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

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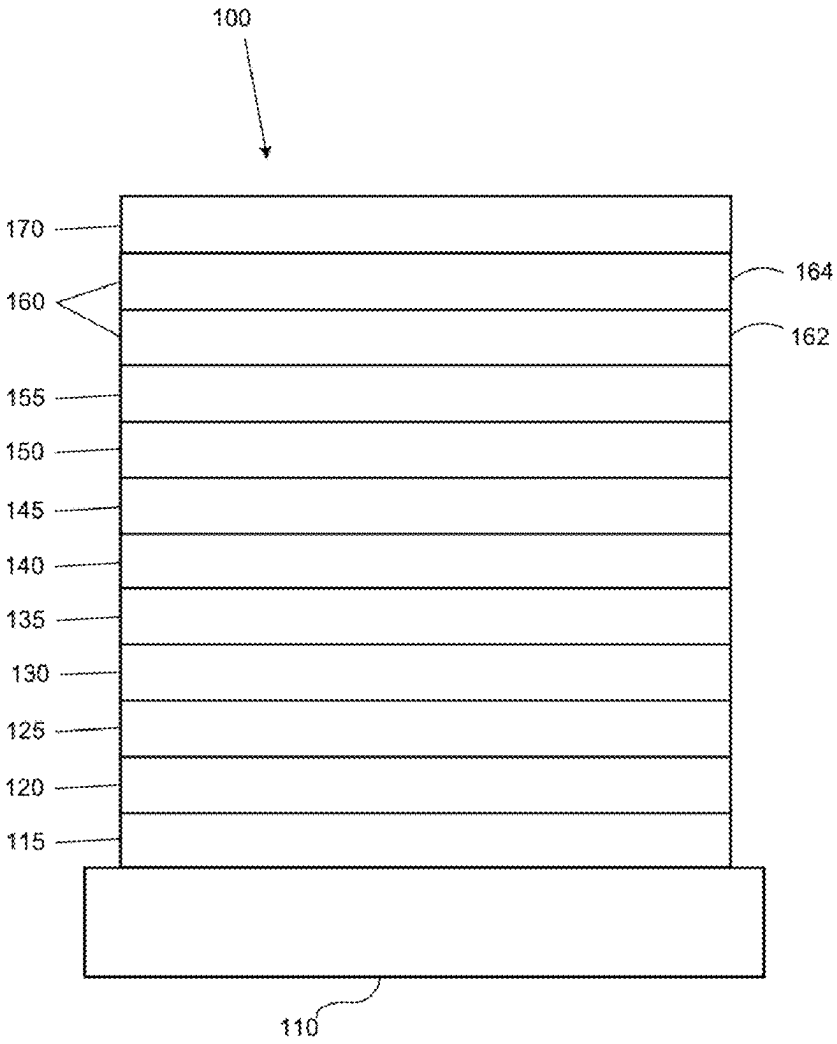
(57) **ABSTRACT**

Provided are organometallic compounds comprising a Pt or Pd atom as the central metal atom, wherein the central metal atom is coordinated by a tetradentate ligand. Also provided are formulations comprising these organometallic compounds. Further provided are organic light emitting devices (OLEDs) as well as related consumer products that utilize these organometallic compounds.



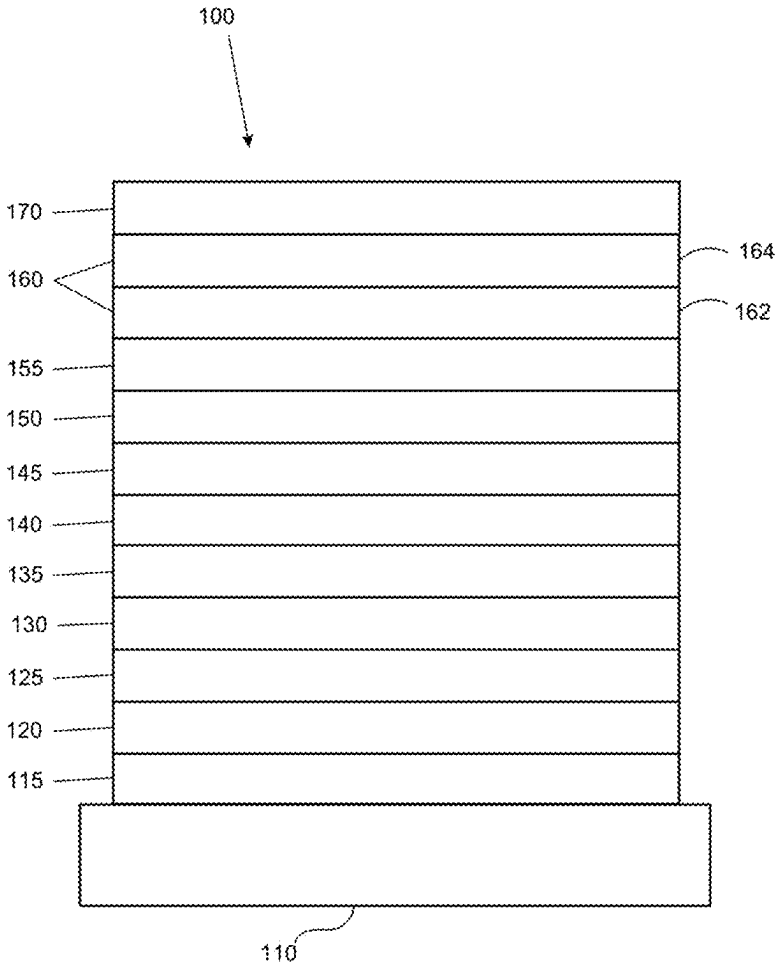

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FIG. 1

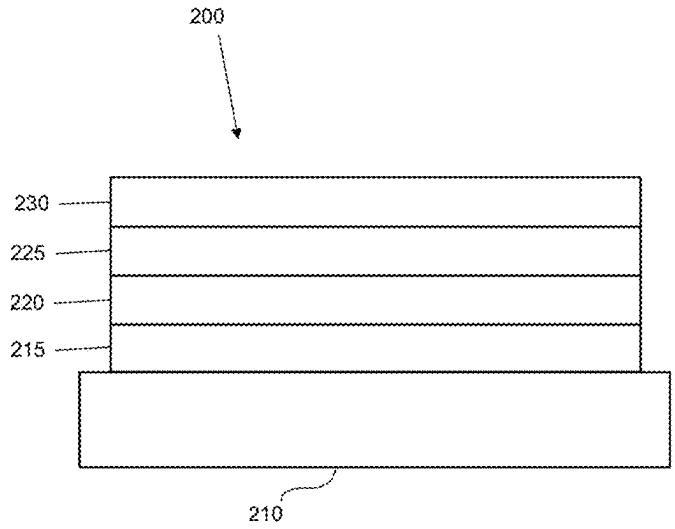
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FIG. 2

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. 63/553,938, filed on Feb. 15, 2024, the entire contents of which are incorporated herein by reference. This application further claims priority under 35 U.S.C. § 119(e) to U.S. Provisional Application No. 63/635,718, filed on Apr. 18, 2024, the entire contents of which are incorporated herein by reference.

FIELD

[0002] The present disclosure generally relates to organic or metal coordination compounds and formulations and their various uses including as emitters, sensitizers, charge transporters, or exciton transporters in devices such as organic light emitting diodes and related electronic devices and consumer products.

BACKGROUND

[0003] Opto-electronic devices that make use of organic materials are becoming increasingly desirable for various 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.

[0004] Examples of organic opto-electronic devices include organic light emitting diodes/devices (OLEDs), organic phototransistors, organic photovoltaic cells, organic scintillators, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials.

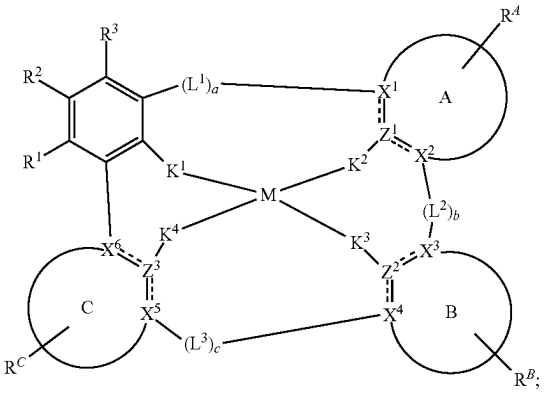
[0005] OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as displays, illumination, and backlighting.

[0006] One application for 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 emissive layer (EML) device or a stack structure. Color may be measured using CIE coordinates, which are well known to the art.

SUMMARY

[0007] In one aspect, the present disclosure provides a compound comprising a structure of Formula I:

Formula I



[0008] wherein moieties A, B, and C are each independently a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered to 10-membered carbocyclic or heterocyclic ring; wherein each L^1, L^2, and L^3 is independently selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR';

[0009] wherein Z^1, Z^2, and Z^3 are each independently C or N;

[0010] wherein M is Pt or Pd;

[0011] wherein X^1-X^6 are each independently C or N;

[0012] wherein each a, b, and c is independently 0 or 1;

[0013] wherein a+b+c=2 or 3;

[0014] wherein each of K^1, K^2, K^3, and K^4 is independently selected from the group consisting of single bond, O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$;

[0015] wherein R^A, R^B, and R^C each independently represent mono to the maximum allowable substitution, or no substitution;

[0016] wherein each R, R', R^α, R^β, R^2, R^3, R^A, R^B, and R^C is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, wherein R^1 is selected from the group consisting of halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, and wherein any two substituents may be joined or fused to form a ring.

[0017] In another aspect, the present disclosure provides a formulation of the compound as described herein.

[0018] In yet another aspect, the present disclosure provides an OLED having an organic layer comprising the compound as described herein.

[0019] In yet another aspect, the present disclosure provides a consumer product comprising an OLED with an organic layer comprising the compound as described herein.

BRIEF DESCRIPTION OF THE DRAWINGS

[0020] FIG. **1** shows an organic light emitting device.

[0021] FIG. **2** shows an inverted organic light emitting device that does not have a separate electron transport layer.

DETAILED DESCRIPTION

A. Terminology

[0022] Unless otherwise specified, the below terms used herein are defined as follows:

[0023] 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.

[0024] As used herein, "solution processable" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

[0025] 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 (TP) 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.

[0026] 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.

[0027] Layers, materials, regions, and devices may be described herein in reference to the color of light they emit. In general, as used herein, an emissive region that is described as producing a specific color of light may include one or more emissive layers disposed over each other in a stack.

[0028] As used herein, a "NIR", "red", "green", "blue", "yellow" layer, material, region, or device refers to a layer, a material, a region, or a device that emits light in the wavelength range of about 700-1500 nm, 580-700 nm, 500-600 nm, 400-500 nm, 540-600 nm, respectively, or a layer, a material, a region, or a device that has a highest peak in its emission spectrum in the respective wavelength region. In some arrangements, separate regions, layers, materials, or devices may provide separate "deep blue" and "light blue" emissions. As used herein, the "deep blue" emission component refers to an emission having a peak emission wavelength that is at least about 4 nm less than the peak emission wavelength of the "light blue" emission component. Typically, a "light blue" emission component has a peak emission wavelength in the range of about 465-500 nm, and a "deep blue" emission component has a peak emission wavelength in the range of about 400-470 nm, though these ranges may vary for some configurations.

[0029] In some arrangements, a color altering layer that converts, modifies, or shifts the color of the light emitted by another layer to an emission having a different wavelength is provided. Such a color altering layer can be formulated to shift wavelength of the light emitted by the other layer by a defined amount, as measured by the difference in the wavelength of the emitted light and the wavelength of the resulting light. In general, there are two classes of color altering layers: color filters that modify a spectrum by removing light of unwanted wavelengths, and color changing layers that convert photons of higher energy to lower energy. For example, a "red" color filter can be present in order to filter an input light to remove light having a wavelength outside the range of about 580-700 nm. A component "of a color" refers to a component that, when activated or used, produces or otherwise emits light having a particular color as previously described. For example, a "first emissive region of a first color" and a "second emissive region of a second color different than the first color" describes two emissive regions that, when activated within a device, emit two different colors as previously described.

[0030] As used herein, emissive materials, layers, and regions may be distinguished from one another and from other structures based upon light initially generated by the material, layer or region, as opposed to light eventually emitted by the same or a different structure. The initial light generation typically is the result of an energy level change resulting in emission of a photon. For example, an organic emissive material may initially generate blue light, which may be converted by a color filter, quantum dot or other structure to red or green light, such that a complete emissive stack or sub-pixel emits the red or green light. In this case the initial emissive material, region, or layer may be referred to as a "blue" component, even though the sub-pixel is a "red" or "green" component.

[0031] In some cases, it may be preferable to describe the color of a component such as an emissive region, sub-pixel, color altering layer, or the like, in terms of 1931 CIE coordinates. For example, a yellow emissive material may have multiple peak emission wavelengths, one in or near an

edge of the "green" region, and one within or near an edge of the "red" region as previously described.

[0032] Accordingly, as used herein, each color term also corresponds to a shape in the 1931 CIE coordinate color space. The shape in 1931 CIE color space is constructed by following the locus between two color points and any additional interior points. For example, interior shape parameters for red, green, blue, and yellow may be defined as shown below:

Color	CIE Shape Parameters
Central Red	Locus: [0.6270, 0.3725]; [0.7347, 0.2653]; Interior: [0.5086, 0.2657]
Central Green	Locus: [0.0326, 0.3530]; [0.3731, 0.6245]; Interior: [0.2268, 0.3321
Central Blue	Locus: [0.1746, 0.0052]; [0.0326, 0.3530]; Interior: [0.2268, 0.3321]
Central Yellow	Locus: [0.3731, 0.6245]; [0.6270, 0.3725]; Interior: [0.3700, 0.4087]; [0.2886, 0.4572]

[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 group (—C(O)—R_s).

[0035] The term "ester" refers to a substituted oxycarbonyl (—O—C(O)—R_s or —C(O)—O—R_s) group.

[0036] The term "ether" refers to an —OR_s group.

[0037] The terms "sulfanyl" or "thio-ether" are used interchangeably and refer to a —SR_s group.

[0038] The term "selenyl" refers to a —SeR_s group.

[0039] The term "sulfinyl" refers to a —S(O)—R_s group.

[0040] The term "sulfonyl" refers to a —SO_2—R_s group.

[0041] The term "phosphino" refers to a group containing at least one phosphorus atom bonded to the relevant structure. Common examples of phosphino groups include, but are not limited to, groups such as a —$P(R_s)_2$ group or a —$PO(R_s)_2$ group, wherein each R_s can be same or different.

[0042] The term "silyl" refers to a group containing at least one silicon atom bonded to the relevant structure. Common examples of silyl groups include, but are not limited to, groups such as a —$Si(R_s)_3$ group, wherein each R_s can be same or different.

[0043] The term "germyl" refers to a group containing at least one germanium atom bonded to the relevant structure. Common examples of germyl groups include, but are not limited to, groups such as a —$Ge(R_s)_3$ group, wherein each R_s can be same or different.

[0044] The term "boryl" refers to a group containing at least one boron atom bonded to the relevant structure. Common examples of boryl groups include, but are not limited to, groups such as a —$B(R_s)_2$ group or its Lewis adduct —$B(R_s)_3$ group, wherein R_s can be same or different.

[0045] In each of the above, R_s can be hydrogen or a substituent selected from the group consisting of the general substituents as defined in this application. Preferred R_s is 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. More preferably R_s is selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combination thereof.

[0046] The term "alkyl" refers to and includes both straight and branched chain alkyl groups having an alkyl carbon atom bonded to the relevant structure. Preferred alkyl groups are those containing from one to fifteen carbon atoms, preferably one to nine carbon atoms, and includes methyl, ethyl, n-propyl, iso-propyl, n-butyl, sec-butyl, iso-butyl, tert-butyl, n-pentyl, 2-methylbutyl, 3-methylbutyl, 2,2-dimethylpropyl, 1,3-dimethylpropyl, 1,1-dimethylpropyl, 2-ethylpropyl, 1,2-dimethylpropyl, n-hexyl, 2-methylpentyl, 3-methylpentyl, 2,2-dimethylbutyl, 2,3-dimethylbutyl, n-heptyl, 2-methylhexyl, 3-methylhexyl, 2,2-dimethylpentyl, 2,3-dimethylpentyl, 2,4-dimethylpentyl, 3,3-dimethylpentyl, 3-ethylpentyl, 2,2,3-trimethylbutyl, and the like. Additionally, the alkyl group can be further substituted.

[0047] The term "cycloalkyl" refers to and includes monocyclic, polycyclic, and spiro alkyl groups having a ring alkyl carbon atom bonded to the relevant structure. 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 can be further substituted.

[0048] The terms "heteroalkyl" or "heterocycloalkyl" refer to an alkyl or a cycloalkyl group, 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, Ge and Se, preferably, O, S or N. Additionally, the heteroalkyl or heterocycloalkyl group can be further substituted.

[0049] The term "alkenyl" refers to and includes both straight and branched chain alkene groups. Alkenyl groups are essentially alkyl groups that include at least one carbon-carbon double bond in the alkyl chain with one carbon atom from the carbon-carbon double bond that is bonded to the relevant structure. 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 group 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, Ge, 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 can be further substituted.

[0050] The term "alkynyl" refers to and includes both straight and branched chain alkyne groups. Alkynyl groups are essentially alkyl groups that include at least one carbon-carbon triple bond in the alkyl chain with one carbon atom from the carbon-carbon triple bond that is bonded to the relevant structure. Preferred alkynyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group can be further substituted.

[0051] The terms "aralkyl" or "arylalkyl" are used interchangeably and refer to an aryl-substituted alkyl group having an alkyl carbon atom bonded to the relevant structure. Additionally, the aralkyl group can be further substituted.

[0052] The term "heterocyclic group" refers to and includes aromatic and non-aromatic cyclic groups containing at least one heteroatom. Optionally the at least one heteroatom is selected from O, S, Se, N, P, B, Si, Ge, and Se, preferably, O, S, N, or B. Hetero-aromatic cyclic groups may

be used interchangeably with heteroaryl. Preferred hetero-non-aromatic cyclic groups are those containing 3 to 10 ring atoms, preferably 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 can be further substituted or fused.

[0053] The term "aryl" refers to and includes both single-ring and polycyclic aromatic hydrocarbyl groups. The polycyclic rings may have two or more rings in which two carbons are common to two adjoining rings (the rings are "fused"). Preferred aryl groups are those containing six to thirty carbon atoms, preferably six to twenty-four carbon atoms, six to eighteen carbon atoms, and more preferably six to twelve carbon atoms. Especially preferred is an aryl group having six carbons, ten carbons, twelve carbons, fourteen carbons, or eighteen carbons. Suitable aryl groups include phenyl, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, pyrene, chrysene, perylene, and azulene, preferably phenyl, biphenyl, triphenyl, triphenylene, and naphthalene. Additionally, the aryl group can be further substituted or fused, such as, without limitation, fluorene.

[0054] 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, Se, N, P, B, Si, Ge, and Se. In many instances, O, S, N, or B 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 aromatic 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. 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-four carbon atoms, three to eighteen carbon atoms, and more preferably three to twelve carbon atoms. Suitable heteroaryl groups include dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, selenophenodipyridine, azaborine, borazine, $5\lambda^2,9\lambda^2$-diaza-13b-boranaphtho[2,3,4-de]anthracene, $5\lambda^2$-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, and 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene; preferably dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, triazine, benzimidazole, $5\lambda^2,9\lambda^2$-diaza-13b-boranaphtho[2,3,4-de]anthracene, $5\lambda^2$-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, and 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene. Additionally, the heteroaryl group can be further substituted or fused.

[0055] Of the aryl and heteroaryl groups listed above, the groups of triphenylene, naphthalene, anthracene, dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, pyrazine, pyrimidine, triazine, benzimidazole, $5\lambda^2,9\lambda^2$-diaza-13b-boranaphtho[2,3,4-de]anthracene, $5\lambda^2$-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene, and the respective aza-analogs of each thereof are of particular interest.

[0056] In many instances, the General Substituents are selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, selenyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0057] In some instances, the Preferred General Substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

[0058] In some instances, the More Preferred General Substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, aryl, heteroaryl, nitrile, sulfanyl, and combinations thereof.

[0059] In some instances, the Even More Preferred General Substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, silyl, aryl, heteroaryl, nitrile, and combinations thereof.

[0060] In yet other instances, the Most Preferred General Substituents are selected from the group consisting of deuterium, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0061] 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 zero or no substitution, R^1, for example, can be a hydrogen for all 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.

[0062] 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.

[0063] 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.

[0064] 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[fh]quinoxaline and dibenzo[fh] 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.

[0065] 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.

[0066] As used herein, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. includes undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also include undeuterated, partially deuterated, and fully deuterated versions thereof. Unless otherwise specified, atoms in chemical structures without valences fully filled by H or D should be considered to include undeuterated, partially deuterated, and fully deuterated versions thereof. For example, the chemical structure of implies to include C_6H_6, C_6D_6, $C_6H_3D_3$, and any other partially deuterated variants thereof. Some common basic partially or fully deuterated group include, without limitation, CD_3, $CD_2C(CH_3)_3$, $C(CD_3)_3$, and C_6D_5.

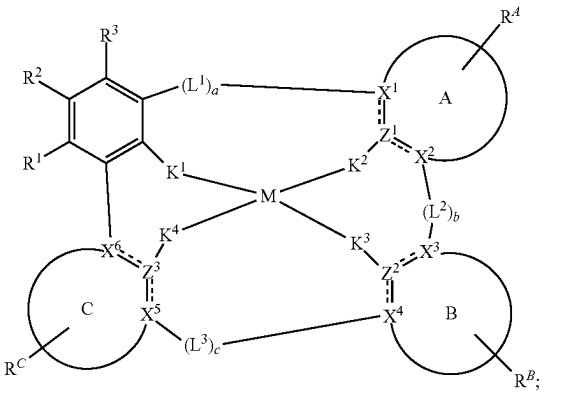
[0067] It is to be understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it were a fragment (e.g. phenyl, phenylene, naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. benzene, naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[0068] In some instances, a pair of substituents in the molecule can be optionally joined or fused into a ring. The preferred ring is a five to nine-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. In yet other instances, a pair of adjacent substituents can be optionally joined or fused into a ring. 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.

B. The Compounds of the Present Disclosure

[0069] In one aspect, the present disclosure provides a compound comprising a structure of Formula I:

Formula I



[0070] wherein moieties A, B, and C are each independently a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered to 10-membered carbocyclic or heterocyclic ring; wherein each L^1, L^2, and L^3 is independently selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR';

[0071] wherein Z^1, Z^2, and Z^3 are each independently C or N;

[0072] wherein M is Pt or Pd;

[0073] wherein X^1-X^6 are each independently C or N;

[0074] wherein each a, b, and c is independently 0 or 1;

[0075] wherein a+b+c=2 or 3;

[0076] wherein each of K^1, K^2, K^3, and K^4 is independently selected from the group consisting of single bond, O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$; wherein R^A, R^B, and R^C each independently represent mono to the maximum allowable substitution, or no substitution;

[0077] wherein each R, R', R^α, R^β, R^2, R^3, R^A, R^B, and R^C is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, wherein R^1 is selected from the group consisting of halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfo-

nyl, phosphino, and combinations thereof, and wherein any two substituents may be joined or fused to form a ring.

[0078] In some embodiments, the compound consists essentially of Formula I.

[0079] In some embodiments, the compound has a structure of Formula I.

[0080] In some embodiments of Formula I, at least one R, R', R^A, R^B, R^C, R^1, R^2, or R^3 is partially or fully deuterated. In some embodiments, at least one R^A is partially or fully deuterated. In some embodiments, at least one R^B is partially or fully deuterated. In some embodiments, at least one R^C is partially or fully deuterated. In some embodiments, at least one R^1 is partially or fully deuterated.

[0081] In some embodiments, at least one R^2 is partially or fully deuterated. In some embodiments, at least one R^3 is partially or fully deuterated. In some embodiments of Formula I, at least R or R' is present and is partially or fully deuterated.

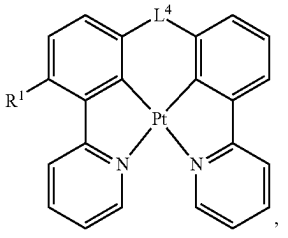
[0082] In some embodiments, at least one R^A, R^B, R^C, R^2, or R^3 is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^A is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^B is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^C is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^2 is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^3 is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^A, R^B, R^C, R^2, or R^3 is selected from the group consisting of the Preferred General Substituents defined herein.

[0083] In some embodiments, if R^1 is tert-butyl, R^3 is not tert-butyl.

[0084] In some embodiments, R^1 and R^2 do not join to form a ring.

[0085] In some embodiments, R^1 and R^C do not join to form a ring.

[0086] In some embodiments, the compound does not comprise:



wherein L^4 is selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

[0087] In some embodiments, each of R, R', R^α, R^β, R^2, R^3, R^A, R^B, and R^C is independently a hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

[0088] In some embodiments, R^1 is selected from the group consisting of fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

[0089] In some embodiments, at least one of X^1—X^6 is N.

[0090] In some embodiments, exactly one of X^1—X^6 is N.

[0091] In some embodiments, at least two of X^1—X^6 are N.

[0092] In some embodiments, all of X^1—X^6 are C.

[0093] In some embodiments, at least two of Z^1-Z^3 are N.

[0094] In some embodiments, exactly two of Z^1-Z^3 are N.

[0095] In some embodiments, Z^1 is N.

[0096] In some embodiments, Z^2 is C.

[0097] In some embodiments, Z^3 is N.

[0098] In some embodiments, at least one of K^1, K^2, K^3, and K^4 is selected from the group consisting of O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$.

[0099] In some embodiments, at least one of K^1, K^2, K^3, and K^4 is O.

[0100] In some embodiments, exactly one of K^1, K^2, K^3, and K^4 is selected from the group consisting of O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$.

[0101] In some embodiments, exactly one of K^1, K^2, K^3, and K^4 is O.

[0102] In some embodiments, K^4 is selected from the group consisting of O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$.

[0103] In some embodiments, K^4 is O.

[0104] In some embodiments, all of K^1, K^2, K^3, and K^4 are direct bonds.

[0105] In some embodiments, when a is 0, L^1 is absent, when a is 1, L^1 is present. In some embodiments, when b is 0, L^2 is absent, when b is 1, L^2 is present. In some embodiments, when c is 0, L^3 is absent, when c is 1, L^3 is present.

[0106] In some embodiments, a+b+c=2.

[0107] In some embodiments, a+b+c=3.

[0108] In some embodiments, a is 1 (L^1 is present).

[0109] In some embodiments, b is 1 (L^2 is present).

[0110] In some embodiments, c is 1 (L^3 is present).

[0111] In some embodiments, c is 0 (L^3 is absent).

[0112] In some embodiments, a is 1, and L^1 is present and is selected from the group consisting of O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

[0113] In some embodiments, a is 1, and L^1 is present and is CR.

[0114] In some embodiments, a is 1, L^1 is present and is CR, and R of CR forms a 6-membered ring which is fused to moiety A.

[0115] In some embodiments, a is 1, L^1 is present and is CR, and R of CR forms a 6-membered aromatic ring which is fused to moiety A.

[0116] In some embodiments, a is 1, L^1 is present and is CR, and R of CR forms a 6-membered carbocyclic aromatic ring which is fused to moiety A.

[0117] In some embodiments, a is 1, and L^1 is present and is a direct bond.

[0118] In some embodiments, b is 1, and L^2 is present and is a direct bond.

[0119] In some embodiments, b is 1, and L^2 is present and is selected from the group consisting of O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

[0120] In some embodiments, b is 1, and L^2 is present and is NR.

[0121] In some embodiments, c is 1, and L^3 is present and is selected from the group consisting of O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

[0122] In some embodiments, c is 1, and L^3 is present and is O.

[0123] In some embodiments, moiety A is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered carbocyclic or heterocyclic ring. In some embodiments, moiety A is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered aryl or heteroaryl ring.

[0124] In some embodiments, moiety A is independently selected from the group consisting of the following Cyclic List: benzene, pyridine, pyrimidine, pyridazine, pyrazine, triazine, imidazole, imidazole-derived carbene, pyrazole, pyrrole, oxazole, furan, thiophene, thiazole, triazole, naphthalene, quinoline, isoquinoline, quinazoline, benzofuran, aza-benzofuran, benzoxazole, aza-benzoxazole, benzothiophene, aza-benzothiophene, benzothiazole, aza-benzothiazole, benzoselenophene, aza-benzoselenophene, indene, aza-indene, indole, aza-indole, benzimidazole, benzimidazole-derived carbene, aza-benzimidazole-derived carbene, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, phenanthro[3,2-b]benzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene. In some embodiments, the aza variant includes one N on a benzo ring. In some embodiments, the aza variant includes one N on a benzo ring and the N is bonded to the metal M.

[0125] In some embodiments, moiety A is a monocyclic ring. In some embodiments, moiety A is selected from the group consisting of benzene, pyridine, pyrimidine, pyridazine, pyrazine, triazine, imidazole, imidazole-derived carbene, pyrazole, pyrrole, oxazole, furan, thiophene, thiazole, and triazole. In some embodiments, moiety A is benzene.

[0126] In some embodiments, moiety A is a polycyclic fused ring system. In some embodiments, moiety A is selected from the group consisting of naphthalene, quinoline, isoquinoline, quinazoline, benzofuran, aza-benzofuran, benzoxazole, aza-benzoxazole, benzothiophene, aza-benzothiophene, benzothiazole, aza-benzothiazole, benzoselenophene, aza-benzoselenophene, indene, aza-indene, indole, aza-indole, benzimidazole, benzimidazole-derived carbene, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, phenanthro[3,2-b]benzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene. In some embodiments, moiety A is selected from the group consisting of naphthalene.

[0127] In some embodiments, moiety A has 3 rings and is selected from the group consisting of carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene.

[0128] In some embodiments, moiety A can be a polycyclic fused ring structure. In some embodiments, moiety A can be a polycyclic fused ring structure comprising at least three fused rings. In some embodiments, the polycyclic fused ring structure has two 6-membered rings and one 5-membered ring. In some such embodiments, the 5-membered ring is fused to the ring coordinated to the Ir atom and the second 6-membered ring is fused to the 5-membered ring. In some embodiments, moiety A can be selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and aza-variants thereof. In some such embodiments, moiety A can be further substituted at the ortho- or meta-position of the O, S, or Se atom by a substituent selected from the group consisting of deuterium, fluorine, nitrile, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof. In some such embodiments, the aza-variants contain exactly one N atom at the 6-position (ortho to the O, S, or Se) with a substituent at the 7-position (meta to the O, S, or Se).

[0129] In some embodiments, moiety A can be a polycyclic fused ring structure comprising at least four fused rings. In some embodiments, the polycyclic fused ring structure comprises three 6-membered rings and one 5-membered ring. In some such embodiments, the 5-membered ring is fused to the ring coordinated to the Ir atom, the second 6-membered ring is fused to the 5-membered ring, and the third 6-membered ring is fused to the second 6-membered ring. In some such embodiments, the third 6-membered ring is further substituted by a substituent selected from the group consisting of deuterium, fluorine, nitrile, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0130] In some embodiments, moiety A can be a polycyclic fused ring structure comprising at least five fused rings. In some embodiments, the polycyclic fused ring structure comprises four 6-membered rings and one 5-membered ring or three 6-membered rings and two 5-membered rings. In some embodiments comprising two 5-membered rings, the 5-membered rings are fused together. In some embodiments comprising two 5-membered rings, the 5-membered rings are separated by at least one 6-membered ring. In some embodiments with one 5-membered ring, the 5-membered ring is fused to the ring coordinated to the Ir atom, the second 6-membered ring is fused to the 5-membered ring, the third 6-membered ring is fused to the second 6-membered ring, and the fourth 6-membered ring is fused to the third 6-membered ring.

[0131] In some embodiments, moiety A can be an aza version of the polycyclic fused rings described above. In some such embodiments, moiety A can contain exactly one aza N atom. In some such embodiments, moiety A contains exactly two aza N atoms, which can be in one ring, or in two different rings. In some such embodiments, the ring having aza N atom is separated by at least two other rings from the Ir atom. In some such embodiments, the ring having aza N atom is separated by at least three other rings from the Ir atom. In some such embodiments, each of the ortho positions of the aza N atom is substituted.

[0132] In some embodiments, moiety B is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered carbocyclic or heterocyclic ring. In some embodiments, moiety B is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered aryl or heteroaryl ring.

[0133] In some embodiments, moiety B is independently selected from the group consisting of the following Cyclic List: benzene, pyridine, pyrimidine, pyridazine, pyrazine, triazine, imidazole, imidazole-derived carbene, pyrazole, pyrrole, oxazole, furan, thiophene, thiazole, triazole, naphthalene, quinoline, isoquinoline, quinazoline, benzofuran, aza-benzofuran, benzoxazole, aza-benzoxazole, benzothiophene, aza-benzothiophene, benzothiazole, aza-benzothiazole, benzoselenophene, aza-benzoselenophene, indene, aza-indene, indole, aza-indole, benzimidazole, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, phenanthro[3,2-b]benzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene. In some embodiments, the aza variant includes one N on a benzo ring. In some embodiments, the aza variant includes one N on a benzo ring and the N is bonded to the metal M.

[0134] In some embodiments, moiety B is a monocyclic ring. In some embodiments, moiety B is selected from the group consisting of benzene, pyridine, pyrimidine, pyridazine, pyrazine, triazine, imidazole, imidazole-derived carbene, pyrazole, pyrrole, oxazole, furan, thiophene, thiazole, and triazole. In some embodiments, moiety B is benzene.

[0135] In some embodiments, moiety B is a polycyclic fused ring system. In some embodiments, moiety B is selected from the group consisting of naphthalene, quinoline, isoquinoline, quinazoline, benzofuran, aza-benzofuran, benzoxazole, aza-benzoxazole, benzothiophene, aza-benzothiophene, benzothiazole, aza-benzothiazole, benzoselenophene, aza-benzoselenophene, indene, aza-indene, indole, aza-indole, benzimidazole, benzimidazole-derived carbene, aza-benzimidazole-derived carbene, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene. In some embodiments, moiety B is selected from the group consisting of naphthalene.

[0136] In some embodiments, moiety B has 3 rings and is selected from the group consisting of carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene.

[0137] In some embodiments, moiety B can be a polycyclic fused ring structure. In some embodiments, moiety B can be a polycyclic fused ring structure comprising at least three fused rings. In some embodiments, the polycyclic fused ring structure has two 6-membered rings and one 5-membered ring. In some such embodiments, the 5-membered ring is fused to the ring coordinated to the Ir atom and the second 6-membered ring is fused to the 5-membered ring. In some embodiments, moiety B can be selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and aza-variants thereof. In some such embodiments, moiety B can be further substituted at the ortho- or meta-position of the O, S, or Se atom by a substituent selected from the group consisting of deuterium, fluorine, nitrile, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof. In some such embodiments, the aza-variants contain exactly one N atom at the 6-position (ortho to the O, S, or Se) with a substituent at the 7-position (meta to the O, S, or Se).

[0138] In some embodiments, moiety B can be a polycyclic fused ring structure comprising at least four fused rings. In some embodiments, the polycyclic fused ring structure comprises three 6-membered rings and one 5-membered ring. In some such embodiments, the 5-membered ring is fused to the ring coordinated to the Ir atom, the second 6-membered ring is fused to the 5-membered ring, and the third 6-membered ring is fused to the second 6-membered ring. In some such embodiments, the third 6-membered ring is further substituted by a substituent selected from the group consisting of deuterium, fluorine, nitrile, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0139] In some embodiments, moiety B can be a polycyclic fused ring structure comprising at least five fused rings. In some embodiments, the polycyclic fused ring structure comprises four 6-membered rings and one 5-membered ring or three 6-membered rings and two 5-membered rings. In some embodiments comprising two 5-membered rings, the 5-membered rings are fused together. In some embodiments comprising two 5-membered rings, the 5-membered rings are separated by at least one 6-membered ring. In some embodiments with one 5-membered ring, the 5-membered ring is fused to the ring coordinated to the Ir atom, the second 6-membered ring is fused to the 5-membered ring, the third 6-membered ring is fused to the second 6-membered ring, and the fourth 6-membered ring is fused to the third 6-membered ring.

[0140] In some embodiments, moiety B can be an aza version of the polycyclic fused rings described above. In some such embodiments, moiety B can contain exactly one aza N atom. In some such embodiments, moiety B contains exactly two aza N atoms, which can be in one ring, or in two different rings. In some such embodiments, the ring having aza N atom is separated by at least two other rings from the Ir atom. In some such embodiments, the ring having aza N atom is separated by at least three other rings from the Ir atom. In some such embodiments, each of the ortho positions of the aza N atom is substituted.

[0141] In some embodiments, moiety C is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered carbocyclic or heterocyclic ring. In some embodiments, moiety C is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered aryl or heteroaryl ring.

[0142] In some embodiments, moiety C is independently selected from the group consisting of the following Cyclic List: benzene, pyridine, pyrimidine, pyridazine, pyrazine, triazine, imidazole, pyrazole, pyrrole, oxazole, furan, thiophene, thiazole, triazole, naphthalene, quinoline, isoquino-

line, quinazoline, benzofuran, aza-benzofuran, benzoxazole, aza-benzoxazole, benzothiophene, aza-benzothiophene, benzothiazole, aza-benzothiazole, benzoselenophene, aza-benzoselenophene, indene, aza-indene, indole, aza-indole, benzimidazole, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, phenanthro[3,2-b]benzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene. In some embodiments, the aza variant includes one N on a benzo ring. In some embodiments, the aza variant includes one N on a benzo ring and the N is bonded to the metal M.

[0143] In some embodiments, moiety C is a monocyclic ring. In some embodiments, moiety C is selected from the group consisting of benzene, pyridine, pyrimidine, pyridazine, pyrazine, triazine, imidazole, pyrazole, pyrrole, oxazole, furan, thiophene, thiazole, and triazole. In some embodiments, moiety C is benzene.

[0144] In some embodiments, moiety C is a polycyclic fused ring system. In some embodiments, moiety C is selected from the group consisting of naphthalene, quinoline, isoquinoline, quinazoline, benzofuran, aza-benzofuran, benzoxazole, aza-benzoxazole, benzothiophene, aza-benzothiophene, benzothiazole, aza-benzothiazole, benzoselenophene, aza-benzoselenophene, indene, aza-indene, indole, aza-indole, benzimidazole, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, phenanthro[3,2-b] benzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene. In some embodiments, moiety C is selected from the group consisting of naphthalene.

[0145] In some embodiments, moiety C has 3 rings and is selected from the group consisting of carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalazine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene.

[0146] In some embodiments, moiety C can be a polycyclic fused ring structure. In some embodiments, moiety C can be a polycyclic fused ring structure comprising at least three fused rings. In some embodiments, the polycyclic fused ring structure has two 6-membered rings and one 5-membered ring. In some such embodiments, the 5-membered ring is fused to the ring coordinated to the Ir atom and the second 6-membered ring is fused to the 5-membered ring. In some embodiments, moiety C can be selected from the group consisting of dibenzofuran, dibenzothiophene, dibenzoselenophene, and aza-variants thereof. In some such embodiments, moiety C can be further substituted at the ortho- or meta-position of the O, S, or Se atom by a substituent selected from the group consisting of deuterium, fluorine, nitrile, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof. In some such embodiments, the aza-variants contain exactly one N atom at the 6-position (ortho to the O, S, or Se) with a substituent at the 7-position (meta to the O, S, or Se).

[0147] In some embodiments, moiety C can be a polycyclic fused ring structure comprising at least four fused rings. In some embodiments, the polycyclic fused ring structure comprises three 6-membered rings and one 5-membered ring. In some such embodiments, the 5-membered ring is fused to the ring coordinated to the Ir atom, the second 6-membered ring is fused to the 5-membered ring, and the third 6-membered ring is fused to the second 6-membered ring. In some such embodiments, the third 6-membered ring is further substituted by a substituent selected from the group consisting of deuterium, fluorine, nitrile, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0148] In some embodiments, moiety C can be a polycyclic fused ring structure comprising at least five fused rings. In some embodiments, the polycyclic fused ring structure comprises four 6-membered rings and one 5-membered ring or three 6-membered rings and two 5-membered rings. In some embodiments comprising two 5-membered rings, the 5-membered rings are fused together. In some embodiments comprising two 5-membered rings, the 5-membered rings are separated by at least one 6-membered ring. In some embodiments with one 5-membered ring, the 5-membered ring is fused to the ring coordinated to the Ir atom, the second 6-membered ring is fused to the 5-membered ring, the third 6-membered ring is fused to the second 6-membered ring, and the fourth 6-membered ring is fused to the third 6-membered ring.

