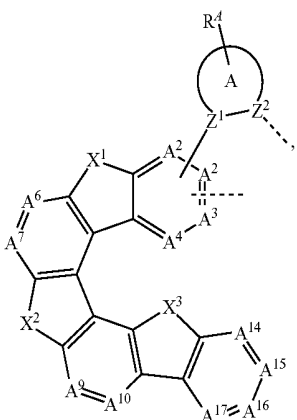
Formula IV



Formula V

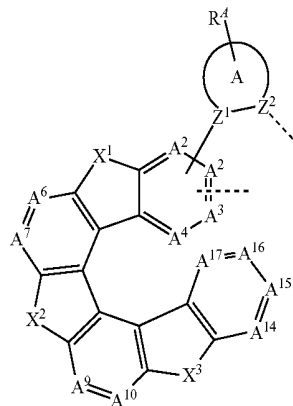


Formula VI



Formula VII

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Formula VIII

and the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X² or X³.

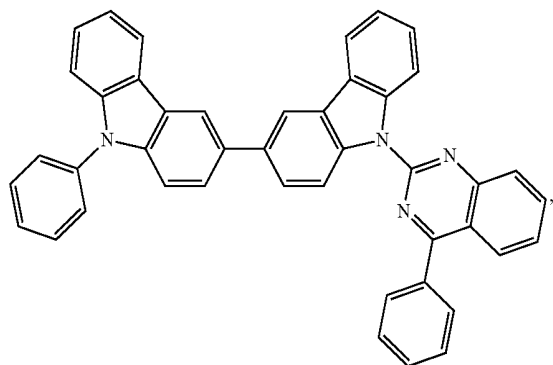
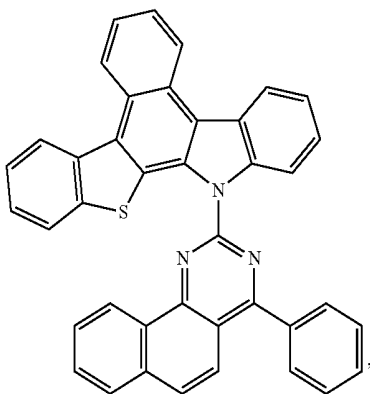
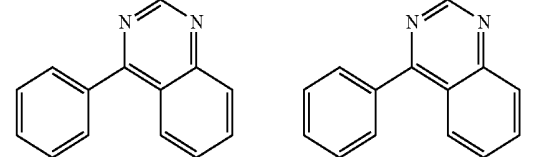
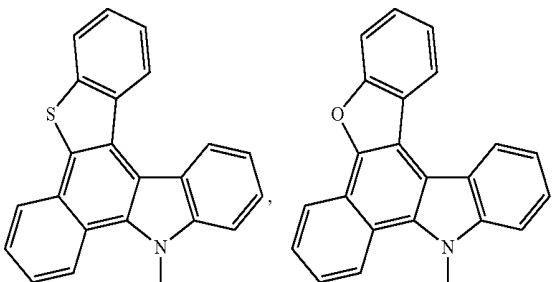
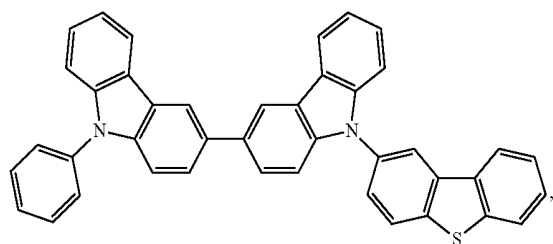
[0093] In some embodiments, the OLED has one or more characteristics selected from the group consisting of being flexible, being rollable, being foldable, being stretchable, and being curved. In some embodiments, the OLED is transparent or semi-transparent. In some embodiments, the OLED further comprises a layer comprising carbon nanotubes.

[0094] 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.

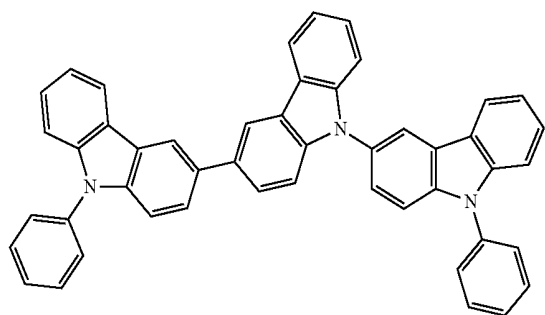
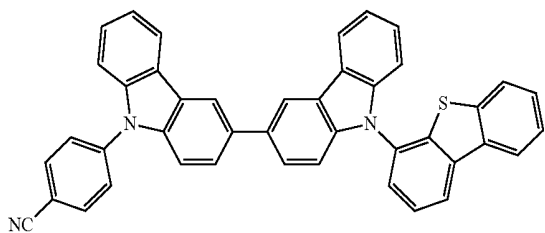
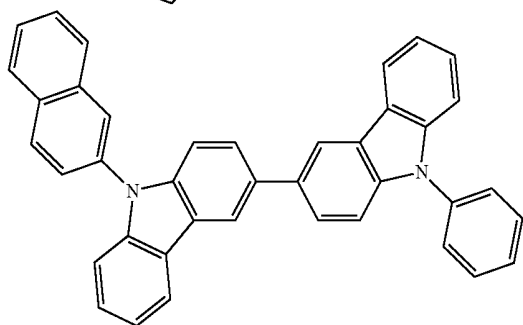
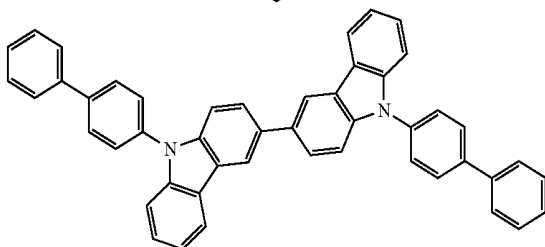
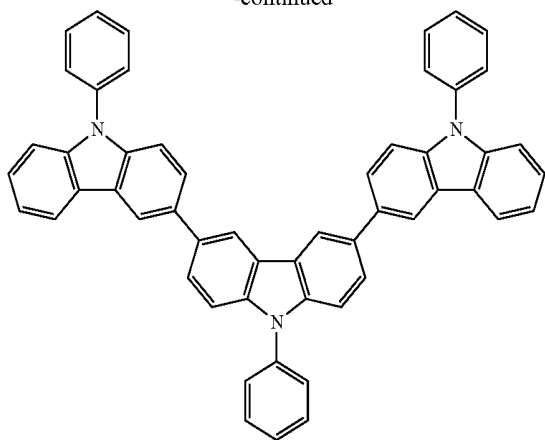
[0095] In some embodiments, the compound can be an emissive dopant. In some embodiments, the compound can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, i.e., TADF (also referred to as E-type delayed fluorescence; see, e.g., U.S. application Ser. No. 15/700,352, published on Mar. 14, 2019 as U.S. patent application publication No. 2019/0081248, 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. In some embodiments, the compound can be homoleptic (each ligand is the same). In some embodiments, the compound can be heteroleptic (at least one ligand is different from others).

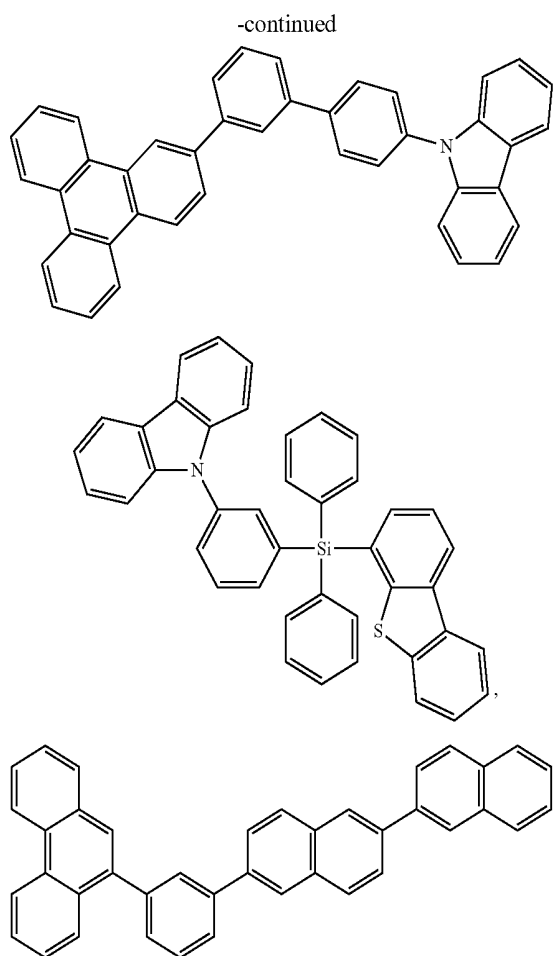
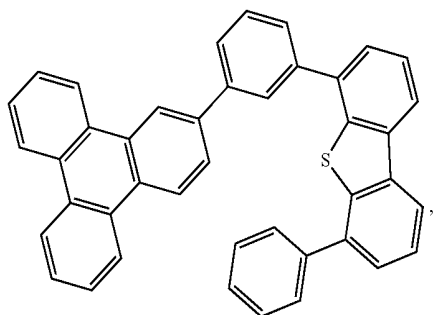
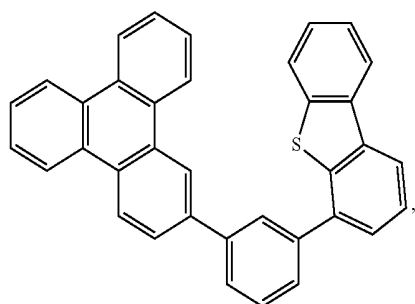
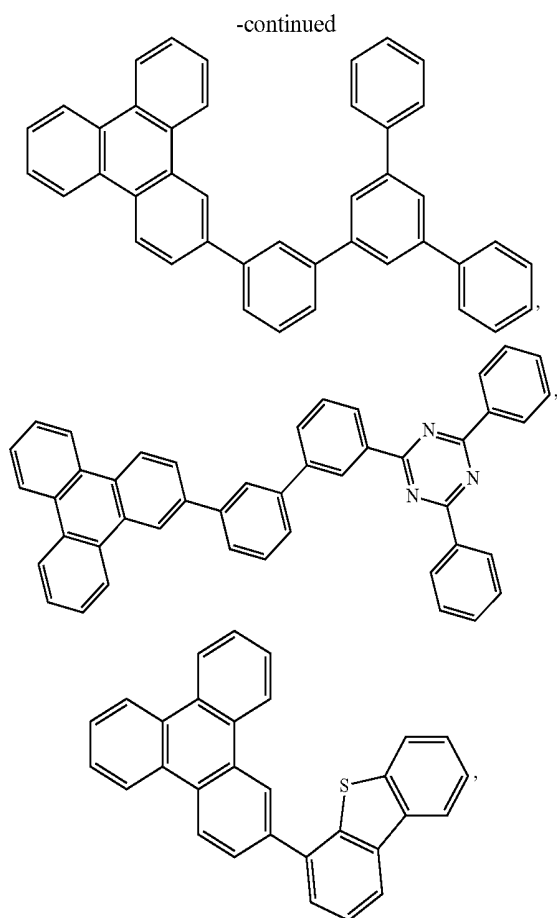
[0096] When there are more than one ligand coordinated to a metal, the ligands can all be the same in some embodiments. In some other embodiments, at least one ligand is different from the other ligand(s). In some embodiments, every ligand can be different from each other. This is also true in embodiments where a ligand being coordinated to a metal can be linked with other ligands being coordinated to that metal to form a tridentate, tetradentate, pentadentate, or hexadentate ligands. Thus, where the coordinating ligands are being linked together, all of the ligands can be the same

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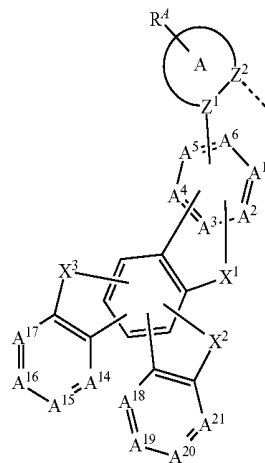


and combinations thereof.

Additional information on possible hosts is provided below.

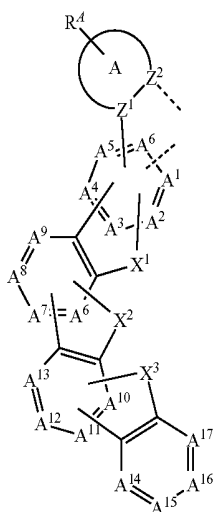
[0102] An emissive region in an organic light emitting device, the emissive region comprising a compound comprising a first ligand L_A selected from the group consisting of

Formula I



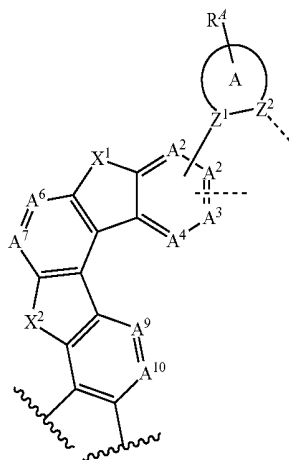
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Formula II

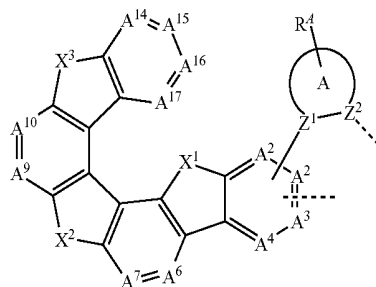
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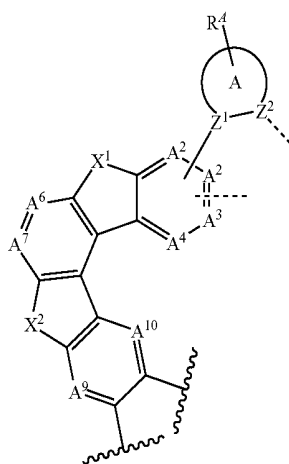
Formula IV

is disclosed, where, L_A is complexed to a metal M to form a 5-membered chelate ring; A is a 5-membered or 6-membered aryl or heteroaryl ring; Z^1 and Z^2 are each independently C or N;

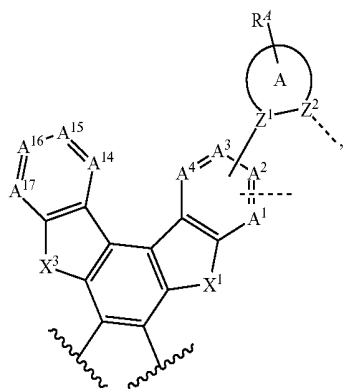
R^4 represents mono to the maximum allowable substitutions, or no substitution; each A^1 to A^{13} is independently C, CR, or N; each A^{14} to A^{21} is independently CR or N; any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ; any of A^1 to A^{13} are C when they are adjacent and fused to a ring; any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring; X^1 , X^2 , and X^3 are each independently selected from the group consisting of O, S, Se, NR', CR'R'', and SiR'R''; each R, R', R'', and R^4 is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined above, and combinations thereof; M is optionally coordinated to other ligands; the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand; any two substituents may be joined or fused together to form a ring; if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ; if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ; where Formulas III through VIII are defined as follows:



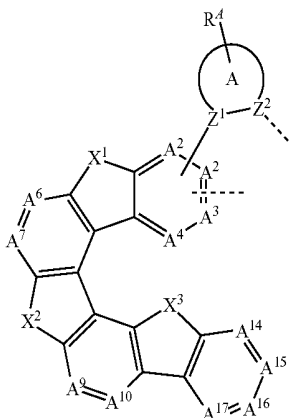
Formula V



Formula VI



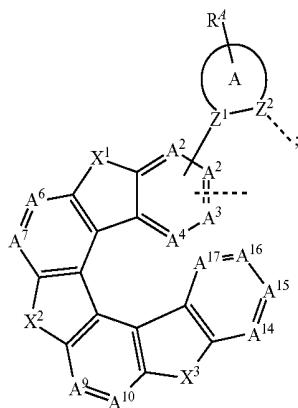
Formula III



Formula VII

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Formula VIII



and the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X^2 or X^3 .

[0103] In some embodiments of the emissive region, the compound is an emissive dopant or a non-emissive dopant.

[0104] In some embodiments of the emissive region, 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.

[0105] In some embodiments of the emissive region, the emissive region further comprises a host, wherein the host is selected from the Host Group defined above.

[0106] 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 material, disclosed herein.

[0107] 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 is can also be incorporated into the supramolecule complex without covalent bonds.

Combination with Other Materials

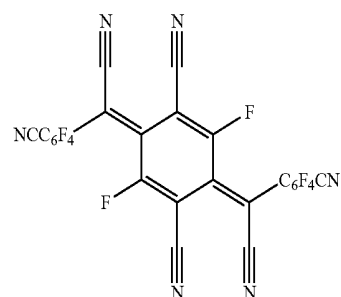
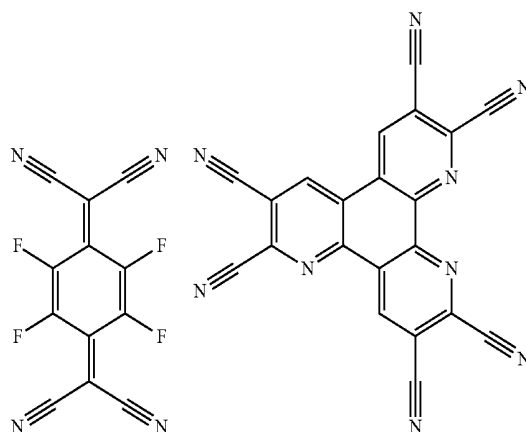
[0108] The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials

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.

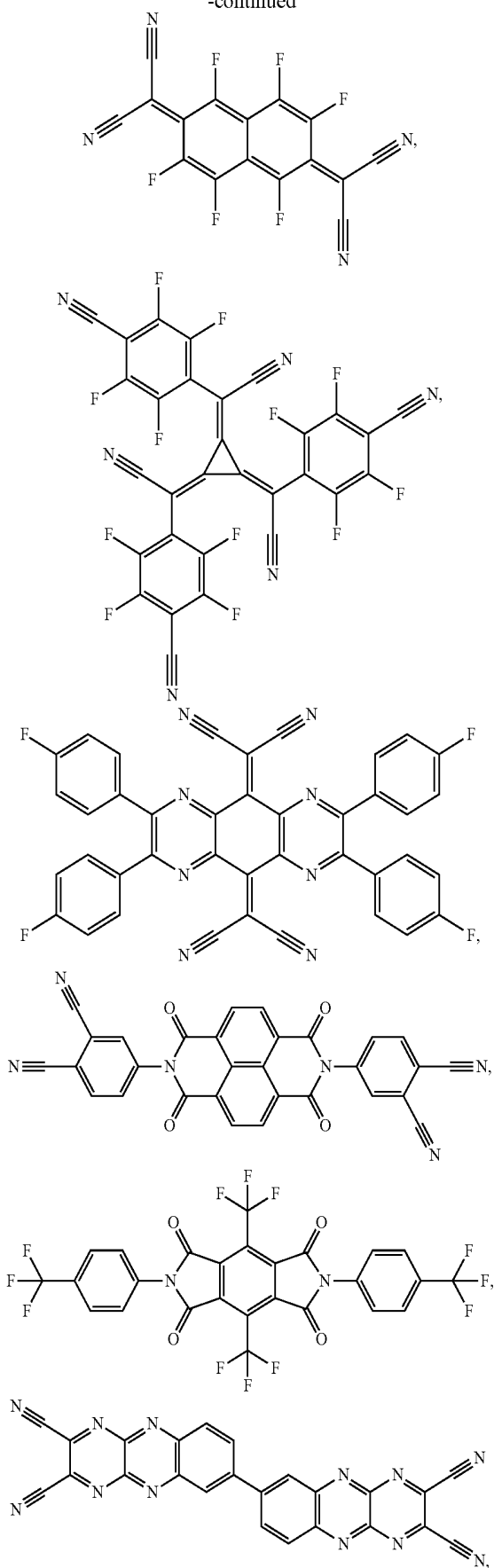
Conductivity Dopants:

[0109] 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.

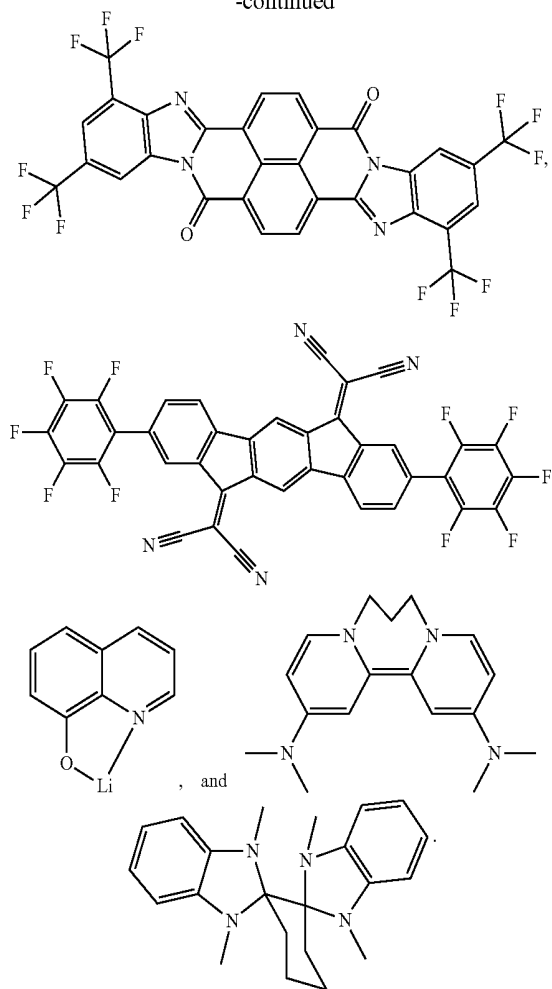
[0110] Non-limiting examples of the conductivity dopants that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: EP01617493, EP01968131, EP2020694, EP2684932, US20050139810, US20070160905, US20090167167, US2010288362, WO06081780, WO2009003455, WO2009008277, WO2009011327, WO2014009310, US2007252140, US2015060804, US20150123047, and US2012146012.



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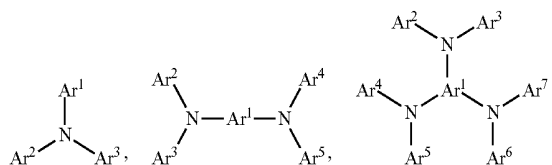
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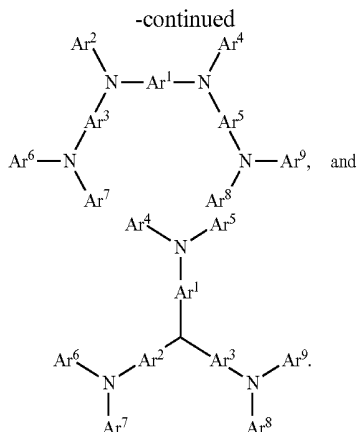


HIL/HTL:

[0111] 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.

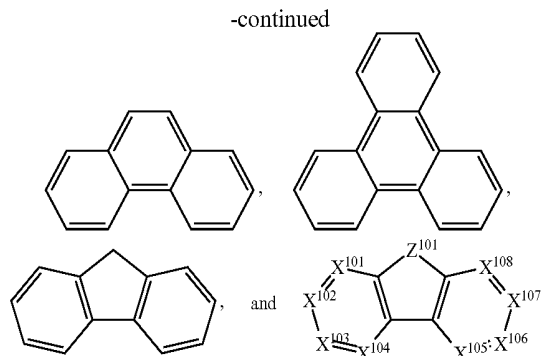
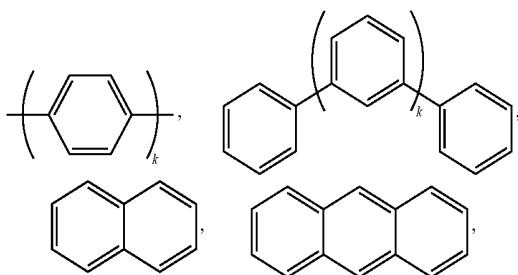
[0112] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:





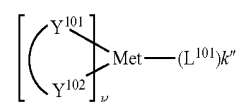
[0113] Each of Ar¹ to Ar⁹ is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothio-*phene*, 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, benzofuro-pyridine, 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.

[0114] In one aspect, Ar¹ to Ar⁹ is independently selected from the group consisting of:



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

[0115] Examples of metal complexes used in HIL or HTL include, but are not limited to the following general formula:

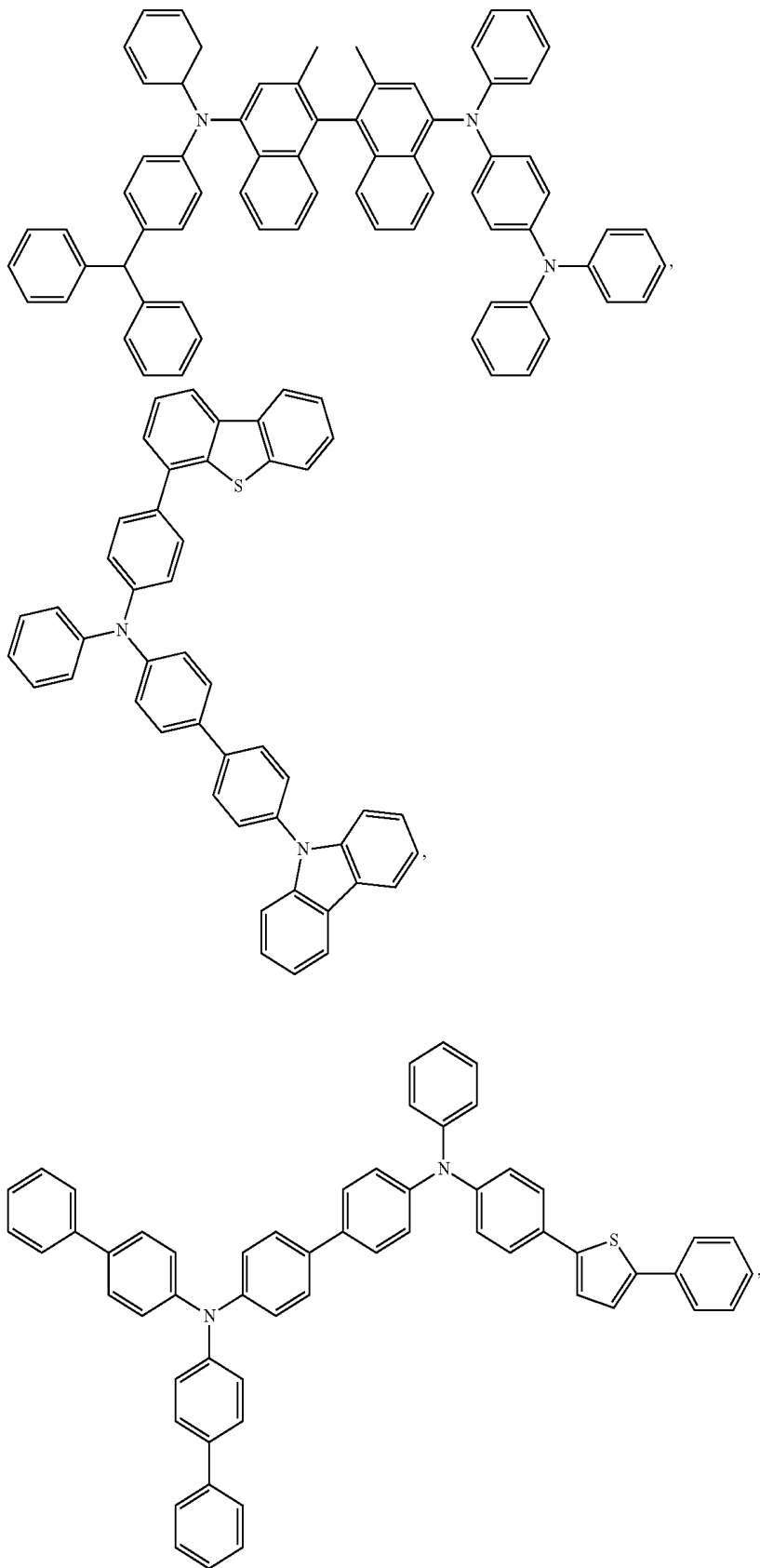


wherein Met is a metal, which can have an atomic weight greater than 40; (Y¹⁰¹-Y¹⁰²) is a bidentate ligand, Y¹⁰¹ and Y¹⁰² are independently selected from C, N, O, P, and S; L¹⁰¹ is an ancillary ligand; *k*' is an integer value from 1 to the maximum number of ligands that may be attached to the metal;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

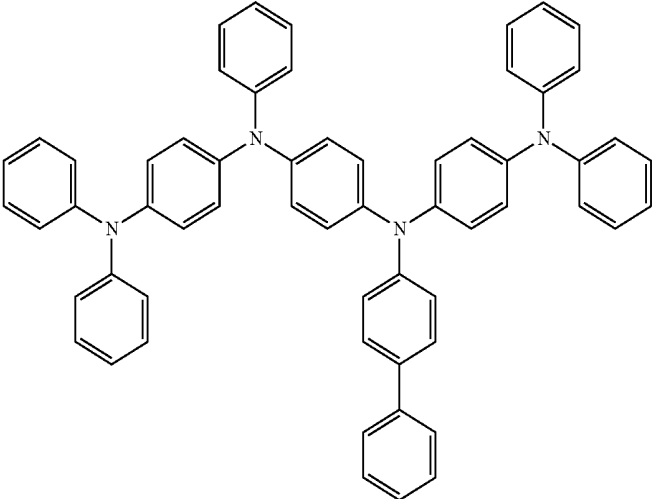
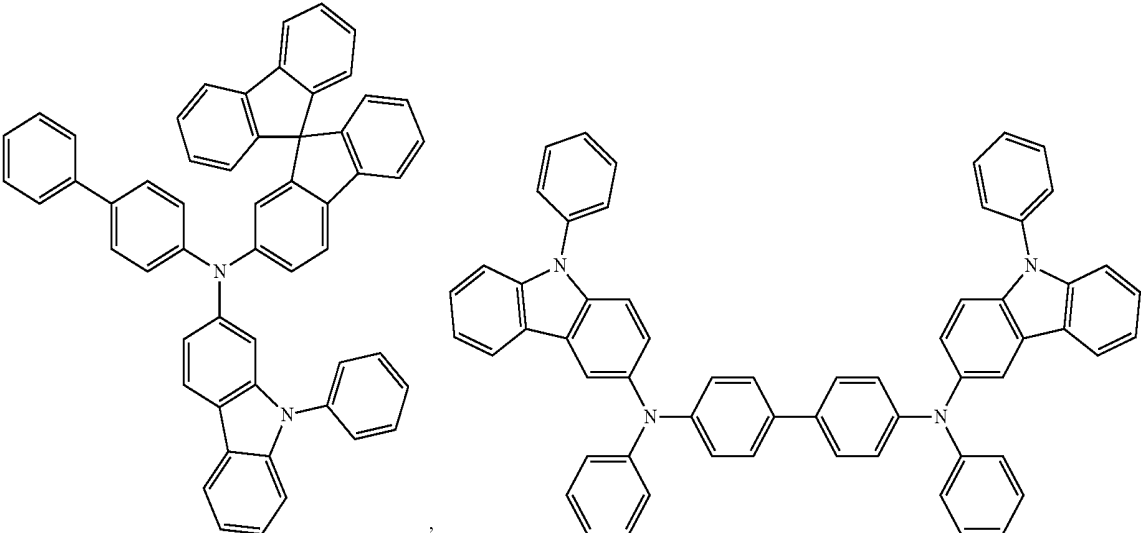
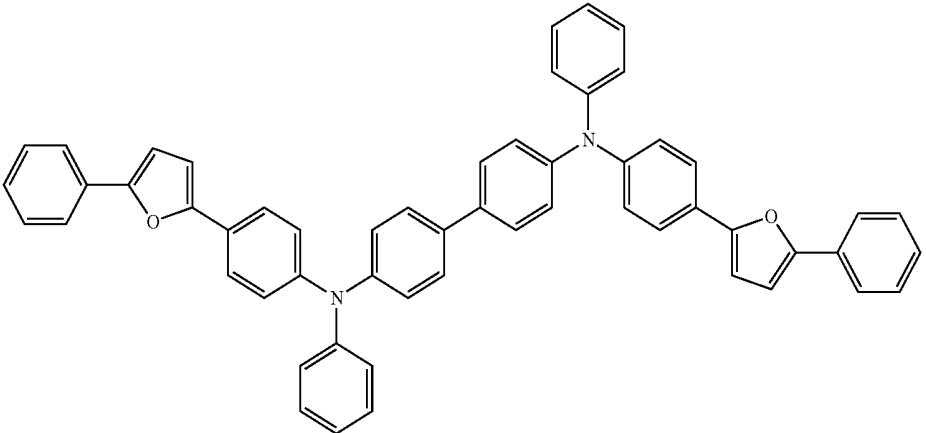
[0116] In one aspect, (Y¹⁰¹-Y¹⁰²) is a 2-phenylpyridine derivative. In another aspect, (Y¹⁰¹-Y¹⁰²) is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc⁺/Fc couple less than about 0.6 V.

