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ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

Abstract

A compound having a first ligand L.sub.A comprising a structure of Formula I,

##STR00001##

is provided. In Formula I, moiety A is a monocyclic ring or a polycyclic fused ring system; each of X.sup.1 to X.sup.12 and Z.sup.1 is C or N; Z is B or N; each of Y.sup.1, Y.sup.2, and Y.sup.3 is absent or a linker, each of K.sup.1 and K.sup.2 is a direct bond or a linker, each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is hydrogen or a General Substituent defined herein; and L.sub.A is coordinated to a metal M. Formulations, OLEDs, and consumer products containing the compound are also provided.

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Background/Summary

CROSS-REFERENCE TO RELATED APPLICATIONS [0001] This application claims priority under 35 U.S.C. § 119(e) to U.S. Provisional Applications No. 63/632,362, filed on Apr. 10, 2024, No. 63/619,914, filed on Jan. 11, 2024, No. 63/619,527, filed on Jan. 10, 2024, No. 63/618,688, filed on Jan. 8, 2024, No. 63/614,848, filed on Dec. 26, 2023, and No. 63/609,996, filed on Dec. 14, 2023, 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. 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.

[0004] OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting.

[0005] One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as “saturated” colors. In particular, these standards call for saturated red, green, and blue pixels. Alternatively, the OLED can be designed to emit white light. In conventional liquid crystal display s 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

[0006] In one aspect, the present disclosure provides a compound having a first ligand L.sub.A comprising a structure of Formula I:

##STR00002##

In Formula I:

[0007] moiety A is a monocyclic ring or a polycyclic fused ring system, wherein the monocyclic ring or each ring of the polycyclic [0008] fused ring system is independently a 5-membered to 10-membered carbocyclic or heterocyclic ring; [0009] each of X.sup.1 to X.sup.12 and Z.sup.1 is independently C or N; [0010] Z is B or N; [0011] each of Y.sup.1, Y.sup.2, and Y.sup.3, if present, is independently selected from the group consisting of O, S, C=O, C=S, C=NR, CRR', and C=CRR', with at least one of them being present; [0012] each of K.sup.1 and K.sup.2 is independently selected from the group consisting of a direct bond, O, S, N(R.sup.α), P(R.sup.α), B(R.sup.α), C(R.sup.α)(R.sup.β), and Si(R.sup.α)(R.sup.β); [0013] each R.sup.A, R.sup.B, R.sup.C, and R.sup.D independently represents mono to the maximum allowable substitution, or no substitution; [0014] each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently a 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, selenyl, and combinations thereof; [0015] L.sub.A is coordinated to a metal M, having an atomic mass of at least 40; [0016] metal M can be coordinated to other ligands; [0017] any two substituents may be joined or fused to form a ring; and [0018] L.sub.A can join with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand.

[0019] In another aspect, the present disclosure provides a formulation comprising a compound having a first ligand L.sub.A comprising a structure of Formula I as described herein.

[0020] In yet another aspect, the present disclosure provides an OLED having an organic layer comprising a compound having a first ligand L.sub.A comprising a structure of Formula I as described herein.

[0021] In yet another aspect, the present disclosure provides a consumer product comprising an OLED with an organic layer comprising a compound having a first ligand L.sub.A comprising a structure of Formula I as described herein.

Description

BRIEF DESCRIPTION OF THE DRAWINGS

[0022] FIG. 1 shows an organic light emitting device.

[0023] FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

DETAILED DESCRIPTION

A. Terminology

[0024] Unless otherwise specified, the below terms used herein are defined as follows:

[0025] 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.

[0026] 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.

[0027] As used herein, and as would be generally understood by one skilled in the art, a first

“Highest Occupied Molecular Orbital” (HOMO) or “Lowest Unoccupied Molecular Orbital” (LUMO) energy level is “greater than” or “higher than” a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level of the same material. A “higher” HOMO or LUMO energy level appears closer to the top of such a diagram than a “lower” HOMO or LUMO energy level.

[0028] 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.

[0029] 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.

[0030] 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.

[0031] 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.

[0032] 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.

[0033] 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. 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:

TABLE-US-00001 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]

[0034] The terms “halo,” “halogen,” and “halide” are used interchangeably and refer to fluorine, chlorine, bromine, and iodine.

[0035] The term “acyl” refers to a substituted carbonyl group (—C(O)—R.sub.s).

[0036] The term “ester” refers to a substituted oxycarbonyl (—O—C(O)—R.sub.s or —C(O)—O—R.sub.s) group.

[0037] The term “ether” refers to an —OR.sub.s group.

[0038] The terms “sulfanyl” or “thio-ether” are used interchangeably and refer to a —SR.sub.s group.

[0039] The term “selenyl” refers to a —SeR.sub.s group.

[0040] The term “sulfinyl” refers to a —S(O)—R.sub.s group.

[0041] The term “sulfonyl” refers to a —SO.sub.2—R.sub.s group.

[0042] 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.sub.s).sub.2 group or a $\text{—PO(R.sub.s).sub.2}$ group, wherein each R.sub.s can be same or different.

[0043] 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 $\text{—Si(R.sub.s).sub.3}$ group, wherein each R.sub.s can be same or different.

[0044] The term “germyl” refers to a group containing at least one germanium atom bonded to the relevant structure. Common examples of germlyl groups include, but are not limited to, groups such as a $\text{—Ge(R.sub.s).sub.3}$ group, wherein each R.sub.s can be same or different.

[0045] 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.sub.s).sub.2 group or its Lewis adduct —B(R.sub.s).sub.3 group, wherein R.sub.s can be same or different.

[0046] In each of the above, R.sub.s can be hydrogen or a substituent selected from the group consisting of the General Substituents as defined in this application. Preferred R.sub.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.sub.s is selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combination thereof.

[0047] 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, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, and the like. Additionally, the alkyl group can be further substituted.

[0048] 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.

[0049] 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.

[0050] 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.

[0051] 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.

[0052] 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.

[0053] 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.

[0054] 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.

[0055] 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, indolocarbazoles, 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, benzofuropyrindine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, selenophenodipyridine, azaborine, borazine, 5 λ .sup.2, 9 λ .sup.2-diaza-13b-boranaphtho[2,3,4-de]anthracene, 5 λ .sup.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 λ .sup.2,9 λ .sup.2-diaza-13b-boranaphtho[2,3,4-de]anthracene, 5 λ .sup.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.

[0056] Of the aryl and heteroaryl groups listed above, the groups of triphenylene, naphthalene, anthracene, dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazoles, imidazole, pyridine, pyrazine, pyrimidine, triazine, benzimidazole, 5 λ .sup.2,9 λ .sup.2-diaza-13b-boranaphtho[2,3,4-de]anthracene, 5 λ .sup.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.

[0057] 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.

[0058] 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.

[0059] 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.

[0060] 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.

[0061] In yet other instances, the Most Preferred General Substituents are selected from the group consisting of deuterium, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.


[0062] 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^{sup.1} represents mono-substitution, then one R^{sup.1} must be other than H (i.e., a substitution). Similarly, when R^{sup.1} represents di-substitution, then two of R^{sup.1} must be other than H. Similarly, when R^{sup.1} represents zero or no substitution, R^{sup.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.

[0063] As used herein, “combinations thereof” indicates that one or more members of the applicable list are combined to form a known or chemically stable arrangement that one of ordinary skill in the art can envision from the applicable list. For example, an alkyl and deuterium can be combined to form a partial or fully deuterated alkyl group; a halogen and alkyl can be combined to form a halogenated alkyl substituent; and a halogen, alkyl, and aryl can be combined to form a halogenated arylalkyl. In one instance, the term substitution includes a combination of two to four of the listed groups. In another instance, the term substitution includes a combination of two to three groups. In yet another instance, the term substitution includes a combination of two groups. Preferred combinations of substituent groups are those that contain up to fifty atoms that are not hydrogen or deuterium, or those which include up to forty atoms that are not hydrogen or deuterium, or those that include up to thirty atoms that are not hydrogen or deuterium. In many instances, a preferred combination of substituent groups will include up to twenty atoms that are not hydrogen or deuterium.

[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[f,h]quinoxaline and dibenzo[f,h]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein.

[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. IS 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  custom-character implies to include C.sub.6H.sub.6, C.sub.6D.sub.6, C.sub.6H.sub.3D.sub.3, and any other partially deuterated variants thereof. Some common basic partially or fully deuterated groups include, without limitation, CD.sub.3, CD.sub.2C(CH.sub.3).sub.3, C(CD.sub.3).sub.3, and C.sub.6D.sub.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 having a first ligand L.sub.A comprising a structure of Formula I:

##STR00003##

In Formula I:

[0070] 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 to 10-membered carbocyclic or heterocyclic ring; [0071] each of X.sup.1 to X.sup.12 and Z.sup.1 is independently C or N; [0072] Z is B or N; [0073] each of Y.sup.1, Y.sup.2, and Y.sup.3, if present, is independently selected from the group consisting of O, S, C=O, C=S, C=NR, CRR', and C=CRR', with at least one of them being present; [0074] each of K.sup.1 and K.sup.2 is independently selected from the group consisting of a direct bond, O, S, N(R.sup.α), P(R.sup.α), B(R.sup.α), C(R.sup.α)(R.sup.β), and Si(R.sup.α)(R.sup.β); [0075] each R.sup.A, R.sup.B, R.sup.C, and R.sup.D independently represents mono to the maximum allowable substitution, or no substitution; [0076] each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently a hydrogen, or a substituent selected from the group consisting of the General Substituents defined herein; [0077] L.sub.A is coordinated to a metal M, having an atomic mass of at least 40; [0078] metal M can be coordinated to other ligands; [0079] any two substituents may be joined or fused to form a ring; and [0080] L.sub.A can join with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand.

[0081] In some embodiments, if M is Ir, Y.sup.2 is present, and Y.sup.3 is absent, then moiety A is joined to X.sup.1 or X.sup.3, and K.sup.2 is joined to X.sup.2.

[0082] In some embodiments, if M is Pt, then Z.sup.1 is not a carbene carbon.

[0083] In some embodiments, the first ligand L.sub.A has a structure of Formula I. In some embodiments, the first ligand L.sub.A consists essentially of a structure of Formula I.

[0084] In some embodiments of Formula I, at least one R, R', R.sup.A, R.sup.B, R.sup.C, and R.sup.D is partially or fully deuterated. In some embodiments, at least one R.sup.A is partially or fully deuterated. In some embodiments, at least one R.sup.B is partially or fully deuterated. In some embodiments, at least one R.sup.C is partially or fully deuterated. In some embodiments, at least one R.sup.D is partially or fully deuterated. In some embodiments, at least one R or R' is partially or fully deuterated. In some embodiments, at least one R.sup.α or R.sup.β is partially or fully deuterated.

[0085] In some embodiments, if Z is B, then each Y.sup.1, Y.sup.2, and Y.sup.3, if present, is independently O or S. In some embodiments, Z is B and each Y.sup.1, Y.sup.2, and Y.sup.3, if present, is independently O or S.

[0086] In some embodiments, if Y.sup.1, Y.sup.2, and Y.sup.3 are O, then moiety A is not pyridine or pyrimidine. In some embodiments Y.sup.1, Y.sup.2, and Y.sup.3 are O, and moiety A is not pyridine or pyrimidine.

[0087] In some embodiments, at least one of Y.sup.1 or Y.sup.2 is present. In some embodiments, Y.sup.3 is present and at least one of Y.sup.1 or Y.sup.2 is present. In some embodiments, both Y.sup.1 and Y.sup.3 are present, and Y.sup.2 is absent. In some embodiments, both Y.sup.2 and Y.sup.3 are present, and Y.sup.1 is absent. In some embodiments, both Y.sup.1 and Y.sup.2 are present, and Y.sup.3 is absent. In some embodiments, each of Y.sup.1, Y.sup.2, and Y.sup.3 is present.

[0088] In some embodiments, two R.sup.D do not join or fuse to form a ring.

[0089] In some embodiments, both Y.sup.1 and Y.sup.2 are present. In some embodiments, both Y.sup.1 and Y.sup.2 are present and Y.sup.3 is absent. In some embodiments, both Y.sup.1 and Y.sup.2 are present and Y.sup.3 is also present. In some embodiments, at least one R.sup.B and at least one R.sup.C is not hydrogen. In some embodiments, at least one R.sup.B and at least one R.sup.C is selected from the group consisting of the General Substituents defined herein.

[0090] In some embodiments, when Z.sup.1 is N, Z is N, and each of X.sup.1, X.sup.2, and X.sup.3 is independently C, then Y.sup.1 is absent if moiety A is attached to the carbon of X.sup.3. In some embodiments, when Z.sup.1 is N, Z is N, and each of X.sup.1, X.sup.2, and X.sup.3 is independently C, then Y.sup.2 is absent if moiety A is attached to the carbon of X.sup.1. In some embodiments, when Z.sup.1 is N, Z is N, and each of X.sup.1, X.sup.2, and X.sup.3 is independently C, both Y.sup.1 and Y.sup.2 are present. In some embodiments, when Z.sup.1 is N, Z is N, and each of X.sup.1, X.sup.2, and X.sup.3 is independently C, at least one R.sup.B and at least one R.sup.C is not hydrogen. In some embodiments, when Z.sup.1 is N, Z is N, and each of X.sup.1, X.sup.2, and X.sup.3 is independently C, at least one R.sup.B and at least one R.sup.C is not hydrogen, at least one R.sup.B and at least one R.sup.C is selected from the group consisting of the General Substituents defined herein. In some such embodiments, moiety A is pyridine. In some such embodiments, moiety A is imidazole. In some such embodiments, moiety A is benzimidazole.

[0091] In some embodiments when Z.sup.1 is C and Z is N, then X.sup.2 is not N. In some embodiments when Z.sup.1 is C, Z is N and X is N, then both Y.sup.1 and Y.sup.2 are present. In some embodiments, when Z.sup.1 is C, Z is N and X is N, then Y.sup.1 is absent if moiety A is attached to X.sup.3 which is carbon. In some embodiments, when Z.sup.1 is C, Z is N and X.sup.2 is N, then Y.sup.2 is absent if moiety A is attached to X.sup.1 which is carbon. In some embodiments, when Z.sup.1 is C, Z is N and X.sup.2 is N, then both Y.sup.1 and Y.sup.2 are present. In some embodiments when Z.sup.1 is C, Z is N and X.sup.2 is N, at least one R.sup.B and at least one R.sup.C is not hydrogen. In some embodiments when Z.sup.1 is C, Z is N and X.sup.2 is N, at least one R.sup.B and at least one R.sup.C is selected from the group consisting of the General Substituents defined herein.

[0092] In some embodiments, moiety A is attached to X.sup.3 which is carbon. In some embodiments when moiety A is attached to X.sup.1 which is carbon and X.sup.2 is N; then Y.sup.1 is present and Y.sup.2 is absent. In some embodiments when moiety A is attached to X.sup.3 which is carbon and X.sup.2 is N; then Y.sup.2 is present and Y.sup.1 is absent. In some embodiments when X.sup.2 is N, both Y.sup.1 and Y.sup.2 are present. In some embodiments when X.sup.2 is N, moiety A is not benzene or naphthalene.

[0093] In some embodiments, each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently hydrogen or a substituent selected from the group consisting of the Preferred General Substituents defined herein. In some embodiments, each R, R', R.sup.α, R.sub.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently hydrogen or a substituent selected from the group consisting of the More Preferred General Substituents defined herein. In some embodiments, each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently hydrogen or a substituent selected from the group consisting of the Most Preferred General Substituents defined herein.

[0094] In some embodiments, at least one R.sup.A, R.sup.B, R.sup.C, or R.sup.D is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.A is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.B is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.C is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.D is a substituent selected from the group consisting of the General Substituents defined herein.

[0095] In some embodiments, metal M is selected from the group consisting of Ir, Rh, Re, Ru, Os,

Pt, Pd, Ag, Au, and Cu. In some embodiments, metal M is Ir. In some embodiments, metal M is Pt or Pd. In some embodiments, metal M is Pt. In some embodiments, metal M is Pd.

[0096] 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.

[0097] In some embodiments, moiety A is independently selected from the group consisting of the following Cyclic Moiety 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, benzimidazole derived carbene, aza-benzimidazole derived carbene, 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, 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.

[0098] 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.

[0099] In some embodiments, moiety A is benzene, pyridine, oxazole, thiazole, or imidazole. In some embodiments, moiety A is benzene. In some embodiments, moiety A is pyridine. In some embodiments, moiety A is oxazole. In some embodiments, moiety A is thiazole. In some embodiments, moiety A is imidazole.