[0149] In some embodiments, moiety C can be an aza version of the polycyclic fused rings described above. In some such embodiments, moiety C can contain exactly one aza N atom. In some such embodiments, moiety C contains exactly two aza N atoms, which can be in one ring, or in two different rings. In some such embodiments, the ring having aza N atom is separated by at least two other rings from the Ir atom. In some such embodiments, the ring having aza N atom is separated by at least three other rings from the Ir atom. In some such embodiments, each of the ortho positions of the aza N atom is substituted.

[0150] In some embodiments, moiety A comprises a 5-membered ring.

[0151] In some embodiments, moiety A comprises a 5-membered heterocyclic ring.

[0152] In some embodiments, moiety A comprises a 5-membered heterocyclic aromatic ring.

[0153] In some embodiments, moiety A comprises an imidazole ring.

[0154] In some embodiments, moiety A comprises a 6-membered ring.

[0155] In some embodiments, moiety B comprises a 6-membered ring.

[0156] In some embodiments, moiety B comprises a 6-membered carbocyclic ring.

[0157] In some embodiments, moiety B comprises a 6-membered carbocyclic aromatic ring.

[0158] In some embodiments, moiety B is a 6-membered ring.

[0159] In some embodiments, moiety B is a 6-membered carbocyclic ring.

[0160] In some embodiments, moiety B is a 6-membered carbocyclic aromatic ring.

[0161] In some embodiments, moiety C comprises a 6-membered ring.

[0162] In some embodiments, moiety C comprises a 6-membered aromatic ring.

[0163] In some embodiments, moiety C comprises a 6-membered heterocyclic aromatic ring.

[0164] In some embodiments, moiety C is a 6-membered ring.

[0165] In some embodiments, moiety C is a 6-membered aromatic ring.

[0166] In some embodiments, moiety C is a 6-membered heterocyclic aromatic ring.

[0167] In some embodiments, R^1 is alkyl.

[0168] In some embodiments, R^1 is partially or fully deuterated alkyl.

[0169] In some embodiments, R^2 is hydrogen.

[0170] In some embodiments, R^3 is hydrogen.

[0171] In some embodiments, the compound comprises a fully deuterated alkyl group.

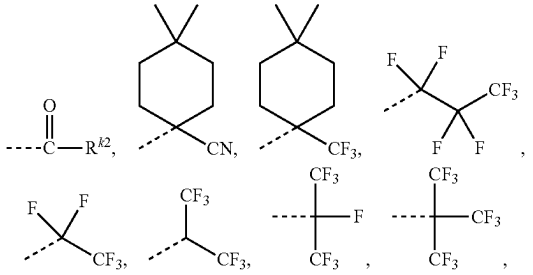
[0172] In some embodiments, the compound comprises a fully deuterated methyl group.

[0173] In some embodiments, the compound comprises a tert-butyl group.

[0174] In some embodiments, the compound comprises a fully deuterated tert-butyl group.

[0175] In some embodiments, the compound comprises an electron-withdrawing group. In some embodiments, the electron-withdrawing group has a Hammett constant larger than 0. In some embodiments, the electron-withdrawing group has a Hammett constant equal or larger than 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, or 1.1.

[0176] In some embodiments, the compound comprises an electron-withdrawing group selected from the group consisting of the following EWG1 LIST: F, CF_3, CN, $COCH_3$, CHO, $COCF_3$, COOMe, $COOCF_3$, NO_2, SF_3, SiF_3, PF_4, SF_5, OCF_3, SCF_3, $SeCF_3$, $SOCF_3$, $SeOCF_3$, SO_2F, SO_2CF_3, SeO_2CF_3, $OSeO_2CF_3$, OCN, SCN, SeCN, NC, $^+N(R^{k2})_3$, $(R^{k2})_2CCN$, $(R^{k2})_2CCF_3$, $CNC(CF_3)_2$, $BR^{k3}R^{k2}$, substituted or unsubstituted dibenzoborole, 1-substituted carbazole, 1,9-substituted carbazole, substituted or unsubstituted carbazole, substituted or unsubstituted pyridine, substituted or unsubstituted pyrimidine, substituted or unsubstituted pyrazine, substituted or unsubstituted pyridoxine, substituted or unsubstituted triazine, substituted or unsubstituted oxazole, substituted or unsubstituted benzoxazole, substituted or unsubstituted thiazole, substituted or unsubstituted benzothiazole, substituted or unsubstituted imidazole, substituted or unsubstituted benzimidazole, ketone, carboxylic acid, ester, nitrile, isonitrile, sulfinyl, sulfonyl, partially and fully fluorinated alkyl, partially and fully fluorinated aryl, partially and fully fluorinated heteroaryl, cyano-containing alkyl, cyano-containing aryl, cyano-containing heteroaryl, isocyanate,



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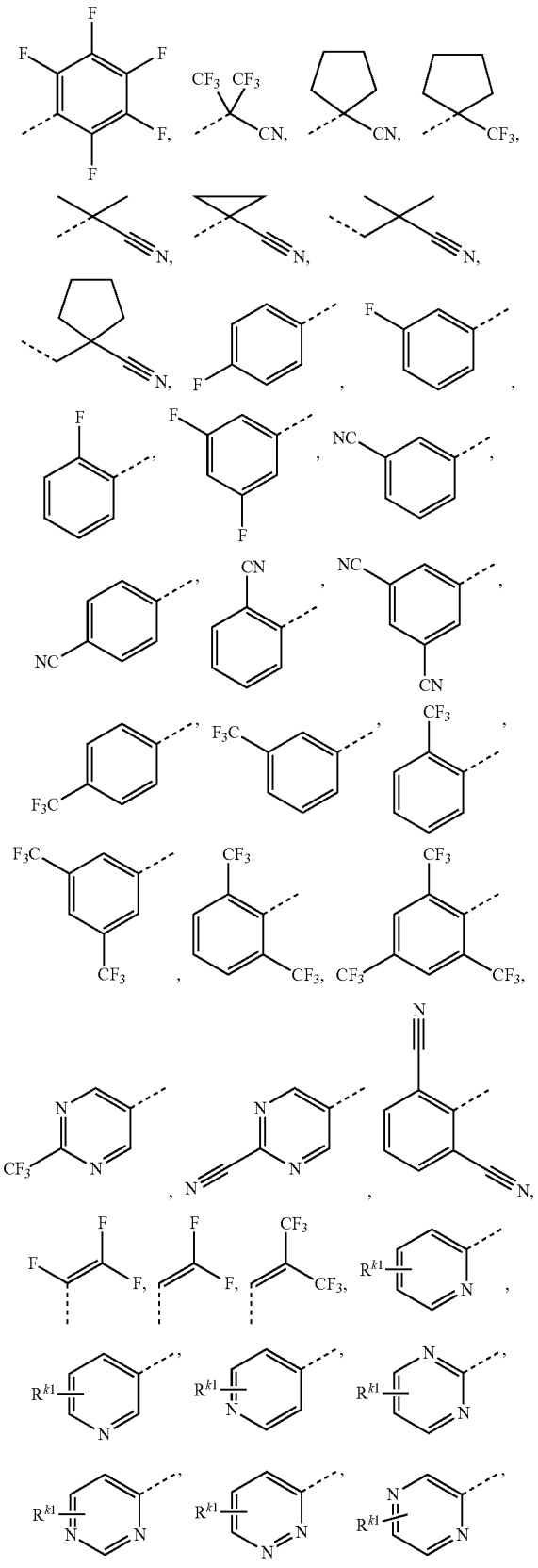

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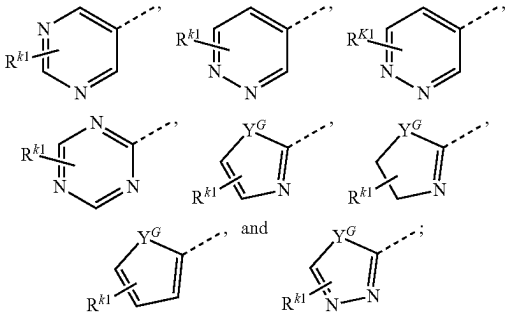


[0177] wherein each R^{k1} represents mono to the maximum allowable substitution, or no substitutions;

[0178] wherein Y^G is selected from the group consisting of BR_e, NR_e, PR_e, O, S, Se, C═O, S═O, SO_2, CR_eR_f, SiR_eR_f, and GeR_eR_f; and wherein each of R^{k1}, R^{k2}, R'3, R_e, and R_f is independently a hydrogen or a substituent selected from the group consisting of the General Substituents defined herein.

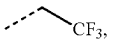
[0179] In some embodiments, the compound comprises an electron-withdrawing group selected from the group consisting of the structures of the following EWG2 List:

E1

E2

E3

E4



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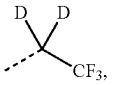

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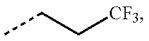

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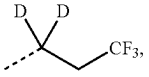

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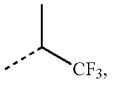

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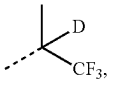

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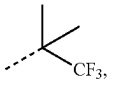

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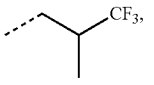

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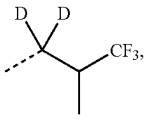

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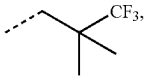

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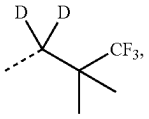

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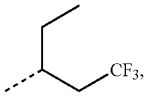

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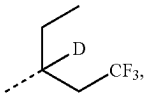

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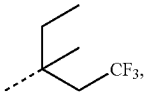

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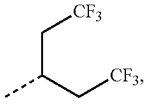

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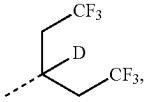

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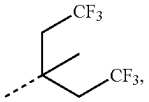

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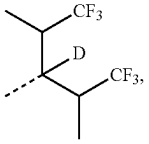

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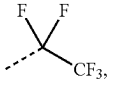

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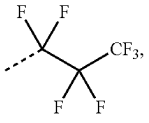

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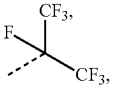

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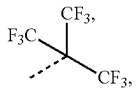

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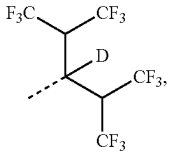

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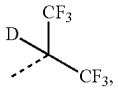

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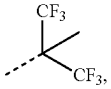

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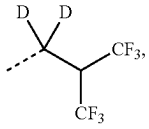

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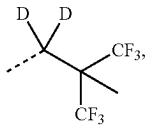

E31

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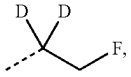

E33

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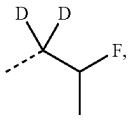

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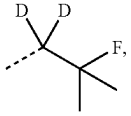

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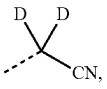

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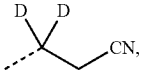

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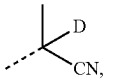

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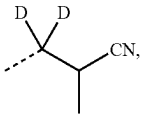

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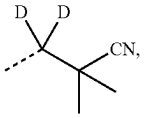

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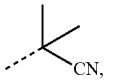

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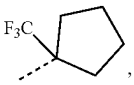

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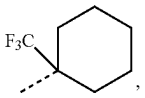

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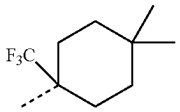

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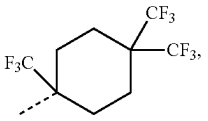

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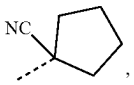

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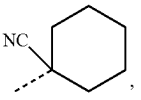

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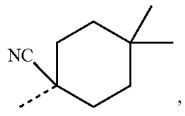

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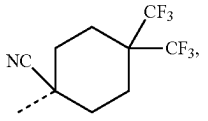

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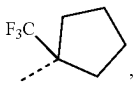

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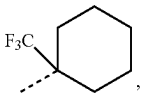

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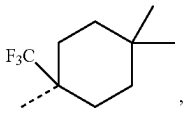

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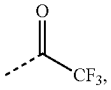

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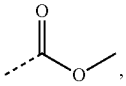

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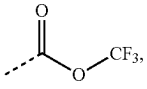

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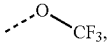

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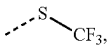

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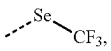

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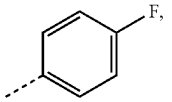

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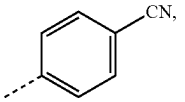

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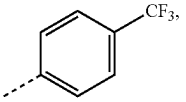

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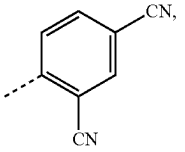

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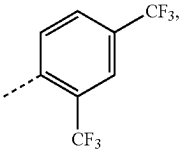

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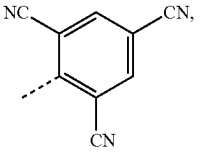

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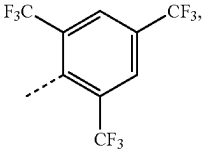

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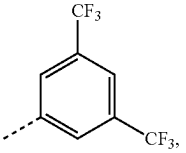

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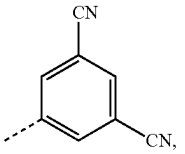

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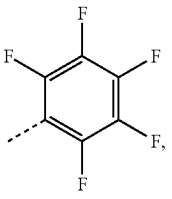

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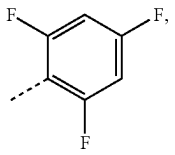

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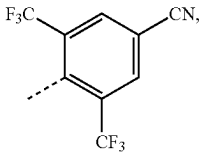

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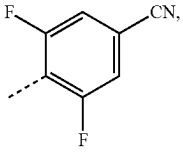

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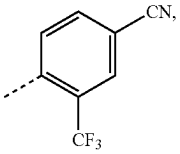

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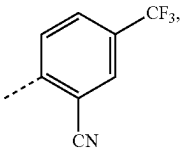

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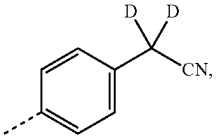

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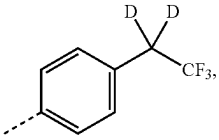

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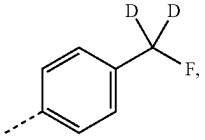

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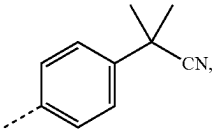

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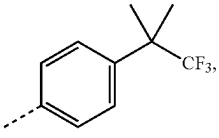

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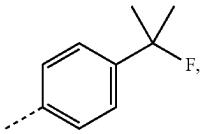

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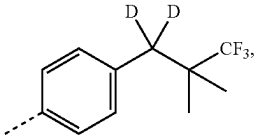

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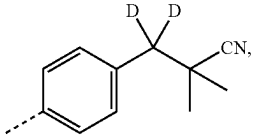

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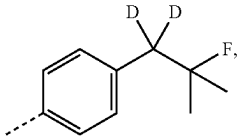

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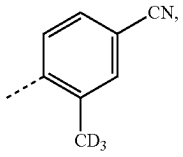

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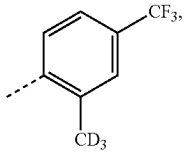

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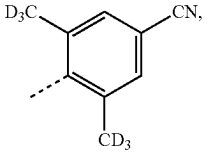

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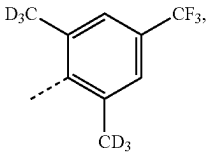

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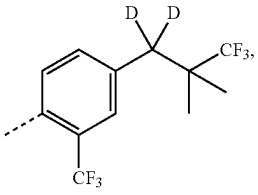

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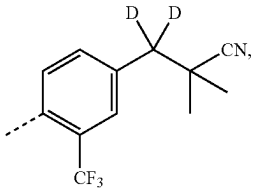

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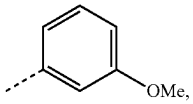

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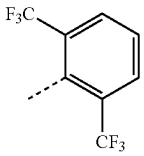

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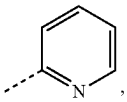

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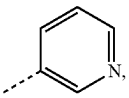

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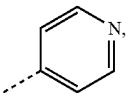

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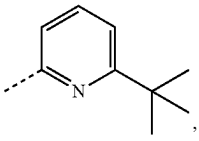

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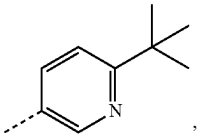

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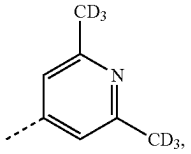

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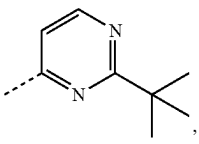

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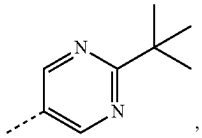

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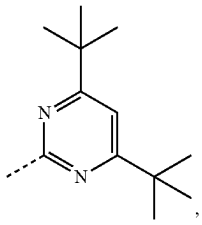

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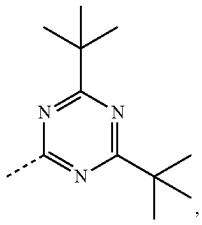

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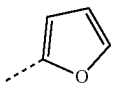

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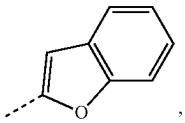

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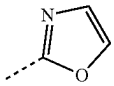

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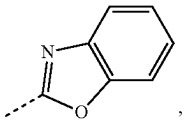

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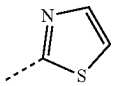

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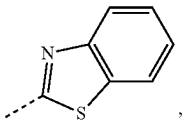

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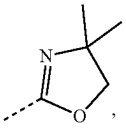

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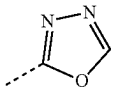

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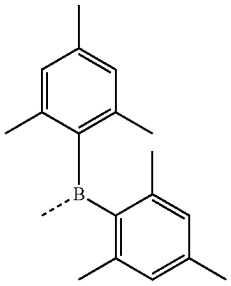

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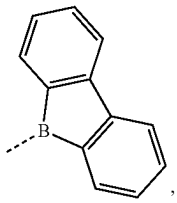

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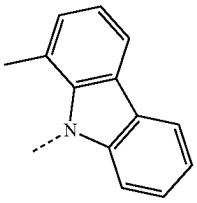

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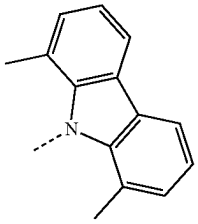

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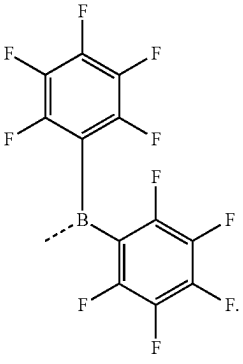


[0180] In some embodiments, the compound comprises an electron-withdrawing group selected from the group consisting of the structures of the following EWG3 LIST:

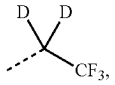
E1

E2

-continued

E3

E5



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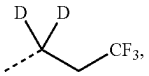

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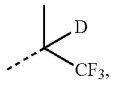

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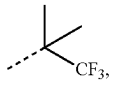

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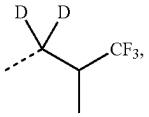

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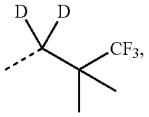

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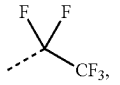

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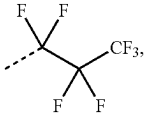

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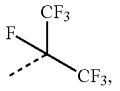

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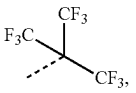

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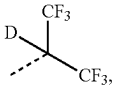

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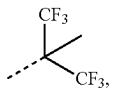

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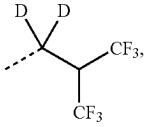

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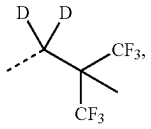

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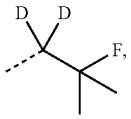

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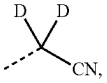

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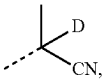

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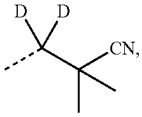

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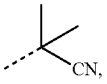

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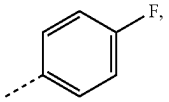

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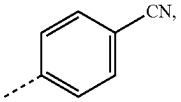

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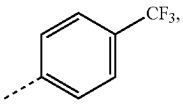

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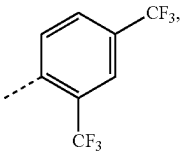

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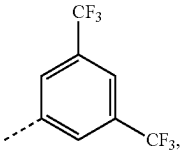

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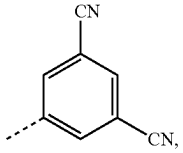

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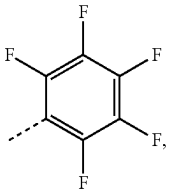

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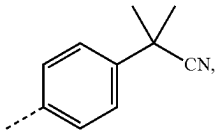

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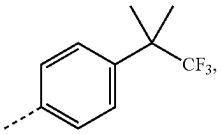

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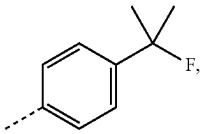

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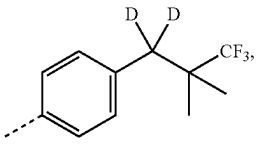

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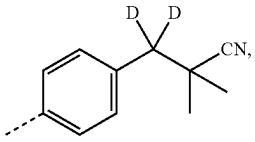

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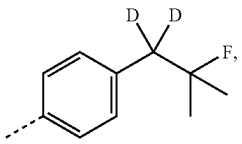

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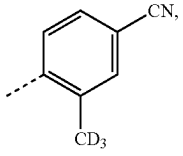

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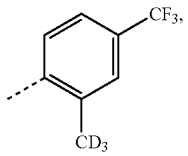

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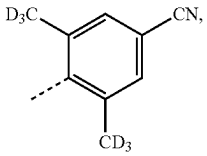

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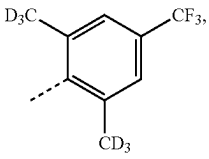

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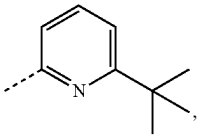

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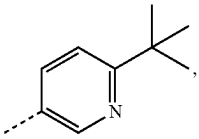
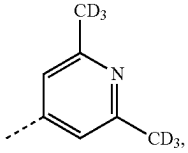


E108



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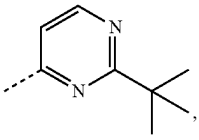

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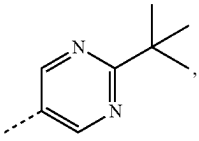

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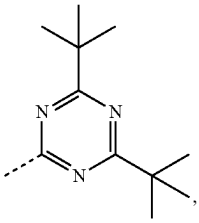

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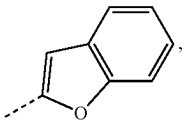
E114



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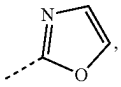
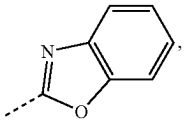
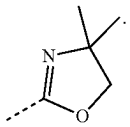


E116



and

E119



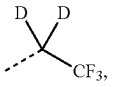
[0181] In some embodiments, the compound comprises an electron-withdrawing group selected from the group consisting of the structures of the following EWG4 LIST:

E1

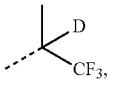
E2

E3

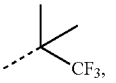
E5



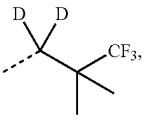
E9



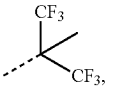
E10



E14



E28



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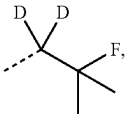

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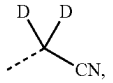
E36



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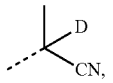

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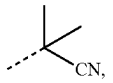

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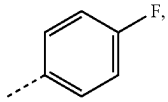

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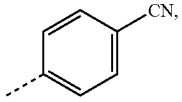

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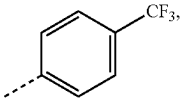

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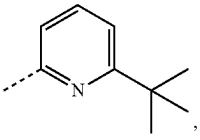

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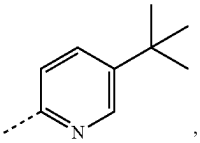

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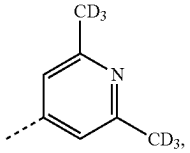

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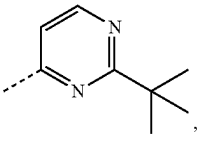

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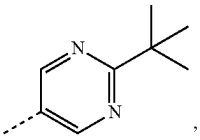

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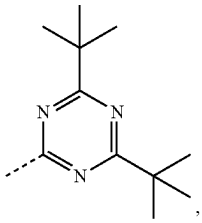

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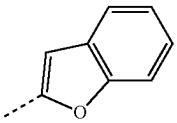

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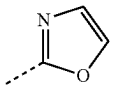

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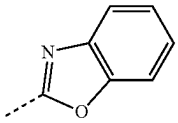
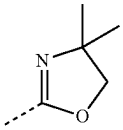
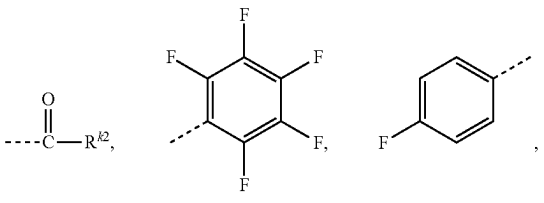


and

E119



[0182] In some embodiments, the compound comprises an electron-withdrawing group that is a 7r-electron deficient electron-withdrawing group. In some embodiments, the 7r-electron deficient electron-withdrawing group is selected from the group consisting of the structures of the following Pi-EWG LIST: CN, $COCH_3$, CHO, $COCF_3$, COOMe, $COOCF_3$, NO_2, SF_3, SiF_3, PF_4, SF_5, OCF_3, SCF_3, $SeCF_3$, $SOCF_3$, $SeOCF_3$, SO_2F, SO_2CF_3, SeO_2CF_3, $OSeO_2CF_3$, OCN, SCN, SeCN, NC, $^+N(R^{k2})_3$, $BR^{k2}R^{k3}$, substituted or unsubstituted dibenzoborole, 1-substituted carbazole, 1,9-substituted carbazole, substituted or unsubstituted carbazole, substituted or unsubstituted pyridine, substituted or unsubstituted pyrimidine, substituted or unsubstituted pyrazine, substituted or unsubstituted pyridazine, substituted or unsubstituted triazine, substituted or unsubstituted oxazole, substituted or unsubstituted benzoxazole, substituted or unsubstituted thiazole, substituted or unsubstituted benzothiazole, substituted or unsubstituted imidazole, substituted or unsubstituted benzimidazole, ketone, carboxylic acid, ester, nitrile, isonitrile, sulfinyl, sulfonyl, partially and fully fluorinated aryl, partially and fully fluorinated heteroaryl, cyano-containing aryl, cyano-containing



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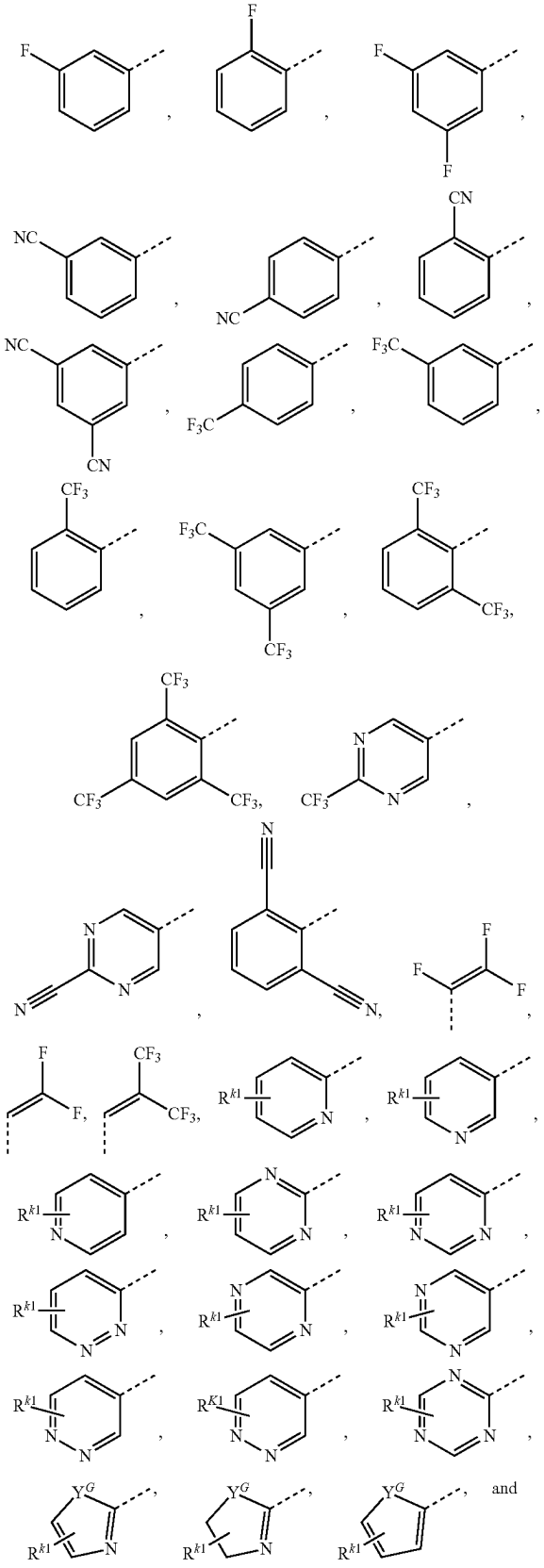

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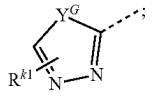


wherein the variables are the same as previously defined.

[0183] In some embodiments, the compound comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, the compound comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, the compound comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, the compound comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, the compound comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0184] In some embodiments, at least one R^A is or comprises an electron-withdrawing group. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0185] In some embodiments, at least one R^B is or comprises an electron-withdrawing group. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0186] In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0187] In some embodiments of Formula I, at least one R', R", R^A, R^B, R^C, R^1, R^2, or R^3 is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R', R", R^A, R^B, R^C, R^1, R^2, or R^3 is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R', R", R^A, R^B, R^C, R^1, R^2, or R^3 is or comprises an electron-withdrawing group from the EWG3

LIST as defined herein. In some embodiments, at least one R', R", R^A, R^B, R^C, R^1, R^2, or R^3 is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R', R", R^A, R^B, R^C, R^1, R^2, or R^3 is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0188] In some embodiments of Formula I, at least one R^A is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^A is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0189] In some embodiments of Formula I, at least one R^B is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^B is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0190] In some embodiments of Formula I, at least one R^C is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^C is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0191] In some embodiments of Formula I, at least one R^1 is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^1 is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^1 is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^1 is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^1 is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0192] In some embodiments of Formula I, at least one R^2 is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^2 is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^2 is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^2 is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^2 is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0193] In some embodiments of Formula I, at least one R^3 is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R^3 is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R^3 is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R^3 is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R^3 is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0194] In some embodiments, Formula I comprises an electron-withdrawing group from the EWG1 LIST as defined herein.

[0195] In some embodiments, Formula I comprises an electron-withdrawing group from the EWG2 LIST as defined herein.

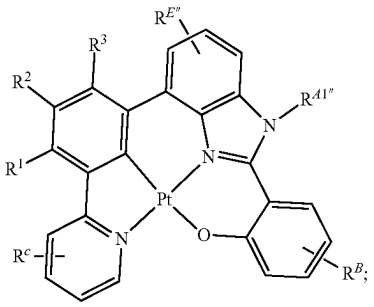
[0196] In some embodiments, Formula I comprises an electron-withdrawing group from the EWG3 LIST as defined herein.

[0197] In some embodiments, Formula I comprises an electron-withdrawing group from the EWG4 LIST as defined herein.

[0198] In some embodiments, Formula I comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0199] In some embodiments, the compound comprises a structure of Formula II

Formula II



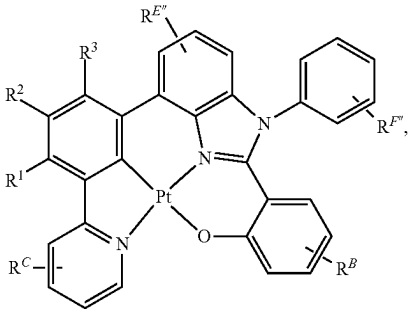
[0200] wherein each of $R^{A1"}$ and $R^{E"}$ is independently a hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, combinations thereof, and

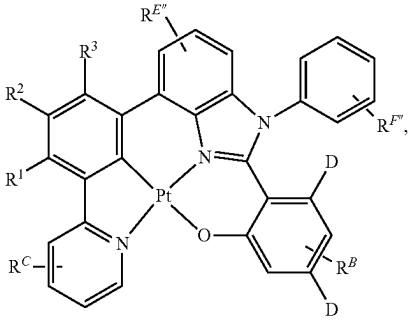
[0201] wherein one or more of the R^B or R^C is D.

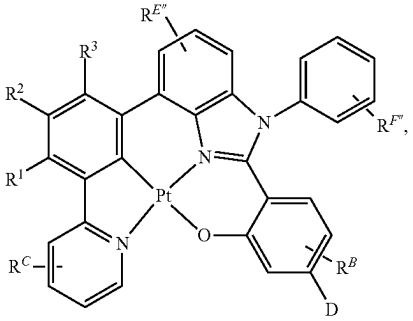
[0202] In some of the above embodiments, exactly one R^B or R^C is D. In some of the above embodiments, two R^B or R^C are D. In some of the above embodiments, D is meta to the N of pyridine. In some of the above embodiments, one R^B is para to the N. In some of the above embodiments, one R^B is selected from the group consisting of aryl, heteroaryl,

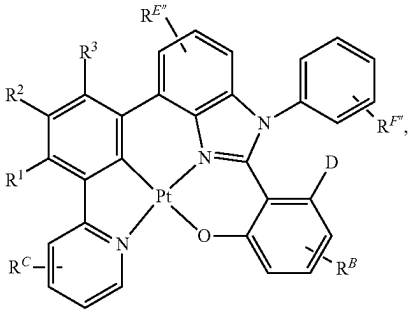
alkyl, cycloalkyl, silyl, partially or fully deuterated variants thereof, partially or fully fluorinated variants thereof, and combinations thereof.

[0203] In some embodiments, the compound has a structure selected from the group consisting of the following (LIST 1):









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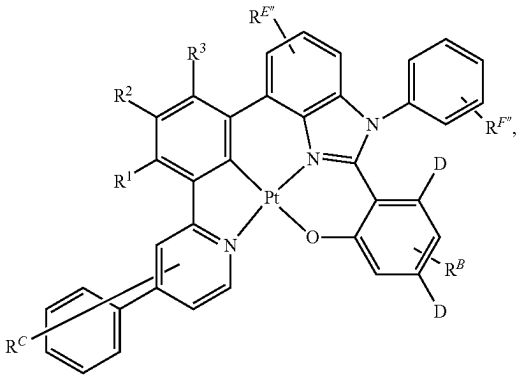

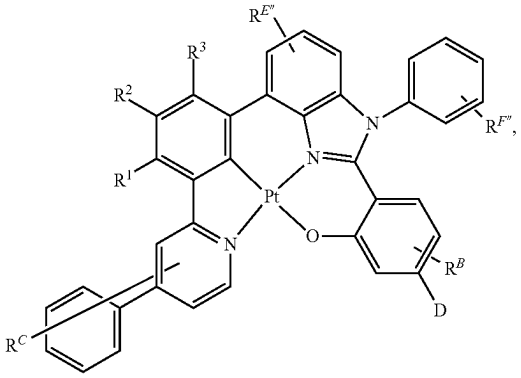

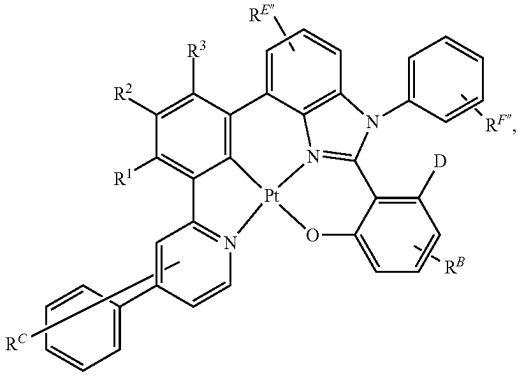

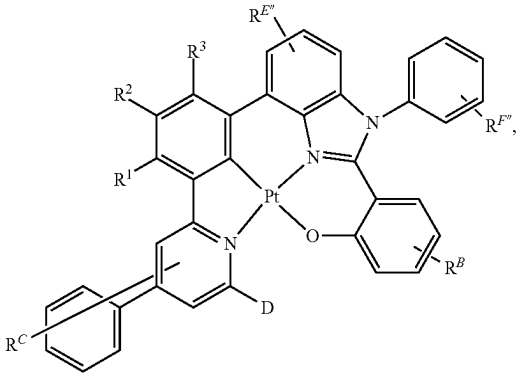

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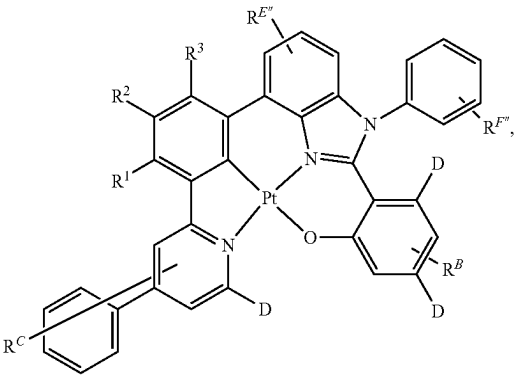

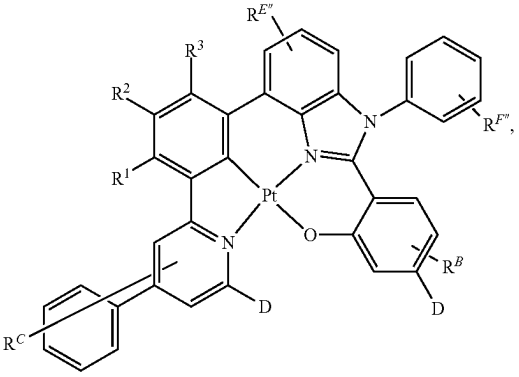

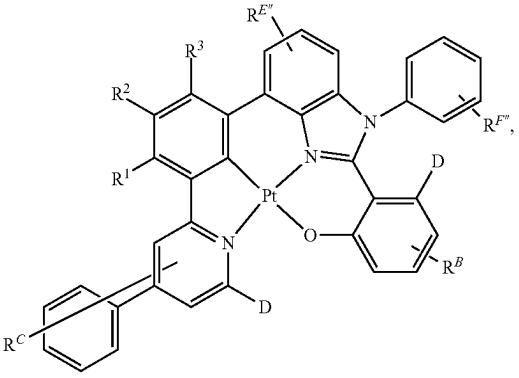

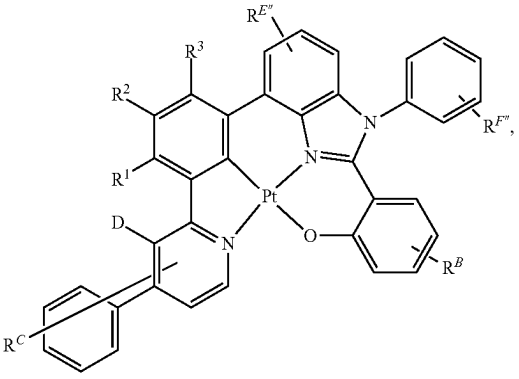

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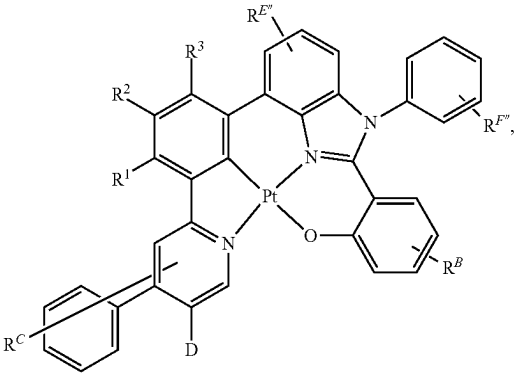