[0117] 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,

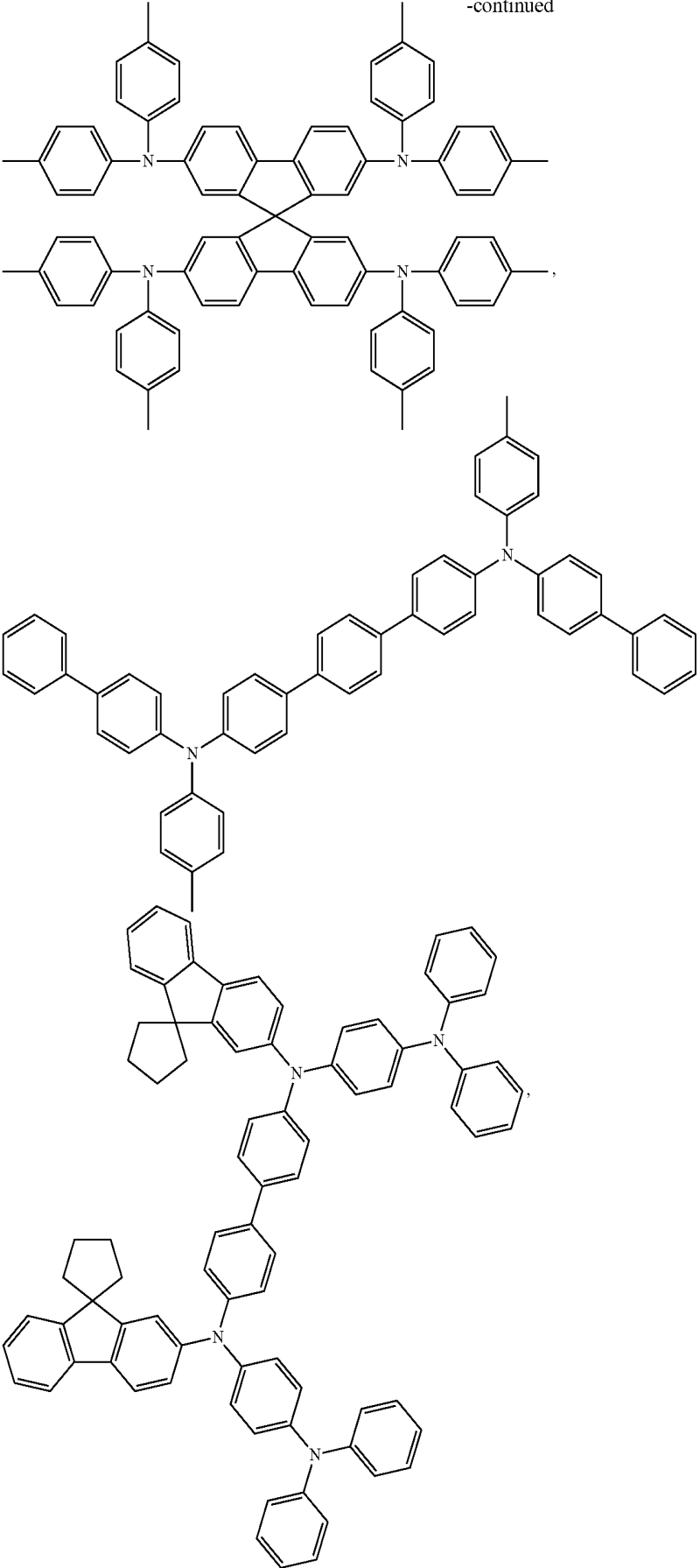
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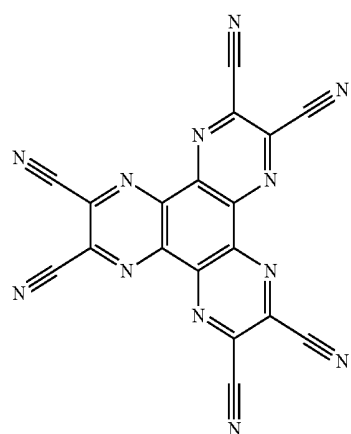
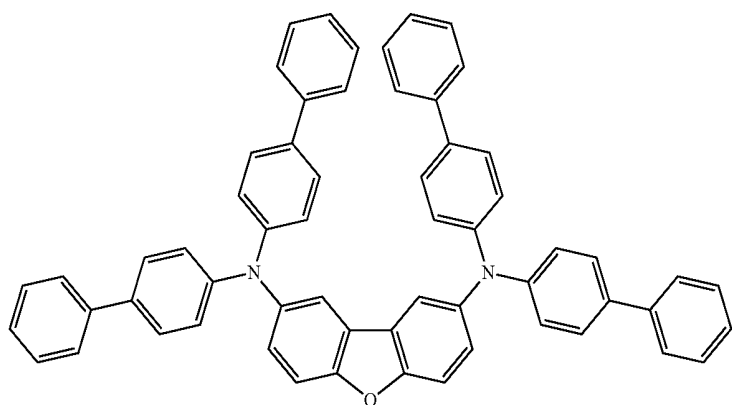
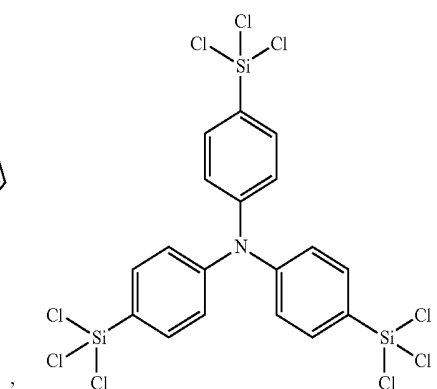
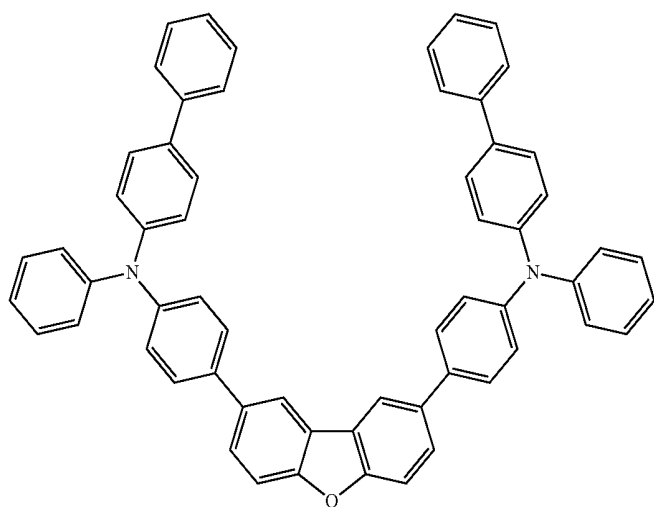
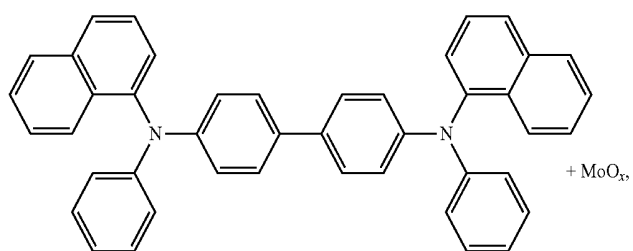
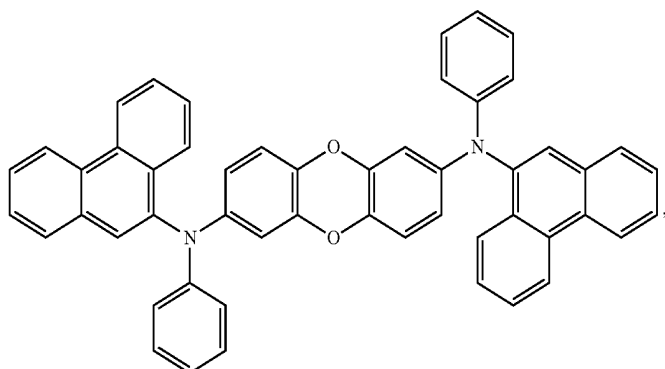
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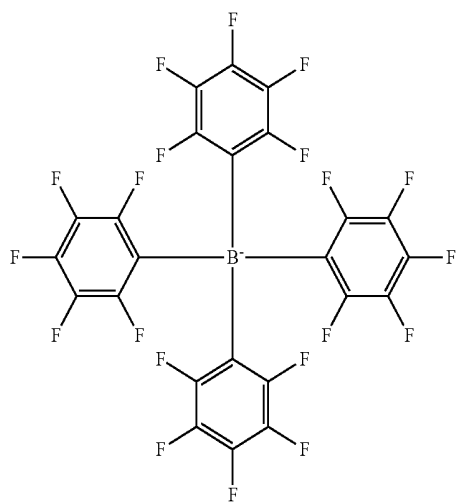
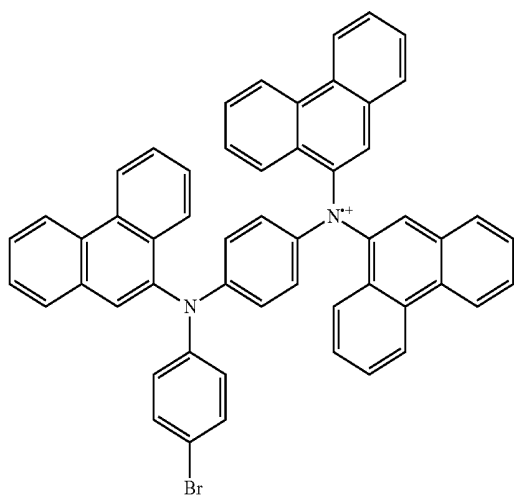
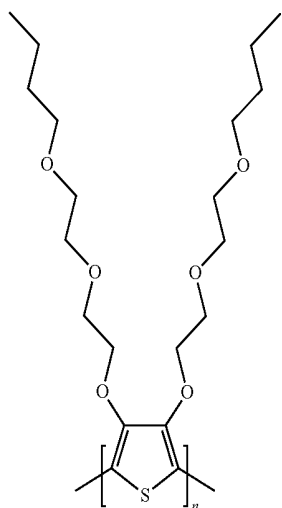
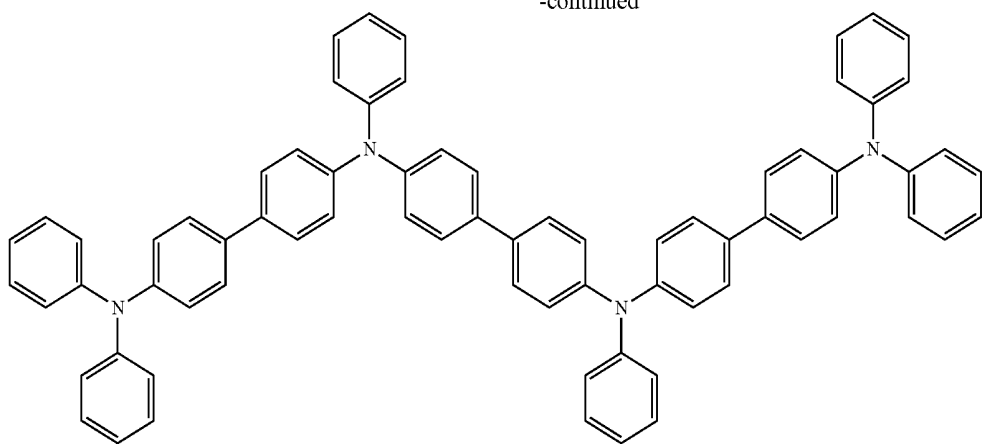
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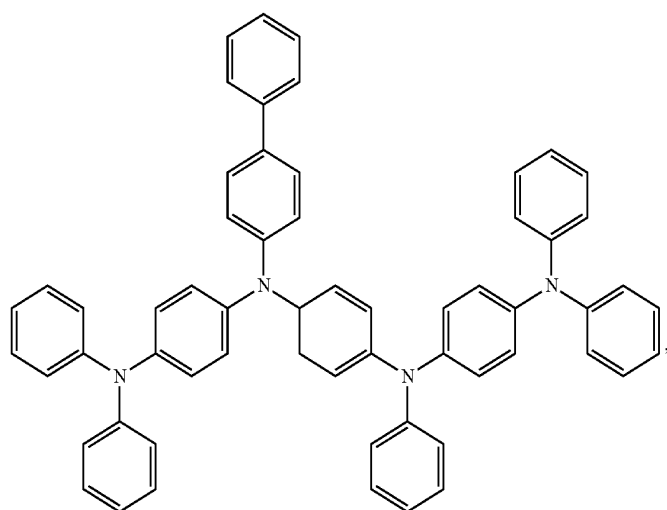
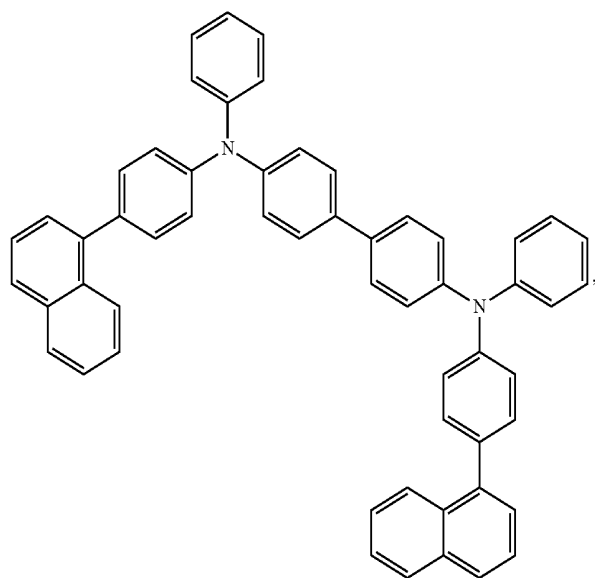
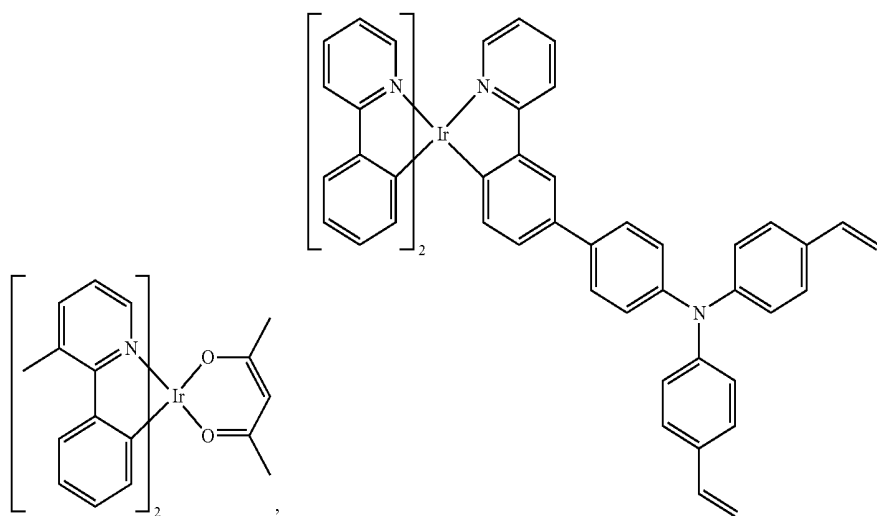
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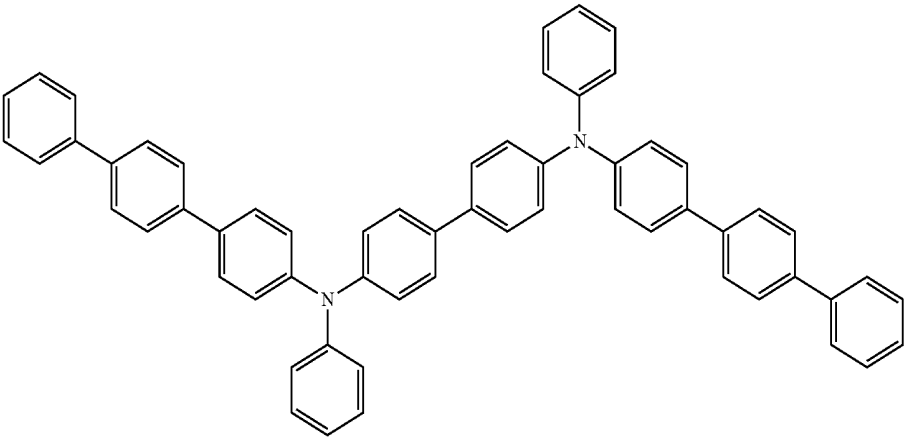
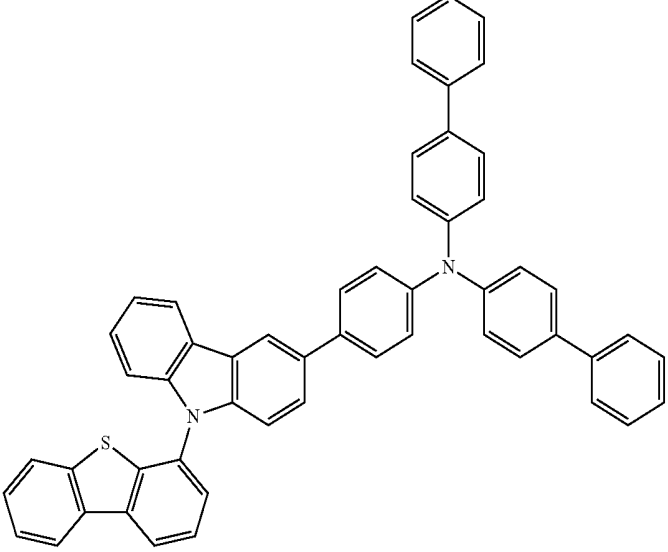
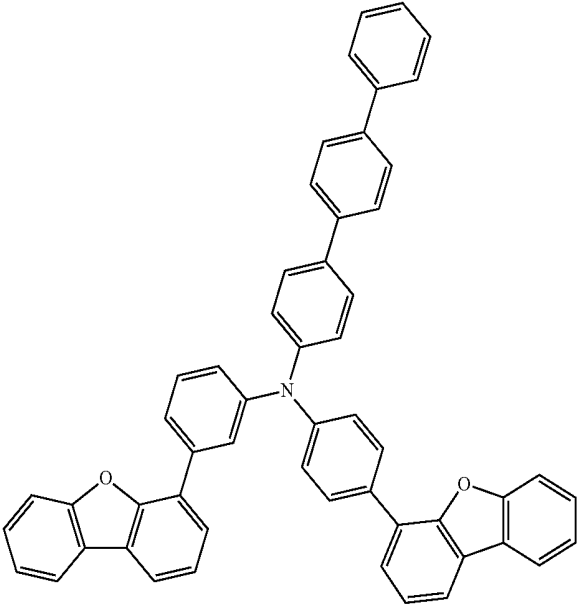
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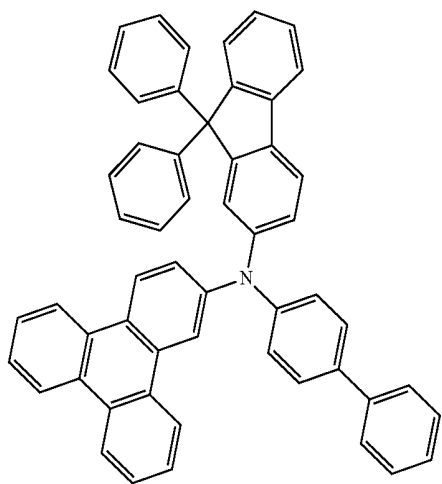
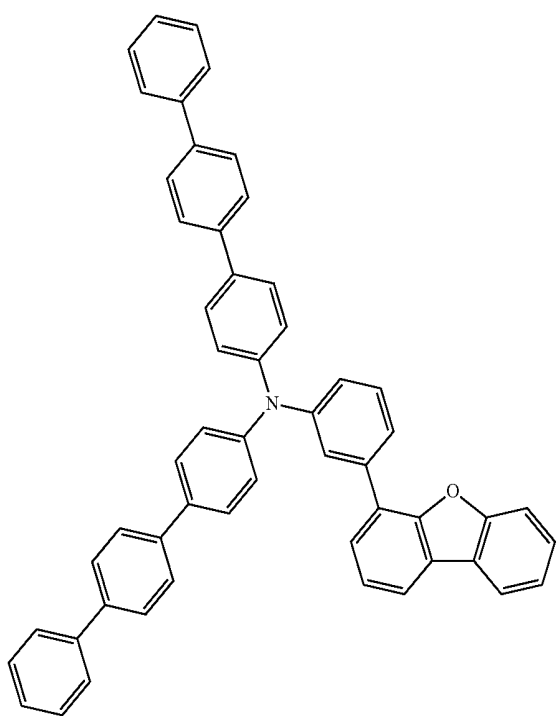
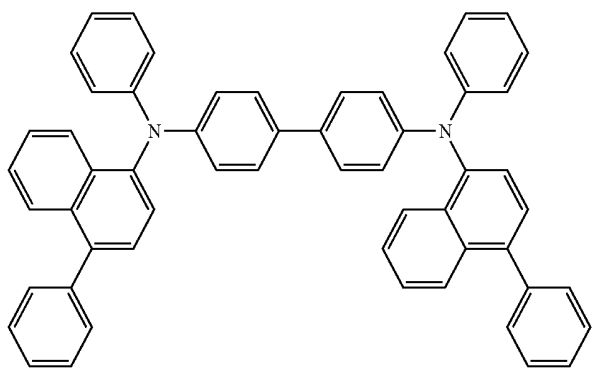
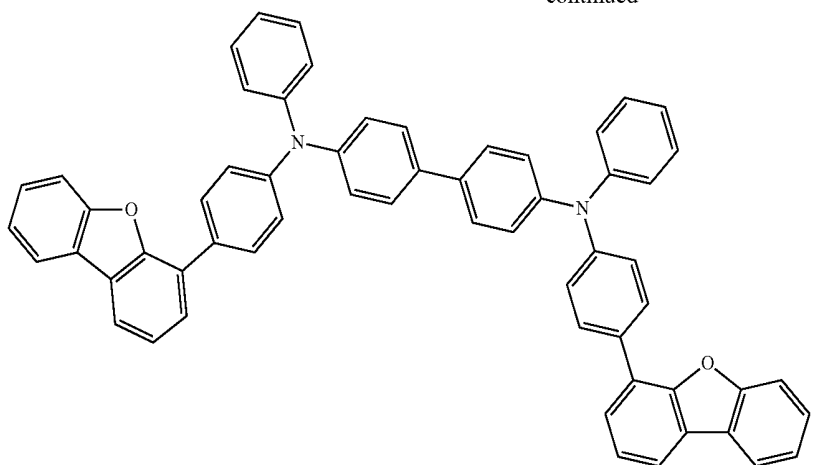
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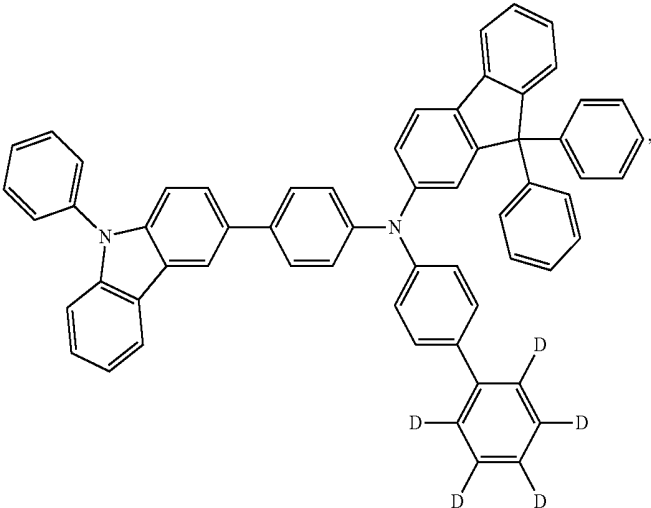
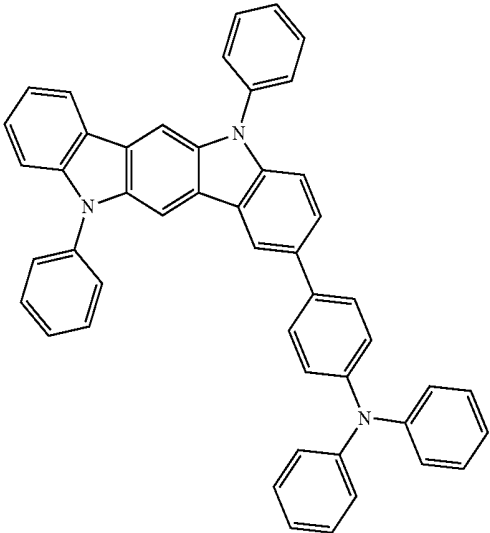
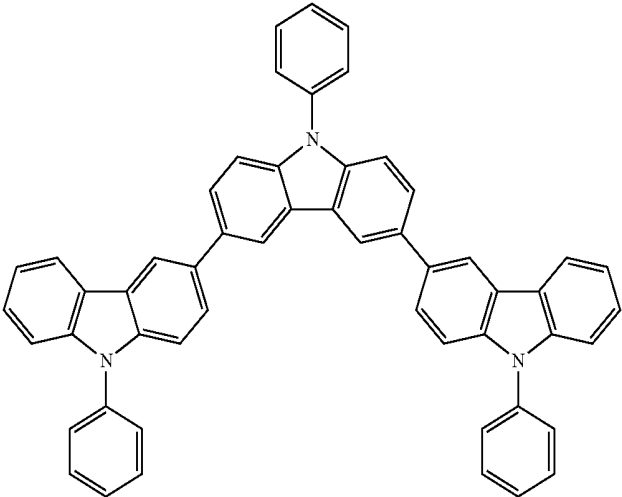
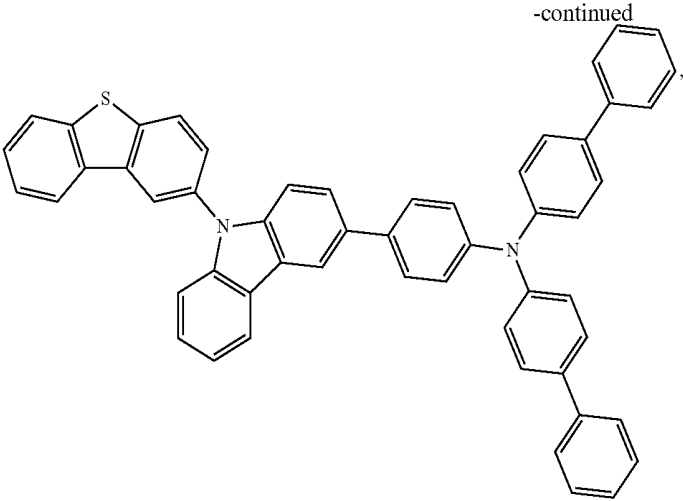
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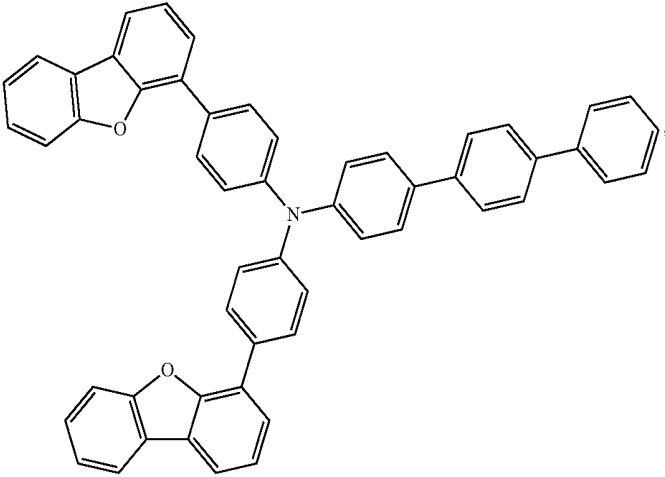
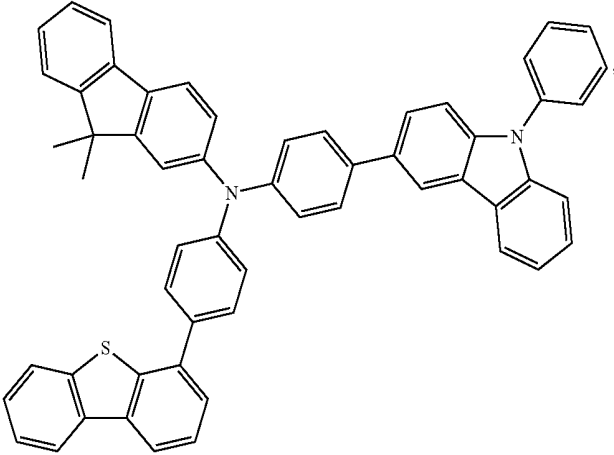
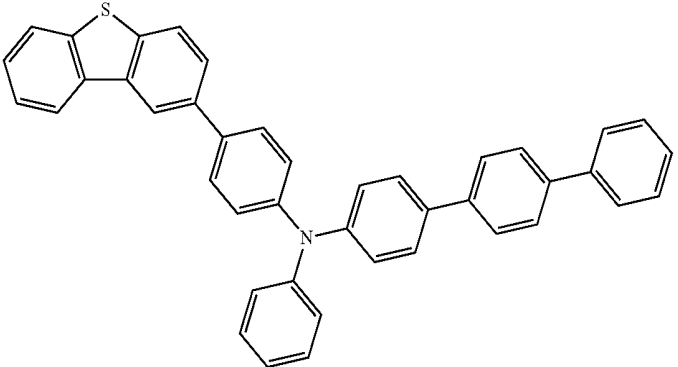
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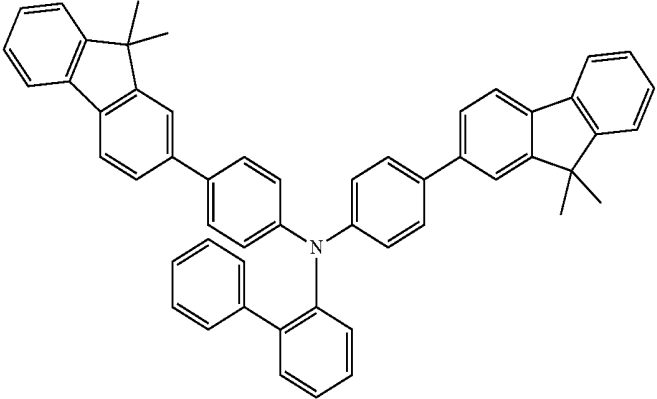
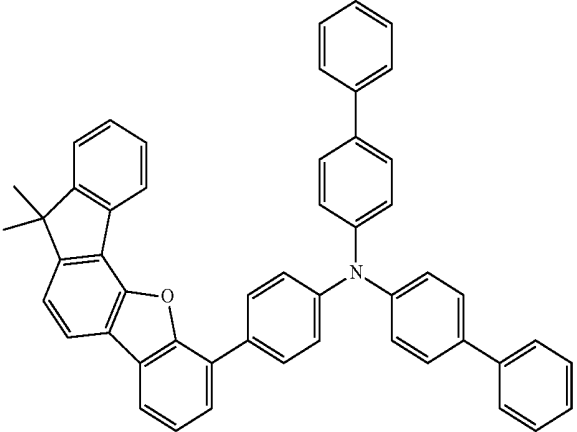
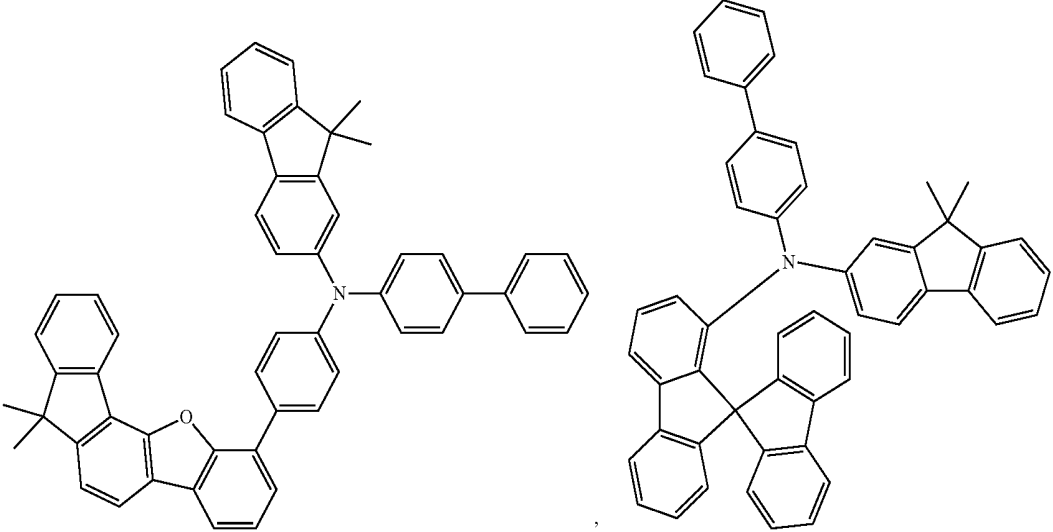
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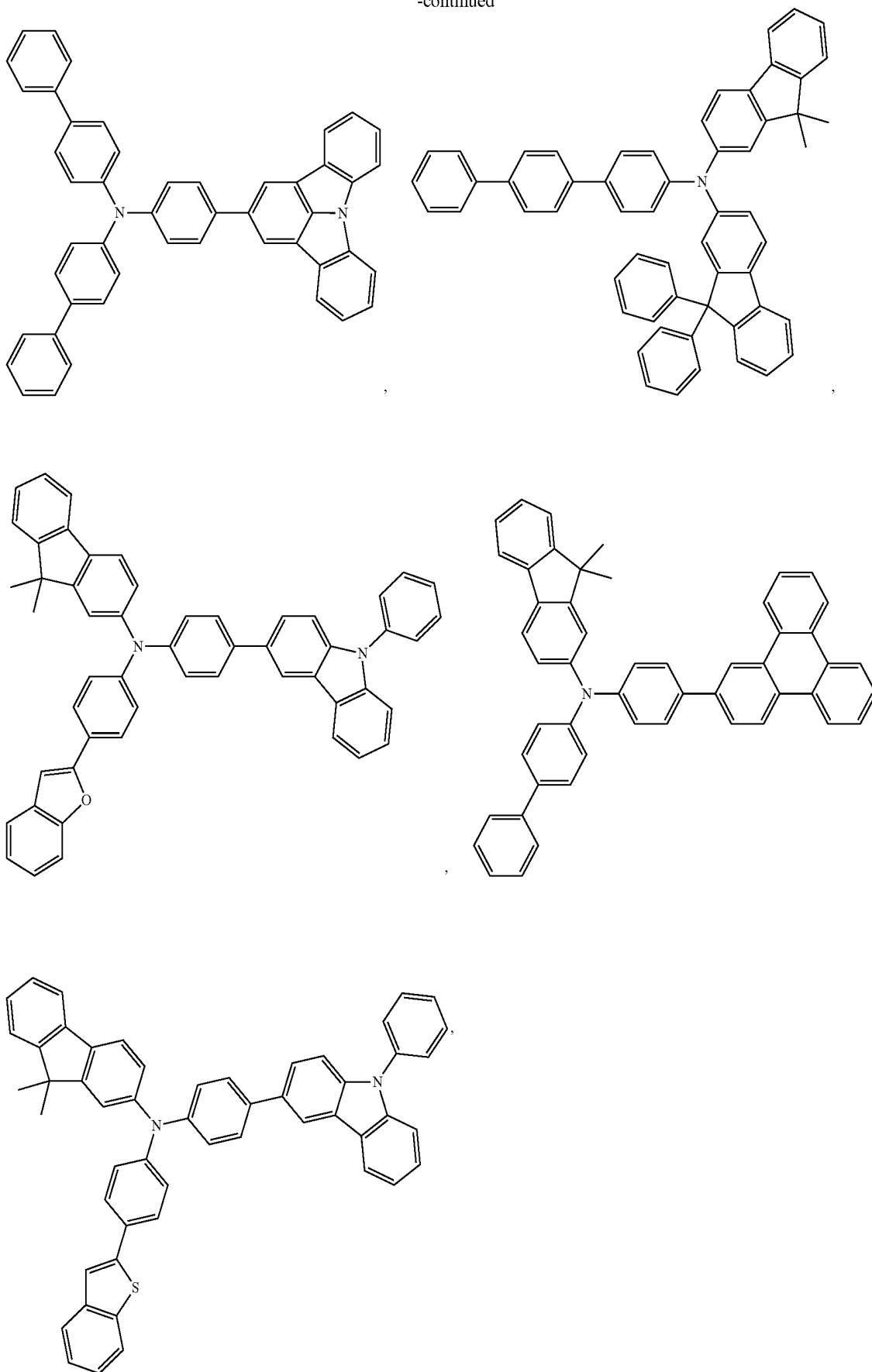
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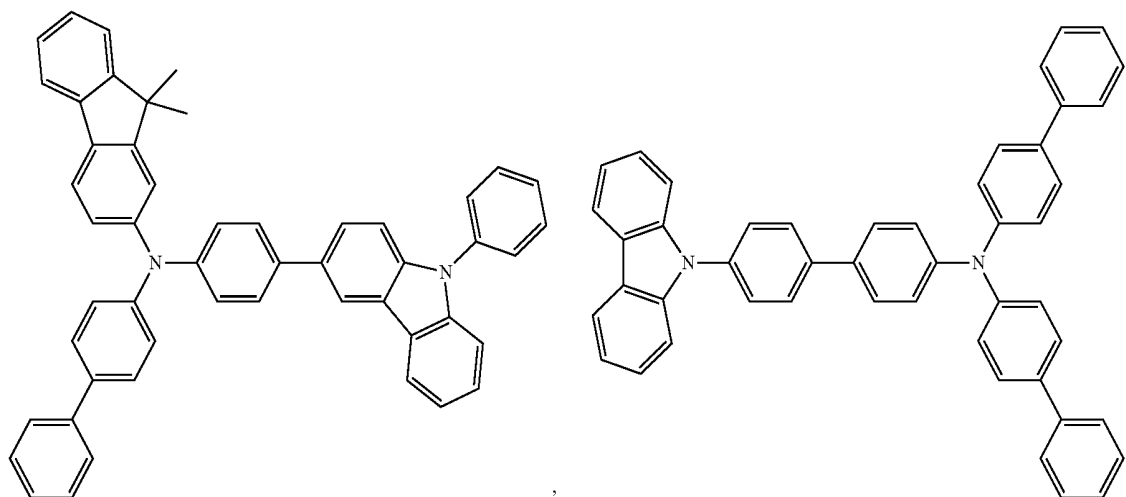
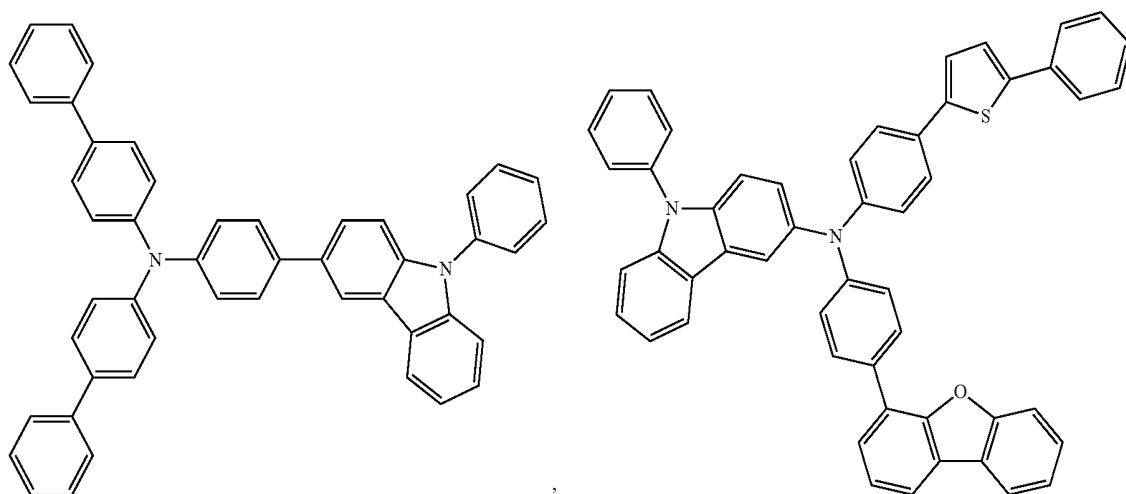
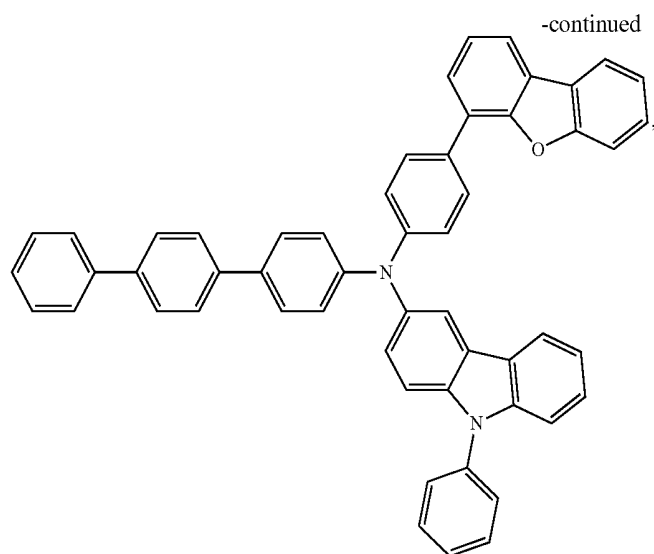


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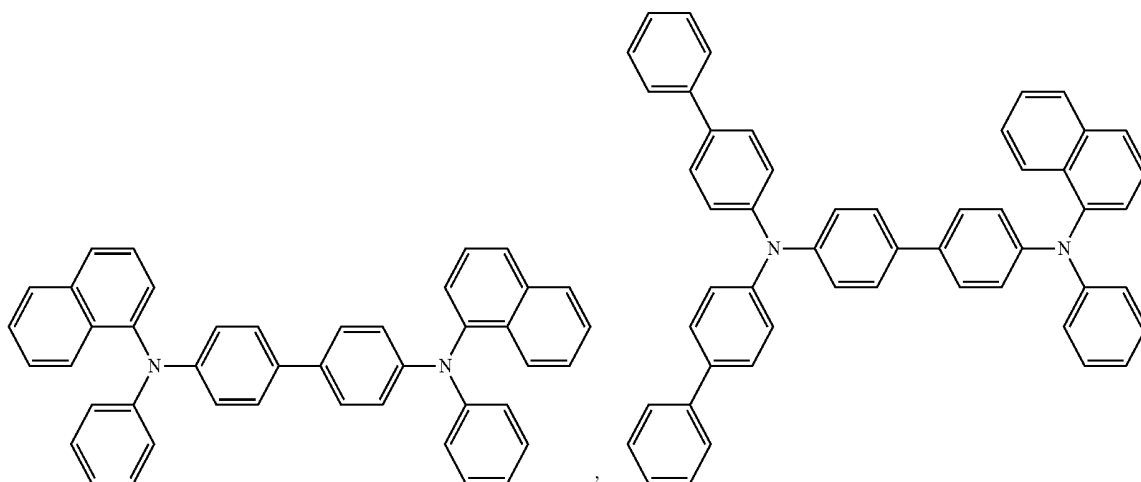
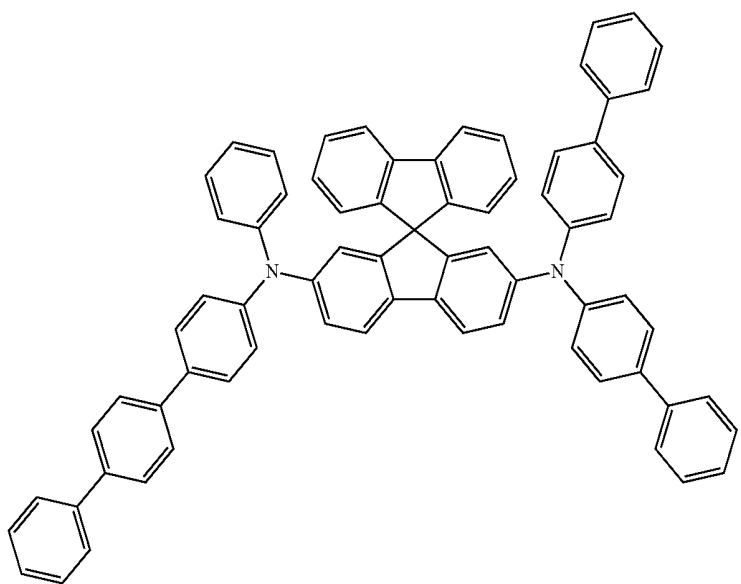
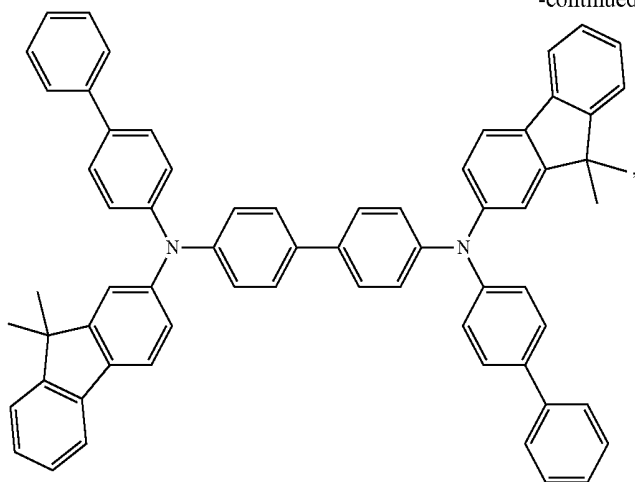


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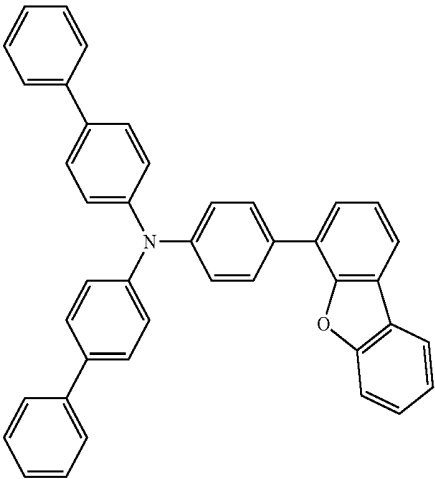
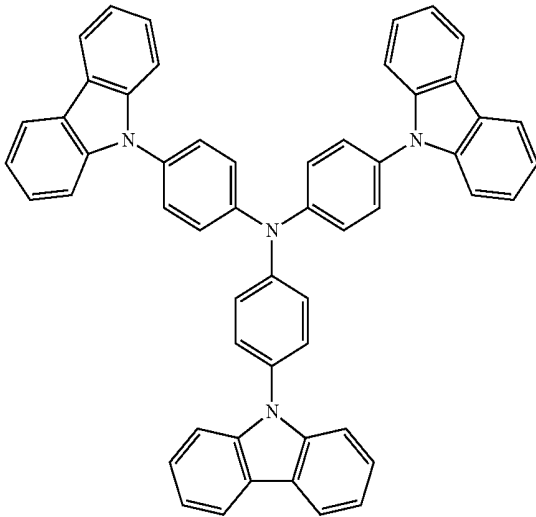
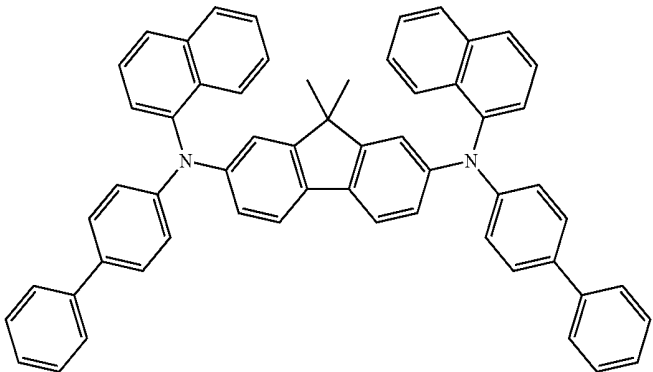
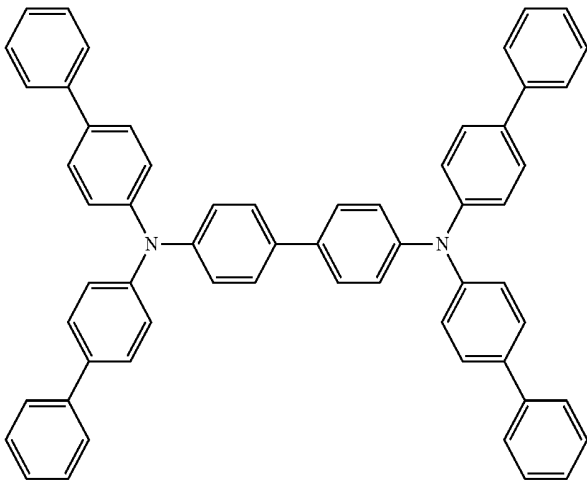


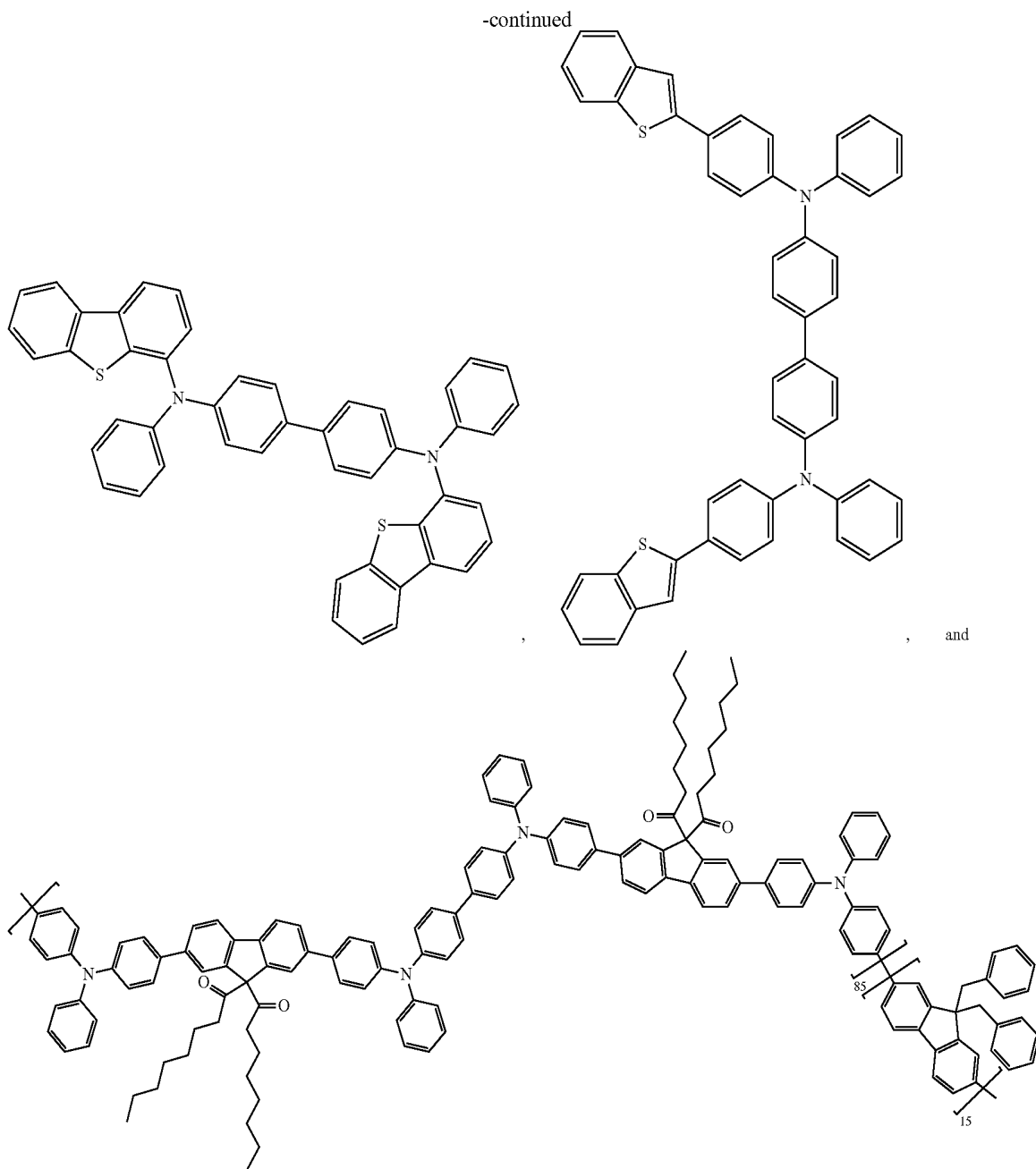


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EBL:

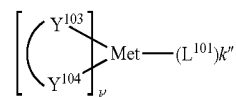
[0118] An electron blocking layer (EBL) may be used to reduce the number of electrons and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies, and/or longer lifetime, as compared to a similar device lacking a blocking 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.

Host:

[0119] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal

complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. Any host material may be used with any dopant so long as the triplet criteria is satisfied.

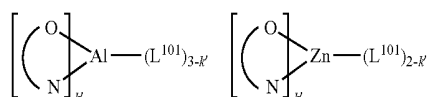
[0120] Examples of metal complexes used as host are preferred to have the following general formula:



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 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.

[0121] In one aspect, the metal complexes are:

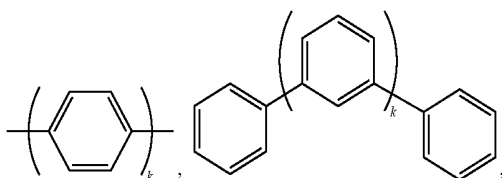


wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

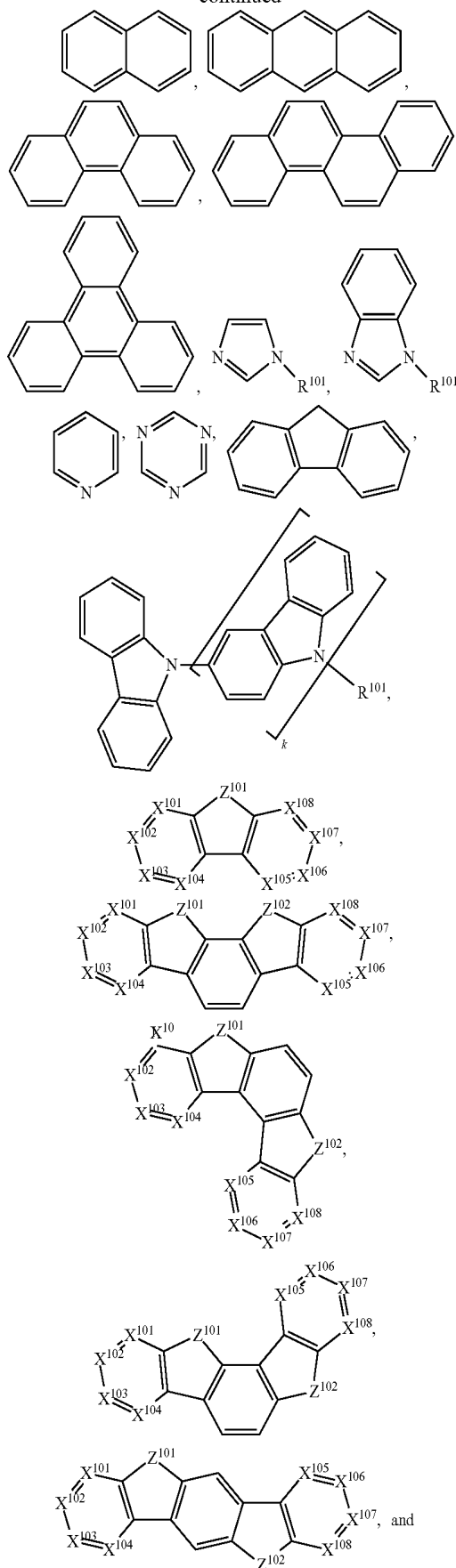
[0122] In another aspect, Met is selected from Ir and Pt. In a further aspect, $(Y^{103}-Y^{104})$ is a carbene ligand.

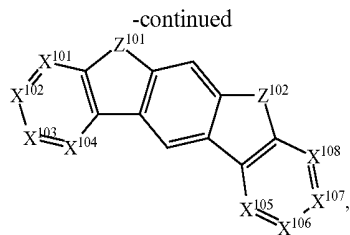
[0123] In one aspect, the host compound contains at least one of the following groups selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, 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, quinoxaline, 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 option within each group 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.

[0124] In one aspect, the host compound contains at least one of the following groups in the molecule:



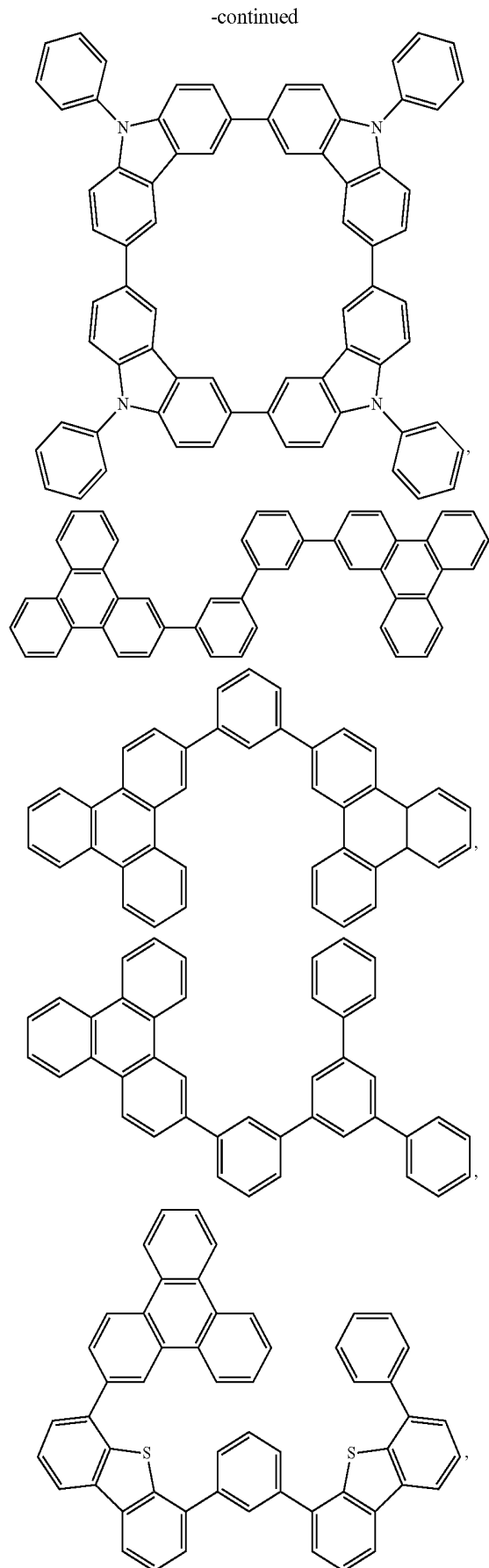
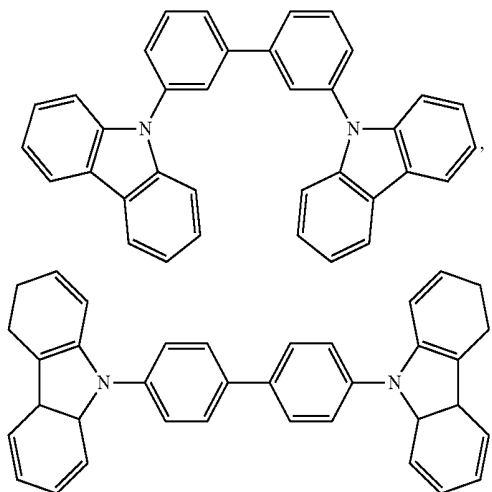
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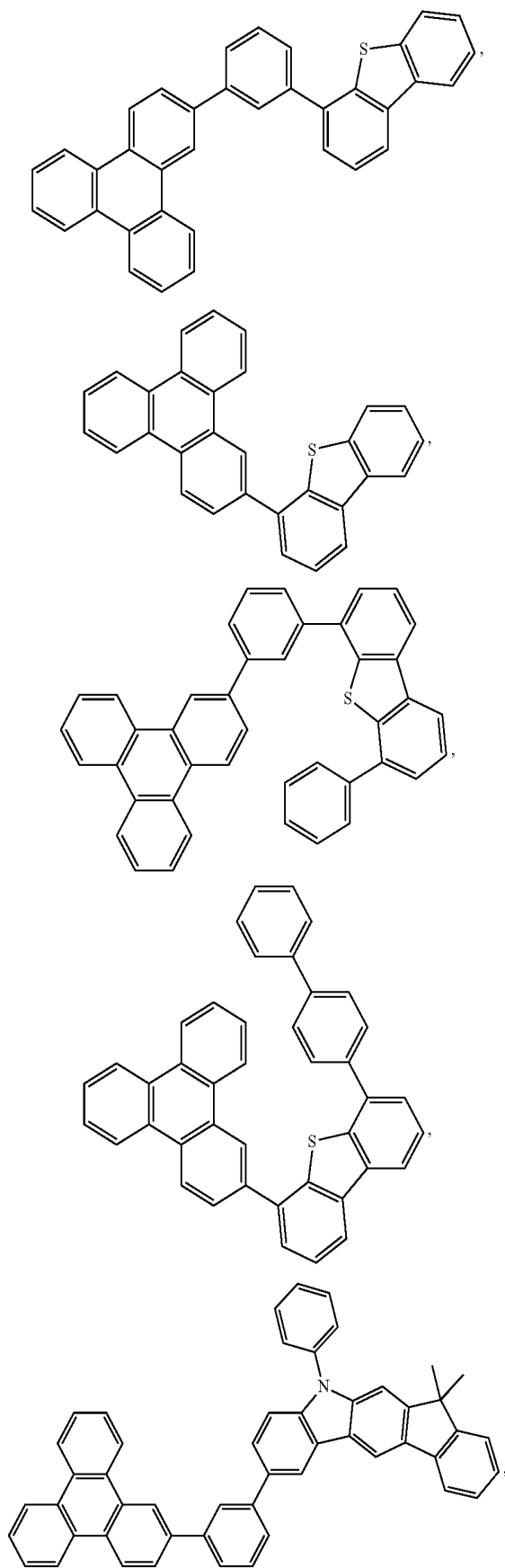


wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, and 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.

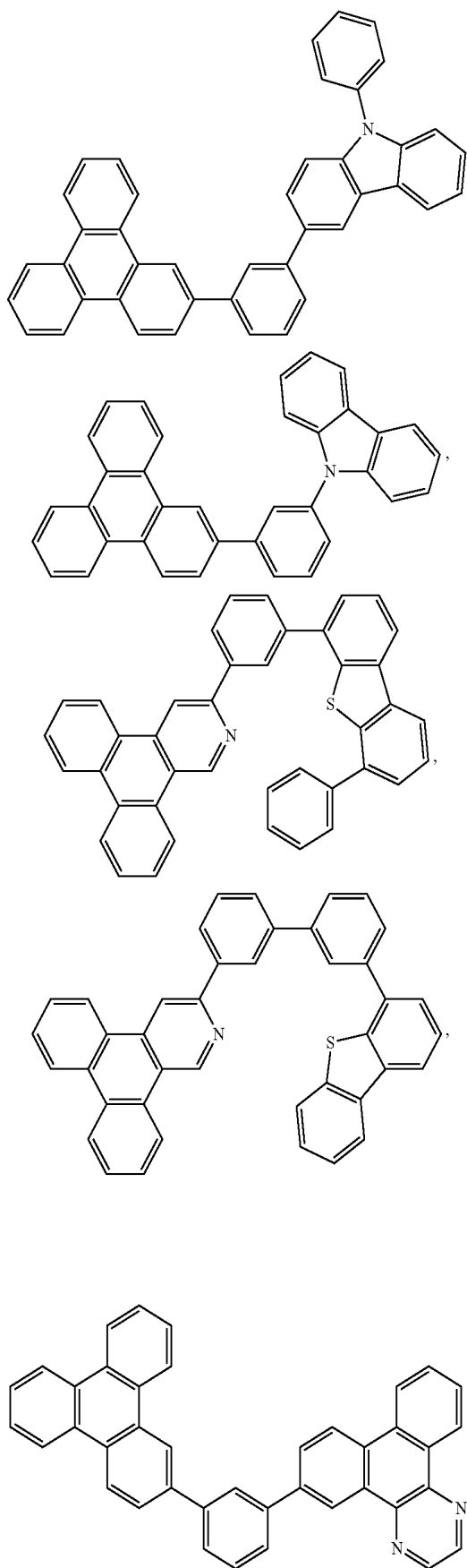
[0125] Non-limiting examples of the host materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: EP2034538, EP2034538A, EP2757608, JP2007254297, KR20100079458, KR20120088644, KR20120129733, KR20130115564, 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,