[0100] 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, aza-benzimidazole, benzobenzimidazole, aza-benzobenzimidazole, benzimidazole derived carbene, aza-benzimidazole derived carbene, 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 A is benzimidazole, benzimidazole derived carbene, benzoxazole, or benzothiazole. In some embodiments, moiety A is benzimidazole. In some embodiments, moiety A is benzimidazole-derived carbene. In some embodiments, moiety A is benzoxazole. In some embodiments, moiety A is benzothiazole.

[0101] 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 metal M 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).

[0102] 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 metal M, 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.

[0103] 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 metal M, 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.

[0104] 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 can contain 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 metal M atom. In some such embodiments, the ring having aza N atom is separated by at least three other rings from the metal M atom. In some such embodiments, each of the ortho positions of the aza N atom is substituted.

[0105] In some embodiments, Z^{sup.1} is N or carbene C. In some embodiments, Z^{sup.1} is N. In some embodiments, Z^{sup.1} is carbene C. In some embodiments, Z^{sup.1} is C, but not a carbene C.

[0106] In some embodiments, Z^{sup.1} is C.

[0107] In some embodiments, each of X^{sup.1} to X^{sup.12} is C.

[0108] In some embodiments, each of X^{sup.1} to X^{sup.3} is C. In some embodiments, at least one of X^{sup.1} to X^{sup.3} is N.

[0109] In some embodiments, the one of X^{sup.1} to X^{sup.3} coordinated to M is N. In some embodiments, the one of X^{sup.1} to X^{sup.3} coordinated to M is C.

[0110] In some embodiments, each of X^{sup.4} to X^{sup.7} is C. In some embodiments, at least one of X^{sup.4} to X^{sup.7} is N. In some embodiments, exactly one of X^{sup.4} to X^{sup.7} is N. In some embodiments, X^{sup.4} is N. In some embodiments, X^{sup.5} is N. In some embodiments, X^{sup.6} is N. In some embodiments, X^{sup.7} is N.

[0111] In some embodiments, each of X^{sup.8} to X^{sup.12} is C. In some embodiments, at least one of X^{sup.8} to X^{sup.12} is N. In some embodiments, exactly one of X^{sup.8} to X^{sup.12} is N. In some embodiments, X^{sup.8} is N. In some embodiments, X^{sup.9} is N. In some embodiments, X^{sup.10} is N. In some embodiments, X^{sup.11} is N. In some embodiments, X^{sup.12} is N.

[0112] In some embodiments, the one of X^{sup.1} to X^{sup.3} bonded to moiety A is C. In some embodiments, X^{sup.1} is bonded to moiety A. In some embodiments, X^{sup.2} is bonded to moiety A. In some embodiments, X^{sup.3} is bonded to moiety A.

[0113] In some embodiments, the one of X^{sup.1} to X^{sup.3} bonded to moiety A is N. In some embodiments, the one of X^{sup.1} to X^{sup.3} connected to K^{sup.2} is C. In some embodiments, the one of X^{sup.1} to X^{sup.3} connected to K^{sup.2} is N.

[0114] In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} is present.

[0115] In some embodiments, exactly two of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} are present. In some embodiments, Y^{sup.1} and Y^{sup.2} are present, and Y^{sup.3} is absent. In some embodiments, Y^{sup.1} and Y^{sup.3} are present, and Y^{sup.2} is absent. In some embodiments, Y^{sup.1} is present, and Y^{sup.2} and Y^{sup.3} are absent.

[0116] In some embodiments, Z is B. In some embodiments, Z is N.

[0117] In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is independently O or S. In some embodiments, at least two of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} are O. In some embodiments, at least two of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} are S. In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} is O. In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} is S.

[0118] In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is O. In some embodiments, each one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} that is present is O.

[0119] In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is S. In some embodiments, each one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} that is present is S.

[0120] In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is C=O, C=S, C=NR, CRR', and C=CRR'. In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is C=O. In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is C=CRR'. In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is CRR'.

[0121] In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is independently selected from the group consisting of C=O, C=S, C=NR, CRR', and C=CRR'. In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is C=O. In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is CRR'. In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is C=CRR'.

[0122] In some embodiments, at least one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} is present and is different than another one of Y^{sup.1}, Y^{sup.2}, or Y^{sup.3} that is present. In some embodiments, each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is the same.

[0123] In some embodiments, K^{sup.1} is a direct bond.

[0124] In some embodiments, K^{sup.1} is O or S. In some embodiments, K^{sup.1} is O. In some embodiments, K^{sup.1} is S. In some embodiments, K^{sup.1} is N(R^{sup.α}), P(R^{sup.α}), or B(R^{sup.α}). In some embodiments, K^{sup.1} is C(R^{sup.α})(R^{sup.β}) or Si(R^{sup.α})(R^{sup.β}).

[0125] In some embodiments, K^{sup.2} is a direct bond.

[0126] In some embodiments, K^{sup.2} is O or S. In some embodiments, K^{sup.2} is O. In some embodiments, K^{sup.2} is S. In some embodiments, K^{sup.2} is N(R^{sup.α}), P(R^{sup.α}), or B(R^{sup.α}). In some embodiments, K^{sup.2} is C(R^{sup.α})(R^{sup.β}) or Si(R^{sup.α})(R^{sup.β}).

[0127] In some embodiments, each of K^{sup.1} and K^{sup.2} is a direct bond.

[0128] In some embodiments, K^{sup.1} is a direct bond, and K^{sup.2} is not a direct bond.

[0129] In some embodiments, K^{sup.2} is a direct bond, and K^{sup.1} is not a direct bond.

[0130] 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.

[0131] In some embodiments, Formula I comprises an electron-withdrawing group selected from the group consisting of the following EWG1 LIST: F, CF₃, CN, COCH₃, CHO, COCF₃, COOMe, COOCF₃, NO₂, SF₃, SiF₃, PF₃, SF₅, OCF₃, SCF₃, SeCF₃, SOCF₃, SeOCF₃, SO₂F, SO₂CF₃, SeO₂CF₃, OSeO₂CF₃, OCN, SCN, SeCN, NC, ⁺N(R^{k2}), ₂(R^{k2}), ₂CCN, (R^{k2}), ₂CCF₃, CNC(CF₃), ₂, BR₃R₂, 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,

##STR00004## ##STR00005## [0132] wherein each R.sup.k1 represents mono to the maximum allowable substitution, or no substitutions; [0133] wherein Y.sup.G is selected from the group consisting of BR.sub.e, NR.sub.e, PR.sub.e, O, S, Se, C=O, S=O, SO.sub.2, CR.sub.eR.sub.f, SiR.sub.eR.sub.f, and GeR.sub.eR.sub.f; and [0134] wherein each of R.sup.k1, R.sup.k2, R.sup.k3, R.sub.e, and R.sub.f is independently a hydrogen or a substituent selected from the group consisting of the General Substituents defined herein.

[0135] In some embodiments, Formula I comprises an electron-withdrawing group selected from the group consisting of the structures of the following EWG2 List:

##STR00006## ##STR00007## ##STR00008## ##STR00009## ##STR00010## ##STR00011## ##STR00012## ##STR00013## ##STR00014## ##STR00015## ##STR00016## ##STR00017##

[0136] In some embodiments, Formula I comprises an electron-withdrawing group selected from the group consisting of the structures of the following EWG3 LIST:

##STR00018## ##STR00019## ##STR00020## ##STR00021## ##STR00022## ##STR00023## ##STR00024##

[0137] In some embodiments, Formula I comprises an electron-withdrawing group selected from the group consisting of the structures of the following EWG4 LIST:

##STR00025## ##STR00026## ##STR00027##

[0138] In some embodiments, Formula I comprises an electron-withdrawing group that is a π -electron deficient electron-withdrawing group. In some embodiments, the π -electron deficient electron-withdrawing group is selected from the group consisting of the structures of the following Pi-EWG LIST: CN, COCH.sub.3, CHO, COCF.sub.3, COOMe, COOCF.sub.3, NO.sub.2, SF.sub.3, SiF.sub.3, PF.sub.4, SF.sub.5, OCF.sub.3, SCF.sub.3, SeCF.sub.3, SOCF.sub.3, SeOCF.sub.3, SO.sub.2F, SO.sub.2CF.sub.3, SeO.sub.2CF.sub.3, OSeO.sub.2CF.sub.3, OCN, SCN, SeCN, NC, .sup.+N(R.sup.k2).sub.3, BR.sup.k2R.sup.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 heteroaryl, isocyanate,

##STR00028## ##STR00029##

wherein the variables are the same as previously defined.

[0139] 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.

[0140] In some embodiments, at least one R.sup.A is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sup.A is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some

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

[0141] In some embodiments, at least one R.sup.B is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sup.B is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sup.B is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sup.B is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R.sup.B is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0142] In some embodiments, at least one R.sup.C is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sup.C is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sup.C is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sup.C is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R.sup.C is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0143] In some embodiments, at least one R.sup.D is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sup.D is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sup.D is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sup.D is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R.sup.D is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0144] In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0145] In some embodiments, at least one R.sup.A is not hydrogen. In some embodiments, at least one R.sup.A comprises at least one C atom. In some embodiments, at least one R.sup.A comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0146] In some embodiments, at least one R.sup.A is not hydrogen. In some embodiments, at least one R.sup.B comprises at least one C atom. In some embodiments, at least one R.sup.B comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0147] In some embodiments, two R.sup.B are joined or fused to form moiety B1, wherein moiety B1 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 to 10-membered carbocyclic or heterocyclic ring. In some embodiments, moiety B1 is selected from the group consisting of the Cyclic Moiety LIST defined herein. In some embodiments, moiety B1 is benzene.

[0148] In some embodiments, at least one R.sup.C is not hydrogen. In some embodiments, at least one R.sup.C comprises at least one C atom. In some embodiments, at least one R.sup.C comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0149] In some embodiments, two R.sup.C are joined or fused to form moiety C1, wherein moiety

C1 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 to 10-membered carbocyclic or heterocyclic ring. In some embodiments, moiety C1 is selected from the group consisting of the Cyclic Moiety LIST defined herein. In some embodiments, moiety C1 is benzene. [0150] In some embodiments, at least one R.sup.D is not hydrogen. In some embodiments, at least one R.sup.D comprises at least one C atom. In some embodiments, at least one R.sup.D comprises at least one heteroatom. In some embodiments, R.sup.D is O and is bonded to another ligand. In some embodiments, at least one R.sup.D comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0151] In some embodiments, M is Ir, Y.sup.2 is present and Y is absent.

[0152] In some embodiments, the ligand L.sub.A is selected from the group consisting of the structures of the following LIST 1:

##STR00030## ##STR00031## ##STR00032## ##STR00033## ##STR00034## ##STR00035##
##STR00036## ##STR00037## ##STR00038## ##STR00039##

wherein: [0153] X.sub.15 to X.sub.29 are each independently C or N; [0154] each of Y.sub.4, Y.sub.5, and Y.sub.6 is independently absent or selected from the group consisting of O, S, C=O, C=S, C=NR, CRR', and C=CRR'; [0155] K1 and K.sup.2 are each independently selected from the group consisting of a direct bond, O, S, N(R.sup.α), P(R.sup.α), B(R.sup.α), C(R.sup.α)(R.sup.β), and Si(R.sup.α)(R.sup.β); [0156] each R.sup.AA, R.sup.BB, R.sup.CC, and R.sup.DD independently represent mono to the maximum allowable substitution, or no substitution; [0157] each R, R', R'', R.sup.AA, R.sup.BB, R.sup.CC, and R.sup.DD is independently a hydrogen, or a substituent selected from the group consisting of the General Substituents defined herein; and [0158] any two substituents can be fused or joined to form a ring.

[0159] In some embodiments where ligand L.sub.A is selected from LIST 1, at least two of Y.sub.4, Y.sub.5, or Y.sub.6 are present. In some embodiments, exactly two of Y.sub.4, Y.sub.5, or Y.sub.6 are present. In some embodiments, all three of Y.sub.4, Y.sub.5, and Y.sub.6 are present.

[0160] In some embodiments where ligand L.sub.A is selected from LIST 1, each of X.sub.15 to X.sub.27 is C. In some embodiments, at least one of X.sub.15 to X.sub.27 is N. In some embodiments, exactly one of X.sub.15 to X.sub.27 is N. In some embodiments, at least two of X.sub.15 to X.sub.27 are N. In some embodiments, exactly two of X.sub.15 to X.sub.27 are N. In some embodiments, each of four of X.sub.15 to X.sub.27 contained in the same ring is independently C. In some embodiments, one of four of X.sub.15 to X.sub.27 contained in the same ring is N. In some embodiments, K.sup.1 is a direct bond. In some embodiments, K.sup.2 is a direct bond.

[0161] In some embodiments, exactly two of Y.sub.4, Y.sub.5, or Y.sub.6 are present. In some embodiments, all three of Y.sub.4, Y.sub.5, and Y.sub.6 are present.

[0162] In some embodiments. In some embodiments, the ligand L.sub.A is selected from the group consisting of the structures of the following LIST 1a:

##STR00040## ##STR00041## ##STR00042## ##STR00043## ##STR00044##

wherein Y.sub.4, Y.sub.5, or Y.sub.6 are all present, and all the remaining variables are the same as previously defined.

[0163] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one R.sup.AA, R.sup.BB, R.sup.CC, or R.sup.DD is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.AA is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.BB is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.CC is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.DD is a substituent selected from the group consisting of the General Substituents defined herein.

[0164] In some embodiments where ligand L.sub.A is selected from LIST 1, at least two R.sup.AA are each a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least two R.sup.BB are each a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least two R.sup.CC are each a substituent selected from the group consisting of the General Substituents defined herein.

[0165] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one of R, R', R'', R.sup.AA, R.sup.BB, R.sup.CC, or R.sup.DD is partially or fully deuterated. In some embodiments, R'' is partially or fully deuterated. In some embodiments, at least one R.sup.AA is partially or fully deuterated. In some embodiments, at least one R.sub.BB is partially or fully deuterated. In some embodiments, at least one R.sup.CC is partially or fully deuterated. In some embodiments, at least one R.sup.DD is partially or fully deuterated. In some embodiments, at least one R or R' is partially or fully deuterated.

[0166] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, R'' is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, R'' is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, R'' is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, R'' is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, R'' is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0167] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one R or R' is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R or R' is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0168] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one R.sup.AA is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sup.AA is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sup.AA is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sup.AA is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R.sup.AA is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0169] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one R.sub.BB is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sub.BB is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sub.BB is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sub.BB is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R.sub.BB is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0170] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one R.sup.CC is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sub.CC is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sub.CC is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sub.CC is or comprises an electron-withdrawing group from the EWG4 LIST as



















defined herein. In some embodiments, at least one R.sub.CC is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.