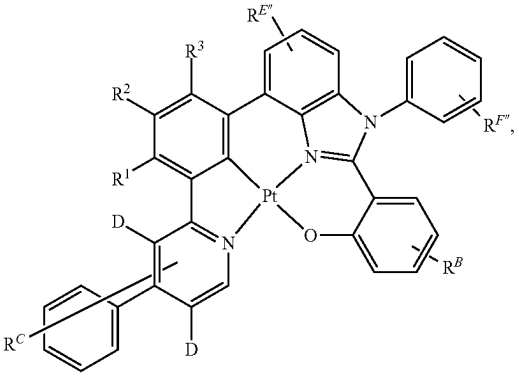

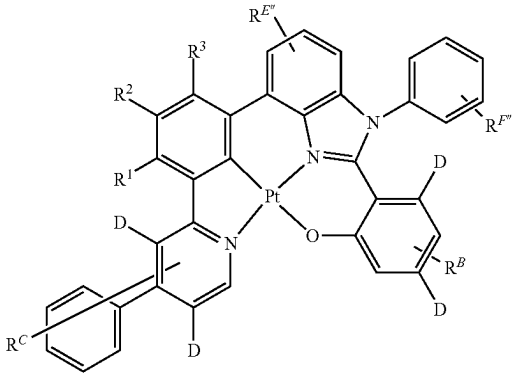

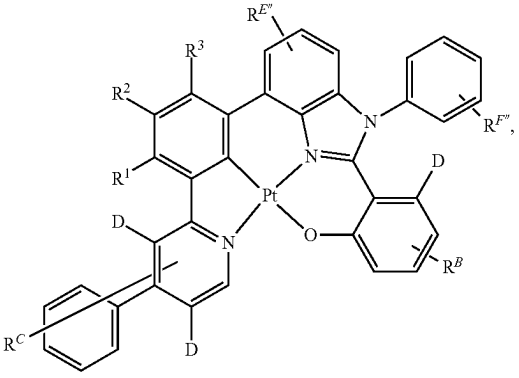

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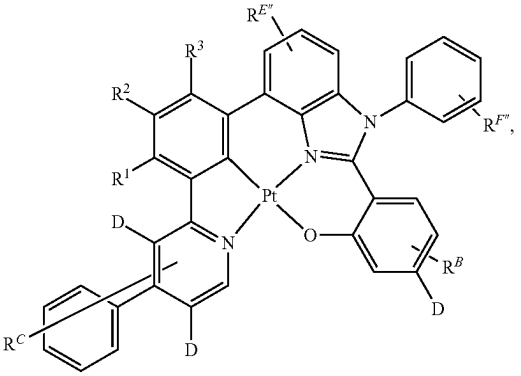

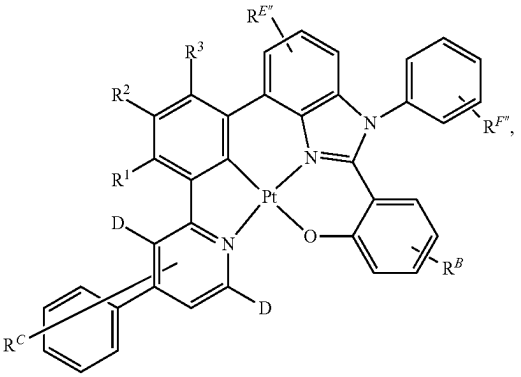

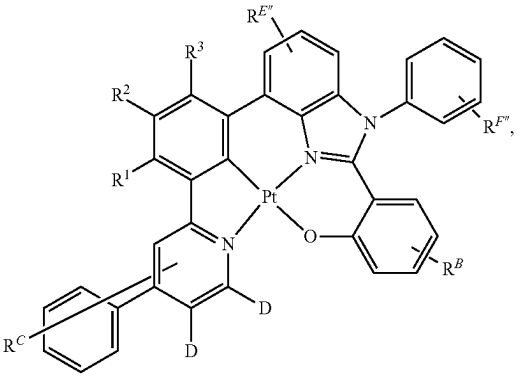

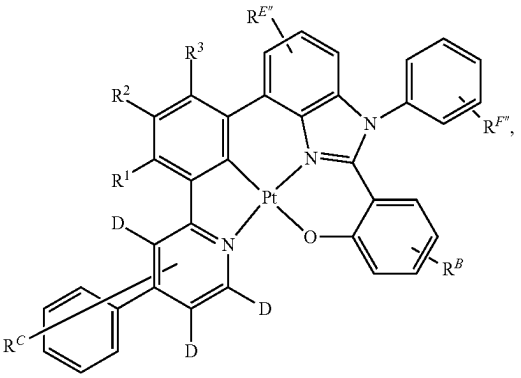

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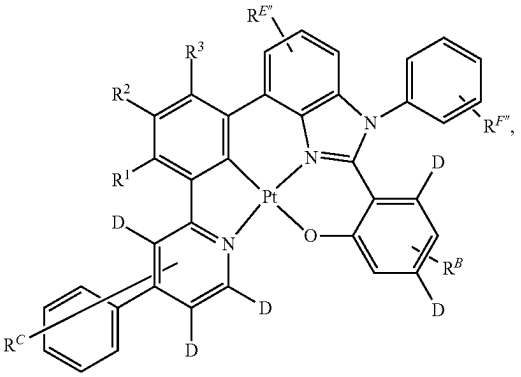

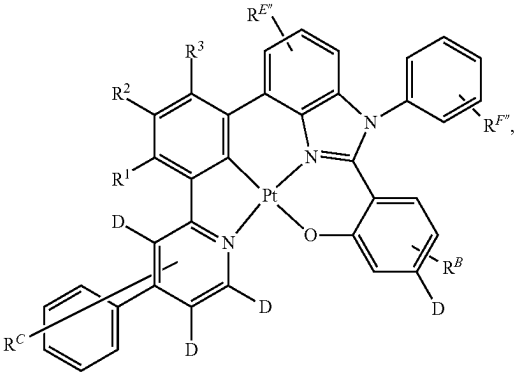

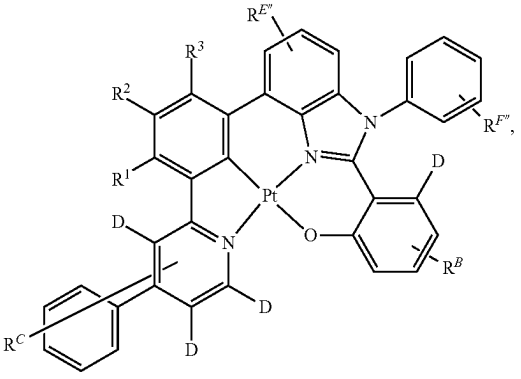

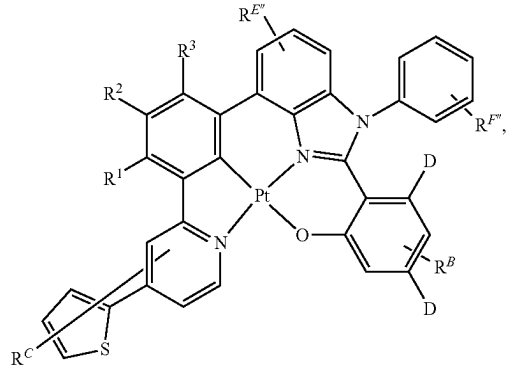

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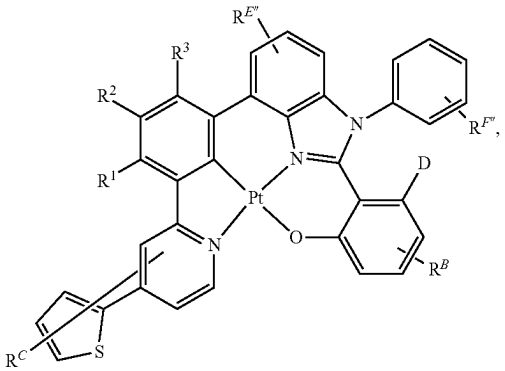

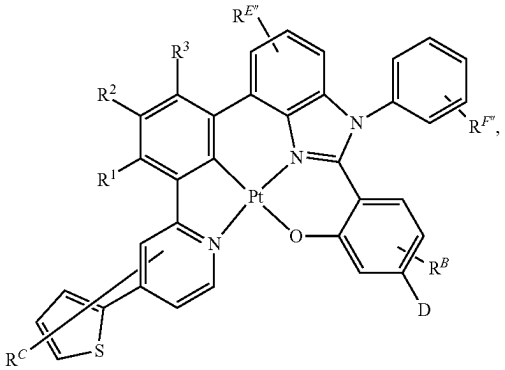

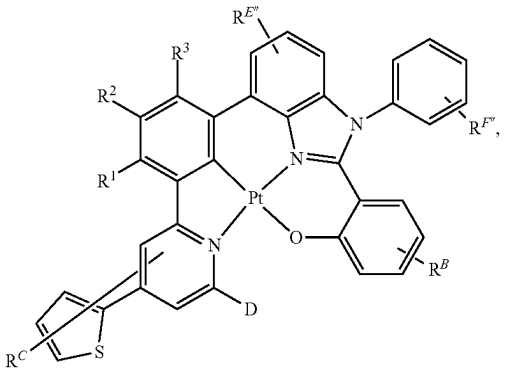

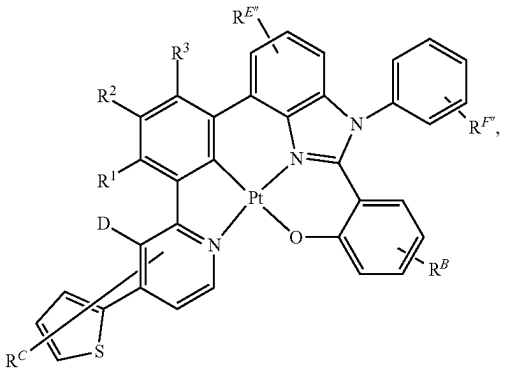

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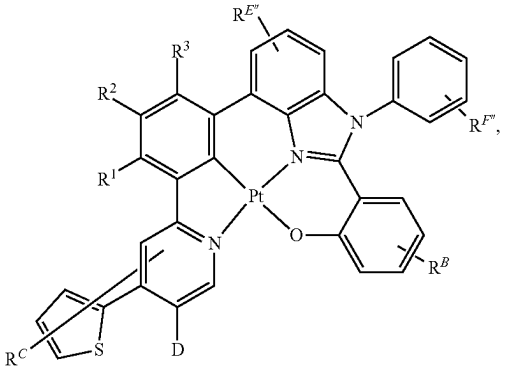

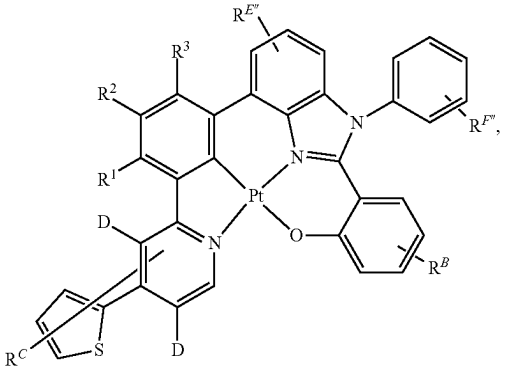

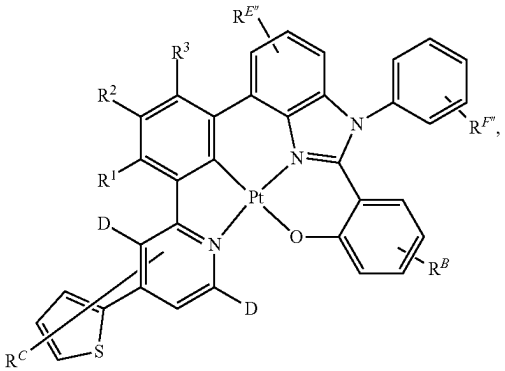

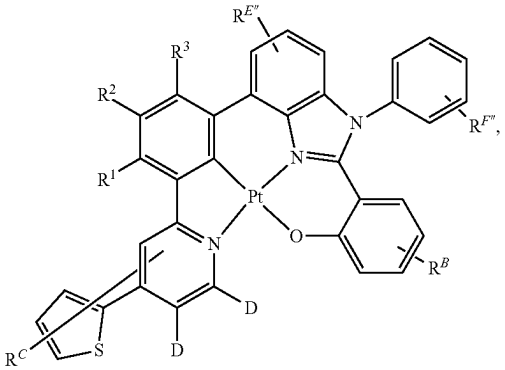

and

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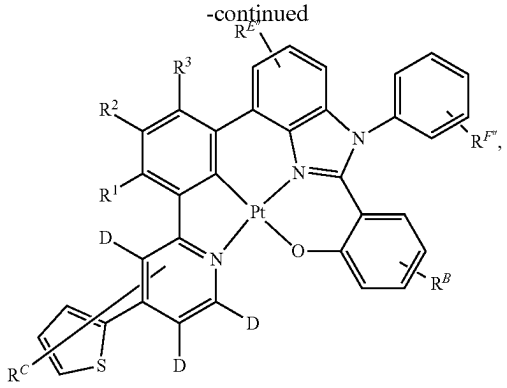


[0204] wherein $R^{F''}$ is independently a hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, combinations thereof; and the rest of variables are the same as previously defined.

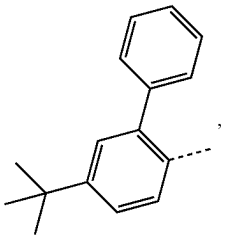
[0205] In some embodiments, in the structures of LIST 1, at least one R^B is D, and at least one R^C is not H or D.

[0206] In some such embodiments, two R^B are D, and the remaining two R^B are not H or D. In some such embodiments, two R^B are D at the meta positions to the carbon atom substituted by the oxygen atom. In some such embodiments, two R^B at the meta positions to the carbon atom bonding to the imidazole ring are alkyl groups having at least two, three, four, or five carbon atoms. In some embodiments, at least one R^C is D, and at least one R^C is not H or D. In some such embodiments, two R^C are D, and one R^C is not H or D. In some such embodiments, two R^C are D at the meta positions to the N atom of the pyridine. In some embodiments, the R^C para to the N of pyridine is a substituted or unsubstituted phenyl. In some of such embodiments, the substituted phenyl can be partially or fully deuterated, or partially or fully fluorinated. In some of such embodiments, the substituted phenyl is substituted by at least one silyl or germyl group.

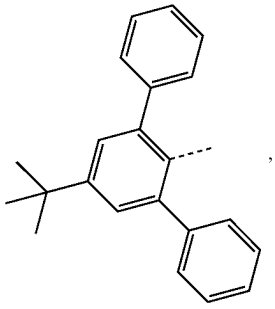
[0207] In some embodiments when the compound is selected from LIST 1, at least one R^B, R^C, $R^{E''}$, $R^{F''}$, R^2, or R^3 is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^B is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^C is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one $R^{E''}$ is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one $R^{F''}$ is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^2 is selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R^3 is selected from the group consisting of the General Substituents defined herein. In some embodiments when the compound is selected from LIST 1, at least one R^B, R^C, $R^{E''}$, $R^{F''}$, R^2, or R^3 is selected from the group consisting of the Preferred General Substituents defined herein.

[0208] In some embodiments, $R^{A1''}$ is selected from $R^{A1''}_{W1}$, wherein W1 is an integer from 1 to 21, wherein $R^{A1''}_1$–$R^{A1''}_{21}$ have the structures in the following LIST 2:

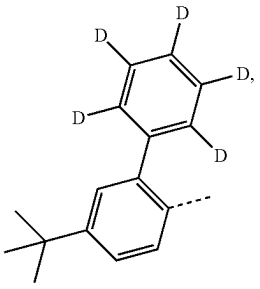
$R^{A1''}_1$



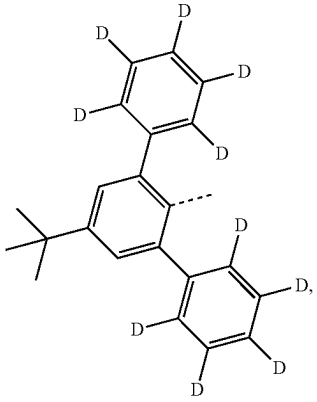
$R^{A1''}_2$



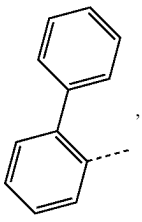
$R^{A1''}_3$



$R^{A1''}_4$



$R^{A1''}_5$



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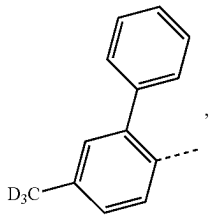
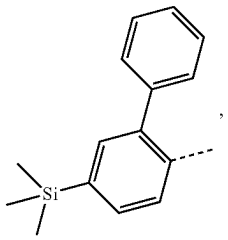
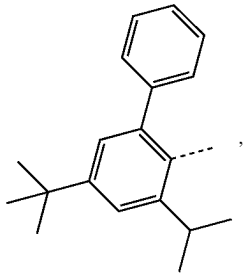
$R^{A1''}_6$



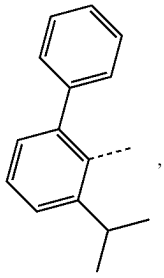
$R^{A1''}_7$



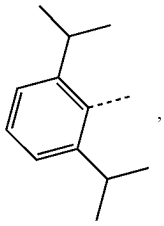
$R^{A1''}_8$



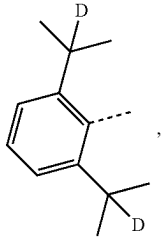
$R^{A1''}_9$



$R^{A1''}_{10}$



$R^{A1''}_{11}$



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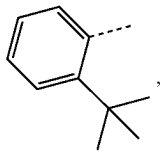
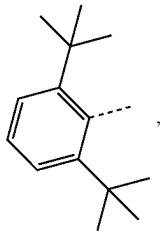
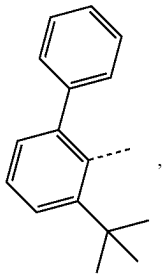
$R^{A1''}_{12}$



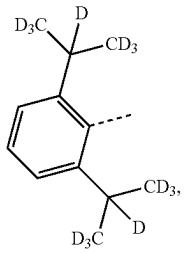
$R^{A1''}_{13}$



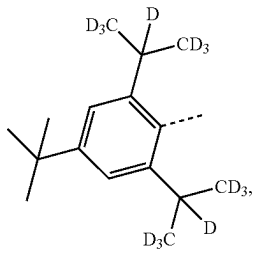
$R^{A1''}_{14}$



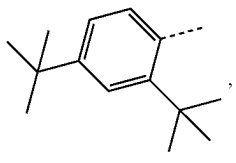
$R^{A1''}_{15}$



$R^{A1''}_{16}$



$R^{A1''}_{17}$



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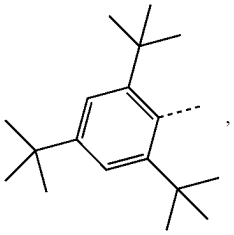
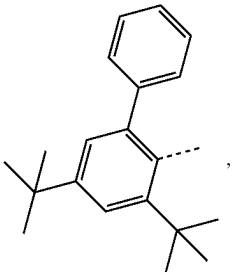
$R^{A1''}_{18}$



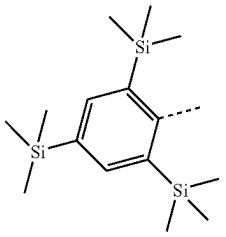
,

$R^{A1''}_{19}$



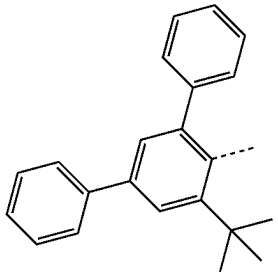
,

$R^{A1''}_{20}$



, and

$R^{A1''}_{21}$



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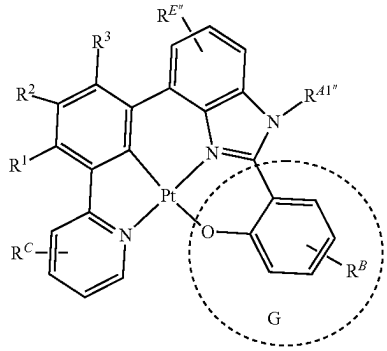
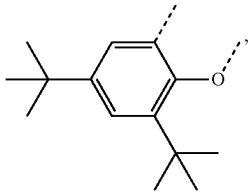
[0209] In some embodiments, the moiety G in Formula II

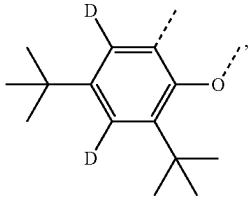


is selected from the group consisting of G_{W2}, wherein W2 is an integer from 1 to 12, and G_1-G_{12} have the following structures:

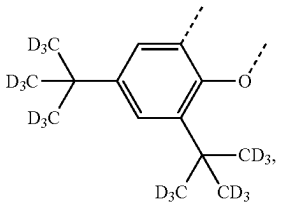
G_1



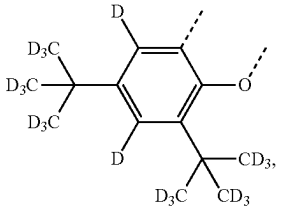
G_2



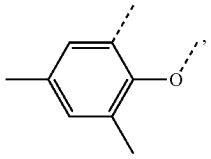
G_3



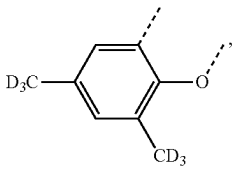
G_4



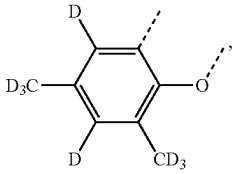
G_5



G_6



G_7



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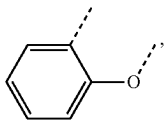
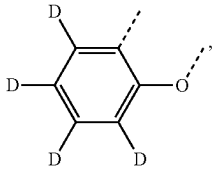
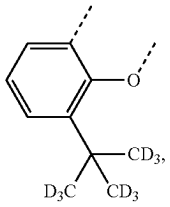
G_8



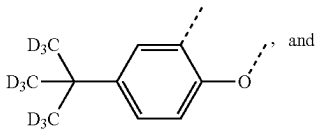
G_9



G_{10}

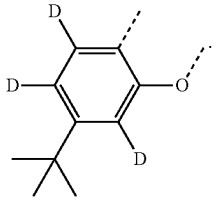


G_{11}

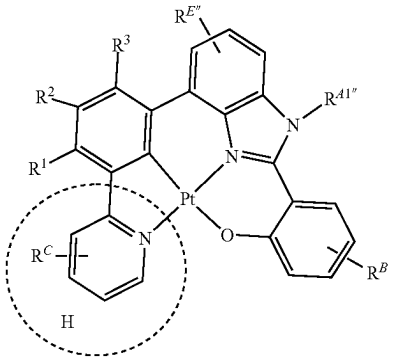


and

G_{12}

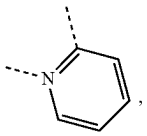


[0210] In some embodiments, the moiety H in Formula II

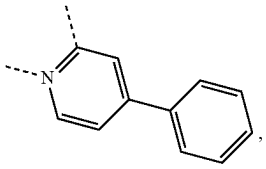


is selected from the group consisting of H_{W3}, wherein W3 is an integer from 1 to 44, and H_1-H_{44} have the structures in the following LIST 3:

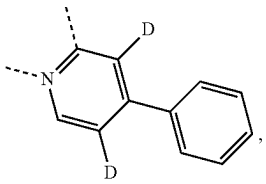
H_1



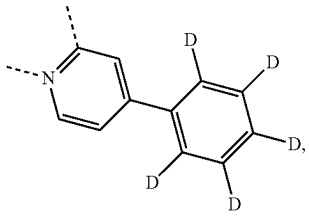
H_2



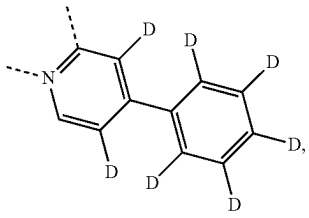
H_3



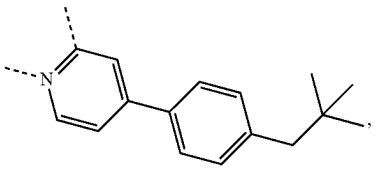
H_4



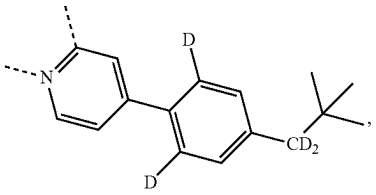
H_5



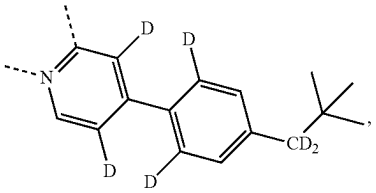
H_7



H_8



H_9



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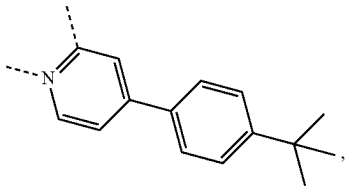
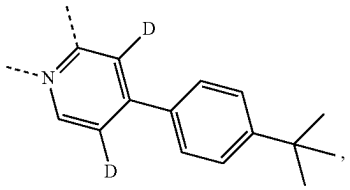
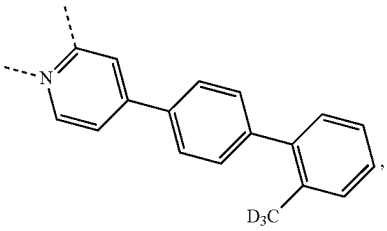
H_{10}



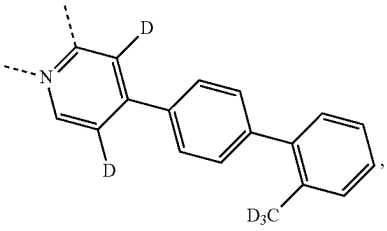
H_{11}



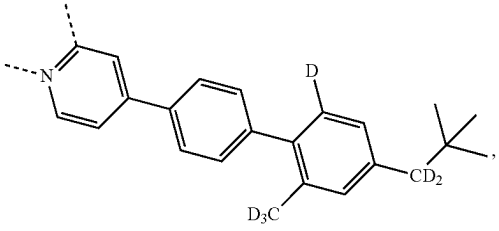
H_{12}



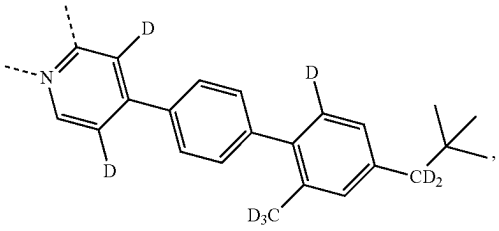
H_{13}



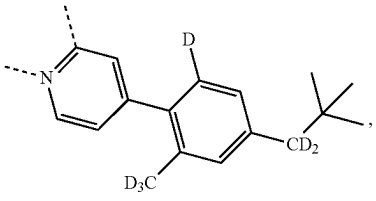
H_{14}



H_{15}



H_{16}



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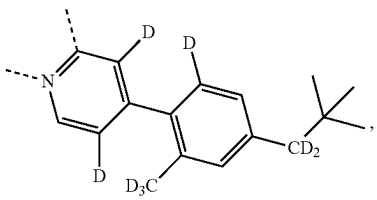
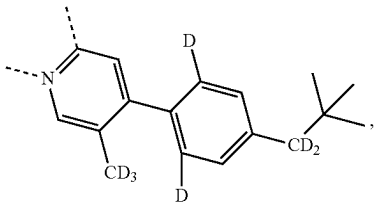
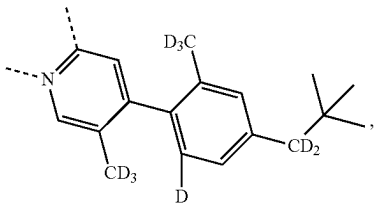
H_{17}



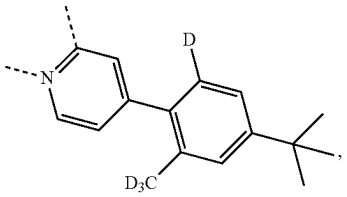
H_{18}



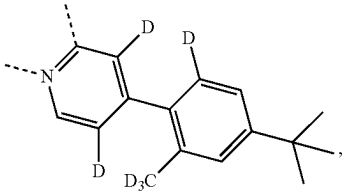
H_{19}



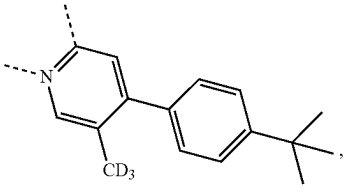
H_{20}



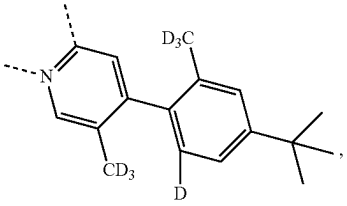
H_{21}



H_{22}



H_{23}



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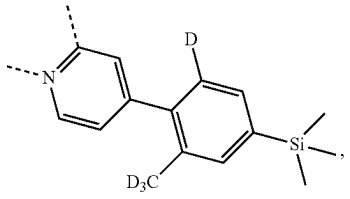
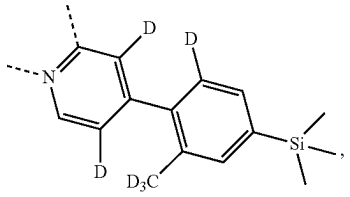
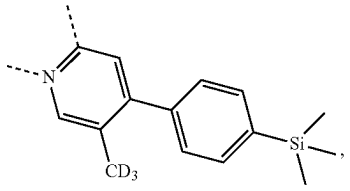
H_{24}



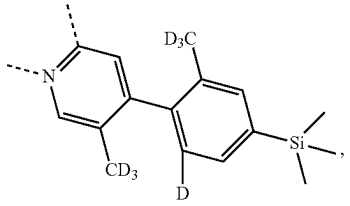
H_{25}



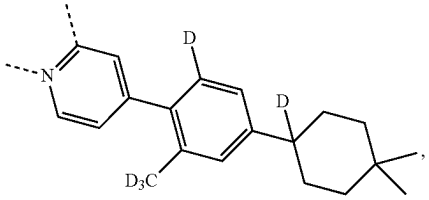
H_{26}



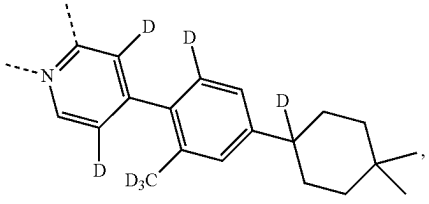
H_{27}



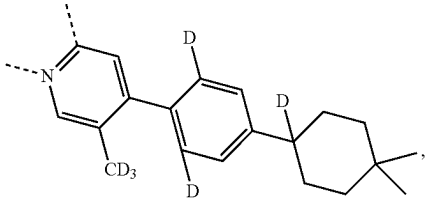
H_{28}



H_{29}



H_{30}



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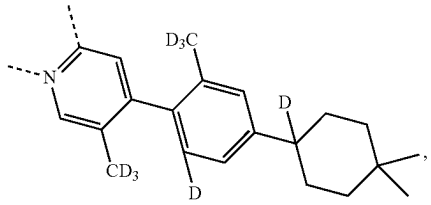
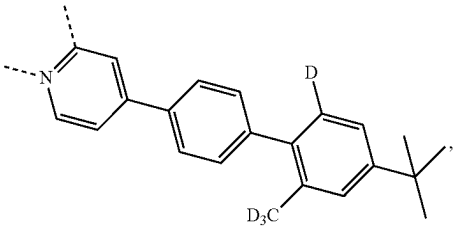
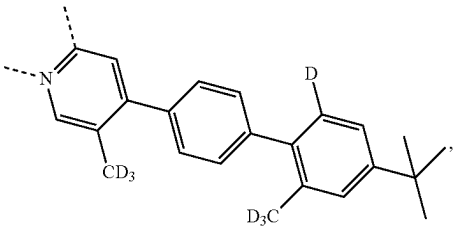
H_{31}



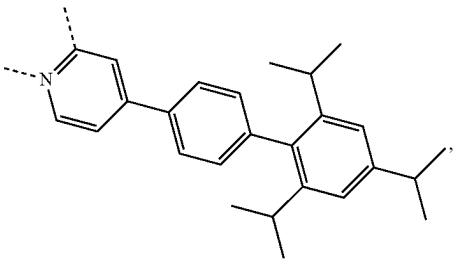
H_{32}



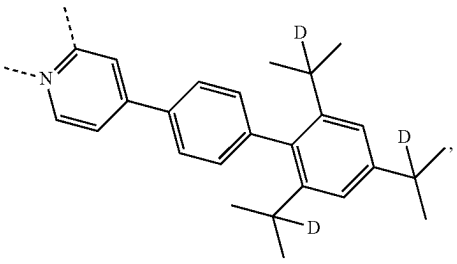
H_{33}



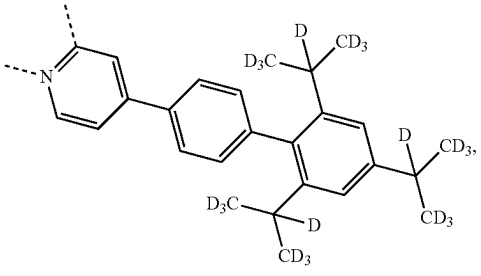
H_{34}



H_{35}



H_{36}



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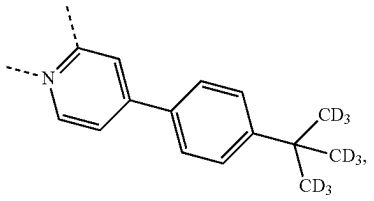
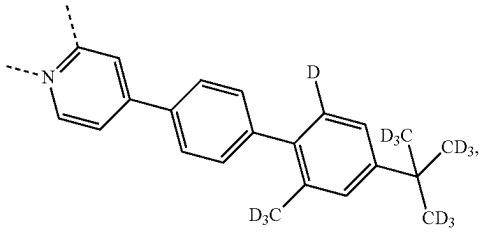
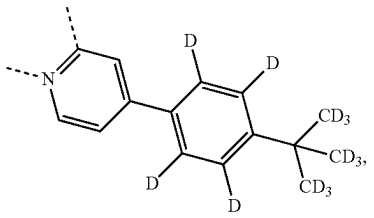
H_{37}



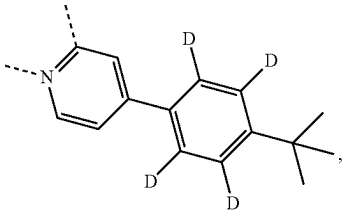
H_{38}



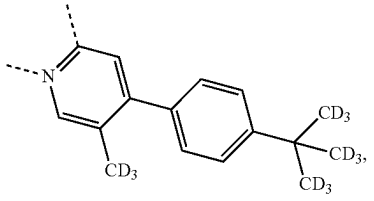
H_{39}



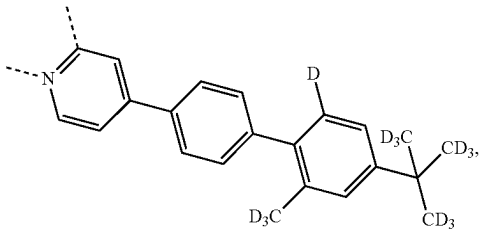
H_{40}



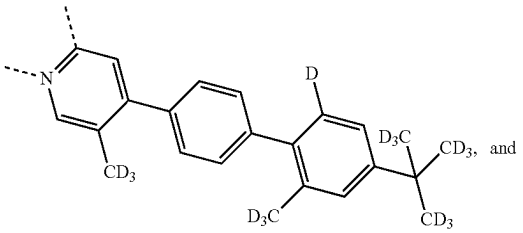
H_{41}



H_{42}



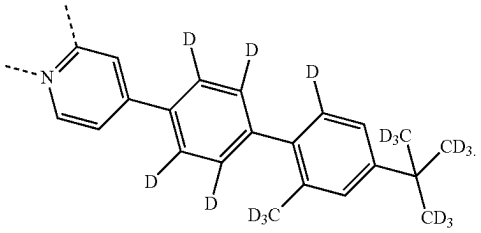
H_{43}



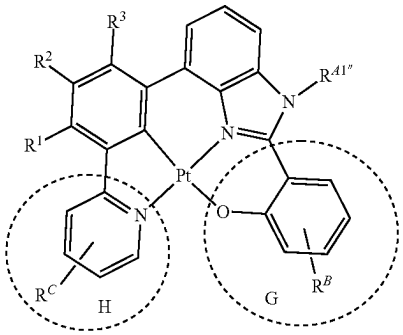
and

-continued

H_{44}



[0211] In some embodiments, the compound has a structure of formula II:

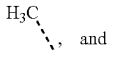


wherein $R^{A1''}$, moiety G, and moiety H are described above, R^3 is selected from the group consisting of R^3_{W4}, wherein W4 is an integer from 1 to 4, and R^3_1-R^3_4 have the structures of:

R^3_1

R^3_2

R^3_3



R^3_4

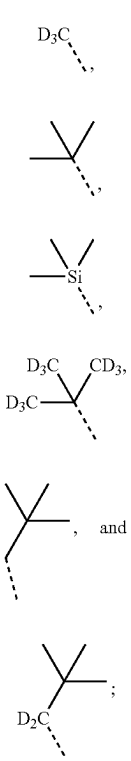
and R^2 is selected from the group consisting of R^2_{W5}, wherein W5 is an integer from 1 to 9, and R^2_1-R^2_9 have the structures of:

R^2_1

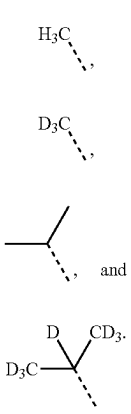
R^2_2

R^2_3

-continued



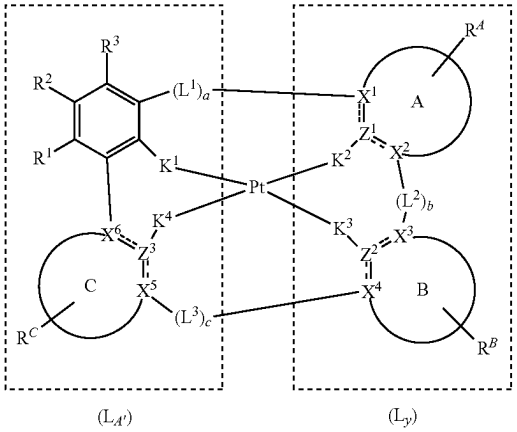
and R^1 is selected from the group consisting of R^1_{W6}, wherein W6 is an integer from 1 to 4, and R^1_1-R^1_4 have the structures of:



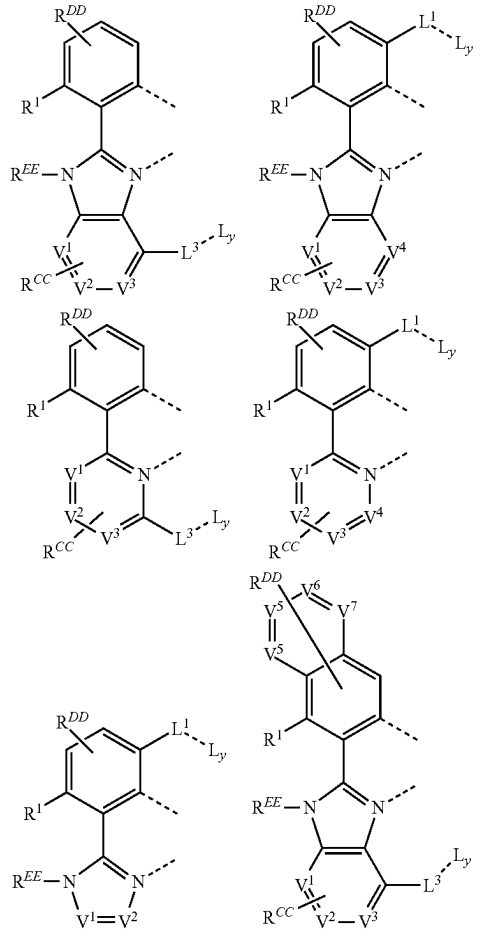
[0212] In some embodiments, the compound has the formula of Pt—$(R^{A1''}_{w1})(G_{w2})(H_{w3})(R^3_{w4})(R^2_{w5})(R^1_{w6})$ corresponding to the above structure; wherein w1 is an integer from 1 to 21, w2 is an integer from 1 to 12, and w3 is an integer from 1 to 44; w4 is an integer from 1 to 4, w5 is an integer from 1 to 9, w6 is an integer from 1 to 4, and the compound is selected from the group consisting of Pt—$(R^{A1''}_1)(G_1)(H_1)(R^3_1)(R^2_1)(R^1_1)$ to Pt—$(R^{A1''}_{21})(G_{12})(H_{44})(R^3_4)(R^2_9)(R^1_4)$.