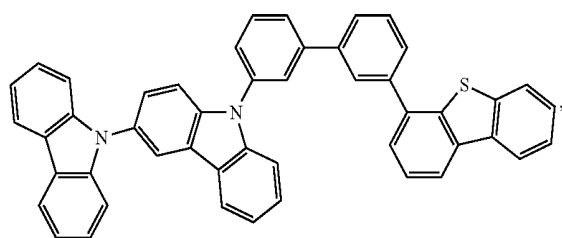
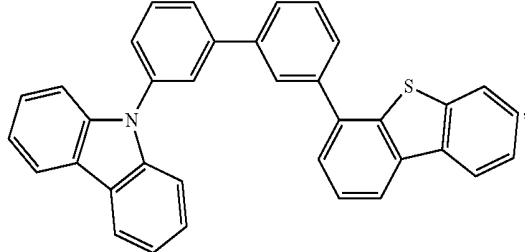
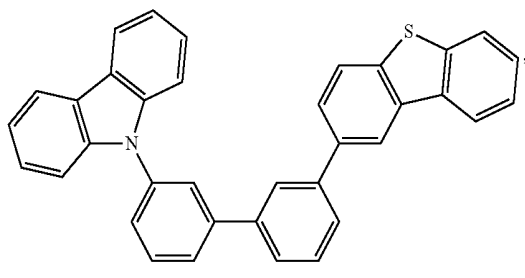
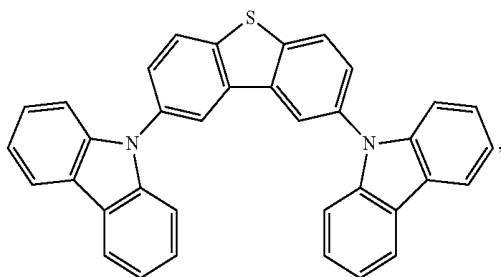
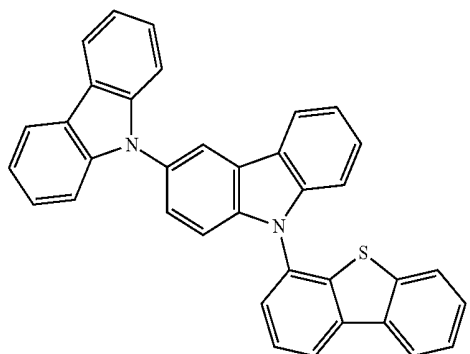
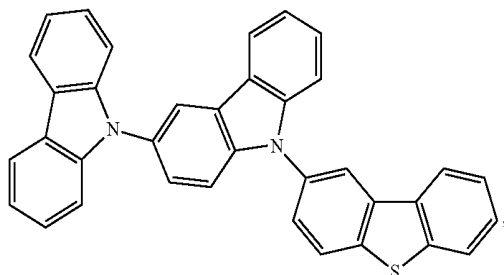
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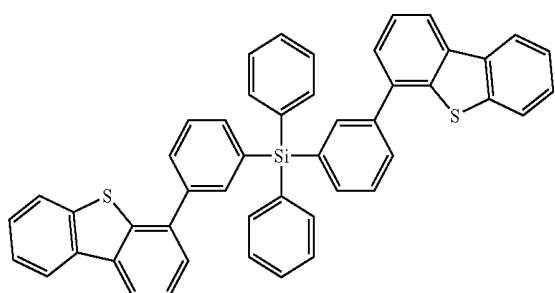
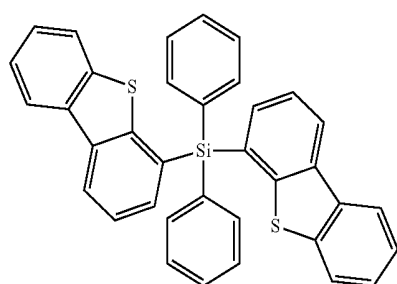
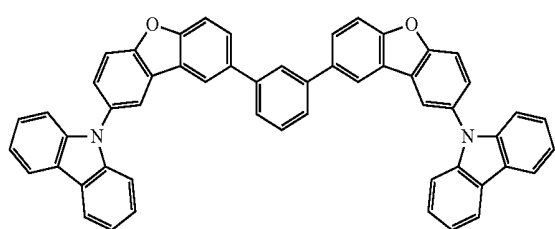
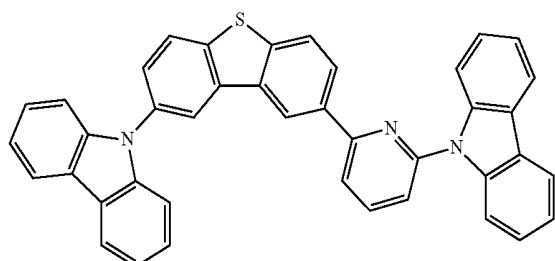
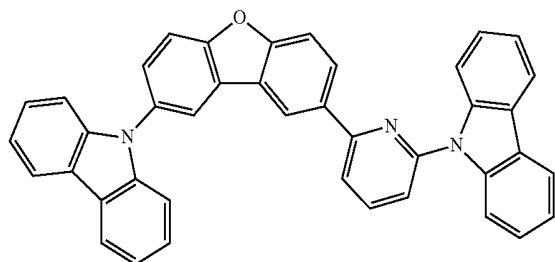
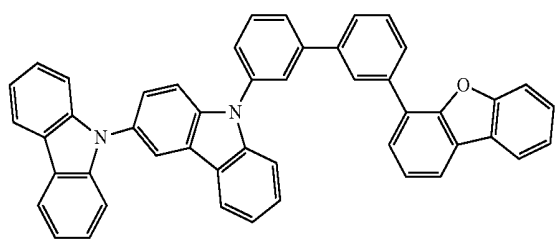
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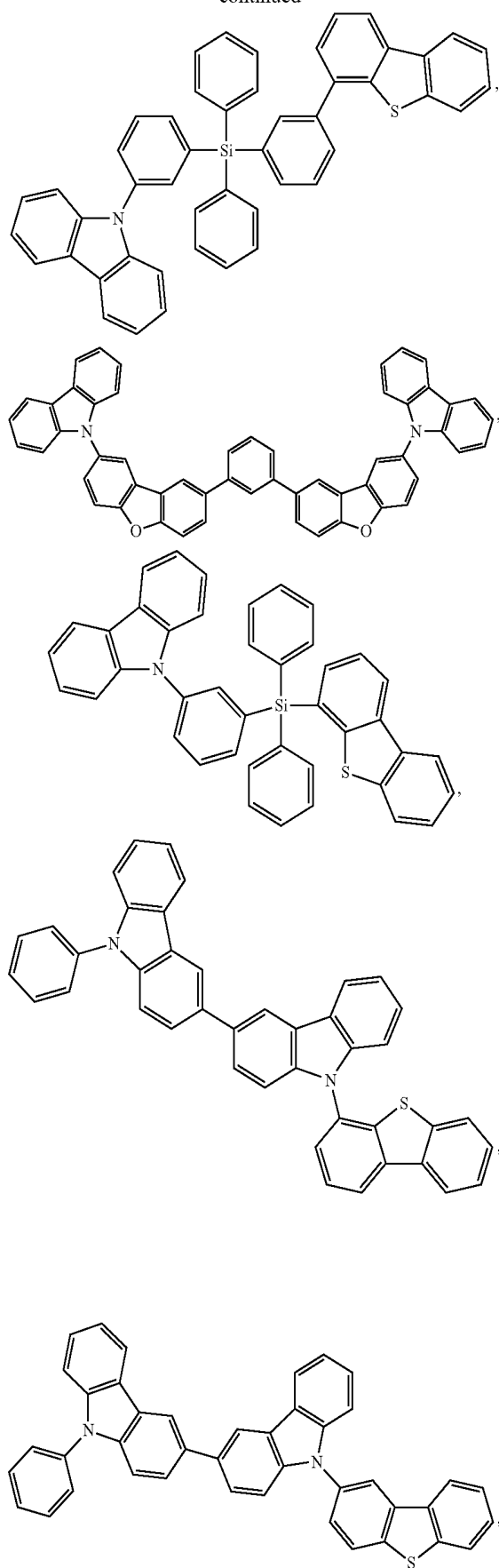
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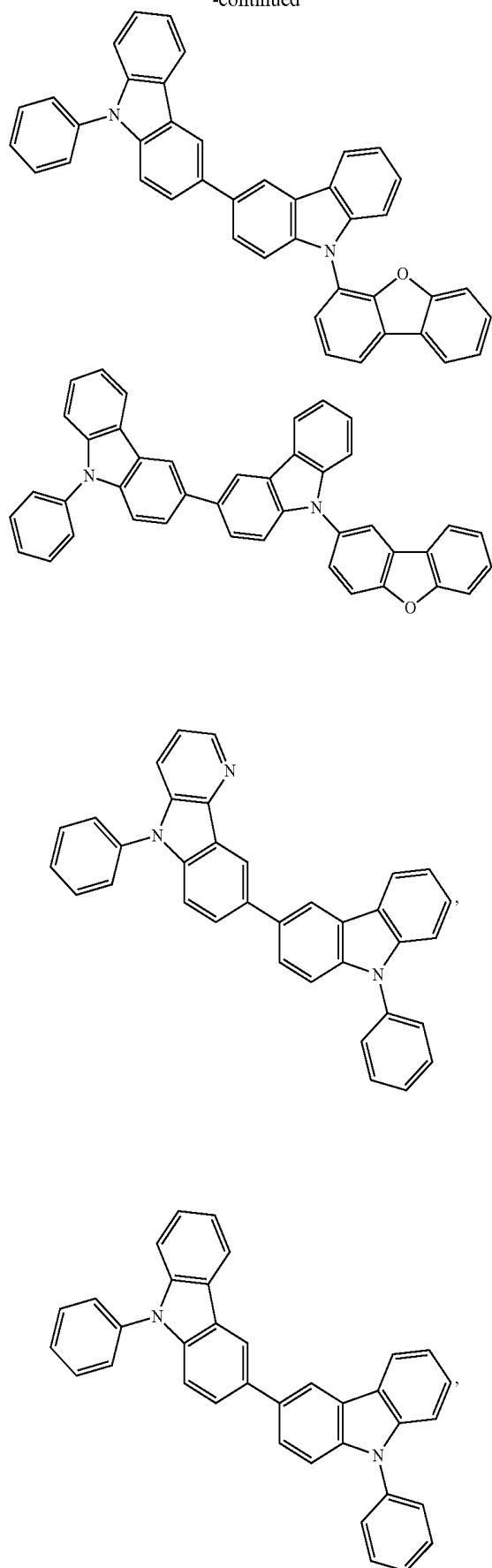
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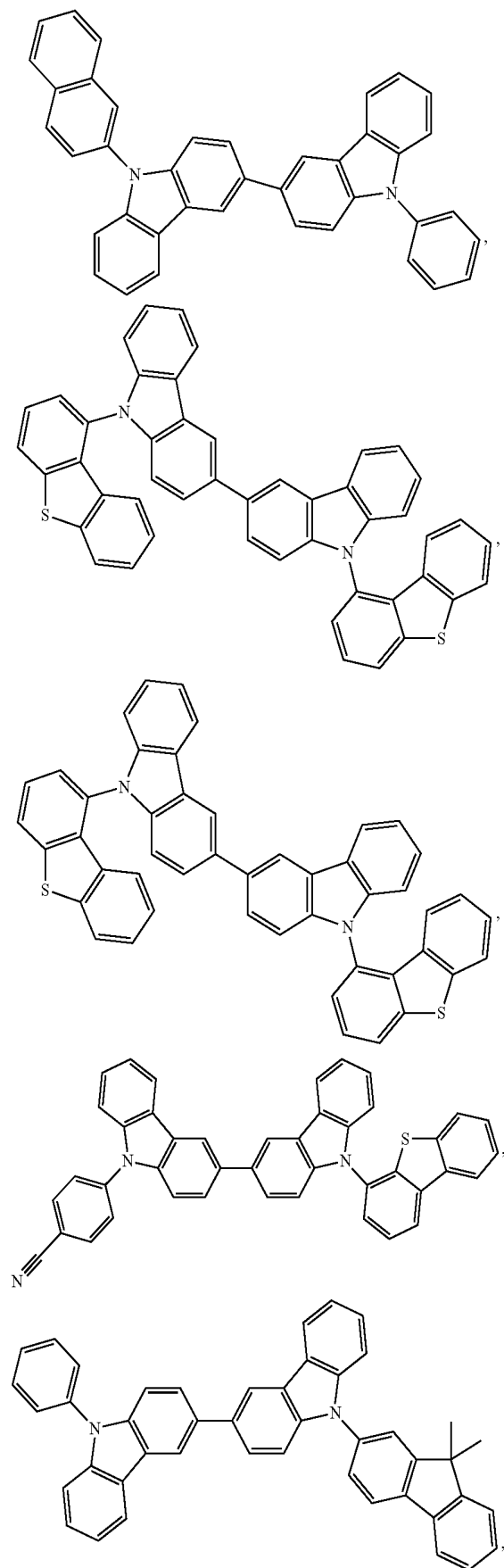
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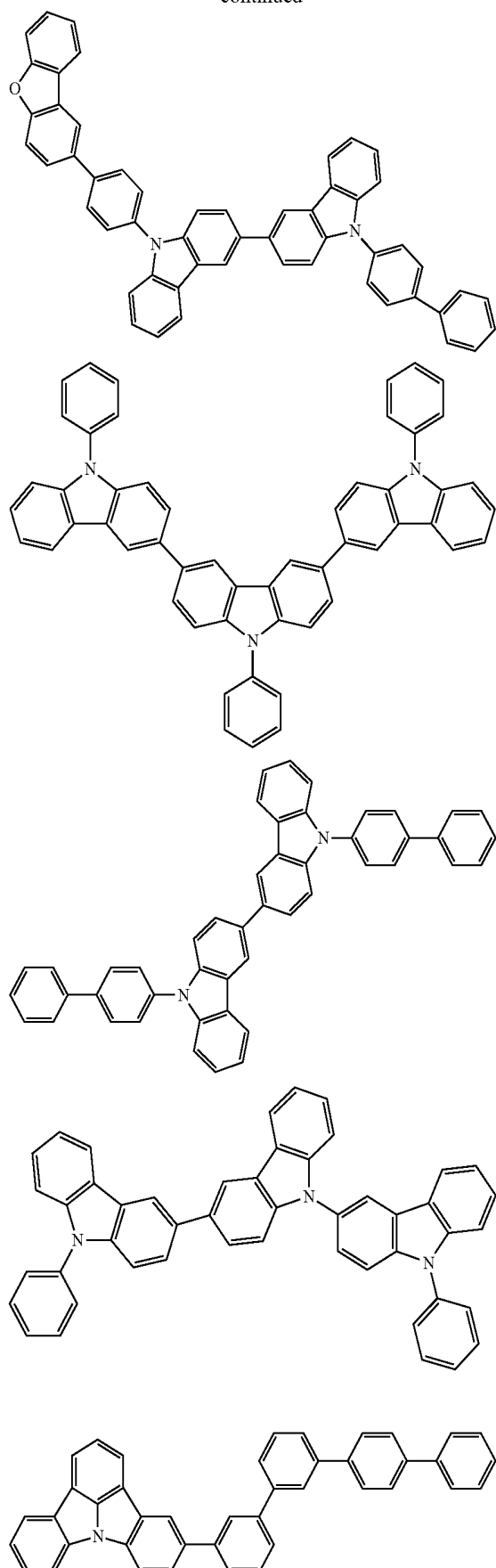
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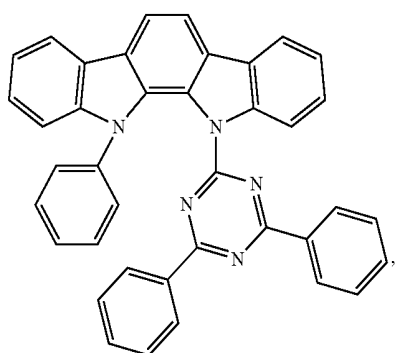
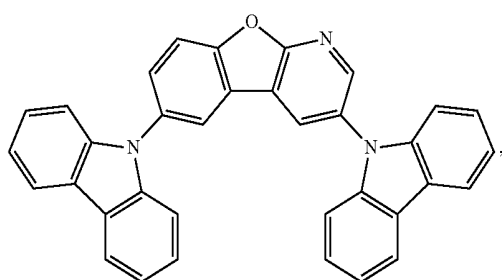
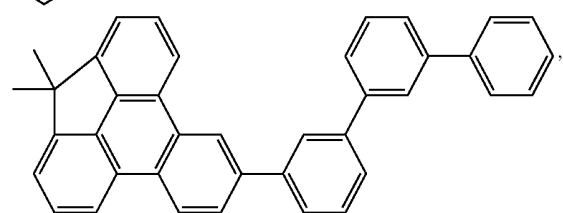
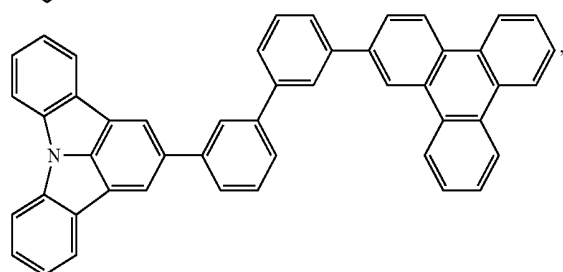
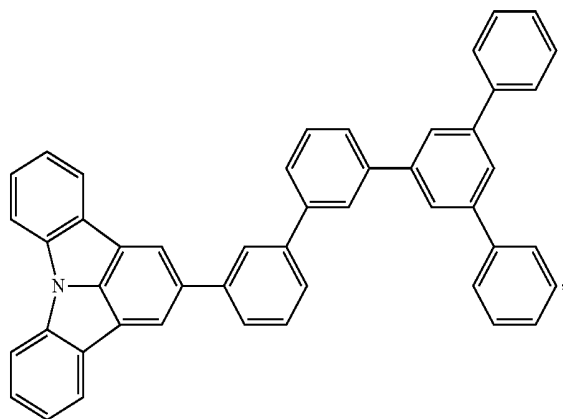
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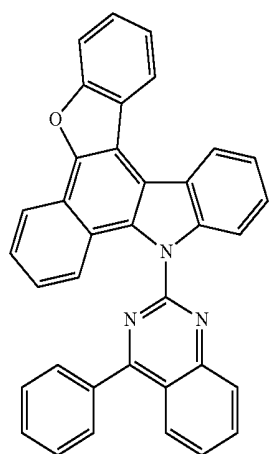
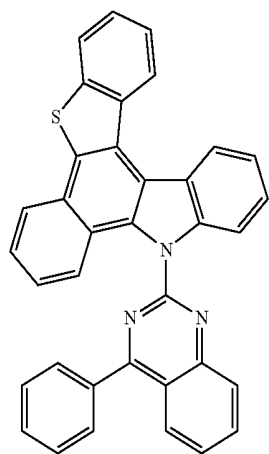
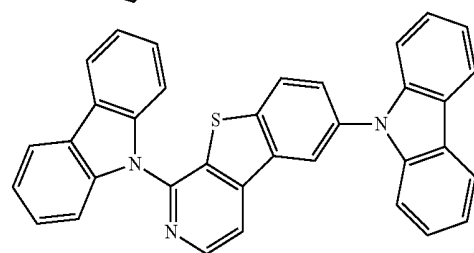
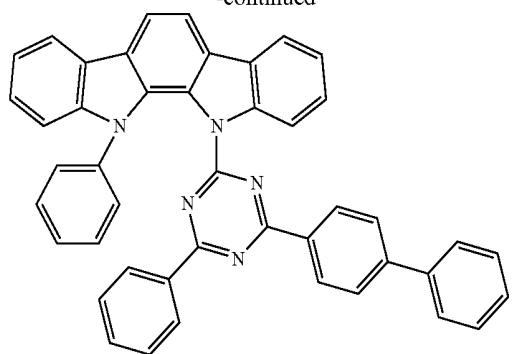
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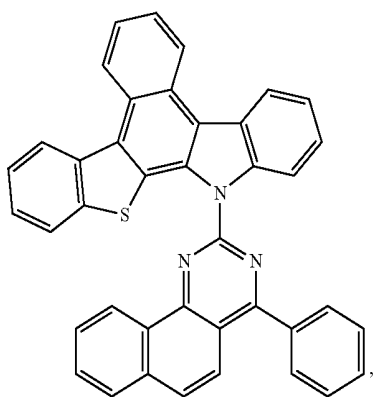
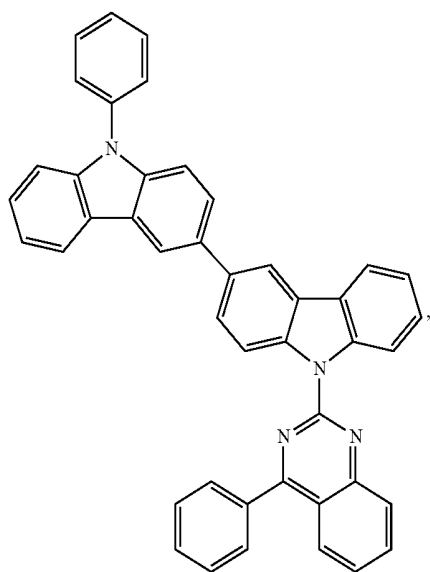
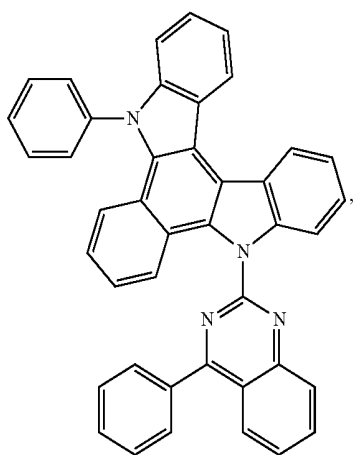
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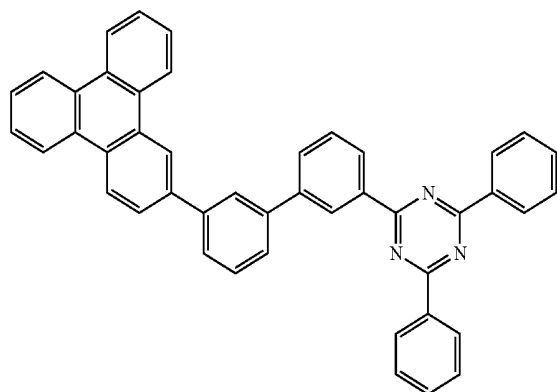
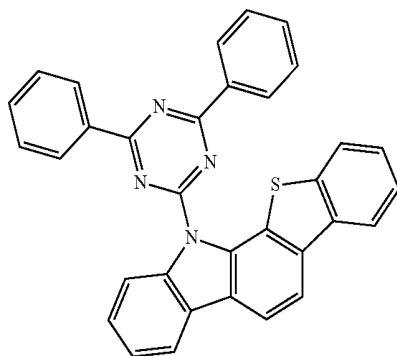
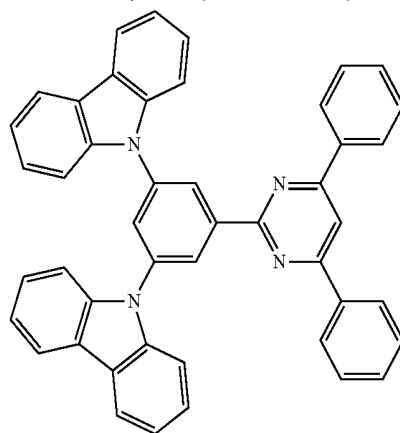
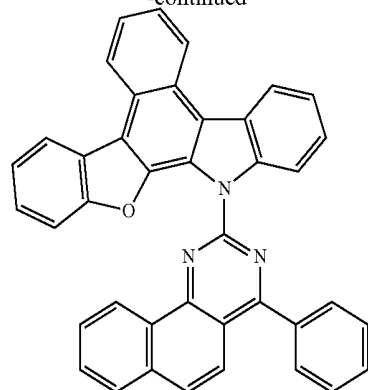
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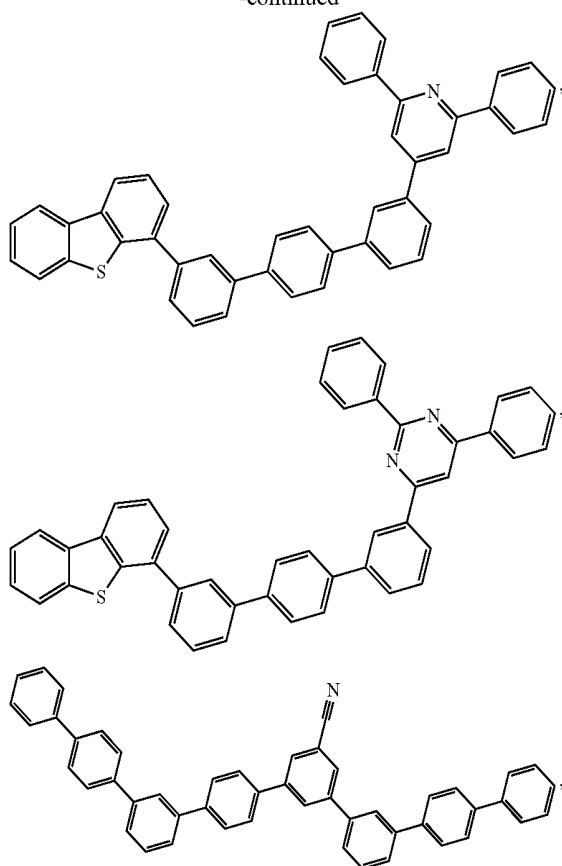
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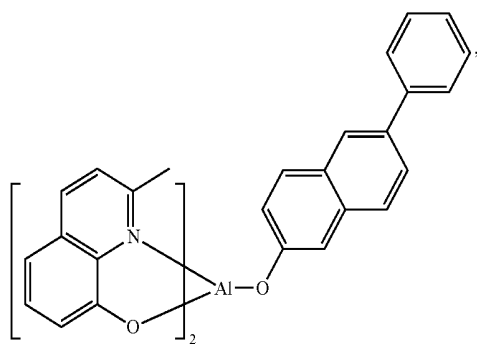
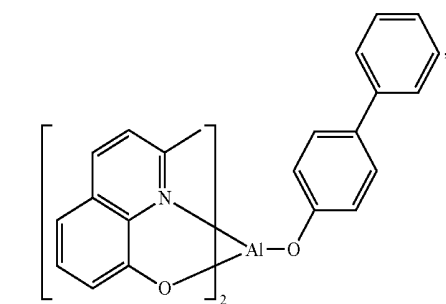
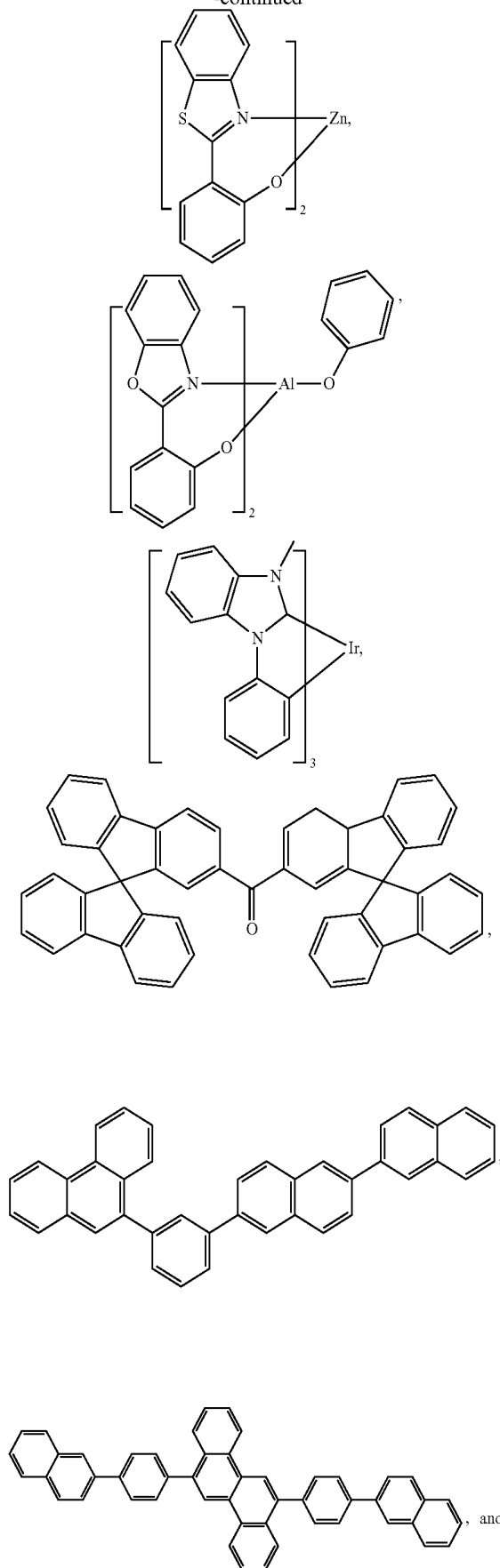
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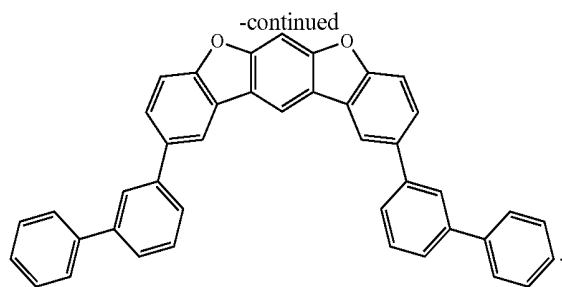
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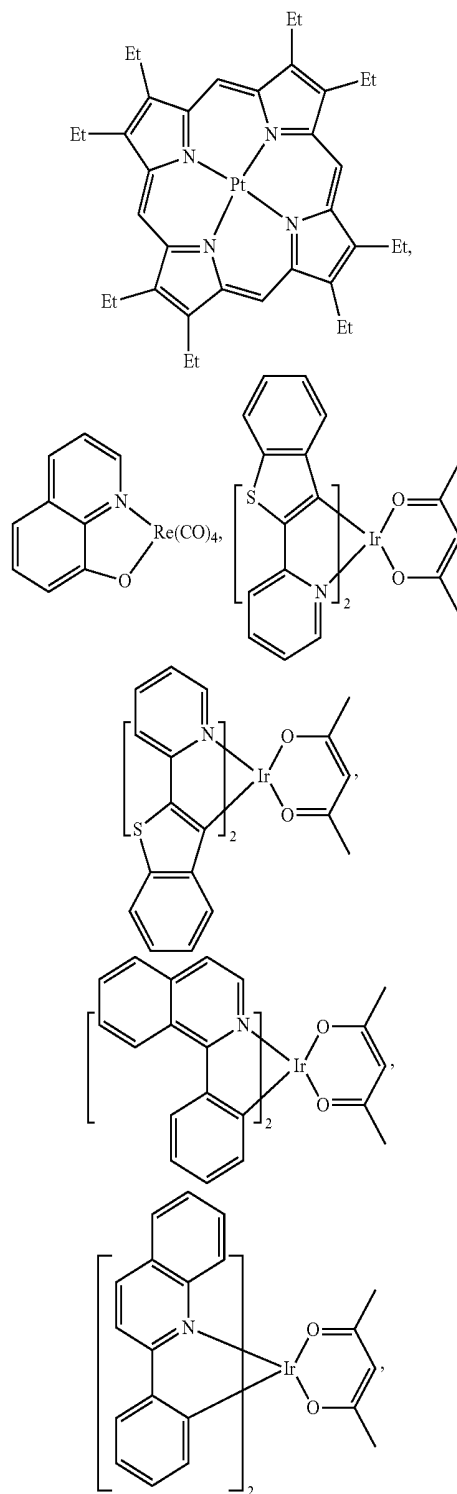


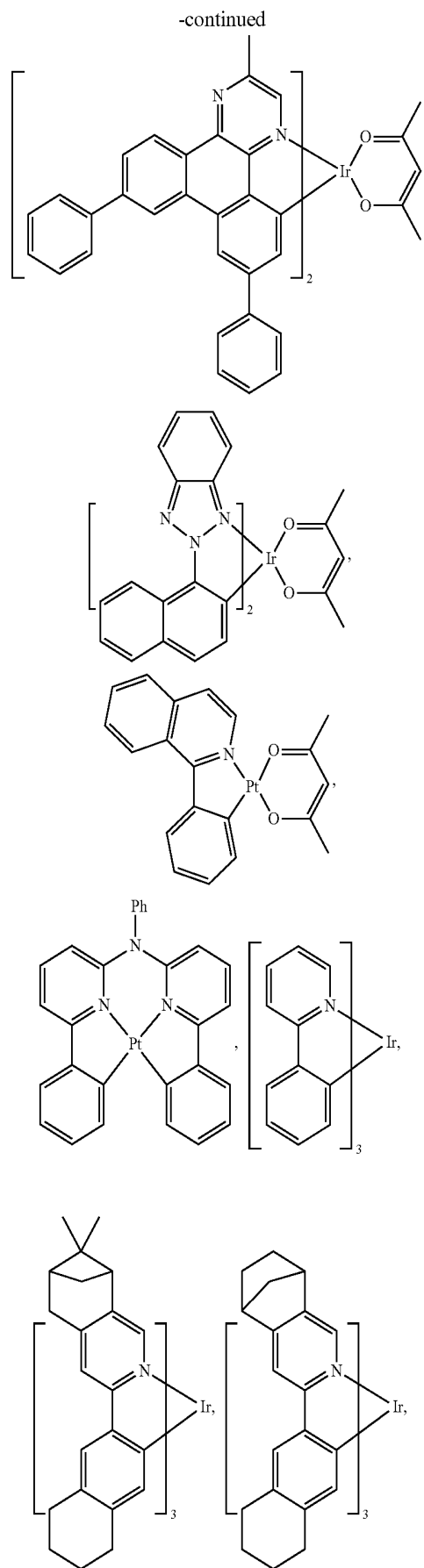
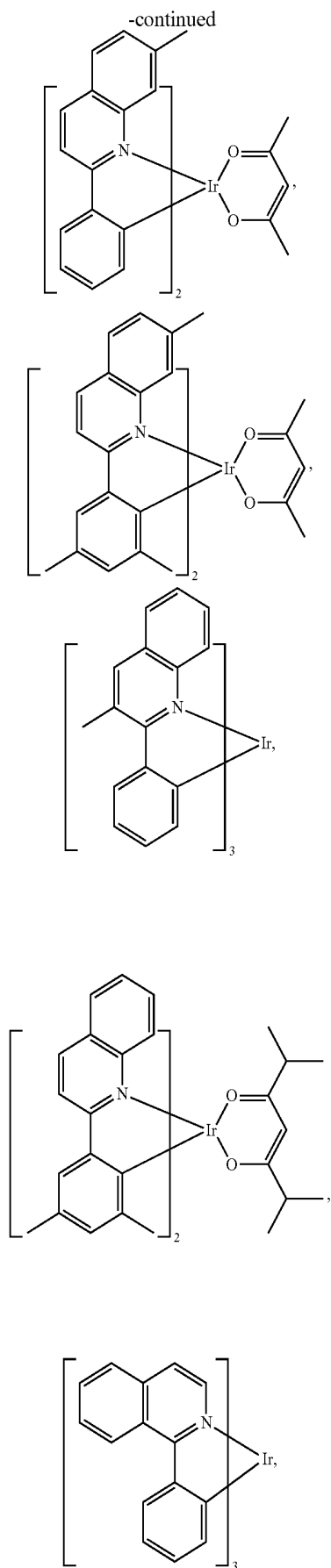
Additional Emitters:

[0126] One or more additional emitter dopants may be used in conjunction with the compound of the present disclosure. Examples of the additional emitter dopants are not particularly limited, and any compounds may be used as long as the compounds are typically used as emitter materials. 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), triplet-triplet annihilation, or combinations of these processes.

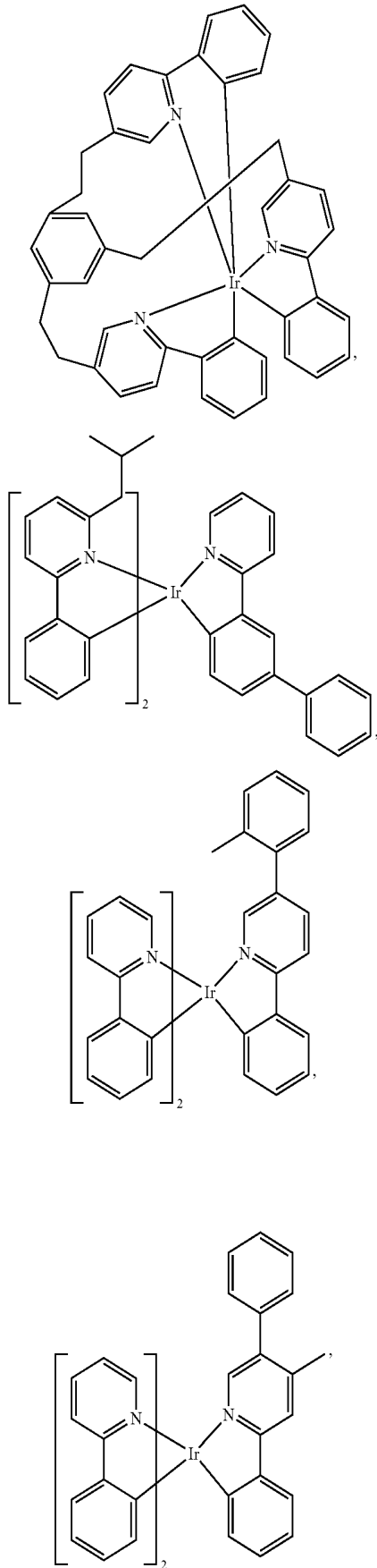
[0127] Non-limiting examples of the emitter materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103694277, CN1696137, EB01238981, EP01239526, EP01961743, EP1239526, EP1244155, EP1642951, EP1647554, 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,

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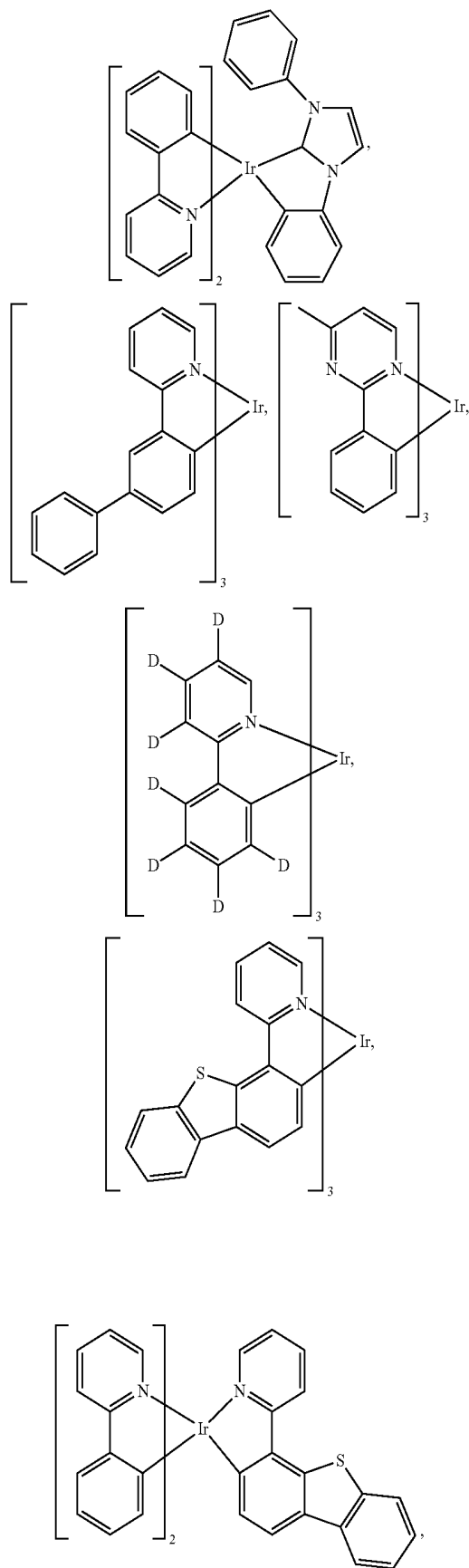


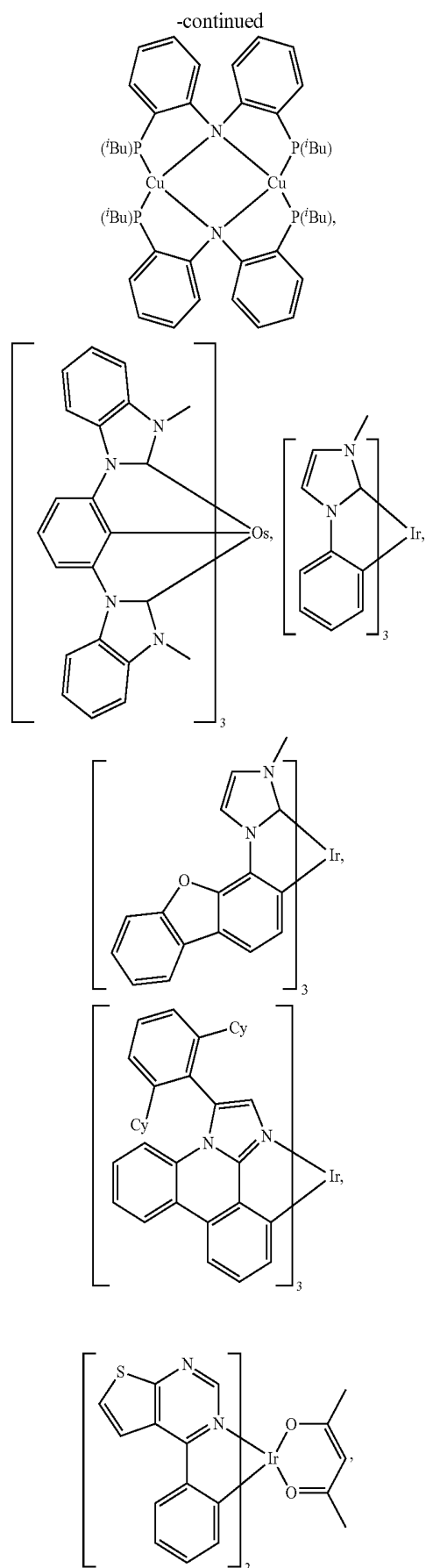
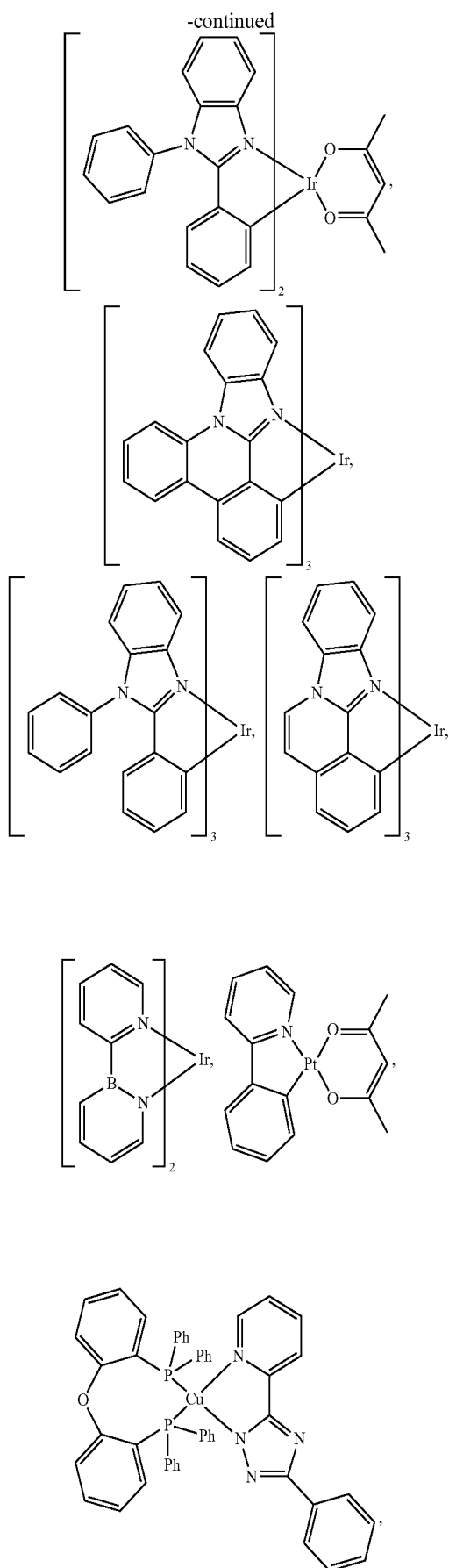


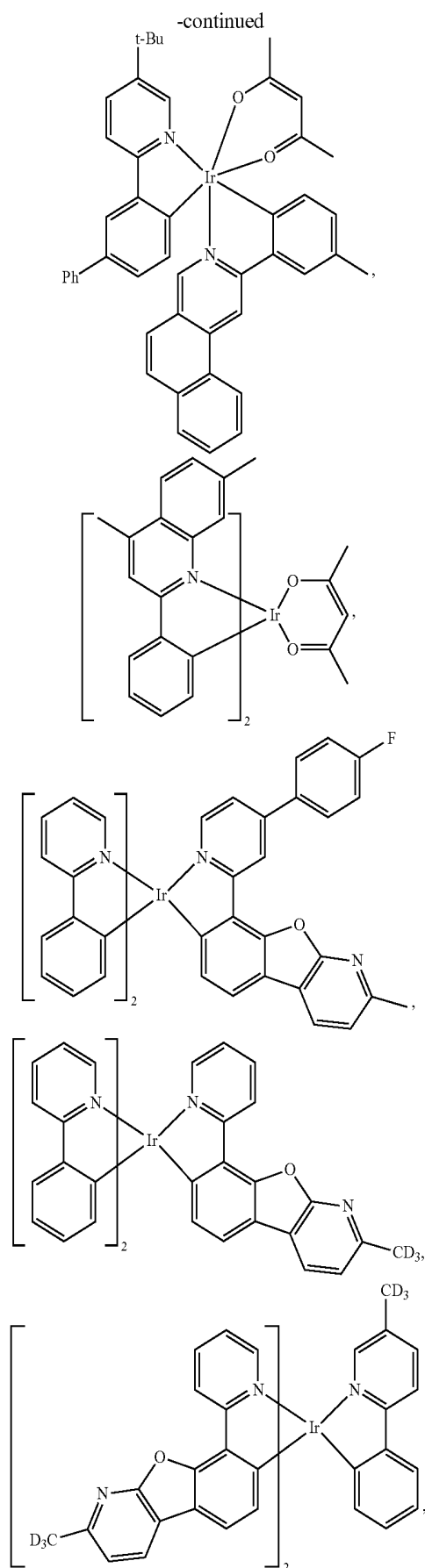
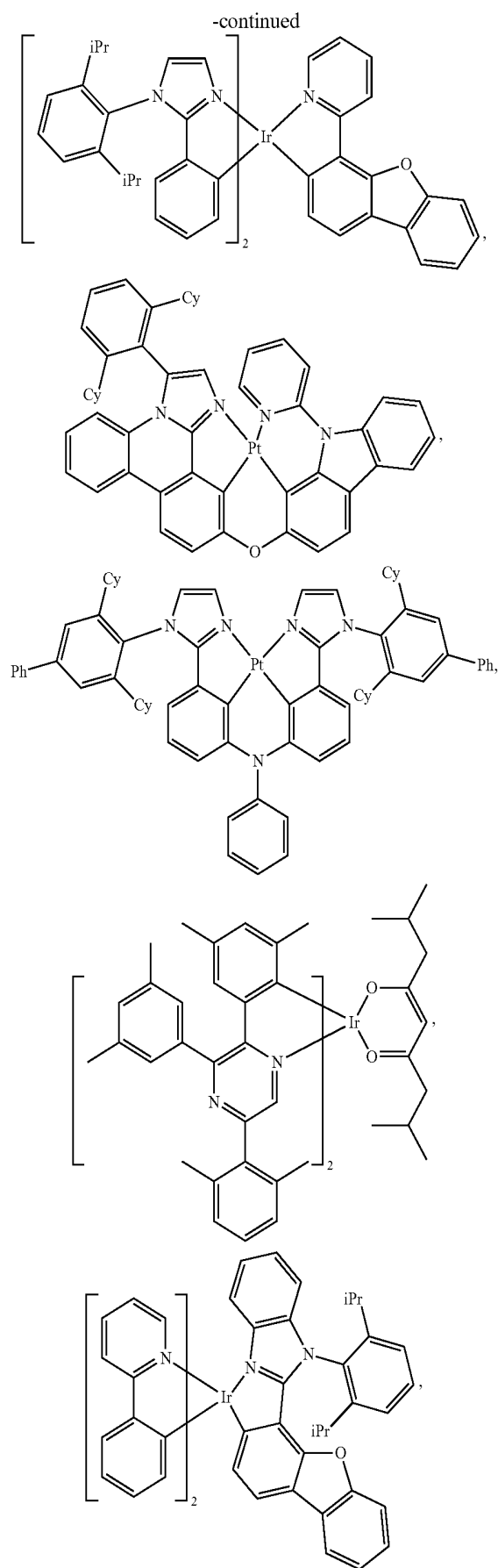
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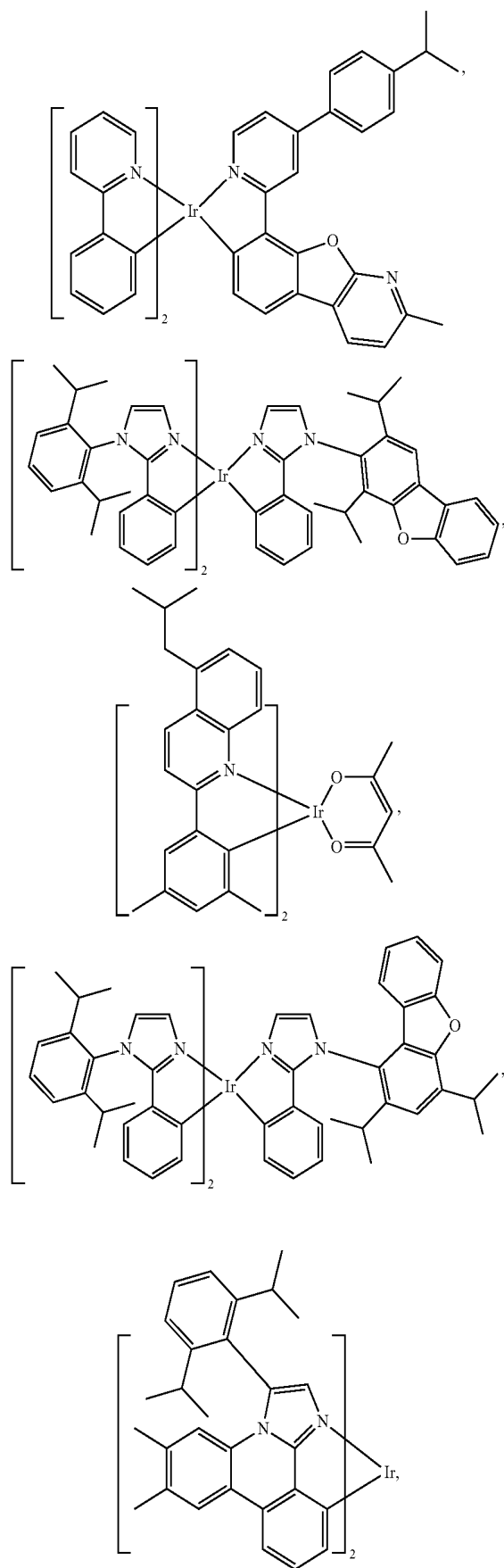
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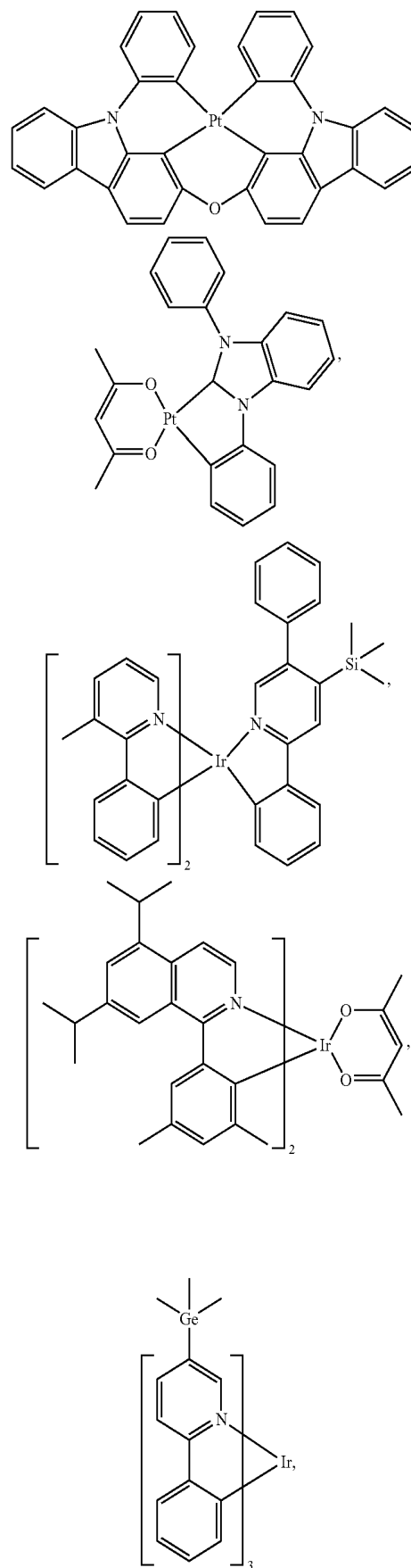




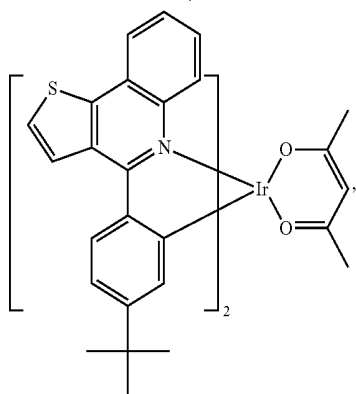
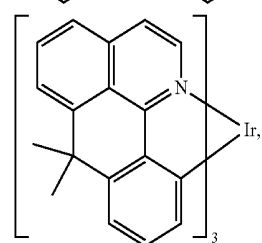
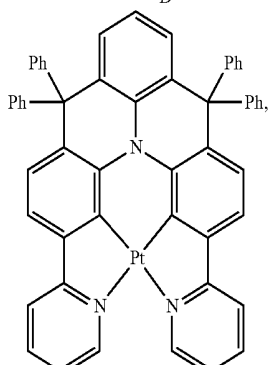
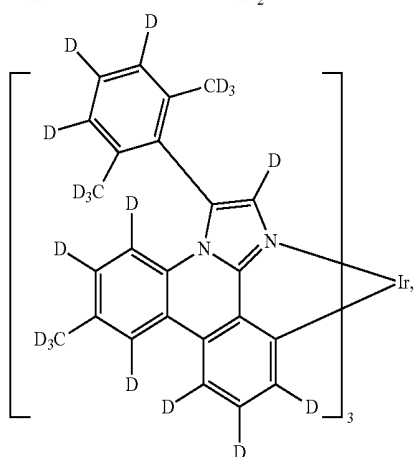
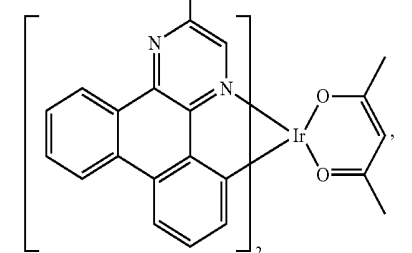
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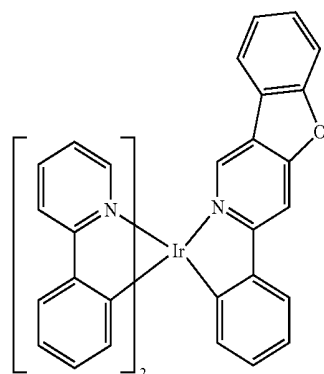
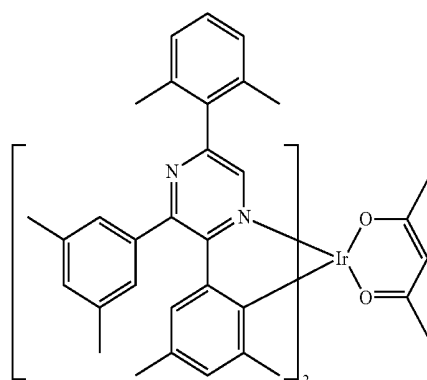
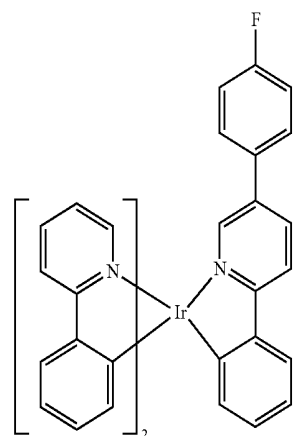
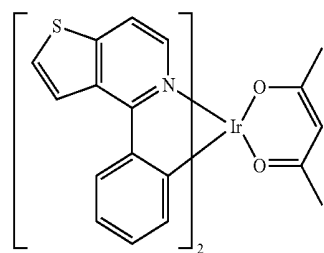
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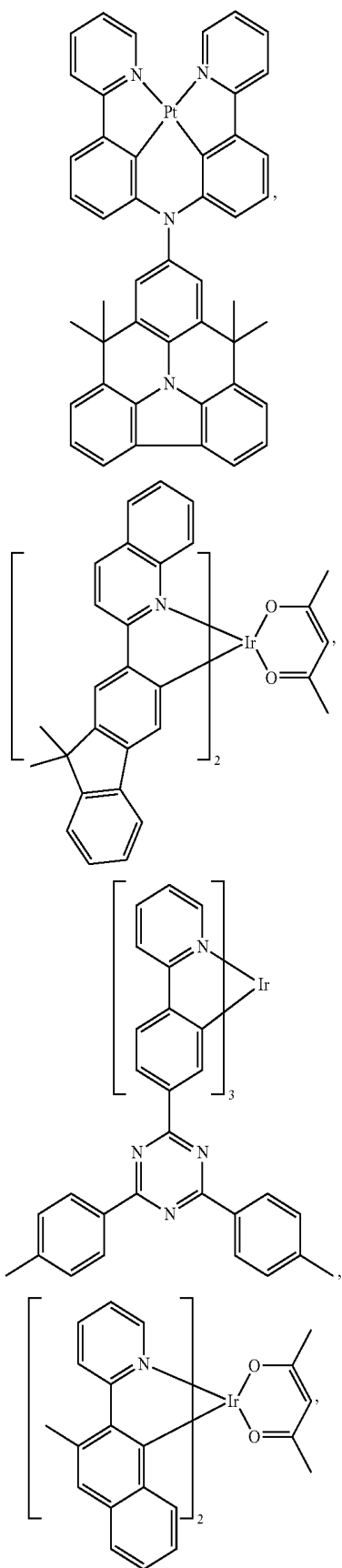
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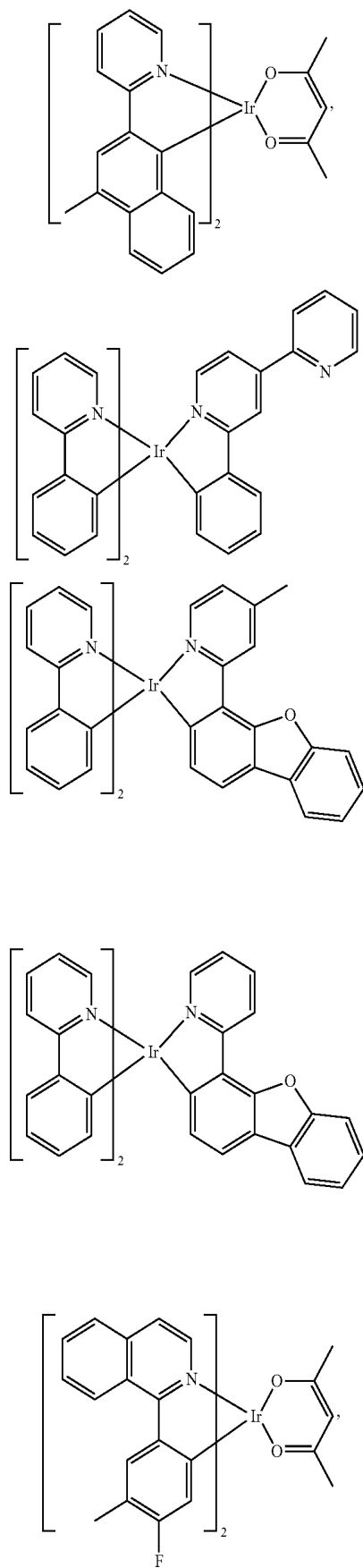
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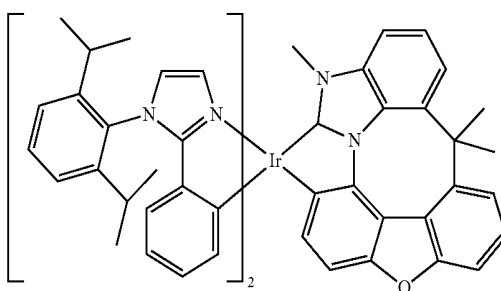
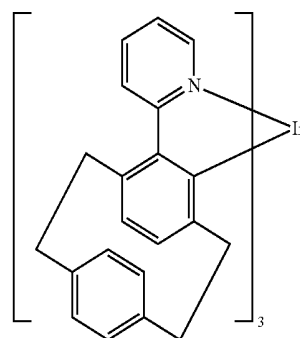
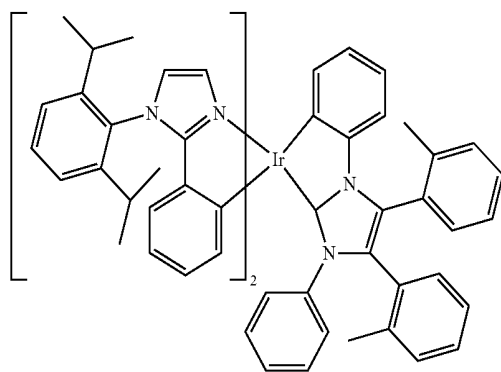
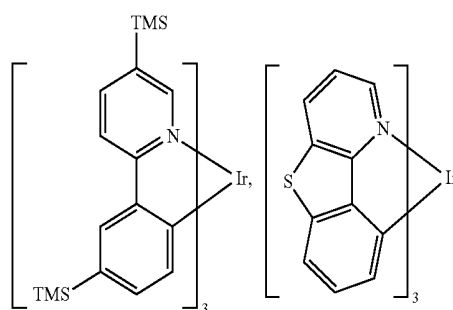
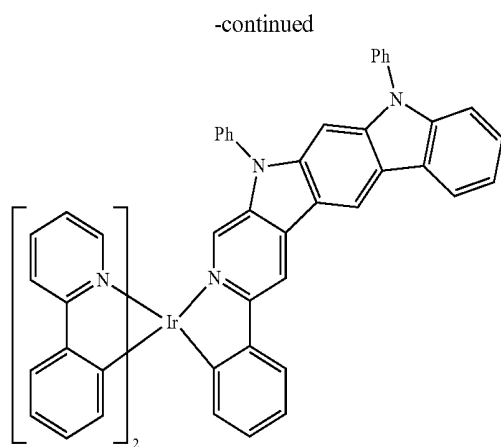
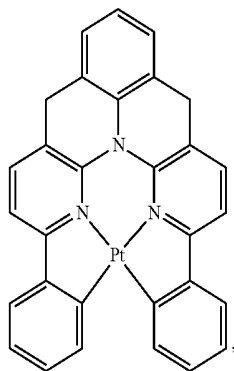
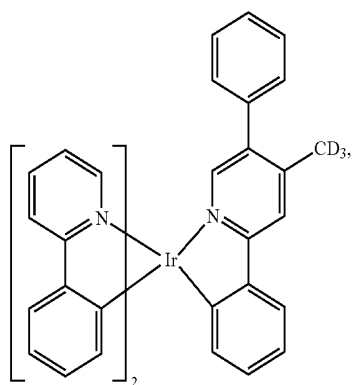
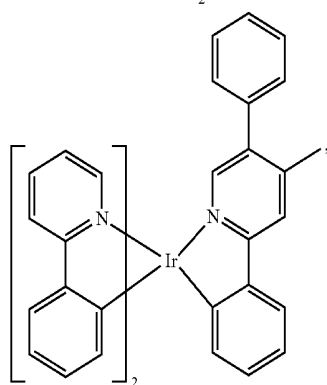
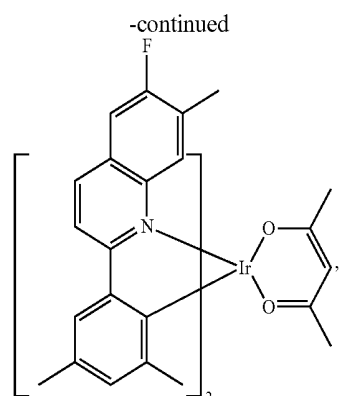