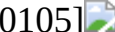


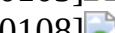


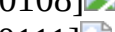


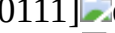


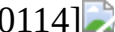


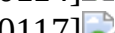


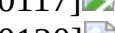


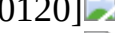


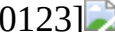


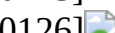


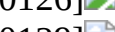


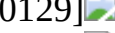


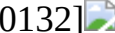


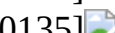


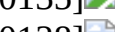


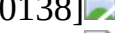


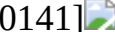





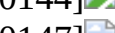


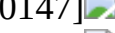





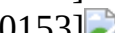


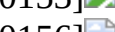


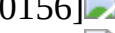





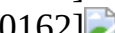


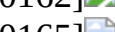


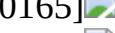




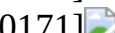
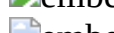

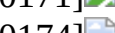







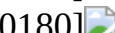




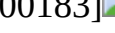
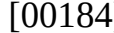


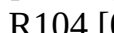
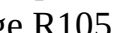
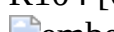
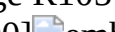
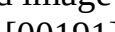


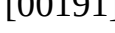
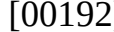

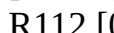
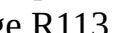

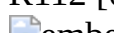
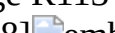
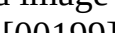
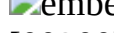

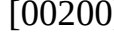


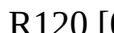


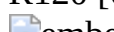
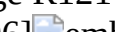
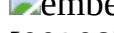

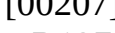
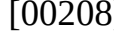


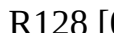

[0171] In some embodiments where ligand L.sub.A is selected from LIST 1 or LIST 1a, at least one R.sub.DD is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R.sub.DD is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, at least one R.sub.DD is or comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, at least one R.sub.DD is or comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, at least one R.sub.DD is or comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0172] In some embodiments, ligand L.sub.A is selected from the group of structures defined by the formula L.sub.Aw-(R_i)(R_j)(R_k)(R_l).sub.Q(Y_m)(Y_n)(Y_o).sub.V, wherein w is an integer from 1 to 38; Q is 1 when w is 1, 3, 4, 5, 6, 7, 10, 11, 12, 13, or 14, otherwise Q is 0, v is 1 when w is 5, 7, 9, 12, 17, 19, 21, 24, 28, 30, 37, or 38, otherwise v is 0; each of R_i, R_j, R_k, and R_l is independently selected from the group consisting of R1 to R468; and each of Y_m and Y_n is independently selected from the group consisting of Y1 to Y3; wherein each of L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A38-(R468)(R468)(R468)(Y3)(Y3)(Y3) is defined in the following LIST 2:

TABLE-US-00002 L.sub.A Structure of L.sub.A L.sub.A1- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A1- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A1- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00045]  L.sub.A2- (R_i)(R_j)(R_k)(Y_m)(Y_n), wherein L.sub.A2- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A2- (R468)(R468)(R468)(Y3)(Y3), have the structure [00046]  L.sub.A3- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A3- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A3- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00047]  L.sub.A4- Y_n), wherein L.sub.A4- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A4- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00048]  L.sub.A5- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n)(Y_o), wherein L.sub.A5- (R1)(R1)(R1)(R1)(Y1)(Y1)(Y1) to L.sub.A5- (R468)(R468)(R468)(R468)(Y3)(Y3)(Y3), have the structure [00049]  L.sub.A6- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A6- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A6- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00050]  L.sub.A7- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n)(Y_o), wherein L.sub.A7- (R1)(R1)(R1)(R1)(Y1)(Y1)(Y1) to L.sub.A7- (R468)(R468)(R468)(R468)(Y3)(Y3)(Y3), have the structure [00051]  L.sub.A8- (R_i)(R_j)(R_k)(Y_m)(Y_n), wherein L.sub.A8- (R1)(R1)(R1)(R1)(R1) to L.sub.A8- (R468)(R468)(R468)(Y3)(Y3), have the structure [00052]  L.sub.A9- (R_i)(R_j)(R_k)(Y_m)(Y_n), (Y_o), wherein L.sub.A9- (R1)(R1)(R1)(Y1)(Y1)(Y1) to L.sub.A9- (R468)(R468)(R468)(Y3)(Y3)(Y3), have the structure [00053]  L.sub.A10- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A10- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A10- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00054]  L.sub.A11- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A11- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A11- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00055]  L.sub.A12- (R_i)(R_f)(R_k)(R_l)(Y_m)(Y_n)(Y_o), wherein L.sub.A12- (R1)(R1)(R1)(R1)(Y1)(Y1)(Y1) to L.sub.A12- (R468)(R468)(R468)(R468)(Y3)(Y3)(Y3), have the structure [00056]  L.sub.A13- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A13- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A13- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00057]  L.sub.A14- (R_i)(R_j)(R_k)(R_l)(Y_m)(Y_n), wherein L.sub.A14- (R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A14- (R468)(R468)(R468)(R468)(Y3)(Y3), have the structure [00058]  L.sub.A15- (R_i)(R_j)(R_k)(Y_m)(Y_n), wherein L.sub.A15- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A15- (R468)(R468)(R468)(Y3)(Y3), have the structure [00059]  L.sub.A16- (R_i)(R_j)(R_k)(Y_m)(Y_n), wherein L.sub.A16- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A16- (R468)(R468)(R468)(Y3)(Y3), have the structure [00060]  L.sub.A17- (R_i)(R_j)(R_k)(Y_m)(Y_n)(Y_o), wherein L.sub.A17-








































(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A17- (R468)(R468)(Y3)(Y3)(Y3), have the structure [00061]  L.sub.A18- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A18- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A18- (R468)(R468)(R468) (Y3)(Y3), have the structure [00062]  L.sub.A19- (Ri)(Rj)(Rk)(Ym)(Yn) (Yo), wherein L.sub.A19- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A19- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00063]  L.sub.A20- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A20- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A20- (R468)(R468)(R468) (Y3)(Y3), have the structure [00064]  L.sub.A21- (Ri)(Rj)(Rk)(Ym)(Yn) (Yo), wherein L.sub.A21- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A21- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00065]  L.sub.A22- (Ri)(Rj)(Rk)(Ym)(Yn) wherein L.sub.A22- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A22- (R468)(R468)(R468) (Y3)(Y3), have the structure [00066]  L.sub.A23- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A23- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A23- (R468)(R468)(R468) (Y3)(Y3), have the structure [00067]  L.sub.A24- (Ri)(Rj)(Rk)(Ym)(Yn), (Yo), wherein L.sub.A24- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A24- (R468)(R468)(R468) (Y3)(Y3) (Y3), have the structure [00068]  L.sub.A25- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A25- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A25- (R468)(R468)(R468) (Y3)(Y3), have the structure [00069]  L.sub.A26- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A26- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A26- (R468)(R468)(R468) (Y3)(Y3), have the structure [00070]  L.sub.A27- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A27- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A27- (R468)(R468)(R468) (Y3)(Y3), have the structure [00071]  L.sub.A28- (Ri)(Rj)(Rk)(Ym)(Yn) (Yo), wherein L.sub.A28- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A28- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00072]  L.sub.A29- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A29- (R1)(R1)(R1)(Y1) (Y1) to L.sub.A29- (R468)(R468)(R468) (Y3)(Y3), have the structure [00073]  L.sub.A30- (Ri)(Rj)(Rk)(Ym)(Yn) (Yo), wherein L.sub.A30- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A30- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00074]  L.sub.A31- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A31- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A31- (R468)(R468)(R468) (Y3)(Y3), have the structure [00075]  L.sub.A32- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A32- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A32- (R468)(R468)(R468) (Y3)(Y3), have the structure [00076]  L.sub.A33- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A33- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A33- (R468)(R468)(R468) (Y3)(Y3), have the structure [00077]  L.sub.A34- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A34- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A34- (R468)(R468)(R468) (Y3)(Y3), have the structure [00078]  L.sub.A35- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A35- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A35- (R468)(R468)(R468) (Y3)(Y3), have the structure [00079]  L.sub.A36- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A36- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A36- (R468)(R468)(R468) (Y3)(Y3), have the structure [00080]  L.sub.A37- (Ri)(Rj)(Rk)(Ym)(Yn) (Yo), wherein L.sub.A37- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A37- (R468)(R468)(R468) (Y3)(Y3) (Y3), have the structure [00081]  L.sub.A38- (Ri)(Rj)(Rk)(Ym)(Yn) (Yo), wherein L.sub.A38- (R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A37- (R468)(R468)(R468) (Y3)(Y3) (Y3), have the structure [00082]   [0173] wherein Y1 is ##STR00083## and [0174] wherein R1 to R468 have the structures defined in the following LIST 3:

TABLE-US-00003 Structure Structure Structure R1 [00084]  R2 [00085]  R3 [00086]  R4 [00087]  R5 [00088]  R6 [00089]  R7 [00090]  R8 [00091]  R9 [00092]  R10 [00093]  R11 [00094]  R12 [00095]  R13 [00096]  R14 [00097]  R15 [00098]  R16 [00099]  R17 [00100]  R18 [00101]  R19 [00102]  R20 [00103]

 R21 [00104] R22 [00105] R23 [00106]
 R24 [00107] R25 [00108] R26 [00109]
 R27 [00110] R28 [00111] R29 [00112]
 R30 [00113] R31 [00114] R32 [00115]
 R33 [00116] R34 [00117] R35 [00118]
 R36 [00119] R37 [00120] R38 [00121]
 R39 [00122] R40 [00123] R41 [00124]
 R42 [00125] R43 [00126] R44 [00127]
 R45 [00128] R46 [00129] R47 [00130]
 R48 [00131] R49 [00132] R50 [00133]
 R51 [00134] R52 [00135] R53 [00136]
 R54 [00137] R55 [00138] R56 [00139]
 R57 [00140] R58 [00141] R59 [00142]
 R60 [00143] R61 [00144] R62 [00145]
 R63 [00146] R64 [00147] R65 [00148]
 R66 [00149] R67 [00150] R68 [00151]
 R69 [00152] R70 [00153] R71 [00154]
 R72 [00155] R73 [00156] R74 [00157]
 R75 [00158] R76 [00159] R77 [00160]
 R78 [00161] R79 [00162] R80 [00163]
 R81 [00164] R82 [00165] R83 [00166]
 R84 [00167] R85 [00168] R86 [00169]
 R87 [00170] R88 [00171] R89 [00172]
 R90 [00173] R91 [00174] R92 [00175]
 R93 [00176] R94 [00177] R95 [00178]
 R96 [00179] R97 [00180] R98 [00181]
 R99 [00182] R100 [00183] R101
[00184] R102 [00185] R103 [00186]
R104 [00187] R105 [00188] R106 [00189]
 R107 [00190] R108 [00191] R109
[00192] R110 [00193] R111 [00194]
R112 [00195] R113 [00196] R114 [00197]
 R115 [00198] R116 [00199] R117
[00200] R118 [00201] R119 [00202]
R120 [00203] R121 [00204] R122 [00205]
 R123 [00206] R124 [00207] R125
[00208] R126 [00209] R127 [00210]
R128 [00211] R129 [00212] R130 [00213]
 R131 [00214] R132 [00215] R133
[00216] R134 [00217] R135 [00218]
R136 [00219] R137 [00220] R138 [00221]
 R139 [00222] R140 [00223] R141
[00224] R142 [00225] R143 [00226]
R144 [00227] R145 [00228] R146 [00229]
 R147 [00230] R148 [00231] R149
[00232] R150 [00233] R151 [00234]
R152 [00235] R153 [00236] R154 [00237]
 R155 [00238] R156 [00239] R157
[00240] R158 [00241] R159 [00242]
R160 [00243] R161 [00244] R162 [00245]

 R163 [00246]  R164 [00247]  R165 [00248]  R166 [00249]  R167 [00250]  R168 [00251]  R169 [00252]  R170 [00253]  R171 [00254]  R172 [00255]  R173 [00256]  R174 [00257]  R175 [00258]  R176 [00259]  R177 [00260]  R178 [00261]  R179 [00262]  R180 [00263]  R181 [00264]  R182 [00265]  R183 [00266]  R184 [00267]  R185 [00268]  R186 [00269]  R187 [00270]  R188 [00271]  R189 [00272]  R190 [00273]  R191 [00274]  R192 [00275]  R193 [00276]  R194 [00277]  R195 [00278]  R196 [00279]  R197 [00280]  R198 [00281]  R199 [00282]  R200 [00283]  R201 [00284]  R202 [00285]  R203 [00286]  R204 [00287]  R205 [00288]  R206 [00289]  R207 [00290]  R208 [00291]  R209 [00292]  R210 [00293]  R211 [00294]  R212 [00295]  R213 [00296]  R214 [00297]  R215 [00298]  R216 [00299]  R217 [00300]  R218 [00301]  R219 [00302]  R220 [00303]  R221 [00304]  R222 [00305]  R223 [00306]  R224 [00307]  R225 [00308]  R226 [00309]  R227 [00310]  R228 [00311]  R229 [00312]  R230 [00313]  R231 [00314]  R232 [00315]  R233 [00316]  R234 [00317]  R235 [00318]  R236 [00319]  R237 [00320]  R238 [00321]  R239 [00322]  R240 [00323]  R241 [00324]  R242 [00325]  R243 [00326]  R244 [00327]  R245 [00328]  R246 [00329]  R247 [00330]  R248 [00331]  R249 [00332]  R250 [00333]  R251 [00334]  R252 [00335]  R253 [00336]  R254 [00337]  R255 [00338]  R256 [00339]  R257 [00340]  R258 [00341]  R259 [00342]  R260 [00343]  R261 [00344]  R262 [00345]  R263 [00346]  R264 [00347]  R265 [00348]  R266 [00349]  R267 [00350]  R268 [00351]  R269 [00352]  R270 [00353]  R271 [00354]  R272 [00355]

R296 [00379]  R297 [00380]  R298 [00381] 
 R299 [00382]  R300 [00383]  R301
[00384]  R302 [00385]  R303 [00386]  R304 [00387]  R305 [00388]  R306 [00389] 
 R307 [00390]  R308 [00391]  R309
[00392]  R310 [00393]  R311 [00394]  R312 [00395]  R313 [00396]  R314 [00397] 
 R315 [00398]  R316 [00399]  R317
[00400]  R318 [00401]  R319 [00402]  R320 [00403]  R321 [00404]  R322 [00405] 
 R323 [00406]  R324 [00407]  R325
[00408]  R326 [00409]  R327 [00410]  R328 [00411]  R329 [00412]  R330 [00413] 
 R331 [00414]  R332 [00415]  R333
[00416]  R334 [00417]  R335 [00418]  R336 [00419]  R337 [00420]  R338 [00421] 
 R339 [00422]  R340 [00423]  R341
[00424]  R342 [00425]  R343 [00426]  R344 [00427]  R345 [00428]  R346 [00429] 
 R347 [00430]  R348 [00431]  R349
[00432]  R350 [00433]  R351 [00434]  R352 [00435]  R353 [00436]  R354 [00437] 
 R355 [00438]  R356 [00439]  R357
[00440]  R358 [00441]  R359 [00442]  R360 [00443]  R361 [00444]  R362 [00445] 
 R363 [00446]  R364 [00447]  R365
[00448]  R366 [00449]  R367 [00450]  R368 [00451]  R369 [00452]  R370 [00453] 
 R371 [00454]  R372 [00455]  R373
[00456]  R374 [00457]  R375 [00458]  R376 [00459]  R377 [00460]  R378 [00461] 
 R379 [00462]  R380 [00463]  R381
[00464]  R382 [00465]  R383 [00466]  R384 [00467]  R385 [00468]  R386 [00469] 
 R387 [00470]  R388 [00471]  R389
[00472]  R390 [00473]  R391 [00474]  R392 [00475]  R393 [00476]  R394 [00477] 
 R395 [00478]  R396 [00479]  R397
[00480]  R398 [00481]  R399 [00482]  R400 [00483]  R401 [00484]  R402 [00485] 
 R403 [00486]  R404 [00487]  R405
[00488]  R406 [00489]  R407 [00490]  R408 [00491]  R409 [00492]  R410 [00493] 
 R411 [00494]  R412 [00495]  R413
[00496]  R414 [00497]  R415 [00498]  R416 [00499]  R417 [00500]  R418 [00501] 
 R419 [00502]  R420 [00503]  R421
[00504]  R422 [00505]  R423 [00506]  R424 [00507]  R425 [00508]  R426 [00509] 
 R427 [00510]  R428 [00511]  R429

[00512]  R430 [00513]  R431 [00514]  R432 [00515]  R433 [00516]  R434 [00517]  R435 [00518]  R436 [00519]  R437 [00520]  R438 [00521]  R439 [00522]  R440 [00523]  R441 [00524]  R442 [00525]  R443 [00526]  R444 [00527]  R445 [00528]  R446 [00529]  R447 [00530]  R448 [00531]  R449 [00532]  R450 [00533]  R451 [00534]  R452 [00535]  R453 [00536]  R454 [00537]  R455 [00538]  R456 [00539]  R457 [00540]  R458 [00541]  R459 [00542]  R460 [00543]  R461 [00544]  R462 [00545]  R463 [00546]  R464 [00547]  R465 [00548]  R466 [00549]  R467 [00550]  R468 [00551]  R469 [00552]

[0175] In some embodiments, the compound has a formula of

$M(L_{sub}A)_{sub.p}(L_{sub}B)_{sub.q}(L_{sub}C)_{sub.r}$ wherein $L_{sub}B$ and $L_{sub}C$ are each a bidentate ligand; and wherein p is 1, 2, or 3; q is 0, 1, or 2; r is 0, 1, or 2; and $p+q+r$ is the oxidation state of the metal M .

[0176] In some embodiments, the compound has a formula selected from the group consisting of $Ir(L_{sub}A)_{sub.3}$, $Ir(L_{sub}A)(L_{sub}B)_{sub.2}$, $Ir(L_{sub}A)_{sub.2}(L_{sub}B)$,

$Ir(L_{sub}A)_{sub.2}(L_{sub}C)$, and $Ir(L_{sub}A)(L_{sub}B)(L_{sub}C)$; and wherein $L_{sub}A$, $L_{sub}B$, and $L_{sub}C$ are different from each other.