[0213] In some embodiments, the compound has the formula $Pt(L_{A'})(Ly)$,

Formula III



[0214] wherein $L_{A'}$ is selected from the group consisting of the structures shown below in the following LIST 4:



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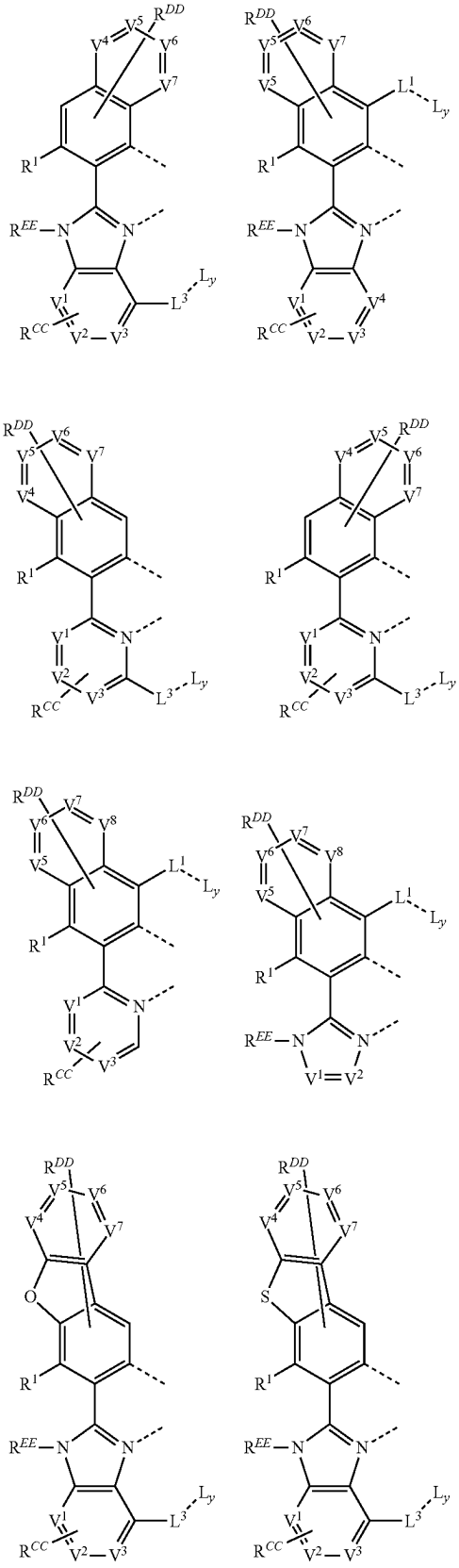

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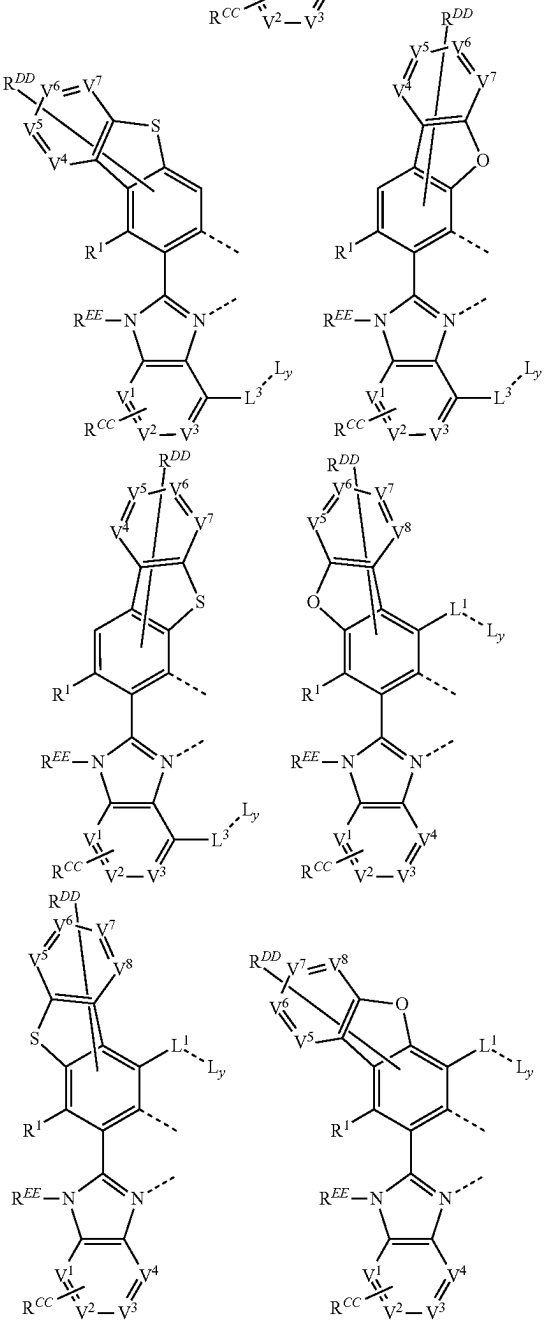

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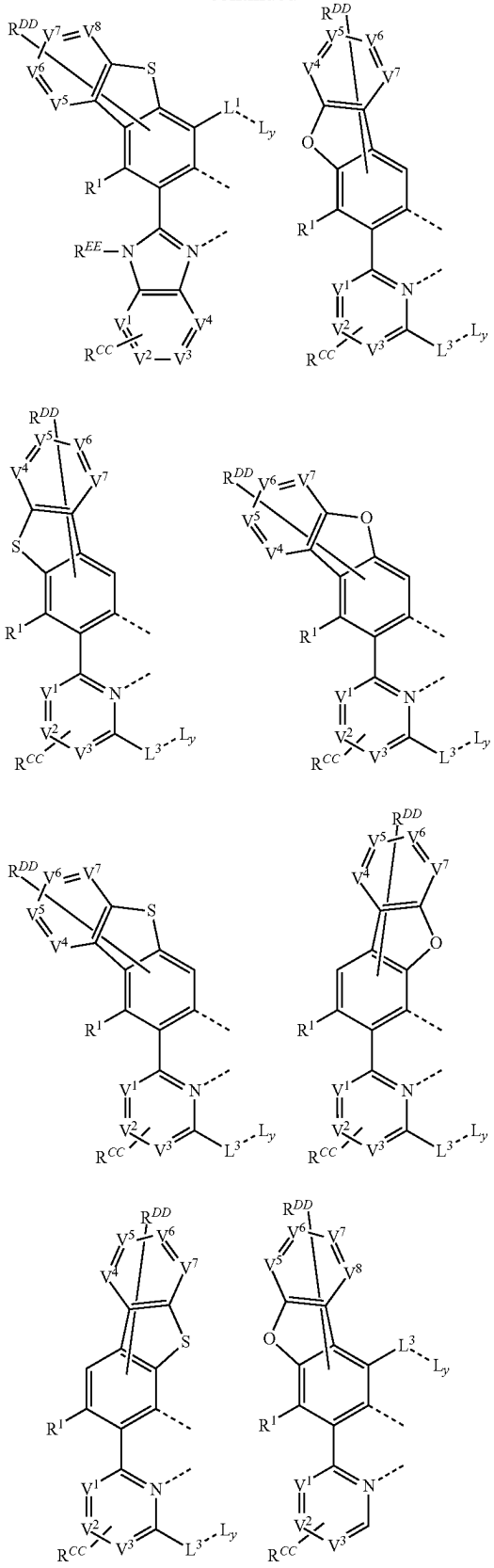

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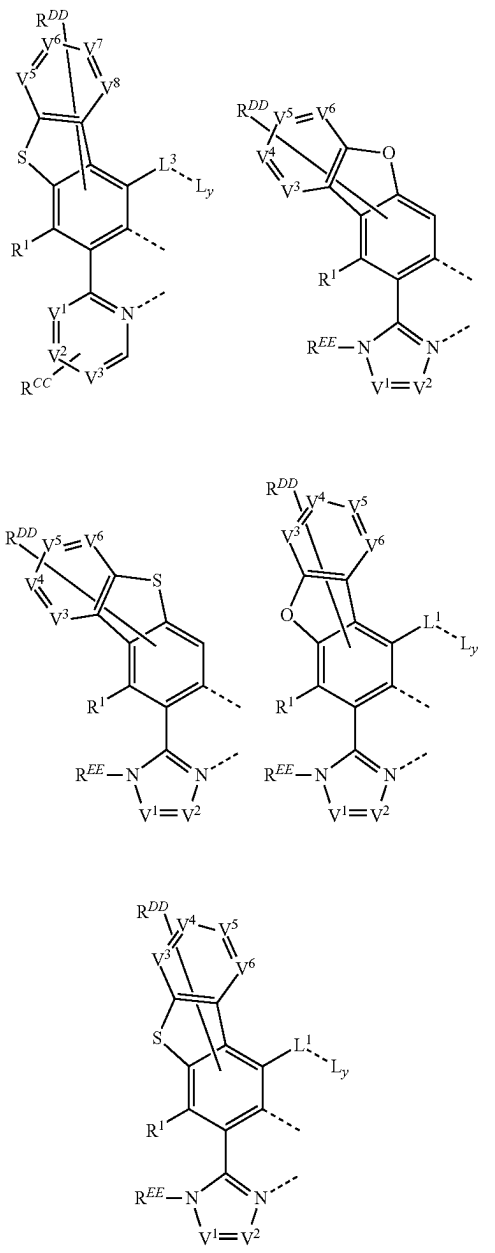
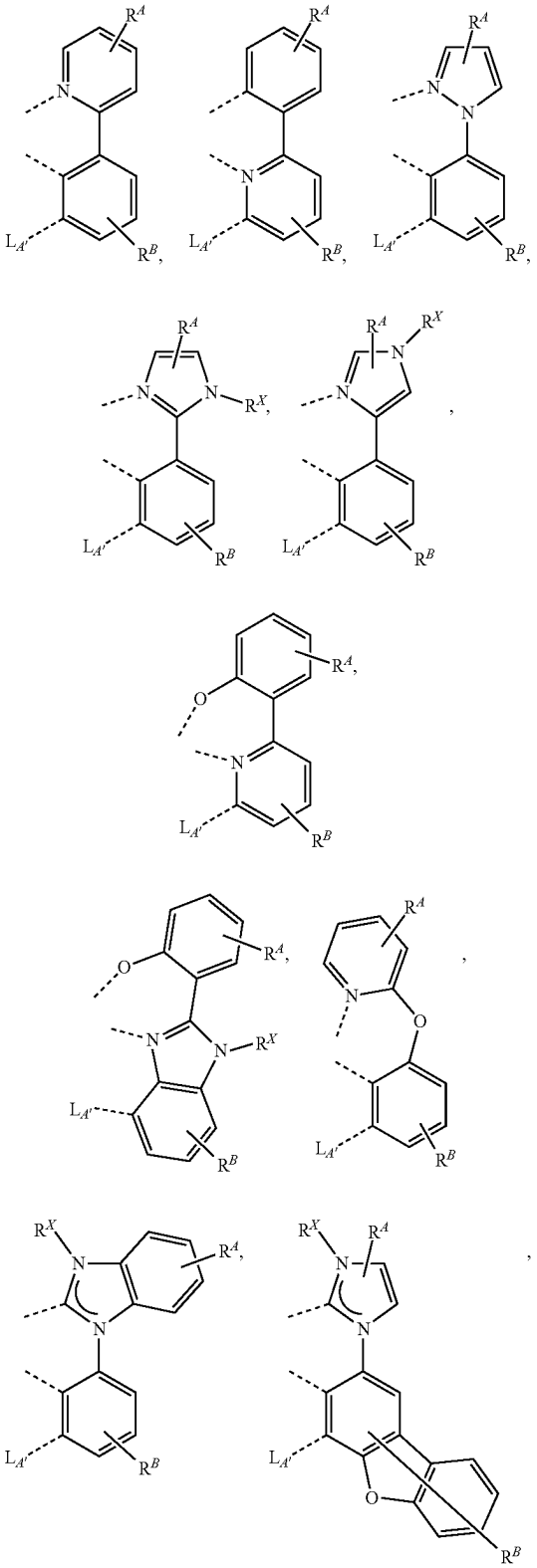


[0215] wherein V^1-V^8 are each independently C or N;

[0216] wherein each of R^{CC} and R^{DD} independently represents mono to the maximum allowable substitution, or no substitution;

[0217] wherein each R^{CC}, R^{DD}, and R^{EE}, is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, selenyl, and combinations thereof,

[0218] wherein L_y is selected from the group consisting of the structures shown below in the following LIST 5:



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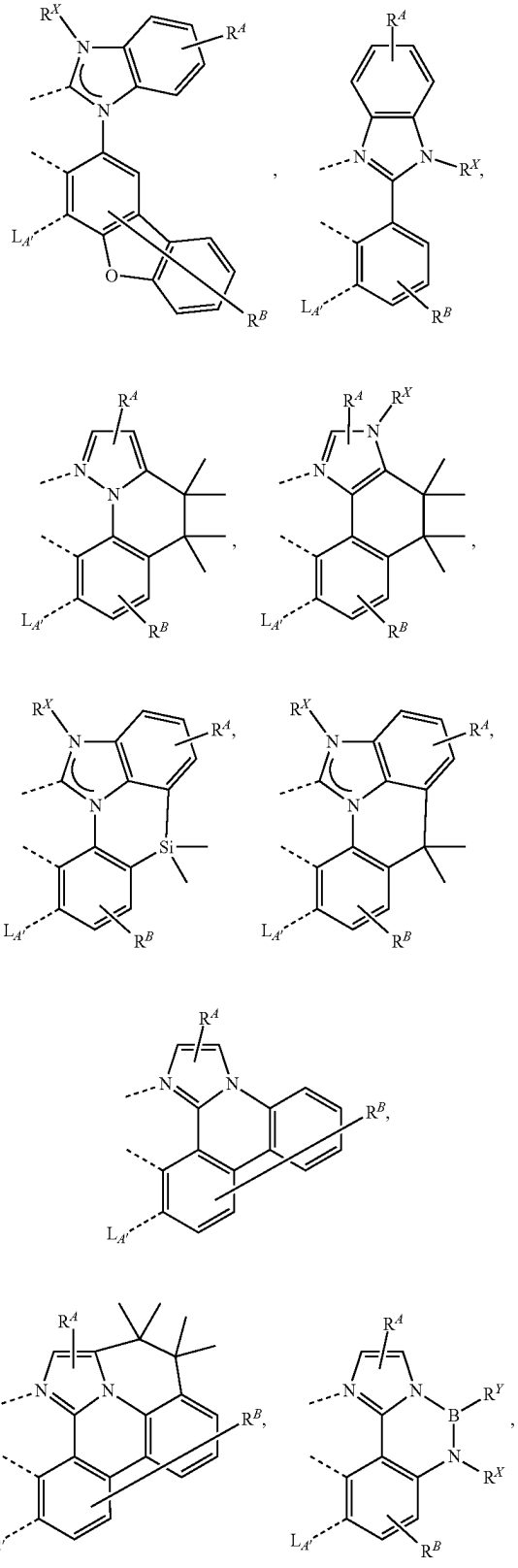

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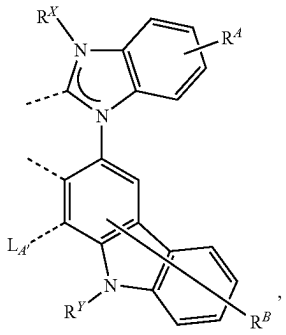

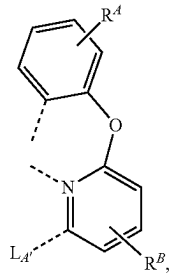

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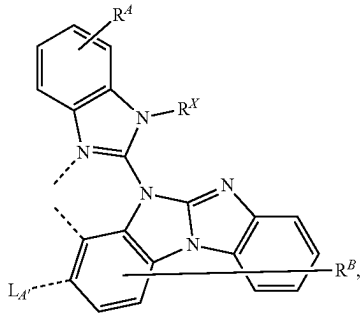

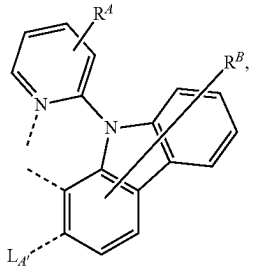

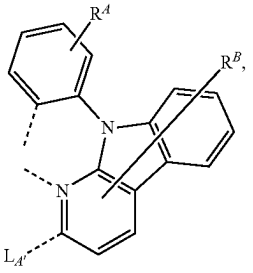

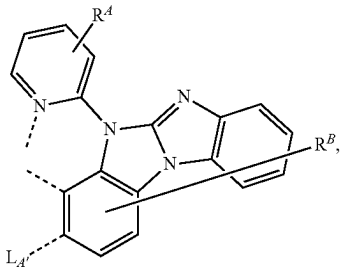

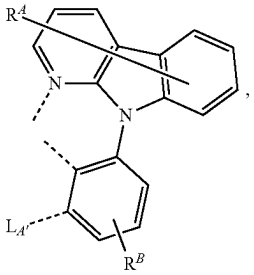

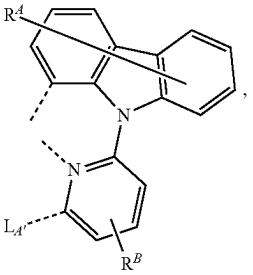

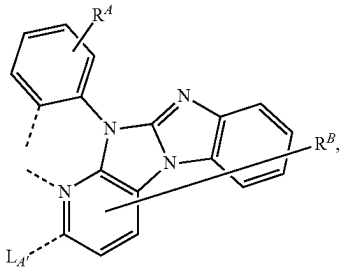

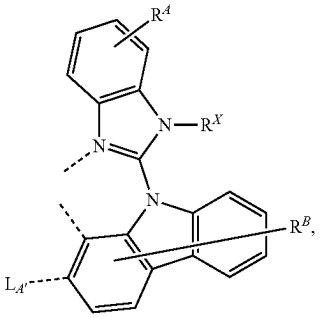

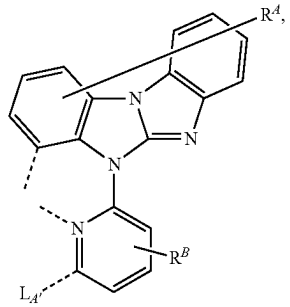

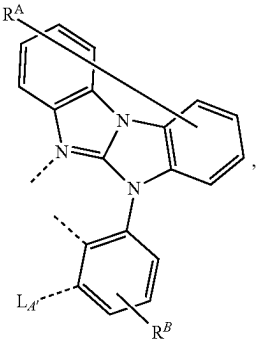

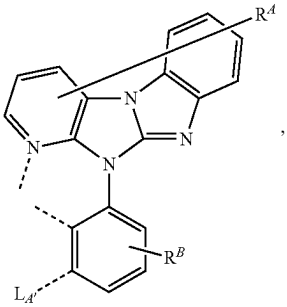

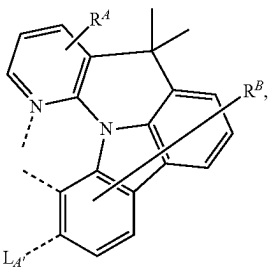

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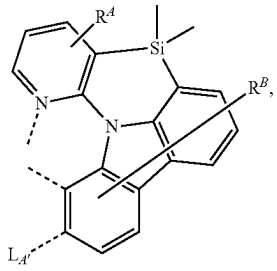

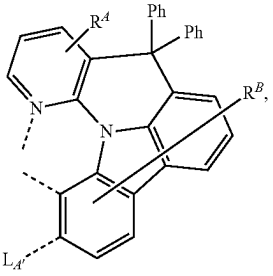

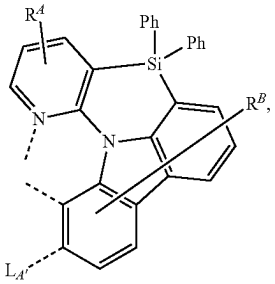

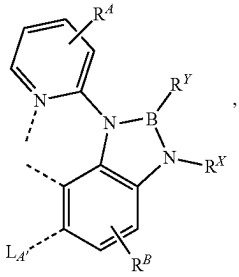

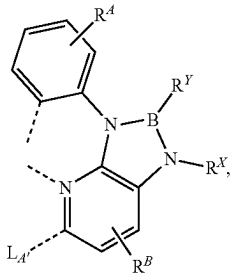

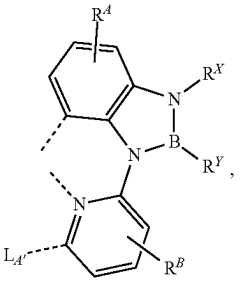

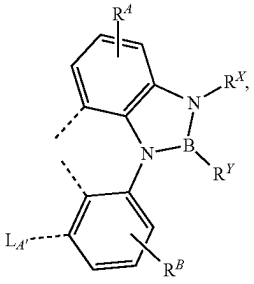

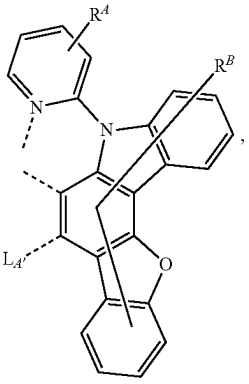

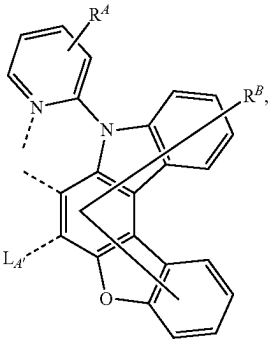

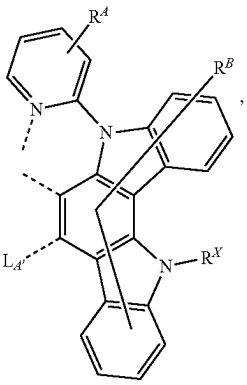

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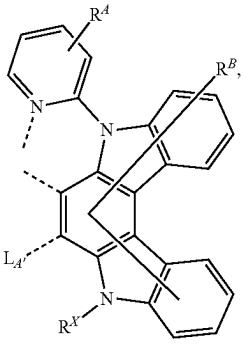

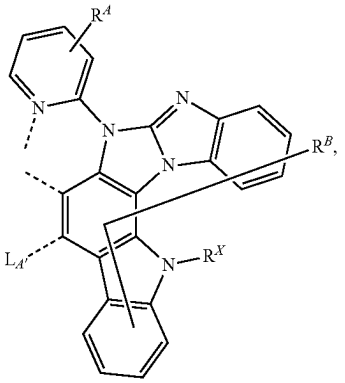

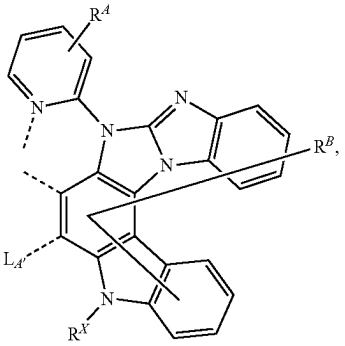

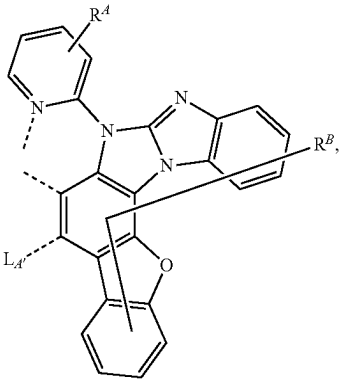

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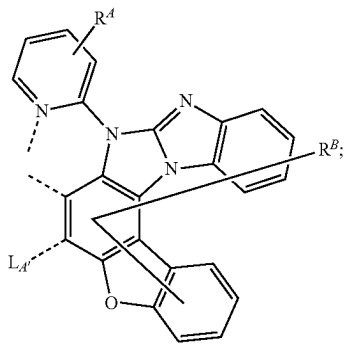
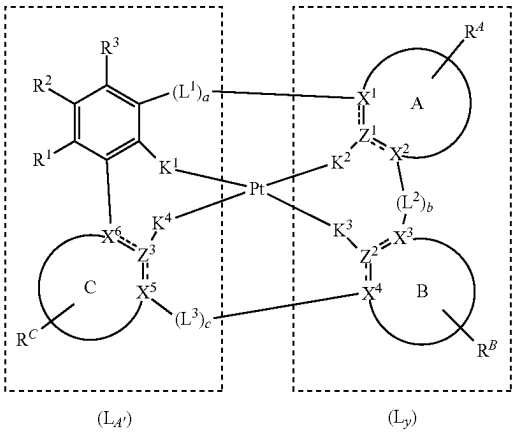


[0219] wherein each R^X and R^Y is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, selenyl, and combinations thereof.

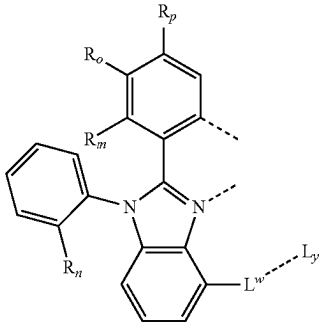
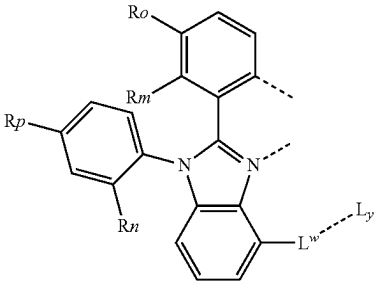
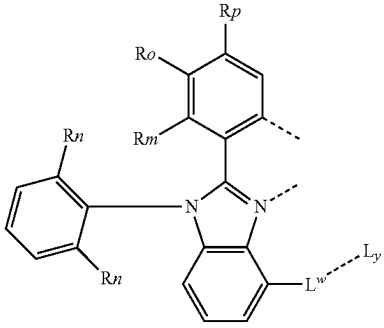
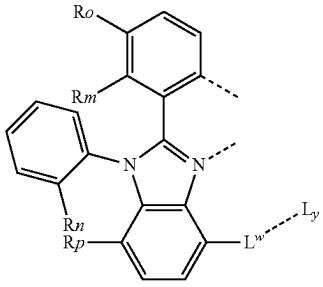
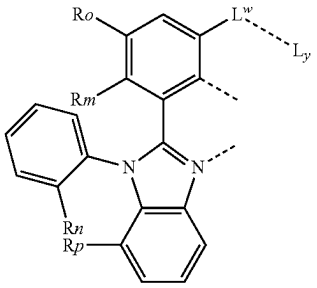
[0220] In some embodiments, the compound is selected from the group consisting of the compounds having the formula of $Pt(L_{A'})(Ly)$,

Formula III



$(L_{A'})$ (L_y)

wherein $L_{A'}$ is selected from $L_{A'}i'$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein i' is an integer from 1 to 57; w is an integer from 1 to 4, m, n, o and p are each an integer from 1 to 466, L^w is selected from L1 to L4; each of Rm, Rn, Ro, and Rp is independently selected from R1 to R466, and each of $L_{A'}1$-(L1)(R1)(R1)(R1)(R1) to $L_{A'}57$-(L4)(R466)(R466)(R466)(R466) is defined in the following LIST 6.

$L_{A'}$	Structure of $L_{A'}$
$L_{A'}1$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein $L_{A'}1$-(L1)(R1)(R1)(R1)(R1) to $L_{A'}1$-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}2$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein $L_{A'}2$-(L1)(R1)(R1)(R1)(R1) to $L_{A'}2$-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}3$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein $L_{A'}3$-(L1)(R1)(R1)(R1)(R1) to $L_{A'}3$-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}4$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein $L_{A'}4$-(L1)(R1)(R1)(R1)(R1) to $L_{A'}4$-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}5$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein $L_{A'}5$-(L1)(R1)(R1)(R1)(R1) to $L_{A'}5$-(L4)(R466)(R466)(R466)(R466), have the structure.	

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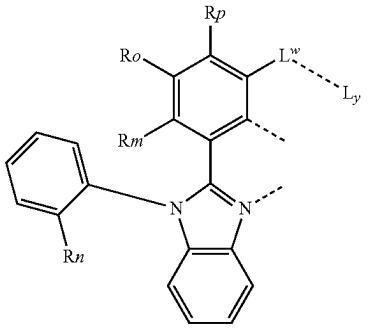
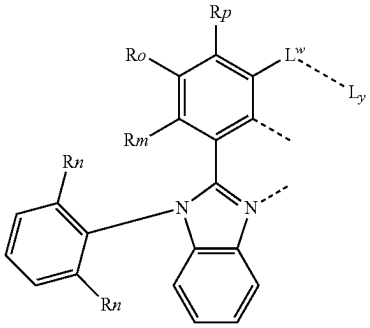
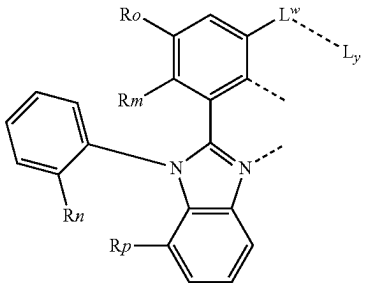
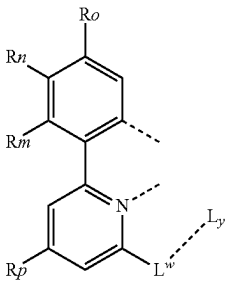
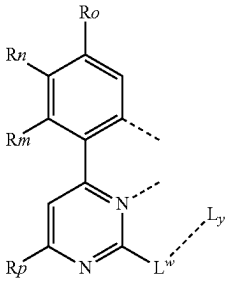
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$6-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$6-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$6-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$7-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$7-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$7-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$8-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$8-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$8-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$9-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$9-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$9-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$10-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$10-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$10-(L4)(R466)(R466)(R466)(R466), have the structure.	

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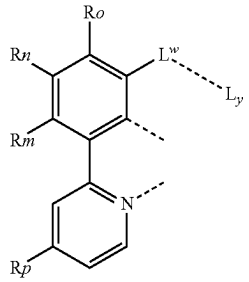
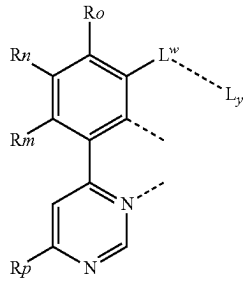
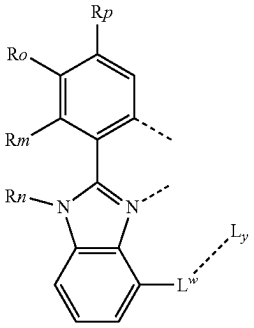
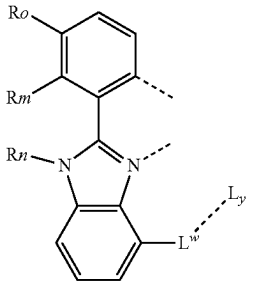
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$11-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$11-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$11-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$12-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$12-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$12-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$13-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$13-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$13-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$14-(L^{w})(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$14-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$14-(L4)(R466)(R466)(R466)(R466), have the structure.	

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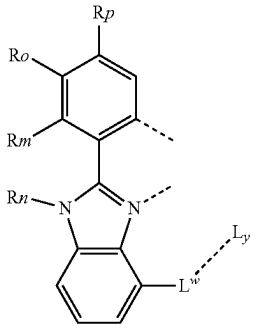
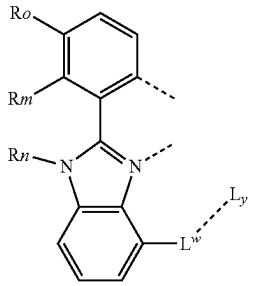
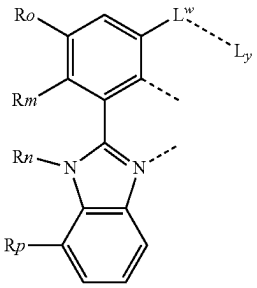
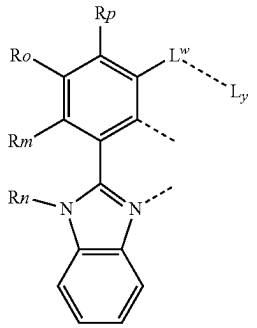
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$15-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$15-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$15-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$16-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$16-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$16-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$17-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$17-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$17-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$18-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$18-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$18-(L4)(R466)(R466)(R466)(R466), have the structure.	

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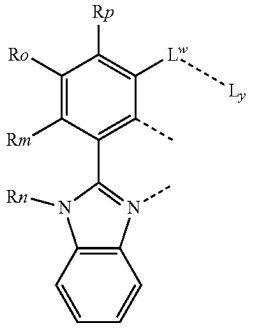
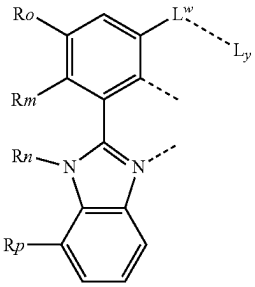
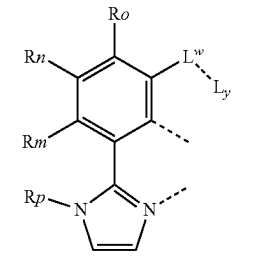
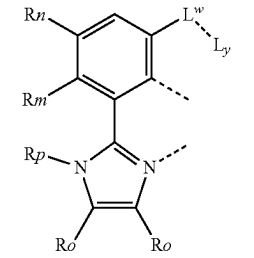
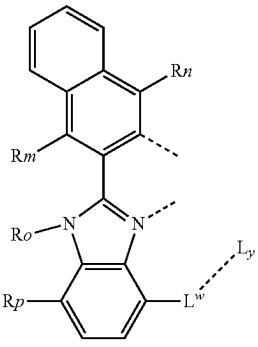
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$19-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$19-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$19-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$20-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$20-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$20-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$21-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$21-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$21-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$22-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$22-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$22-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$23-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$23-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$23-(L4)(R466)(R466)(R466)(R466), have the structure.	

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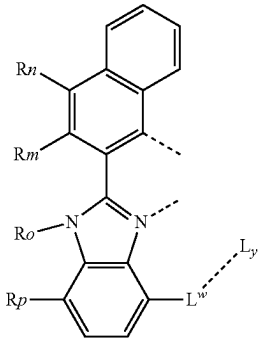
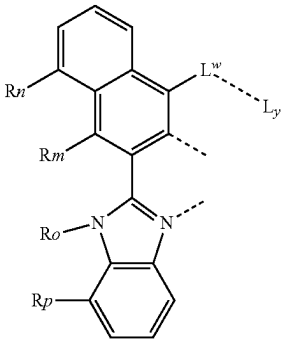
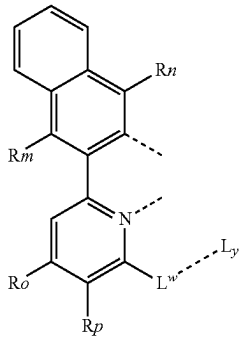
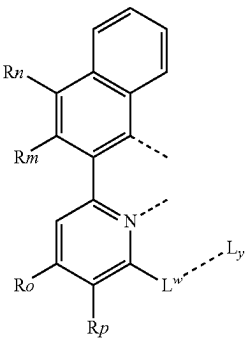
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$24-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$24-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$24-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$25-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$25-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$25-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$26-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$26-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$26-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$27-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$27-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$27-(L4)(R466)(R466)(R466)(R466), have the structure.	

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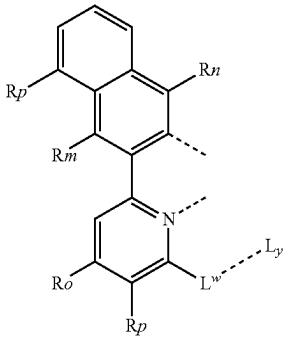
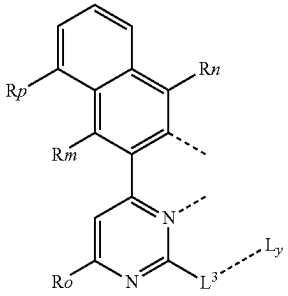
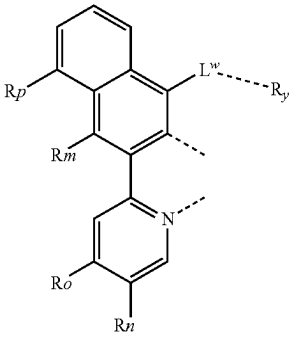
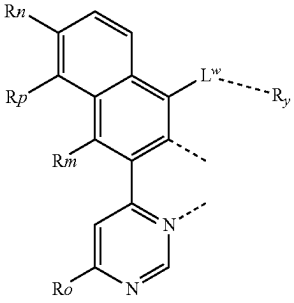
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$28-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$28-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$28-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$29-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$29-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$29-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$30-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$30-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$30-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$31-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$31-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$31-(L4)(R466)(R466)(R466)(R466), have the structure.	

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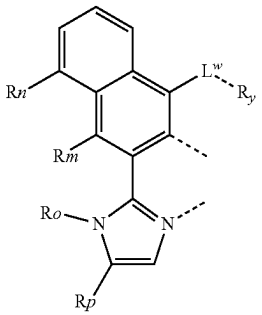
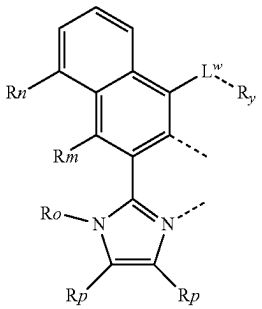
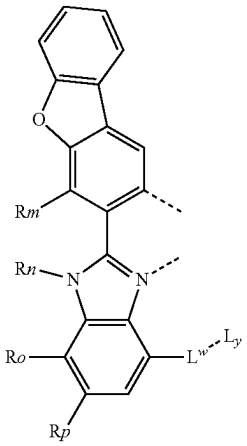
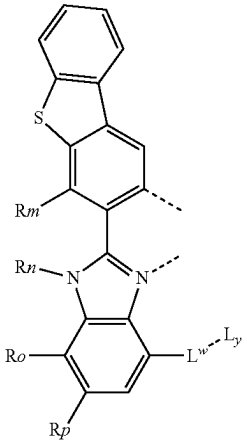
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$32-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$32-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$32-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$33-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$33-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$33-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$34-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$34-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$34-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$35-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$35-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$35-(L4)(R466)(R466)(R466)(R466), have the structure.	

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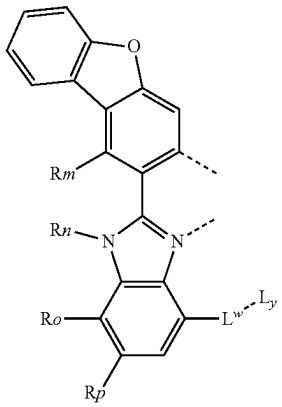
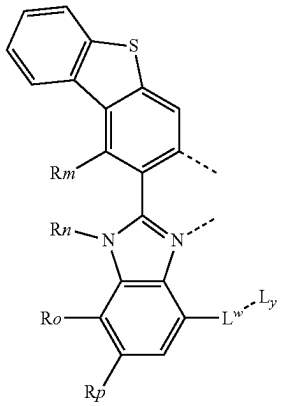
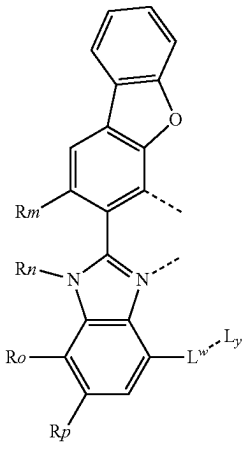
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$36-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$36-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$36-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$37-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$37-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$37-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$38-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$38-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$38-(L4)(R466)(R466)(R466)(R466), have the structure.	

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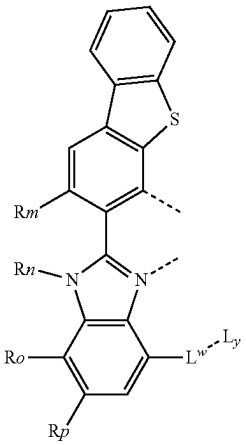
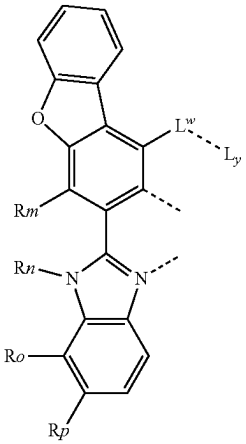
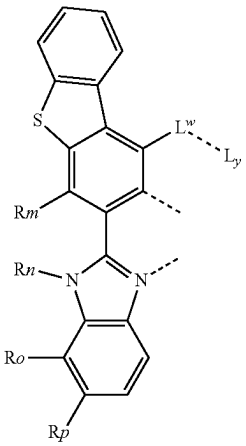
$L_{A'}$	Structure of $L_{A'}$
L_A39-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A39-(L1)(R1)(R1)(R1)(R1) to L_A39-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A40-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A40-(L1)(R1)(R1)(R1)(R1) to L_A40-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A41-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A41-(L1)(R1)(R1)(R1)(R1) to L_A41-(L4)(R466)(R466)(R466)(R466), have the structure.	