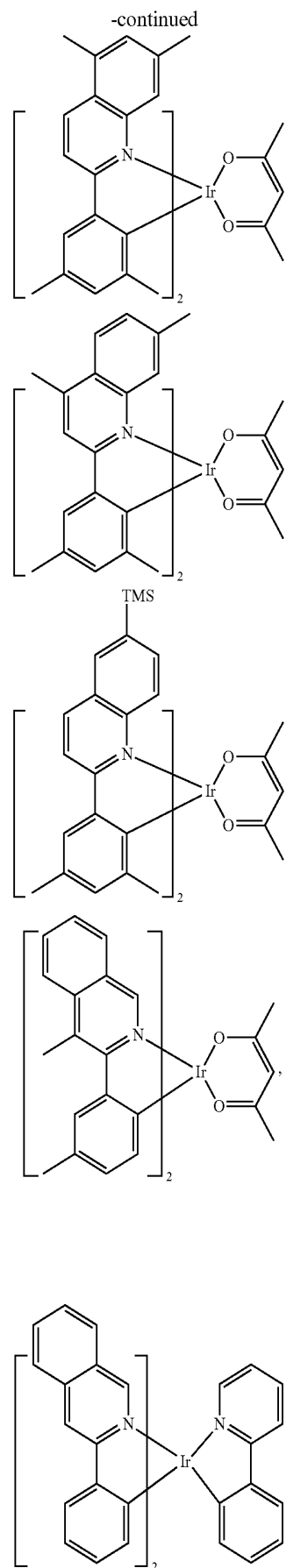
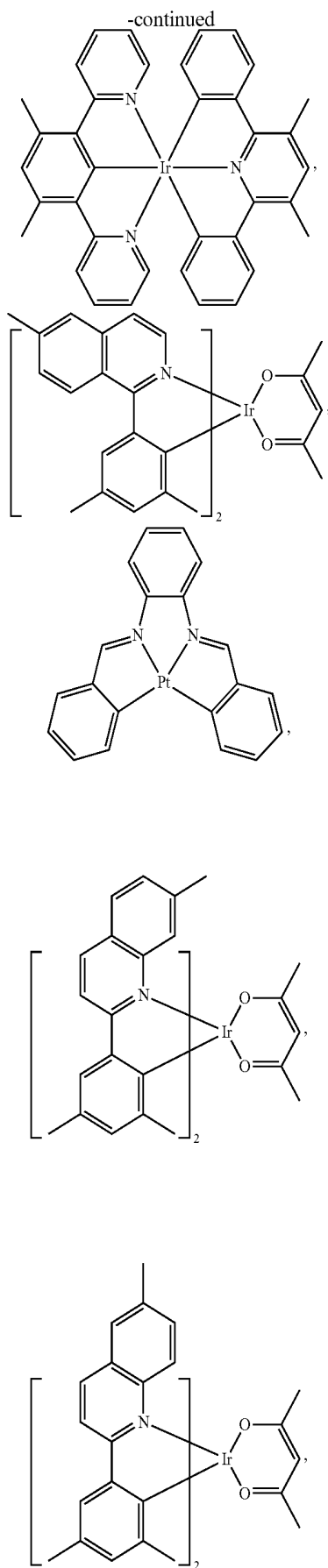
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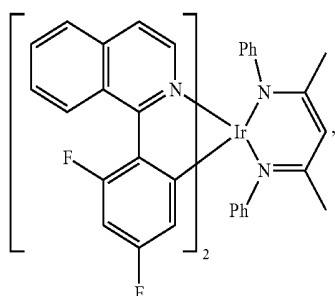
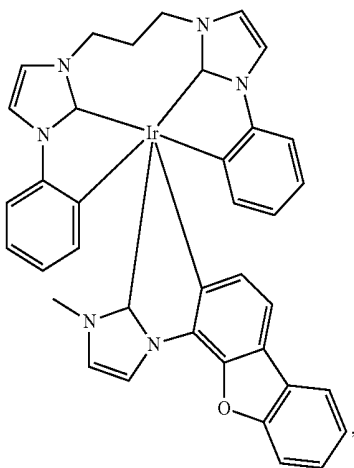
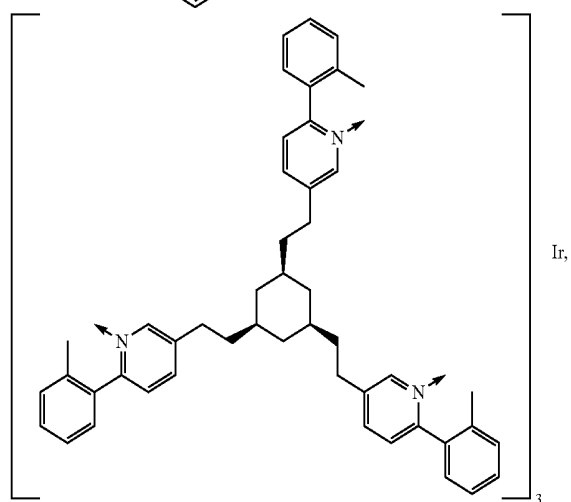
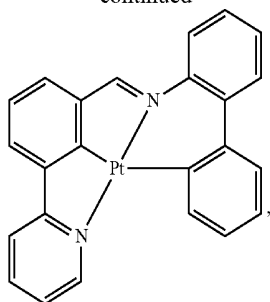
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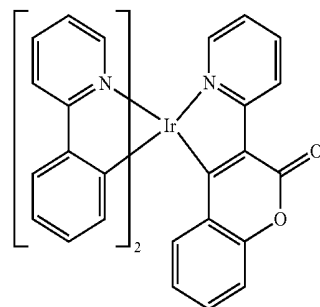
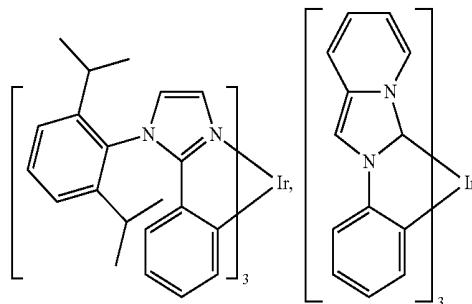
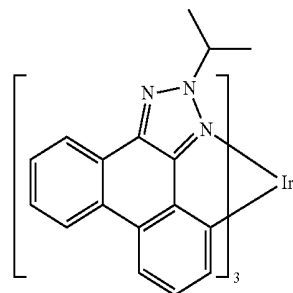
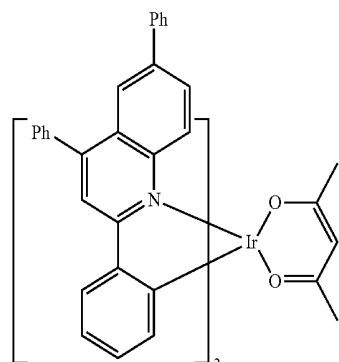
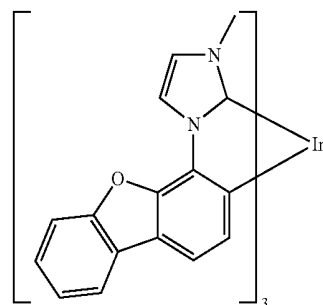


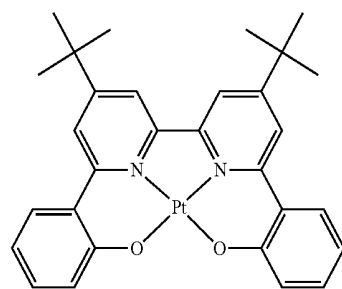
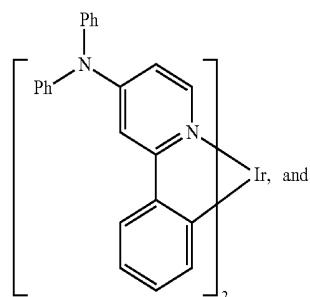
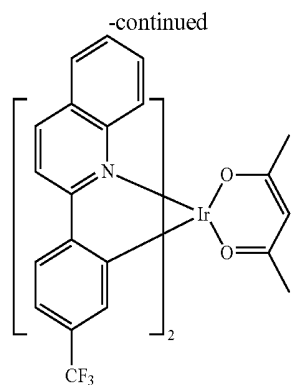
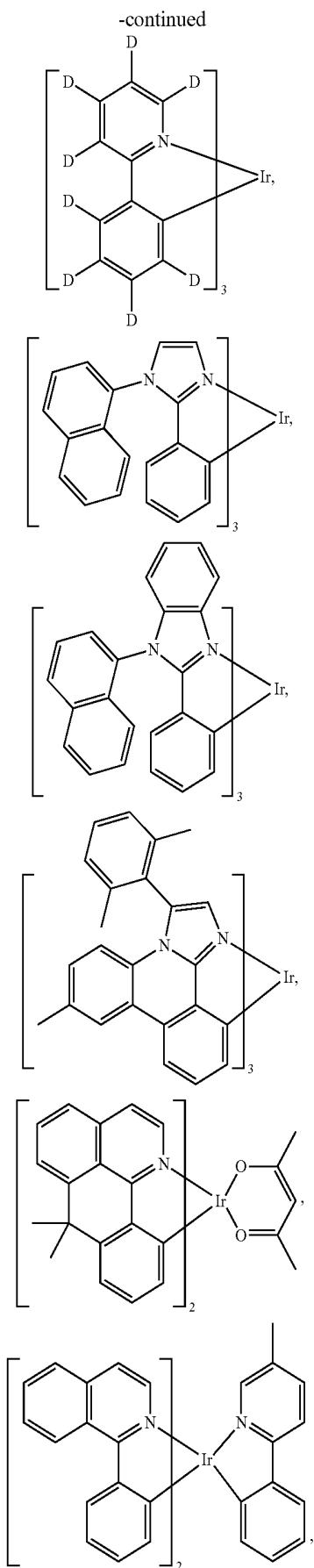


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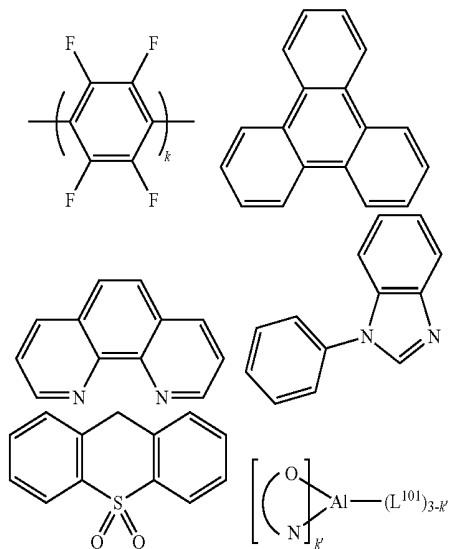


HBL:

[0128] 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.

[0129] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

[0130] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

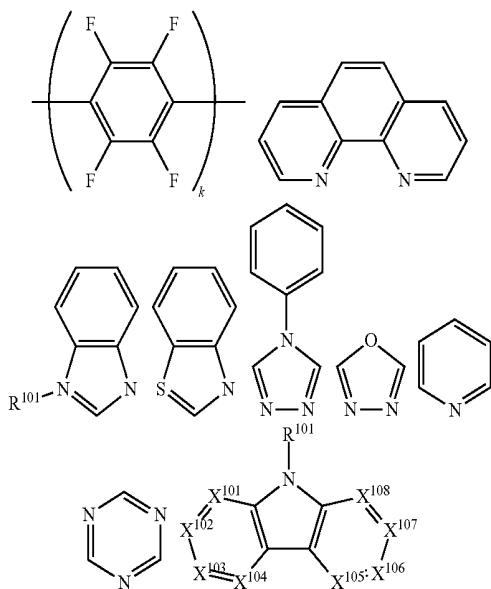


wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

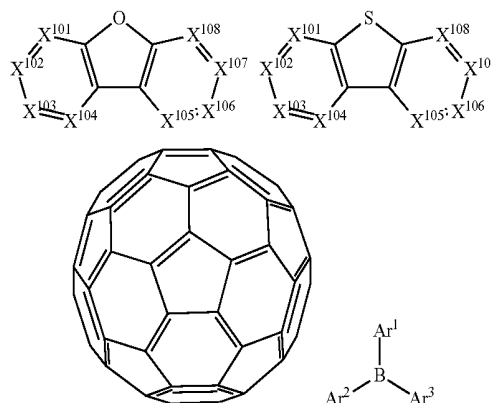
ETL:

[0131] 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.

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

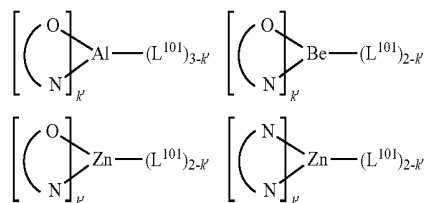


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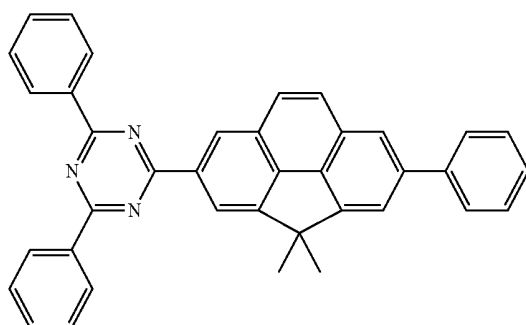
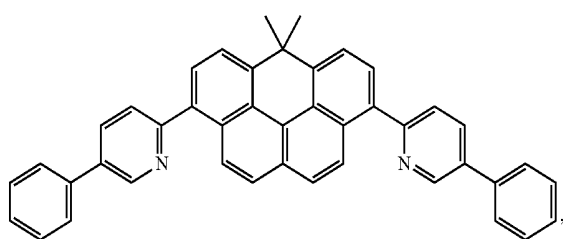
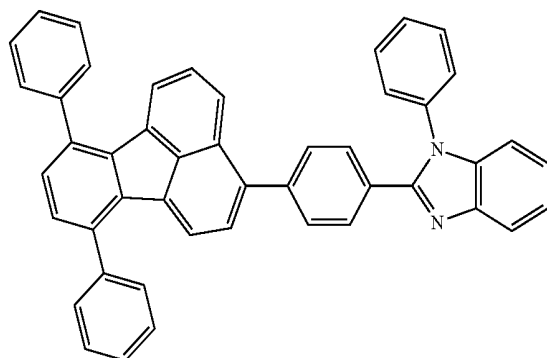
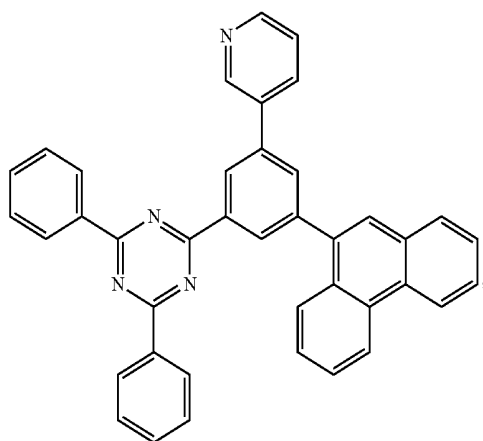
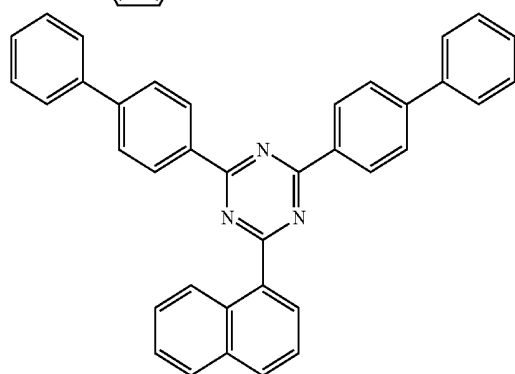
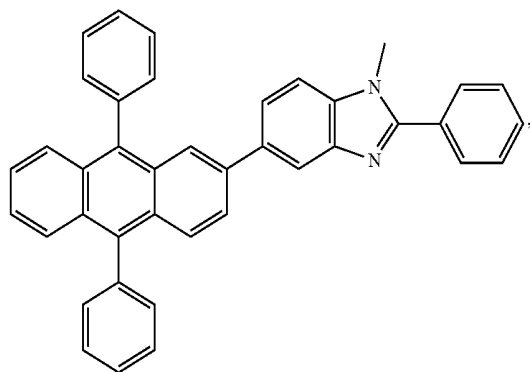
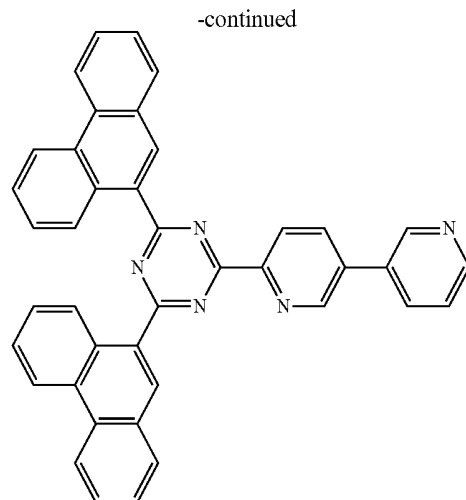
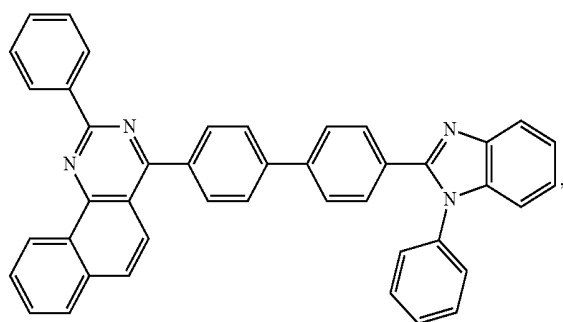
wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alk- enyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, 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.

[0133] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

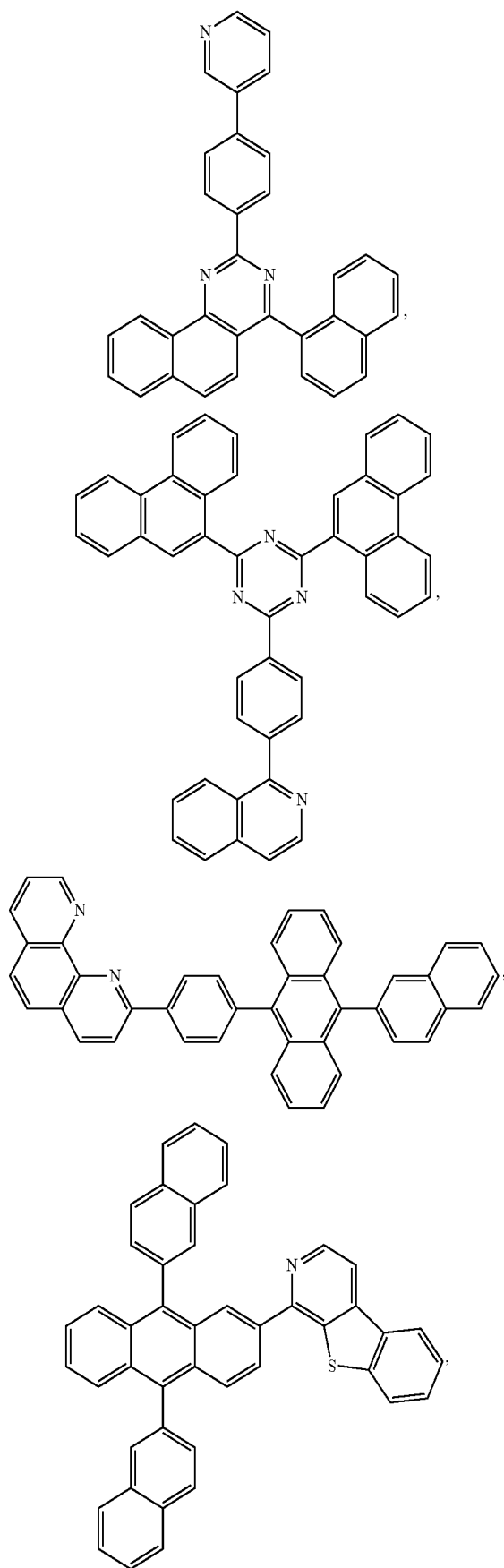


wherein (O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L^{101} is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

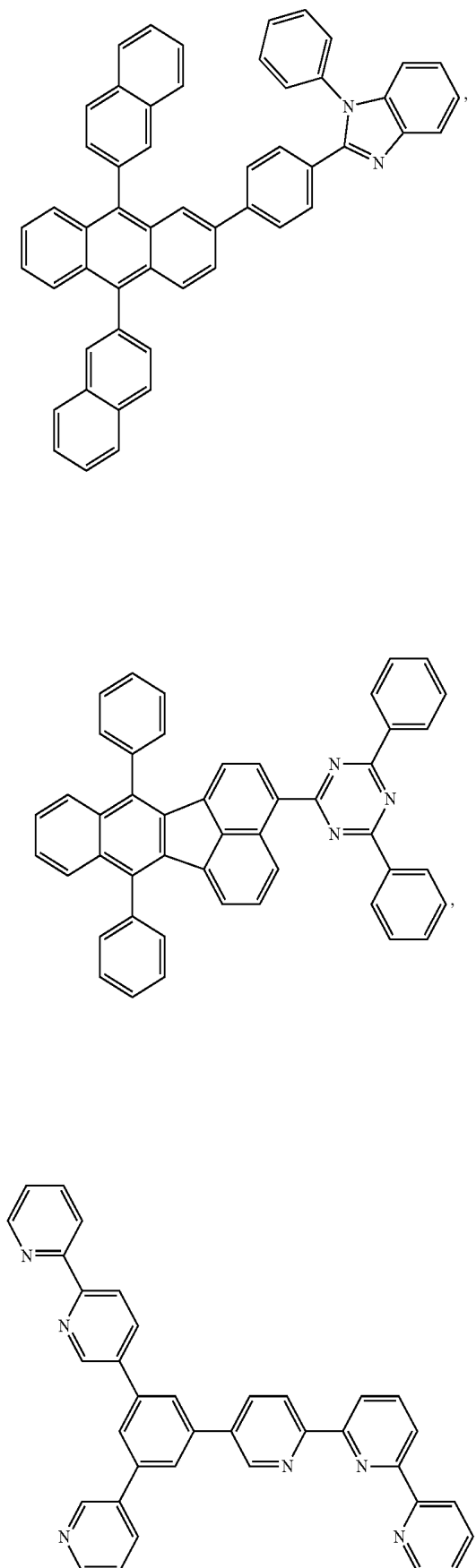
[0134] Non-limiting examples of the ETL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103508940, EP01602648, EP01734038, EP01956007, JP2004-022334, JP2005149918, JP2005-268199, KR0117693, 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,



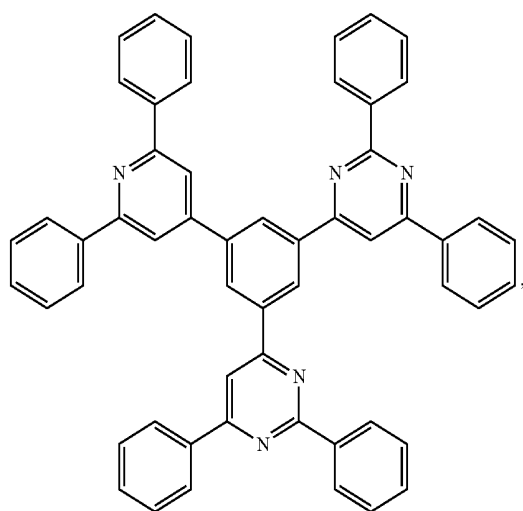
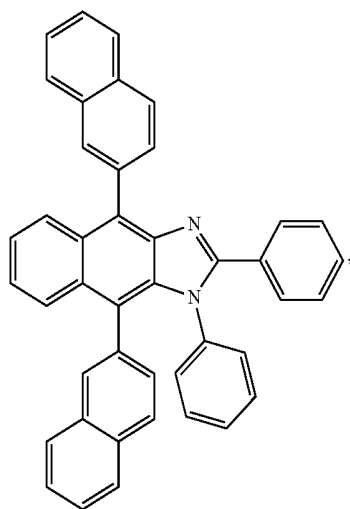
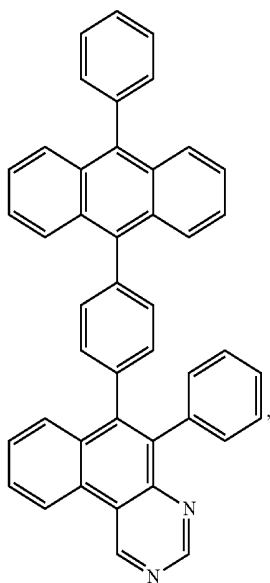
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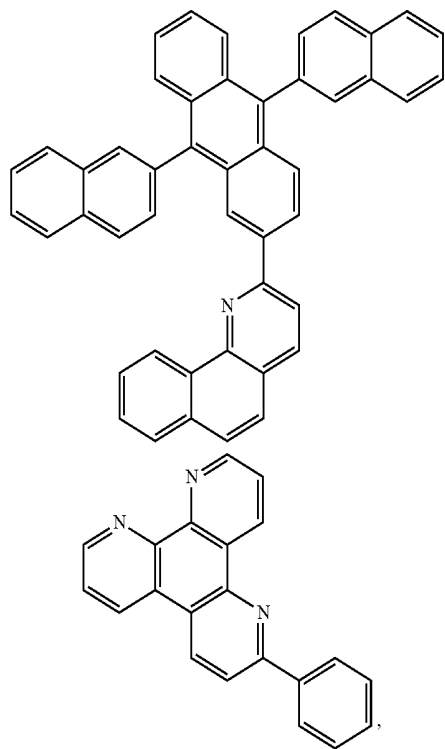
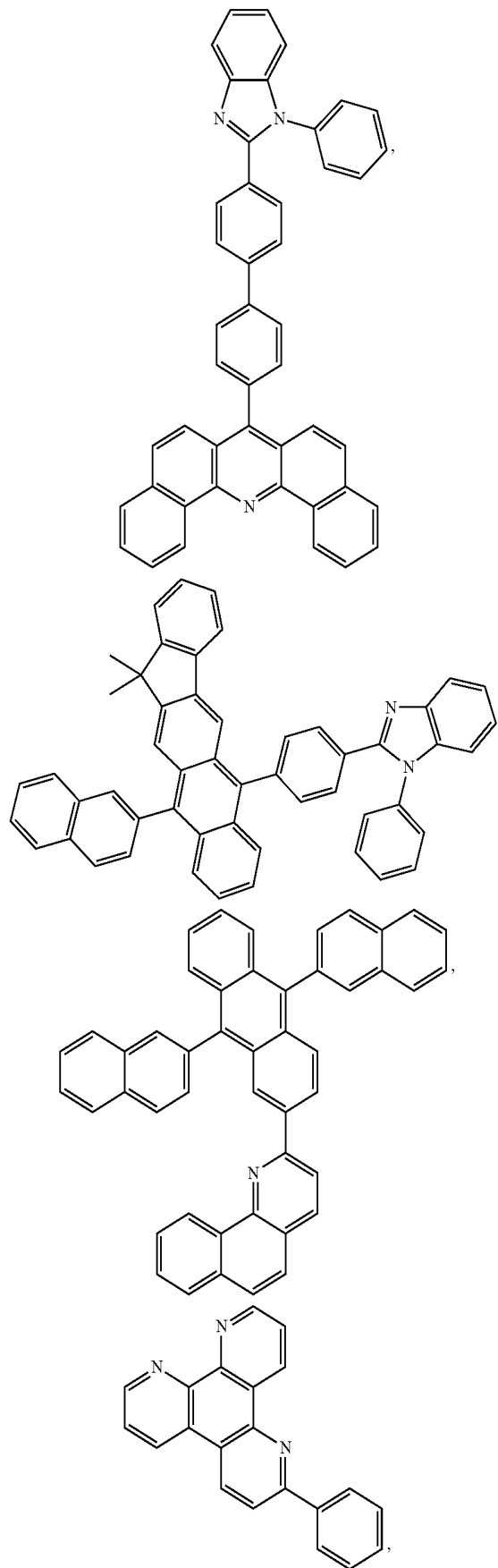
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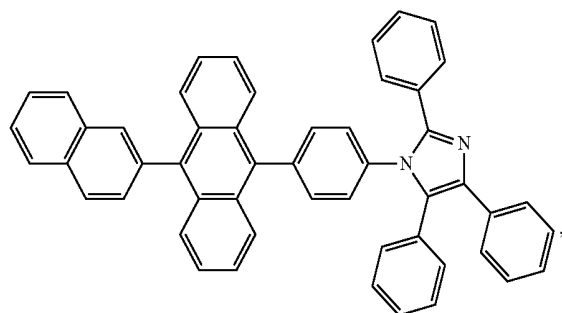
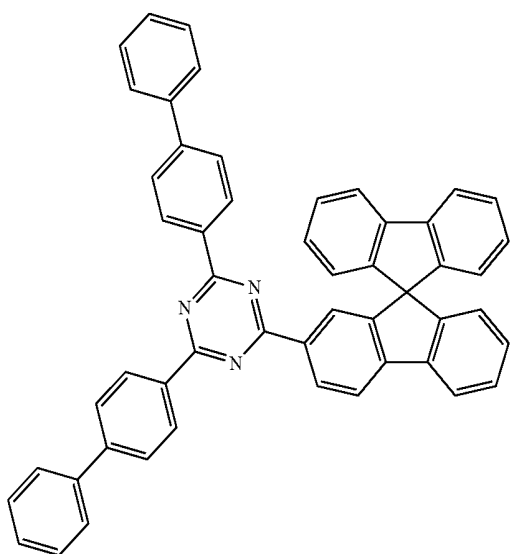
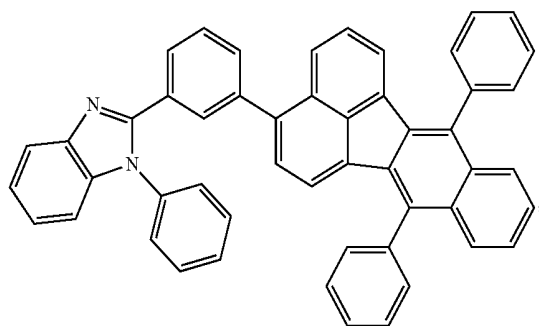
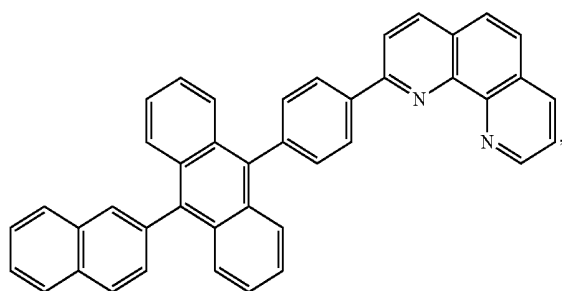
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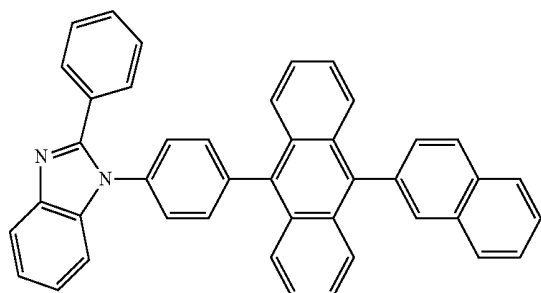
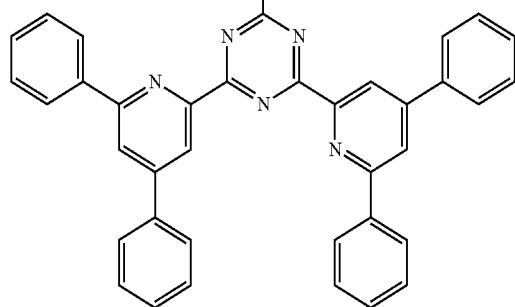
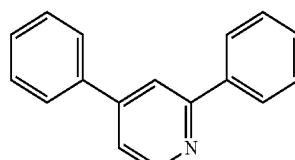
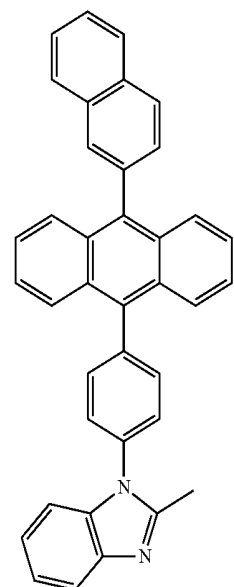
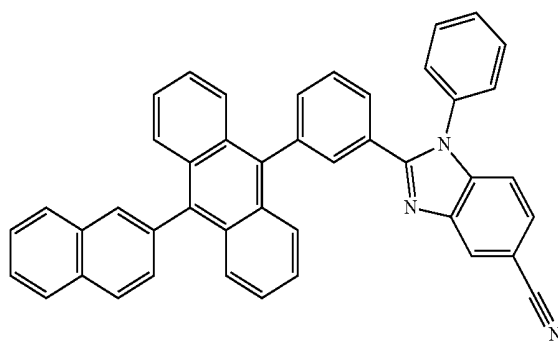
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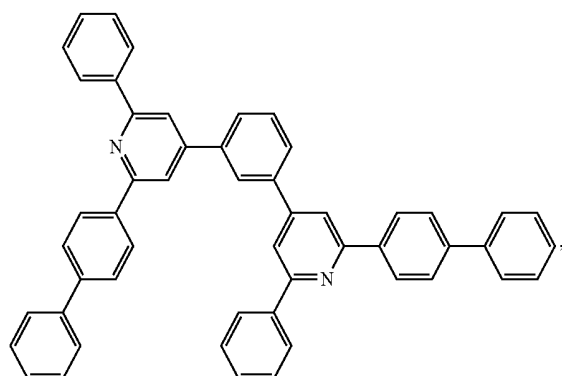
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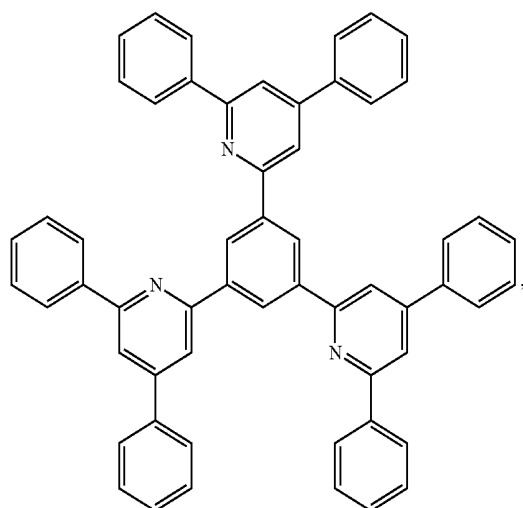
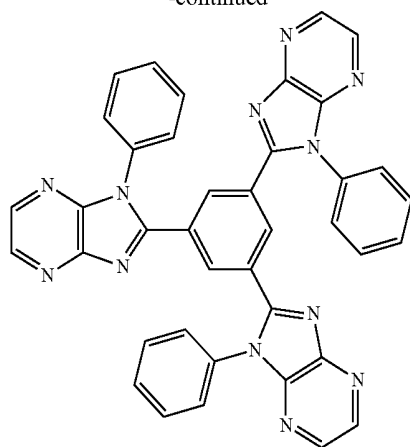
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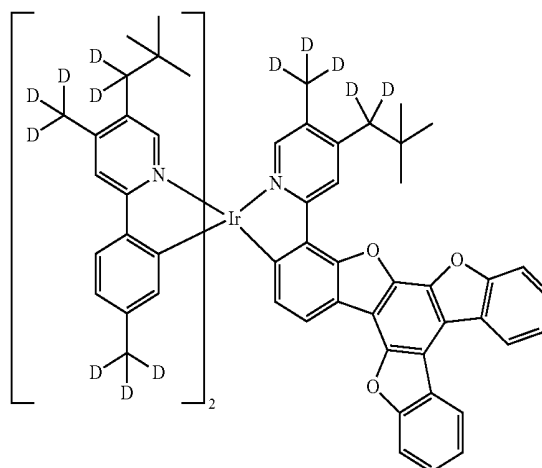
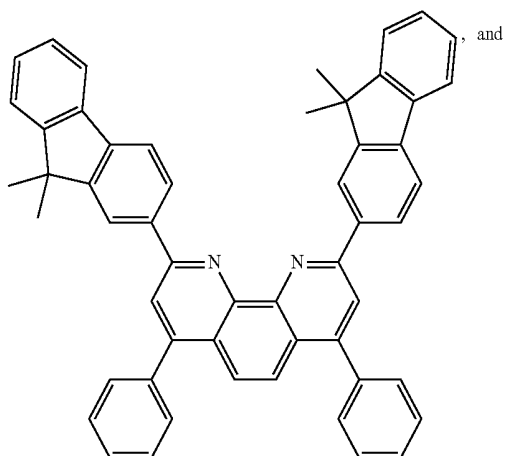
Charge Generation Layer (CGL)

[0135] 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. 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. may be undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also may be undeuterated, partially deuterated, and fully deuterated versions thereof.

EXPERIMENTAL

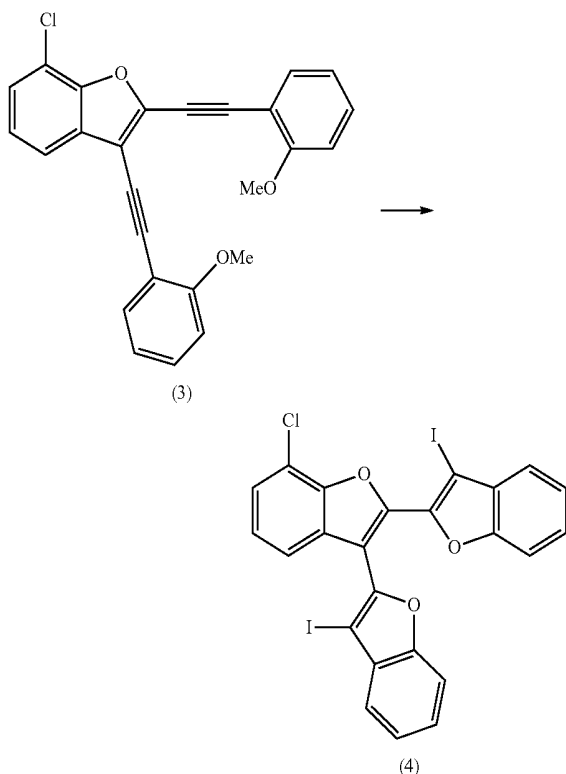
Synthesis of Inventive Compound

[0136]



[0146] Step 4

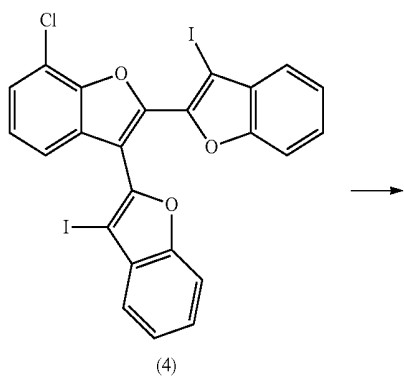
7'-Chloro-3,3"-diiodo-2,2':3',2"-terbenzofuran (4)

[0147]

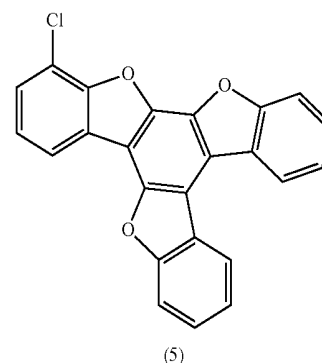
[0148] To a solution of 7-chloro-2,3-bis(2-methoxyphenyl)benzofuran (3) (18.6 g, 45.1 mmol) in DCM (500 mL) was added iodine (45.7 g, 180 mmol) and the mixture was stirred at RT for 6 hours. The reaction was quenched by addition of 10% Na₂S₂O₃ solution (500 mL), the layers were separated and the aqueous was extracted with DCM (100 mL). The combined organic extracts were filtered through a phase separator cartridge and concentrated in vacuo to provide 7'-chloro-3,3"-diiodo-2,2':3',2"-terbenzofuran (4) (29.5 g, 40.8 mmol, 91% yield, 88% LCMS purity) as a pale yellow solid.

[0149] Step 5

7-Chlorobenzo[1,2-b:3,4-b':6,5-b'']trisenbenzofuran (5)

[0150]

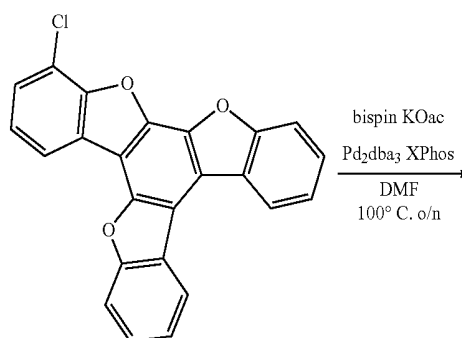
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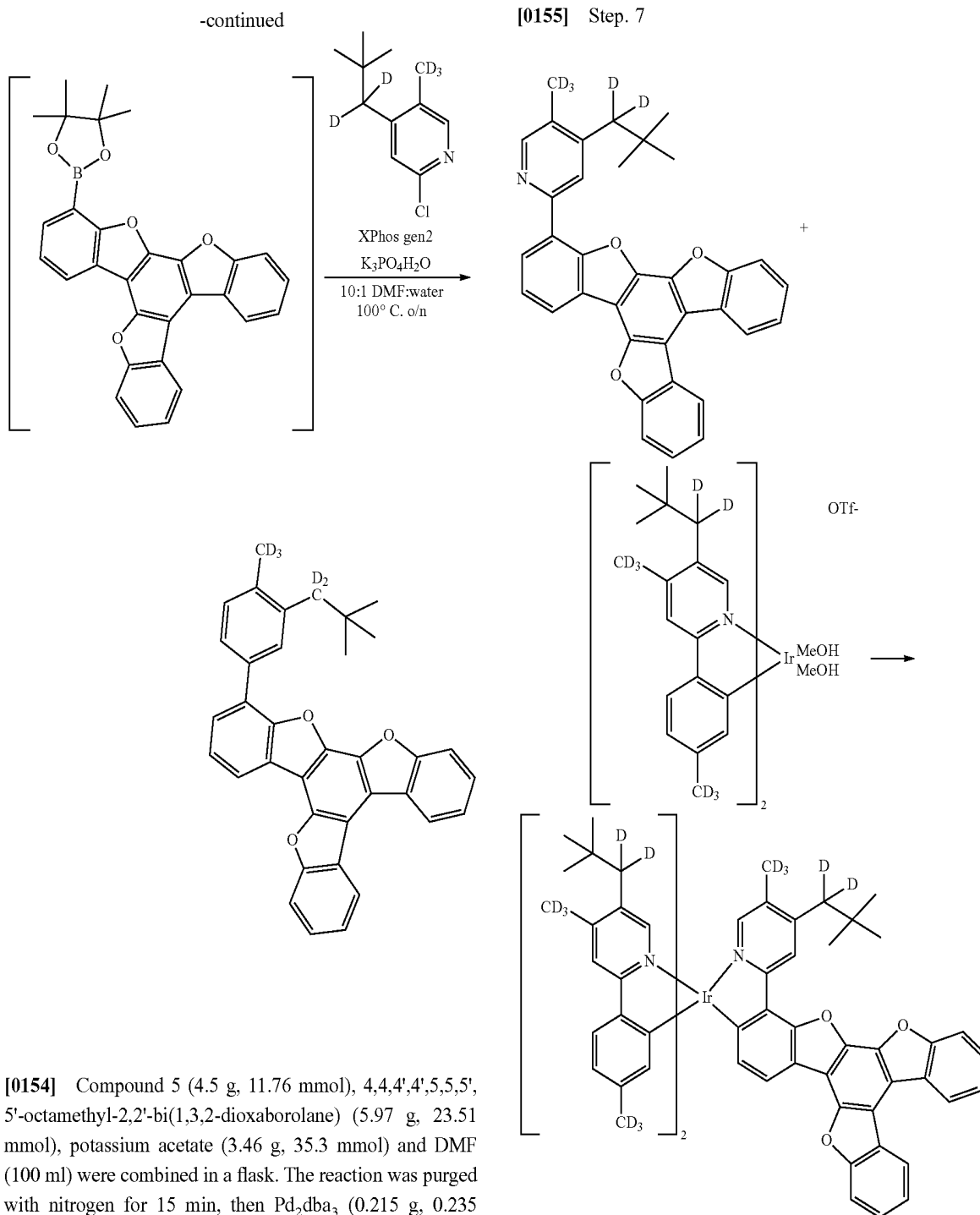


[0151] A mixture of 7'-chloro-3,3"-diiodo-2,2':3',2"-terbenzofuran (4) (28.7 g, 45.1 mmol) and potassium acetate (22.1 g, 226 mmol) in DMF (150 mL) was degassed with bubbling N₂ for 30 min. 1,1'-Bis(diphenylphosphino)ferrocenepalladium(II) dichloride, dichloromethane complex (7.37 g, 9.02 mmol) was added and the mixture was stirred at 100° C. for 64 hours. The reaction mixture was cooled to room temperature, diluted with MeOH (100 mL) and water (100 mL) and stirred for 3 hours. The precipitate was collected by filtration and rinsed with water (3×200 mL), MeOH (3×150 mL) and TBME (150 mL). The solid was re-suspended in toluene (500 mL), heated at reflux for 30 min and then stirred at room temperature for 16.5 hours. The solid was collected by filtration and rinsed with toluene (100 mL) and TBME (100 mL). The solid was re-suspended in toluene (400 mL), heated at reflux for 30 min and then stirred at room temperature for 2 hours. The solid was collected by filtration and rinsed with toluene (100 mL) and TBME (100 mL). The solid was re-suspended in toluene (400 mL), heated at reflux for 16 hours and cooled to room temperature. The solid was collected by filtration, washed with MeOH (100 mL) and TBME (100 mL), and dried in vacuo to provide 7-chlorobenzo[1,2-b:3,4-b':6,5-b'']trisenbenzofuran (5) (16.2 g, 42.3 mmol, 94% yield based on 99.91% HPLC purity) as a grey solid.

[0152] Step 6

2-(2-tribenzofuran)-4-(2,2-dimethylpropyl)-1,1-d2)-5-(methyl-d3)pyridine

[0153]



[0154] Compound 5 (4.5 g, 11.76 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (5.97 g, 23.51 mmol), potassium acetate (3.46 g, 35.3 mmol) and DMF (100 ml) were combined in a flask. The reaction was purged with nitrogen for 15 min, then Pd₂dba₃ (0.215 g, 0.235 mmol) and dicyclohexyl(2',4',6'-triisopropyl-[1,1'-biphenyl]-2-yl)phosphane (XPhos) (0.448 g, 0.940 mmol) were added. The reaction was heated in an oil bath set at 100° C. under nitrogen overnight. The reaction was cooled, then 2-chloro-4-(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridine (2.264 g, 11.17 mmol), potassium phosphate monohydrate (7.49 g, 35.3 mmol), Xphos-Pd Gen2 (0.462 g, 0.588 mmol) and 10 ml water were added. The reaction was heated in an oil bath set at 100° C. overnight. The desired compound is purified by column chromatography (2.43 g, 40% yield).