[0177] In some embodiments, $L_{sub}B$ comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, $L_{sub}B$ comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, $L_{sub}B$ comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, $L_{sub}B$ comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, $L_{sub}B$ comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0178] In some embodiments, $L_{sub}C$ comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, $L_{sub}C$ comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some embodiments, $L_{sub}C$ comprises an electron-withdrawing group from the EWG3 LIST as defined herein. In some embodiments, $L_{sub}C$ comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, $L_{sub}C$ comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.

[0179] In some embodiments, $L_{sub}B$ is a substituted or unsubstituted phenylpyridine, and $L_{sub}C$ is a substituted or unsubstituted acetylacetonate.

[0180] In some embodiments, the compound has a formula of $Pt(L_{sub}A)(L_{sub}B)$; and wherein $L_{sub}A$ and $L_{sub}B$ can be same or different. In some embodiments, $L_{sub}A$ and $L_{sub}B$ are connected to form a tetradentate ligand.

[0181] In some embodiments, $L_{sub}B$ and $L_{sub}C$ are each independently selected from the group consisting of the structures of the following LIST 4:

##STR00552## ##STR00553## ##STR00554## ##STR00555## ##STR00556##

wherein: [0182] T is selected from the group consisting of B, Al, Ga, and In, [0183] $K_{sup.1'}$ is

selected from the group consisting of a single bond, O, S, $NR_{sub.e}$, $PR_{sub.e}$, $BR_{sub.e}$,

$CR_{sub.e}$, $SiR_{sub.e}$, and $SiR_{sub.e}R_{sub.f}$, [0184] each of $Y_{sup.1}$ to $Y_{sup.13}$ is independently

selected from the group consisting of C and N; [0185] Y' is selected from the group consisting of

$BR_{sub.e}$, $BR_{sub.e}R_{sub.f}$, $NR_{sub.e}$, $PR_{sub.e}$, $P(O)R_{sub.e}$, O, S, Se, C=O, C=S, C=Se,

C=NR.sub.e, C=CR.sub.eR.sub.e, S=O, SO.sub.2, CR.sub.eR.sub.f, SiR.sub.eR.sub.f, and GeR.sub.eR.sub.f; [0186] R.sub.e and R.sub.f can be fused or joined to form a ring; [0187] each R.sub.a, R.sub.b, R.sub.c, and R.sub.d independently represents from mono to the maximum allowed number of substitutions, or no substitution; [0188] each of R.sub.a1, R.sub.b1, R.sub.c1, R.sub.d1, R.sub.a, R.sub.b, R.sub.c, R.sub.d, R.sub.e, and R.sub.f is independently a hydrogen or a substituent selected from the group consisting of the General Substituents defined herein; and [0189] any two substituents of R.sub.a1, R.sub.b1, R.sub.c1, R.sub.d1, R.sub.a, R.sub.b, R.sub.c, and R.sub.d can be fused or joined to form a ring or form a multidentate ligand.

[0190] In some embodiments, L.sub.B and L.sub.C are each independently selected from the group consisting of the structures of the following LIST 5:

##STR00557## ##STR00558## ##STR00559## ##STR00560## ##STR00561## ##STR00562##
##STR00563## ##STR00564## ##STR00565## ##STR00566## ##STR00567## ##STR00568##
##STR00569## ##STR00570## ##STR00571## ##STR00572## [0191] wherein: [0192] R.sub.a', R.sub.b', R.sub.c', R.sub.d', and R.sub.e' each independently represents zero, mono, or up to a maximum allowed number of substitution to its associated ring. [0193] R.sub.a', R.sub.b', R.sub.c', R.sub.d', and R.sub.e' each independently hydrogen or a substituent selected from the group consisting of the General Substituents defined herein; and [0194] two substituents of R.sub.a', R.sub.b', R.sub.c', R.sub.d', and R.sub.e' can be fused or joined to form a ring or form a multidentate ligand.

[0195] In some embodiments, L.sub.B comprises a structure of

##STR00573##

wherein the variables are the same as previously defined. In some embodiments, each of Y.sup.1 to Y.sup.4 is independently carbon. In some embodiments, at least one of Y.sup.1 to Y.sup.4 is N. In some embodiments, exactly one of Y.sup.1 to Y.sup.4 is N. In some embodiments, Y.sup.1 is N. In some embodiments, Y.sup.2 is N. In some embodiments, Y.sup.3 is N. In some embodiments, Y.sup.4 is N. In some embodiments, at least one of R.sub.a is a tertiary alkyl, silyl or germyl. In some embodiments, at least one of R.sub.a is a tertiary alkyl. In some embodiments, Y.sup.3 is C and the R.sub.a attached thereto is a tertiary alkyl, silyl or germyl. In some embodiments, Y.sup.1 to Y.sup.3 is C, Y.sup.1 is N, and the R.sub.a attached to Y.sup.3 is a tertiary alkyl, silyl or germyl. In some embodiments, Y.sup.1 to Y.sup.3 is C, Y.sup.4 is N. and the R.sub.a attached to Y.sup.2 is a tertiary alkyl, silyl or germyl. In some embodiments, at least one of R.sub.b is a tertiary alkyl, silyl, or germyl. In some embodiments, the tertiary alkyl is tert-butyl. In some embodiments, at least one pair of R.sub.a, one pair of R.sub.b, or one pair of R.sub.a and R.sub.b are joined or fused into a ring.

[0196] In some embodiments, the compound has formula Ir(L.sub.A).sub.3, formula Ir(L.sub.A)(L.sub.Bk).sub.2, formula Ir(L.sub.A).sub.2(L.sub.Bk), formula Ir(L.sub.A).sub.2(L.sub.Cj-I), or Ir(L.sub.A).sub.2(L.sub.Cj-II); [0197] wherein L.sub.A is according to any embodiment disclosed herein, including L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3); [0198] wherein k is an integer from 1 to 836, and each L.sub.Bk has the structure defined in the following LIST 6:

##STR00574## ##STR00575## ##STR00576## ##STR00577## ##STR00578## ##STR00579##
##STR00580## ##STR00581## ##STR00582## ##STR00583## ##STR00584## ##STR00585##
##STR00586## ##STR00587## ##STR00588## ##STR00589## ##STR00590## ##STR00591##
##STR00592## ##STR00593## ##STR00594## ##STR00595## ##STR00596## ##STR00597##
##STR00598## ##STR00599## ##STR00600## ##STR00601## ##STR00602## ##STR00603##
##STR00604## ##STR00605## ##STR00606## ##STR00607## ##STR00608## ##STR00609##
##STR00610## ##STR00611## ##STR00612## ##STR00613## ##STR00614## ##STR00615##
##STR00616##

##STR00617## ##STR00618## ##STR00619## ##STR00620## ##STR00621## ##STR00622##
##STR00623## ##STR00624## ##STR00625## ##STR00626## ##STR00627## ##STR00628##

##STR00630## ##STR00631## ##STR00632## ##STR00633## ##STR00634##
##STR00635## ##STR00636## ##STR00637## ##STR00638## ##STR00639## ##STR00640##
##STR00641## ##STR00642## ##STR00643## ##STR00644## ##STR00645## ##STR00646##
##STR00647## ##STR00648## ##STR00649## ##STR00650##
##STR00651## ##STR00652## ##STR00653## ##STR00654## ##STR00655## ##STR00656##
##STR00657## ##STR00658## ##STR00659## ##STR00660## ##STR00661## ##STR00662##
##STR00663## ##STR00664## ##STR00665## ##STR00666## ##STR00667## ##STR00668##
##STR00669## ##STR00670## ##STR00671##
##STR00672## ##STR00673## ##STR00674## ##STR00675## ##STR00676## ##STR00677##
##STR00678## ##STR00679## ##STR00680## ##STR00681## ##STR00682## ##STR00683##
##STR00684## ##STR00685## ##STR00686## ##STR00687## ##STR00688## ##STR00689##
##STR00690## ##STR00691## ##STR00692## ##STR00693## ##STR00694## ##STR00695##
##STR00696## ##STR00697## ##STR00698## ##STR00699##
##STR00700## ##STR00701## ##STR00702## ##STR00703## ##STR00704## ##STR00705##
##STR00706## ##STR00707## ##STR00708## ##STR00709## ##STR00710## ##STR00711##
##STR00712## ##STR00713## ##STR00714## ##STR00715## ##STR00716## ##STR00717##
##STR00718## ##STR00719## ##STR00720## ##STR00721## ##STR00722## ##STR00723##
##STR00724## ##STR00725## ##STR00726## ##STR00727##
##STR00728## ##STR00729## ##STR00730## ##STR00731## ##STR00732## [0199] wherein

each L.sub.Cj-I has a structure based on formula

##STR00733##

and [0200] each L.sub.Cj-II has a structure based on formula

##STR00734##

wherein for each L.sub.Cj in L.sub.Cj-I and L.sub.Cj-II, R.sup.201 and R.sup.202 are defined in the following LIST 7:

TABLE-US-00004 L.sub.Cj R.sup.201 R.sup.202 L.sub.Cj R.sup.201 R.sup.202 L.sub.Cj
R.sup.201 R.sup.202 L.sub.Cj R.sup.201 R.sup.202 L.sub.C1 R.sup.D1 R.sup.D1 L.sub.C193
R.sup.D1 R.sup.D3 L.sub.C385 R.sup.D17 R.sup.D40 L.sub.C577 R.sup.D143 R.sup.D120
L.sub.C2 R.sup.D2 R.sup.D2 L.sub.C194 R.sup.D1 R.sup.D4 L.sub.C386 R.sup.D17 R.sup.D41
L.sub.C578 R.sup.D143 R.sup.D133 L.sub.C3 R.sup.D3 R.sup.D3 L.sub.C195 R.sup.D1 R.sup.D5
L.sub.C387 R.sup.D17 R.sup.D42 L.sub.C579 R.sup.D143 R.sup.D134 L.sub.C4 R.sup.D4
R.sup.D4 L.sub.C196 R.sup.D1 R.sup.D9 L.sub.C388 R.sup.D17 R.sup.D43 L.sub.C580
R.sup.D143 R.sup.D135 L.sub.C5 R.sup.D5 R.sup.D5 L.sub.C197 R.sup.D1 R.sup.D10
L.sub.C389 R.sup.D17 R.sup.D48 L.sub.C581 R.sup.D143 R.sup.D136 L.sub.C6 R.sup.D6
R.sup.D6 L.sub.C198 R.sup.D1 R.sup.D17 L.sub.C390 R.sup.D17 R.sup.D49 L.sub.C582
R.sup.D143 R.sup.D144 L.sub.C7 R.sup.D7 R.sup.D7 L.sub.C199 R.sup.D1 R.sup.D18
L.sub.C391 R.sup.D17 R.sup.D50 L.sub.C583 R.sup.D143 R.sup.D145 L.sub.C8 R.sup.D8
R.sup.D8 L.sub.C200 R.sup.D1 R.sup.D20 L.sub.C392 R.sup.D17 R.sup.D54 L.sub.C584
R.sup.D143 R.sup.D146 L.sub.C9 R.sup.D9 R.sup.D9 L.sub.C201 R.sup.D1 R.sup.D22
L.sub.C393 R.sup.D17 R.sup.D55 L.sub.C585 R.sup.D143 R.sup.D147 L.sub.C10 R.sup.D10
R.sup.D10 L.sub.C202 R.sup.D1 R.sup.D37 L.sub.C394 R.sup.D17 R.sup.D58 L.sub.C586
R.sup.D143 R.sup.D149 L.sub.C11 R.sup.D11 R.sup.D11 L.sub.C203 R.sup.D1 R.sup.D40
L.sub.C395 R.sup.D17 R.sup.D59 L.sub.C587 R.sup.D143 R.sup.D151 L.sub.C12 R.sup.D12
R.sup.D12 L.sub.C204 R.sup.D1 R.sup.D41 L.sub.C396 R.sup.D17 R.sup.D78 L.sub.C588
R.sup.D143 R.sup.D154 L.sub.C13 R.sup.D13 R.sup.D13 L.sub.C205 R.sup.D1 R.sup.D42
L.sub.C397 R.sup.D17 R.sup.D79 L.sub.C589 R.sup.D143 R.sup.D155 L.sub.C14 R.sup.D14
R.sup.D14 L.sub.C206 R.sup.D1 R.sup.D43 L.sub.C398 R.sup.D17 R.sup.D81 L.sub.C590
R.sup.D143 R.sup.D161 L.sub.C15 R.sup.D15 R.sup.D15 L.sub.C207 R.sup.D1 R.sup.D48
L.sub.C399 R.sup.D17 R.sup.D87 L.sub.C591 R.sup.D143 R.sup.D175 L.sub.C16 R.sup.D16
R.sup.D16 L.sub.C208 R.sup.D1 R.sup.D49 L.sub.C400 R.sup.D17 R.sup.D88 L.sub.C592

R.sup.D1 R.sup.D13 L.sub.C17 R.sup.D17 R.sup.D17 L.sub.C209 R.sup.D1 R.sup.D50
L.sub.C401 R.sup.D17 R.sup.D89 L.sub.C593 R.sup.D144 R.sup.D5 L.sub.C18 R.sup.D18
R.sup.D18 L.sub.C210 R.sup.D1 R.sup.D54 L.sub.C402 R.sup.D17 R.sup.D93 L.sub.C594
R.sup.D144 R.sup.D17 L.sub.C19 R.sup.D19 R.sup.D19 L.sub.C211 R.sup.D1 R.sup.D55
L.sub.C403 R.sup.D17 R.sup.D116 L.sub.C595 R.sup.D144 R.sup.D18 L.sub.C20 R.sup.D20
R.sup.D20 L.sub.C212 R.sup.D1 R.sup.D58 L.sub.C404 R.sup.D17 R.sup.D117 L.sub.C596
R.sup.D144 R.sup.D20 L.sub.C21 R.sup.D21 R.sup.D21 L.sub.C213 R.sup.D1 R.sup.D59
L.sub.C405 R.sup.D17 R.sup.D118 L.sub.C597 R.sup.D144 R.sup.D22 L.sub.C22 R.sup.D22
R.sup.D22 L.sub.C214 R.sup.D1 R.sup.D78 L.sub.C406 R.sup.D17 R.sup.D119 L.sub.C598
R.sup.D144 R.sup.D37 L.sub.C23 R.sup.D23 R.sup.D23 L.sub.C215 R.sup.D1 R.sup.D79
L.sub.C407 R.sup.D17 R.sup.D120 L.sub.C599 R.sup.D144 R.sup.D40 L.sub.C24 R.sup.D24
R.sup.D24 L.sub.C216 R.sup.D1 R.sup.D81 L.sub.C408 R.sup.D17 R.sup.D133 L.sub.C600
R.sup.D144 R.sup.D41 L.sub.C25 R.sup.D25 R.sup.D25 L.sub.C217 R.sup.D1 R.sup.D87
L.sub.C409 R.sup.D17 R.sup.D134 L.sub.C601 R.sup.D144 R.sup.D42 L.sub.C26 R.sup.D26
R.sup.D26 L.sub.C218 R.sup.D1 R.sup.D88 L.sub.C410 R.sup.D17 R.sup.D135 L.sub.C602
R.sup.D144 R.sup.D43 L.sub.C27 R.sup.D27 R.sup.D27 L.sub.C219 R.sup.D1 R.sup.D89
L.sub.C411 R.sup.D17 R.sup.D136 L.sub.C603 R.sup.D144 R.sup.D48 L.sub.C28 R.sup.D28
R.sup.D28 L.sub.C220 R.sup.D1 R.sup.D93 L.sub.C412 R.sup.D17 R.sup.D143 L.sub.C604
R.sup.D144 R.sup.D49 L.sub.C29 R.sup.D29 R.sup.D29 L.sub.C221 R.sup.D1 R.sup.D116
L.sub.C413 R.sup.D17 R.sup.D144 L.sub.C605 R.sup.D144 R.sup.D54 L.sub.C30 R.sup.D30
R.sup.D30 L.sub.C222 R.sup.D1 R.sup.D117 L.sub.C414 R.sup.D17 R.sup.D145 L.sub.C606
R.sup.D144 R.sup.D58 L.sub.C31 R.sup.D31 R.sup.D31 L.sub.C223 R.sup.D1 R.sup.D118
L.sub.C415 R.sup.D17 R.sup.D146 L.sub.C607 R.sup.D144 R.sup.D59 L.sub.C32 R.sup.D32
R.sup.D32 L.sub.C224 R.sup.D1 R.sup.D119 L.sub.C416 R.sup.D17 R.sup.D147 L.sub.C608
R.sup.D144 R.sup.D78 L.sub.C33 R.sup.D33 R.sup.D33 L.sub.C225 R.sup.D1 R.sup.D120
L.sub.C417 R.sup.D17 R.sup.D149 L.sub.C609 R.sup.D144 R.sup.D79 L.sub.C34 R.sup.D34
R.sup.D34 L.sub.C226 R.sup.D1 R.sup.D133 L.sub.C418 R.sup.D17 R.sup.D151 L.sub.C610
R.sup.D144 R.sup.D81 L.sub.C35 R.sup.D35 R.sup.D35 L.sub.C227 R.sup.D1 R.sup.D134
L.sub.C419 R.sup.D17 R.sup.D154 L.sub.C611 R.sup.D144 R.sup.D87 L.sub.C36 R.sup.D36
R.sup.D36 L.sub.C228 R.sup.D1 R.sup.D135 L.sub.C420 R.sup.D17 R.sup.D155 L.sub.C612
R.sup.D144 R.sup.D88 L.sub.C37 R.sup.D37 R.sup.D37 L.sub.C229 R.sup.D1 R.sup.D136
L.sub.C421 R.sup.D17 R.sup.D161 L.sub.C613 R.sup.D144 R.sup.D89 L.sub.C38 R.sup.D38
R.sup.D38 L.sub.C230 R.sup.D1 R.sup.D143 L.sub.C422 R.sup.D17 R.sup.D175 L.sub.C614
R.sup.D144 R.sup.D93 L.sub.C39 R.sup.D39 R.sup.D39 L.sub.C231 R.sup.D1 R.sup.D144
L.sub.C423 R.sup.D50 R.sup.D3 L.sub.C615 R.sup.D144 R.sup.D116 L.sub.C40 R.sup.D40
R.sup.D40 L.sub.C232 R.sup.D1 R.sup.D145 L.sub.C424 R.sup.D50 R.sup.D5 L.sub.C616
R.sup.D144 R.sup.D117 L.sub.C41 R.sup.D41 R.sup.D41 L.sub.C233 R.sup.D1 R.sup.D146
L.sub.C425 R.sup.D50 R.sup.D18 L.sub.C617 R.sup.D144 R.sup.D118 L.sub.C42 R.sup.D42
R.sup.D42 L.sub.C234 R.sup.D1 R.sup.D147 L.sub.C426 R.sup.D50 R.sup.D20 L.sub.C618
R.sup.D144 R.sup.D119 L.sub.C43 R.sup.D43 R.sup.D43 L.sub.C235 R.sup.D1 R.sup.D149
L.sub.C427 R.sup.D50 R.sup.D22 L.sub.C619 R.sup.D144 R.sup.D120 L.sub.C44 R.sup.D44
R.sup.D44 L.sub.C236 R.sup.D1 R.sup.D151 L.sub.C428 R.sup.D50 R.sup.D37 L.sub.C620
R.sup.D144 R.sup.D133 L.sub.C45 R.sup.D45 R.sup.D45 L.sub.C237 R.sup.D1 R.sup.D154
L.sub.C429 R.sup.D50 R.sup.D40 L.sub.C621 R.sup.D144 R.sup.D134 L.sub.C46 R.sup.D46
R.sup.D46 L.sub.C238 R.sup.D1 R.sup.D155 L.sub.C430 R.sup.D50 R.sup.D41 L.sub.C622
R.sup.D144 R.sup.D135 L.sub.C47 R.sup.D47 R.sup.D47 L.sub.C239 R.sup.D1 R.sup.D161
L.sub.C431 R.sup.D50 R.sup.D42 L.sub.C623 R.sup.D144 R.sup.D136 L.sub.C48 R.sup.D48
R.sup.D48 L.sub.C240 R.sup.D1 R.sup.D175 L.sub.C432 R.sup.D50 R.sup.D43 L.sub.C624
R.sup.D144 R.sup.D145 L.sub.C49 R.sup.D49 R.sup.D49 L.sub.C241 R.sup.D4 R.sup.D3
L.sub.C433 R.sup.D50 R.sup.D48 L.sub.C625 R.sup.D144 R.sup.D146 L.sub.C50 R.sup.D50