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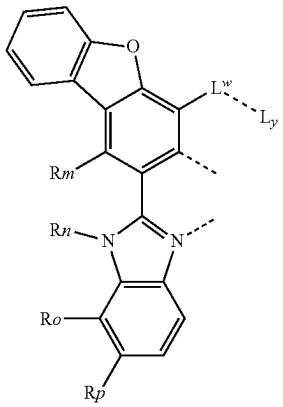
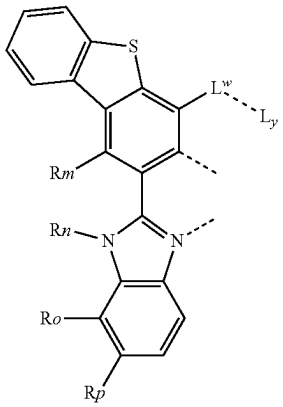
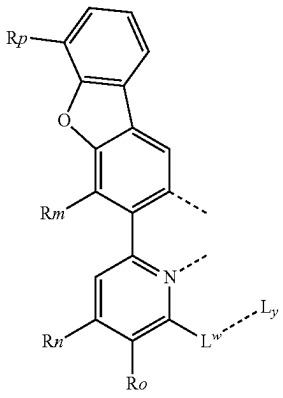
$L_{A'}$	Structure of $L_{A'}$
L_A42-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A42-(L1)(R1)(R1)(R1)(R1) to L_A42-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A43-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A43-(L1)(R1)(R1)(R1)(R1) to L_A43-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A44-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A44-(L1)(R1)(R1)(R1)(R1) to L_A44-(L4)(R466)(R466)(R466)(R466), have the structure.	

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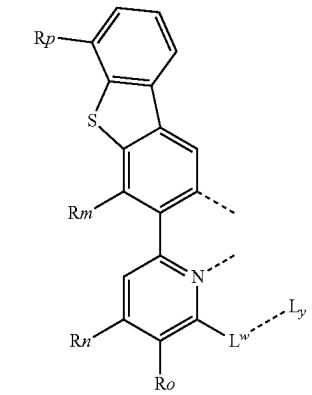
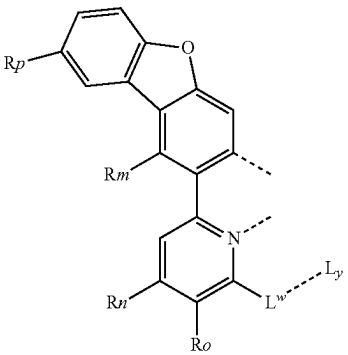
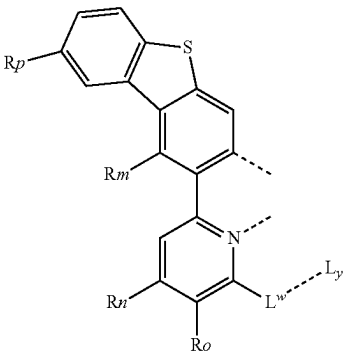
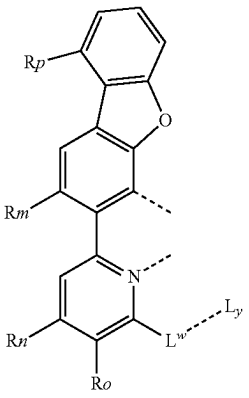
$L_{A'}$	Structure of $L_{A'}$
L_A45-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A45-(L1)(R1)(R1)(R1)(R1) to L_A45-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A46-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A46-(L1)(R1)(R1)(R1)(R1) to L_A46-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A47-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A47-(L1)(R1)(R1)(R1)(R1) to L_A47-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A48-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A48-(L1)(R1)(R1)(R1)(R1) to L_A48-(L4)(R466)(R466)(R466)(R466), have the structure.	

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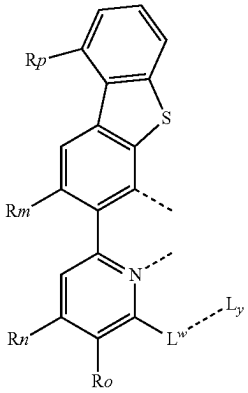
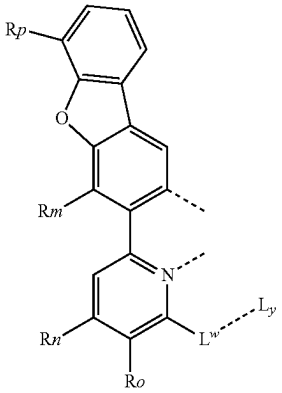
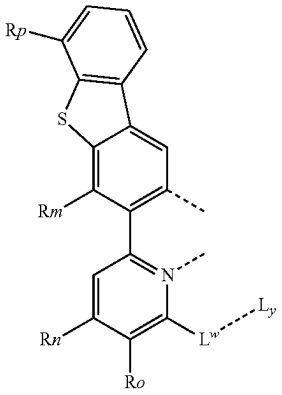
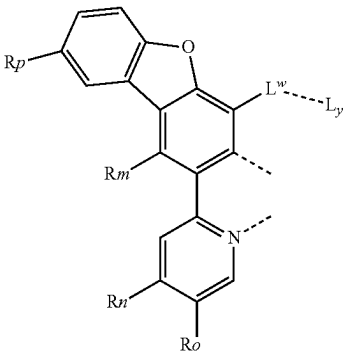
$L_{A'}$	Structure of $L_{A'}$
L_A49-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A49-(L1)(R1)(R1)(R1)(R1) to L_A49-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A50-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A50-(L1)(R1)(R1)(R1)(R1) to L_A50-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A51-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A51-(L1)(R1)(R1)(R1)(R1) to L_A51-(L4)(R466)(R466)(R466)(R466), have the structure.	
L_A52-(L^w)(Rm)(Rn)(Ro)(Rp), wherein L_A52-(L1)(R1)(R1)(R1)(R1) to L_A52-(L4)(R466)(R466)(R466)(R466), have the structure.	

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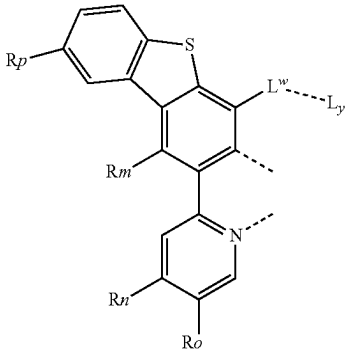
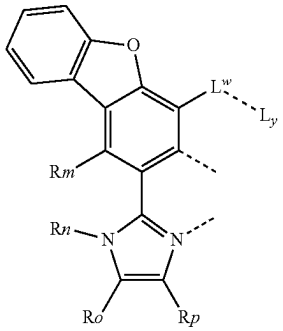
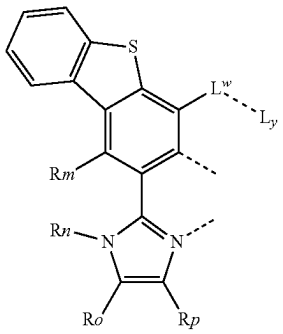
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$53-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$53-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$53-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$54-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$54-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$54-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$55-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$55-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$55-(L4)(R466)(R466)(R466)(R466), have the structure.	

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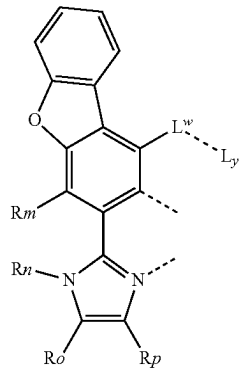
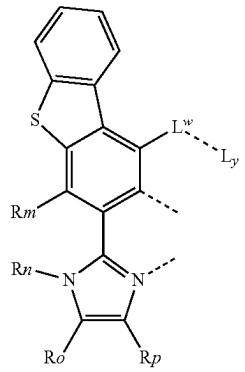
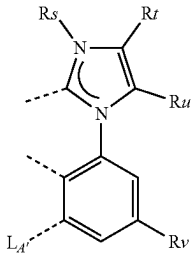
$L_{A'}$	Structure of $L_{A'}$
$L_{A'}$56-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$56-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$56-(L4)(R466)(R466)(R466)(R466), have the structure.	
$L_{A'}$57-(L^w)(Rm)(Rn)(Ro)(Rp), wherein $L_{A'}$57-(L1)(R1)(R1)(R1)(R1) to $L_{A'}$57-(L4)(R466)(R466)(R466)(R466), have the structure.	

[0221] wherein $L_{y'}$ is selected from L_{y}j-(Rs)(Rt)(Ru)(Rv), wherein j is an integer from to 52; each of s, t, u, and v is an integer from 1 to 466, each of Rs, Rt, Ru, and Rv is independently selected from R1 to R466, and each of L_{y}1-(R1)(R1)(R1)(R1) to L_{y}52-(R466)(R466)(R466) (R466) is defined in the following LIST 7:

L_y	Structure of L_y
L_y1-(Rs)(Rt)(Ru)(Rv), wherein L_y1-(R1)(R1)(R1)(R1) to L_y1-(R466)(R466)(R466)(R466) have the structure	

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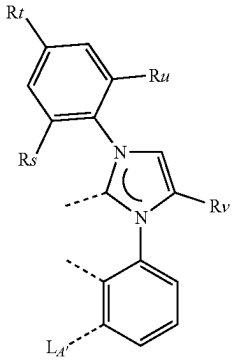
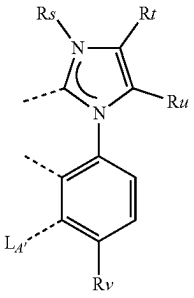
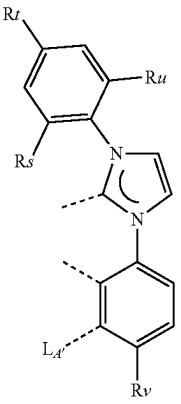
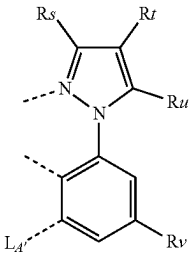
L_y	Structure of L_y
L_y2-(Rs)(Rt)(Ru)(Rv), wherein L_y2-(R1)(R1)(R1)(R1) to L_y2-(R466)(R466)(R466)(R466) have the structure	
L_y3-(Rs)(Rt)(Ru)(Rv), wherein L_y3-(R1)(R1)(R1)(R1) to L_y3-(R466)(R466)(R466)(R466) have the structure	
L_y4-(Rs)(Rt)(Ru)(Rv), wherein L_y4-(R1)(R1)(R1)(R1) to L_y4-(R466)(R466)(R466)(R466) have the structure	
L_y5-(Rs)(Rt)(Ru)(Rv), wherein L_y5-(R1)(R1)(R1)(R1) to L_y5-(R466)(R466)(R466)(R466) have the structure	

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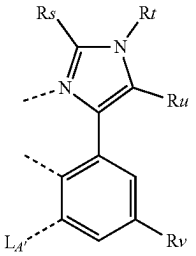
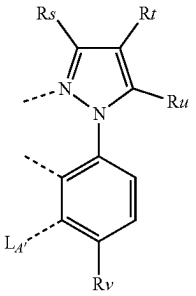
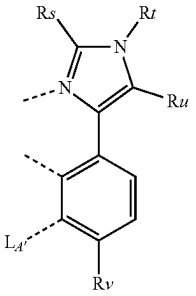
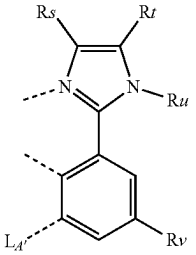
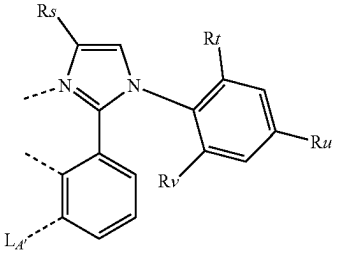
L_y	Structure of L_y
L_y6-(Rs)(Rt)(Ru)(Rv), wherein L_y6-(R1)(R1)(R1)(R1) to L_y6-(R466)(R466)(R466)(R466) have the structure	
L_y7-(Rs)(Rt)(Ru)(Rv), wherein L_y7-(R1)(R1)(R1)(R1) to L_y7-(R466)(R466)(R466)(R466) have the structure	
L_y8-(Rs)(Rt)(Ru)(Rv), wherein L_y8-(R1)(R1)(R1)(R1) to L_y8-(R466)(R466)(R466)(R466) have the structure	
L_y9-(Rs)(Rt)(Ru)(Rv), wherein L_y9-(R1)(R1)(R1)(R1) to L_y9-(R466)(R466)(R466)(R466) have the structure	
L_y10-(Rs)(Rt)(Ru)(Rv), wherein L_y10-(R1)(R1)(R1)(R1) to L_y10-(R466)(R466)(R466)(R466) have the structure	

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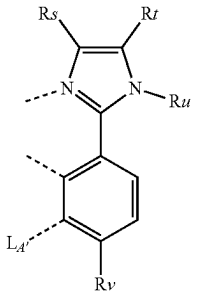
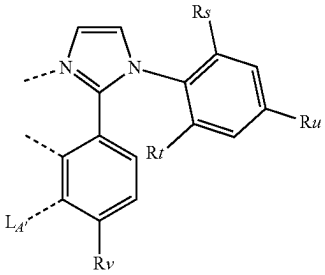
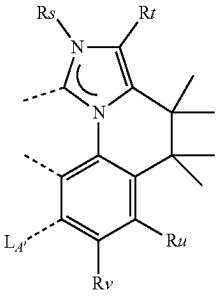
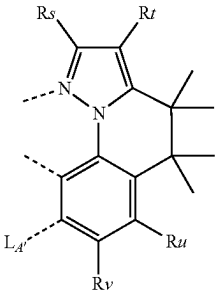
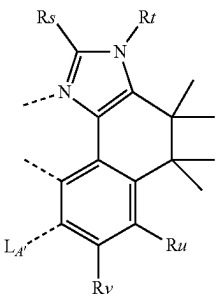
L_y	Structure of L_y
L_y11-(Rs)(Rt)(Ru)(Rv), wherein L_y11-(R1)(R1)(R1)(R1) to L_y11-(R466)(R466)(R466)(R466) have the structure	
L_y12-(Rs)(Rt)(Ru)(Rv), wherein L_y12-(R1)(R1)(R1)(R1) to L_y12-(R466)(R466)(R466)(R466) have the structure	
L_y13-(Rs)(Rt)(Ru)(Rv), wherein L_y13-(R1)(R1)(R1)(R1) to L_y13-(R466)(R466)(R466)(R466) have the structure	
L_y14-(Rs)(Rt)(Ru)(Rv), wherein L_y14-(R1)(R1)(R1)(R1) to L_y14-(R466)(R466)(R466)(R466) have the structure	
L_y15-(Rs)(Rt)(Ru)(Rv), wherein L_y15-(R1)(R1)(R1)(R1) to L_y15-(R466)(R466)(R466)(R466) have the structure	

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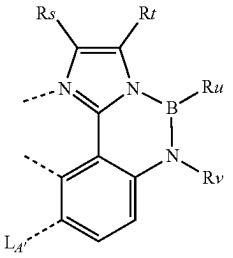
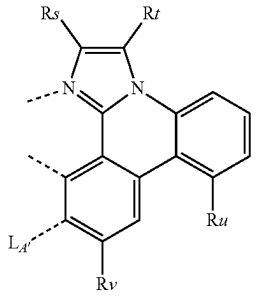
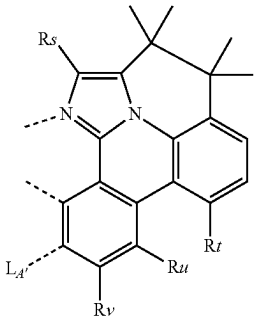
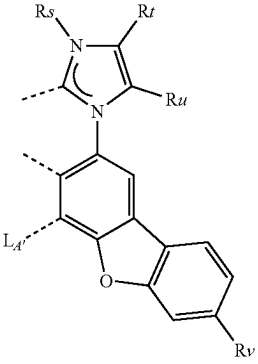
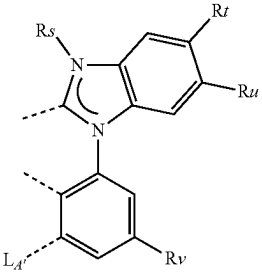
L_y	Structure of L_y
L_y16-(Rs)(Rt)(Ru)(Rv), wherein L_y16-(R1)(R1)(R1)(R1) to L_y16-(R466)(R466)(R466)(R466) have the structure	
L_y17-(Rs)(Rt)(Ru)(Rv), wherein L_y17-(R1)(R1)(R1)(R1) to L_y17-(R466)(R466)(R466)(R466) have the structure	
L_y18-(Rs)(Rt)(Ru)(Rv), wherein L_y18-(R1)(R1)(R1)(R1) to L_y18-(R466)(R466)(R466)(R466) have the structure	
L_y19-(Rs)(Rt)(Ru)(Rn), wherein L_y19-(R1)(R1)(R1)(R1) to L_y19-(R466)(R466)(R466)(R466) have the structure	
L_y20-(Rs)(Rt)(Ru)(Rv), wherein L_y20-(R1)(R1)(R1)(R1) to L_y20-(R466)(R466)(R466)(R466) have the structure	

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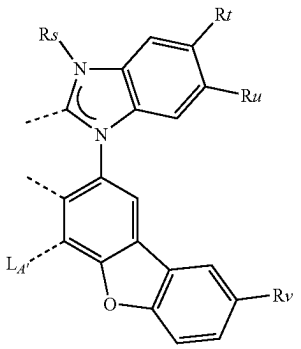
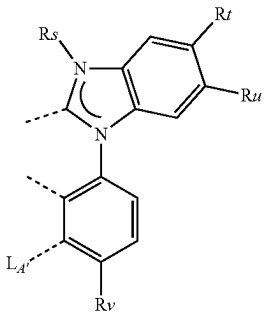
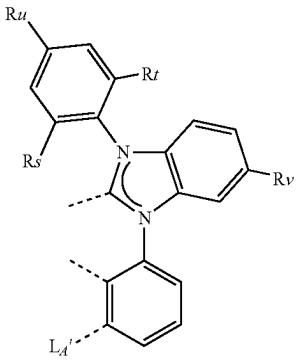
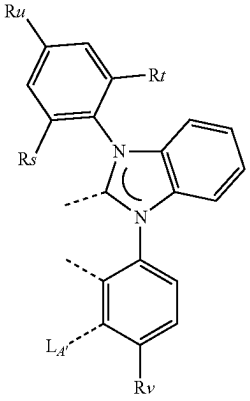
L_y	Structure of L_y
L_y21-(Rs)(Rt)(Ru)(Rv), wherein L_y21-(R1)(R1)(R1)(R1) to L_y21-(R466)(R466)(R466)(R466) have the structure	
L_y22-(Rs)(Rt)(Ru)(Rv), wherein L_y22-(R1)(R1)(R1)(R1) to L_y22-(R466)(R466)(R466)(R466) have the structure	
L_y23-(Rs)(Rt)(Ru)(Rv), wherein L_y23-(R1)(R1)(R1)(R1) to L_y23-(R466)(R466)(R466)(R466) have the structure	
L_y24-(Rs)(Rt)(Ru)(Rv), wherein L_y24-(R1)(R1)(R1)(R1) to L_y24-(R466)(R466)(R466)(R466) have the structure	

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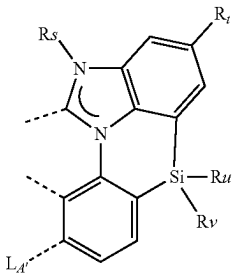
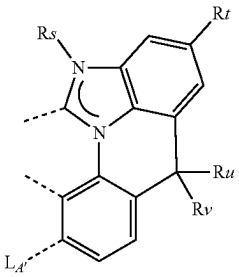
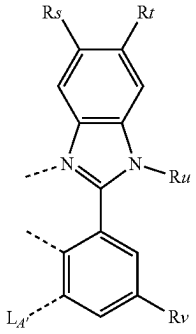
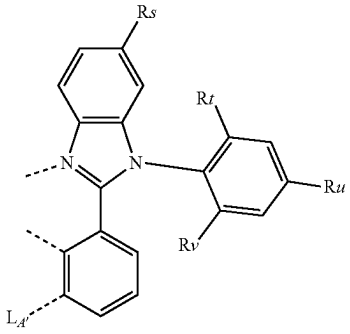
L_y	Structure of L_y
L_y25-(Rs)(Rt)(Ru)(Rv), wherein L_y25-(R1)(R1)(R1)(R1) to L_y25-(R466)(R466)(R466)(R466) have the structure	
L_y26-(Rs)(Rt)(Ru)(Rv), wherein L_y26-(R1)(R1)(R1)(R1) to L_y26-(R466)(R466)(R466)(R466) have the structure	
L_y27-(Rs)(Rt)(Ru)(Rv), wherein L_y27-(R1)(R1)(R1)(R1) to L_y27-(R466)(R466)(R466)(R466) have the structure	
L_y28-(Rs)(Rt)(Ru)(Rv), wherein L_y28-(R1)(R1)(R1)(R1) to L_y28-(R466)(R466)(R466)(R466) have the structure	

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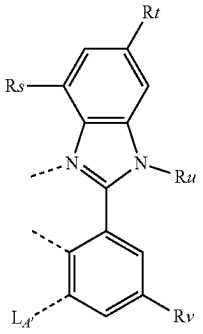
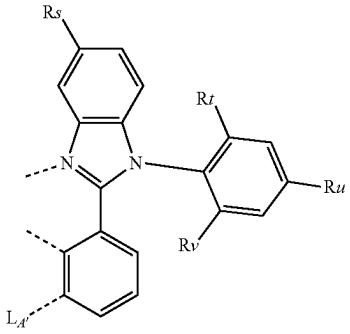
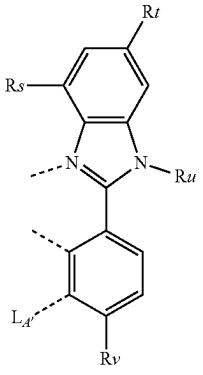
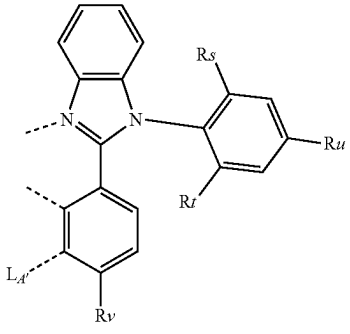
L_y	Structure of L_y
L_y29-(Rs)(Rt)(Ru)(Rv), wherein L_y29-(R1)(R1)(R1)(R1) to L_y29-(R466)(R466)(R466)(R466) have the structure	
L_y30-(Rs)(Rt)(Ru)(Rv), wherein L_y30-(R1)(R1)(R1)(R1) to L_y30-(R466)(R466)(R466)(R466) have the structure	
L_y31-(Rs)(Rt)(Ru)(Rv), wherein L_y31-(R1)(R1)(R1)(R1) to L_y31-(R466)(R466)(R466)(R466) have the structure	
L_y32-(Rs)(Rt)(Ru)(Rv), wherein L_y32-(R1)(R1)(R1)(R1) to L_y32-(R466)(R466)(R466)(R466) have the structure	

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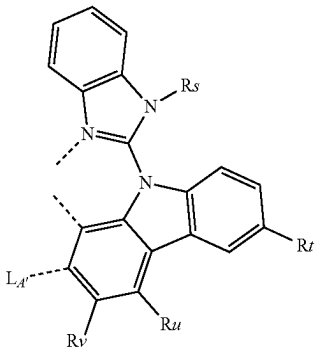
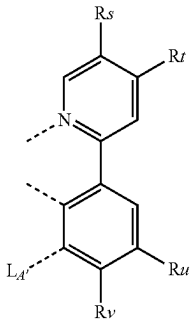
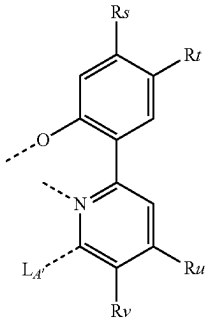
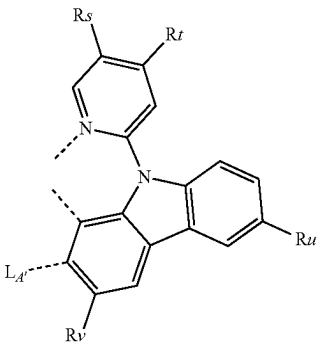
L_y	Structure of L_y
L_y33-(Rs)(Rt)(Ru)(Rv), wherein L_y33-(R1)(R1)(R1)(R1) to L_y33-(R466)(R466)(R466)(R466) have the structure	
L_y34-(Rs)(Rt)(Ru)(Rv), wherein L_y34-(R1)(R1)(R1)(R1) to L_y34-(R466)(R466)(R466)(R466) have the structure	
L_y35-(Rs)(Rt)(Ru)(Rv), wherein L_y35-(R1)(R1)(R1)(R1) to L_y35-(R466)(R466)(R466)(R466) have the structure	
L_y36-(Rs)(Rt)(Ru)(Rv), wherein L_y36-(R1)(R1)(R1)(R1) to L_y36-(R466)(R466)(R466)(R466) have the structure	

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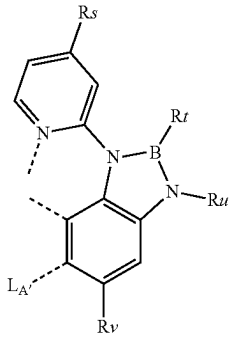
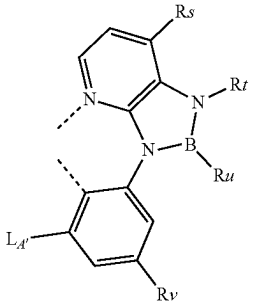
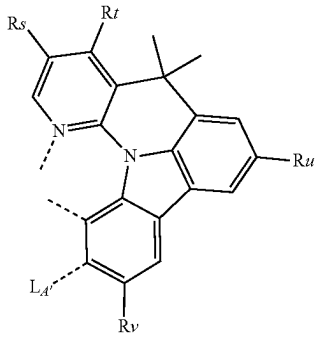
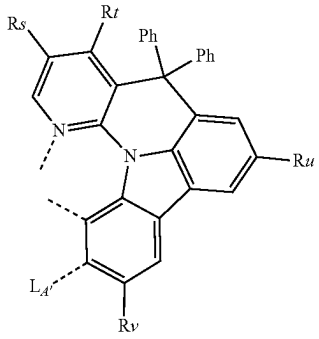
L_y	Structure of L_y
L_y37-(Rs)(Rt)(Ru)(Rv), wherein L_y37-(R1)(R1)(R1)(R1) to L_y37-(R466)(R466)(R466)(R466) have the structure	
L_y38-(Rs)(Rt)(Ru)(Rn), wherein L_y38-(R1)(R1)(R1)(R1) to L_y38-(R466)(R466)(R466)(R466) have the structure	
L_y39-(Rs)(Rt)(Ru)(Rv), wherein L_y39-(R1)(R1)(R1)(R1) to L_y39-(R466)(R466)(R466)(R466) have the structure	
L_y40-(Rs)(Rt)(Ru)(Rv), wherein L_y40-(R1)(R1)(R1)(R1) to L_y40-(R466)(R466)(R466)(R466) have the structure	

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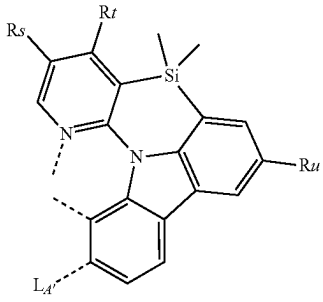
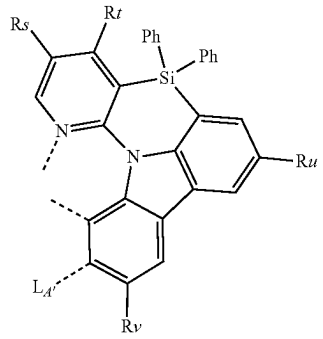
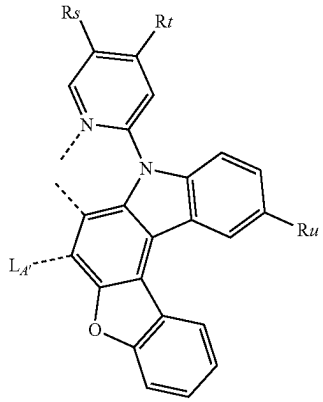
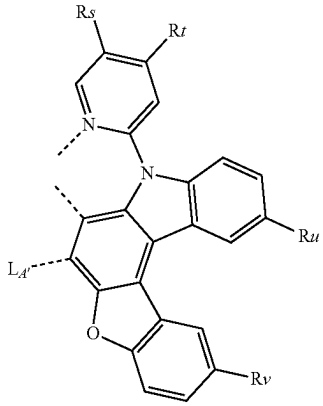
L_y	Structure of L_y
L_y41-(Rs)(Rt)(Ru)(Rv), wherein L_y41-(R1)(R1)(R1)(R1) to L_y41-(R466)(R466)(R466)(R466) have the structure	
L_y42-(Rs)(Rt)(Ru)(Rv), wherein L_y42-(R1)(R1)(R1)(R1) to L_y42-(R466)(R466)(R466)(R466) have the structure	
L_y43-(Rs)(Rt)(Ru)(Rv), wherein L_y43-(R1)(R1)(R1)(R1) to L_y43-(R466)(R466)(R466)(R466) have the structure	
L_y44-(Rs)(Rt)(Ru)(Rv), wherein L_y44-(R1)(R1)(R1)(R1) to L_y44-(R466)(R466)(R466)(R466) have the structure	

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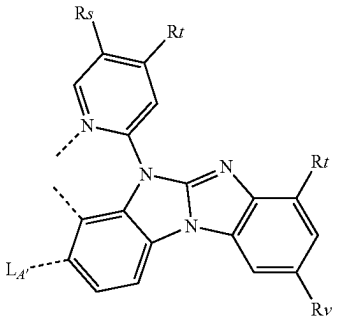
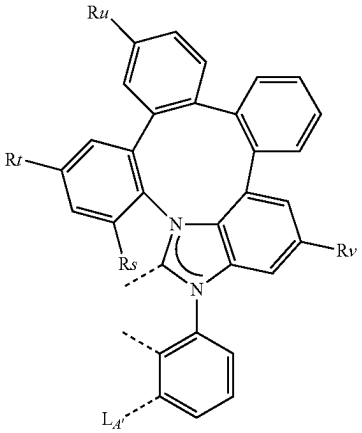
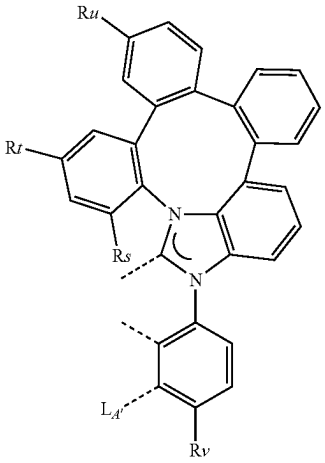
L_y	Structure of L_y
L_y45-(Rs)(Rt)(Ru)(Rv), wherein L_y45-(R1)(R1)(R1)(R1) to L_y45-(R466)(R466)(R466)(R466) have the structure	
L_y46-(Rs)(Rt)(Ru)(Rv), wherein L_y46-(R1)(R1)(R1)(R1) to L_y46-(R466)(R466)(R466)(R466) have the structure	
L_y47-(Rs)(Rt)(Ru)(Rv), wherein L_y47-(R1)(R1)(R1)(R1) to L_y47-(R466)(R466)(R466)(R466) have the structure	

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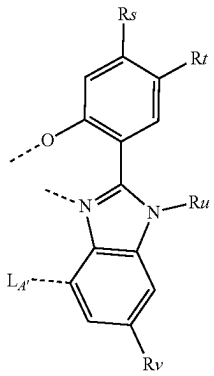
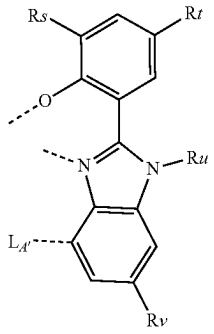
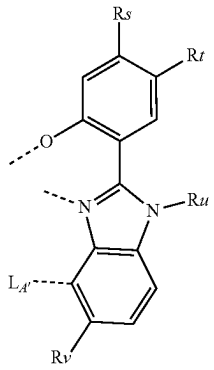
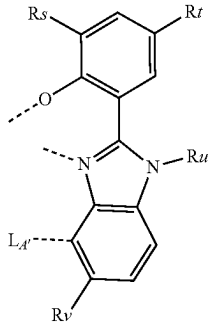
L_y	Structure of L_y
L_y48-(Rs)(Rt)(Ru)(Rv), wherein L_y48-(R1)(R1)(R1)(R1) to L_y48-(R466)(R466)(R466)(R466) have the structure	
L_y49-(Rs)(Rt)(Ru)(Rv), wherein L_y49-(R1)(R1)(R1)(R1) to L_y49-(R466)(R466)(R466)(R466) have the structure	
L_y50-(Rs)(Rt)(Ru)(Rv), wherein L_y50-(R1)(R1)(R1)(R1) to L_y50-(R466)(R466)(R466)(R466) have the structure	
L_y51-(Rs)(Rt)(Ru)(Rv), wherein L_y51-(R1)(R1)(R1)(R1) to L_y51-(R466)(R466)(R466)(R466) have the structure	

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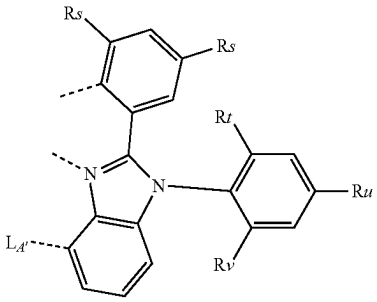
L_y	Structure of L_y
L_y52-(Rs)(Rt)(Ru)(Rv), wherein L_y52-(R1)(R1)(R1)(R1) to L_y52-(R466)(R466)(R466)(R466) have the structure	

[0222] wherein L1 is direct bond, L2 is O, L3 is S, and L4 is NPh;

[0223] wherein when $L_{A'}$ is $L_{A'}9$ or $L_{A'}11$, L_y is not L_y34;

[0224] wherein R1 to R466 have the following structures as defined in the following LIST 8:

Structure	Structure	Structure
R1	R2	R3
R4	R5	R6
R7	R8	R9
R10	R11	R12
R13	R14	R15
R16	R17	R18

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	Structure		Structure		Structure
R19		R20		R21	
R22		R23		R24	
R25		R26		R27	
R28		R29		R30	
R31		R32		R33	
R34		R35		R36	

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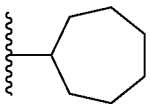
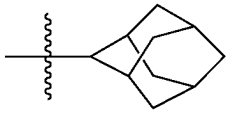
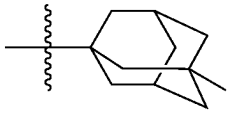
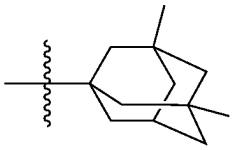
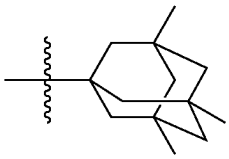
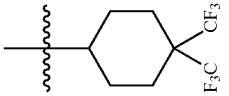
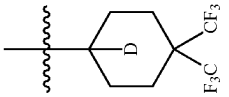
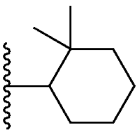
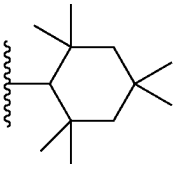
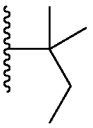
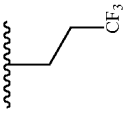
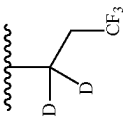
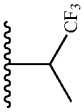
	Structure		Structure		Structure
R37		R38		R39	
R40		R41		R42	
R43		R44		R45	
R46		R47		R48	
R49		R50		R51	

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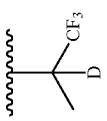
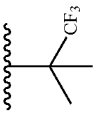
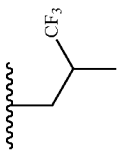
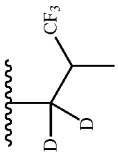
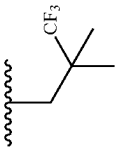
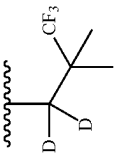
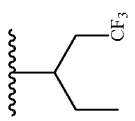
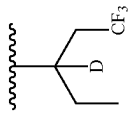
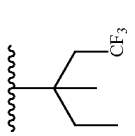
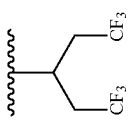
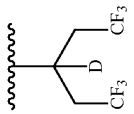
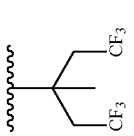
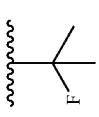
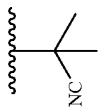
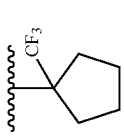
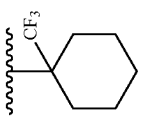
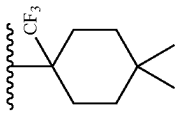
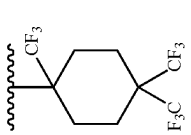
R52		R53		R54	
R55		R56		R57	
R58		R59		R60	
R61		R62		R63	
R64		R65		R66	
R67		R68		R69	

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	Structure		Structure		Structure
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R73		R74		R75	
R76		R77		R78	
R79		R80		R81	
R82		R83		R84	

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Structure	Structure	Structure
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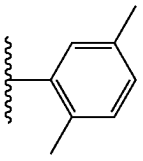	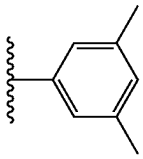	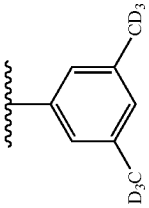
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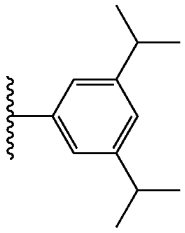	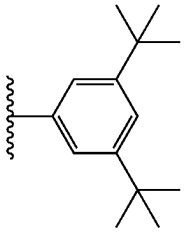	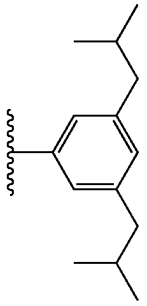
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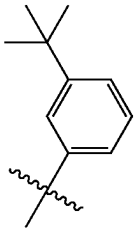	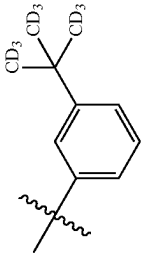	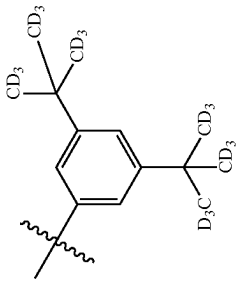
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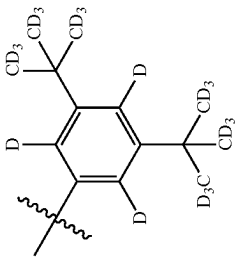
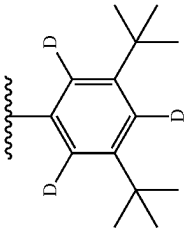
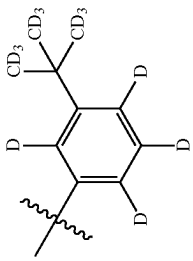
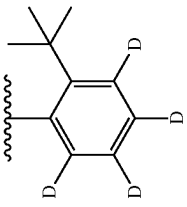
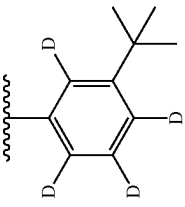
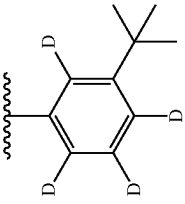
		
R97	R98	R99
		

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	Structure		Structure		Structure
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R103		R104		R105	
R106		R107		R108	
R109		R110		R111	
R112		R113		R114	