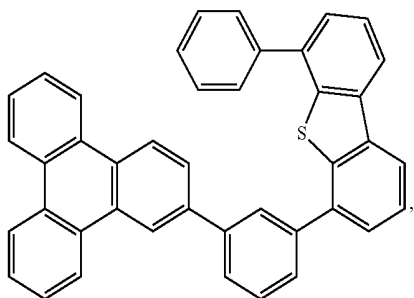
Bis[5-(2,2-dimethylpropyl-1,1-d₂)-4-(methyl-d₃)-2-(4-(methyl-d₃)-[1'-phenyl]-2'-yl)pyridin-1-yl)]bis(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridin-2-yl-1'-yl)-(tris(benzofurano)[3,2-b:2',3'-d:3'', 2''-f]benzen-2-yl)]iridium(III) (2019-ADS-UDC-Ir474)

[0156] A solution of 1-(4-(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridin-2-yl)-tris(benzofurano)[3,2-b:2',3'-d:3'', 2''-f]benzene (1 g, 1.94 mmol, 2.0 equiv) in 2-ethoxyethanol (12.5 mL) and N,N-dimethylformamide (12.5 mL) was sparged with nitrogen for 15 minutes. [Ir(5-(2,2-dimethylpropyl-1,1-d₂)-4-(methyl-d₃)-2-(4-(methyl-d₃)phenyl-2'-

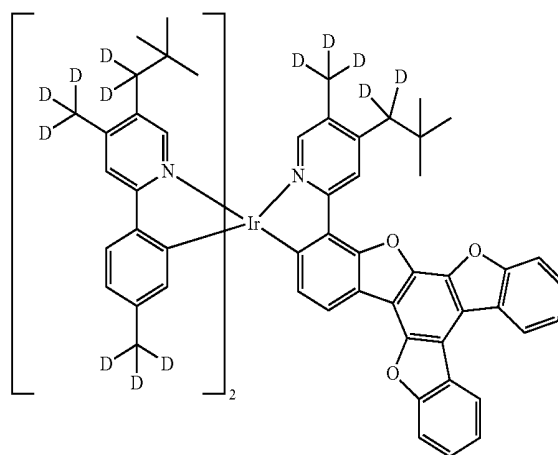
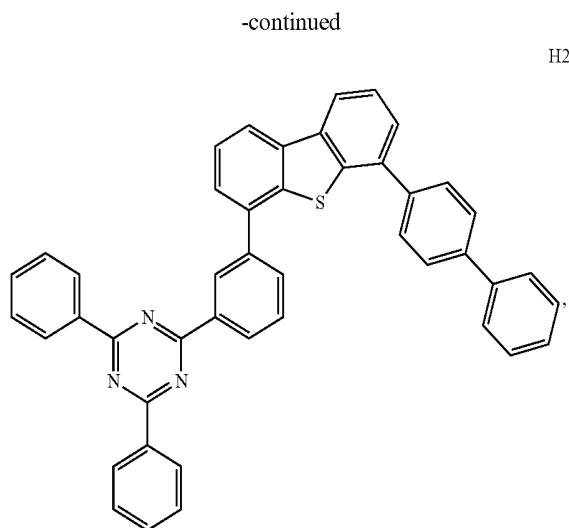
yl)pyridin-1-yl)(-1H)₂(MeOH)₂](trifluoro-methanesulfonate) (0.9 g, 0.97 mmol, 1.0 equiv) was added and the reaction mixture heated at 100° C. for 40 hours. The reaction mixture was cooled to room temperature and filtered. The solids combined with those from a front-run reaction (0.78 mmol scale). The solids were dissolved/suspended in dichloromethane and purified twice on an Interchim automated system (120 g silica gel cartridge atop a 40 g basic alumina cartridge), eluting with 65% dichloromethane in heptanes. The recovered material (1.46 g) was further purified by recrystallization from dichloromethane/hexane to give bis [(5-(2,2-dimethylpropyl-1,1-d₂)-4-(methyl-d₃)-2-(4-(methyl-d₃)-[1'-phenyl]-2'-yl)pyridin-1-yl)](((1-(4-(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridin-2-yl)-1'-yl)-(tris (benzo-furano)[3,2-b:2',3'-d:3'',2''-f]benzen-2-yl)]iridium (III) (0.8 g, 96.4% UPLC purity) and 0.17 g of less pure material (45% combined yield) as yellow solids.

DEVICE EXAMPLES

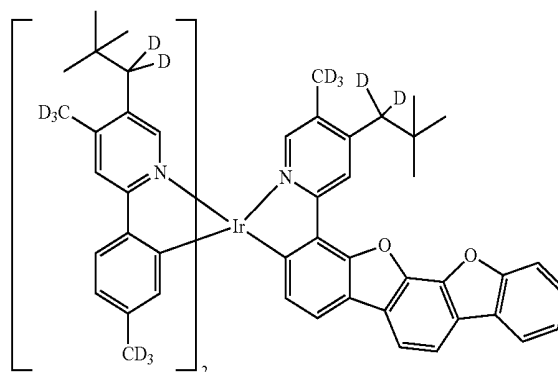
[0157] All example devices were fabricated by forming the layers by high vacuum (<10⁻⁷ Torr) thermal evaporation. The anode electrode was 800 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of Liq (8-hydroxyquinoline lithium) followed by 1,000 Å of Al. All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H₂O and O₂) immediately after fabrication with a moisture getter incorporated inside the package. Referring to Table 1 below, the organic stack of the device examples consisted of sequentially, from the ITO Surface: 100 Å of HAT-CN as the hole injection layer (HIL); 450 Å of HTM as a hole transporting layer (HTL); emissive layer (EML) with thickness 400 Å; emissive layer containing H-host (H1): E-host (H2) in 6:4 ratio and 12 weight % of green emitter; 350 Å of Liq (8-hydroxyquinoline lithium) doped with 40% of ETM as the electron transporting layer (ETL); 10 Å of Liq as the electron injection layer (EIL). The chemical structures of the device materials are shown below.



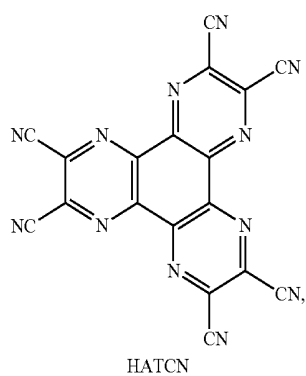
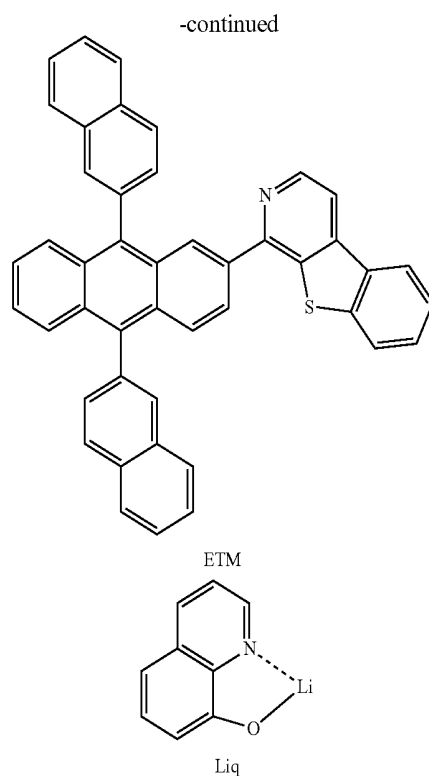
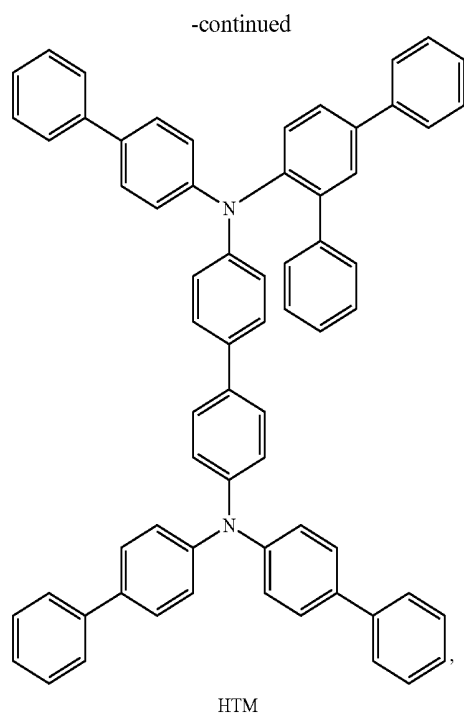
H1



Inventive example



Comparative example



[0158] Provided in Table 2 below is a summary of the device data including emission color, voltage, luminous efficiency (LE), external quantum efficiency (EQE) and power efficiency (PE), recorded at 1000 nits for device examples. The data is normalized to the comparative compound.

TABLE 1

| schematic device structure | | |
|----------------------------|----------------|---------------|
| Layer | Material | Thickness [Å] |
| Anode | ITO | 800 |
| HIL | HAT-CN | 100 |
| HTL | HTM | 450 |
| Green | H1:H2: example | 400 |
| EML | dopant | |
| ETL | Liq:ETM 40% | 350 |
| EIL | Liq | 10 |
| Cathode | Al | 1,000 |

TABLE 2

| Device performance data | | | | | | | | |
|-------------------------|-------|-------|--------------------------|-----------|-------------|-----------|---------|-----------|
| 1931 CIE | | | At 10 mA/cm ² | | | | | |
| Emitter | x | y | λ max [nm] | FWHM [nm] | Voltage [V] | LE [cd/A] | EQE [%] | PE [lm/W] |
| Inventive example | 0.339 | 0.634 | 527 | 52 | 0.97* | 1.03* | 1.01* | 1.05* |
| Comparative Example | 0.334 | 0.633 | 524 | 58 | 1.00 | 1.00 | 1.00 | 1.00 |

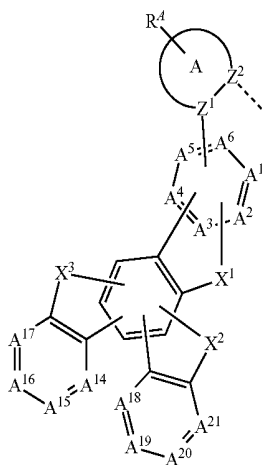
*The value is normalized to the Comparative Example

Comparing the performance data of the inventive example with the comparative example; the external quantum efficiency (EQE) and power efficiency (PE) of the inventive example is higher than the comparative example. Furthermore; inventive example has narrower line shape than the comparative example. (52 nm v.s. 58 nm for FWHM). Inventors believe that the highly conjugated fuse ring system of the inventive emitter compound make the molecule to have less geometry change during the electronic transition process, which has resulted in the narrower line shape.

[0159] 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.

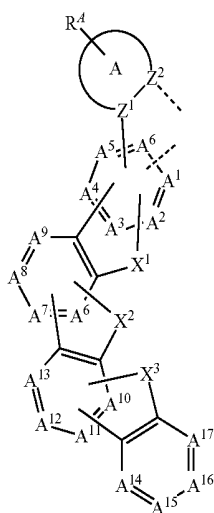
We claim:

1. A compound comprising a first ligand L_A selected from the group consisting of



Formula I

and



Formula II

wherein,

L_A is complexed to a metal M to form a 5-membered chelate ring;

A is a 5-membered or 6-membered aryl or heteroaryl ring;

Z^1 and Z^2 are each independently C or N;

R^4 represents mono to the maximum allowable substitutions, or no substitution;

each A^1 to A^{13} is independently C, CR, or N;

each A^{14} to A^{21} is independently CR or N;

maximum number of N atoms that can connect to each other within a ring is two;

any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ;

any of A^1 to A^{13} are C when they are adjacent and fused to a ring;

any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring; X^1 , X^2 , and X^3 are each independently selected from the group consisting of O, S, Se, NR^1 , CR^1R^2 , and SiR^1R^2 ;

each R, R^1 , R^2 , and R^4 is independently a 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 acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

M is optionally coordinated to other ligands;

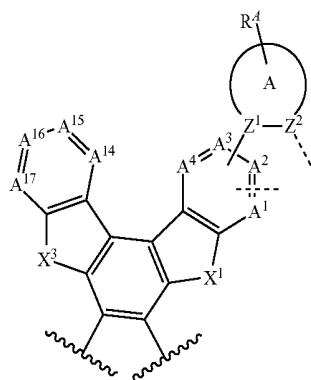
the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand;

any two substituents may be joined or fused together to form a ring;

if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ;

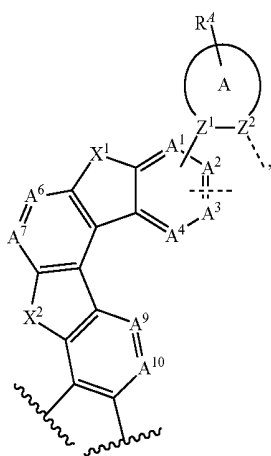
if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ;

Formulas III through VIII are defined as



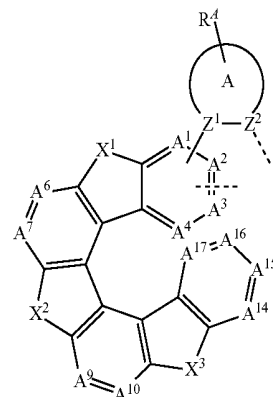
Formula III

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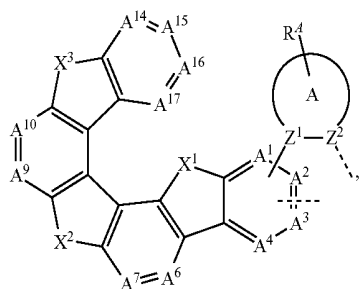


Formula IV

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Formula VIII



Formula V

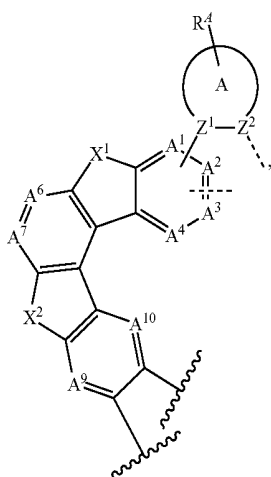
and

the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X² or X³.

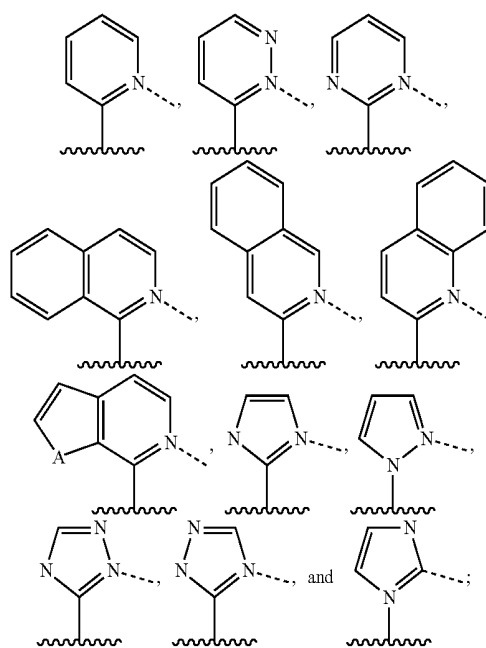
2. The compound of claim 1, wherein each R, R', R'', and R⁴ is independently hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

3. The compound of claim 1, wherein M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pd, Pt, Au, and Cu.

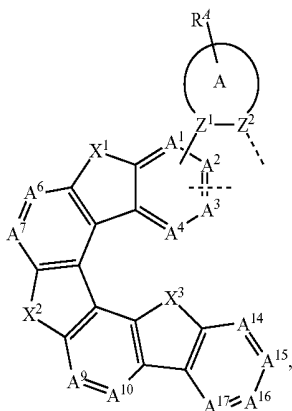
4. The compound of claim 1, wherein ring A is selected from the group consisting of



Formula VI



Formula VII



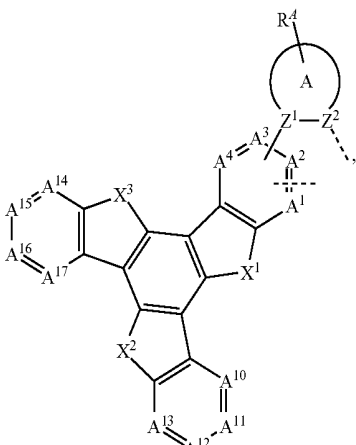
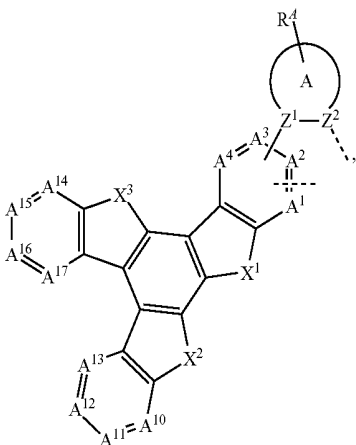
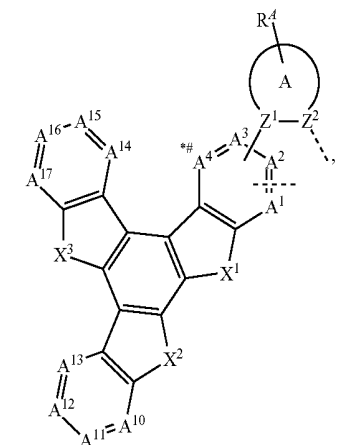
wherein A is O or S;
wherein the dashed line indicates a direct bond to M; and
wherein the wavy line indicates a bond to A¹, A², A³, or A⁴.

5. The compound of claim 1, wherein each X¹, X², and X³ is O.

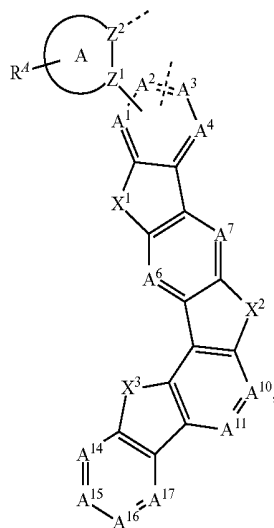
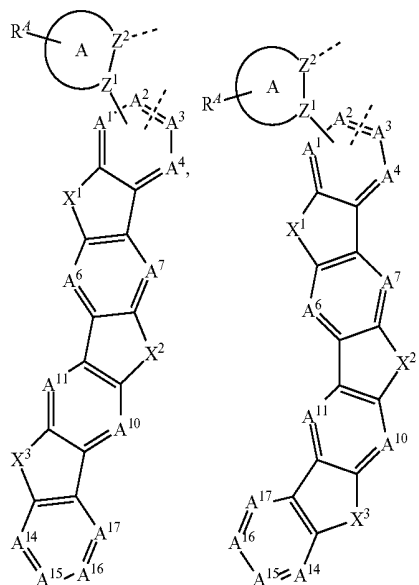
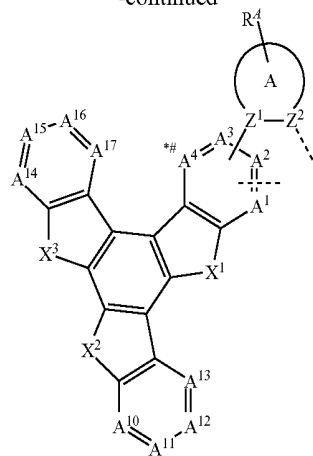
6. The compound of claim 1, wherein each A^1 to A^{13} is C or CR.

7. The compound of claim 1, wherein at least one of A^1 to A^{21} is N.

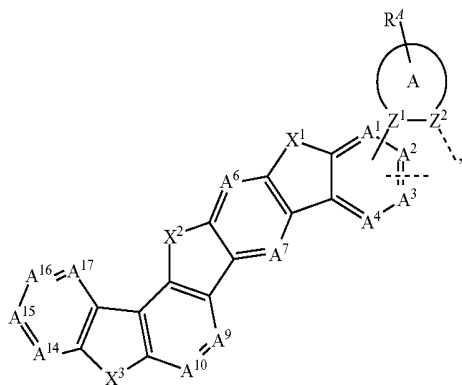
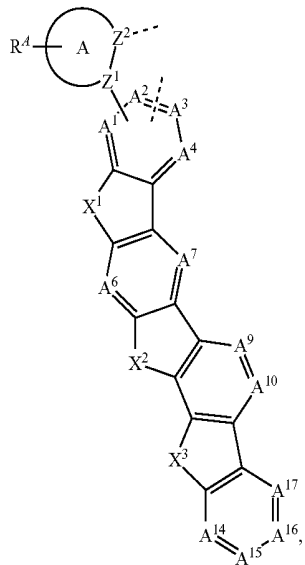
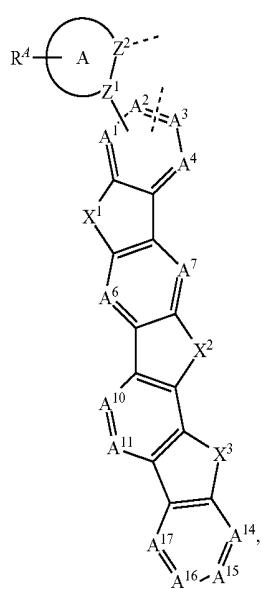
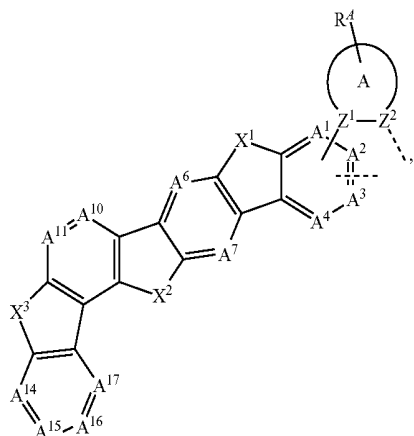
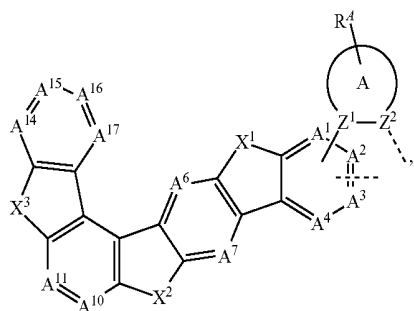
8. The compound of claim 1, wherein the first ligand L_A is selected from the group consisting of:



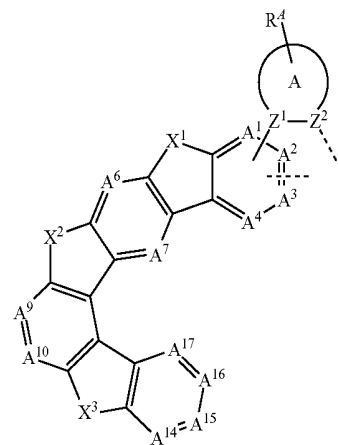
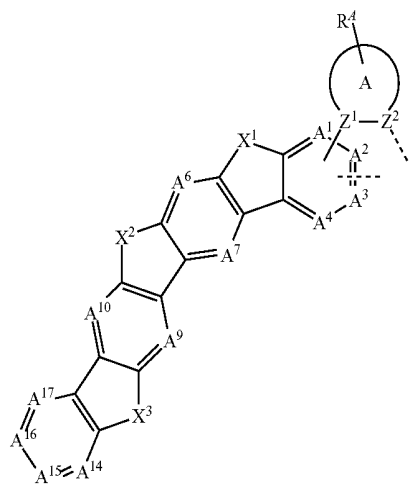
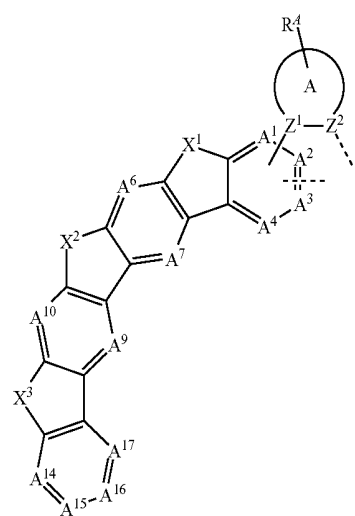
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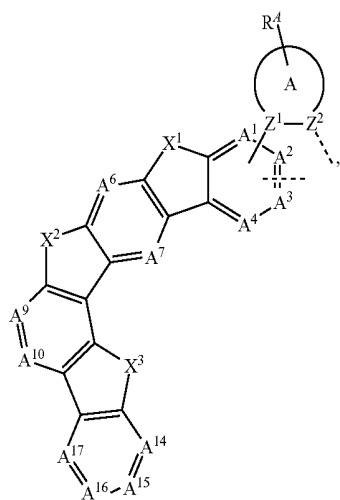
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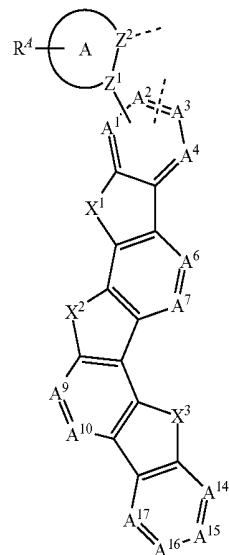
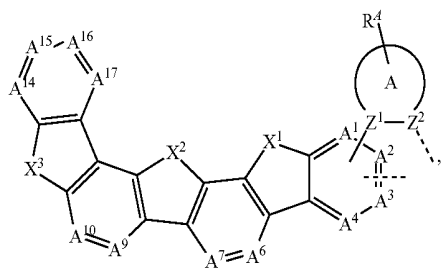
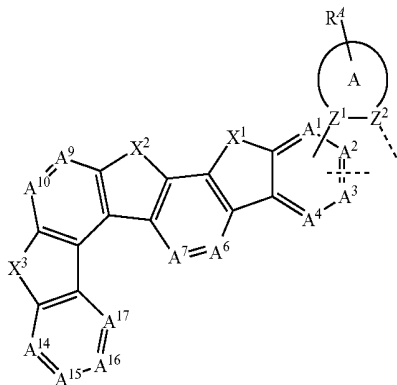
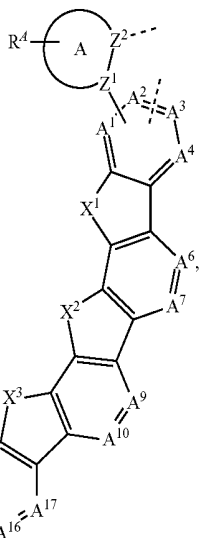
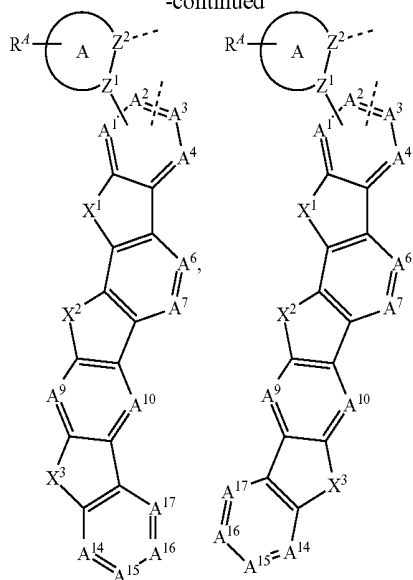
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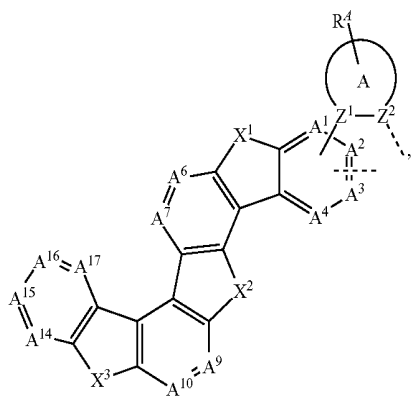
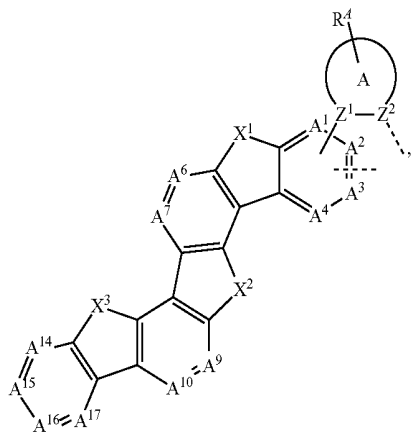
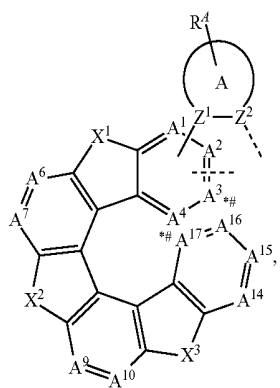
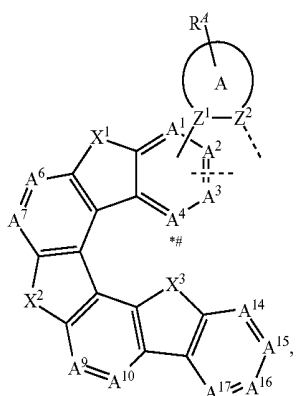
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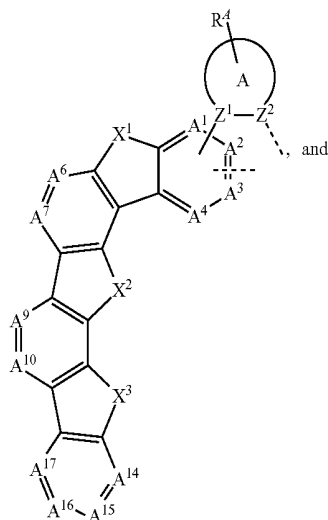
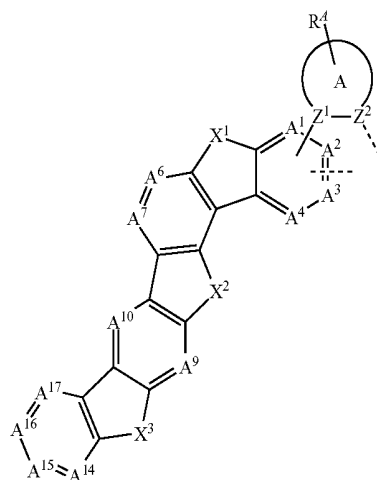
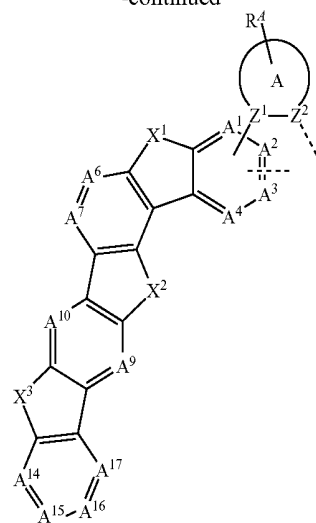
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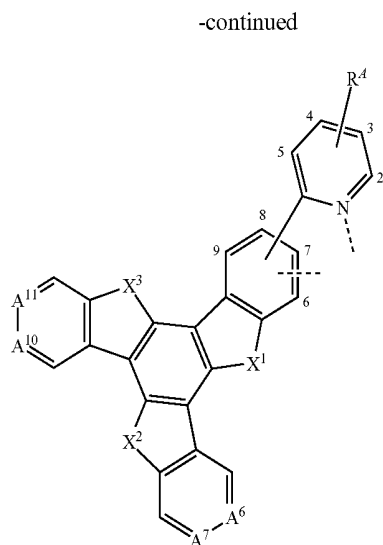
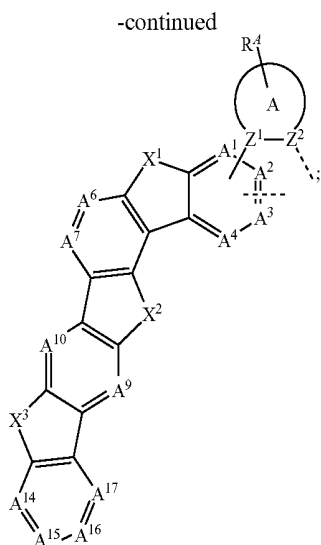


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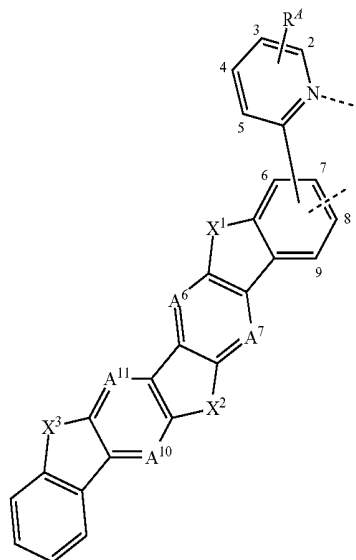
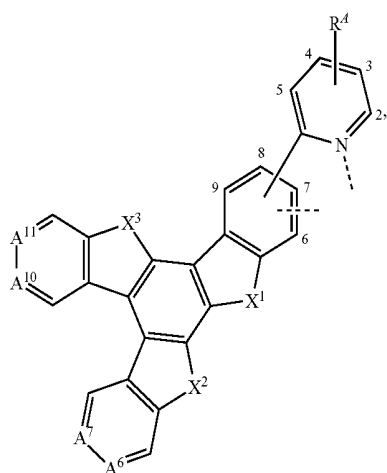
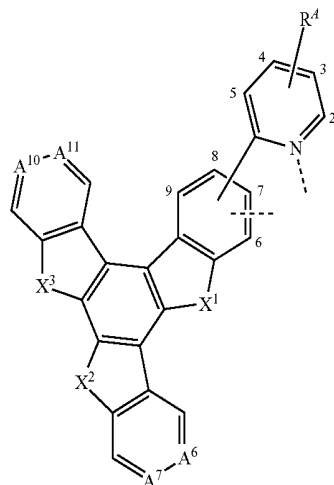
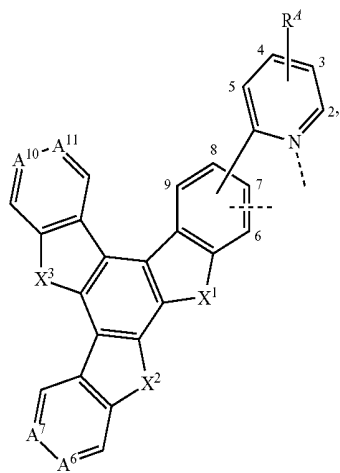




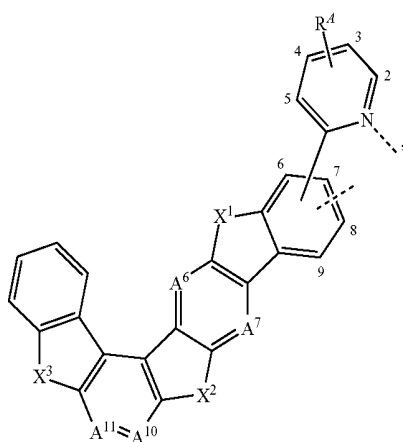
Formula 3-m

wherein M does not form a direct bond to A³ or A⁴ if it is marked with an asterisk (*), and wherein Z¹ does not form a direct bond to A³ or A⁴ if it is marked with a hashtag (#).

9. The compound of claim 1, wherein the first ligand L_A is selected from the group consisting of L_{A1-1-1} to L_{A38-6-67} based on the formula of L_{Aⁿ-m-1}, wherein n is an integer from 1 to 38 and for each n, the first ligand L_{Aⁿ-m-1} has a structure according to Formula 1-m to Formula 38-m shown below:

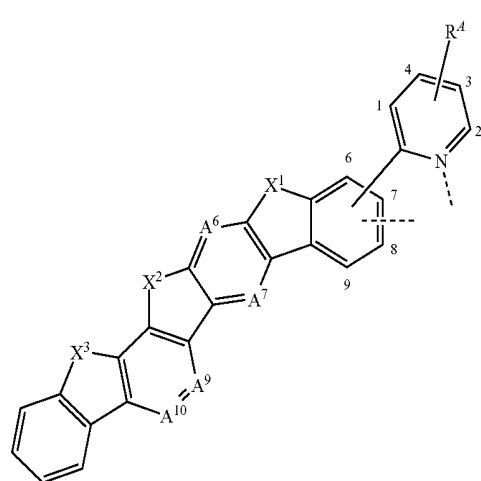


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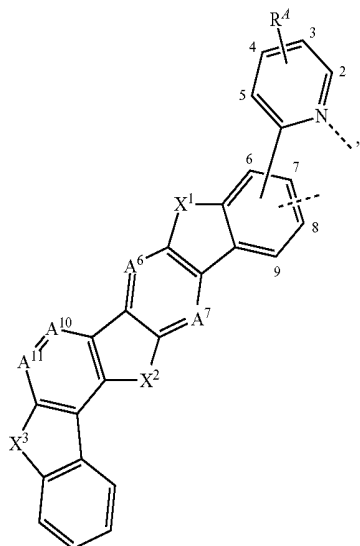
Formula 6-m

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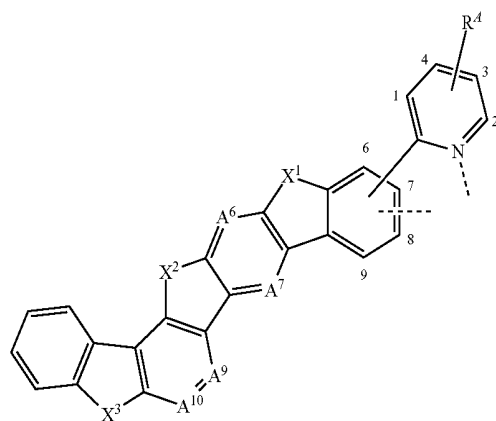


Formula 9-m

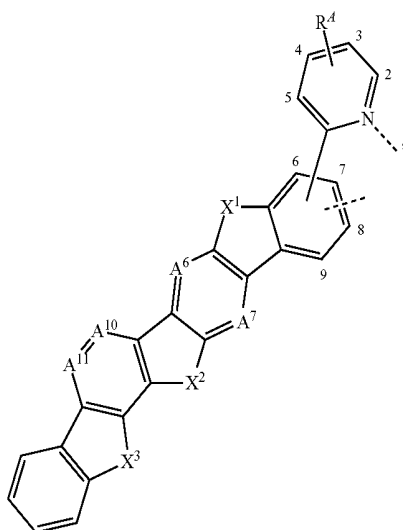
Formula 7-m



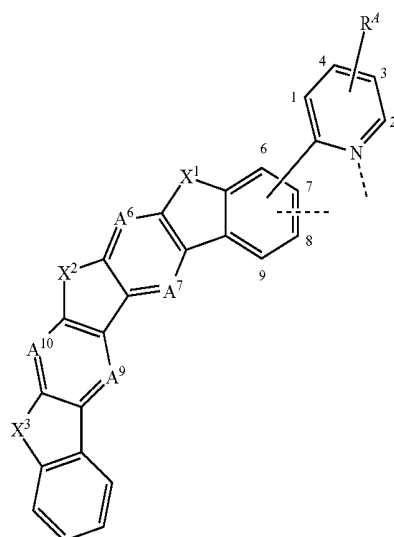
Formula 10-m



Formula 8-m

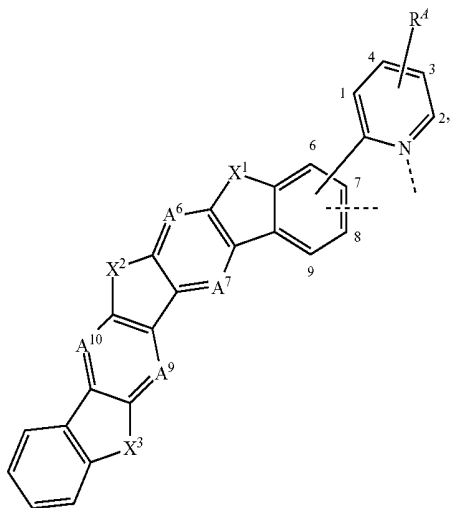


Formula 11-m



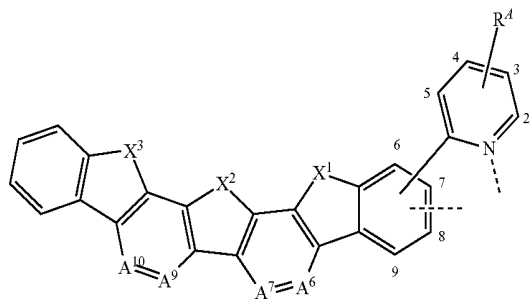
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Formula 12-m

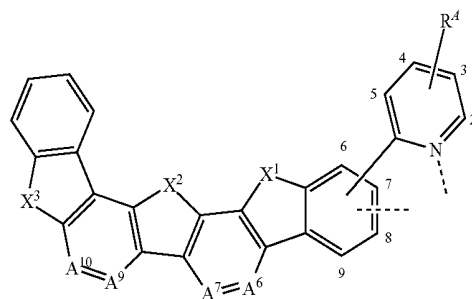


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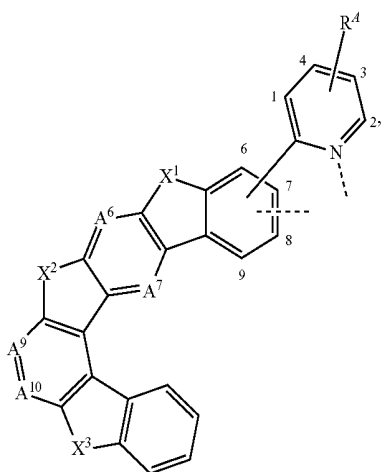
Formula 15-m



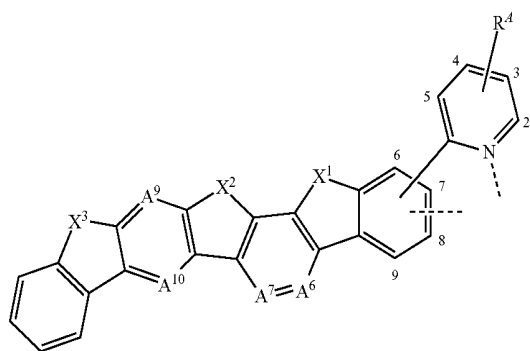
Formula 16-m



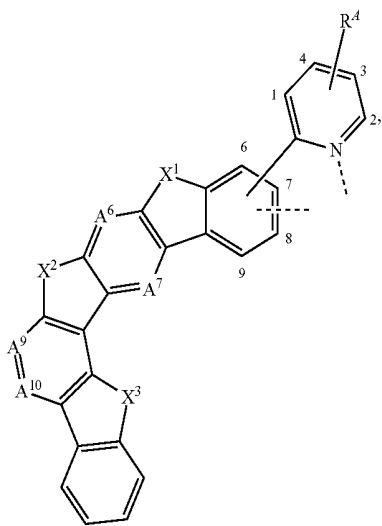
Formula 13-m



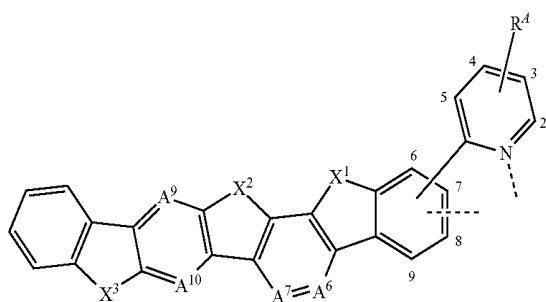
Formula 17-m



Formula 14-m

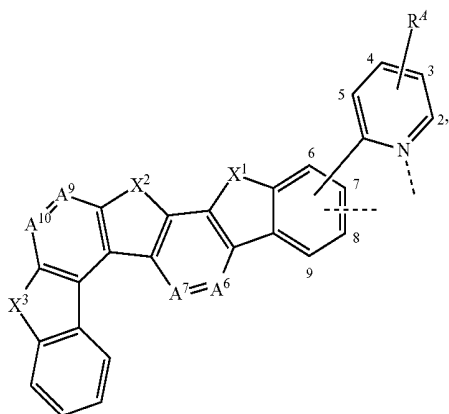


Formula 18-m

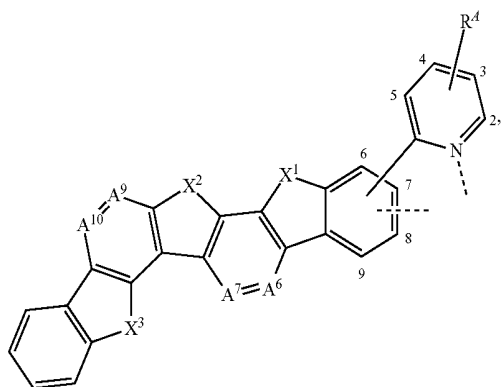


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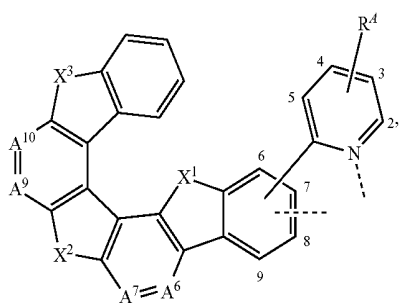
Formula 19-m



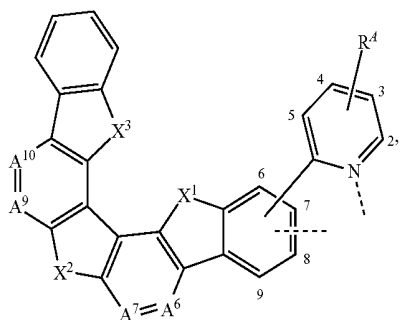
Formula 20-m



Formula 21-m

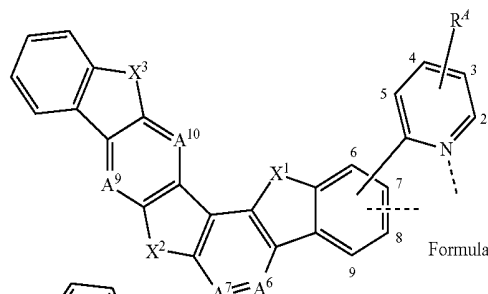


Formula 22-m

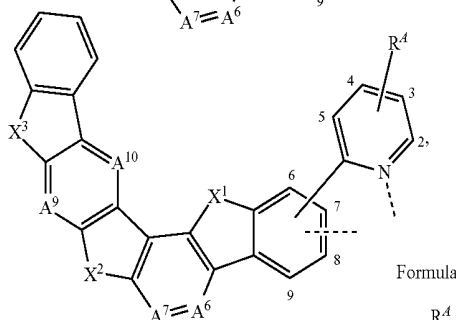


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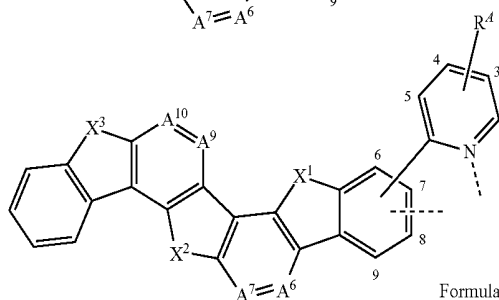
Formula 23-m



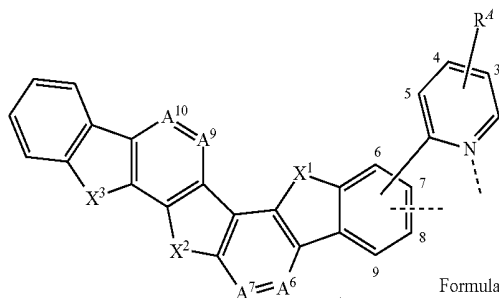
Formula 24-m



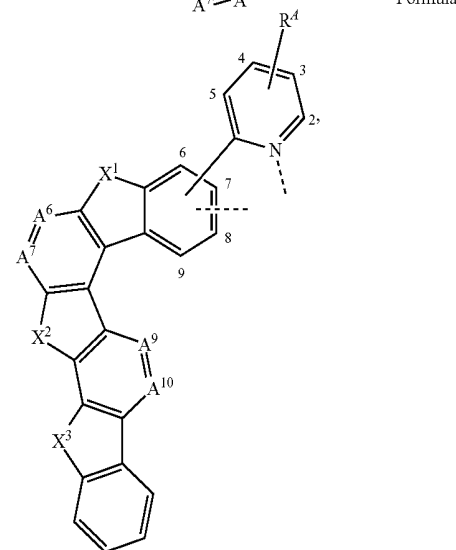
Formula 25-m



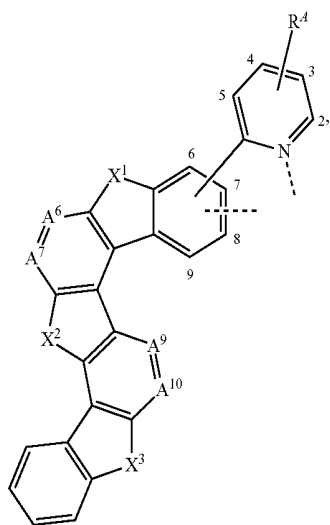
Formula 26-m



Formula 27-m

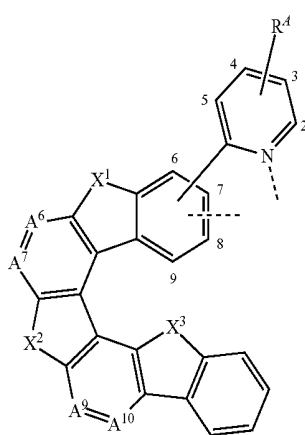


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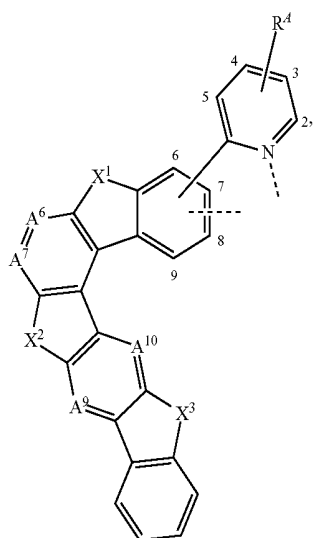
Formula 28-m

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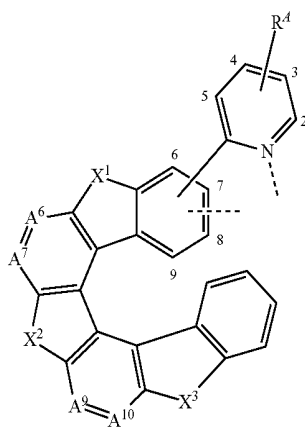


Formula 31-m

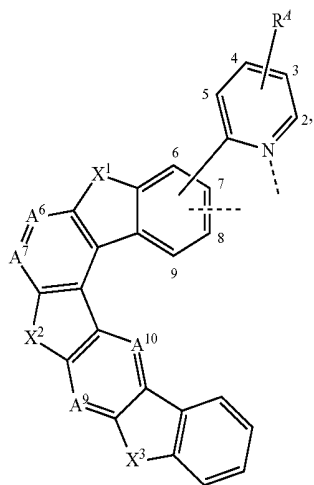
Formula 29-m



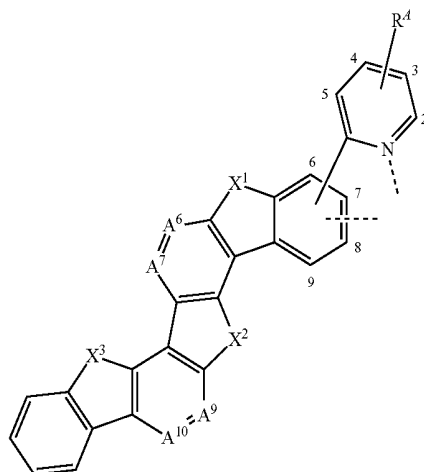
Formula 32-m



Formula 30-m

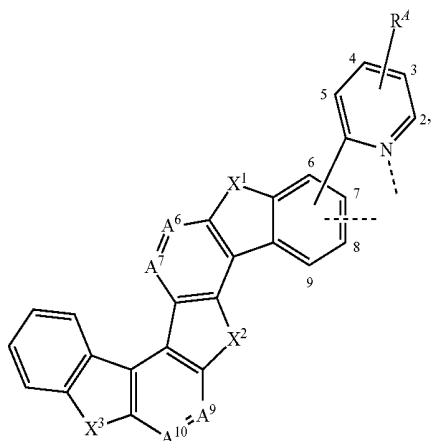


Formula 33-m



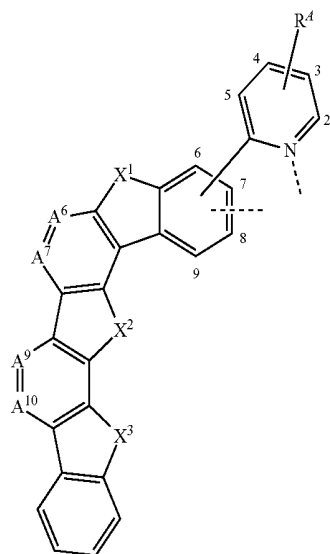
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Formula 34-m

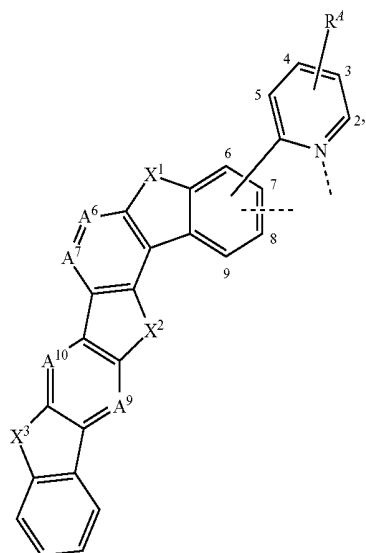


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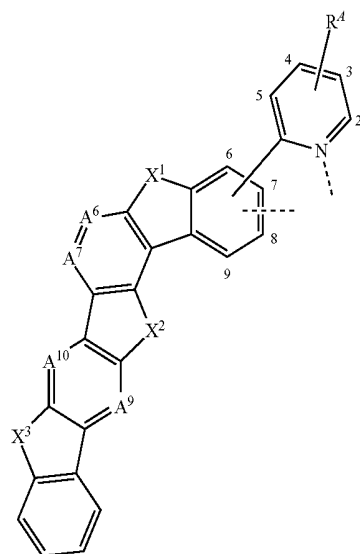
Formula 37-m



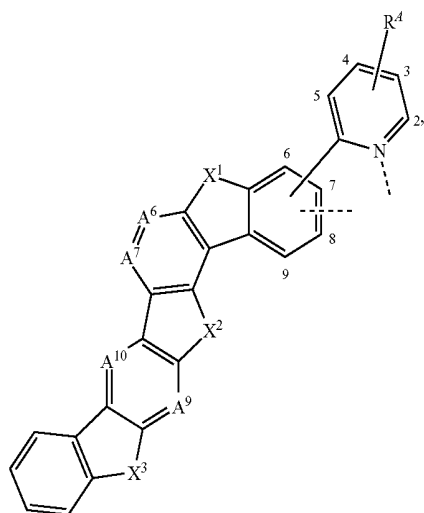
Formula 35-m



Formula 38-m



Formula 36-m



wherein in each Formula n-m, X¹, X², and X³ are defined as follows identified by m, an integer from 1 to 6:

| m | X ¹ | X ² | X ³ |
|---|----------------|------------------|------------------|
| 1 | O | O | O |
| 2 | O | CMe ₂ | O |
| 3 | O | O | CMe ₂ |
| 4 | O | CMe ₂ | CMe ₂ |
| 5 | O | S | O |
| 6 | O | O | S |

wherein for each n-m, there are 67 types of substitution patterns identified by the variable l, wherein l is an integer from 1 to 67, and for each l, the substitution variables in Formula n-m are defined as provided below:

| I # | R ^A | ** | *** | A ⁶ | A ⁷ | A ¹⁰ | A ¹¹ |
|------|--|----|-----|------------------|------------------|------------------|------------------|
| 68. | 3-Me | 6 | 7 | CH | CH | CH | CH |
| 69. | 3-Me | 6 | 7 | CMe | CH | CH | CH |
| 70. | 3-Me | 6 | 7 | CH | CMe | CH | CH |
| 71. | 3-Me | 6 | 7 | CH | CH | CMe | CH |
| 72. | 3-Me | 6 | 7 | CH | CH | CH | CMe |
| 73. | 3-Me | 6 | 7 | N | CH | CH | CH |
| 74. | 3-Me | 6 | 7 | CH | N | CH | CH |
| 75. | 3-Me | 6 | 7 | CH | CH | N | CH |
| 76. | 3-Me | 6 | 7 | CH | CH | CH | N |
| 77. | 3-i-Pr | 6 | 7 | CH | CH | CH | CH |
| 78. | 3-i-Pr | 6 | 7 | N | CH | CH | CH |
| 79. | 3-i-Pr | 6 | 7 | CH | N | CH | CH |
| 80. | 3-i-Pr | 6 | 7 | CH | CH | N | CH |
| 81. | 3-i-Pr | 6 | 7 | CH | CH | CH | N |
| 82. | 3-t-Bu | 6 | 7 | CH | CH | CH | N |
| 83. | 4-Me | 6 | 7 | CH | CH | CH | CH |
| 84. | 4-t-Bu | 6 | 7 | CH | CH | CH | CH |
| 85. | 3-CH ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 86. | 3,4-Me | 6 | 7 | CH | CH | CH | CH |
| 87. | 3-CH ₂ CMe ₃ , 4-CH ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 88. | 4-CH ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 89. | 3-CH ₂ CMe ₃ , 4-Me | 6 | 7 | CH | CH | CH | CH |
| 90. | 4-CH ₂ CMe ₃ , 3-Me | 6 | 7 | CH | CH | CH | CH |
| 91. | H | 6 | 7 | CH | CH | CH | CH |
| 92. | 3-CH ₂ CMe ₃ | 7 | 8 | CH | CH | CH | CH |
| 93. | 3,4-Me | 7 | 8 | CH | CH | CH | CH |
| 94. | 3-CH ₂ CMe ₃ | 8 | 7 | CH | CH | CH | CH |
| 95. | 3,4-Me | 8 | 7 | CH | CH | CH | CH |
| 96. | 3,4-Me | 6 | 7 | N | CH | CH | CH |
| 97. | 3,4-Me | 6 | 7 | CH | N | CH | CH |
| 98. | 3,4-Me | 6 | 7 | CH | CH | N | CH |
| 99. | 3,4-Me | 6 | 7 | CH | CH | CH | N |
| 100. | 3-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 101. | 3-CD ₃ | 6 | 7 | N | CH | CH | CH |
| 102. | 3-CD ₃ | 6 | 7 | CH | N | CH | CH |
| 103. | 3-CD ₃ | 6 | 7 | CH | CH | N | CH |
| 104. | 3-CD ₃ | 6 | 7 | CH | CH | CH | N |
| 105. | 3-CD(CMe) ₂ | 6 | 7 | CH | CH | CH | CH |
| 106. | 3-CD(CMe) ₂ | 6 | 7 | N | CH | CH | CH |
| 107. | 3-CD(CMe) ₂ | 6 | 7 | CH | N | CH | CH |
| 108. | 3-CD(CMe) ₂ | 6 | 7 | CH | CH | N | CH |
| 109. | 3-CD(CMe) ₂ | 6 | 7 | CH | CH | CH | N |
| 110. | 4-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 111. | 3-CD ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 112. | 3,4-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 113. | 3-CD ₂ CMe ₃ , 4-CD ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 114. | 4-CD ₂ CMe ₃ | 6 | 7 | CH | CH | CH | CH |
| 115. | 3-CD ₂ CMe ₃ , 4-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 116. | 4-CD ₂ CMe ₃ , 3-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 117. | H | 6 | 7 | CH | CH | CH | CH |
| 118. | 3-CD ₂ CMe ₃ | 7 | 8 | CH | CH | CH | CH |
| 119. | 3,4-CD ₃ | 7 | 8 | CH | CH | CH | CH |
| 120. | 3-CD ₂ CMe ₃ | 8 | 7 | CH | CH | CH | CH |
| 121. | 3,4-CD ₃ | 8 | 7 | CH | CH | CH | CH |
| 122. | 3,4-CD ₃ | 6 | 7 | N | CH | CH | CH |
| 123. | 3,4-CD ₃ | 6 | 7 | CH | N | CH | CH |
| 124. | 3,4-CD ₃ | 6 | 7 | CH | CH | N | CH |
| 125. | 3,4-CD ₃ | 6 | 7 | CH | CH | CH | N |
| 126. | 3-CD ₃ | 6 | 7 | CH | CH | CH | CH |
| 127. | 3,4-CD ₃ | 6 | 7 | CCD ₃ | CH | CH | CH |
| 128. | 3,4-CD ₃ | 6 | 7 | CH | CCD ₃ | N | CH |
| 129. | 3,4-CD ₃ | 6 | 7 | CH | CH | CCD ₃ | CH |
| 130. | 3-CD ₃ | 6 | 7 | CH | CH | CH | CCD ₃ |
| 131. | 3-CD ₃ | 6 | 7 | N | CH | CH | CH |
| 132. | 3-CD ₃ | 6 | 7 | CH | N | CH | CH |
| 133. | 3-CD ₃ | 6 | 7 | CH | CH | N | CH |
| 134. | 3-CD ₃ | 6 | 7 | CH | CH | CH | N |

wherein ** represents pyridine ring attachment position, and *** represents ligation position.