R.sup.D50 L.sub.C242 R.sup.D4 R.sup.D5 L.sub.C434 R.sup.D50 R.sup.D49 L.sub.C626
R.sup.D144 R.sup.D147 L.sub.C51 R.sup.D51 R.sup.D51 L.sub.C243 R.sup.D4 R.sup.D9
L.sub.C435 R.sup.D50 R.sup.D54 L.sub.C627 R.sup.D144 R.sup.D149 L.sub.C52 R.sup.D52
R.sup.D52 L.sub.C244 R.sup.D4 R.sup.D10 L.sub.C436 R.sup.D50 R.sup.D55 L.sub.C628
R.sup.D144 R.sup.D151 L.sub.C53 R.sup.D53 R.sup.D53 L.sub.C245 R.sup.D4 R.sup.D17
L.sub.C437 R.sup.D50 R.sup.D58 L.sub.C629 R.sup.D144 R.sup.D154 L.sub.C54 R.sup.D54
R.sup.D54 L.sub.C246 R.sup.D4 R.sup.D18 L.sub.C438 R.sup.D50 R.sup.D59 L.sub.C630
R.sup.D144 R.sup.D155 L.sub.C55 R.sup.D55 R.sup.D55 L.sub.C247 R.sup.D4 R.sup.D20
L.sub.C439 R.sup.D50 R.sup.D78 L.sub.C631 R.sup.D144 R.sup.D161 L.sub.C56 R.sup.D56
R.sup.D56 L.sub.C248 R.sup.D4 R.sup.D22 L.sub.C440 R.sup.D50 R.sup.D79 L.sub.C632
R.sup.D144 R.sup.D175 L.sub.C57 R.sup.D57 R.sup.D57 L.sub.C249 R.sup.D4 R.sup.D37
L.sub.C441 R.sup.D50 R.sup.D81 L.sub.C633 R.sup.D145 R.sup.D3 L.sub.C58 R.sup.D58
R.sup.D58 L.sub.C250 R.sup.D4 R.sup.D40 L.sub.C442 R.sup.D50 R.sup.D87 L.sub.C634
R.sup.D145 R.sup.D5 L.sub.C59 R.sup.D59 R.sup.D59 L.sub.C251 R.sup.D4 R.sup.D41
L.sub.C443 R.sup.D50 R.sup.D88 L.sub.C635 R.sup.D145 R.sup.D17 L.sub.C60 R.sup.D60
R.sup.D60 L.sub.C252 R.sup.D4 R.sup.D42 L.sub.C444 R.sup.D50 R.sup.D89 L.sub.C636
R.sup.D145 R.sup.D18 L.sub.C61 R.sup.D61 R.sup.D61 L.sub.C253 R.sup.D4 R.sup.D43
L.sub.C445 R.sup.D50 R.sup.D93 L.sub.C637 R.sup.D145 R.sup.D20 L.sub.C62 R.sup.D62
R.sup.D62 L.sub.C254 R.sup.D4 R.sup.D48 L.sub.C446 R.sup.D50 R.sup.D116 L.sub.C638
R.sup.D145 R.sup.D22 L.sub.C63 R.sup.D63 R.sup.D63 L.sub.C255 R.sup.D4 R.sup.D49
L.sub.C447 R.sup.D50 R.sup.D117 L.sub.C639 R.sup.D145 R.sup.D37 L.sub.C64 R.sup.D64
R.sup.D64 L.sub.C256 R.sup.D4 R.sup.D50 L.sub.C448 R.sup.D50 R.sup.D118 L.sub.C640
R.sup.D145 R.sup.D40 L.sub.C65 R.sup.D65 R.sup.D65 L.sub.C257 R.sup.D4 R.sup.D54
L.sub.C449 R.sup.D50 R.sup.D119 L.sub.C641 R.sup.D145 R.sup.D41 L.sub.C66 R.sup.D66
R.sup.D66 L.sub.C258 R.sup.D4 R.sup.D55 L.sub.C450 R.sup.D50 R.sup.D120 L.sub.C642
R.sup.D145 R.sup.D42 L.sub.C67 R.sup.D67 R.sup.D67 L.sub.C259 R.sup.D4 R.sup.D58
L.sub.C451 R.sup.D50 R.sup.D133 L.sub.C643 R.sup.D145 R.sup.D43 L.sub.C68 R.sup.D68
R.sup.D68 L.sub.C260 R.sup.D4 R.sup.D59 L.sub.C452 R.sup.D50 R.sup.D134 L.sub.C644
R.sup.D145 R.sup.D48 L.sub.C69 R.sup.D69 R.sup.D69 L.sub.C261 R.sup.D4 R.sup.D78
L.sub.C453 R.sup.D50 R.sup.D135 L.sub.C645 R.sup.D145 R.sup.D49 L.sub.C70 R.sup.D70
R.sup.D70 L.sub.C262 R.sup.D4 R.sup.D79 L.sub.C454 R.sup.D50 R.sup.D136 L.sub.C646
R.sup.D145 R.sup.D54 L.sub.C71 R.sup.D71 R.sup.D71 L.sub.C263 R.sup.D4 R.sup.D81
L.sub.C455 R.sup.D50 R.sup.D143 L.sub.C647 R.sup.D145 R.sup.D58 L.sub.C72 R.sup.D72
R.sup.D72 L.sub.C264 R.sup.D4 R.sup.D87 L.sub.C456 R.sup.D50 R.sup.D144 L.sub.C648
R.sup.D145 R.sup.D59 L.sub.C73 R.sup.D73 R.sup.D73 L.sub.C265 R.sup.D4 R.sup.D88
L.sub.C457 R.sup.D50 R.sup.D145 L.sub.C649 R.sup.D145 R.sup.D78 L.sub.C74 R.sup.D74
R.sup.D74 L.sub.C266 R.sup.D4 R.sup.D89 L.sub.C458 R.sup.D50 R.sup.D146 L.sub.C650
R.sup.D145 R.sup.D79 L.sub.C75 R.sup.D75 R.sup.D75 L.sub.C267 R.sup.D4 R.sup.D93
L.sub.C459 R.sup.D50 R.sup.D147 L.sub.C651 R.sup.D145 R.sup.D81 L.sub.C76 R.sup.D76
R.sup.D76 L.sub.C268 R.sup.D4 R.sup.D116 L.sub.C460 R.sup.D50 R.sup.D149 L.sub.C652
R.sup.D145 R.sup.D87 L.sub.C77 R.sup.D77 R.sup.D77 L.sub.C269 R.sup.D4 R.sup.D117
L.sub.C461 R.sup.D50 R.sup.D151 L.sub.C653 R.sup.D145 R.sup.D88 L.sub.C78 R.sup.D78
R.sup.D78 L.sub.C270 R.sup.D4 R.sup.D118 L.sub.C462 R.sup.D50 R.sup.D154 L.sub.C654
R.sup.D145 R.sup.D89 L.sub.C79 R.sup.D79 R.sup.D79 L.sub.C271 R.sup.D4 R.sup.D119
L.sub.C463 R.sup.D50 R.sup.D155 L.sub.C655 R.sup.D145 R.sup.D93 L.sub.C80 R.sup.D80
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R.sup.D145 R.sup.D116 L.sub.C81 R.sup.D81 R.sup.D81 L.sub.C273 R.sup.D4 R.sup.D133
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R.sup.D145 R.sup.D118 L.sub.C83 R.sup.D83 R.sup.D83 L.sub.C275 R.sup.D4 R.sup.D135

L.sub.C467 R.sup.D55 R.sup.D5 L.sub.C659 R.sup.D145 R.sup.D119 L.sub.C84 R.sup.D84
R.sup.D84 L.sub.C276 R.sup.D4 R.sup.D136 L.sub.C468 R.sup.D55 R.sup.D18 L.sub.C660
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L.sub.C477 R.sup.D55 R.sup.D49 L.sub.C669 R.sup.D145 R.sup.D154 L.sub.C94 R.sup.D94
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R.sup.D145 R.sup.D175 L.sub.C97 R.sup.D97 R.sup.D97 L.sub.C289 R.sup.D9 R.sup.D5
L.sub.C481 R.sup.D55 R.sup.D78 L.sub.C673 R.sup.D146 R.sup.D3 L.sub.C98 R.sup.D98
R.sup.D98 L.sub.C290 R.sup.D9 R.sup.D10 L.sub.C482 R.sup.D55 R.sup.D79 L.sub.C674
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L.sub.C483 R.sup.D55 R.sup.D81 L.sub.C675 R.sup.D146 R.sup.D17 L.sub.C100 R.sup.D100
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L.sub.C501 R.sup.D55 R.sup.D147 L.sub.C693 R.sup.D146 R.sup.D88 L.sub.C118 R.sup.D118
R.sup.D118 L.sub.C310 R.sup.D9 R.sup.D87 L.sub.C502 R.sup.D55 R.sup.D149 L.sub.C694
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L.sub.C513 R.sup.D116 R.sup.D22 L.sub.C705 R.sup.D146 R.sup.D147 L.sub.C130 R.sup.D130
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L.sub.C537 R.sup.D116 R.sup.D135 L.sub.C729 R.sup.D133 R.sup.D79 L.sub.C154 R.sup.D154
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L.sub.C541 R.sup.D116 R.sup.D145 L.sub.C733 R.sup.D133 R.sup.D89 L.sub.C158 R.sup.D158
R.sup.D158 L.sub.C350 R.sup.D10 R.sup.D58 L.sub.C542 R.sup.D116 R.sup.D146 L.sub.C734
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L.sub.C543 R.sup.D116 R.sup.D147 L.sub.C735 R.sup.D133 R.sup.D117 L.sub.C160 R.sup.D160
R.sup.D160 L.sub.C352 R.sup.D10 R.sup.D78 L.sub.C544 R.sup.D116 R.sup.D149 L.sub.C736
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L.sub.C545 R.sup.D116 R.sup.D151 L.sub.C737 R.sup.D133 R.sup.D119 L.sub.C162 R.sup.D162
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L.sub.C547 R.sup.D116 R.sup.D155 L.sub.C739 R.sup.D133 R.sup.D133 L.sub.C164 R.sup.D164
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L.sub.C549 R.sup.D116 R.sup.D175 L.sub.C741 R.sup.D133 R.sup.D135 L.sub.C166 R.sup.D166
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R.sup.D210 L.sub.C1164 R.sup.D168 R.sup.D210 L.sub.C841 R.sup.D17 R.sup.D211 L.sub.C949
R.sup.D50 R.sup.D211 L.sub.C1057 R.sup.D145 R.sup.D211 L.sub.C1165 R.sup.D168
R.sup.D211 L.sub.C842 R.sup.D17 R.sup.D212 L.sub.C950 R.sup.D50 R.sup.D212 L.sub.C1058
R.sup.D145 R.sup.D212 L.sub.C1166 R.sup.D168 R.sup.D212 L.sub.C843 R.sup.D17 R.sup.D213
L.sub.C951 R.sup.D50 R.sup.D213 L.sub.C1059 R.sup.D145 R.sup.D213 L.sub.C1167
R.sup.D168 R.sup.D213 L.sub.C844 R.sup.D17 R.sup.D214 L.sub.C952 R.sup.D50 R.sup.D214
L.sub.C1060 R.sup.D145 R.sup.D214 L.sub.C1168 R.sup.D168 R.sup.D214 L.sub.C845
R.sup.D17 R.sup.D215 L.sub.C953 R.sup.D50 R.sup.D215 L.sub.C1061 R.sup.D145 R.sup.D215
L.sub.C1169 R.sup.D168 R.sup.D215 L.sub.C846 R.sup.D17 R.sup.D216 L.sub.C954 R.sup.D50
R.sup.D216 L.sub.C1062 R.sup.D145 R.sup.D216 L.sub.C1170 R.sup.D168 R.sup.D216
L.sub.C847 R.sup.D17 R.sup.D217 L.sub.C955 R.sup.D50 R.sup.D217 L.sub.C1063 R.sup.D145
R.sup.D217 L.sub.C1171 R.sup.D168 R.sup.D217 L.sub.C848 R.sup.D17 R.sup.D218 L.sub.C956
R.sup.D50 R.sup.D218 L.sub.C1064 R.sup.D145 R.sup.D218 L.sub.C1172 R.sup.D168
R.sup.D218 L.sub.C849 R.sup.D17 R.sup.D219 L.sub.C957 R.sup.D50 R.sup.D219 L.sub.C1065
R.sup.D145 R.sup.D219 L.sub.C1173 R.sup.D168 R.sup.D219 L.sub.C850 R.sup.D17 R.sup.D220
L.sub.C958 R.sup.D50 R.sup.D220 L.sub.C1066 R.sup.D145 R.sup.D220 L.sub.C1174
R.sup.D168 R.sup.D220 L.sub.C851 R.sup.D17 R.sup.D221 L.sub.C959 R.sup.D50 R.sup.D221
L.sub.C1067 R.sup.D145 R.sup.D221 L.sub.C1175 R.sup.D168 R.sup.D221 L.sub.C852
R.sup.D17 R.sup.D222 L.sub.C960 R.sup.D50 R.sup.D222 L.sub.C1068 R.sup.D145 R.sup.D222
L.sub.C1176 R.sup.D168 R.sup.D222 L.sub.C853 R.sup.D17 R.sup.D223 L.sub.C961 R.sup.D50
R.sup.D223 L.sub.C1069 R.sup.D145 R.sup.D223 L.sub.C1177 R.sup.D168 R.sup.D223
L.sub.C854 R.sup.D17 R.sup.D224 L.sub.C962 R.sup.D50 R.sup.D224 L.sub.C1070 R.sup.D145
R.sup.D224 L.sub.C1178 R.sup.D168 R.sup.D224 L.sub.C855 R.sup.D17 R.sup.D225 L.sub.C963
R.sup.D50 R.sup.D225 L.sub.C1071 R.sup.D145 R.sup.D225 L.sub.C1179 R.sup.D168
R.sup.D225 L.sub.C856 R.sup.D17 R.sup.D226 L.sub.C964 R.sup.D50 R.sup.D226 L.sub.C1072
R.sup.D145 R.sup.D226 L.sub.C1180 R.sup.D168 R.sup.D226 L.sub.C857 R.sup.D17 R.sup.D227
L.sub.C965 R.sup.D50 R.sup.D227 L.sub.C1073 R.sup.D145 R.sup.D227 L.sub.C1181