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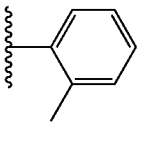
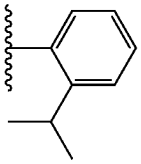
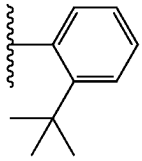
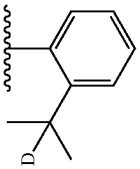
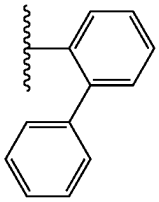
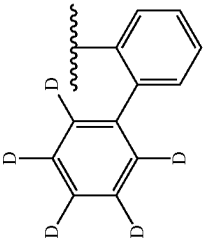
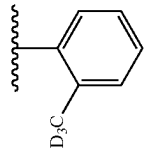
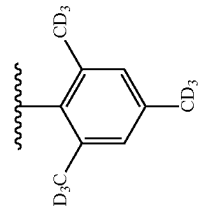
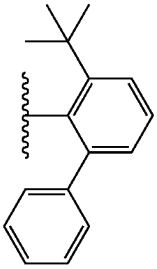
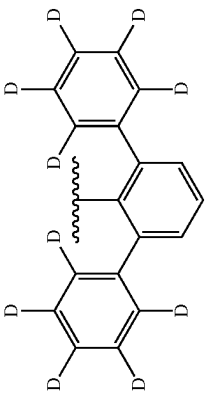
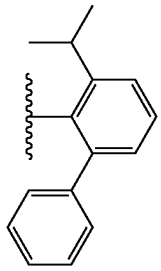
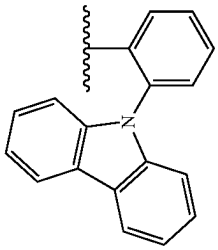
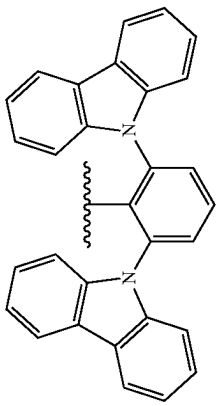
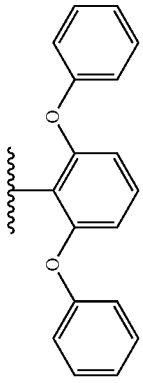
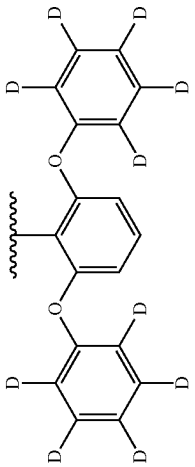
	Structure		Structure		Structure
R115		R116		R117	
R118		R119		R120	
R121		R122		R123	
R124		R125		R126	
R127		R128		R129	

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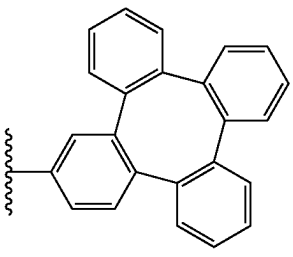
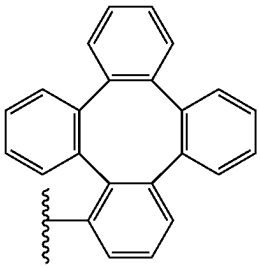
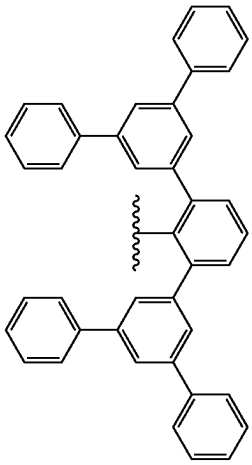
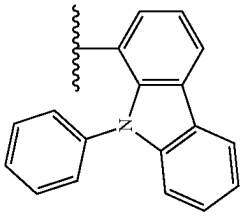
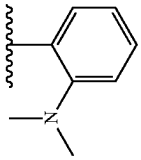
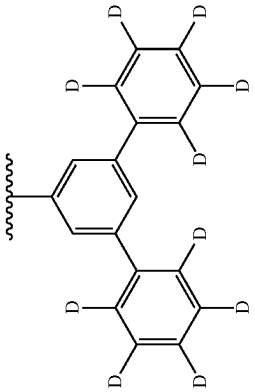
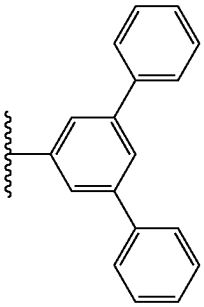
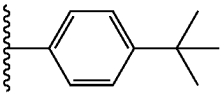
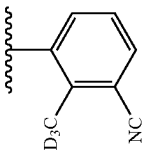
R130		R131		R132	
R133		R134		R135	
R136		R137		R138	

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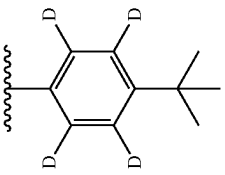
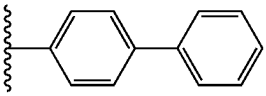
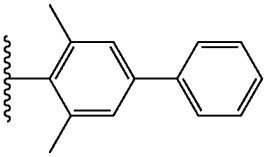
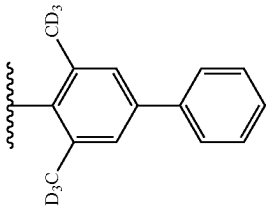
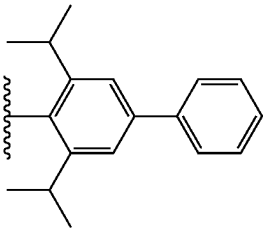
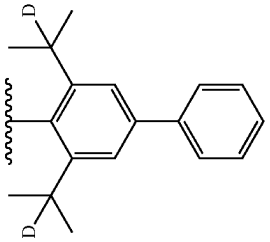
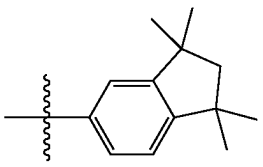
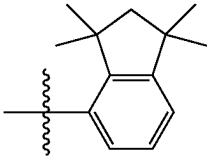
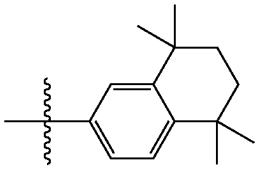
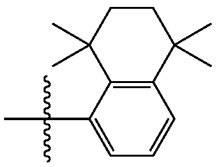
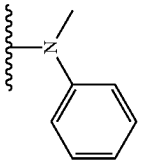
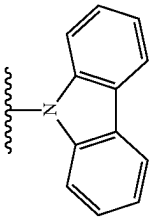
R139		R140		R141	
R142		R143		R144	
R145		R146		R147	
R148		R149		R150	

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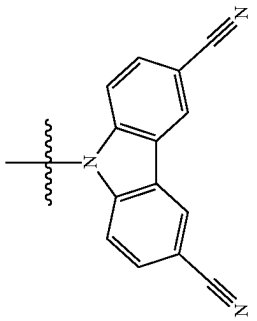
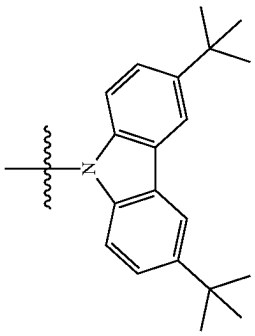
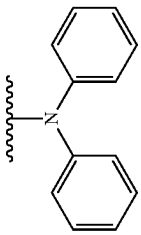
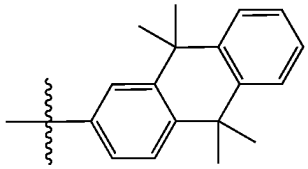
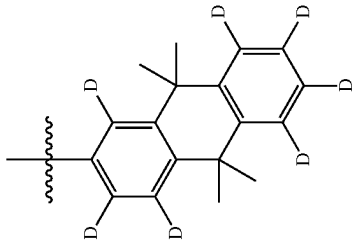
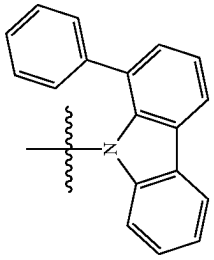
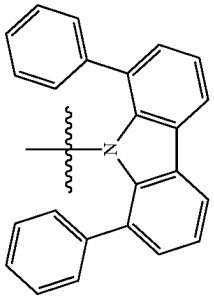
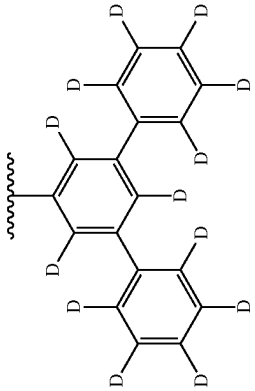
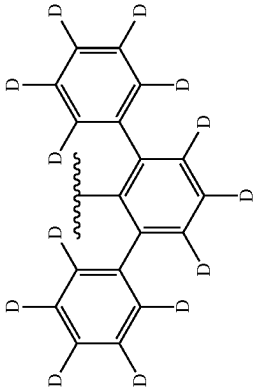
R151		R152		R153	
R154		R155		R156	
R157		R158		R159	

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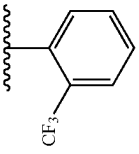
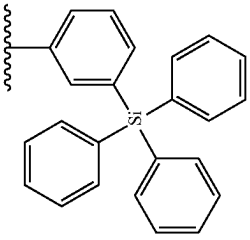
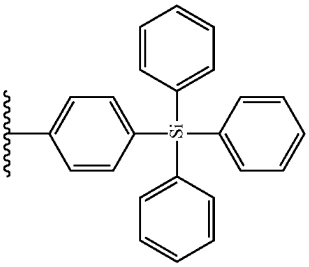
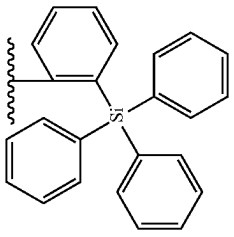
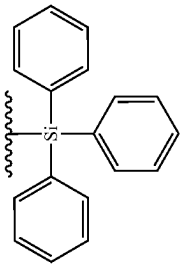
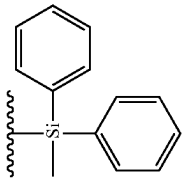
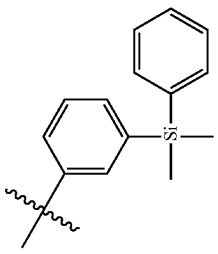
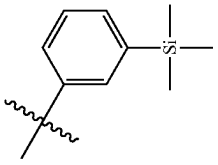
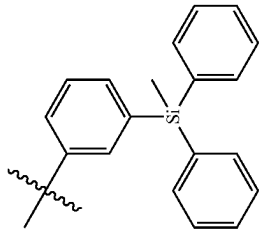
R160		R161		R162	
R163		R164		R165	
R166		R167		R168	

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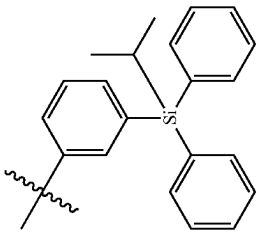
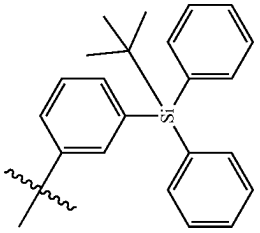
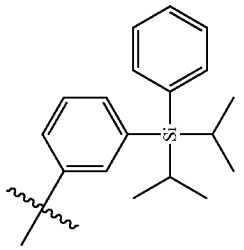
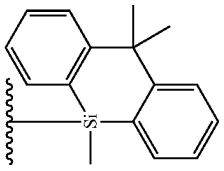
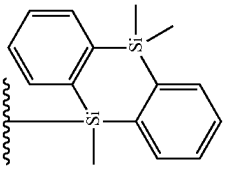
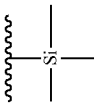
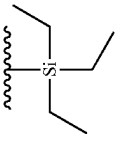
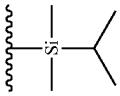
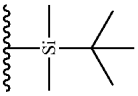
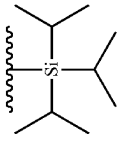
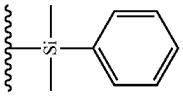
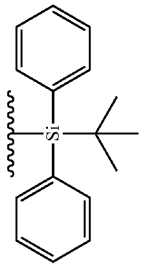
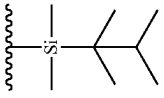
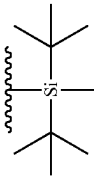
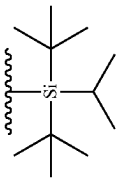
R169		R170		R171	
R172		R173		R174	
R175		R176		R177	
R178		R179		R180	
R181		R182		R183	

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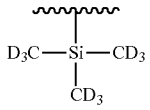
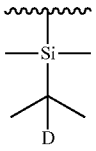
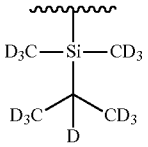
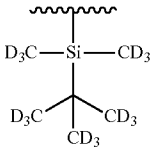
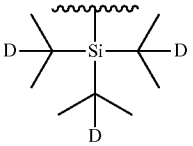
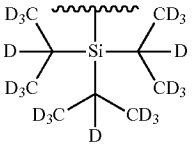
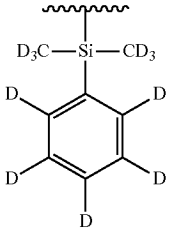
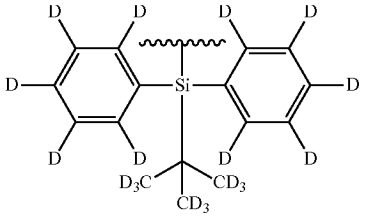
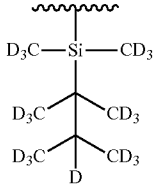
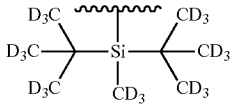
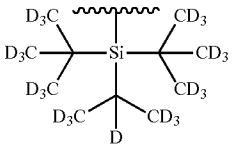
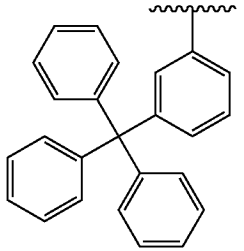
R184		R185		R186	
R187		R188		R189	
R190		R191		R192	
R193		R194		R195	

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R202		R203		R204	

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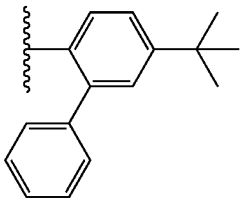
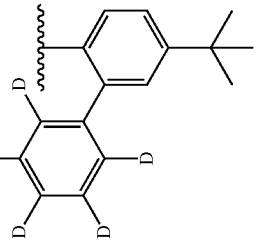
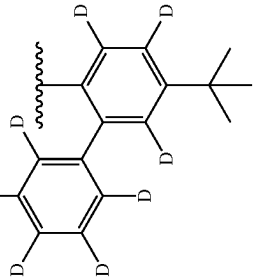
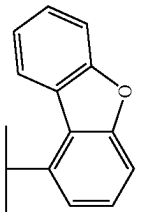
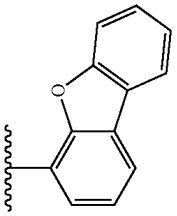
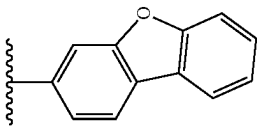
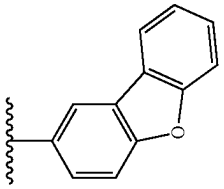
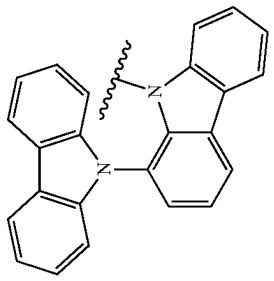
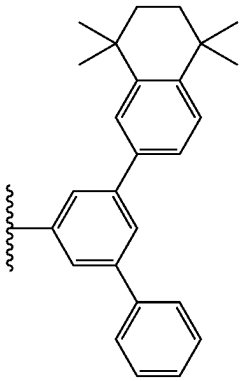
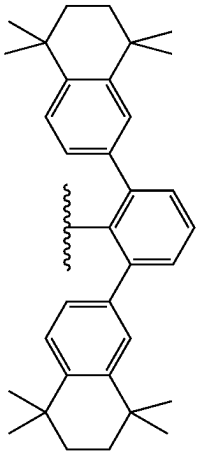
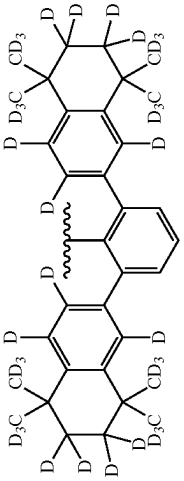
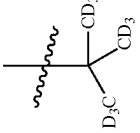
R205		R206		R207	
R208		R209		R210	
R211		R212		R213	
R214		R215		R216	

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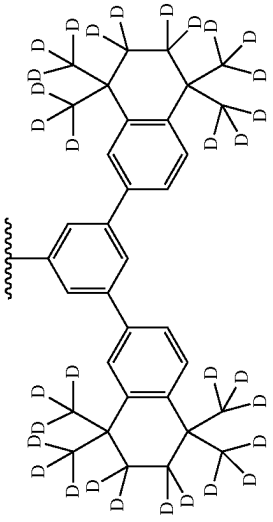
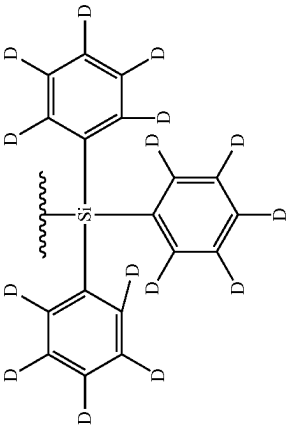
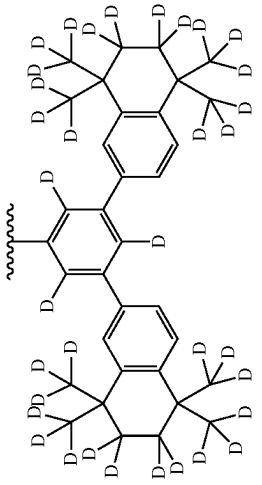
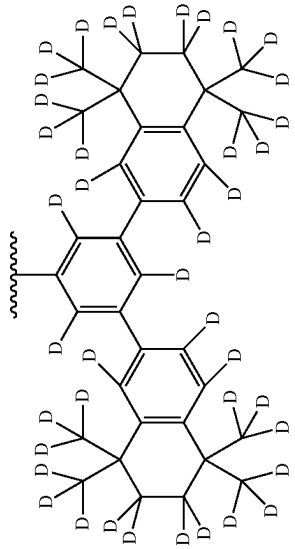
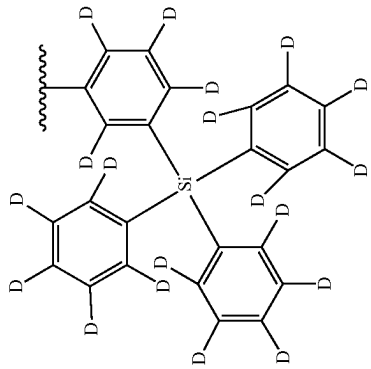
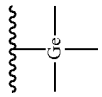
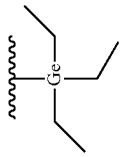
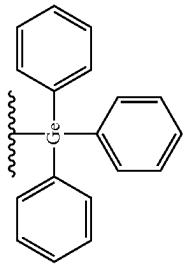
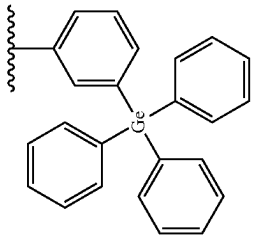
R226		R227		R228	
R229		R230		R231	
R232		R233		R234	

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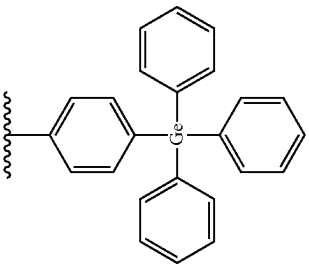
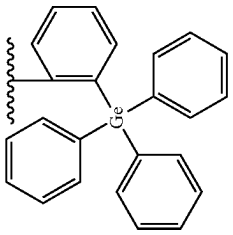
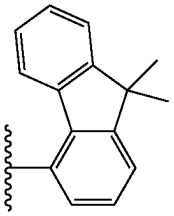
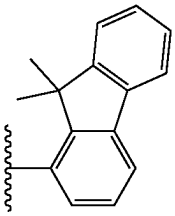
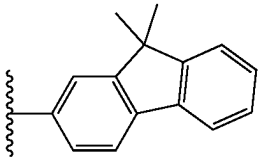
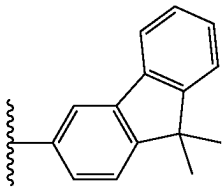
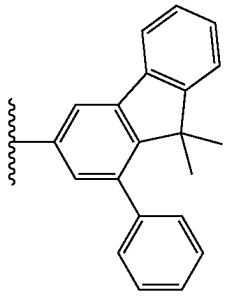
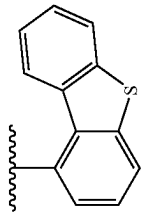
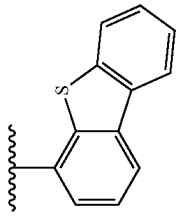
R235		R236		R237	
R238		R239		R240	
R241		R242		R243	

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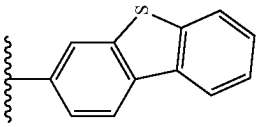
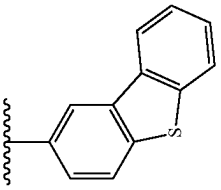
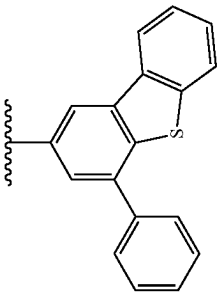
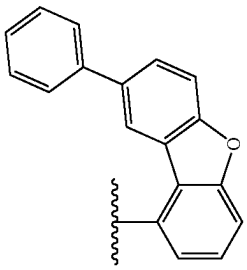
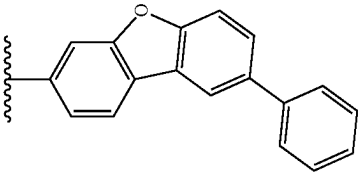
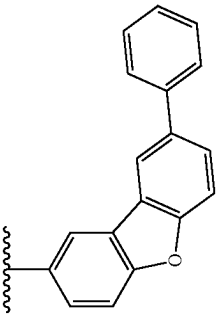
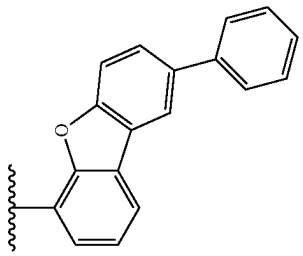
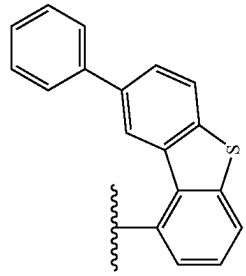
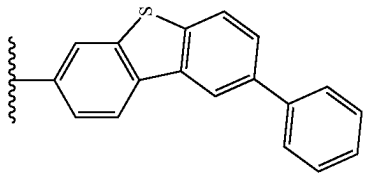
R244		R245		R246	
R247		R248		R249	
R250		R251		R252	

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Structure	Structure	Structure
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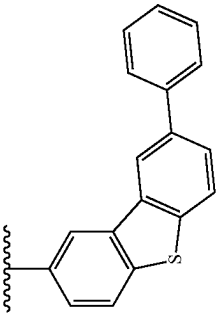	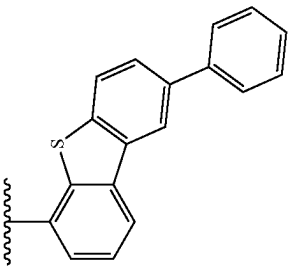	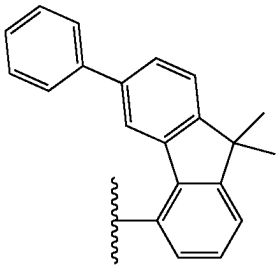
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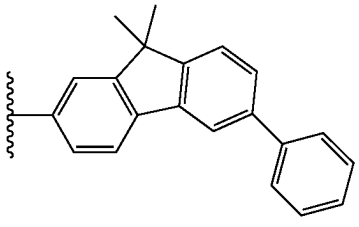	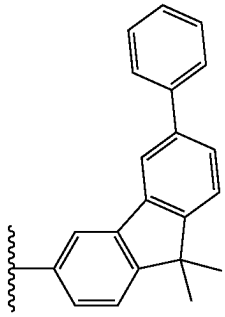	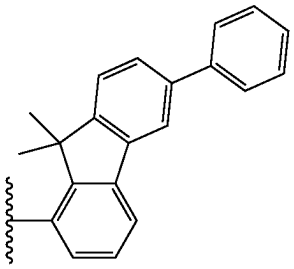
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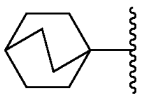	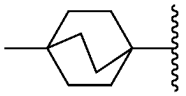	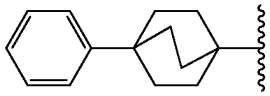

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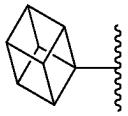
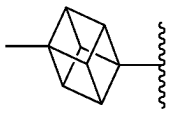
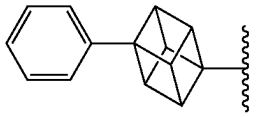
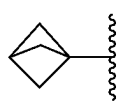
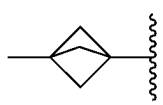
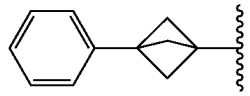
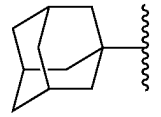
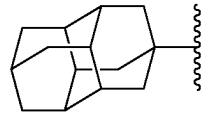
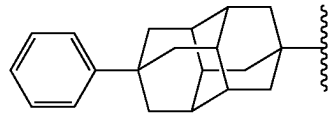
R262		R263		R264	
R265		R266		R267	
R268		R269		R270	

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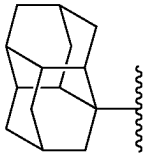
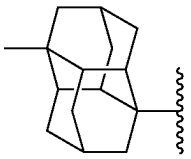
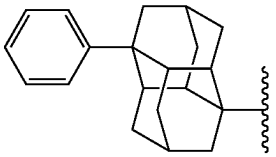
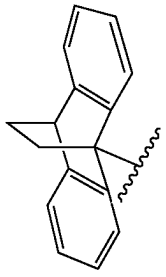
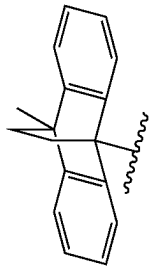
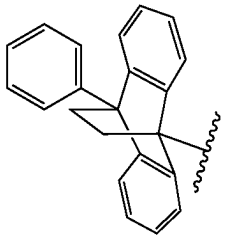
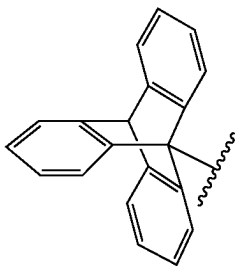
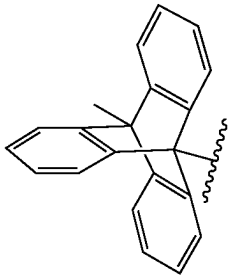
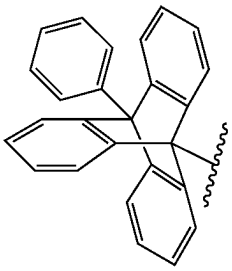
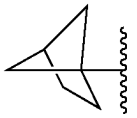
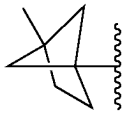
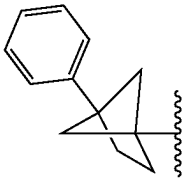
R271		R272		R273	
R274		R275		R276	
R277		R278		R279	
R280		R281		R282	

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Structure	Structure	Structure
R283	R284	R285
R286	R287	R288
R289	R290	R291
R292	R293	R294
R295	R296	R297

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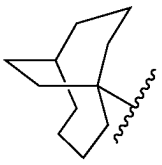
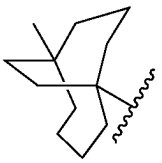
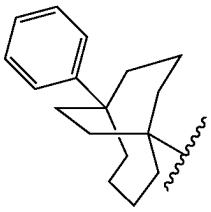
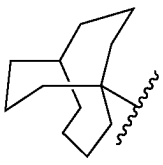
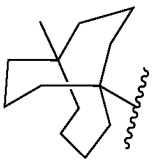
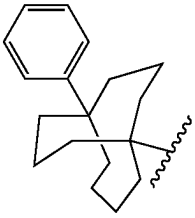
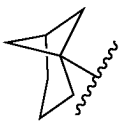
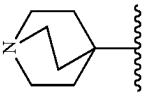
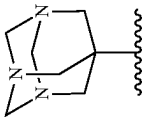
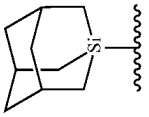
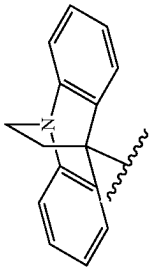
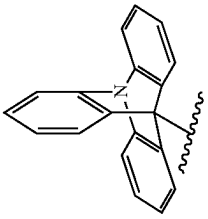
	Structure		Structure		Structure
R298		R299		R300	
R301		R302		R303	
R304		R305		R306	
R307		R308		R309	

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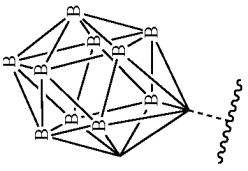
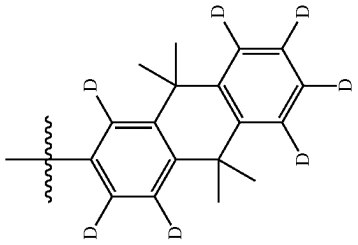
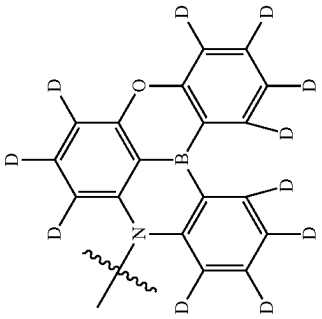
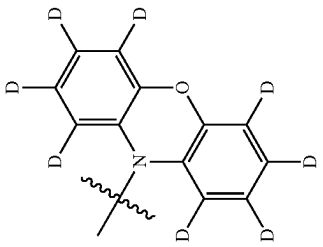
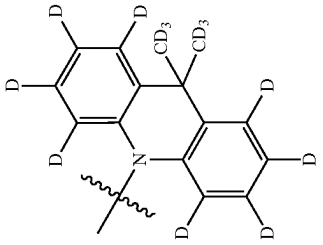
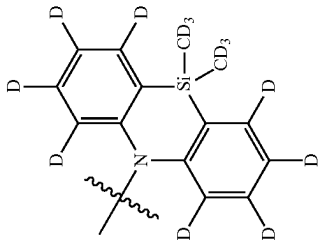
R310	
R311	
R312	
R313	
R314	
R315	

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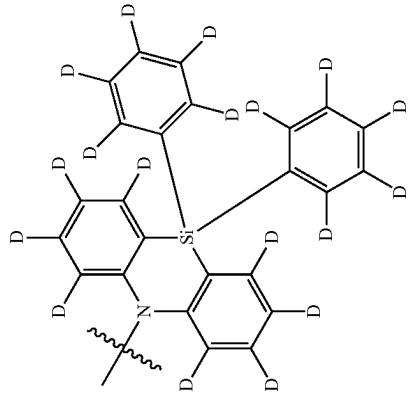
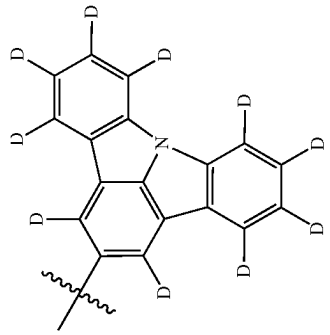
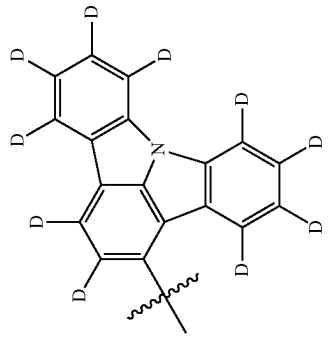
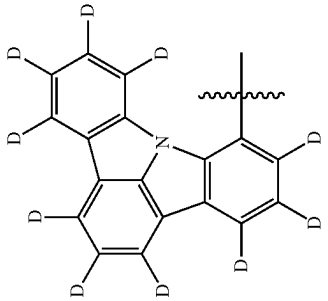
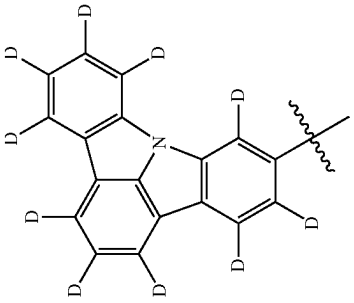
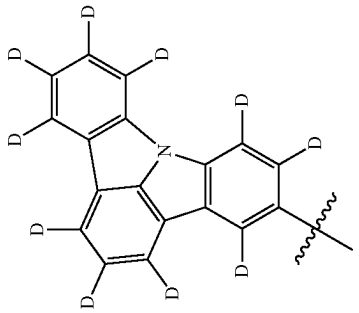
R316	
R317	
R318	
R319	
R320	
R321	

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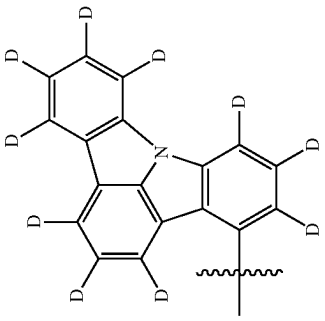
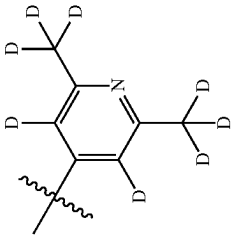
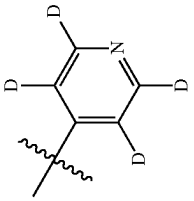
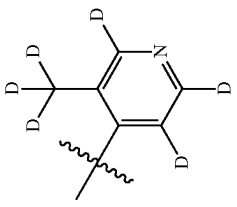
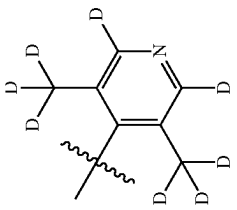
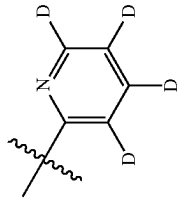
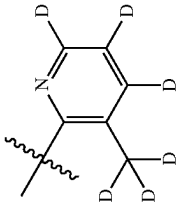
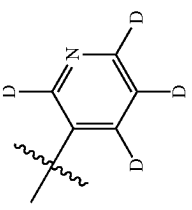
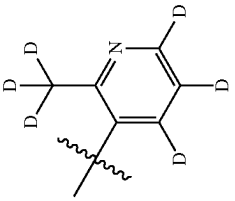
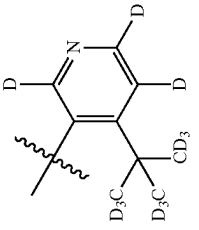
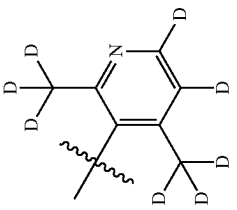
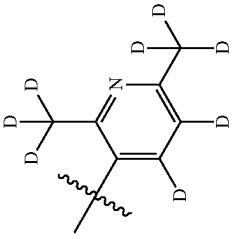
R322		R323		R324	
R325		R326		R327	
R328		R329		R330	
R331		R332		R333	

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Structure	Structure	Structure
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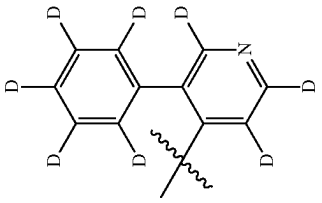	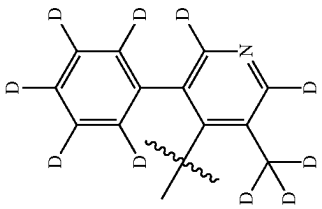	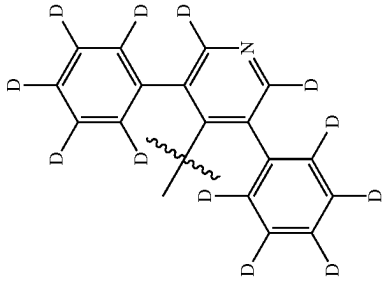
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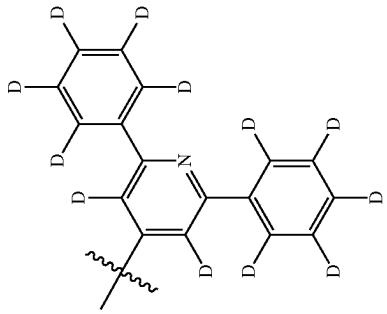	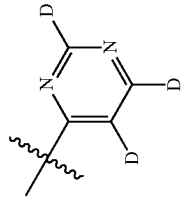	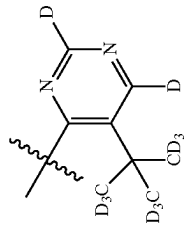
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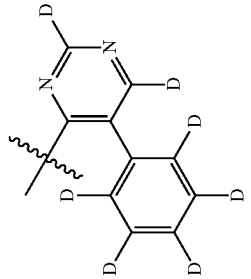	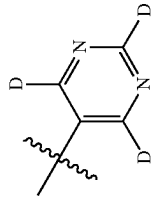	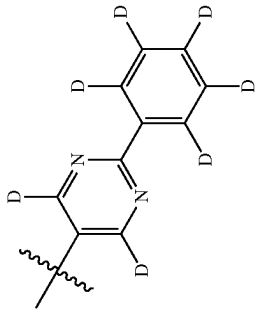

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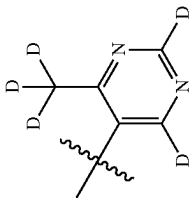
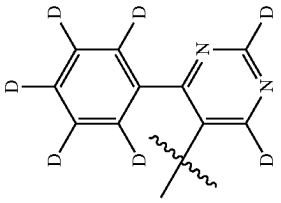
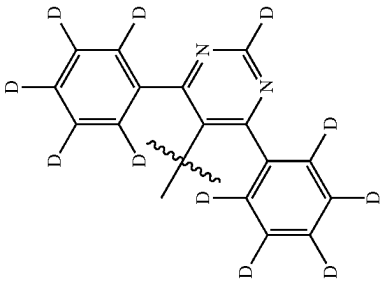
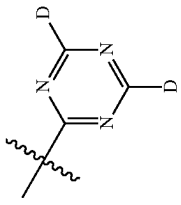
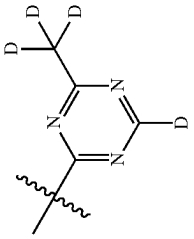
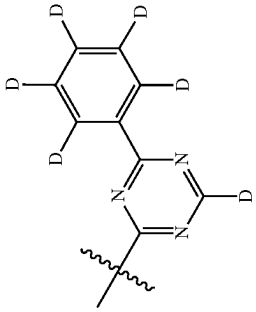
R343	
R344	
R345	
R346	
R347	
R348	

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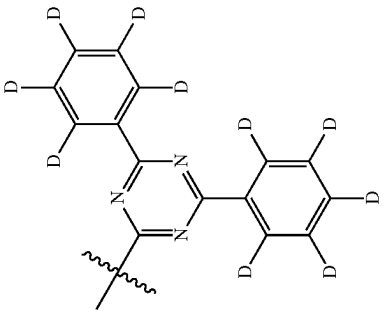
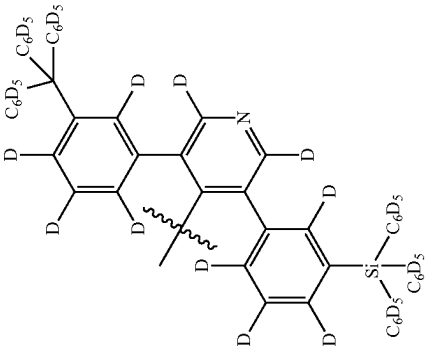
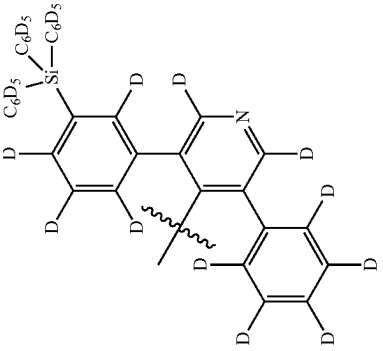
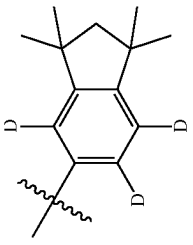
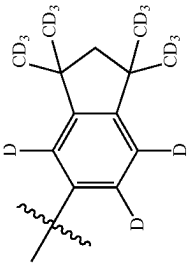
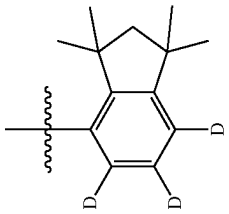
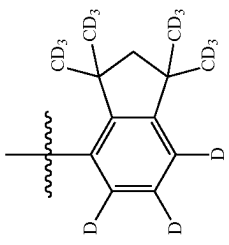
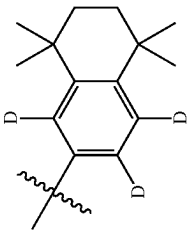
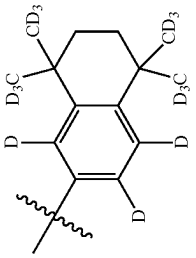
R349		R350		R351	
R352		R353		R354	
R355		R356		R357	