10. The compound of claim 1, wherein the compound has a formula of $M(L_A)_x(L_B)_y(L_C)_z$, wherein L_B and L_C are each a bidentate ligand;

x is 1, 2, or 3;

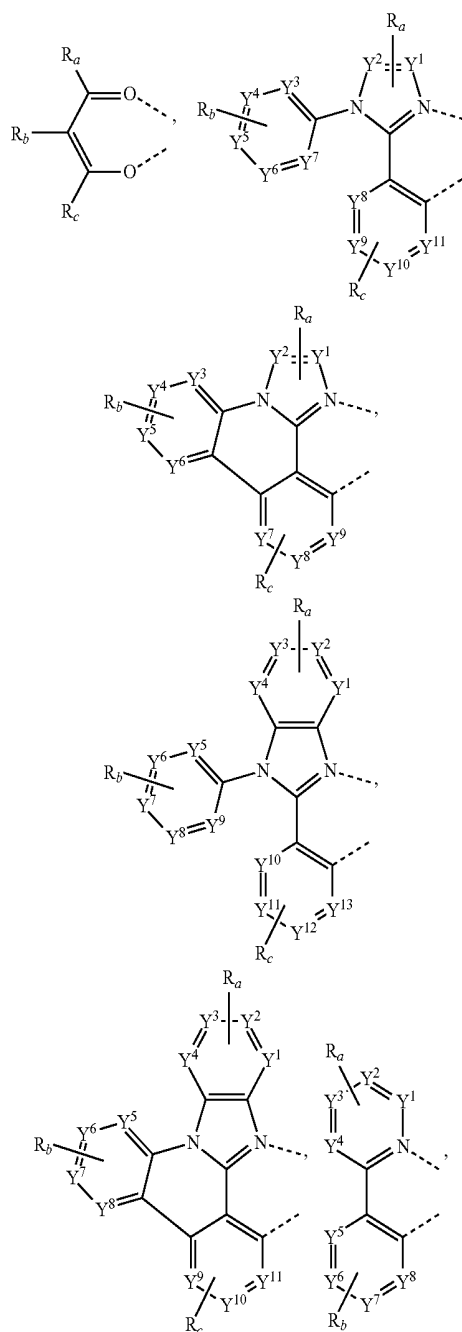
y is 0, 1, or 2;

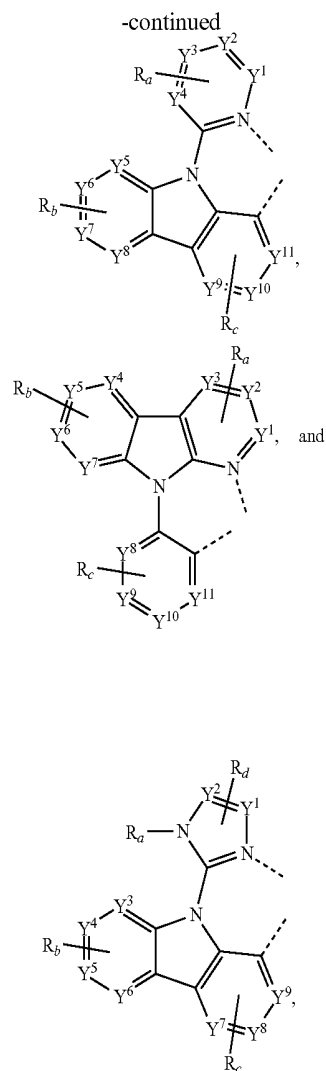
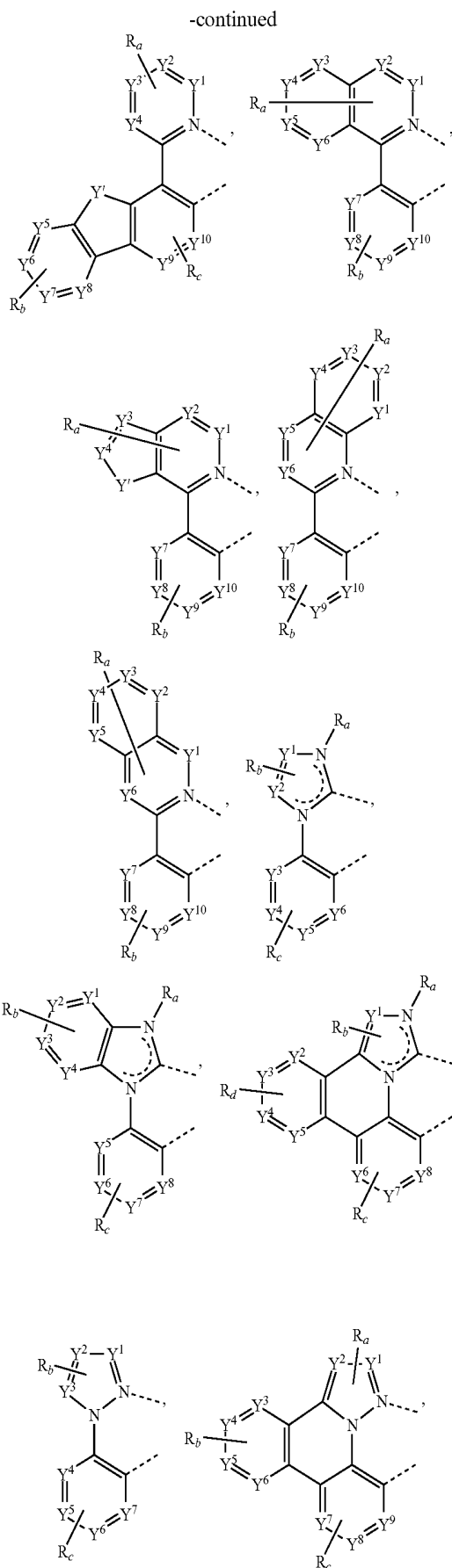
z is 0, 1, or 2; and

x+y+z is the oxidation state of the metal M.

11. The compound of claim 10, wherein the compound has a formula selected from the group consisting of $Ir(L_A)_3$, $Ir(L_A)(L_B)_2$, $Ir(L_A)_2(L_B)$, $Ir(L_A)_2(L_C)$, and $Ir(L_A)(L_B)(L_C)$; wherein L_A , L_B , and L_C are different from each other; or wherein the compound has a formula of $Pt(L_A)(L_B)$; wherein L_A and L_B can be the same or different.

12. The compound of claim 10, wherein L_B and L_C are each independently selected from the group consisting of:





wherein

each Y^1 to Y^{13} is independently selected from the group consisting of C and N;

Y^1 is selected from the group consisting of B R_e , N R_e , P R_e , O, S, Se, C=O, S=O, SO_2 , CR_eR_f , SiR_eR_f , and GeR_eR_f ;

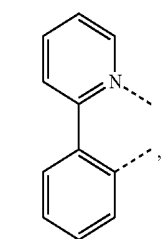
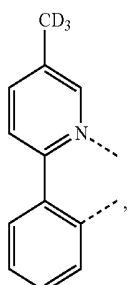
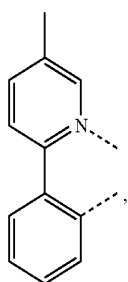
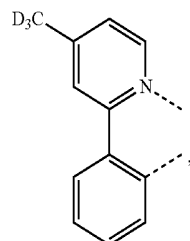
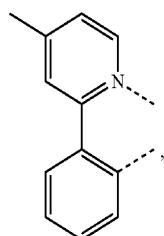
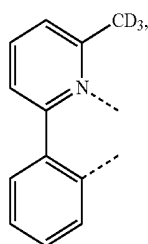
R_e and R_f are optionally fused or joined to form a ring;

each R_a , R_b , R_d , and R_d independently represents from mono substitution to the maximum possible number of substitutions, or no substitution;

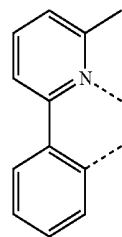
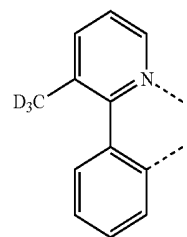
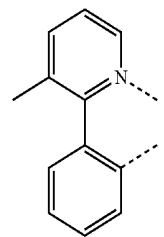
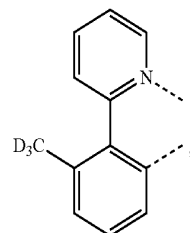
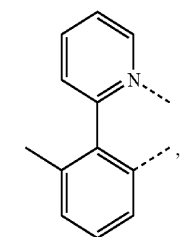
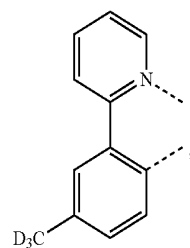
each R_a , R_b , R_d , R_d , R_e , and R_f is independently hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, aryl, alkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, 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.

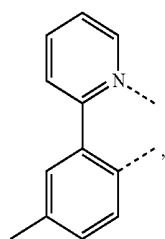
13. The compound of claim 10, wherein L_B is selected from the group consisting of:

 L_{B1}  L_{B2}  L_{B3}  L_{B4}  L_{B5}  L_{B6}

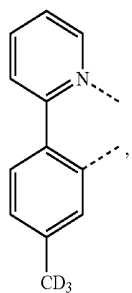
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 L_{B7}  L_{B8}  L_{B9}  L_{B10}  L_{B11}  L_{B12}

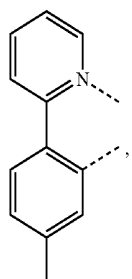
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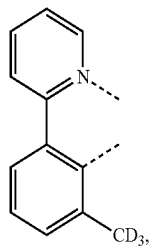
L_{B13}



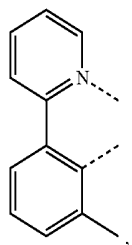
L_{B14}



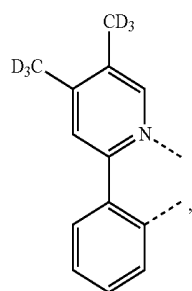
L_{B15}



L_{B16}

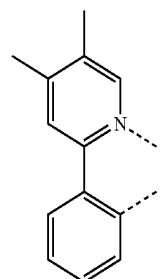


L_{B17}

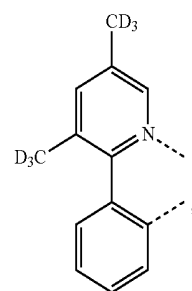


L_{B18}

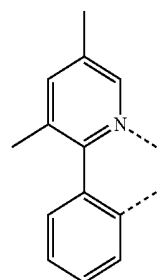
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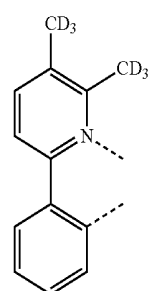
L_{B19}



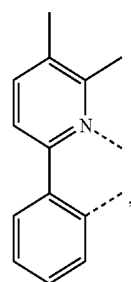
L_{B20}



L_{B21}

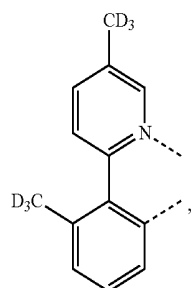


L_{B22}

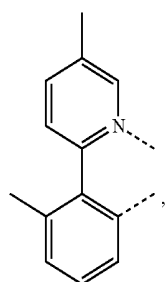


L_{B23}

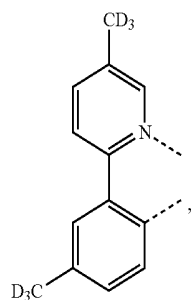
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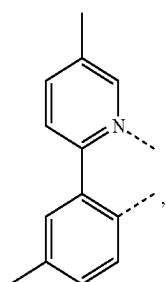
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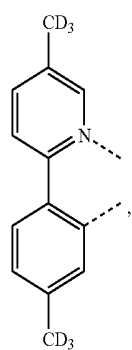
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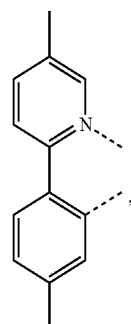


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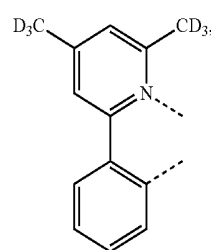


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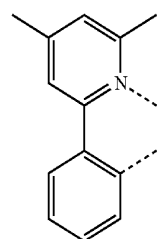
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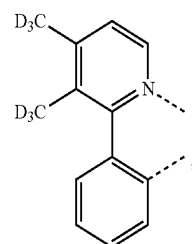
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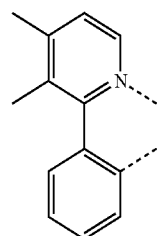
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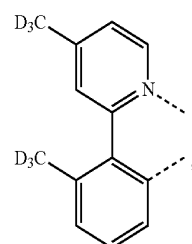
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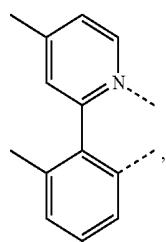


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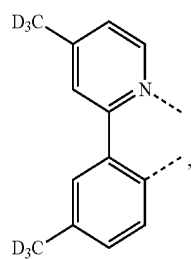


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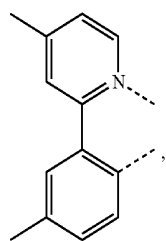
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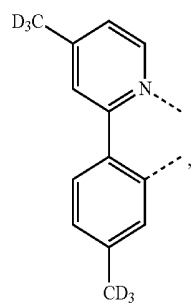
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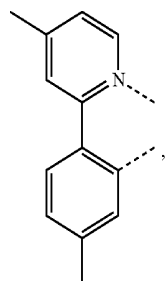
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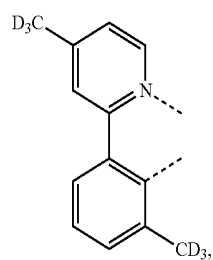
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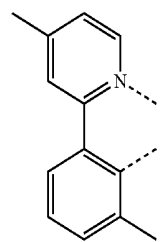


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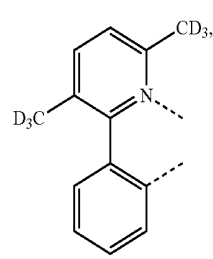


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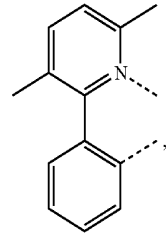
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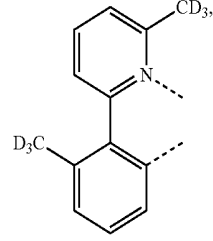
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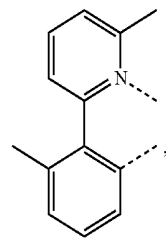
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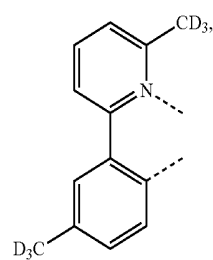
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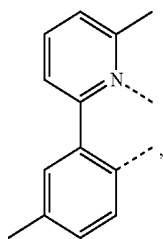


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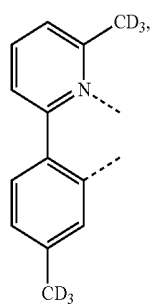


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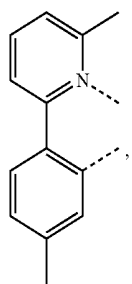
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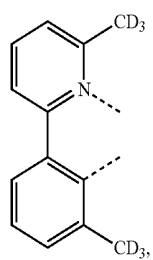
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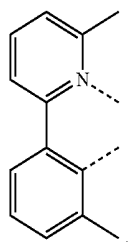
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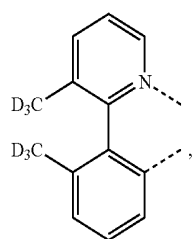
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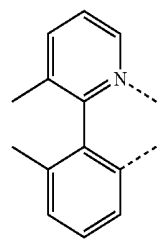


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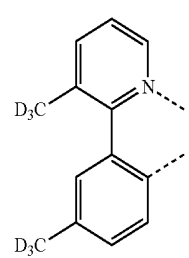


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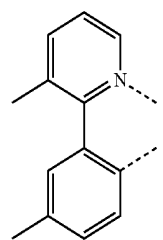
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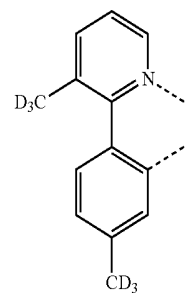
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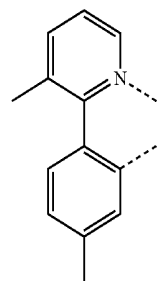
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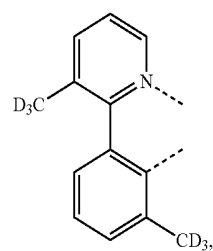
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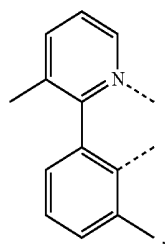


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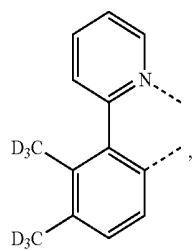


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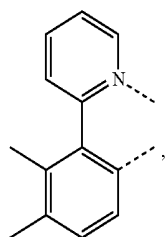
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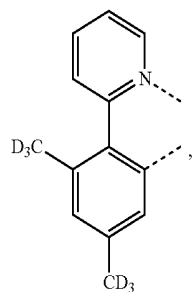
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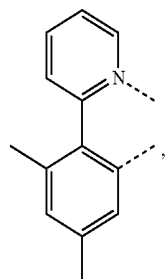
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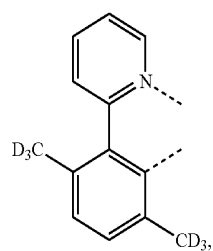
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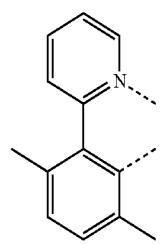


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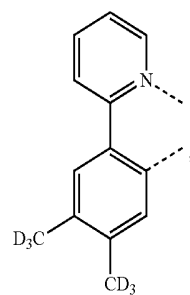


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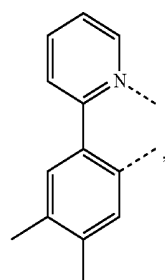
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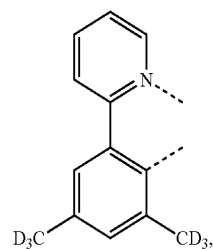
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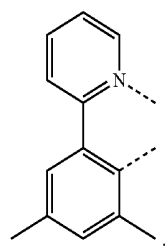
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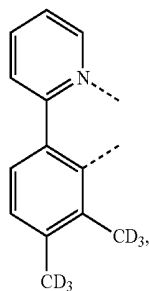


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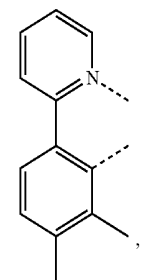


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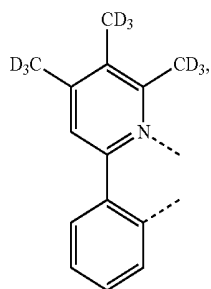
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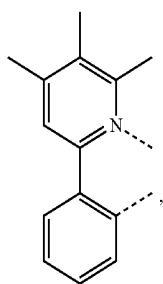
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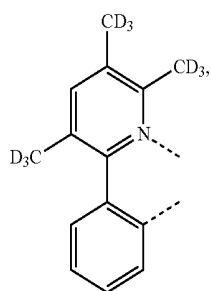
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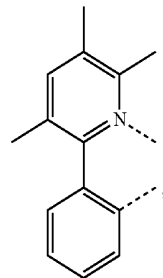


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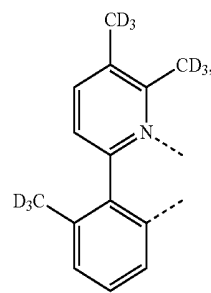


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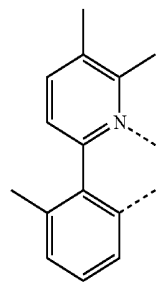
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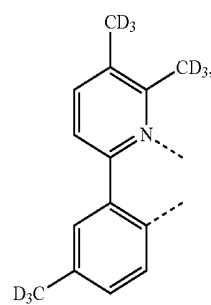
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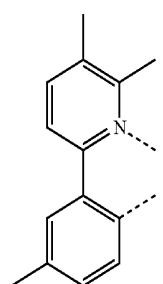
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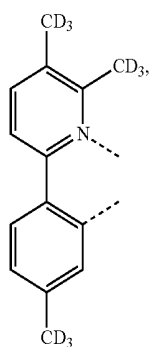


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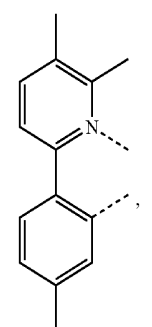


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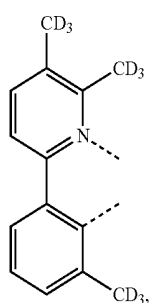
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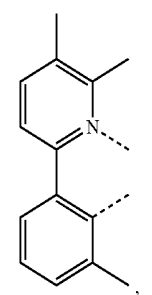
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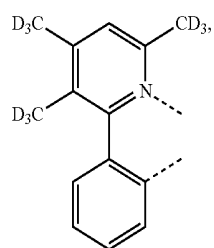
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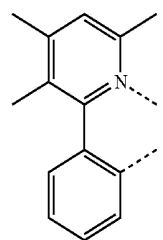


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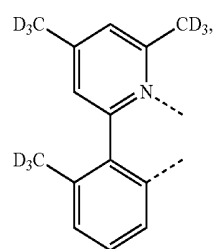


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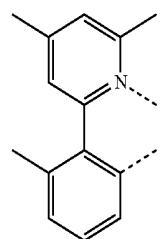
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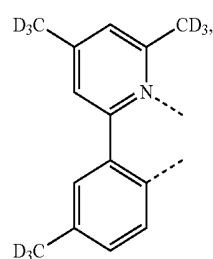
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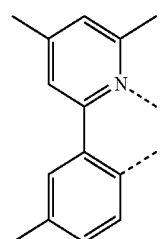
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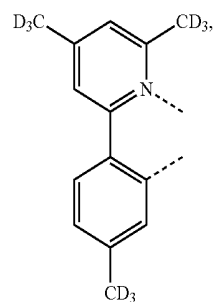
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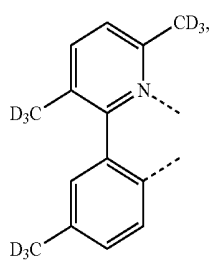
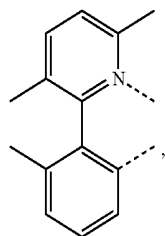
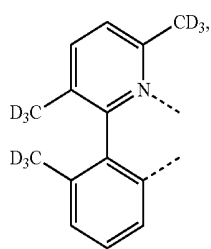
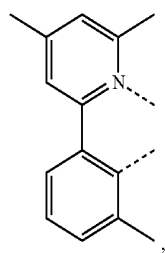
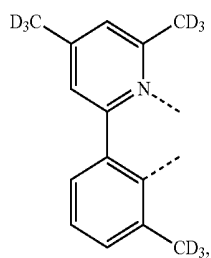
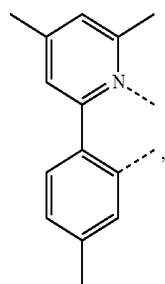


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L_{B91}

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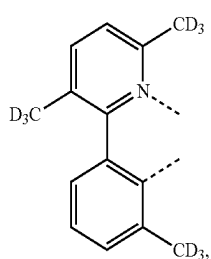
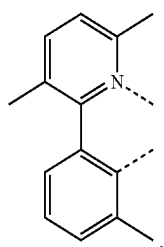
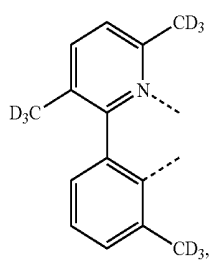
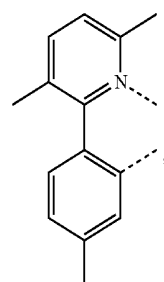
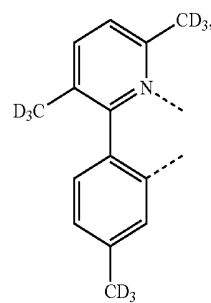
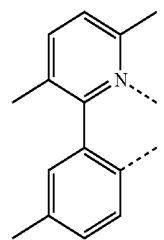
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L_{B97}

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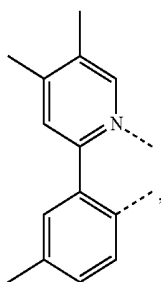
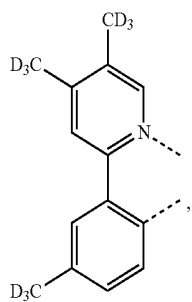
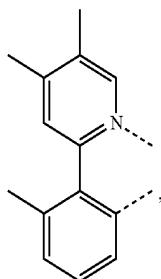
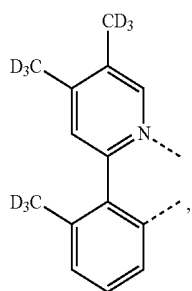
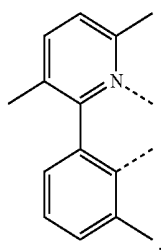
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L_{B103}

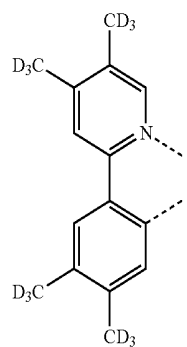
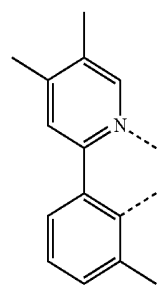
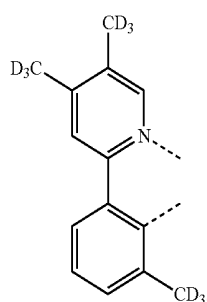
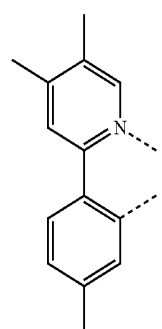
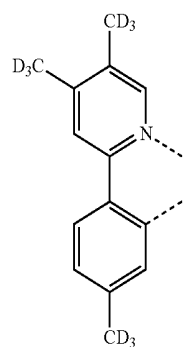
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L_{B108}

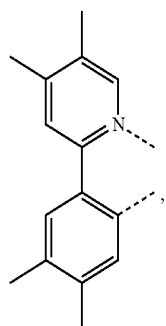
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L_{B110}

L_{B111}

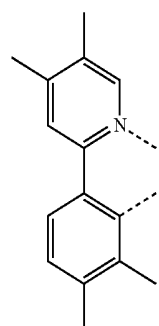
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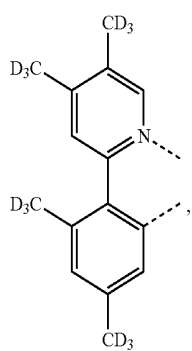


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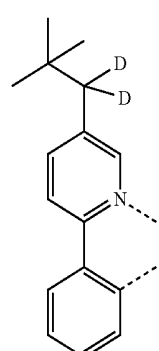
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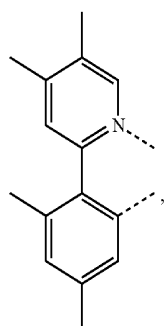
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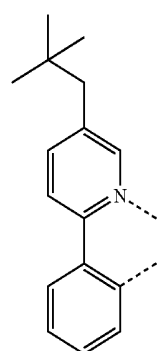
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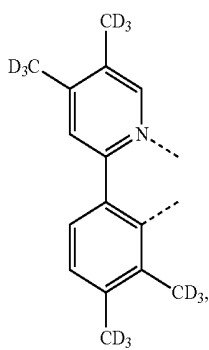
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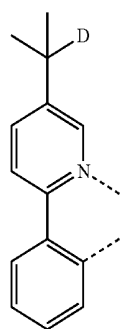
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L_{B119}

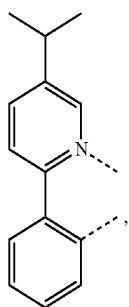


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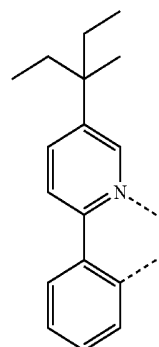
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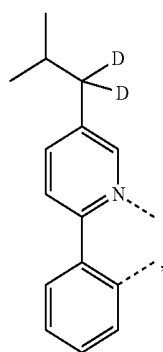


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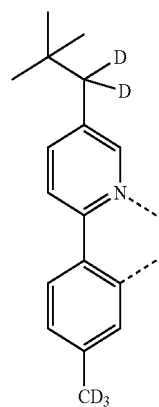
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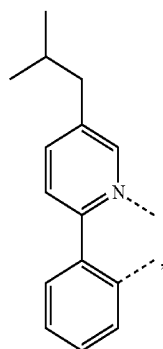
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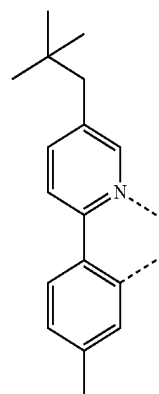
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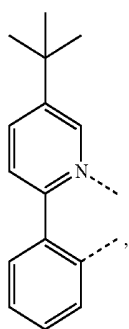
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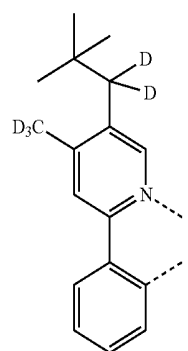
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LB127

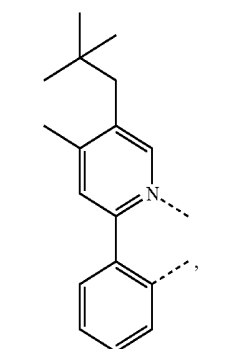


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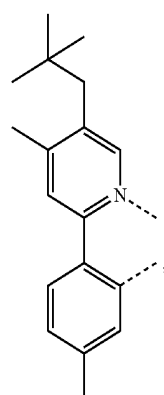
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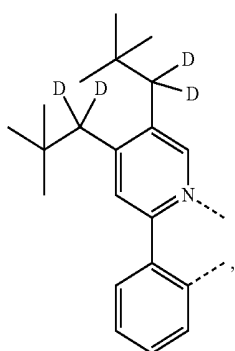


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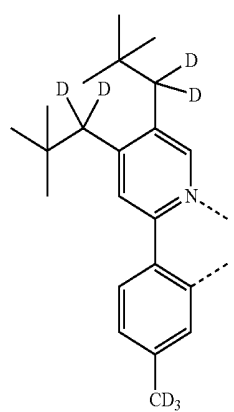
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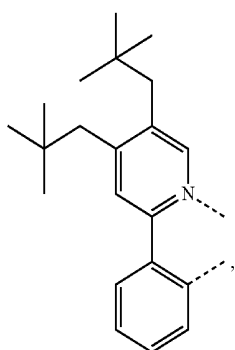
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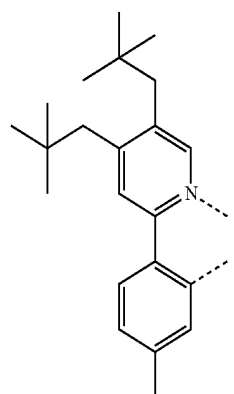
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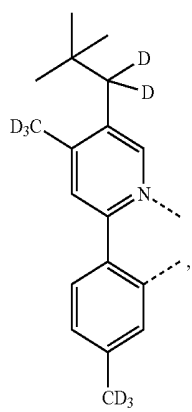
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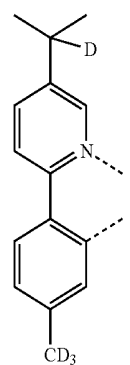
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LB135

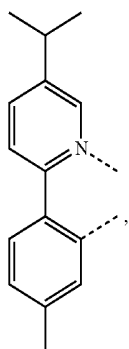


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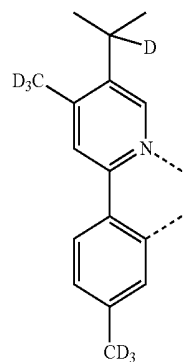
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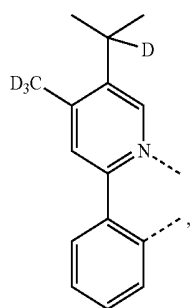


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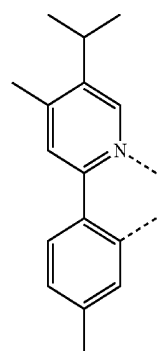
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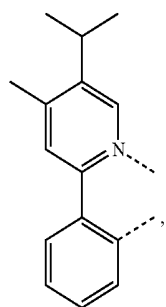
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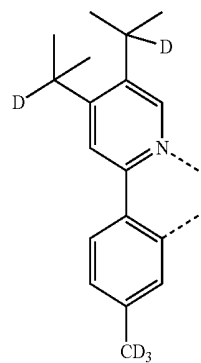
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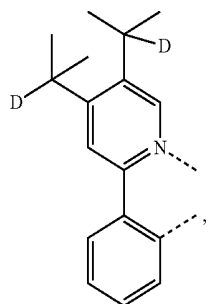
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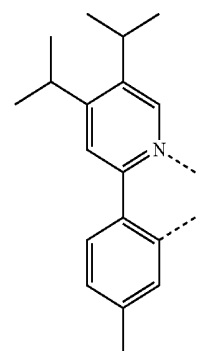
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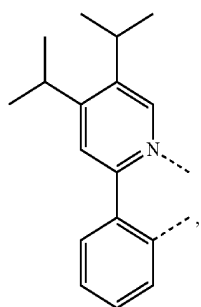
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LB140

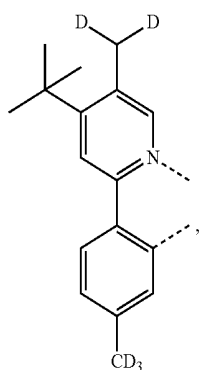


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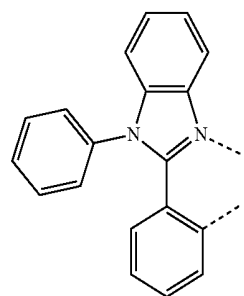
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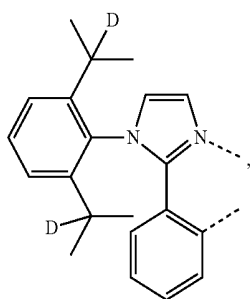


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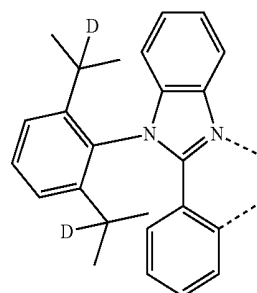
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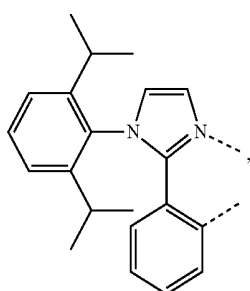
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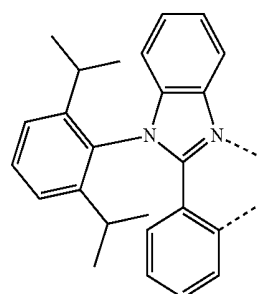
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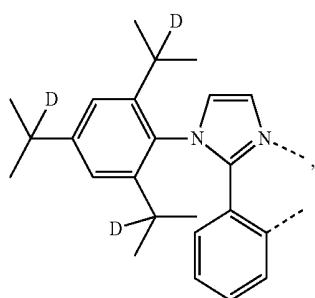
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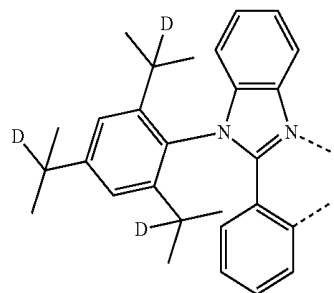
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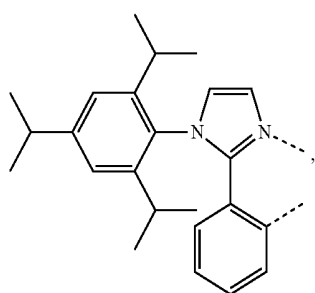
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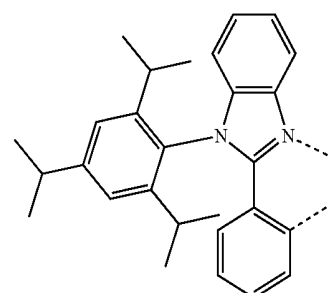
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L_{B154}

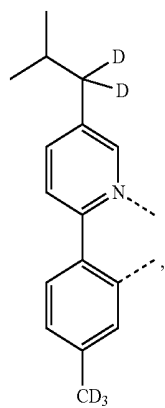


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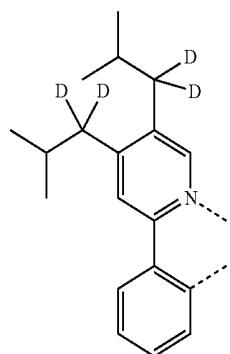
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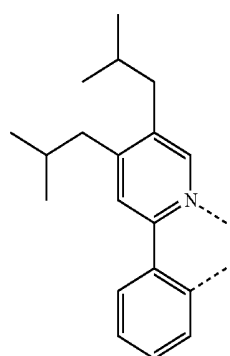
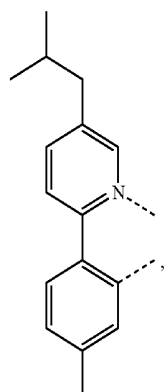
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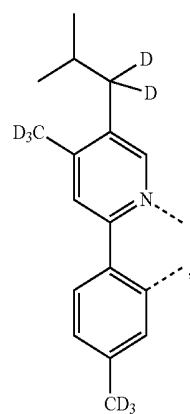
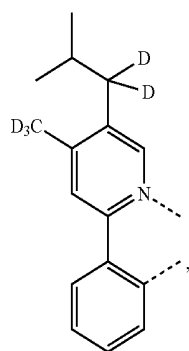
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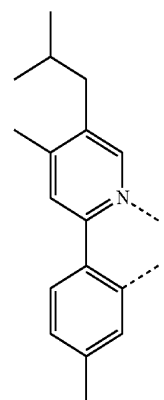
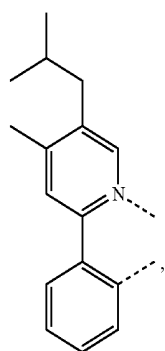
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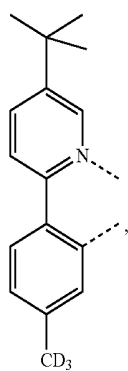
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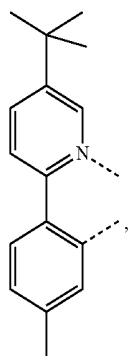


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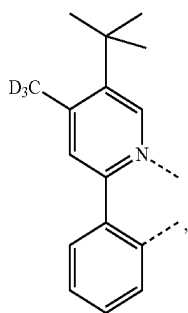
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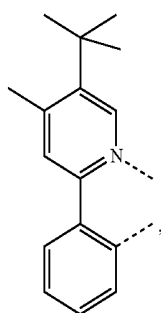
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LB165

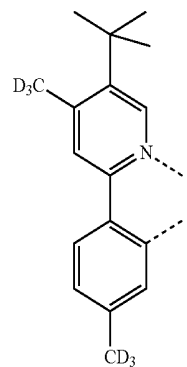


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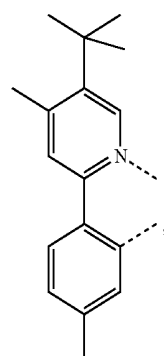


LB167

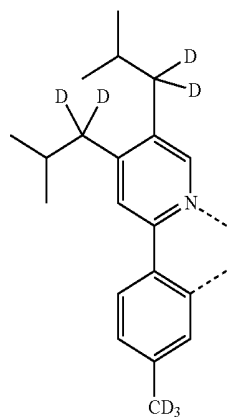
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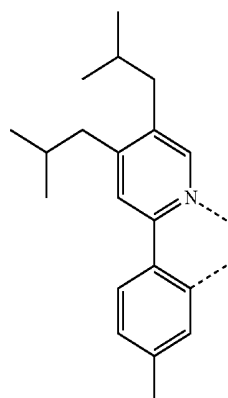
LB168



LB169

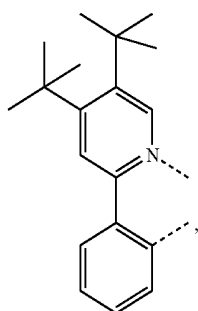


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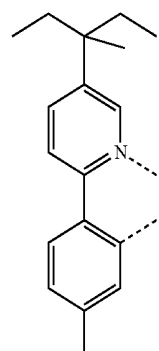
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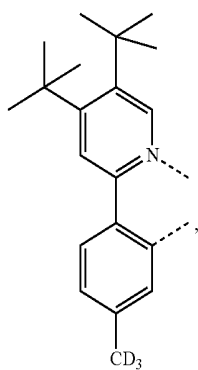


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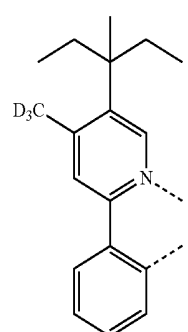
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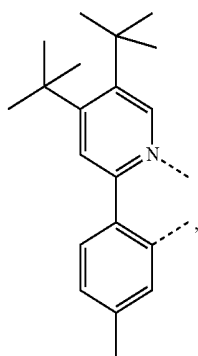
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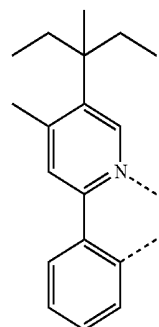
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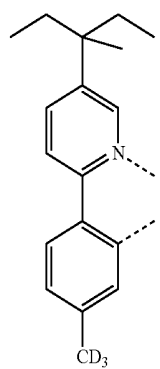
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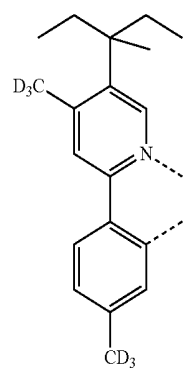
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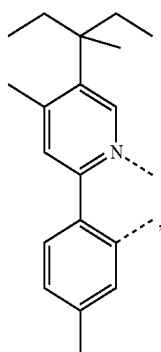


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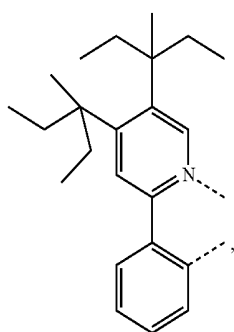


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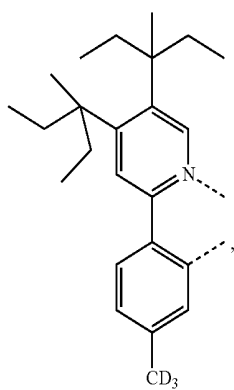
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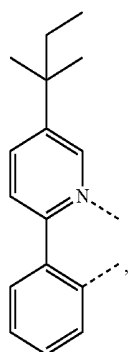
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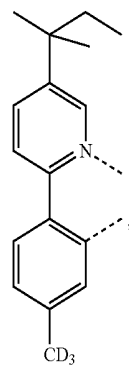


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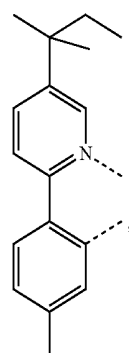


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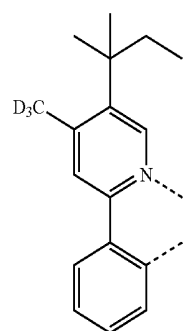
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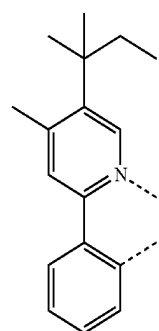
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L_{B185}

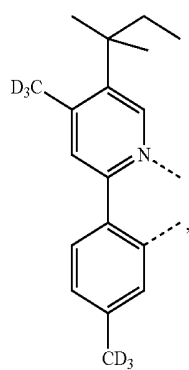


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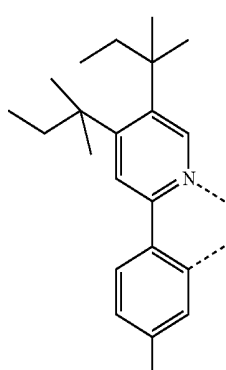
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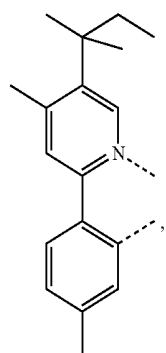


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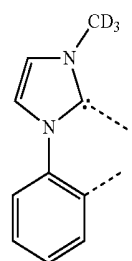
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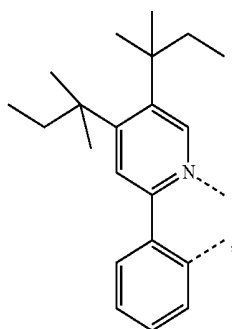
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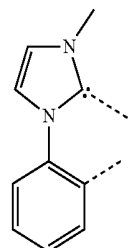
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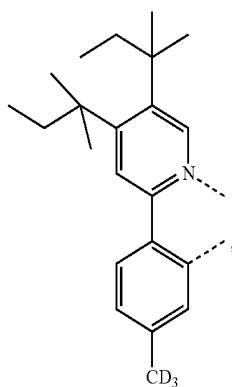
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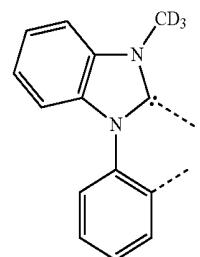
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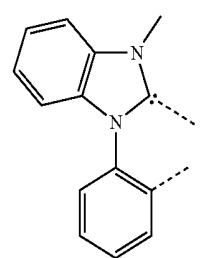
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LB191