R.sup.D168 R.sup.D227 L.sub.C858 R.sup.D17 R.sup.D228 L.sub.C966 R.sup.D50 R.sup.D228
L.sub.C1074 R.sup.D145 R.sup.D228 L.sub.C1182 R.sup.D168 R.sup.D228 L.sub.C859
R.sup.D17 R.sup.D229 L.sub.C967 R.sup.D50 R.sup.D229 L.sub.C1075 R.sup.D145 R.sup.D229
L.sub.C1183 R.sup.D168 R.sup.D229 L.sub.C860 R.sup.D17 R.sup.D230 L.sub.C968 R.sup.D50
R.sup.D230 L.sub.C1076 R.sup.D145 R.sup.D230 L.sub.C1184 R.sup.D168 R.sup.D230
L.sub.C861 R.sup.D17 R.sup.D231 L.sub.C969 R.sup.D50 R.sup.D231 L.sub.C1077 R.sup.D145
R.sup.D231 L.sub.C1185 R.sup.D168 R.sup.D231 L.sub.C862 R.sup.D17 R.sup.D232 L.sub.C970
R.sup.D50 R.sup.D232 L.sub.C1078 R.sup.D145 R.sup.D232 L.sub.C1186 R.sup.D168
R.sup.D232 L.sub.C863 R.sup.D17 R.sup.D233 L.sub.C971 R.sup.D50 R.sup.D233 L.sub.C1079
R.sup.D145 R.sup.D233 L.sub.C1187 R.sup.D168 R.sup.D233 L.sub.C864 R.sup.D17 R.sup.D234
L.sub.C972 R.sup.D50 R.sup.D234 L.sub.C1080 R.sup.D145 R.sup.D234 L.sub.C1188
R.sup.D168 R.sup.D234 L.sub.C865 R.sup.D17 R.sup.D235 L.sub.C973 R.sup.D50 R.sup.D235
L.sub.C1081 R.sup.D145 R.sup.D235 L.sub.C1189 R.sup.D168 R.sup.D235 L.sub.C866
R.sup.D17 R.sup.D236 L.sub.C974 R.sup.D50 R.sup.D236 L.sub.C1082 R.sup.D145 R.sup.D236
L.sub.C1190 R.sup.D168 R.sup.D236 L.sub.C867 R.sup.D17 R.sup.D237 L.sub.C975 R.sup.D50
R.sup.D237 L.sub.C1083 R.sup.D145 R.sup.D237 L.sub.C1191 R.sup.D168 R.sup.D237
L.sub.C868 R.sup.D17 R.sup.D238 L.sub.C976 R.sup.D50 R.sup.D238 L.sub.C1084 R.sup.D145
R.sup.D238 L.sub.C1192 R.sup.D168 R.sup.D238 L.sub.C869 R.sup.D17 R.sup.D239 L.sub.C977
R.sup.D50 R.sup.D239 L.sub.C1085 R.sup.D145 R.sup.D239 L.sub.C1193 R.sup.D168
R.sup.D239 L.sub.C870 R.sup.D17 R.sup.D240 L.sub.C978 R.sup.D50 R.sup.D240 L.sub.C1086
R.sup.D145 R.sup.D240 L.sub.C1194 R.sup.D168 R.sup.D240 L.sub.C871 R.sup.D17 R.sup.D241
L.sub.C979 R.sup.D50 R.sup.D241 L.sub.C1087 R.sup.D145 R.sup.D241 L.sub.C1195
R.sup.D168 R.sup.D241 L.sub.C872 R.sup.D17 R.sup.D242 L.sub.C980 R.sup.D50 R.sup.D242
L.sub.C1088 R.sup.D145 R.sup.D242 L.sub.C1196 R.sup.D168 R.sup.D242 L.sub.C873
R.sup.D17 R.sup.D243 L.sub.C981 R.sup.D50 R.sup.D243 L.sub.C1089 R.sup.D145 R.sup.D243
L.sub.C1197 R.sup.D168 R.sup.D243 L.sub.C874 R.sup.D17 R.sup.D244 L.sub.C982 R.sup.D50
R.sup.D244 L.sub.C1090 R.sup.D145 R.sup.D244 L.sub.C1198 R.sup.D168 R.sup.D244
L.sub.C875 R.sup.D17 R.sup.D245 L.sub.C983 R.sup.D50 R.sup.D245 L.sub.C1091 R.sup.D145
R.sup.D245 L.sub.C1199 R.sup.D168 R.sup.D245 L.sub.C876 R.sup.D17 R.sup.D246 L.sub.C984
R.sup.D50 R.sup.D246 L.sub.C1092 R.sup.D145 R.sup.D246 L.sub.C1200 R.sup.D168
R.sup.D246 L.sub.C1201 R.sup.D10 R.sup.D193 L.sub.C1255 R.sup.D55 R.sup.D193
L.sub.C1309 R.sup.D37 R.sup.D193 L.sub.C1363 R.sup.D143 R.sup.D193 L.sub.C1202
R.sup.D10 R.sup.D194 L.sub.C1256 R.sup.D55 R.sup.D194 L.sub.C1310 R.sup.D37 R.sup.D194
L.sub.C1364 R.sup.D143 R.sup.D194 L.sub.C1203 R.sup.D10 R.sup.D195 L.sub.C1257
R.sup.D55 R.sup.D195 L.sub.C1311 R.sup.D37 R.sup.D195 L.sub.C1365 R.sup.D143 R.sup.D195
L.sub.C1204 R.sup.D10 R.sup.D196 L.sub.C1258 R.sup.D55 R.sup.D196 L.sub.C1312 R.sup.D37
R.sup.D196 L.sub.C1366 R.sup.D143 R.sup.D196 L.sub.C1205 R.sup.D10 R.sup.D197
L.sub.C1259 R.sup.D55 R.sup.D197 L.sub.C1313 R.sup.D37 R.sup.D197 L.sub.C1367
R.sup.D143 R.sup.D197 L.sub.C1206 R.sup.D10 R.sup.D198 L.sub.C1260 R.sup.D55 R.sup.D198
L.sub.C1314 R.sup.D37 R.sup.D198 L.sub.C1368 R.sup.D143 R.sup.D198 L.sub.C1207
R.sup.D10 R.sup.D199 L.sub.C1261 R.sup.D55 R.sup.D199 L.sub.C1315 R.sup.D37 R.sup.D199
L.sub.C1369 R.sup.D143 R.sup.D199 L.sub.C1208 R.sup.D10 R.sup.D200 L.sub.C1262
R.sup.D55 R.sup.D200 L.sub.C1316 R.sup.D37 R.sup.D200 L.sub.C1370 R.sup.D143 R.sup.D200
L.sub.C1209 R.sup.D10 R.sup.D201 L.sub.C1263 R.sup.D55 R.sup.D201 L.sub.C1317 R.sup.D37
R.sup.D201 L.sub.C1371 R.sup.D143 R.sup.D201 L.sub.C1210 R.sup.D10 R.sup.D202
L.sub.C1264 R.sup.D55 R.sup.D202 L.sub.C1318 R.sup.D37 R.sup.D202 L.sub.C1372
R.sup.D143 R.sup.D202 L.sub.C1211 R.sup.D10 R.sup.D203 L.sub.C1265 R.sup.D55 R.sup.D203
L.sub.C1319 R.sup.D37 R.sup.D203 L.sub.C1373 R.sup.D143 R.sup.D203 L.sub.C1212
R.sup.D10 R.sup.D204 L.sub.C1266 R.sup.D55 R.sup.D204 L.sub.C1320 R.sup.D37 R.sup.D204
L.sub.C1374 R.sup.D143 R.sup.D204 L.sub.C1213 R.sup.D10 R.sup.D205 L.sub.C1267

R.sup.D55 R.sup.D205 L.sub.C1321 R.sup.D205 L.sub.C1375 R.sup.D205 L.sub.C1375 R.sup.D205
L.sub.C1214 R.sup.D10 R.sup.D206 L.sub.C1268 R.sup.D55 R.sup.D206 L.sub.C1322 R.sup.D37
R.sup.D206 L.sub.C1376 R.sup.D143 R.sup.D206 L.sub.C1215 R.sup.D10 R.sup.D207
L.sub.C1269 R.sup.D55 R.sup.D207 L.sub.C1323 R.sup.D37 R.sup.D207 L.sub.C1377
R.sup.D143 R.sup.D207 L.sub.C1216 R.sup.D10 R.sup.D208 L.sub.C1270 R.sup.D55 R.sup.D208
L.sub.C1324 R.sup.D37 R.sup.D208 L.sub.C1378 R.sup.D143 R.sup.D208 L.sub.C1217
R.sup.D10 R.sup.D209 L.sub.C1271 R.sup.D55 R.sup.D209 L.sub.C1325 R.sup.D37 R.sup.D209
L.sub.C1379 R.sup.D143 R.sup.D209 L.sub.C1218 R.sup.D10 R.sup.D210 L.sub.C1272
R.sup.D55 R.sup.D210 L.sub.C1326 R.sup.D37 R.sup.D210 L.sub.C1380 R.sup.D143 R.sup.D210
L.sub.C1219 R.sup.D10 R.sup.D211 L.sub.C1273 R.sup.D55 R.sup.D211 L.sub.C1327 R.sup.D37
R.sup.D211 L.sub.C1381 R.sup.D143 R.sup.D211 L.sub.C1220 R.sup.D10 R.sup.D212
L.sub.C1274 R.sup.D55 R.sup.D212 L.sub.C1328 R.sup.D37 R.sup.D212 L.sub.C1382
R.sup.D143 R.sup.D212 L.sub.C1221 R.sup.D10 R.sup.D213 L.sub.C1275 R.sup.D55 R.sup.D213
L.sub.C1329 R.sup.D37 R.sup.D213 L.sub.C1383 R.sup.D143 R.sup.D213 L.sub.C1222
R.sup.D10 R.sup.D214 L.sub.C1276 R.sup.D55 R.sup.D214 L.sub.C1330 R.sup.D37 R.sup.D214
L.sub.C1384 R.sup.D143 R.sup.D214 L.sub.C1223 R.sup.D10 R.sup.D215 L.sub.C1277
R.sup.D55 R.sup.D215 L.sub.C1331 R.sup.D37 R.sup.D215 L.sub.C1385 R.sup.D143 R.sup.D215
L.sub.C1224 R.sup.D10 R.sup.D216 L.sub.C1278 R.sup.D55 R.sup.D216 L.sub.C1332 R.sup.D37
R.sup.D216 L.sub.C1386 R.sup.D143 R.sup.D216 L.sub.C1225 R.sup.D10 R.sup.D217
L.sub.C1279 R.sup.D55 R.sup.D217 L.sub.C1333 R.sup.D37 R.sup.D217 L.sub.C1387
R.sup.D143 R.sup.D217 L.sub.C1226 R.sup.D10 R.sup.D218 L.sub.C1280 R.sup.D55 R.sup.D218
L.sub.C1334 R.sup.D37 R.sup.D218 L.sub.C1388 R.sup.D143 R.sup.D218 L.sub.C1227
R.sup.D10 R.sup.D219 L.sub.C1281 R.sup.D55 R.sup.D219 L.sub.C1335 R.sup.D37 R.sup.D219
L.sub.C1389 R.sup.D143 R.sup.D219 L.sub.C1228 R.sup.D10 R.sup.D220 L.sub.C1282
R.sup.D55 R.sup.D220 L.sub.C1336 R.sup.D37 R.sup.D220 L.sub.C1390 R.sup.D143 R.sup.D220
L.sub.C1229 R.sup.D10 R.sup.D221 L.sub.C1283 R.sup.D55 R.sup.D221 L.sub.C1337 R.sup.D37
R.sup.D221 L.sub.C1391 R.sup.D143 R.sup.D221 L.sub.C1230 R.sup.D10 R.sup.D222
L.sub.C1284 R.sup.D55 R.sup.D222 L.sub.C1338 R.sup.D37 R.sup.D222 L.sub.C1392
R.sup.D143 R.sup.D222 L.sub.C1231 R.sup.D10 R.sup.D223 L.sub.C1285 R.sup.D55 R.sup.D223
L.sub.C1339 R.sup.D37 R.sup.D223 L.sub.C1393 R.sup.D143 R.sup.D223 L.sub.C1232
R.sup.D10 R.sup.D224 L.sub.C1286 R.sup.D55 R.sup.D224 L.sub.C1340 R.sup.D37 R.sup.D224
L.sub.C1394 R.sup.D143 R.sup.D224 L.sub.C1233 R.sup.D10 R.sup.D225 L.sub.C1287
R.sup.D55 R.sup.D225 L.sub.C1341 R.sup.D37 R.sup.D225 L.sub.C1395 R.sup.D143 R.sup.D225
L.sub.C1234 R.sup.D10 R.sup.D226 L.sub.C1288 R.sup.D55 R.sup.D226 L.sub.C1342 R.sup.D37
R.sup.D226 L.sub.C1396 R.sup.D143 R.sup.D226 L.sub.C1235 R.sup.D10 R.sup.D227
L.sub.C1289 R.sup.D55 R.sup.D227 L.sub.C1343 R.sup.D37 R.sup.D227 L.sub.C1397
R.sup.D143 R.sup.D227 L.sub.C1236 R.sup.D10 R.sup.D228 L.sub.C1290 R.sup.D55 R.sup.D228
L.sub.C1344 R.sup.D37 R.sup.D228 L.sub.C1398 R.sup.D143 R.sup.D228 L.sub.C1237
R.sup.D10 R.sup.D229 L.sub.C1291 R.sup.D55 R.sup.D229 L.sub.C1345 R.sup.D37 R.sup.D229
L.sub.C1399 R.sup.D143 R.sup.D229 L.sub.C1238 R.sup.D10 R.sup.D230 L.sub.C1292
R.sup.D55 R.sup.D230 L.sub.C1346 R.sup.D37 R.sup.D230 L.sub.C1400 R.sup.D143 R.sup.D230
L.sub.C1239 R.sup.D10 R.sup.D231 L.sub.C1293 R.sup.D55 R.sup.D231 L.sub.C1347 R.sup.D37
R.sup.D231 L.sub.C1401 R.sup.D143 R.sup.D231 L.sub.C1240 R.sup.D10 R.sup.D232
L.sub.C1294 R.sup.D55 R.sup.D232 L.sub.C1348 R.sup.D37 R.sup.D232 L.sub.C1402
R.sup.D143 R.sup.D232 L.sub.C1241 R.sup.D10 R.sup.D233 L.sub.C1295 R.sup.D55 R.sup.D233
L.sub.C1349 R.sup.D37 R.sup.D233 L.sub.C1403 R.sup.D143 R.sup.D233 L.sub.C1242
R.sup.D10 R.sup.D234 L.sub.C1296 R.sup.D55 R.sup.D234 L.sub.C1350 R.sup.D37 R.sup.D234
L.sub.C1404 R.sup.D143 R.sup.D234 L.sub.C1243 R.sup.D10 R.sup.D235 L.sub.C1297
R.sup.D55 R.sup.D235 L.sub.C1351 R.sup.D37 R.sup.D235 L.sub.C1405 R.sup.D143 R.sup.D235
L.sub.C1244 R.sup.D10 R.sup.D236 L.sub.C1298 R.sup.D55 R.sup.D236 L.sub.C1352 R.sup.D37