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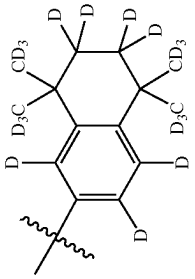
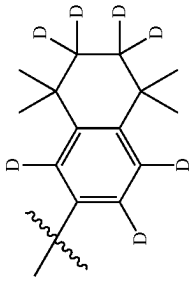
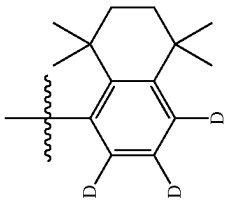
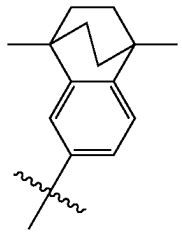
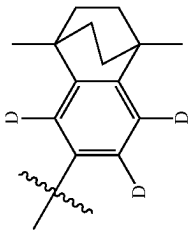
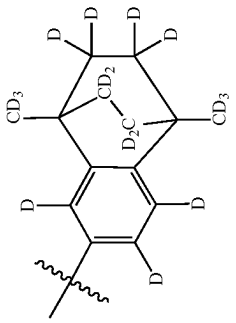
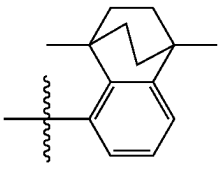
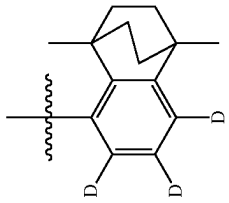
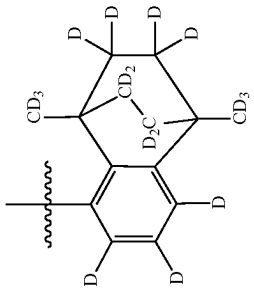
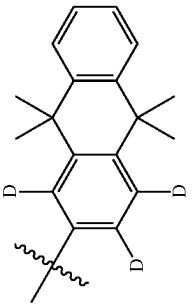
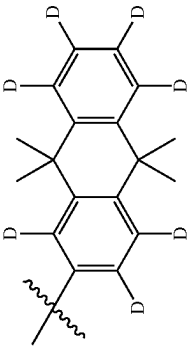
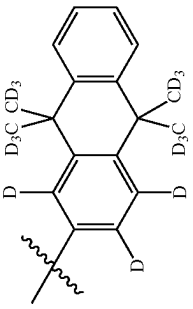
R358		R359		R360	
R361		R362		R363	
R364		R365		R366	
R367		R368		R369	

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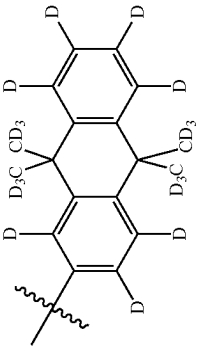
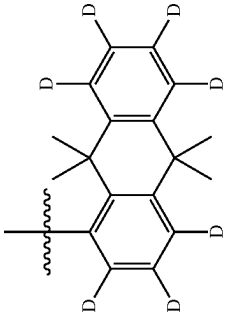
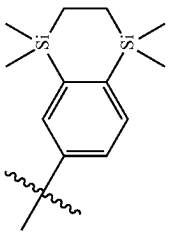
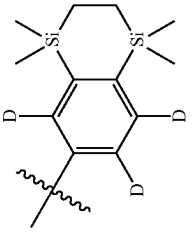
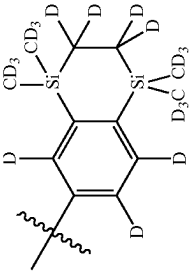
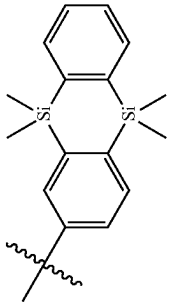
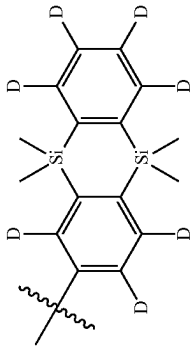
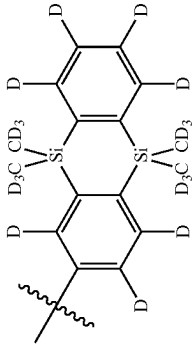
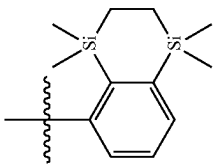
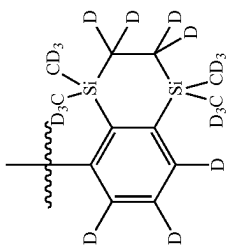
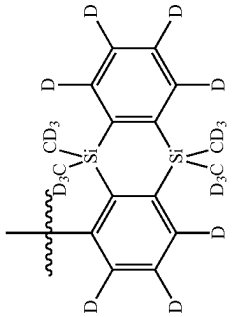
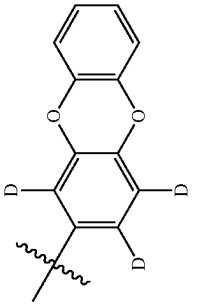
R370		R371		R372	
R373		R374		R375	
R376		R377		R378	
R379		R380		R381	

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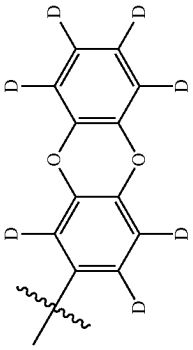
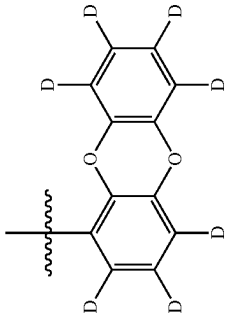
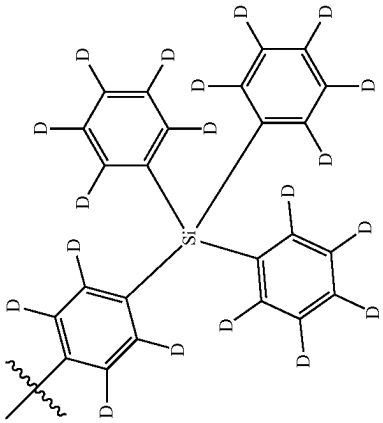
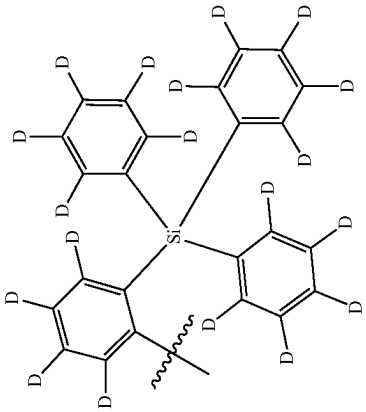
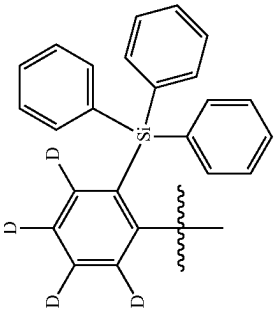
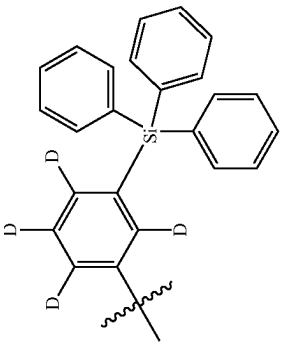
R382	
R383	
R384	
R385	
R386	
R387	

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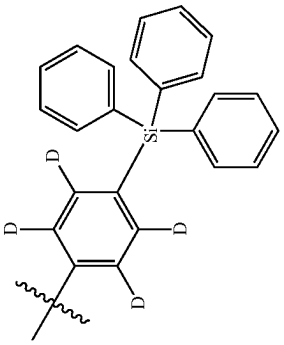
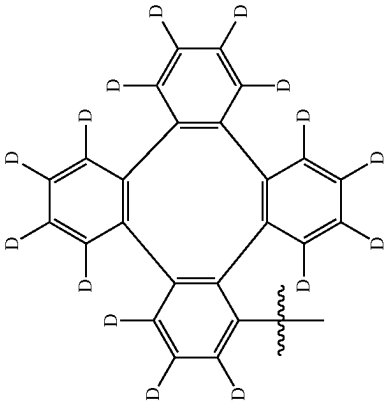
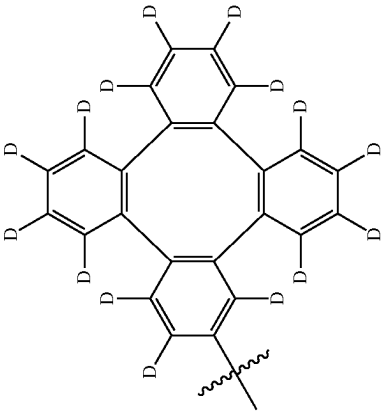
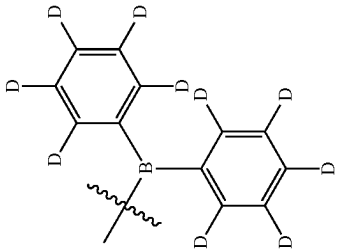
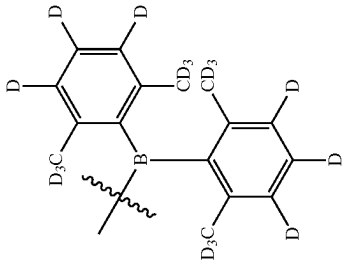
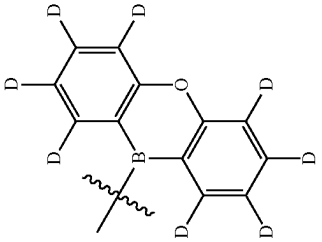
R388	
R389	
R390	
R391	
R392	
R393	

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Structure	Structure	Structure
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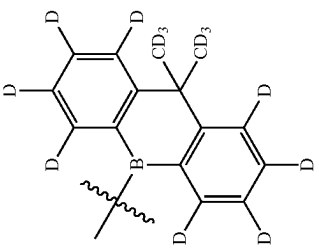
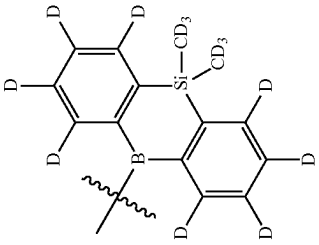
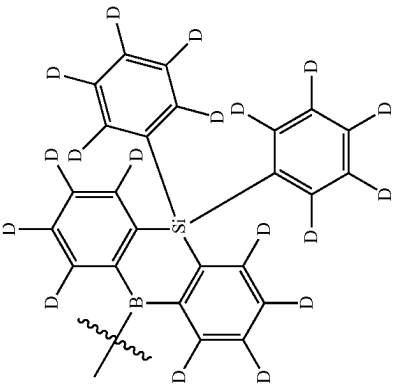
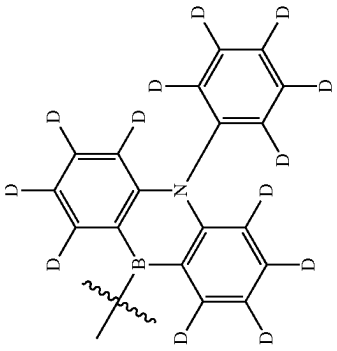
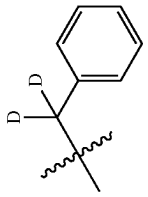
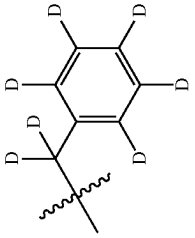
		
R397	R398	R399
		
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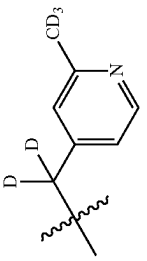	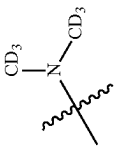	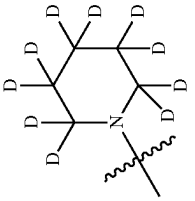

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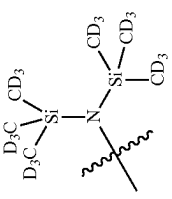
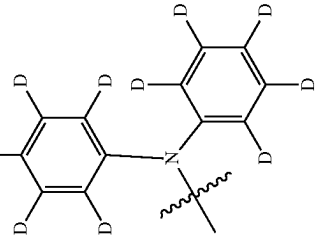
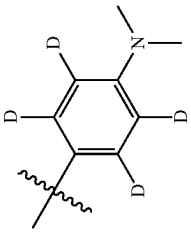
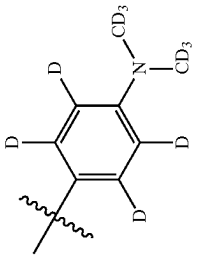
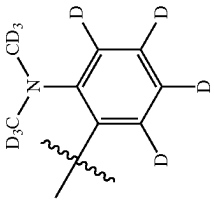
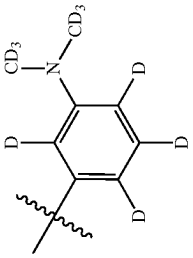
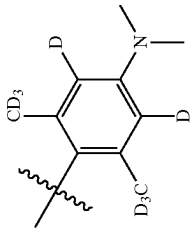
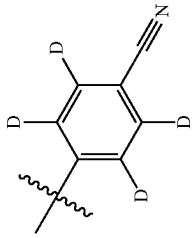
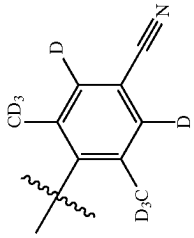
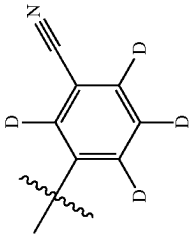
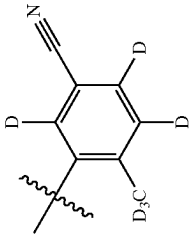
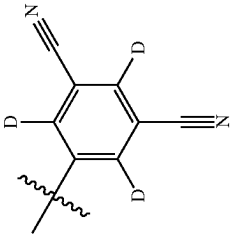
	Structure		Structure		Structure
R403		R404		R405	
R406		R407		R408	
R409		R410		R411	
R412		R413		R414	

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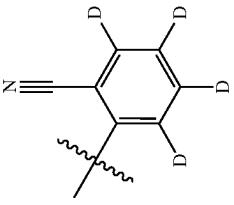
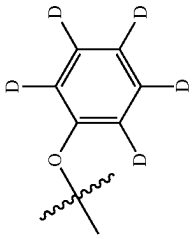
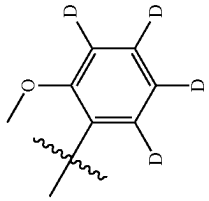
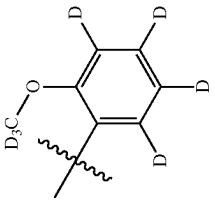
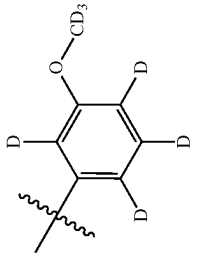
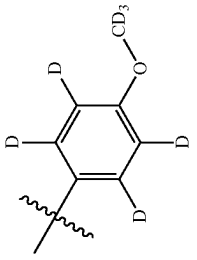
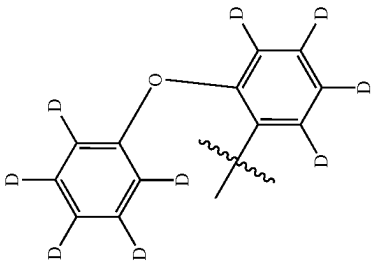
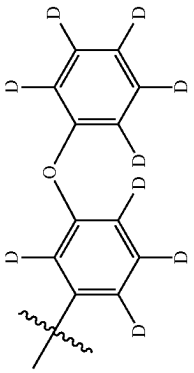
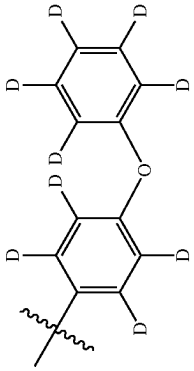
R415	
R416	
R417	
R418	
R419	
R420	
R421	
R422	
R423	

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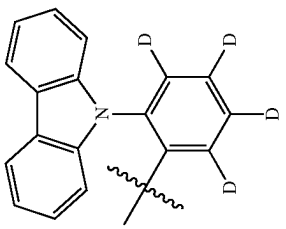
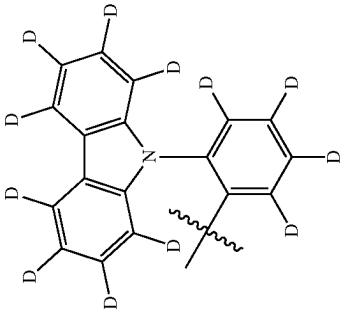
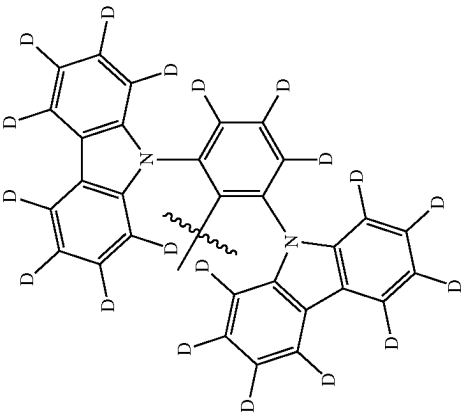
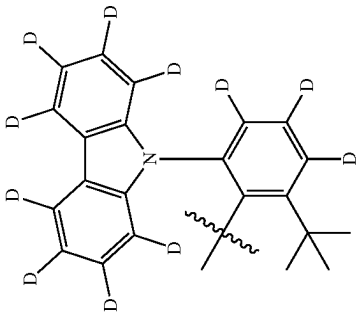
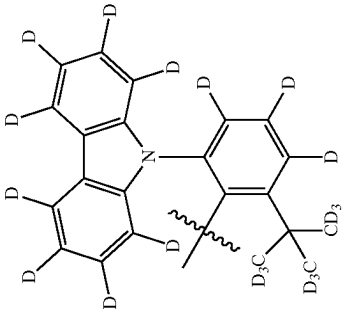
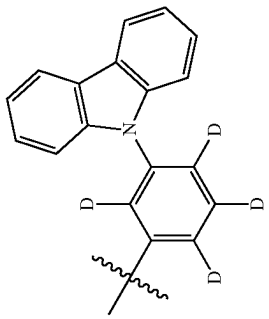
R424	
R425	
R426	
R427	
R428	
R429	

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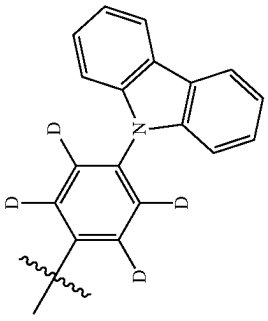
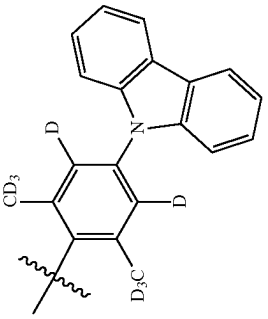
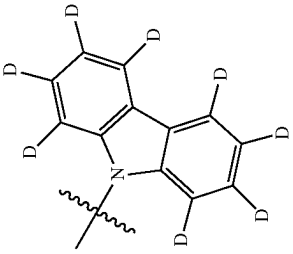
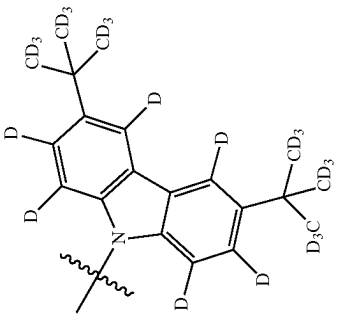
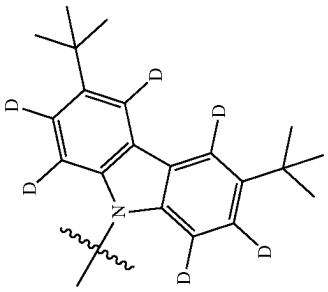
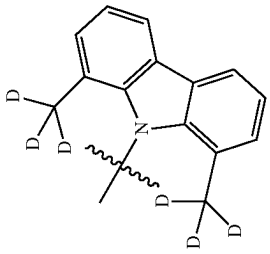
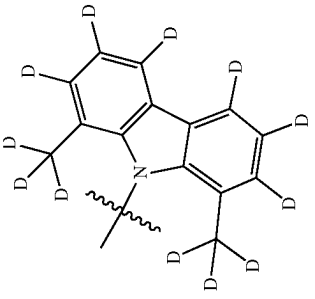
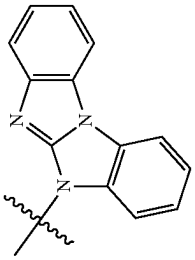
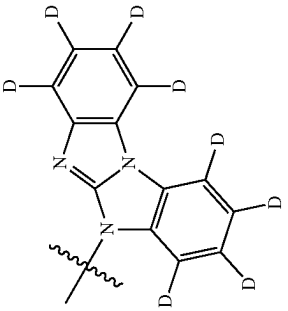
R430	
R431	
R432	
R433	
R434	
R435	
R436	
R437	
R438	

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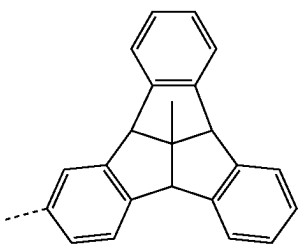
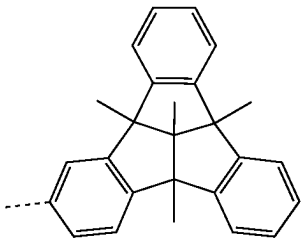
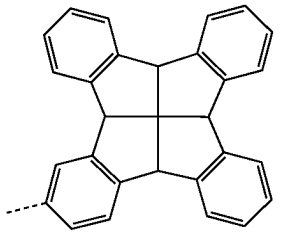
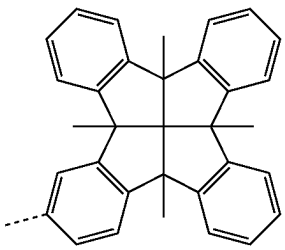
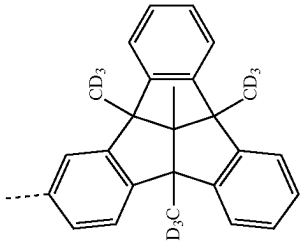
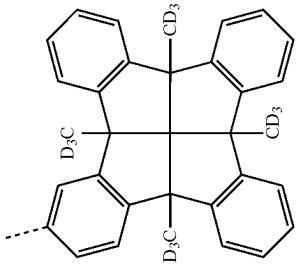
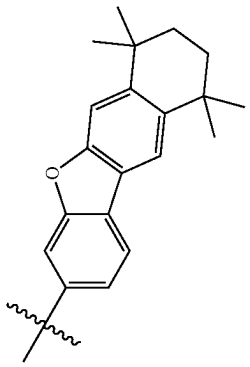
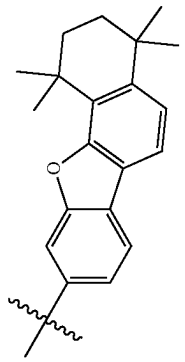
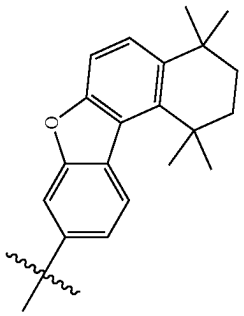
R439		R440		R441	
R442		R443		R444	
R445		R446		R447	

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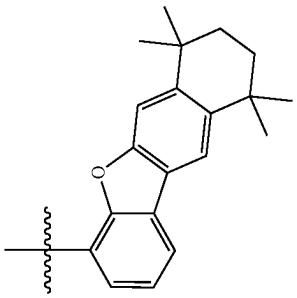	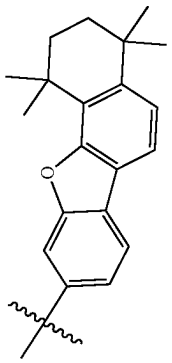	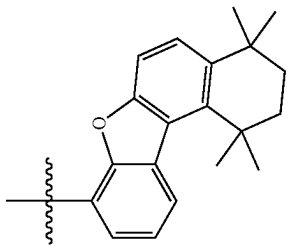
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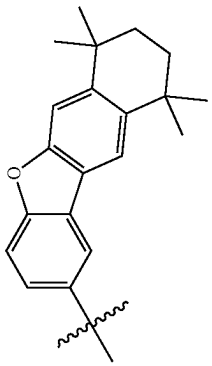	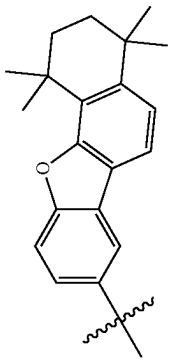	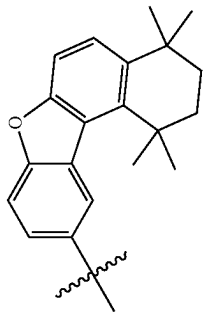
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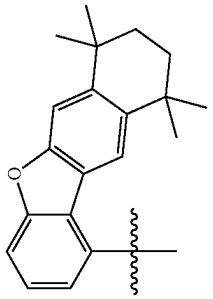
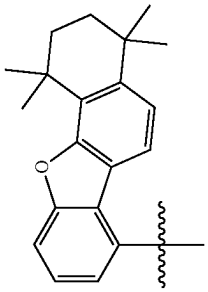
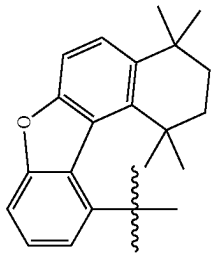
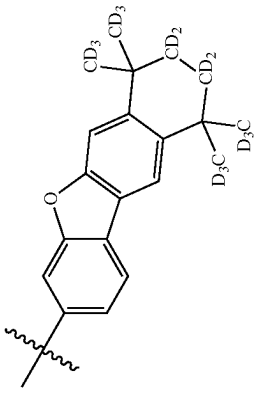
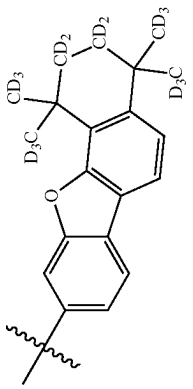
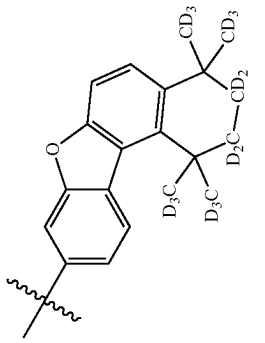
		
R457	R458	R459
		

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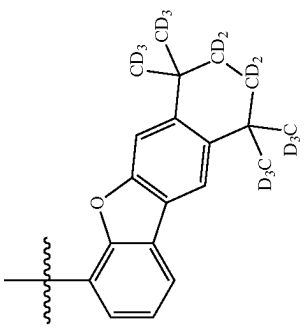
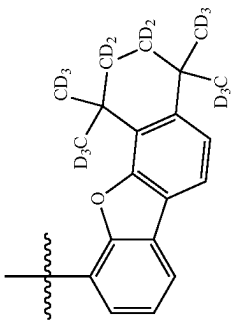
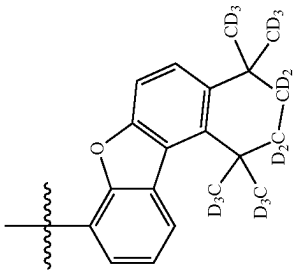
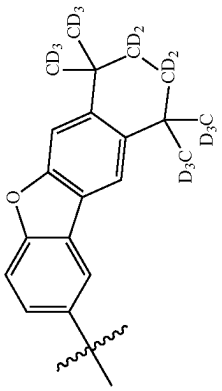
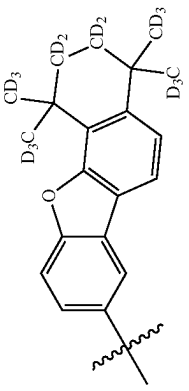
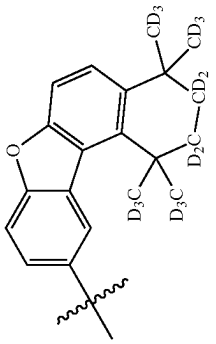
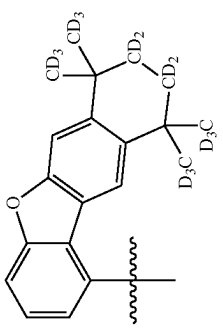
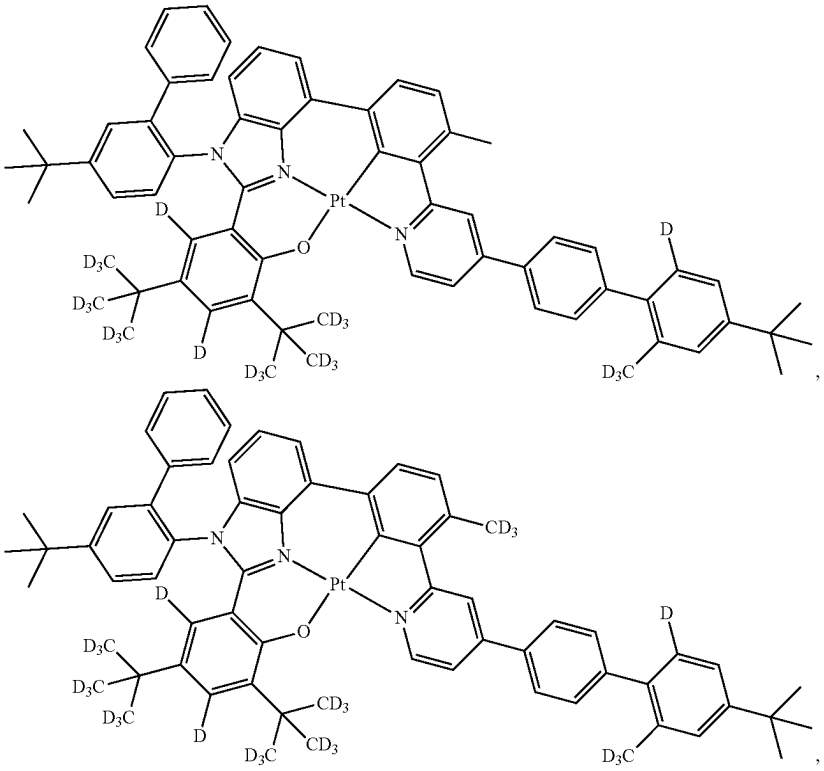
	Structure		Structure		Structure
R460		R461		R462	
R463		R464		R465	
R466					

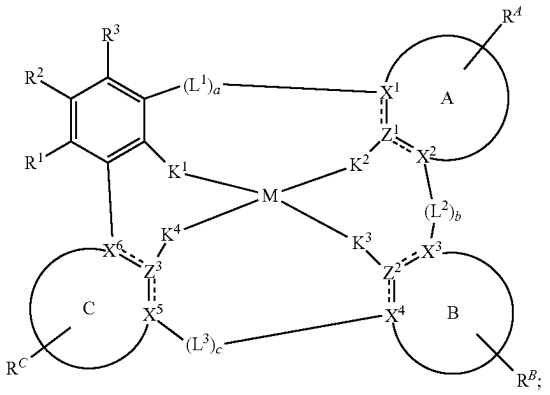
[0225] In some embodiments, the compound is selected from the group consisting of the structures from the following LIST 9:



What is claimed is:

1. A compound comprising a structure of Formula I:

Formula I



wherein moieties A, B, and C are each independently a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered to 10-membered carbocyclic or heterocyclic ring;

wherein each L^1, L^2, and L^3 is independently selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR';

wherein Z^1, Z^2, and Z^3 are each independently C or N;

wherein M is Pt or Pd;

wherein X^1-X^6 are each independently C or N;

wherein each a, b, and c is independently 0 or 1;

wherein a+b+c=2 or 3;

wherein each of K^1, K^2, K^3, and K^4 is independently selected from the group consisting of single bond, O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$;

wherein R^A, R^B, and R^C each independently represent mono to the maximum allowable substitution, or no substitution;

wherein each R, R', R^α, R^β, R^2, R^3, R^A, R^B, and R^C is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, wherein R^1 is selected from the group consisting of halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof,

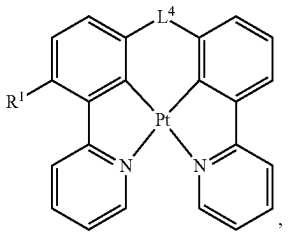
wherein any two substituents may be joined or fused to form a ring;

with the proviso that if R^1 is tert-butyl, R^3 is not tert-butyl;

with the proviso that R^1 and R^2 do not join to form a ring;

with the proviso that R^1 and R^C do not join to form a ring; and

with the proviso that the compound does not comprise:



wherein L^4 is selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

2. The compound of claim **1**, wherein each of R, R', R^{α}, R^{β}, R^2, R^3, R^A, R^B, and R^C is independently a hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

3. The compound of claim **1**, wherein R^1 is selected from the group consisting of fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

4. The compound of claim **1**, wherein all of X^1—X^6 are C.

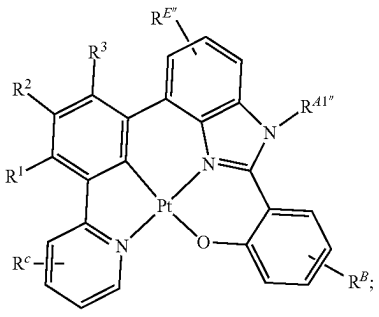
5. The compound of claim **1**, wherein exactly two of Z^1-Z^3 are N.

6. The compound of claim **1**, wherein at least one of K^1, K^2, K^3, and K^4 is O.

7. The compound of claim **1**, wherein the compound comprises a fully deuterated alkyl group.

8. The compound of claim **1**, wherein the compound comprises a structure of Formula II

Formula II



wherein each of $R^{A1''}$ and $R^{E''}$ is independently a hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, aryloxy, alkoxy, aryloxy, amino, silyl, germyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, combinations thereof, and

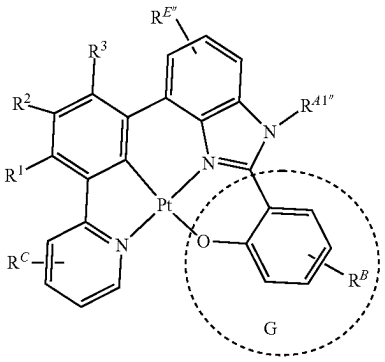
wherein one or more of the R^B or R^C is D.

9. The compound of claim **1**, wherein the compound has a structure selected from the group consisting of the following structures of LIST 1 as defined herein;

wherein $R^{E''}$ is independently a hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, combinations thereof, and the rest of variables are the same as previously defined.

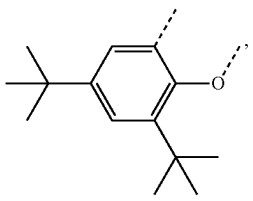
10. The compound of claim **8**, wherein $R^{A1''}$ is selected from the group consisting of the structures from the LIST 2 as defined herein.

11. The compound of claim **1**, wherein the moiety G in Formula II

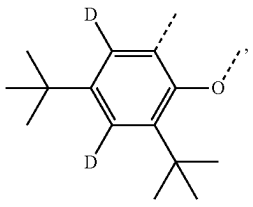


is selected from the group consisting of G_{W2}, W2 is an integer from 1 to 12, wherein G_1-G_{12} having the following structures:

G_1



G_2



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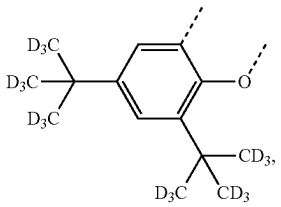

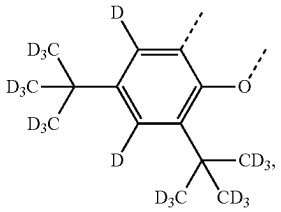

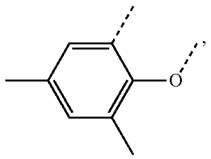

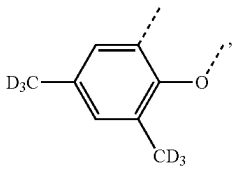

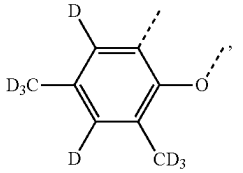

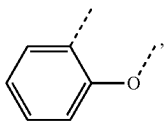

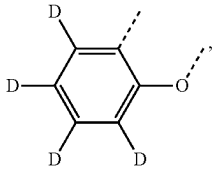

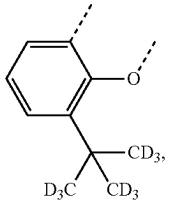

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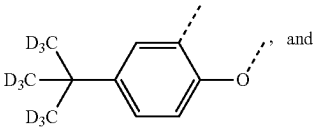
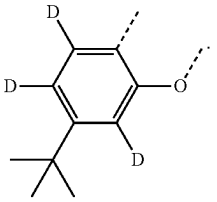
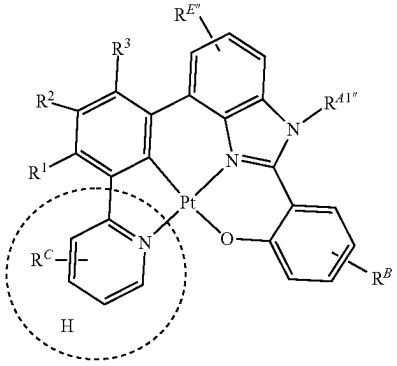


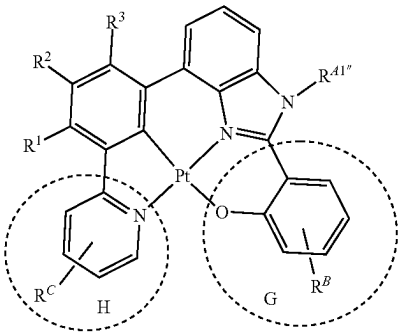


12. The compound of claim **1**, wherein the moiety H in Formula II

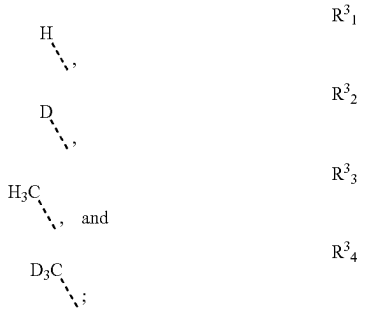


is selected from the group consisting of the structures from LIST 3 as defined herein.