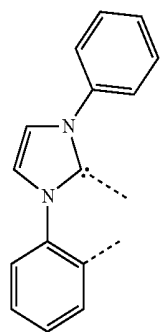


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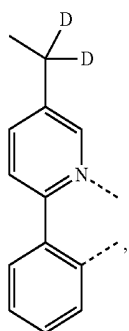


LB196

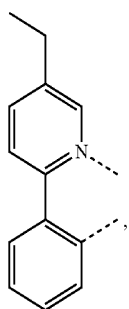
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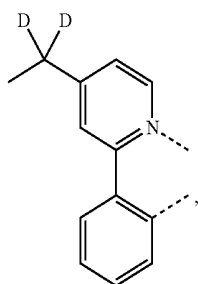
LB197



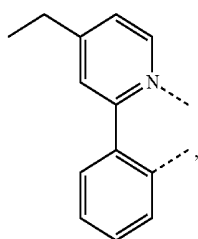
LB198



LB199

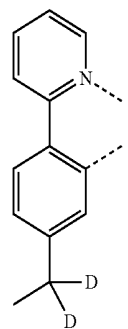


LB200

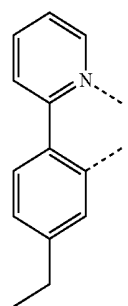


LB201

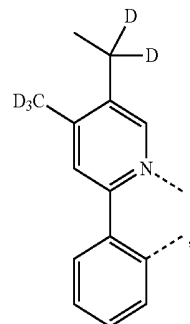
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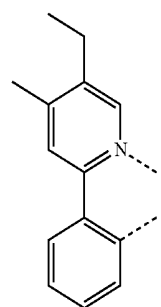
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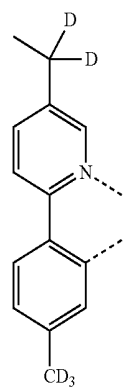
LB203



LB204

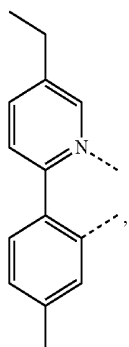


LB205



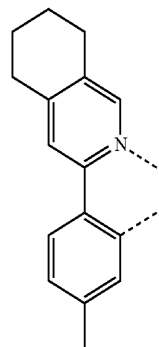
LB206

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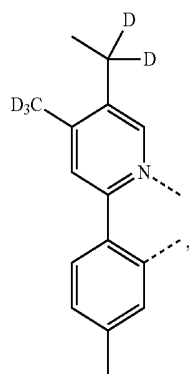


L_{B207}

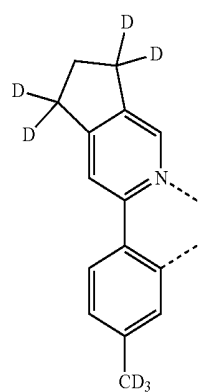
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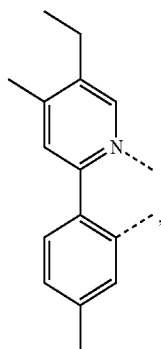
L_{B211}



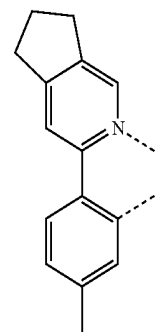
L_{B208}



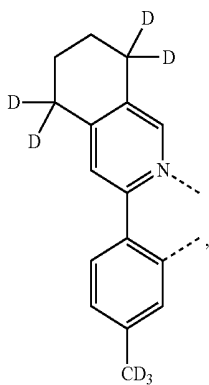
L_{B212}



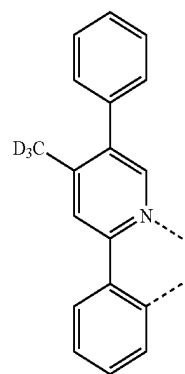
L_{B209}



L_{B213}

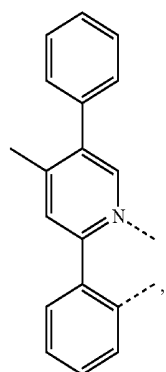


L_{B210}

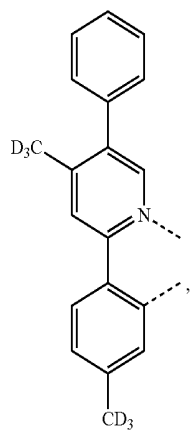


L_{B214}

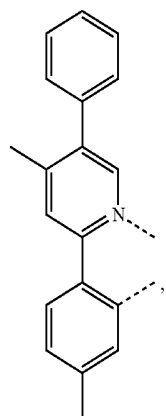
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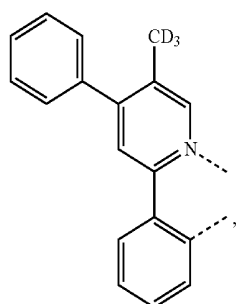
L_{B215}



L_{B216}

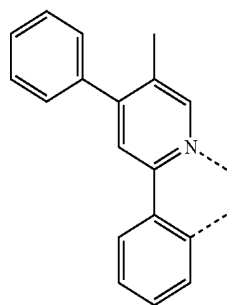


L_{B217}

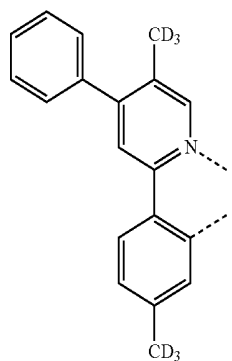


L_{B218}

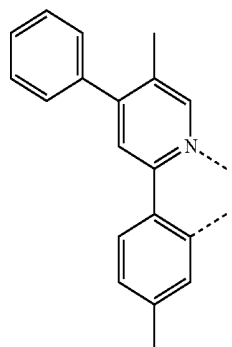
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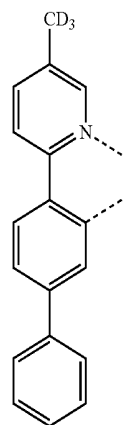
L_{B219}



L_{B220}

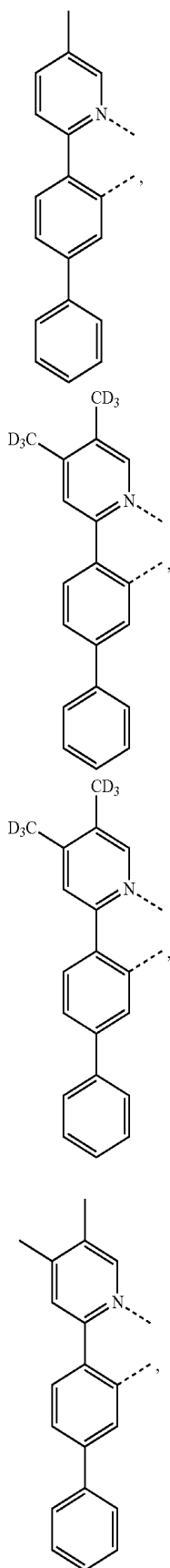


L_{B221}



L_{B222}

-continued



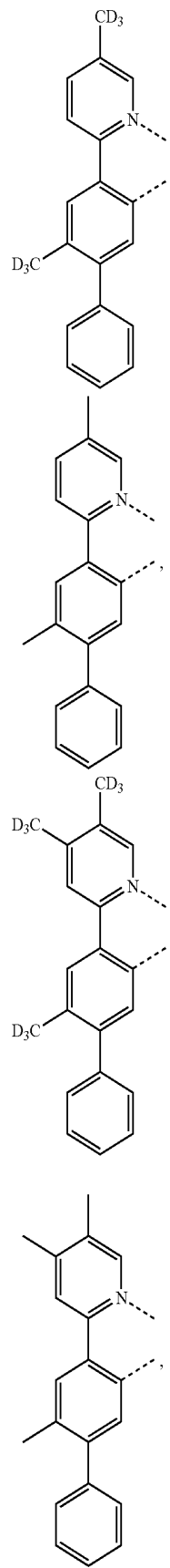
LB223

LB224

LB225

LB226

-continued



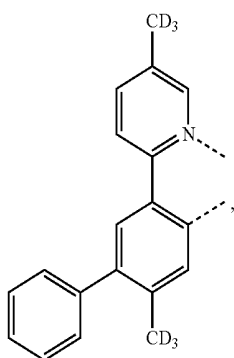
LB227

LB228

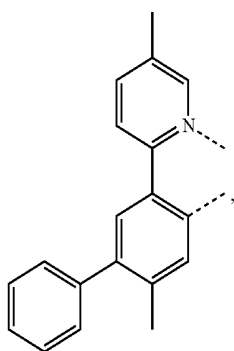
LB229

LB230

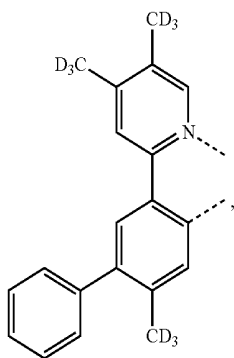
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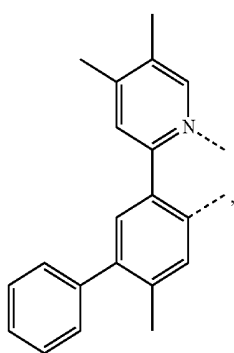
L_{B231}



L_{B232}

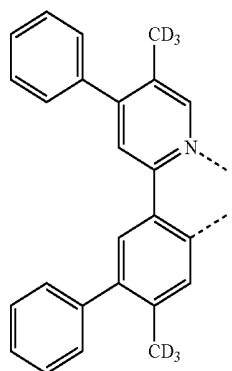


L_{B233}

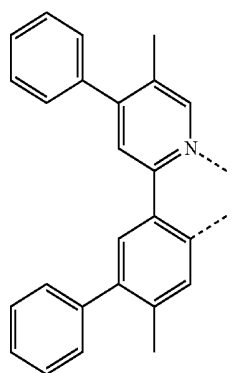


L_{B234}

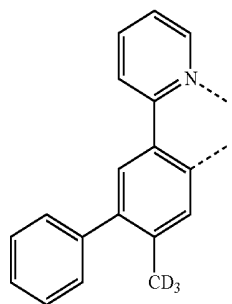
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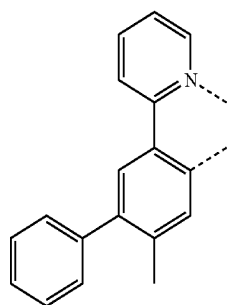
L_{B235}



L_{B236}

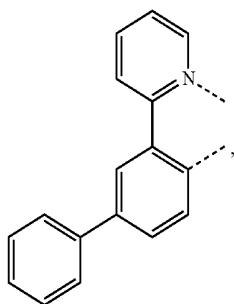


L_{B237}

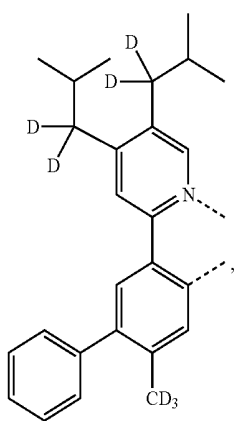


L_{B238}

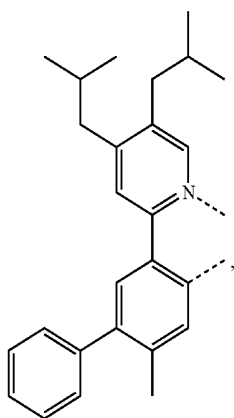
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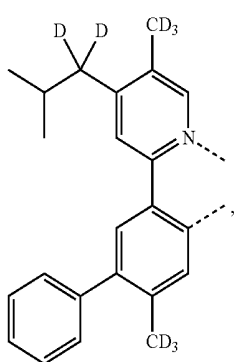
L_{B239}



L_{B240}

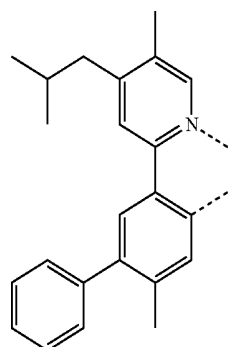


L_{B241}

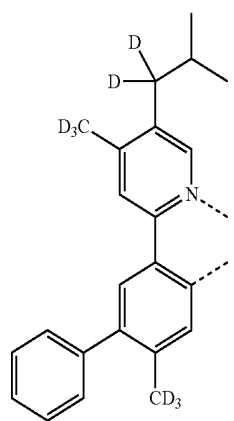


L_{B242}

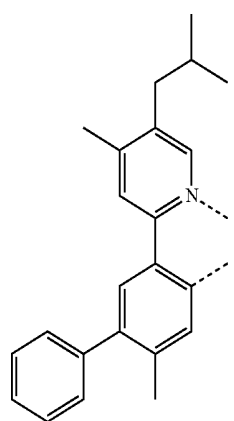
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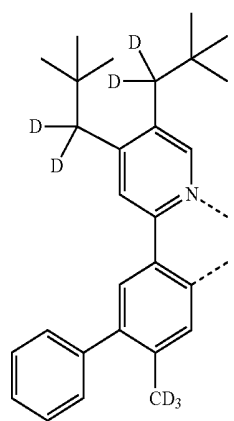
L_{B243}



L_{B244}

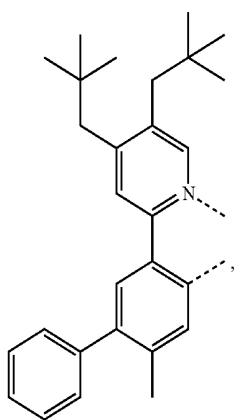


L_{B245}



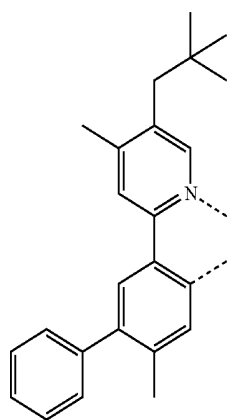
L_{B246}

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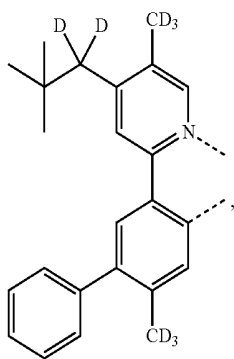


L_{B247}

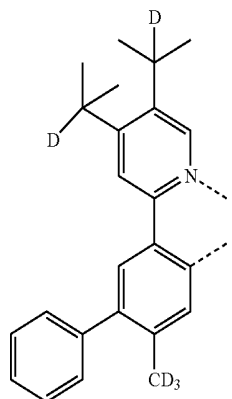
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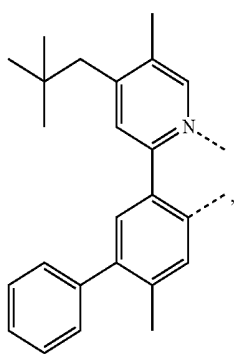
L_{B251}



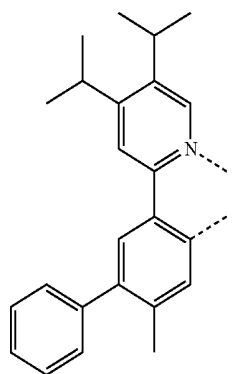
L_{B248}



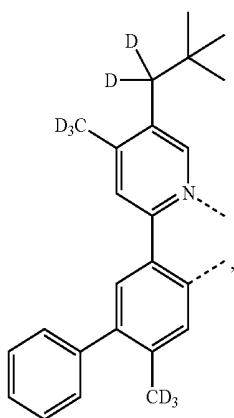
L_{B252}



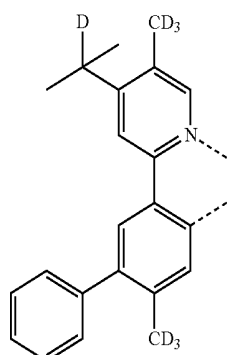
L_{B249}



L_{B253}

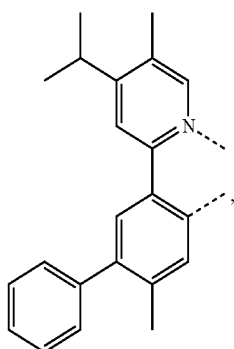


L_{B250}



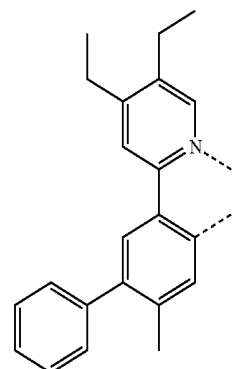
L_{B254}

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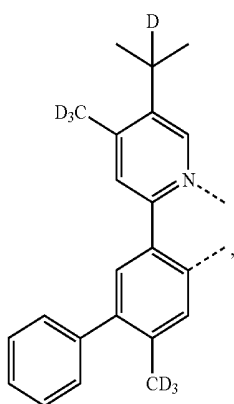


L_{B255}

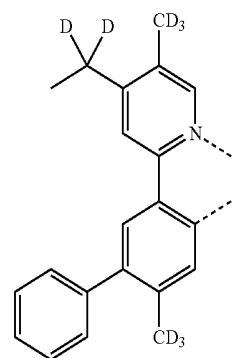
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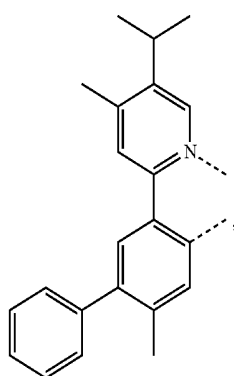
L_{B259}



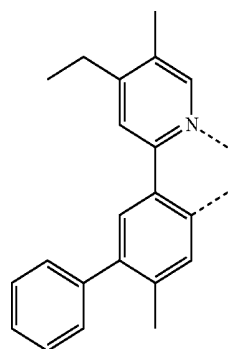
L_{B256}



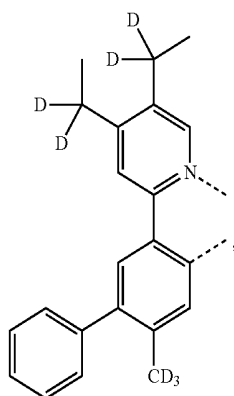
L_{B260}



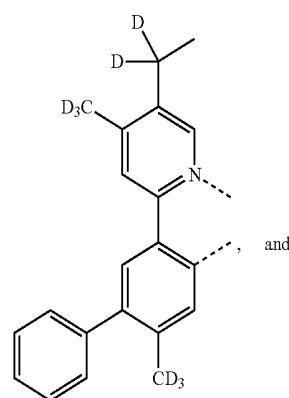
L_{B257}



L_{B261}



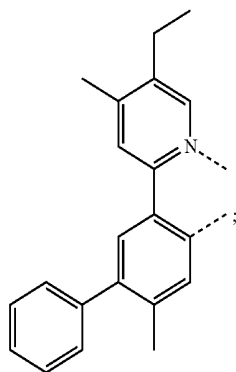
L_{B258}



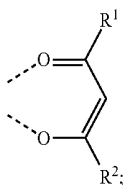
L_{B262}

and

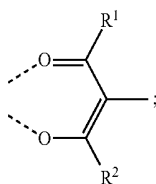
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and wherein L_C is selected from the group consisting of L_{C1-I} through L_{C768-I} with general numbering formula L_{Cj-I} (j is an integer of 1 to 768) based on a structure of



L_{C1-II} through $L_{C768-II}$ with general numbering formula L_{Cj-II} based on a structure of



wherein for each L_{Cj} , R^1 and R^2 are defined as:

| Ligand | R^1 | R^2 |
|-----------|-----------|-----------|
| L_{C1} | R^{D1} | R^{D1} |
| L_{C2} | R^{D2} | R^{D2} |
| L_{C3} | R^{D3} | R^{D3} |
| L_{C4} | R^{D4} | R^{D4} |
| L_{C5} | R^{D5} | R^{D5} |
| L_{C6} | R^{D6} | R^{D6} |
| L_{C7} | R^{D7} | R^{D7} |
| L_{C8} | R^{D8} | R^{D8} |
| L_{C9} | R^{D9} | R^{D9} |
| L_{C10} | R^{D10} | R^{D10} |
| L_{C11} | R^{D11} | R^{D11} |
| L_{C12} | R^{D12} | R^{D12} |
| L_{C13} | R^{D13} | R^{D13} |
| L_{C14} | R^{D14} | R^{D14} |
| L_{C15} | R^{D15} | R^{D15} |
| L_{C16} | R^{D16} | R^{D16} |
| L_{C17} | R^{D17} | R^{D17} |
| L_{C18} | R^{D18} | R^{D18} |
| L_{C19} | R^{D19} | R^{D19} |
| L_{C20} | R^{D20} | R^{D20} |
| L_{C21} | R^{D21} | R^{D21} |

L_{B263}

-continued

| Ligand | R^1 | R^2 |
|-----------|-----------|-----------|
| L_{C22} | R^{D22} | R^{D22} |
| L_{C23} | R^{D23} | R^{D23} |
| L_{C24} | R^{D24} | R^{D24} |
| L_{C25} | R^{D25} | R^{D25} |
| L_{C26} | R^{D26} | R^{D26} |
| L_{C27} | R^{D27} | R^{D27} |
| L_{C28} | R^{D28} | R^{D28} |
| L_{C29} | R^{D29} | R^{D29} |
| L_{C30} | R^{D30} | R^{D30} |
| L_{C31} | R^{D31} | R^{D31} |
| L_{C32} | R^{D32} | R^{D32} |
| L_{C33} | R^{D33} | R^{D33} |
| L_{C34} | R^{D34} | R^{D34} |
| L_{C35} | R^{D35} | R^{D35} |
| L_{C36} | R^{D36} | R^{D36} |
| L_{C37} | R^{D37} | R^{D37} |
| L_{C38} | R^{D38} | R^{D38} |
| L_{C39} | R^{D39} | R^{D39} |
| L_{C40} | R^{D40} | R^{D40} |
| L_{C41} | R^{D41} | R^{D41} |
| L_{C42} | R^{D42} | R^{D42} |
| L_{C43} | R^{D43} | R^{D43} |
| L_{C44} | R^{D44} | R^{D44} |
| L_{C45} | R^{D45} | R^{D45} |
| L_{C46} | R^{D46} | R^{D46} |
| L_{C47} | R^{D47} | R^{D47} |
| L_{C48} | R^{D48} | R^{D48} |
| L_{C49} | R^{D49} | R^{D49} |
| L_{C50} | R^{D50} | R^{D50} |
| L_{C51} | R^{D51} | R^{D51} |
| L_{C52} | R^{D52} | R^{D52} |
| L_{C53} | R^{D53} | R^{D53} |
| L_{C54} | R^{D54} | R^{D54} |
| L_{C55} | R^{D55} | R^{D55} |
| L_{C56} | R^{D56} | R^{D56} |
| L_{C57} | R^{D57} | R^{D57} |
| L_{C58} | R^{D58} | R^{D58} |
| L_{C59} | R^{D59} | R^{D59} |
| L_{C60} | R^{D60} | R^{D60} |
| L_{C61} | R^{D61} | R^{D61} |
| L_{C62} | R^{D62} | R^{D62} |
| L_{C63} | R^{D63} | R^{D63} |
| L_{C64} | R^{D64} | R^{D64} |
| L_{C65} | R^{D65} | R^{D65} |
| L_{C66} | R^{D66} | R^{D66} |
| L_{C67} | R^{D67} | R^{D67} |
| L_{C68} | R^{D68} | R^{D68} |
| L_{C69} | R^{D69} | R^{D69} |
| L_{C70} | R^{D70} | R^{D70} |
| L_{C71} | R^{D71} | R^{D71} |
| L_{C72} | R^{D72} | R^{D72} |
| L_{C73} | R^{D73} | R^{D73} |
| L_{C74} | R^{D74} | R^{D74} |
| L_{C75} | R^{D75} | R^{D75} |
| L_{C76} | R^{D76} | R^{D76} |
| L_{C77} | R^{D77} | R^{D77} |
| L_{C78} | R^{D78} | R^{D78} |
| L_{C79} | R^{D79} | R^{D79} |
| L_{C80} | R^{D80} | R^{D80} |
| L_{C81} | R^{D81} | R^{D81} |
| L_{C82} | R^{D82} | R^{D82} |
| L_{C83} | R^{D83} | R^{D83} |
| L_{C84} | R^{D84} | R^{D84} |
| L_{C85} | R^{D85} | R^{D85} |
| L_{C86} | R^{D86} | R^{D86} |
| L_{C87} | R^{D87} | R^{D87} |
| L_{C88} | R^{D88} | R^{D88} |
| L_{C89} | R^{D89} | R^{D89} |
| L_{C90} | R^{D90} | R^{D90} |
| L_{C91} | R^{D91} | R^{D91} |
| L_{C92} | R^{D92} | R^{D92} |
| L_{C93} | R^{D93} | R^{D93} |
| L_{C94} | R^{D94} | R^{D94} |
| L_{C95} | R^{D95} | R^{D95} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|-------------------|-------------------|
| L _{C96} | R ^{D96} | R ^{D96} |
| L _{C97} | R ^{D97} | R ^{D97} |
| L _{C98} | R ^{D98} | R ^{D98} |
| L _{C99} | R ^{D99} | R ^{D99} |
| L _{C100} | R ^{D100} | R ^{D100} |
| L _{C101} | R ^{D101} | R ^{D101} |
| L _{C102} | R ^{D102} | R ^{D102} |
| L _{C103} | R ^{D103} | R ^{D103} |
| L _{C104} | R ^{D104} | R ^{D104} |
| L _{C105} | R ^{D105} | R ^{D105} |
| L _{C106} | R ^{D106} | R ^{D106} |
| L _{C107} | R ^{D107} | R ^{D107} |
| L _{C108} | R ^{D108} | R ^{D108} |
| L _{C109} | R ^{D109} | R ^{D109} |
| L _{C110} | R ^{D110} | R ^{D110} |
| L _{C111} | R ^{D111} | R ^{D111} |
| L _{C112} | R ^{D112} | R ^{D112} |
| L _{C113} | R ^{D113} | R ^{D113} |
| L _{C114} | R ^{D114} | R ^{D114} |
| L _{C115} | R ^{D115} | R ^{D115} |
| L _{C116} | R ^{D116} | R ^{D116} |
| L _{C117} | R ^{D117} | R ^{D117} |
| L _{C118} | R ^{D118} | R ^{D118} |
| L _{C119} | R ^{D119} | R ^{D119} |
| L _{C120} | R ^{D120} | R ^{D120} |
| L _{C121} | R ^{D121} | R ^{D121} |
| L _{C122} | R ^{D122} | R ^{D122} |
| L _{C123} | R ^{D123} | R ^{D123} |
| L _{C124} | R ^{D124} | R ^{D124} |
| L _{C125} | R ^{D125} | R ^{D125} |
| L _{C126} | R ^{D126} | R ^{D126} |
| L _{C127} | R ^{D127} | R ^{D127} |
| L _{C128} | R ^{D128} | R ^{D128} |
| L _{C129} | R ^{D129} | R ^{D129} |
| L _{C130} | R ^{D130} | R ^{D130} |
| L _{C131} | R ^{D131} | R ^{D131} |
| L _{C132} | R ^{D132} | R ^{D132} |
| L _{C133} | R ^{D133} | R ^{D133} |
| L _{C134} | R ^{D134} | R ^{D134} |
| L _{C135} | R ^{D135} | R ^{D135} |
| L _{C136} | R ^{D136} | R ^{D136} |
| L _{C137} | R ^{D137} | R ^{D137} |
| L _{C138} | R ^{D138} | R ^{D138} |
| L _{C139} | R ^{D139} | R ^{D139} |
| L _{C140} | R ^{D140} | R ^{D140} |
| L _{C141} | R ^{D141} | R ^{D141} |
| L _{C142} | R ^{D142} | R ^{D142} |
| L _{C143} | R ^{D143} | R ^{D143} |
| L _{C144} | R ^{D144} | R ^{D144} |
| L _{C145} | R ^{D145} | R ^{D145} |
| L _{C146} | R ^{D146} | R ^{D146} |
| L _{C147} | R ^{D147} | R ^{D147} |
| L _{C148} | R ^{D148} | R ^{D148} |
| L _{C149} | R ^{D149} | R ^{D149} |
| L _{C150} | R ^{D150} | R ^{D150} |
| L _{C151} | R ^{D151} | R ^{D151} |
| L _{C152} | R ^{D152} | R ^{D152} |
| L _{C153} | R ^{D153} | R ^{D153} |
| L _{C154} | R ^{D154} | R ^{D154} |
| L _{C155} | R ^{D155} | R ^{D155} |
| L _{C156} | R ^{D156} | R ^{D156} |
| L _{C157} | R ^{D157} | R ^{D157} |
| L _{C158} | R ^{D158} | R ^{D158} |
| L _{C159} | R ^{D159} | R ^{D159} |
| L _{C160} | R ^{D160} | R ^{D160} |
| L _{C161} | R ^{D161} | R ^{D161} |
| L _{C162} | R ^{D162} | R ^{D162} |
| L _{C163} | R ^{D163} | R ^{D163} |
| L _{C164} | R ^{D164} | R ^{D164} |
| L _{C165} | R ^{D165} | R ^{D165} |
| L _{C166} | R ^{D166} | R ^{D166} |
| L _{C167} | R ^{D167} | R ^{D167} |
| L _{C168} | R ^{D168} | R ^{D168} |
| L _{C169} | R ^{D169} | R ^{D169} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|-------------------|-------------------|
| L _{C170} | R ^{D170} | R ^{D170} |
| L _{C171} | R ^{D171} | R ^{D171} |
| L _{C172} | R ^{D172} | R ^{D172} |
| L _{C173} | R ^{D173} | R ^{D173} |
| L _{C174} | R ^{D174} | R ^{D174} |
| L _{C175} | R ^{D175} | R ^{D175} |
| L _{C176} | R ^{D176} | R ^{D176} |
| L _{C177} | R ^{D177} | R ^{D177} |
| L _{C178} | R ^{D178} | R ^{D178} |
| L _{C179} | R ^{D179} | R ^{D179} |
| L _{C180} | R ^{D180} | R ^{D180} |
| L _{C181} | R ^{D181} | R ^{D181} |
| L _{C182} | R ^{D182} | R ^{D182} |
| L _{C183} | R ^{D183} | R ^{D183} |
| L _{C184} | R ^{D184} | R ^{D184} |
| L _{C185} | R ^{D185} | R ^{D185} |
| L _{C186} | R ^{D186} | R ^{D186} |
| L _{C187} | R ^{D187} | R ^{D187} |
| L _{C188} | R ^{D188} | R ^{D188} |
| L _{C189} | R ^{D189} | R ^{D189} |
| L _{C180} | R ^{D180} | R ^{D180} |
| L _{C191} | R ^{D191} | R ^{D191} |
| L _{C192} | R ^{D192} | R ^{D192} |
| L _{C193} | R ^{D1} | R ^{D3} |
| L _{C194} | R ^{D1} | R ^{D4} |
| L _{C195} | R ^{D1} | R ^{D5} |
| L _{C196} | R ^{D1} | R ^{D9} |
| L _{C197} | R ^{D1} | R ^{D10} |
| L _{C198} | R ^{D1} | R ^{D17} |
| L _{C199} | R ^{D1} | R ^{D18} |
| L _{C200} | R ^{D1} | R ^{D20} |
| L _{C201} | R ^{D1} | R ^{D22} |
| L _{C202} | R ^{D1} | R ^{D37} |
| L _{C203} | R ^{D1} | R ^{D40} |
| L _{C204} | R ^{D1} | R ^{D41} |
| L _{C205} | R ^{D1} | R ^{D42} |
| L _{C206} | R ^{D1} | R ^{D43} |
| L _{C207} | R ^{D1} | R ^{D48} |
| L _{C208} | R ^{D1} | R ^{D49} |
| L _{C209} | R ^{D1} | R ^{D50} |
| L _{C210} | R ^{D1} | R ^{D54} |
| L _{C211} | R ^{D1} | R ^{D55} |
| L _{C212} | R ^{D1} | R ^{D58} |
| L _{C213} | R ^{D1} | R ^{D59} |
| L _{C214} | R ^{D1} | R ^{D78} |
| L _{C215} | R ^{D1} | R ^{D79} |
| L _{C216} | R ^{D1} | R ^{D81} |
| L _{C217} | R ^{D1} | R ^{D87} |
| L _{C218} | R ^{D1} | R ^{D88} |
| L _{C219} | R ^{D1} | R ^{D89} |
| L _{C220} | R ^{D1} | R ^{D93} |
| L _{C221} | R ^{D1} | R ^{D116} |
| L _{C222} | R ^{D1} | R ^{D117} |
| L _{C223} | R ^{D1} | R ^{D118} |
| L _{C224} | R ^{D1} | R ^{D119} |
| L _{C225} | R ^{D1} | R ^{D120} |
| L _{C226} | R ^{D1} | R ^{D133} |
| L _{C227} | R ^{D1} | R ^{D134} |
| L _{C228} | R ^{D1} | R ^{D135} |
| L _{C229} | R ^{D1} | R ^{D136} |
| L _{C230} | R ^{D1} | R ^{D143} |
| L _{C231} | R ^{D1} | R ^{D144} |
| L _{C232} | R ^{D1} | R ^{D145} |
| L _{C233} | R ^{D1} | R ^{D146} |
| L _{C234} | R ^{D1} | R ^{D147} |
| L _{C235} | R ^{D1} | R ^{D149} |
| L _{C236} | R ^{D1} | R ^{D151} |
| L _{C237} | R ^{D1} | R ^{D154} |
| L _{C238} | R ^{D1} | R ^{D155} |
| L _{C239} | R ^{D1} | R ^{D161} |
| L _{C240} | R ^{D1} | R ^{D175} |
| L _{C241} | R ^{D4} | R ^{D3} |
| L _{C242} | R ^{D4} | R ^{D5} |
| L _{C243} | R ^{D4} | R ^{D9} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|-----------------|-------------------|
| L _{C244} | R ^{D4} | R ^{D10} |
| L _{C245} | R ^{D4} | R ^{D17} |
| L _{C246} | R ^{D4} | R ^{D18} |
| L _{C247} | R ^{D4} | R ^{D20} |
| L _{C248} | R ^{D4} | R ^{D22} |
| L _{C249} | R ^{D4} | R ^{D37} |
| L _{C250} | R ^{D4} | R ^{D40} |
| L _{C251} | R ^{D4} | R ^{D41} |
| L _{C252} | R ^{D4} | R ^{D42} |
| L _{C253} | R ^{D4} | R ^{D43} |
| L _{C254} | R ^{D4} | R ^{D48} |
| L _{C255} | R ^{D4} | R ^{D49} |
| L _{C256} | R ^{D4} | R ^{D50} |
| L _{C257} | R ^{D4} | R ^{D54} |
| L _{C258} | R ^{D4} | R ^{D55} |
| L _{C259} | R ^{D4} | R ^{D58} |
| L _{C260} | R ^{D4} | R ^{D59} |
| L _{C261} | R ^{D4} | R ^{D78} |
| L _{C262} | R ^{D4} | R ^{D79} |
| L _{C263} | R ^{D4} | R ^{D81} |
| L _{C264} | R ^{D4} | R ^{D87} |
| L _{C265} | R ^{D4} | R ^{D88} |
| L _{C266} | R ^{D4} | R ^{D89} |
| L _{C267} | R ^{D4} | R ^{D93} |
| L _{C268} | R ^{D4} | R ^{D116} |
| L _{C269} | R ^{D4} | R ^{D117} |
| L _{C270} | R ^{D4} | R ^{D118} |
| L _{C271} | R ^{D4} | R ^{D119} |
| L _{C272} | R ^{D4} | R ^{D120} |
| L _{C273} | R ^{D4} | R ^{D133} |
| L _{C274} | R ^{D4} | R ^{D134} |
| L _{C275} | R ^{D4} | R ^{D135} |
| L _{C276} | R ^{D4} | R ^{D136} |
| L _{C277} | R ^{D4} | R ^{D143} |
| L _{C278} | R ^{D4} | R ^{D144} |
| L _{C279} | R ^{D4} | R ^{D145} |
| L _{C280} | R ^{D4} | R ^{D146} |
| L _{C281} | R ^{D4} | R ^{D147} |
| L _{C282} | R ^{D4} | R ^{D149} |
| L _{C283} | R ^{D4} | R ^{D151} |
| L _{C284} | R ^{D4} | R ^{D154} |
| L _{C285} | R ^{D4} | R ^{D155} |
| L _{C286} | R ^{D4} | R ^{D161} |
| L _{C287} | R ^{D4} | R ^{D175} |
| L _{C288} | R ^{D9} | R ^{D3} |
| L _{C289} | R ^{D9} | R ^{D5} |
| L _{C280} | R ^{D9} | R ^{D10} |
| L _{C291} | R ^{D9} | R ^{D17} |
| L _{C292} | R ^{D9} | R ^{D18} |
| L _{C293} | R ^{D9} | R ^{D20} |
| L _{C294} | R ^{D9} | R ^{D22} |
| L _{C295} | R ^{D9} | R ^{D37} |
| L _{C296} | R ^{D9} | R ^{D40} |
| L _{C297} | R ^{D9} | R ^{D41} |
| L _{C298} | R ^{D9} | R ^{D42} |
| L _{C299} | R ^{D9} | R ^{D43} |
| L _{C300} | R ^{D9} | R ^{D48} |
| L _{C301} | R ^{D9} | R ^{D49} |
| L _{C302} | R ^{D9} | R ^{D50} |
| L _{C303} | R ^{D9} | R ^{D54} |
| L _{C304} | R ^{D9} | R ^{D55} |
| L _{C305} | R ^{D9} | R ^{D58} |
| L _{C306} | R ^{D9} | R ^{D59} |
| L _{C307} | R ^{D9} | R ^{D78} |
| L _{C308} | R ^{D9} | R ^{D79} |
| L _{C309} | R ^{D9} | R ^{D81} |
| L _{C310} | R ^{D9} | R ^{D87} |
| L _{C311} | R ^{D9} | R ^{D88} |
| L _{C312} | R ^{D9} | R ^{D89} |
| L _{C313} | R ^{D9} | R ^{D93} |
| L _{C314} | R ^{D9} | R ^{D116} |
| L _{C315} | R ^{D9} | R ^{D117} |
| L _{C316} | R ^{D9} | R ^{D118} |
| L _{C317} | R ^{D9} | R ^{D119} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|------------------|-------------------|
| L _{C318} | R ^{D9} | R ^{D120} |
| L _{C319} | R ^{D9} | R ^{D133} |
| L _{C320} | R ^{D9} | R ^{D134} |
| L _{C321} | R ^{D9} | R ^{D135} |
| L _{C322} | R ^{D9} | R ^{D136} |
| L _{C323} | R ^{D9} | R ^{D143} |
| L _{C324} | R ^{D9} | R ^{D144} |
| L _{C325} | R ^{D9} | R ^{D145} |
| L _{C326} | R ^{D9} | R ^{D146} |
| L _{C327} | R ^{D9} | R ^{D147} |
| L _{C328} | R ^{D9} | R ^{D149} |
| L _{C329} | R ^{D9} | R ^{D151} |
| L _{C330} | R ^{D9} | R ^{D154} |
| L _{C331} | R ^{D9} | R ^{D155} |
| L _{C332} | R ^{D9} | R ^{D161} |
| L _{C333} | R ^{D9} | R ^{D175} |
| L _{C334} | R ^{D10} | R ^{D3} |
| L _{C335} | R ^{D10} | R ^{D5} |
| L _{C336} | R ^{D10} | R ^{D17} |
| L _{C337} | R ^{D10} | R ^{D18} |
| L _{C338} | R ^{D10} | R ^{D20} |
| L _{C339} | R ^{D10} | R ^{D22} |
| L _{C340} | R ^{D10} | R ^{D37} |
| L _{C341} | R ^{D10} | R ^{D40} |
| L _{C342} | R ^{D10} | R ^{D41} |
| L _{C343} | R ^{D10} | R ^{D42} |
| L _{C344} | R ^{D10} | R ^{D43} |
| L _{C345} | R ^{D10} | R ^{D48} |
| L _{C346} | R ^{D10} | R ^{D49} |
| L _{C347} | R ^{D10} | R ^{D50} |
| L _{C348} | R ^{D10} | R ^{D54} |
| L _{C349} | R ^{D10} | R ^{D55} |
| L _{C350} | R ^{D10} | R ^{D58} |
| L _{C351} | R ^{D10} | R ^{D59} |
| L _{C352} | R ^{D10} | R ^{D78} |
| L _{C353} | R ^{D10} | R ^{D79} |
| L _{C354} | R ^{D10} | R ^{D81} |
| L _{C355} | R ^{D10} | R ^{D87} |
| L _{C356} | R ^{D10} | R ^{D88} |
| L _{C357} | R ^{D10} | R ^{D89} |
| L _{C358} | R ^{D10} | R ^{D93} |
| L _{C359} | R ^{D10} | R ^{D116} |
| L _{C360} | R ^{D10} | R ^{D117} |
| L _{C361} | R ^{D10} | R ^{D118} |
| L _{C362} | R ^{D10} | R ^{D119} |
| L _{C363} | R ^{D10} | R ^{D120} |
| L _{C364} | R ^{D10} | R ^{D133} |
| L _{C365} | R ^{D10} | R ^{D134} |
| L _{C366} | R ^{D10} | R ^{D135} |
| L _{C367} | R ^{D10} | R ^{D136} |
| L _{C368} | R ^{D10} | R ^{D143} |
| L _{C369} | R ^{D10} | R ^{D144} |
| L _{C370} | R ^{D10} | R ^{D145} |
| L _{C371} | R ^{D10} | R ^{D146} |
| L _{C372} | R ^{D10} | R ^{D147} |
| L _{C373} | R ^{D10} | R ^{D149} |
| L _{C374} | R ^{D10} | R ^{D151} |
| L _{C375} | R ^{D10} | R ^{D154} |
| L _{C376} | R ^{D10} | R ^{D155} |
| L _{C377} | R ^{D10} | R ^{D161} |
| L _{C378} | R ^{D10} | R ^{D175} |
| L _{C379} | R ^{D17} | R ^{D3} |
| L _{C380} | R ^{D17} | R ^{D5} |
| L _{C381} | R ^{D17} | R ^{D18} |
| L _{C382} | R ^{D17} | R ^{D20} |
| L _{C383} | R ^{D17} | R ^{D22} |
| L _{C384} | R ^{D17} | R ^{D37} |
| L _{C385} | R ^{D17} | R ^{D40} |
| L _{C386} | R ^{D17} | R ^{D41} |
| L _{C387} | R ^{D17} | R ^{D42} |
| L _{C388} | R ^{D17} | R ^{D43} |
| L _{C389} | R ^{D17} | R ^{D48} |
| L _{C380} | R ^{D17} | R ^{D49} |
| L _{C391} | R ^{D17} | R ^{D50} |

-continued

| Ligand | R ¹ | R ² |
|--------|------------------|-------------------|
| LC392 | R ^{D17} | R ^{D54} |
| LC393 | R ^{D17} | R ^{D55} |
| LC394 | R ^{D17} | R ^{D58} |
| LC395 | R ^{D17} | R ^{D59} |
| LC396 | R ^{D17} | R ^{D78} |
| LC397 | R ^{D17} | R ^{D79} |
| LC398 | R ^{D17} | R ^{D81} |
| LC399 | R ^{D17} | R ^{D87} |
| LC400 | R ^{D17} | R ^{D88} |
| LC401 | R ^{D17} | R ^{D89} |
| LC402 | R ^{D17} | R ^{D93} |
| LC403 | R ^{D17} | R ^{D116} |
| LC404 | R ^{D17} | R ^{D117} |
| LC405 | R ^{D17} | R ^{D118} |
| LC406 | R ^{D17} | R ^{D119} |
| LC407 | R ^{D17} | R ^{D120} |
| LC408 | R ^{D17} | R ^{D133} |
| LC409 | R ^{D17} | R ^{D134} |
| LC410 | R ^{D17} | R ^{D135} |
| LC411 | R ^{D17} | R ^{D136} |
| LC412 | R ^{D17} | R ^{D143} |
| LC413 | R ^{D17} | R ^{D144} |
| LC414 | R ^{D17} | R ^{D145} |
| LC415 | R ^{D17} | R ^{D146} |
| LC416 | R ^{D17} | R ^{D147} |
| LC417 | R ^{D17} | R ^{D149} |
| LC418 | R ^{D17} | R ^{D151} |
| LC419 | R ^{D17} | R ^{D154} |
| LC420 | R ^{D17} | R ^{D155} |
| LC421 | R ^{D17} | R ^{D161} |
| LC422 | R ^{D17} | R ^{D175} |
| LC423 | R ^{D50} | R ^{D3} |
| LC424 | R ^{D50} | R ^{D5} |
| LC425 | R ^{D50} | R ^{D18} |
| LC426 | R ^{D50} | R ^{D20} |
| LC427 | R ^{D50} | R ^{D22} |
| LC428 | R ^{D50} | R ^{D37} |
| LC429 | R ^{D50} | R ^{D40} |
| LC430 | R ^{D50} | R ^{D41} |
| LC431 | R ^{D50} | R ^{D42} |
| LC432 | R ^{D50} | R ^{D43} |
| LC433 | R ^{D50} | R ^{D48} |
| LC434 | R ^{D50} | R ^{D49} |
| LC435 | R ^{D50} | R ^{D54} |
| LC436 | R ^{D50} | R ^{D55} |
| LC437 | R ^{D50} | R ^{D58} |
| LC438 | R ^{D50} | R ^{D59} |
| LC439 | R ^{D50} | R ^{D78} |
| LC440 | R ^{D50} | R ^{D79} |
| LC441 | R ^{D50} | R ^{D81} |
| LC442 | R ^{D50} | R ^{D87} |
| LC443 | R ^{D50} | R ^{D88} |
| LC444 | R ^{D50} | R ^{D89} |
| LC445 | R ^{D50} | R ^{D93} |
| LC446 | R ^{D50} | R ^{D116} |
| LC447 | R ^{D50} | R ^{D117} |
| LC448 | R ^{D50} | R ^{D118} |
| LC449 | R ^{D50} | R ^{D119} |
| LC450 | R ^{D50} | R ^{D120} |
| LC451 | R ^{D50} | R ^{D133} |
| LC452 | R ^{D50} | R ^{D134} |
| LC453 | R ^{D50} | R ^{D135} |
| LC454 | R ^{D50} | R ^{D136} |
| LC455 | R ^{D50} | R ^{D143} |
| LC456 | R ^{D50} | R ^{D144} |
| LC457 | R ^{D50} | R ^{D145} |
| LC458 | R ^{D50} | R ^{D146} |
| LC459 | R ^{D50} | R ^{D147} |
| LC460 | R ^{D50} | R ^{D149} |
| LC461 | R ^{D50} | R ^{D151} |
| LC462 | R ^{D50} | R ^{D154} |
| LC463 | R ^{D50} | R ^{D155} |
| LC464 | R ^{D50} | R ^{D161} |
| LC465 | R ^{D50} | R ^{D175} |

-continued

| Ligand | R ¹ | R ² |
|--------|-------------------|-------------------|
| LC466 | R ^{D55} | R ^{D3} |
| LC467 | R ^{D55} | R ^{D5} |
| LC468 | R ^{D55} | R ^{D18} |
| LC469 | R ^{D55} | R ^{D20} |
| LC470 | R ^{D55} | R ^{D22} |
| LC471 | R ^{D55} | R ^{D37} |
| LC472 | R ^{D55} | R ^{D40} |
| LC473 | R ^{D55} | R ^{D41} |
| LC474 | R ^{D55} | R ^{D42} |
| LC475 | R ^{D55} | R ^{D43} |
| LC476 | R ^{D55} | R ^{D48} |
| LC477 | R ^{D55} | R ^{D49} |
| LC478 | R ^{D55} | R ^{D54} |
| LC479 | R ^{D55} | R ^{D58} |
| LC480 | R ^{D55} | R ^{D59} |
| LC481 | R ^{D55} | R ^{D78} |
| LC482 | R ^{D55} | R ^{D79} |
| LC483 | R ^{D55} | R ^{D81} |
| LC484 | R ^{D55} | R ^{D87} |
| LC485 | R ^{D55} | R ^{D88} |
| LC486 | R ^{D55} | R ^{D89} |
| LC487 | R ^{D55} | R ^{D93} |
| LC488 | R ^{D55} | R ^{D116} |
| LC489 | R ^{D55} | R ^{D117} |
| LC490 | R ^{D55} | R ^{D118} |
| LC491 | R ^{D55} | R ^{D119} |
| LC492 | R ^{D55} | R ^{D120} |
| LC493 | R ^{D55} | R ^{D133} |
| LC494 | R ^{D55} | R ^{D134} |
| LC495 | R ^{D55} | R ^{D135} |
| LC496 | R ^{D55} | R ^{D136} |
| LC497 | R ^{D55} | R ^{D143} |
| LC498 | R ^{D55} | R ^{D144} |
| LC499 | R ^{D55} | R ^{D145} |
| LC500 | R ^{D55} | R ^{D146} |
| LC501 | R ^{D55} | R ^{D147} |
| LC502 | R ^{D55} | R ^{D149} |
| LC503 | R ^{D55} | R ^{D151} |
| LC504 | R ^{D55} | R ^{D154} |
| LC505 | R ^{D55} | R ^{D155} |
| LC506 | R ^{D55} | R ^{D161} |
| LC507 | R ^{D55} | R ^{D175} |
| LC508 | R ^{D116} | R ^{D3} |
| LC509 | R ^{D116} | R ^{D5} |
| LC510 | R ^{D116} | R ^{D17} |
| LC511 | R ^{D116} | R ^{D18} |
| LC512 | R ^{D116} | R ^{D20} |
| LC513 | R ^{D116} | R ^{D22} |
| LC514 | R ^{D116} | R ^{D37} |
| LC515 | R ^{D116} | R ^{D40} |
| LC516 | R ^{D116} | R ^{D41} |
| LC517 | R ^{D116} | R ^{D42} |
| LC518 | R ^{D116} | R ^{D43} |
| LC519 | R ^{D116} | R ^{D48} |
| LC520 | R ^{D116} | R ^{D49} |
| LC521 | R ^{D116} | R ^{D54} |
| LC522 | R ^{D116} | R ^{D58} |
| LC523 | R ^{D116} | R ^{D59} |
| LC524 | R ^{D116} | R ^{D78} |
| LC525 | R ^{D116} | R ^{D79} |
| LC526 | R ^{D116} | R ^{D81} |
| LC527 | R ^{D116} | R ^{D87} |
| LC528 | R ^{D116} | R ^{D88} |
| LC529 | R ^{D116} | R ^{D89} |
| LC530 | R ^{D116} | R ^{D93} |
| LC531 | R ^{D116} | R ^{D117} |
| LC532 | R ^{D116} | R ^{D118} |
| LC533 | R ^{D116} | R ^{D119} |
| LC534 | R ^{D116} | R ^{D120} |
| LC535 | R ^{D116} | R ^{D133} |
| LC536 | R ^{D116} | R ^{D134} |
| LC537 | R ^{D116} | R ^{D135} |
| LC538 | R ^{D116} | R ^{D136} |
| LC539 | R ^{D116} | R ^{D143} |