R.sup.D236 L.sub.C1406 R.sup.D143 R.sup.D236 L.sub.C1245 R.sup.D10 R.sup.D237
L.sub.C1299 R.sup.D55 R.sup.D237 L.sub.C1353 R.sup.D37 R.sup.D237 L.sub.C1407
R.sup.D143 R.sup.D237 L.sub.C1246 R.sup.D10 R.sup.D238 L.sub.C1300 R.sup.D55 R.sup.D238
L.sub.C1354 R.sup.D37 R.sup.D238 L.sub.C1408 R.sup.D143 R.sup.D238 L.sub.C1247
R.sup.D10 R.sup.D239 L.sub.C1301 R.sup.D55 R.sup.D239 L.sub.C1355 R.sup.D37 R.sup.D239
L.sub.C1409 R.sup.D143 R.sup.D239 L.sub.C1248 R.sup.D10 R.sup.D240 L.sub.C1302
R.sup.D55 R.sup.D240 L.sub.C1356 R.sup.D37 R.sup.D240 L.sub.C1410 R.sup.D143 R.sup.D240
L.sub.C1249 R.sup.D10 R.sup.D241 L.sub.C1303 R.sup.D55 R.sup.D241 L.sub.C1357 R.sup.D37
R.sup.D241 L.sub.C1411 R.sup.D143 R.sup.D241 L.sub.C1250 R.sup.D10 R.sup.D242
L.sub.C1304 R.sup.D55 R.sup.D242 L.sub.C1358 R.sup.D37 R.sup.D242 L.sub.C1412
R.sup.D143 R.sup.D242 L.sub.C1251 R.sup.D10 R.sup.D243 L.sub.C1305 R.sup.D55 R.sup.D243
L.sub.C1359 R.sup.D37 R.sup.D243 L.sub.C1413 R.sup.D143 R.sup.D243 L.sub.C1252
R.sup.D10 R.sup.D244 L.sub.C1306 R.sup.D55 R.sup.D244 L.sub.C1360 R.sup.D37 R.sup.D244
L.sub.C1414 R.sup.D143 R.sup.D244 L.sub.C1253 R.sup.D10 R.sup.D245 L.sub.C1307
R.sup.D55 R.sup.D245 L.sub.C1361 R.sup.D37 R.sup.D245 L.sub.C1415 R.sup.D143 R.sup.D245
L.sub.C1254 R.sup.D10 R.sup.D246 L.sub.C1308 R.sup.D55 R.sup.D246 L.sub.C1362 R.sup.D37
R.sup.D246 L.sub.C1416 R.sup.D143 R.sup.D246 [0201] wherein R.sup.D1 to R.sup.D246 have
the structures defined in the following LIST 8:

##STR00735## ##STR00736## ##STR00737## ##STR00738## ##STR00739## ##STR00740##
##STR00741## ##STR00742## ##STR00743## ##STR00744## ##STR00745## ##STR00746##
##STR00747## ##STR00748## ##STR00749## ##STR00750## ##STR00751## ##STR00752##
##STR00753## ##STR00754## ##STR00755##

[0202] In some embodiments, the compound is selected from the group consisting of only those compounds whose L.sub.Bk corresponds to one of the following: L.sub.B1, L.sub.B2, L.sub.B18, L.sub.B28, L.sub.B38, L.sub.B108, L.sub.B118, L.sub.B122, L.sub.B124, L.sub.B126, L.sub.B128, L.sub.B130, L.sub.B132, L.sub.B134, L.sub.B136, L.sub.B138, L.sub.B140, L.sub.B142, L.sub.B144, L.sub.B156, L.sub.B158, L.sub.B160, L.sub.B162, L.sub.B164, L.sub.B168, L.sub.B172, L.sub.B175, L.sub.B204, L.sub.B206, L.sub.B214, L.sub.B214, L.sub.B216, L.sub.B218, L.sub.B220, L.sub.B222, L.sub.B231, L.sub.B233, L.sub.B235, L.sub.B327, L.sub.B240, L.sub.B242, L.sub.B244, L.sub.B246, L.sub.B248, L.sub.B250, L.sub.B252, L.sub.B254, L.sub.B256, L.sub.B258, L.sub.B260, L.sub.B262, L.sub.B264, L.sub.B265, L.sub.B266, L.sub.B267, L.sub.B268, L.sub.B269, and L.sub.B270.

[0203] In some embodiments, the compound is selected from the group consisting of only those compounds whose L.sub.Bk, corresponds to one of the following: L.sub.B1, L.sub.B2, L.sub.B18, L.sub.B28, L.sub.B38, L.sub.B108, L.sub.B118, L.sub.B122, L.sub.B126, L.sub.B128, L.sub.B132, L.sub.B136, L.sub.B138, L.sub.B142, L.sub.B156, L.sub.B162, L.sub.B204, L.sub.B206, L.sub.B214, L.sub.B214, L.sub.B216, L.sub.B218, L.sub.B220, L.sub.B231, L.sub.B233, L.sub.B327, L.sub.B264, L.sub.B265, L.sub.B266, L.sub.B267, L.sub.B268, L.sub.B269, and L.sub.B270.

[0204] In some embodiments, the compound is selected from the group consisting of only those compounds having L.sub.Cj-I or L.sub.Cj-II ligand whose corresponding R.sup.201 and R.sup.202 are defined to be one of the following structures: R.sup.D1, R.sup.D3, R.sup.D4, R.sub.D5, R.sup.D9, R.sup.D10, R.sup.D17, R.sup.D18, R.sup.D20, R.sup.D22, R.sup.D37, R.sup.D40, R.sup.D41, R.sup.D42, R.sup.D43, R.sup.D48, R.sup.D49, R.sup.D50, R.sup.D54, R.sup.D55, R.sup.D58, R.sup.D78, R.sup.D79, R.sup.D81, R.sup.D87, R.sup.D88, R.sup.D89, R.sup.D93, R.sup.D116, R.sup.D117, R.sup.D118, R.sup.D119, R.sup.D120, R.sup.D133, R.sup.D134, R.sup.D135, R.sup.D136, R.sup.D143, R.sup.D144, R.sup.D145, R.sup.D146, R.sup.D147, R.sup.D149, R.sup.D151, R.sup.D154, R.sup.D155, R.sup.D161, R.sup.D175, R.sup.D190, R.sup.D193, R.sup.D200, R.sup.D201, R.sup.D206, R.sup.D210, R.sup.D214, R.sup.D215, R.sup.D216, R.sup.D218, R.sup.D219, R.sup.D220, R.sup.D227, R.sup.D237, R.sup.D241,

R.sup.D242, R.sup.D245, and R.sup.D246.

[0205] In some embodiments, the compound is selected from the group consisting of only those compounds having L.sub.Cj-I or L.sub.Cj-II ligand whose corresponding R.sup.201 and R.sup.202 are defined to be one of selected from the following structures: R.sup.D1, R.sup.D3, R.sup.D4, R.sup.D5, R.sup.D9, R.sup.D10, R.sup.D17, R.sup.D22, R.sup.D43, R.sup.D50, R.sup.D78, R.sup.D116, R.sup.D118, R.sup.D133, R.sup.D134, R.sup.D135, R.sup.D136, R.sup.D143, R.sup.D144, R.sup.D145, R.sup.D146, R.sup.D149, R.sup.D151, R.sup.D154, R.sup.D155, R.sup.D190, R.sup.D193, R.sup.D200, R.sup.D201, R.sup.D206, R.sup.D210, R.sup.D214, R.sup.D215, R.sup.D216, R.sup.D218, R.sup.D219, R.sup.D220, R.sup.D227, R.sup.D237, R.sup.D241, R.sup.D242, R.sup.D245, and R.sup.D246.

[0206] In some embodiments, the compound is selected from the group consisting of only those compounds having one of the structures of the following LIST 9 for the L.sub.Cj-I ligand:

##STR00756## ##STR00757## ##STR00758## ##STR00759## ##STR00760##

[0207] In some embodiments, the compound has a formula selected from the group consisting of Ir(L.sub.A).sub.3, Ir(L.sub.A).sub.2(L.sub.B), Ir(L.sub.A)(L.sub.B).sub.2, Ir(L.sub.A).sub.2(L.sub.C), and Ir(L.sub.A)(L.sub.B)(L.sub.C). In some embodiments, L.sub.A is selected from the group consisting of the structures of LIST 1, LIST 1a, and LIST 2, L.sub.B is selected from the group consisting of the structures of LIST 4, LIST 5, and LIST 6 (L.sub.Bk), and L.sub.C is selected from the group consisting of the structures of L.sub.Cj-I and L.sub.Cj-II defined herein.

[0208] In some embodiments, L.sub.A is selected from the group consisting of the structures of LIST 1 and L.sub.B is selected from the group consisting of the structures of L.sub.Bk. In some embodiments, L.sub.A is selected from the group consisting of the structures of LIST 1a and L.sub.B is selected from the group consisting of the structures of L.sub.Bk. In some embodiments, L.sub.A is selected from LIST 2 defined herein, and L.sub.B is selected from the group consisting of the structures of L.sub.Bk wherein k is an integer from 1 to 836. In some embodiments, L.sub.A is selected from LIST 2 defined herein, and L.sub.C is selected from the group consisting of the structures of L.sub.Cj-I and L.sub.Cj-II wherein j is an integer from 1 to 1416.

[0209] In some embodiments, the compound can have the formula Ir(L.sub.Aw-(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V).sub.3 consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1)).sub.3 to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3)).sub.3, the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V)(L.sub.B).sub.2, the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V).sub.2(L.sub.B), the formula Ir(L.sub.A)(L.sub.Bk).sub.2, the formula Ir(L.sub.A).sub.2(L.sub.Bk), the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V)(L.sub.Bk).sub.2 consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1))(L.sub.Bk).sub.2 to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3))(L.sub.B836).sub.2, the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V).sub.2(L.sub.Bk) consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1)).sub.2(L.sub.B1) to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3)).sub.2(L.sub.B836), the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V).sub.2(L.sub.Cj-I) consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1)).sub.2(L.sub.Cl-I) to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3)).sub.2(L.sub.C1416-I), the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V).sub.2(L.sub.Cj-II) consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1)).sub.2(L.sub.Cl-II) to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3)).sub.2(L.sub.C1416-II), the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V)(L.sub.Bk)(L.sub.Cj-I) consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1))(L.sub.Bl)(L.sub.Cl-I) to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3))(L.sub.B836)(L.sub.C1416-I), or the formula Ir(L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V)(L.sub.Bk)(L.sub.Cj-II) consisting of the compounds of Ir(L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1))(L.sub.Bl)(L.sub.Cl-II) to Ir(L.sub.A37-(R468)(R468)(R468)(Y3)(Y3)(Y3))(L.sub.B836)

(L.sub.Cl143-II), wherein L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V, L.sub.Bk, and L.sub.Cj-I and L.sub.Cj-II are all defined herein.

[0210] In some embodiments, the compound is selected from the group consisting of the structures of the following LIST 10:

##STR00761## ##STR00762## ##STR00763## ##STR00764## ##STR00765## ##STR00766##
##STR00767## ##STR00768## ##STR00769##

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

##STR00770##

wherein: [0212] M.sup.1 is Pd or Pt; [0213] moieties E and F are each independently monocyclic or polycyclic ring structure, 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; [0214] Z.sup.3 and Z.sup.4 are each independently C or N; [0215] K.sup.1, K.sup.2, K.sup.3, and K.sup.4 are each independently selected from the group consisting of a direct bond, O, and S, wherein at least two of them are direct bonds; [0216] L.sup.1, L.sup.2, and L.sup.3 are each independently absent or selected from the group consisting of a direct bond, BR, BRR', NR, PR, P(O)R, O, S, Se, C=O, C=S, C=Se, C=NR, C=CRR', S=O, SO.sub.2, CRR', SiRR', GeRR', alkylene, cycloalkyl, aryl, cycloalkylene, arylene, heteroarylene, and combinations thereof, wherein at least one of L.sup.1 and L.sup.2 is present; [0217] R.sup.E and R.sup.F each independently represents zero, mono, or up to a maximum allowed number of substitutions; [0218] each of R, R', R.sup.E, and R.sup.F is independently a hydrogen or a substituent selected from the group consisting of the General Substituents defined herein; and [0219] two adjacent R.sup.A, R.sup.B, R.sup.C, R.sup.E, and R.sup.F can be joined or fused together to form a ring where chemically feasible.

[0220] In some embodiments of Formula II, each of R, R', R.sup.E, and R.sup.F is independently a hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

[0221] In some embodiments of Formula II, moieties E and F are each independently monocyclic or polycyclic ring structures, wherein the monocyclic ring or each ring of the polycyclic fused ring system is independently a 5-membered or 6-membered carbocyclic or heterocyclic rings.

[0222] In some embodiments of Formula II, at least one R, R', R.sup.A, R.sup.B, R.sup.C, R.sup.E, or R.sup.F is partially or fully deuterated. In some embodiments, at least one R.sup.A is partially or fully deuterated. In some embodiments, at least one R.sup.B is partially or fully deuterated. In some embodiments, at least one R.sup.C is partially or fully deuterated. In some embodiments, at least one R.sup.E is partially or fully deuterated. In some embodiments, at least one R.sup.F is partially or fully deuterated. In some embodiments of Formula II, at least R or R' is present and is partially or fully deuterated.

[0223] In some embodiments of Formula II, at least one R.sup.A, R.sup.B, R.sup.C, R.sup.E, or R.sup.F is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one R.sup.A is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one at least one R.sup.B is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one at least one R.sup.C is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one at least one R.sup.E is a substituent selected from the group consisting of the General Substituents defined herein. In some embodiments, at least one at least one R.sup.F is a substituent selected from the group consisting of the General Substituents defined herein.

[0224] In some embodiments of Formula II, at least one R, R', R.sup.A, R.sup.B, R.sup.C, R.sup.E, or R.sup.F is or comprises an electron-withdrawing group from the EWG1 LIST as defined herein. In some embodiments, at least one R, R', R.sup.A, R.sup.B, R.sup.C, R.sup.E, or R.sup.F is or comprises an electron-withdrawing group from the EWG2 LIST as defined herein. In some

embodiments, Formula II comprises an electron-withdrawing group from the EWG4 LIST as defined herein. In some embodiments, Formula II comprises an electron-withdrawing group from the Pi-EWG LIST as defined herein.]

[0231] In some embodiments of Formula II, moiety E and moiety F are both 6-membered aromatic rings.

[0232] In some embodiments of Formula II, moiety F is a 5-membered or 6-membered heteroaromatic ring.

[0233] In some embodiments of Formula II, L^{sup.1} is O or CRR'.

[0234] In some embodiments of Formula II, Z^{sup.4} is N and Z^{sup.3} is C. In some embodiments of Formula II, Z^{sup.4} is C and Z^{sup.3} is N.

[0235] In some embodiments of Formula II, L^{sup.2} is a direct bond. In some embodiments of Formula II, L^{sup.2} is NR.

[0236] In some embodiments of Formula II, K^{sup.1}, K^{sup.2}, K^{sup.3}, and K^{sup.4} are all direct bonds. In some embodiments of Formula II, one of K^{sup.1}, K^{sup.2}, K^{sup.3}, and K^{sup.4} is O.

[0237] In some embodiments of Formula II, the compound is selected from the group consisting of compounds having the formula of Pt(L_{sub}.A')(Ly):

##STR00771## [0238] wherein L_{sub}.A' is selected from the group consisting of the structures shown in the following LIST 11:

##STR00772## ##STR00773## ##STR00774## ##STR00775## ##STR00776## [0239] wherein L_{sub}.y is selected from the group consisting of the structures shown in the following LIST 12:

##STR00777## ##STR00778## ##STR00779## ##STR00780## ##STR00781## ##STR00782## ##STR00783## ##STR00784## ##STR00785## ##STR00786##
























wherein: [0240] Z' is B or N; [0241] each of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'} is independently absent or selected from the group consisting of BR, BRR', NR, PR, P(O)R, O, S, Se, C=O, C=S, C=Se, C=NR, C=CRR', S=O, SO_{sub}.2, CRR', SiRR', and GeRR'; [0242] each of L_{sub}.Z and L_{sub}.Z' is independently a direct bond, O, or S; [0243] R^{sup.AA}, R^{sup.BB}, R^{sup.CC}, and R^{sup.G} each independently represents zero, mono, or up to a maximum allowed number of substitutions; [0244] each of R^{sup.AA}, R^{sup.BB}, R^{sup.CC}, R^{sup.G}, R^{sup.N}, R^{sup.X}, and R^{sup.Y} is independently a hydrogen or a substituent selected from the group consisting of the General Substituents defined herein; and [0245] any two substituents can be joined or fused to form a ring.