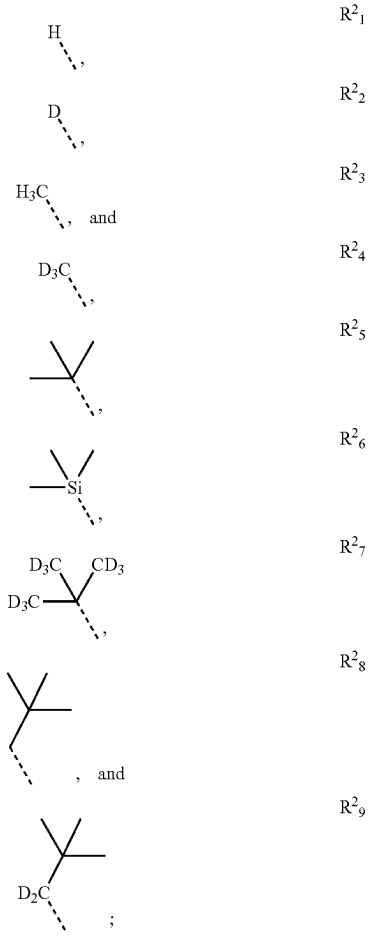
13. The compound of claim **1**, wherein the compound has a structure of Formula II:



wherein $R^{A1''}$, moiety G, and moiety H are described above, R^3 is selected from the group consisting of R^3_{W4}, wherein W4 is an integer from 1 to 4, and R^3_1-R^3_4 have the structures of:



and R^2 is selected from the group consisting of R^2_{W5}, wherein W5 is an integer from 1 to 9, and R^2_1-R^2_9 have the structures of:



and R^1 is selected from the group consisting of R^1_{W6}, wherein W6 is an integer from 1 to 4, and R^1_1—R^1_4 have the structures of:

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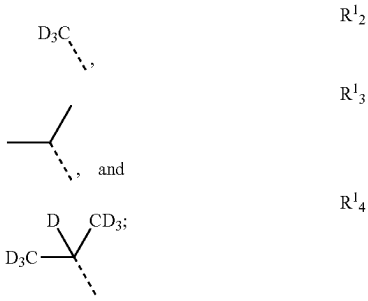
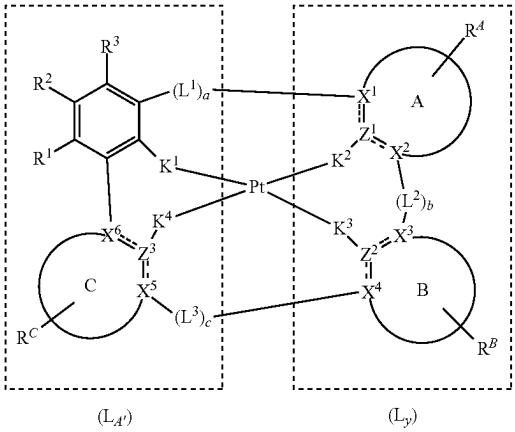


14. The compound of claim **1**, wherein the compound has the formula $Pt(L_{A'})(Ly)$,

Formula III



wherein $L_{A'}$ is selected from the group consisting of the structures shown in LIST 4 as defined herein;

wherein V^1-V^8 are each independently C or N;

wherein each of R^{CC} and R^{DD} independently represents mono to the maximum allowable substitution, or no substitution;

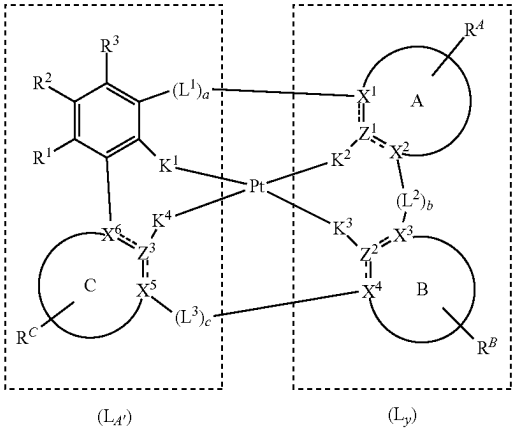
wherein each R^{CC}, R^{DD}, and R^{EE}, is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, selenyl, and combinations thereof;

wherein Ly is selected from the group consisting of the structures shown in LIST 5 as defined herein;

wherein each R^X and R^Y is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, selenyl, and combinations thereof.

15. The compound of claim **1**, wherein the compound is selected from the group consisting of the compounds having the formula of $Pt(L_{A'})(Ly)$,

Formula III

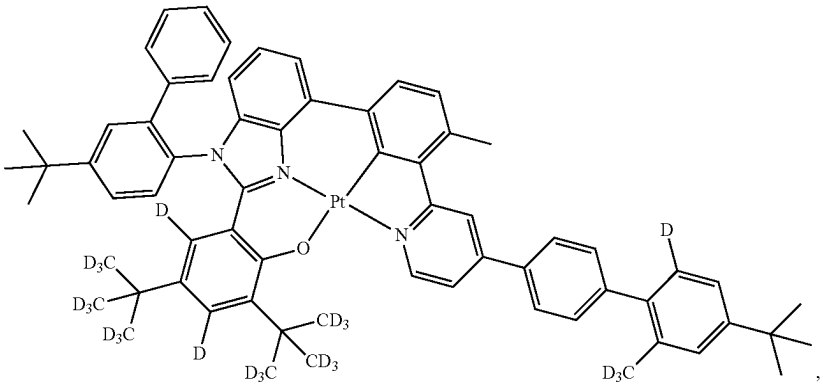


wherein $L_{A'}$ is selected from $L_A i'$-$(L^w)(Rm)(Rn)(Ro)(Rp)$, wherein i' is an integer from 1 to 57; w is an integer from 1 to 4, m, n, o and p are each an integer from 1 to 466, L^w is selected from L1 to L4; each of Rm, Rn, Ro, and Rp is independently selected from R1 to R466, and each of $L_A i$-(L1)(R1)(R1)(R1)(R1) to $L_A 57$-(L4)(R466)(R466)(R466)(R466) is defined in LIST 6; wherein $L_{y'}$ is selected from $L_y j$-(Rs)(Rt)(Ru)(Rv), wherein j is an integer from 1 to 52; each of s, t, u, and v is an integer from 1 to 466, each of Rs, Rt, Ru, and Rv is independently selected from R1 to R466, and each of $L_y 1$-(R1)(R1)(R1)(R1) to $L_y 52$-(R466)(R466)(R466)(R466) is defined in LIST 7; wherein L1 is direct bond, L2 is 0, L3 is S, and L4 is NPh;

wherein when $L_{A'}$ is $L_A 9$ or $L_A 11$, L_y is not $L_y 34$;

wherein R1 to R466 have the structures as defined in LIST 8.

16. The compound of claim **1**, wherein the compound is selected from the group consisting of the structures from the following LIST 9:



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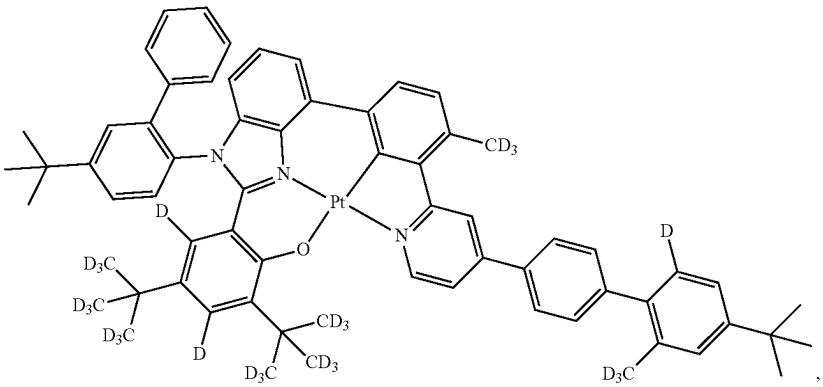

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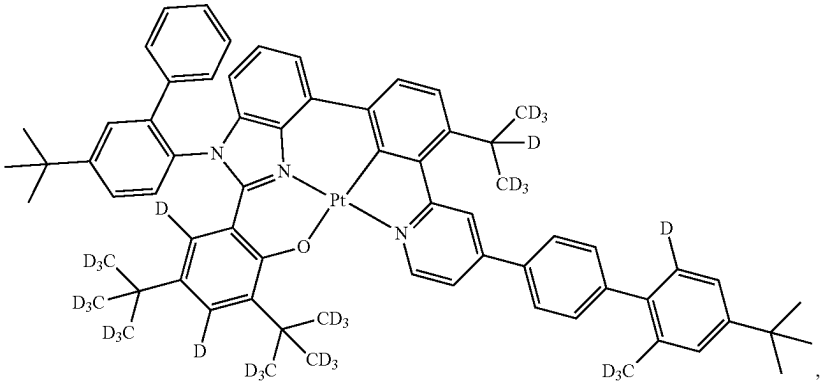

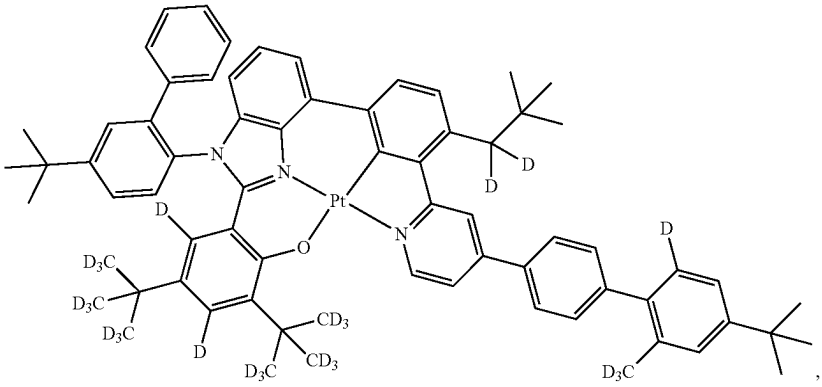

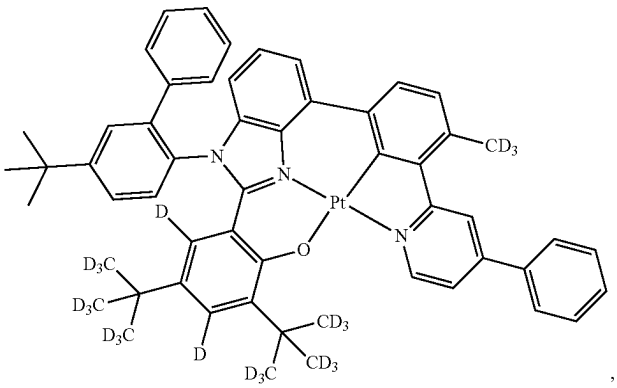

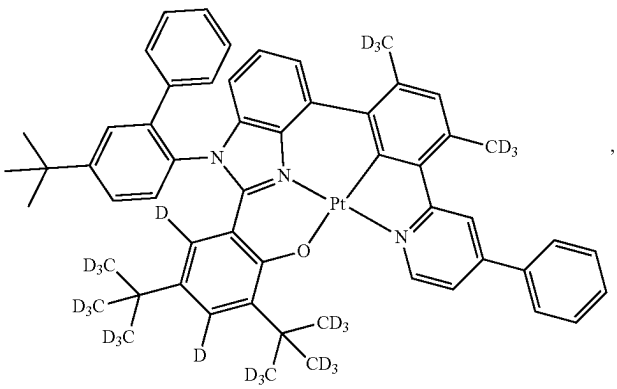

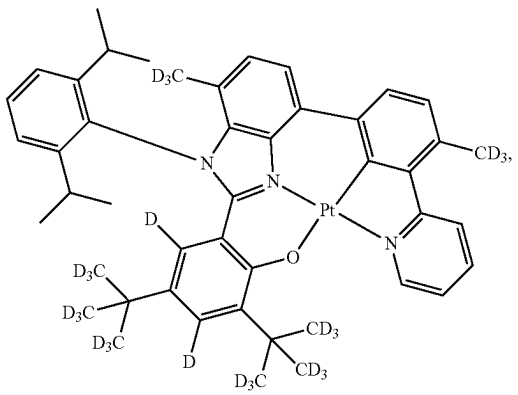

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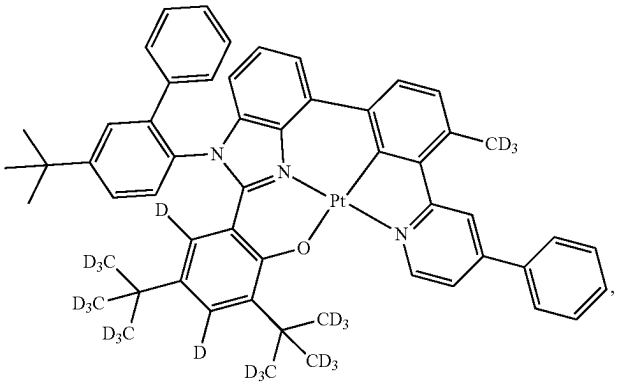

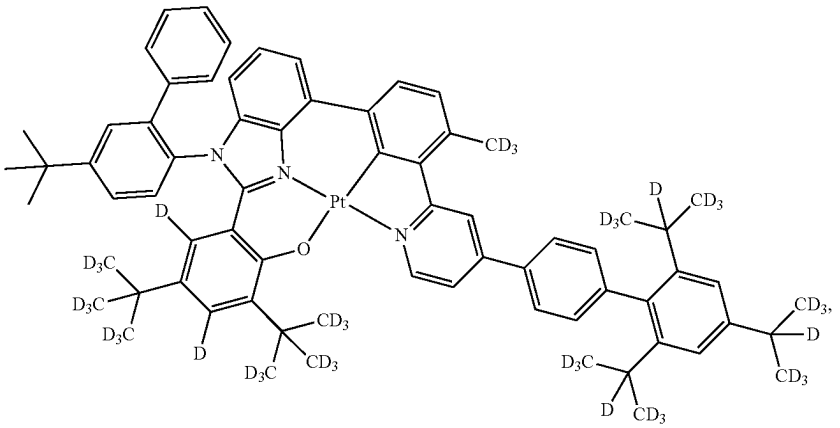

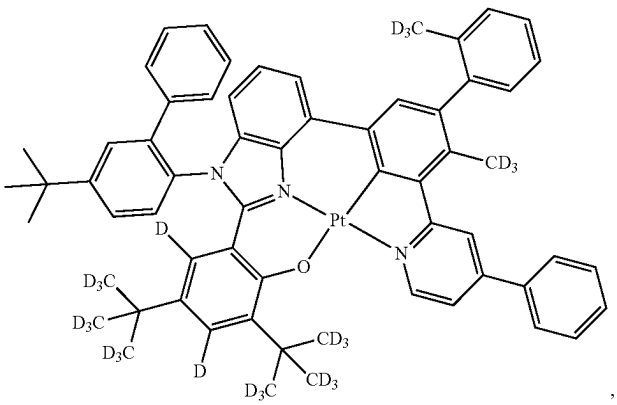

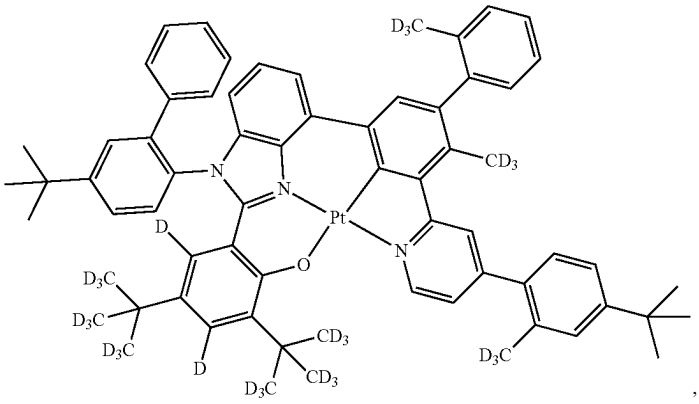

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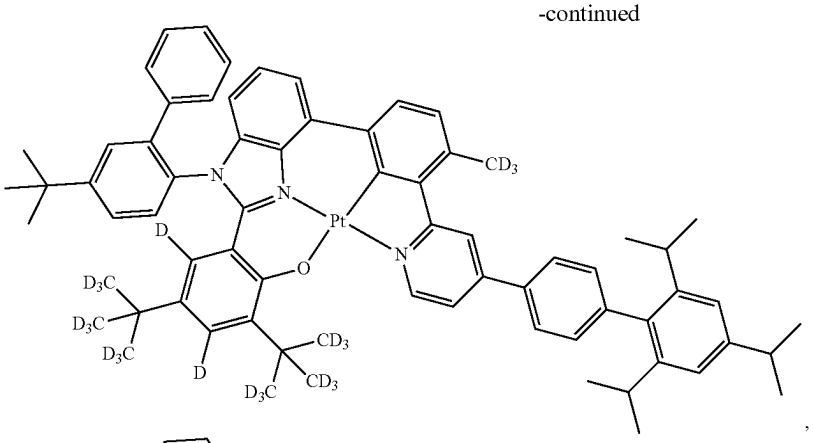

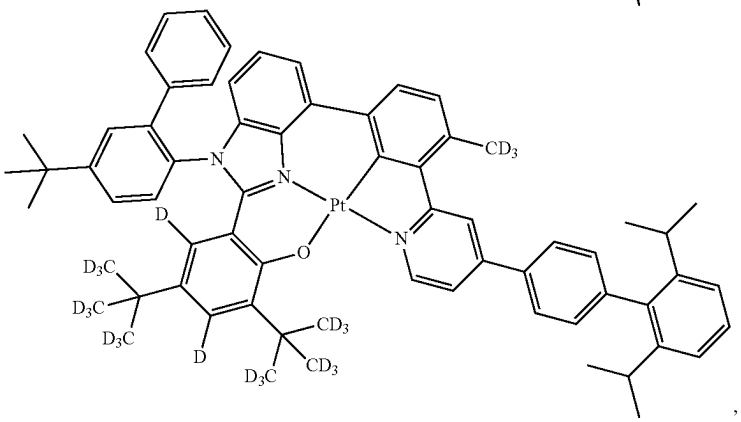

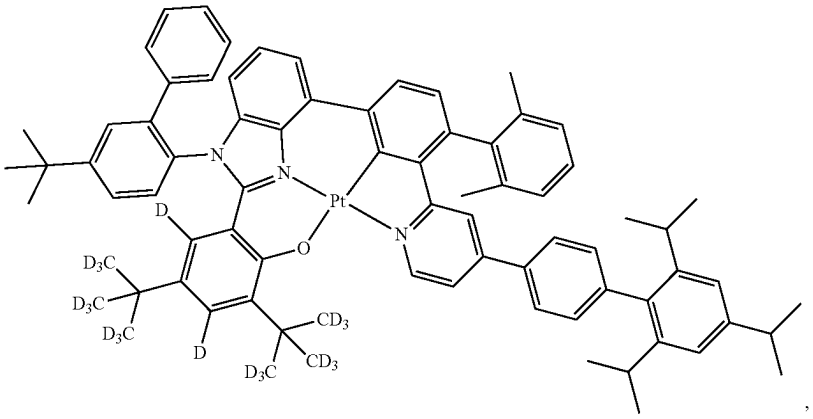

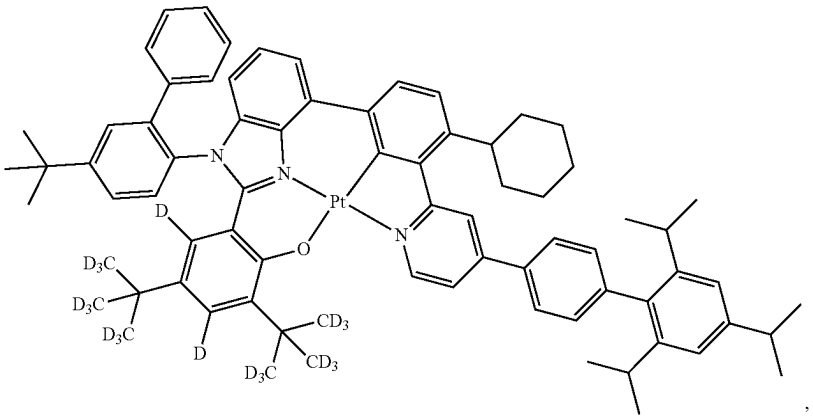

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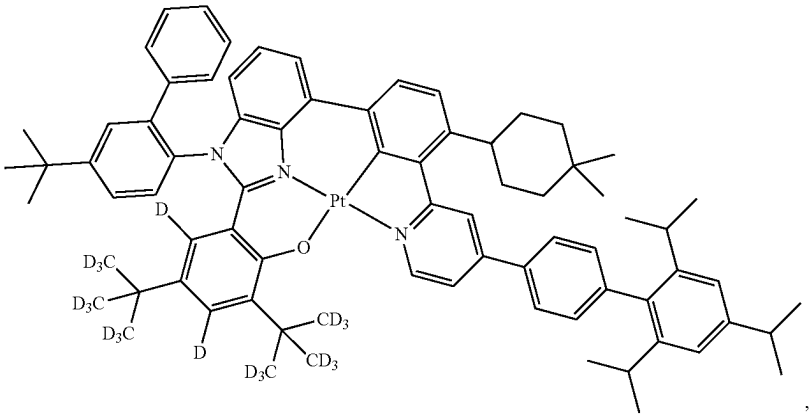

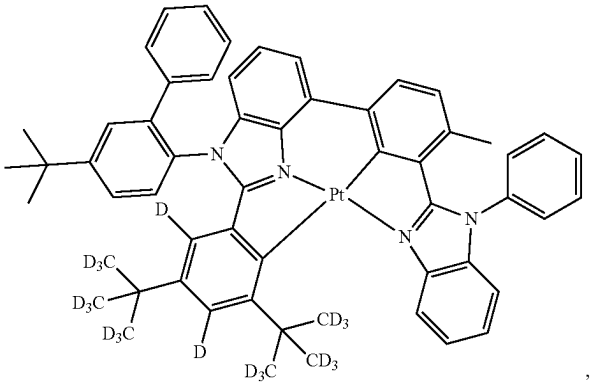

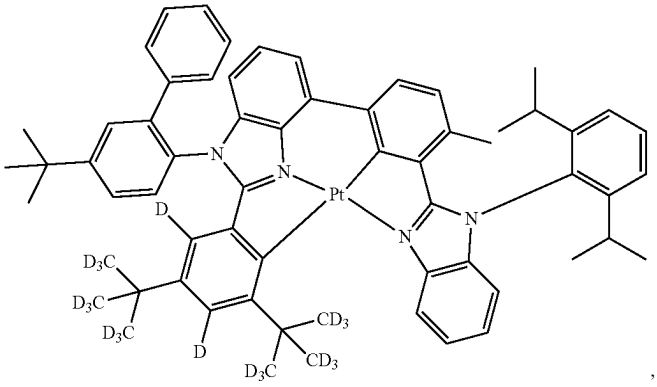

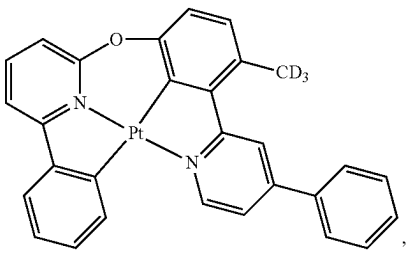

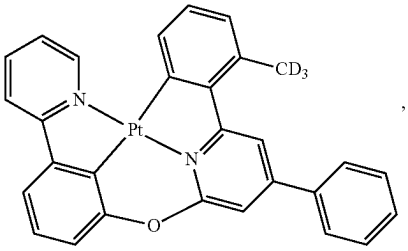

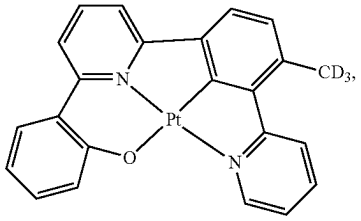

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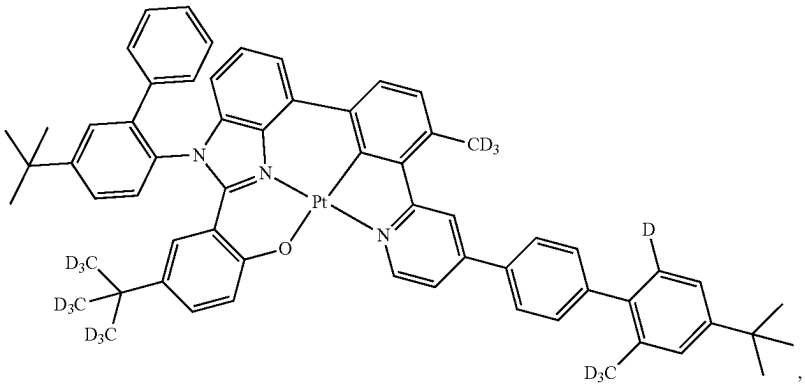

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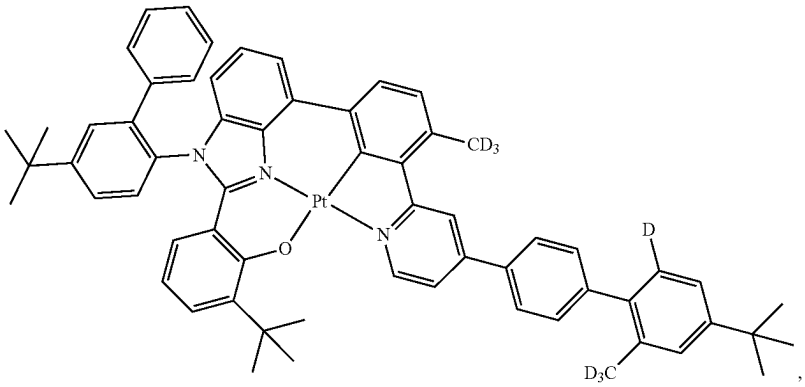

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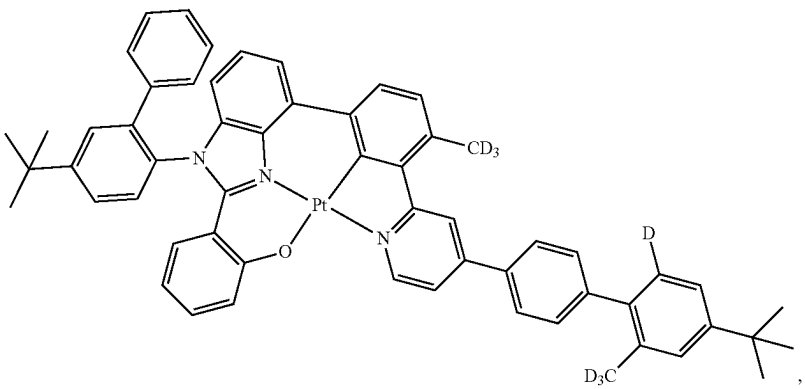

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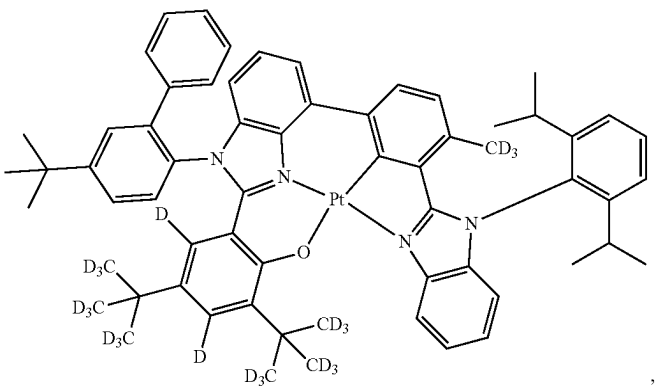

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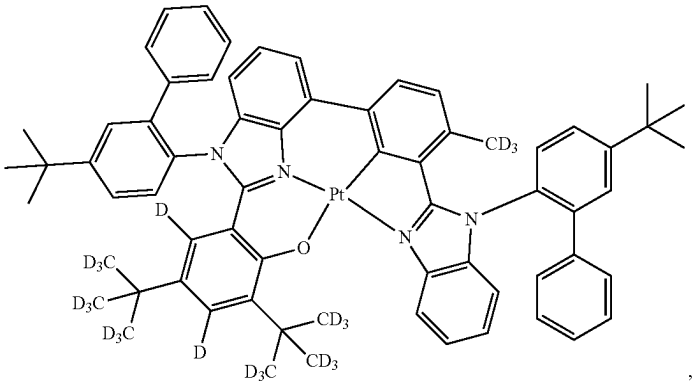

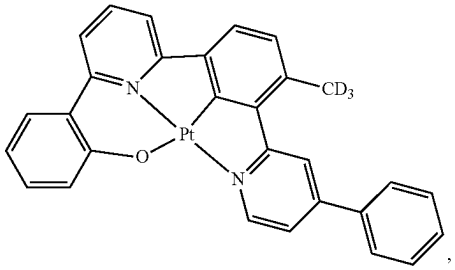

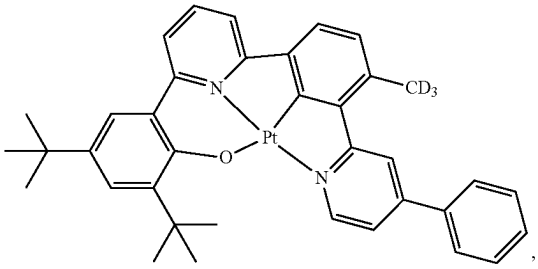

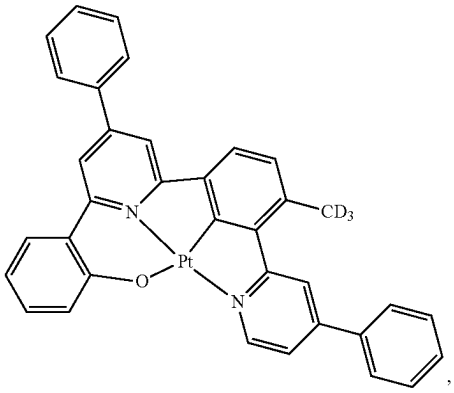

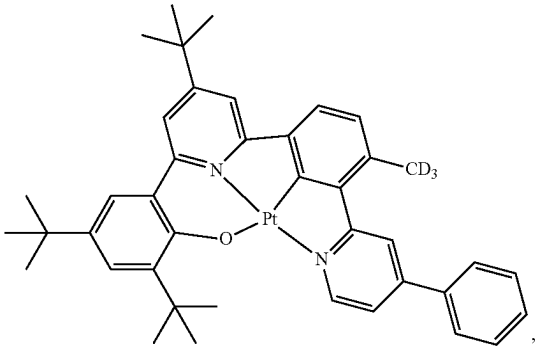

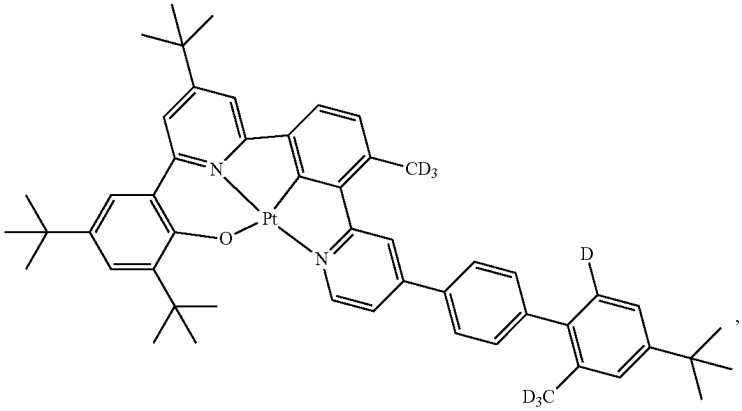

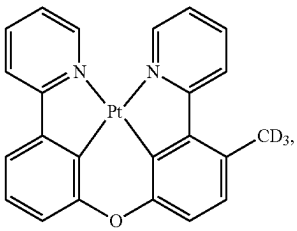

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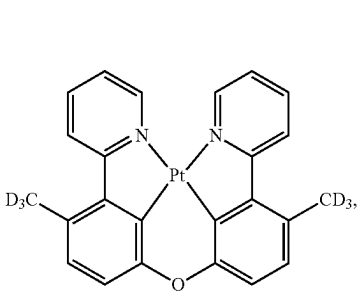

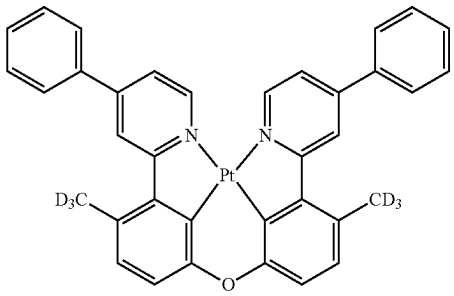

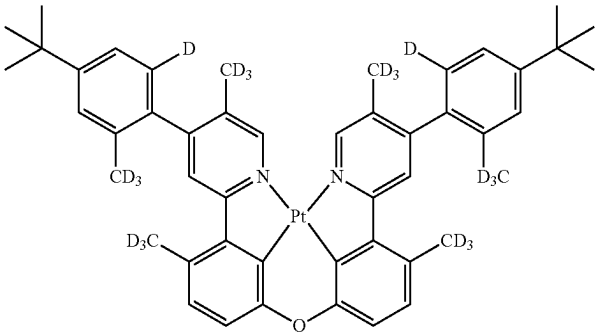

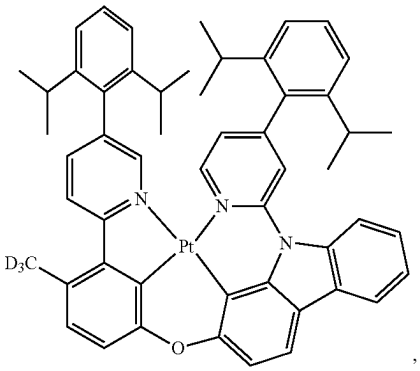

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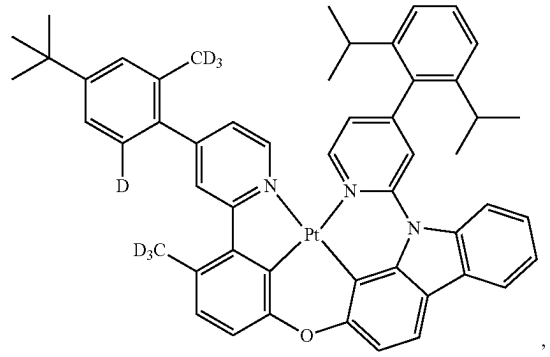
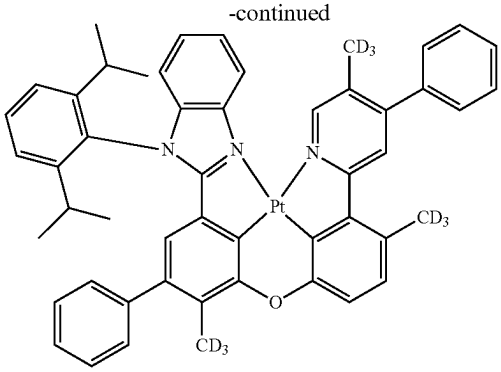
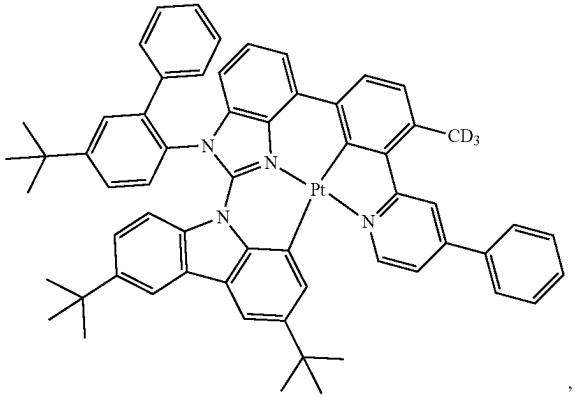
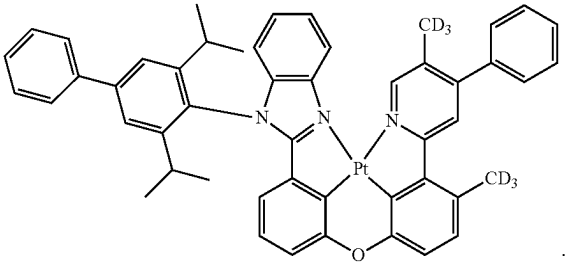








17. An organic light emitting device (OLED) comprising:

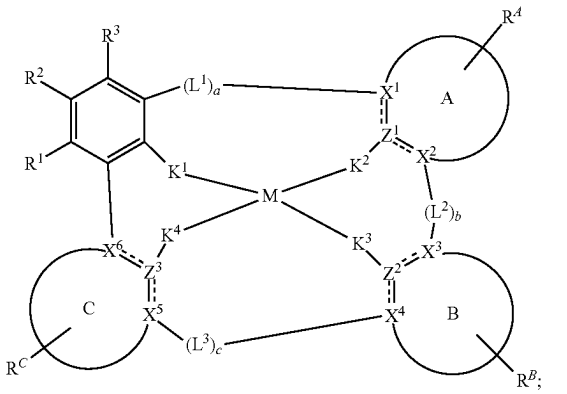
an anode;

a cathode; and

an organic layer disposed between the anode and the cathode,

wherein the organic layer comprises a compound comprising a structure of Formula I:

Formula I



wherein moieties A, B, and C are each independently a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered to 10-membered carbocyclic or heterocyclic ring;

wherein each L^1, L^2, and L^3 is independently selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR';

wherein Z^1, Z^2, and Z^3 are each independently C or N;

wherein M is Pt or Pd;

wherein X^1-X^6 are each independently C or N;

wherein each a, b, and c is independently 0 or 1;

wherein a+b+c=2 or 3;

wherein each of K^1, K^2, K^3, and K^4 is independently selected from the group consisting of single bond, O, S, $N(R^\alpha)$, $P(R^\alpha)$, $B(R^\alpha)$, $C(R^\alpha)(R^\beta)$, and $Si(R^\alpha)(R^\beta)$;

wherein R^A, R^B, and R^C each independently represent mono to the maximum allowable substitution, or no substitution;

wherein each R, R', R^α, R^β, R^2, R^3, R^A, R^B, and R^C is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof,

wherein R^1 is selected from the group consisting of halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof,

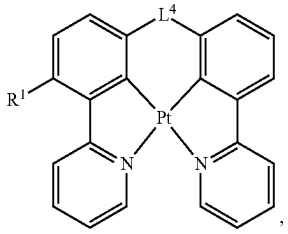
wherein any two substituents may be joined or fused to form a ring;

with the proviso that if R^1 is tert-butyl, R^3 is not tert-butyl;

with the proviso that R^1 and R^2 do not join to form a ring;

with the proviso that R^1 and R^C do not join to form a ring; and

with the proviso that the compound does not comprise:



wherein L^4 is selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

18. The OLED of claim **17**, wherein the organic layer further comprises a host, wherein the host comprises at least one chemical moiety selected from the group consisting of triphenylene, carbazole, indolocarbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, $5\lambda^2$-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene, azaborinine, oxaborinine, dihydroacridine, xanthene, dihydrobenzoazasiline, dibenzooxasiline, phenoxazine, phenoxathiine, phenothiazine, dihydrophenazine, fluorene, naphthalene, anthracene, phenanthrene, phenanthroline, benzoquinoline, quinoline, isoquinoline, quinazoline, pyrimidine, pyrazine, pyridine, triazine, boryl, silyl, aza-triphenylene, aza-carbazole, aza-indolocarbazole, aza-dibenzothiophene, aza-dibenzofuran, aza-dibenzoselenophene, aza-$5\lambda^2$-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, and aza-(5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene).

19. The OLED of claim **18**, wherein the host is selected from the group consisting of HOST GROUP 1 as defined herein.

20. A consumer product comprising an organic light-emitting device (OLED) comprising:

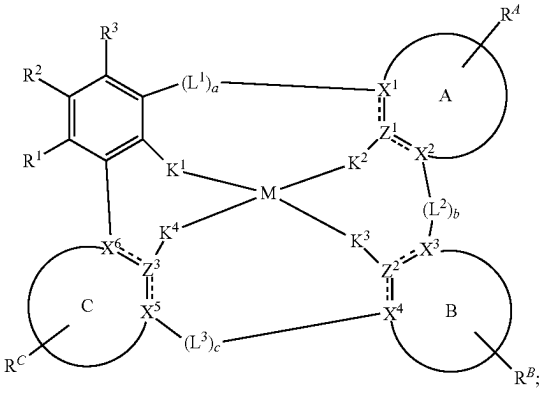
an anode;

a cathode; and

an organic layer disposed between the anode and the cathode,

wherein the organic layer comprises a compound comprising a structure of Formula I:

Formula I



wherein moieties A, B, and C are each independently a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered to 10-membered carbocyclic or heterocyclic ring;

wherein each L^1, L^2, and L^3 is independently selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR';

wherein Z^1, Z^2, and Z^3 are each independently C or N;

wherein M is Pt or Pd;

wherein X^1-X^6 are each independently C or N;

wherein each a, b, and c is independently 0 or 1;

wherein a+b+c=2 or 3;

wherein each of K^1, K^2, K^3, and K^4 is independently selected from the group consisting of single bond, O, S, $N(R^{\alpha})$, $P(R^{\alpha})$, $B(R^{\alpha})$, $C(R^{\alpha})(R^{\beta})$, and $Si(R^{\alpha})(R^{\beta})$;

wherein R^A, R^B, and R^C each independently represent mono to the maximum allowable substitution, or no substitution;

wherein each R, R', R^{α}, R^{β}, R^2, R^3, R^A, R^B, and R^C is independently hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof,

wherein R^1 is selected from the group consisting of halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof,

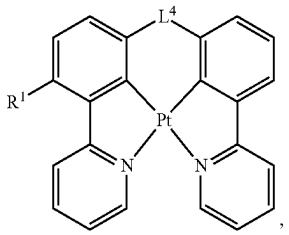
wherein any two substituents may be joined or fused to form a ring;

with the proviso that if R^1 is tert-butyl, R^3 is not tert-butyl;

with the proviso that R^1 and R^2 do not join to form a ring;

with the proviso that R^1 and R^C do not join to form a ring; and

with the proviso that the compound does not comprise:



,

wherein L^4 is selected from the group consisting of a direct bond, O, S, Se, NR, BR, BRR', PR, CR, C═O, C═NR, C═CRR', C═S, CRR', SO, SO_2, P(O)R, SiRR', and GeRR'.

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