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| Ligand | R ¹ | R ² |
|--------|-------------------|-------------------|
| LC540 | R ^{D116} | R ^{D144} |
| LC541 | R ^{D116} | R ^{D145} |
| LC542 | R ^{D116} | R ^{D146} |
| LC543 | R ^{D116} | R ^{D147} |
| LC544 | R ^{D116} | R ^{D149} |
| LC545 | R ^{D116} | R ^{D151} |
| LC546 | R ^{D116} | R ^{D154} |
| LC547 | R ^{D116} | R ^{D155} |
| LC548 | R ^{D116} | R ^{D161} |
| LC549 | R ^{D116} | R ^{D175} |
| LC550 | R ^{D143} | R ^{D3} |
| LC551 | R ^{D143} | R ^{D5} |
| LC552 | R ^{D143} | R ^{D17} |
| LC553 | R ^{D143} | R ^{D18} |
| LC554 | R ^{D143} | R ^{D20} |
| LC555 | R ^{D143} | R ^{D22} |
| LC556 | R ^{D143} | R ^{D37} |
| LC557 | R ^{D143} | R ^{D40} |
| LC558 | R ^{D143} | R ^{D41} |
| LC559 | R ^{D143} | R ^{D42} |
| LC560 | R ^{D143} | R ^{D43} |
| LC561 | R ^{D143} | R ^{D48} |
| LC562 | R ^{D143} | R ^{D49} |
| LC563 | R ^{D143} | R ^{D54} |
| LC564 | R ^{D143} | R ^{D58} |
| LC565 | R ^{D143} | R ^{D59} |
| LC566 | R ^{D143} | R ^{D78} |
| LC567 | R ^{D143} | R ^{D79} |
| LC568 | R ^{D143} | R ^{D81} |
| LC569 | R ^{D143} | R ^{D87} |
| LC570 | R ^{D143} | R ^{D88} |
| LC571 | R ^{D143} | R ^{D89} |
| LC572 | R ^{D143} | R ^{D93} |
| LC573 | R ^{D143} | R ^{D116} |
| LC574 | R ^{D143} | R ^{D117} |
| LC575 | R ^{D143} | R ^{D118} |
| LC576 | R ^{D143} | R ^{D119} |
| LC577 | R ^{D143} | R ^{D120} |
| LC578 | R ^{D143} | R ^{D133} |
| LC579 | R ^{D143} | R ^{D134} |
| LC580 | R ^{D143} | R ^{D135} |
| LC581 | R ^{D143} | R ^{D136} |
| LC582 | R ^{D143} | R ^{D144} |
| LC583 | R ^{D143} | R ^{D145} |
| LC584 | R ^{D143} | R ^{D146} |
| LC585 | R ^{D143} | R ^{D147} |
| LC586 | R ^{D143} | R ^{D149} |
| LC587 | R ^{D143} | R ^{D151} |
| LC588 | R ^{D143} | R ^{D154} |
| LC589 | R ^{D143} | R ^{D155} |
| LC580 | R ^{D143} | R ^{D161} |
| LC591 | R ^{D143} | R ^{D175} |
| LC592 | R ^{D144} | R ^{D3} |
| LC593 | R ^{D144} | R ^{D5} |
| LC594 | R ^{D144} | R ^{D17} |
| LC595 | R ^{D144} | R ^{D18} |
| LC596 | R ^{D144} | R ^{D20} |
| LC597 | R ^{D144} | R ^{D22} |
| LC598 | R ^{D144} | R ^{D37} |
| LC599 | R ^{D144} | R ^{D40} |
| LC600 | R ^{D144} | R ^{D41} |
| LC601 | R ^{D144} | R ^{D42} |
| LC602 | R ^{D144} | R ^{D43} |
| LC603 | R ^{D144} | R ^{D48} |
| LC604 | R ^{D144} | R ^{D49} |
| LC605 | R ^{D144} | R ^{D54} |
| LC606 | R ^{D144} | R ^{D58} |
| LC607 | R ^{D144} | R ^{D59} |
| LC608 | R ^{D144} | R ^{D78} |
| LC609 | R ^{D144} | R ^{D79} |
| LC610 | R ^{D144} | R ^{D81} |
| LC611 | R ^{D144} | R ^{D87} |
| LC612 | R ^{D144} | R ^{D88} |
| LC613 | R ^{D144} | R ^{D89} |

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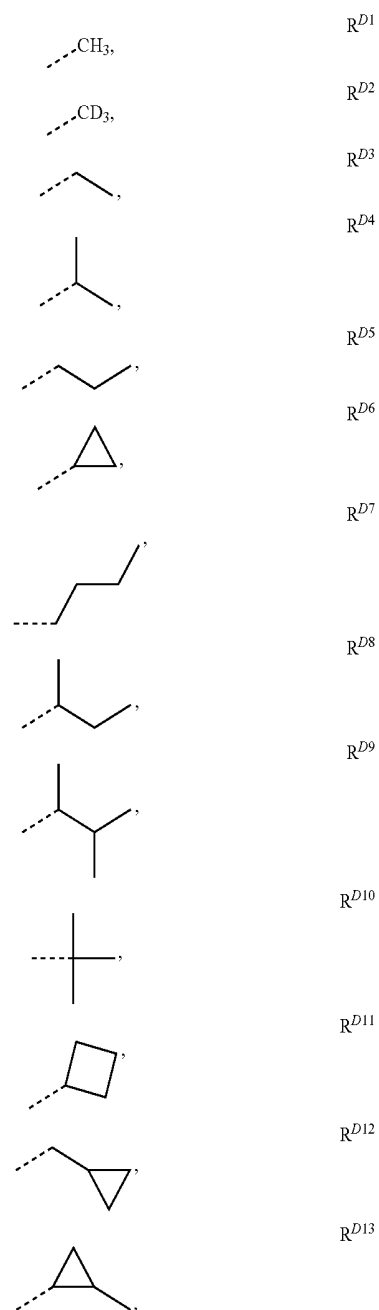
| Ligand | R ¹ | R ² |
|--------|-------------------|-------------------|
| LC614 | R ^{D144} | R ^{D93} |
| LC615 | R ^{D144} | R ^{D116} |
| LC616 | R ^{D144} | R ^{D117} |
| LC617 | R ^{D144} | R ^{D118} |
| LC618 | R ^{D144} | R ^{D119} |
| LC619 | R ^{D144} | R ^{D120} |
| LC620 | R ^{D144} | R ^{D133} |
| LC621 | R ^{D144} | R ^{D134} |
| LC622 | R ^{D144} | R ^{D135} |
| LC623 | R ^{D144} | R ^{D136} |
| LC624 | R ^{D144} | R ^{D145} |
| LC625 | R ^{D144} | R ^{D146} |
| LC626 | R ^{D144} | R ^{D147} |
| LC627 | R ^{D144} | R ^{D149} |
| LC628 | R ^{D144} | R ^{D151} |
| LC629 | R ^{D144} | R ^{D154} |
| LC630 | R ^{D144} | R ^{D155} |
| LC631 | R ^{D144} | R ^{D161} |
| LC632 | R ^{D144} | R ^{D175} |
| LC633 | R ^{D145} | R ^{D3} |
| LC634 | R ^{D145} | R ^{D5} |
| LC635 | R ^{D145} | R ^{D17} |
| LC636 | R ^{D145} | R ^{D18} |
| LC637 | R ^{D145} | R ^{D20} |
| LC638 | R ^{D145} | R ^{D22} |
| LC639 | R ^{D145} | R ^{D37} |
| LC640 | R ^{D145} | R ^{D40} |
| LC641 | R ^{D145} | R ^{D41} |
| LC642 | R ^{D145} | R ^{D42} |
| LC643 | R ^{D145} | R ^{D43} |
| LC644 | R ^{D145} | R ^{D48} |
| LC645 | R ^{D145} | R ^{D49} |
| LC646 | R ^{D145} | R ^{D54} |
| LC647 | R ^{D145} | R ^{D58} |
| LC648 | R ^{D145} | R ^{D59} |
| LC649 | R ^{D145} | R ^{D78} |
| LC650 | R ^{D145} | R ^{D79} |
| LC651 | R ^{D145} | R ^{D81} |
| LC652 | R ^{D145} | R ^{D87} |
| LC653 | R ^{D145} | R ^{D88} |
| LC654 | R ^{D145} | R ^{D89} |
| LC655 | R ^{D145} | R ^{D93} |
| LC656 | R ^{D145} | R ^{D116} |
| LC657 | R ^{D145} | R ^{D117} |
| LC658 | R ^{D145} | R ^{D118} |
| LC659 | R ^{D145} | R ^{D119} |
| LC660 | R ^{D145} | R ^{D120} |
| LC661 | R ^{D145} | R ^{D133} |
| LC662 | R ^{D145} | R ^{D134} |
| LC663 | R ^{D145} | R ^{D135} |
| LC664 | R ^{D145} | R ^{D136} |
| LC665 | R ^{D145} | R ^{D146} |
| LC666 | R ^{D145} | R ^{D147} |
| LC667 | R ^{D145} | R ^{D149} |
| LC668 | R ^{D145} | R ^{D151} |
| LC669 | R ^{D145} | R ^{D154} |
| LC670 | R ^{D145} | R ^{D155} |
| LC671 | R ^{D145} | R ^{D161} |
| LC672 | R ^{D145} | R ^{D175} |
| LC673 | R ^{D146} | R ^{D3} |
| LC674 | R ^{D146} | R ^{D5} |
| LC675 | R ^{D146} | R ^{D17} |
| LC676 | R ^{D146} | R ^{D18} |
| LC677 | R ^{D146} | R ^{D20} |
| LC678 | R ^{D146} | R ^{D22} |
| LC679 | R ^{D146} | R ^{D37} |
| LC680 | R ^{D146} | R ^{D40} |
| LC681 | R ^{D146} | R ^{D41} |
| LC682 | R ^{D146} | R ^{D42} |
| LC683 | R ^{D146} | R ^{D43} |
| LC684 | R ^{D146} | R ^{D48} |
| LC685 | R ^{D146} | R ^{D49} |
| LC686 | R ^{D146} | R ^{D54} |
| LC687 | R ^{D146} | R ^{D58} |

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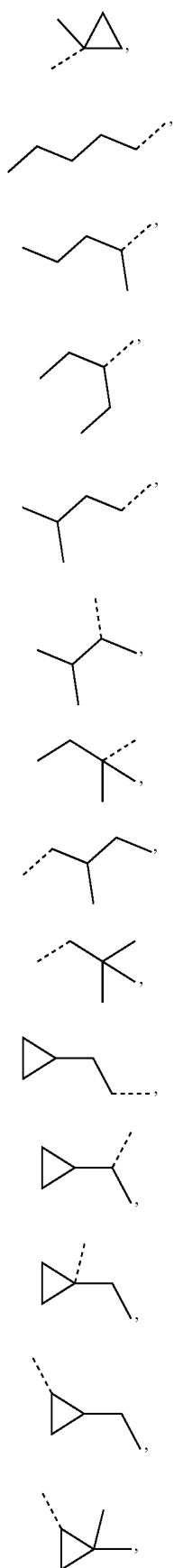
| Ligand | R ¹ | R ² |
|-------------------|-------------------|-------------------|
| L _{C688} | R ^{D146} | R ^{D59} |
| L _{C689} | R ^{D146} | R ^{D78} |
| L _{C680} | R ^{D146} | R ^{D79} |
| L _{C691} | R ^{D146} | R ^{D81} |
| L _{C692} | R ^{D146} | R ^{D87} |
| L _{C693} | R ^{D146} | R ^{D88} |
| L _{C694} | R ^{D146} | R ^{D89} |
| L _{C695} | R ^{D146} | R ^{D93} |
| L _{C696} | R ^{D146} | R ^{D117} |
| L _{C697} | R ^{D146} | R ^{D118} |
| L _{C698} | R ^{D146} | R ^{D119} |
| L _{C699} | R ^{D146} | R ^{D120} |
| L _{C700} | R ^{D146} | R ^{D133} |
| L _{C701} | R ^{D146} | R ^{D134} |
| L _{C702} | R ^{D146} | R ^{D135} |
| L _{C703} | R ^{D146} | R ^{D136} |
| L _{C704} | R ^{D146} | R ^{D146} |
| L _{C705} | R ^{D146} | R ^{D147} |
| L _{C706} | R ^{D146} | R ^{D149} |
| L _{C707} | R ^{D146} | R ^{D151} |
| L _{C708} | R ^{D146} | R ^{D154} |
| L _{C709} | R ^{D146} | R ^{D155} |
| L _{C710} | R ^{D146} | R ^{D161} |
| L _{C711} | R ^{D146} | R ^{D175} |
| L _{C712} | R ^{D133} | R ^{D3} |
| L _{C713} | R ^{D133} | R ^{D5} |
| L _{C714} | R ^{D133} | R ^{D3} |
| L _{C715} | R ^{D133} | R ^{D18} |
| L _{C716} | R ^{D133} | R ^{D20} |
| L _{C717} | R ^{D133} | R ^{D22} |
| L _{C718} | R ^{D133} | R ^{D37} |
| L _{C719} | R ^{D133} | R ^{D40} |
| L _{C720} | R ^{D133} | R ^{D41} |
| L _{C721} | R ^{D133} | R ^{D42} |
| L _{C722} | R ^{D133} | R ^{D43} |
| L _{C723} | R ^{D133} | R ^{D48} |
| L _{C724} | R ^{D133} | R ^{D49} |
| L _{C725} | R ^{D133} | R ^{D54} |
| L _{C726} | R ^{D133} | R ^{D58} |
| L _{C727} | R ^{D133} | R ^{D59} |
| L _{C728} | R ^{D133} | R ^{D78} |
| L _{C729} | R ^{D133} | R ^{D79} |
| L _{C730} | R ^{D133} | R ^{D81} |
| L _{C731} | R ^{D133} | R ^{D87} |
| L _{C732} | R ^{D133} | R ^{D88} |
| L _{C733} | R ^{D133} | R ^{D89} |
| L _{C734} | R ^{D133} | R ^{D93} |
| L _{C735} | R ^{D133} | R ^{D117} |
| L _{C736} | R ^{D133} | R ^{D118} |
| L _{C737} | R ^{D133} | R ^{D119} |
| L _{C738} | R ^{D133} | R ^{D120} |
| L _{C739} | R ^{D133} | R ^{D133} |
| L _{C740} | R ^{D133} | R ^{D134} |
| L _{C741} | R ^{D133} | R ^{D135} |
| L _{C742} | R ^{D133} | R ^{D136} |
| L _{C743} | R ^{D133} | R ^{D146} |
| L _{C744} | R ^{D133} | R ^{D147} |
| L _{C745} | R ^{D133} | R ^{D149} |
| L _{C746} | R ^{D133} | R ^{D151} |
| L _{C747} | R ^{D133} | R ^{D154} |
| L _{C748} | R ^{D133} | R ^{D155} |
| L _{C749} | R ^{D133} | R ^{D161} |
| L _{C750} | R ^{D133} | R ^{D175} |
| L _{C751} | R ^{D175} | R ^{D3} |
| L _{C752} | R ^{D175} | R ^{D5} |
| L _{C753} | R ^{D175} | R ^{D18} |
| L _{C754} | R ^{D175} | R ^{D20} |
| L _{C755} | R ^{D175} | R ^{D22} |
| L _{C756} | R ^{D175} | R ^{D37} |
| L _{C757} | R ^{D175} | R ^{D40} |
| L _{C758} | R ^{D175} | R ^{D41} |
| L _{C759} | R ^{D175} | R ^{D42} |
| L _{C760} | R ^{D175} | R ^{D43} |
| L _{C761} | R ^{D175} | R ^{D48} |

-continued

| Ligand | R ¹ | R ² |
|-------------------|-------------------|------------------|
| L _{C762} | R ^{D175} | R ^{D49} |
| L _{C763} | R ^{D175} | R ^{D54} |
| L _{C764} | R ^{D175} | R ^{D58} |
| L _{C765} | R ^{D175} | R ^{D59} |
| L _{C766} | R ^{D175} | R ^{D78} |
| L _{C767} | R ^{D175} | R ^{D79} |
| L _{C768} | R ^{D175} | R ^{D81} |

wherein R^{D1} to R^{D192} have the following structures:

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R^{D14}

R^{D15}

R^{D16}

R^{D17}

R^{D18}

R^{D19}

R^{D20}

R^{D21}

R^{D22}

R^{D23}

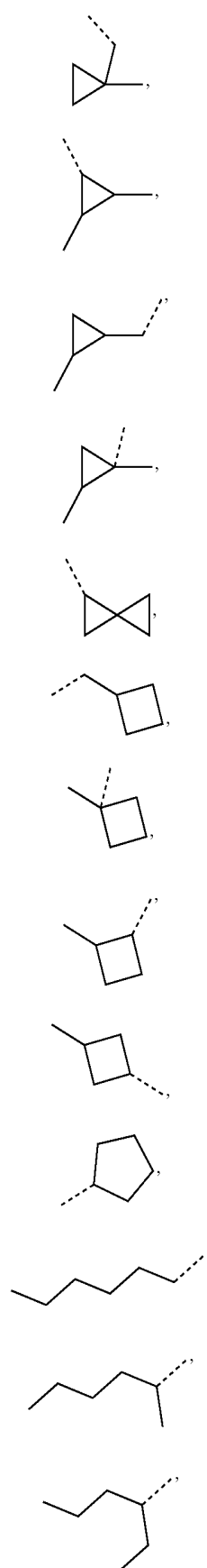
R^{D24}

R^{D25}

R^{D26}

R^{D27}

-continued



R^{D28}

R^{D29}

R^{D30}

R^{D31}

R^{D32}

R^{D33}

R^{D34}

R^{D35}

R^{D36}

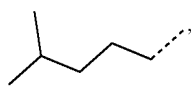
R^{D37}

R^{D38}

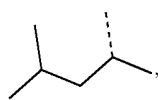
R^{D39}

R^{D40}

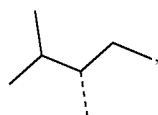
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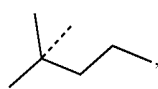
R^{D41}



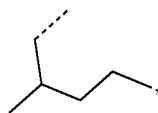
R^{D42}



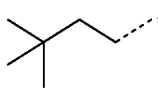
R^{D43}



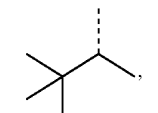
R^{D44}



R^{D45}



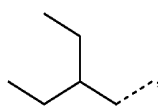
R^{D46}



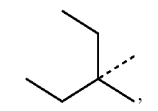
R^{D46}



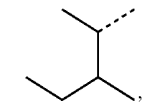
R^{D48}



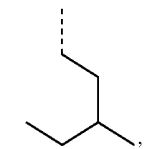
R^{D49}



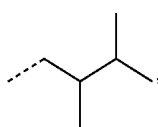
R^{D50}



R^{D51}

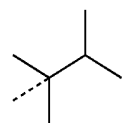


R^{D52}

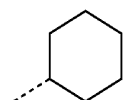


R^{D53}

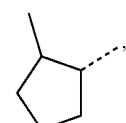
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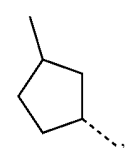
R^{D54}



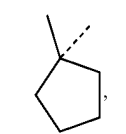
R^{D55}



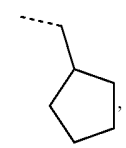
R^{D56}



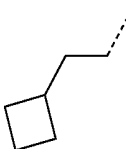
R^{D57}



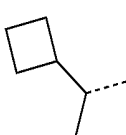
R^{D58}



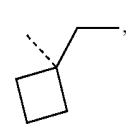
R^{D59}



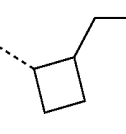
R^{D60}



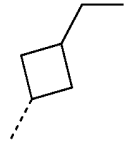
R^{D61}



R^{D62}

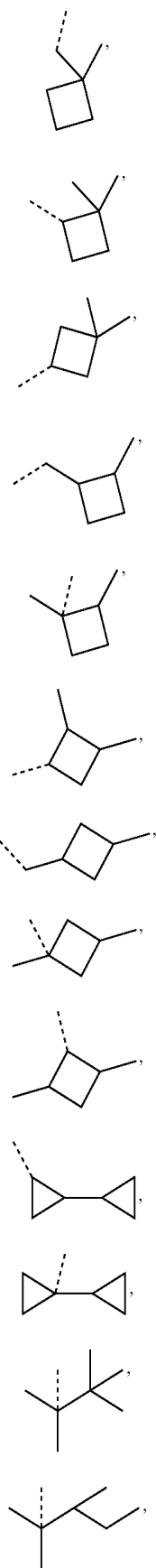


R^{D63}



R^{D64}

-continued



R^{D65}

R^{D66}

R^{D67}

R^{D68}

R^{D69}

R^{D70}

R^{D71}

R^{D72}

R^{D73}

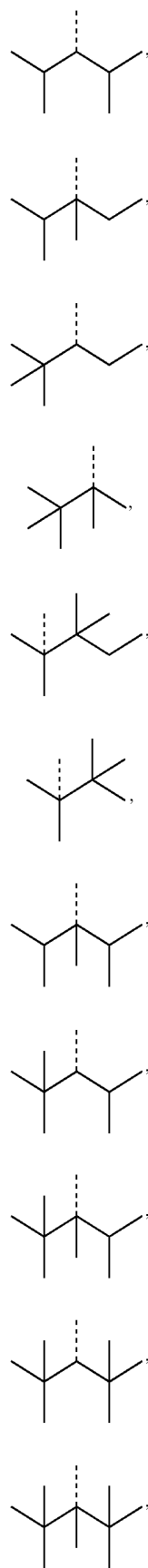
R^{D74}

R^{D75}

R^{D76}

R^{D77}

-continued



R^{D78}

R^{D79}

R^{D80}

R^{D81}

R^{D82}

R^{D83}

R^{D84}

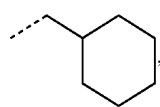
R^{D85}

R^{D86}

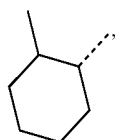
R^{D87}

R^{D88}

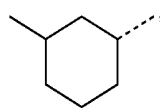
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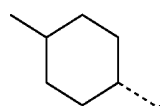
R^{D89}



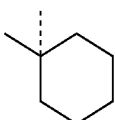
R^{D90}



R^{D91}



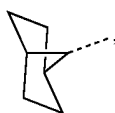
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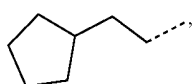
R^{D93}



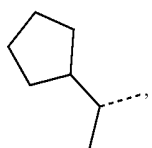
R^{D94}



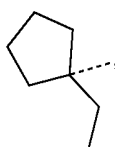
R^{D95}



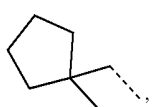
R^{D96}



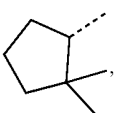
R^{D97}



R^{D98}

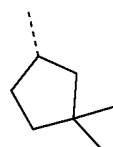


R^{D99}

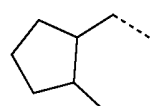


R^{D100}

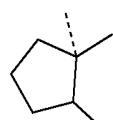
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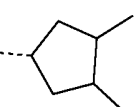
R^{D101}



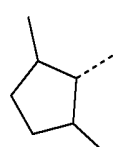
R^{D102}



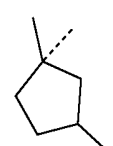
R^{D103}



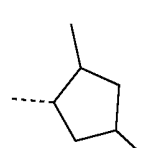
R^{D104}



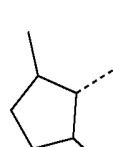
R^{D105}



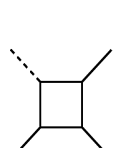
R^{D106}



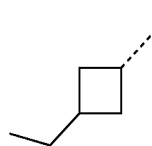
R^{D107}



R^{D108}

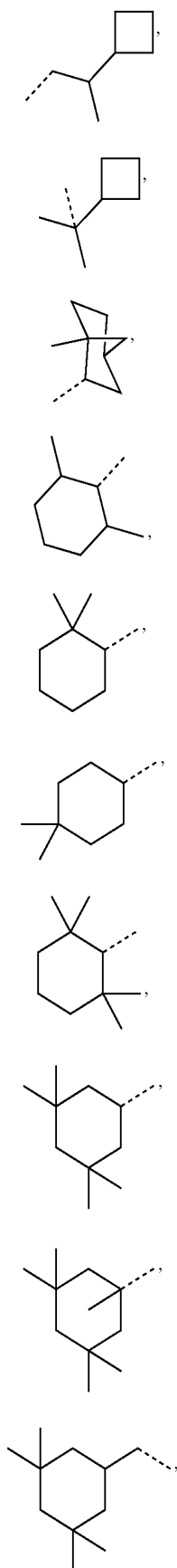


R^{D109}

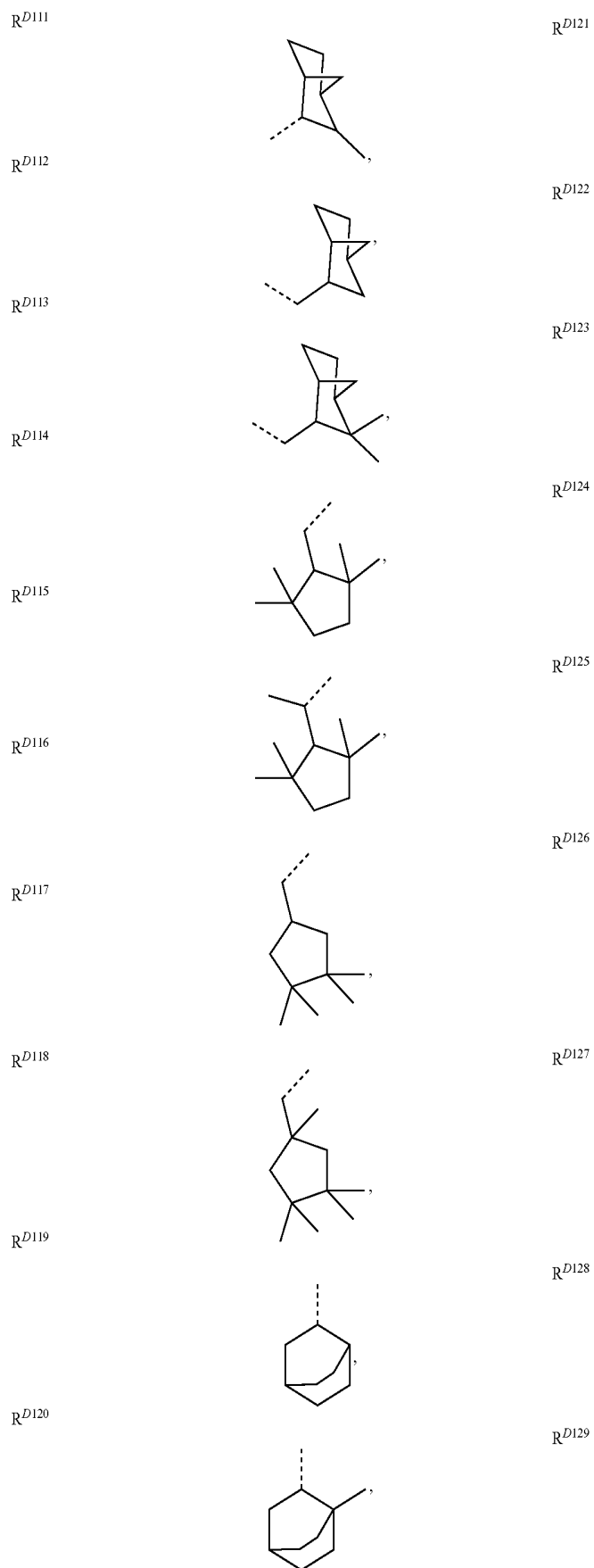


R^{D110}

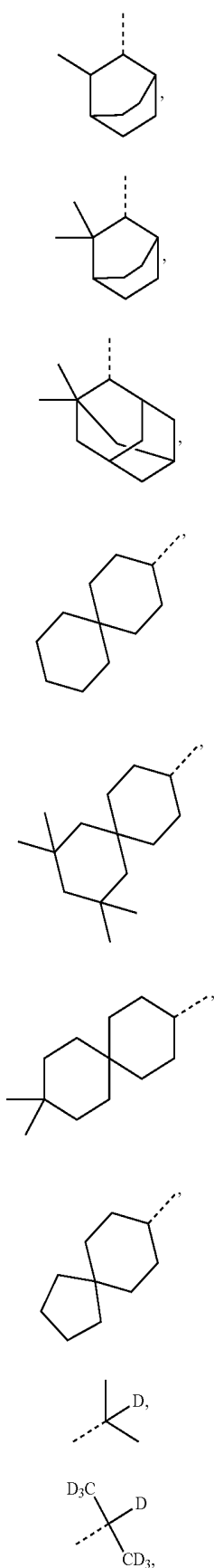
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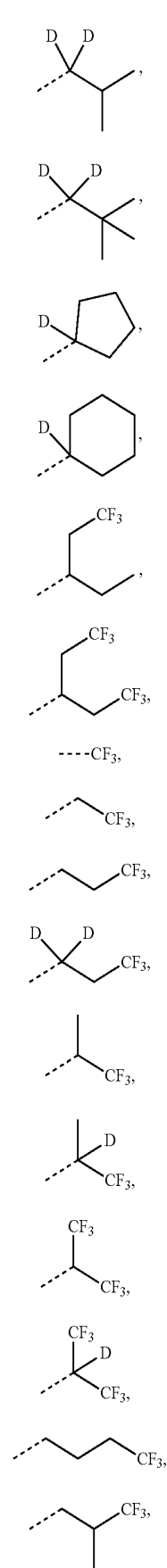
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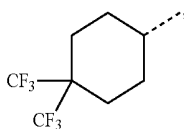
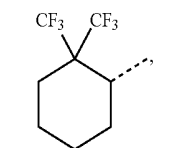
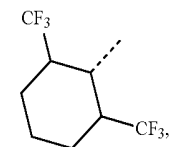
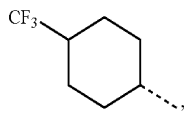
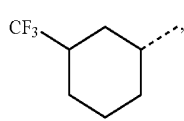
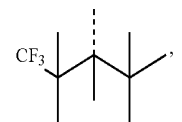
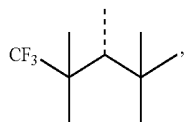
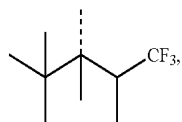
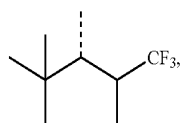
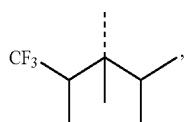
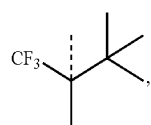
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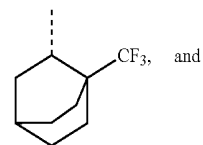
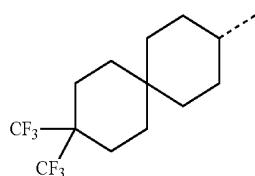
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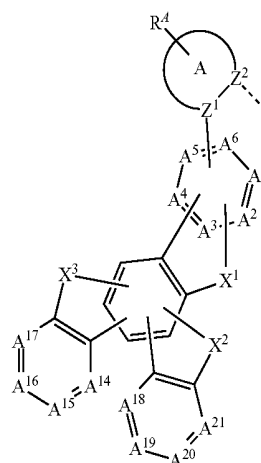
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R^{D180}R^{D191}R^{D181}R^{D192}R^{D182}R^{D183}

14. An organic light emitting device (OLED) comprising:
 an anode;
 a cathode; and an organic layer, disposed between the anode and the cathode, comprising a compound comprising a first ligand L_A selected from the group consisting of

R^{D184}

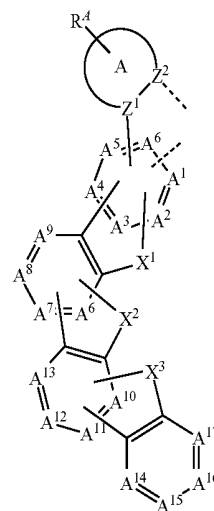
Formula I

R^{D185}R^{D186}R^{D187}

and

R^{D188}

Formula II

R^{D189}R^{D190}

wherein

L_A is complexed to a metal M to form a 5-membered chelate ring;

A is a 5-membered or 6-membered aryl or heteroaryl ring;

Z^1 and Z^2 are each independently C or N;

R^4 represents mono to the maximum allowable substitutions, or no substitution;

each A^1 to A^{13} is independently C, CR, or N;

each A^{14} to A^{21} is independently CR or N;

maximum number of N atoms that can connect to each other within a ring is two;

any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ;

any of A^1 to A^{13} are C when they are adjacent and fused to a ring;

any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring;

X^1 , X^2 , and X^3 are each independently selected from the group consisting of O, S, NR', CR'R'', and SiR'R'';

each R, R', R'', and R^4 is independently a 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 acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

M is optionally coordinated to other ligands;

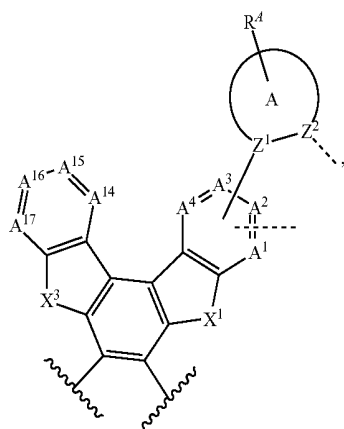
the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand;

any two substituents may be joined or fused together to form a ring;

if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ;

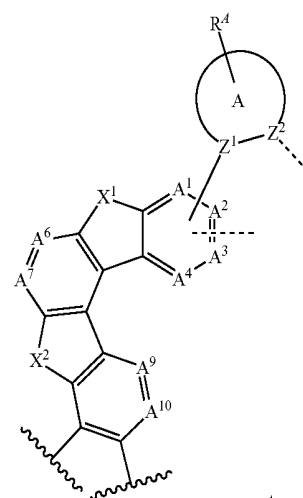
if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ;

Formulas III through VIII are defined as

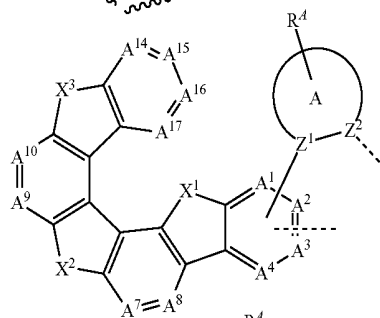


Formula III

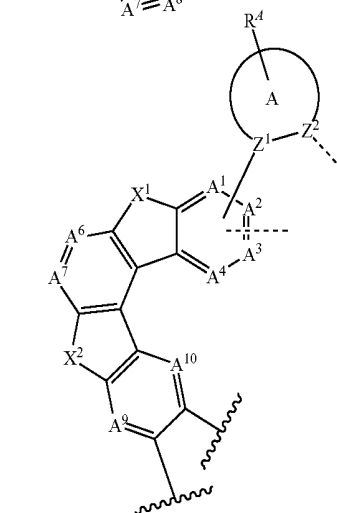
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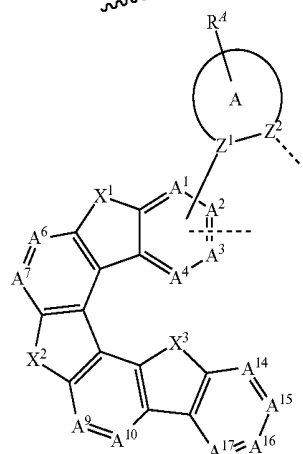
Formula IV



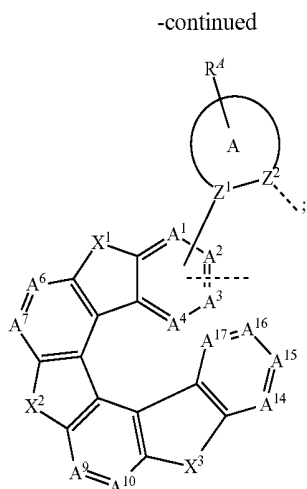
Formula V



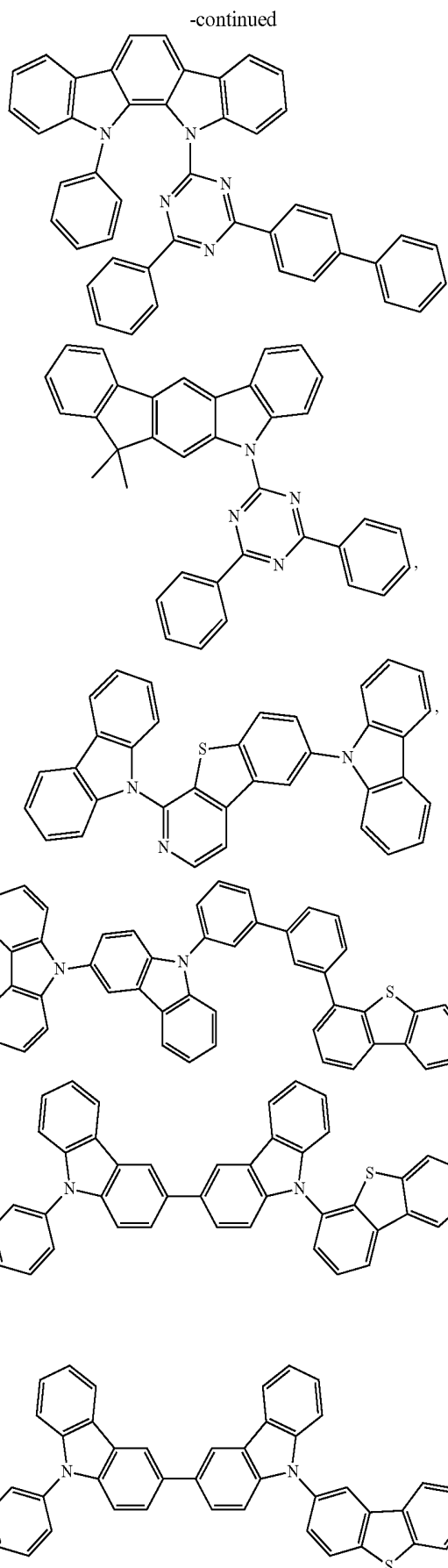
Formula VI



Formula VII



Formula VIII



and

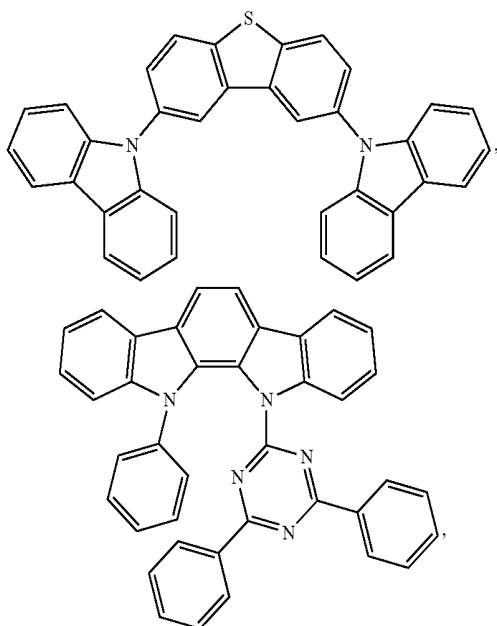
the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X^2 or X^3 .

15. The OLED of claim 14, wherein the compound is a sensitizer and the OLED further comprises an acceptor; and wherein the acceptor is selected from the group consisting of fluorescent emitter, delayed fluorescence emitter, and combination thereof.

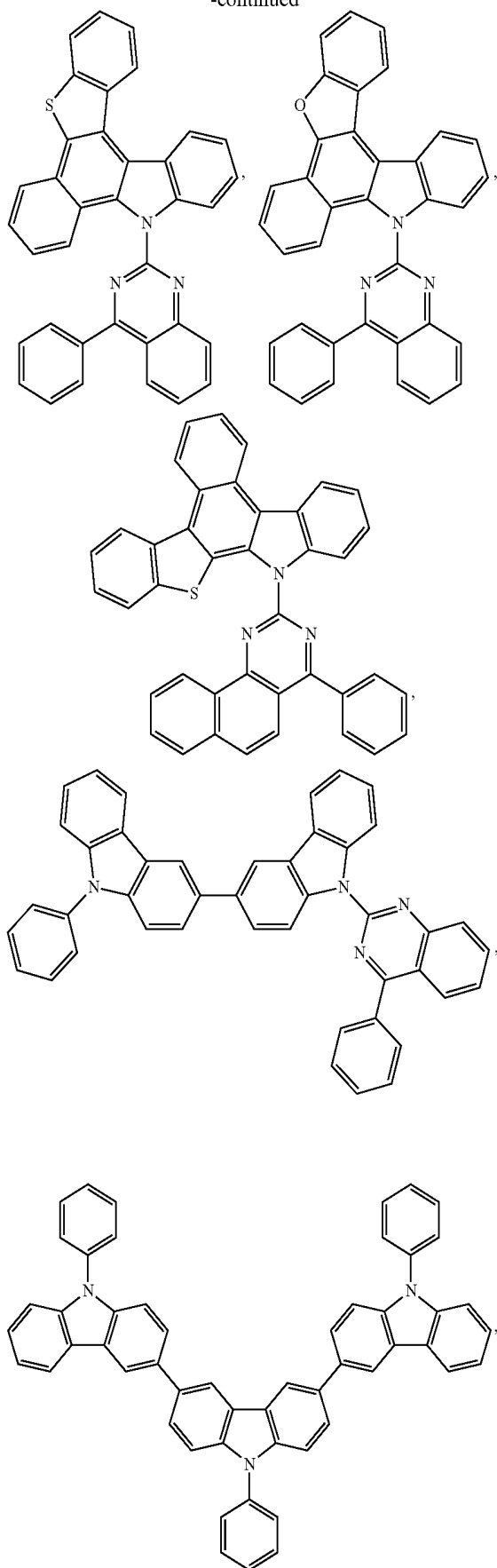
16. The OLED of claim 14, wherein the organic layer is an emissive layer and the compound is an emissive dopant or a non-emissive dopant.

17. The OLED of claim 14, wherein the organic layer further comprises a host, wherein host comprises at least one chemical group selected from the group consisting of triphenylene, carbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, azatriphenylene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene.

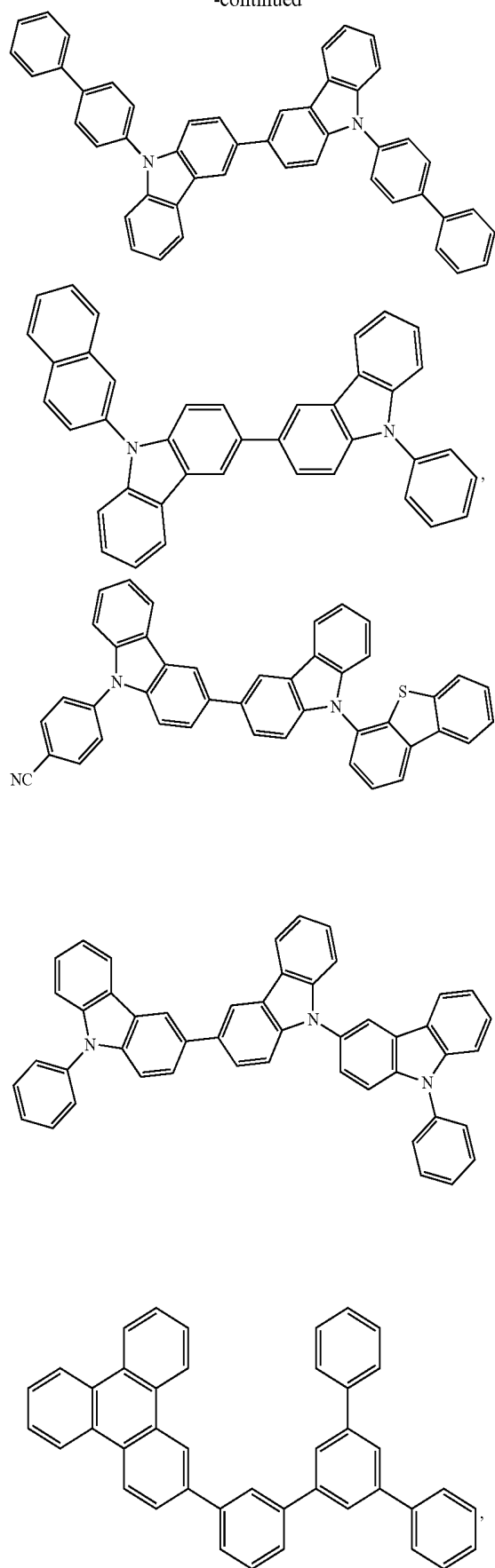
18. The OLED of claim 14, wherein the host is selected from the group consisting of:



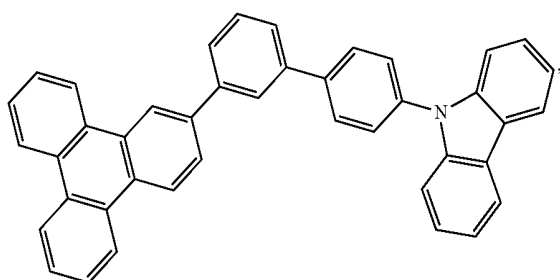
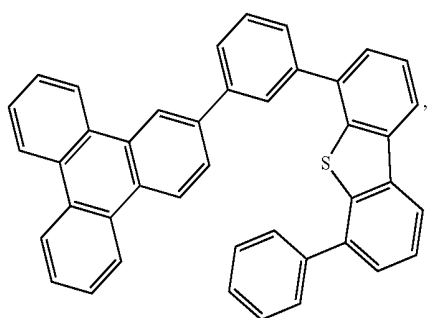
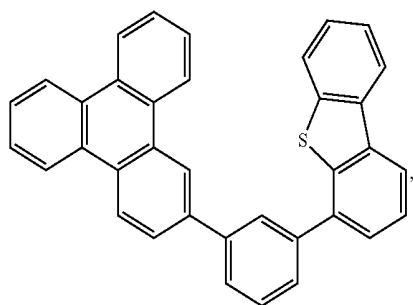
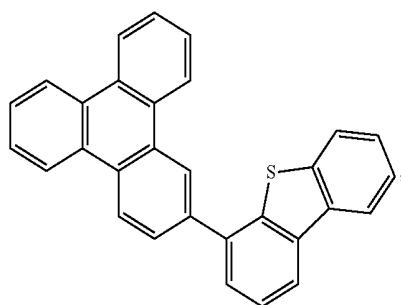
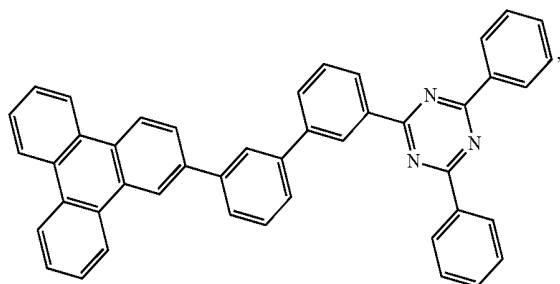
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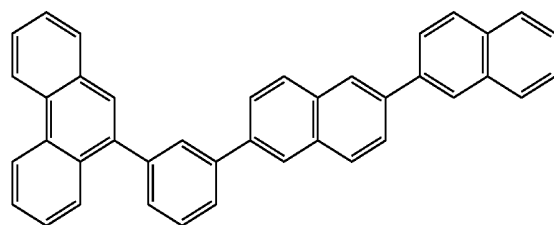
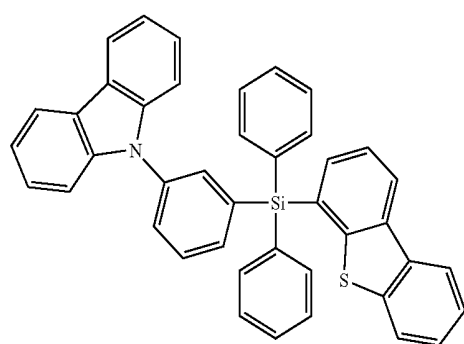
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and combinations thereof.

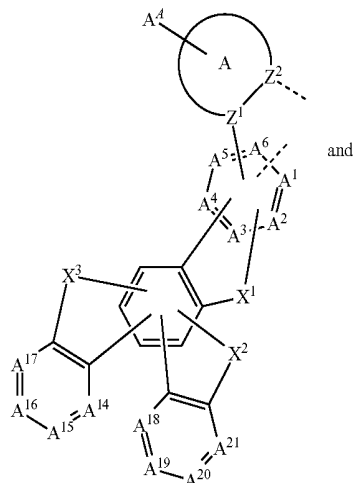
19. A consumer product comprising an organic light-emitting device comprising:

an anode;

a cathode; and

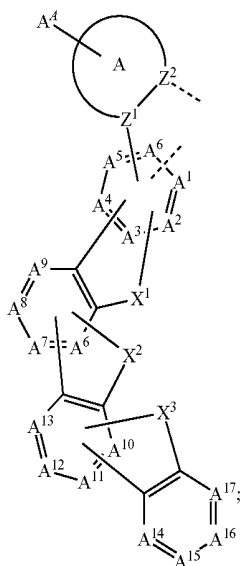
an organic layer, disposed between the anode and the cathode, comprising a compound comprising a first ligand L_A selected from the group consisting of

Formula I



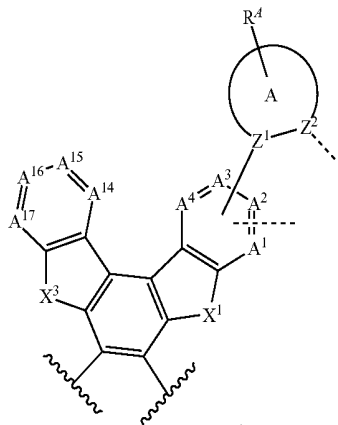
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Formula II

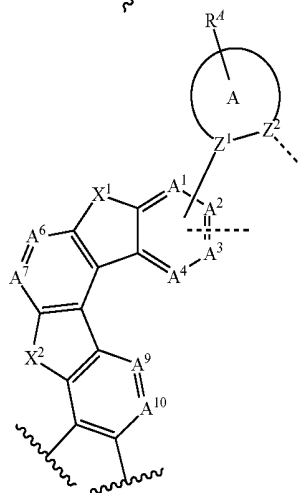


Formulas III through VIII are defined as

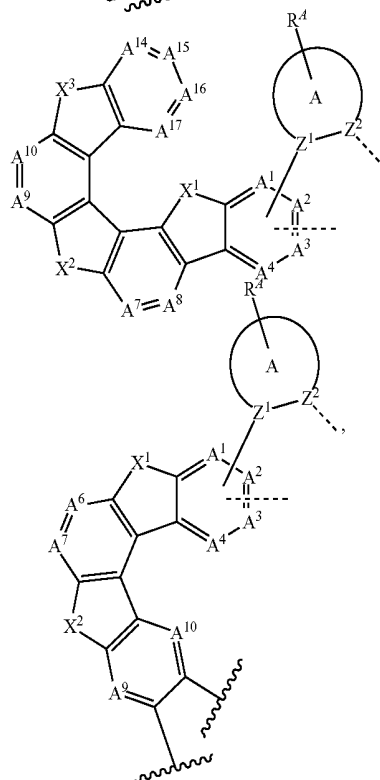
Formula III



Formula IV



Formula V



Formula VI

wherein

L_A is complexed to a metal M to form a 5-membered chelate ring;

A is a 5-membered or 6-membered aryl or heteroaryl ring;

Z^1 and Z^2 are each independently C or N;

R^A represents mono to the maximum allowable substitutions, or no substitution;

each A^1 to A^{13} is independently C, CR, or N;

each A^{14} to A^{21} is independently CR or N;

maximum number of N atoms that can connect to each other within a ring is two;

any of A^1 to A^6 is C when it forms a direct bond to M or Z^1 ;

any of A^1 to A^{13} are C when they are adjacent and fused to a ring;

any ring comprising X^1 , X^2 , and X^3 is a 5-membered ring;

X^1 , X^2 , and X^3 are each independently selected from the group consisting of O, S, NR', CR'R'', and SiR'R'';

each R, R', R'', and R^A is independently a 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 acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

M is optionally coordinated to other ligands;

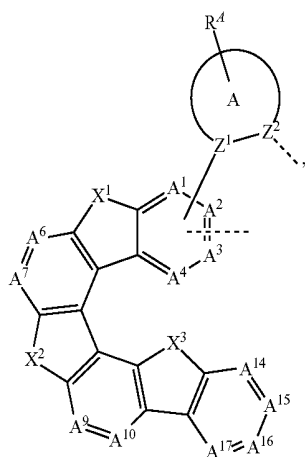
the ligand L_A is optionally linked with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand;

any two substituents may be joined or fused together to form a ring;

if the first ligand L_A comprises a structure of Formula III through VII, then neither Z^1 nor M forms a direct bond to A^4 ;

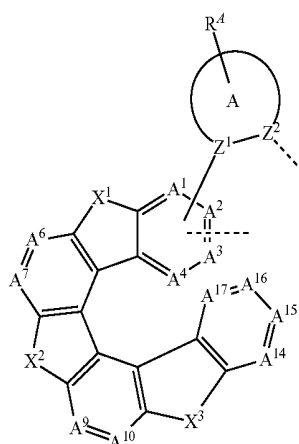
if the first ligand L_A comprises a structure of Formula VIII, then neither Z^1 nor M forms a direct bond to A^3 or A^4 ;

-continued



Formula VII

-continued



Formula VIII

and

the wavy lines in Formulas III, IV, and VI indicate the point of attachment to a 5-membered ring comprising X² or X³.

20. A formulation comprising the compound of claim 1.

* * * * *

| | | | |
|----------------|---|---------|------------|
| 专利名称(译) | 有机电致发光材料和器件 | | |
| 公开(公告)号 | US20200083465A1 | 公开(公告)日 | 2020-03-12 |
| 申请号 | US16/560542 | 申请日 | 2019-09-04 |
| [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 | TSAI JUI YI FELDMAN JERALD DYATKIN ALEXEY BORISOVICH JI ZHIQIANG BOUDREAUULT PIERRE LUC T | | |
| 发明人 | TSAI, JUI-YI FELDMAN, JERALD DYATKIN, ALEXEY BORISOVICH JI, ZHIQIANG BOUDREAUULT, PIERRE-LUC T. | | |
| IPC分类号 | H01L51/00 C07F15/00 C09K11/06 | | |
| CPC分类号 | C07F15/0033 C09K2211/185 C07B2200/05 H01L51/0085 C09K2211/1029 C09K11/06 H01L51/5016 C09K2211/1033 H01L51/5012 H01L51/0054 H01L51/0067 H01L51/0074 H01L2251/5384 | | |
| 优先权 | 62/727721 2018-09-06 US | | |
| 外部链接 | Espacenet USPTO | | |

摘要(译)

本公开涉及包含具有独特稠环的新型配体的环金属化金属化合物。预期本发明的化合物表现出独特的光物理和电子性质，并且可用于有机电致发光器件中以改善性能。