[0246] In some of the above embodiments of Ly where there is a structure containing Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'}, each of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'}, if present, is independently selected from the group consisting of O, S, C=O, C=S, C=NR, CRR', and C=CRR'. In some such embodiments, at least one of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'} is present. In some such embodiments, exactly one of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'} is present. In some such embodiments, at least two of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'} are present. In some such embodiments, exactly two of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'} are present. In some such embodiments, all three of Y^{sup.1'}, Y^{sup.2'}, and Y^{sup.3'} are present.

[0247] In some embodiments, the compound is selected from the group consisting of the compounds having the formula of Pt(L_{sub}.A')(Ly):

##STR00787## [0248] ligand L_{sub}.A' is selected from L_{sub}.A'^{i'}-(Lw)_{sub}.A(Lz)_{sub}.B(Rp)(Rq)(Rr)(Ym)(Yn)(Yo)_{sub}.C, wherein i' is an integer from 1 to 46; A is 1 when i' is 1, 3, 4, 5, 6, 10, 11, 14, 15, 16, 17, 18, 24, 25, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, or 46, otherwise A is 0; B is 1 when i' is 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, or 26, otherwise B is 0; C is 1 when i' is 6, 9, 11, 13, 16, 21, 23, 32, 35, 40, 43, 45, or 46, otherwise C is 0; each of Rp, Rq, and Rr is independently selected from the group consisting of R1 to R468; each of Lw and Lz is independently selected from the group consisting of L1 and L2, where L1 is a direct bond and L2 is O; and each of Yin, Yn, and Yo is independently selected from the group consisting of Y1 to Y3; wherein each of L_{sub}.A'¹-(L1)(L1)(R1)(R1)(R1)(Y1)(Y1) to L_{sub}.A'⁴⁶-(L2)(R468)(R468)(R468)(Y3)(Y3)(Y3) is defined in the following LIST

TABLE-US-00005 L.sub.A' Structure of L.sub.A' L.sub.A'1- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'1- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'1- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00788]  L.sub.A'2- (Lz)(Rp)(Rq)(Rr)(Ym)(Yn), wherein L.sub.A'2- (L1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A'2- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00789]  L.sub.A'3- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'3- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'3- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00790]  L.sub.A'4- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'4- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'4- (L2)(L2)(R468)(R468) (R468) (Y3)(Y3), have the structure [00791]  L.sub.A'5- (Lw)(Lz)(Rp)(Rq)(Rr) (Ym) (Yn), wherein L.sub.A'5- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'5- (L2)(L2)(R468) (R468)(R468) (Y3)(Y3), have the structure [00792]  L.sub.A'6- (Lw)(Lz)(Rp) (Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'6- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'6- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00793]  L.sub.A'7- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'7- (L1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A'7- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00794]  L.sub.A'8- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'8- (L1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A'8- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00795]  L.sub.A'9- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'9- (L1)(R1)(R1)(R1)(Y1)(Y1) (Y1) to L.sub.A'9- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00796]  L.sub.A'10- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'10- (L1)(L1) (R1)(R1)(R1)(Y1) (Y1) to L.sub.A'10- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00797]  L.sub.A'11- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'11- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'11- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00798]  L.sub.A'12- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'12- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'12- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00799]  L.sub.A'13- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'13- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'13- (L2)(L2)(R468)(R468) (R468) (Y3)(Y3)(Y3), have the structure [00800]  L.sub.A'14- (Lw)(Lz)(Rp) (Rq)(Rr)(Ym) (Yn), wherein L.sub.A'14- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'14- (L2)(L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00801]  L.sub.A'15- (Lw) (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'15- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'15- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00802]  L.sub.A'16- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'16- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'16- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00803]  L.sub.A'17- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'17- (L1)(L1) (R1)(R1)(R1)(Y1) (Y1) to L.sub.A'17- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00804]  L.sub.A'18- (Lw)(Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'18- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'18- (L2)(L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00805]  L.sub.A'19- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'19- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'19- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00806]  L.sub.A'20- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'20- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'20- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00807]  L.sub.A'21- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'21- (L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'21- (L2)(R468)(R468)(R468) (Y3)(Y3) (Y3), have the structure [00808]  L.sub.A'22- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'22- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'22- (L2)(R468)(R468)(R468) (Y3) (Y3), have the structure [00809]  L.sub.A'23- (Lz)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'23- (L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'23- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00810]  L.sub.A'24- (Lw)(Lz)(Rp)(Rq)(Rr)

(Ym) (Yn), wherein L.sub.A'24- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'24- (L2)(L2)(R468) (R468)(R468) (Y3)(Y3), have the structure [00811]  embedded image L.sub.A'25- (Lw)(Lz)(Rp) (Rq)(Rr)(Ym) (Yn), wherein L.sub.A'25- (L1)(L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'25- (L2)(L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00812]  embedded image L.sub.A'26- (Lz) (Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'26- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'26- (L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00813]  embedded image L.sub.A'27- (Lw) (Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'27- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'27- (L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00814]  embedded image L.sub.A'28- (Lw) (Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'28- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'28- (L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00815]  embedded image L.sub.A'29- (Lw) (Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'29- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'29- (L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00816]  embedded image L.sub.A'30- (Lw) (Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'30- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'30- (L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00817]  embedded image L.sub.A'31- (Lw) (Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'31- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'31- (L2) (R468)(R468)(R468) (Y3)(Y3), have the structure [00818]  embedded image L.sub.A'32- (Lw) (Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'32- (L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'32- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00819]  embedded image L.sub.A'33- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'33- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'33- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00820]  embedded image L.sub.A'34- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'34- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'34- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00821]  embedded image L.sub.A'35- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'35- (L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'35- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00822]  embedded image L.sub.A'36- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'36- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'36- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00823]  embedded image L.sub.A'37- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'37- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'37- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00824]  embedded image L.sub.A'38- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'38- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'38- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00825]  embedded image L.sub.A'39- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'39- (L1)(R1)(R1)(R1)(Y1) (Y1) to L.sub.A'39- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00826]  embedded image L.sub.A'40- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'40- (L1)(R1)(R1)(R1)(Y1) (Y1) (Y1) to L.sub.A'40- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00827]  embedded image L.sub.A'41- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'41- (L1)(R1)(R1) (R1)(Y1) (Y1) to L.sub.A'41- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00828]  embedded image L.sub.A'42- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'42- (L1)(R1)(R1) (R1)(Y1) (Y1) to L.sub.A'42- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00829]  embedded image L.sub.A'43- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'43- (L1)(R1) (R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'43- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00830]  embedded image L.sub.A'44- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn), wherein L.sub.A'44- (L1) (R1)(R1)(R1)(Y1) (Y1) to L.sub.A'44- (L2)(R468)(R468)(R468) (Y3)(Y3), have the structure [00831]  embedded image L.sub.A'45- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'45- (L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'45- (L2)(R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure [00832]  embedded image L.sub.A'46- (Lw)(Rp)(Rq)(Rr)(Ym) (Yn)(Yo), wherein L.sub.A'46- (L1)(R1)(R1)(R1)(Y1) (Y1)(Y1) to L.sub.A'46- (L2)(R468)(R468)(R468) (Y3)(Y3) (Y3), have the structure [00833]  embedded image [0249] wherein ligand L.sub.y is selected from the group consisting of L.sub.yj-(Rs)(Rt)(Ru)(Rv), wherein j is an integer from 1 to 52; each of Rs, Rt, Ru, and Rv is independently selected from the group consisting of R1 to R468; wherein each of L.sub.y1-(R1)(R1)(R1)(R1) to L.sub.y52-(R468)(R468)(R468)(R468) is defined in the following

LIST 14:

TABLE-US-00006 L.sub.y Structure of L.sub.y L.sub.y1-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y1-(R1)(R1)(R1) to L.sub.y1- (R468)(R468)(R468)(R468) have the structure [00834]

 L.sub.y2-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y2-(R1)(R1)(R1)(R1) to L.sub.y2-(R468)(R468)(R468)(R468) have the structure [00835]  L.sub.y3-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y3-(R1)(R1)(R1)(R1) to L.sub.y3- (R468)(R468)(R468)(R468) have the structure [00836]  L.sub.y4-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y4-(R1)(R1)(R1)(R1) to L.sub.y4- (R468)(R468)(R468)(R468) have the structure [00837]  L.sub.y5-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y5-(R1)(R1)(R1)(R1) to L.sub.y5- (R468)(R468)(R468)(R468) have the structure [00838]  L.sub.y6-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y6-(R1)(R1)(R1)(R1) to L.sub.y6- (R468)(R468)(R468)(R468) have the structure [00839]  L.sub.y7-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y7-(R1)(R1)(R1)(R1) to L.sub.y7- (R468)(R468)(R468)(R468) have the structure [00840]  L.sub.y8-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y8-(R1)(R1)(R1)(R1) to L.sub.y8- (R468)(R468)(R468)(R468) have the structure [00841]  L.sub.y9-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y9-(R1)(R1)(R1)(R1) to L.sub.y9- (R468)(R468)(R468)(R468) have the structure [00842]  L.sub.y10-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y10-(R1)(R1)(R1)(R1) to L.sub.y10- (R468)(R468)(R468)(R468) have the structure [00843]  L.sub.y11-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y11-(R1)(R1)(R1)(R1) to L.sub.y11- (R468)(R468)(R468)(R468) have the structure [00844]  L.sub.y12-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y12-(R1)(R1)(R1)(R1) to L.sub.y12- (R468)(R468)(R468)(R468) have the structure [00845]  L.sub.y13-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y13-(R1)(R1)(R1)(R1) to L.sub.y13- (R468)(R468)(R468)(R468) have the structure [00846]  L.sub.y14-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y14-(R1)(R1)(R1)(R1) to L.sub.y14- (R468)(R468)(R468)(R468) have the structure [00847]  L.sub.y15-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y15-(R1)(R1)(R1)(R1) to L.sub.y15- (R468)(R468)(R468)(R468) have the structure [00848]  L.sub.y16-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y16-(R1)(R1)(R1)(R1) to L.sub.y16- (R468)(R468)(R468)(R468) have the structure [00849]  L.sub.y17-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y17-(R1)(R1)(R1)(R1) to L.sub.y17- (R468)(R468)(R468)(R468) have the structure [00850]  L.sub.y18-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y18-(R1)(R1)(R1)(R1) to L.sub.y18- (R468)(R468)(R468)(R468) have the structure [00851]  L.sub.y19-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y19-(R1)(R1)(R1)(R1) to L.sub.y19- (R468)(R468)(R468)(R468) have the structure [00852]  L.sub.y20-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y20-(R1)(R1)(R1)(R1) to L.sub.y20- (R468)(R468)(R468)(R468) have the structure [00853]  L.sub.y21-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y21-(R1)(R1)(R1)(R1) to L.sub.y21- (R468)(R468)(R468)(R468) have the structure [00854]  L.sub.y22-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y22-(R1)(R1)(R1)(R1) to L.sub.y22- (R468)(R468)(R468)(R468) have the structure [00855]  L.sub.y23-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y23-(R1)(R1)(R1)(R1) to L.sub.y23- (R468)(R468)(R468)(R468) have the structure [00856]  L.sub.y24-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y24-(R1)(R1)(R1)(R1) to L.sub.y24- (R468)(R468)(R468)(R468) have the structure [00857]  L.sub.y25-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y25-(R1)(R1)(R1)(R1) to L.sub.y25- (R468)(R468)(R468)(R468) have the structure [00858]  L.sub.y26-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y26-(R1)(R1)(R1)(R1) to L.sub.y26- (R468)(R468)(R468)(R468) have the structure [00859]  L.sub.y27-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y27-(R1)(R1)(R1)(R1) to L.sub.y27- (R468)(R468)(R468)(R468) have the structure [00860]  L.sub.y28-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y28-(R1)(R1)(R1)(R1) to L.sub.y28- (R468)(R468)(R468)(R468) have the structure [00861]  L.sub.y29-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y29-(R1)(R1)(R1)(R1) to L.sub.y29- (R468)(R468)(R468)(R468) have the structure [00862]  L.sub.y30-(Rs)(Rt)(Ru)(Rv), wherein L.sub.y30-(R1)(R1)(R1)(R1) to

L.sub.y30- (R468)(R468)(R468) have the structure [00863]  embedded image L.sub.y31- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y31- (R1)(R1)(R1)(R1) to L.sub.y31- (R468)(R468)(R468)(R468) have the structure [00864]  embedded image L.sub.y32- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y32- (R1)(R1)(R1)(R1) to L.sub.y32- (R468)(R468)(R468)(R468) have the structure [00865]  embedded image L.sub.y33- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y33- (R1)(R1)(R1)(R1) to L.sub.y33- (R468)(R468)(R468)(R468) have the structure [00866]  embedded image L.sub.y34- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y34- (R1)(R1)(R1)(R1) to L.sub.y34- (R468)(R468)(R468)(R468) have the structure [00867]  embedded image L.sub.y35- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y35- (R1)(R1)(R1)(R1) to L.sub.y35- (R468)(R468)(R468)(R468) have the structure [00868]  embedded image L.sub.y36- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y36- (R1)(R1)(R1)(R1) to L.sub.y36- (R468)(R468)(R468)(R468) have the structure [00869]  embedded image L.sub.y37- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y37- (R1)(R1)(R1)(R1) to L.sub.y37- (R468)(R468)(R468)(R468) have the structure [00870]  embedded image L.sub.y38- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y38- (R1)(R1)(R1)(R1) to L.sub.y38- (R468)(R468)(R468)(R468) have the structure [00871]  embedded image L.sub.y39- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y39- (R1)(R1)(R1)(R1) to L.sub.y39- (R468)(R468)(R468)(R468) have the structure [00872]  embedded image L.sub.y40- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y40- (R1)(R1)(R1)(R1) to L.sub.y40- (R468)(R468)(R468)(R468) have the structure [00873]  embedded image L.sub.y41- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y41- (R1)(R1)(R1)(R1) to L.sub.y41- (R468)(R468)(R468)(R468) have the structure [00874]  embedded image L.sub.y42- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y42- (R1)(R1)(R1)(R1) to L.sub.y42- (R468)(R468)(R468)(R468) have the structure [00875]  embedded image L.sub.y43- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y43- (R1)(R1)(R1)(R1) to L.sub.y43- (R468)(R468)(R468)(R468) have the structure [00876]  embedded image L.sub.y44- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y44- (R1)(R1)(R1)(R1) to L.sub.y44- (R468)(R468)(R468)(R468) have the structure [00877]  embedded image L.sub.y45- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y45- (R1)(R1)(R1)(R1) to L.sub.y45- (R468)(R468)(R468)(R468) have the structure [00878]  embedded image L.sub.y46- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y46- (R1)(R1)(R1)(R1) to L.sub.y46- (R468)(R468)(R468)(R468) have the structure [00879]  embedded image L.sub.y47- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y47- (R1)(R1)(R1)(R1) to L.sub.y47- (R468)(R468)(R468)(R468) have the structure [00880]  embedded image L.sub.y48- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y48- (R1)(R1)(R1)(R1) to L.sub.y48- (R468)(R468)(R468)(R468) have the structure [00881]  embedded image L.sub.y49- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y49- (R1)(R1)(R1)(R1) to L.sub.y49- (R468)(R468)(R468)(R468) have the structure [00882]  embedded image L.sub.y50- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y50- (R1)(R1)(R1)(R1) to L.sub.y50- (R468)(R468)(R468)(R468) have the structure [00883]  embedded image L.sub.y51- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y51- (R1)(R1)(R1)(R1) to L.sub.y51- (R468)(R468)(R468)(R468) have the structure [00884]  embedded image L.sub.y52- (Rs)(Rt)(Ru)(Rv), wherein L.sub.y52- (R1)(R1)(R1)(R1) to L.sub.y52- (R468)(R468)(R468)(R468) have the structure [00885]  embedded image [0250] wherein Y1 is

##STR00886##

and [0251] wherein each of R1 to R468 have the structures defined in LIST 3 defined herein.

[0252] In some embodiments, the compound is selected from the group consisting of the structures of the following LIST 15:

##STR00887## ##STR00888## ##STR00889## ##STR00890## ##STR00891## ##STR00892##

[0253] In some embodiments, the compound having a first ligand L.sub.A of Formula I described herein can be at least 30% deuterated, at least 40% deuterated, at least 50% deuterated, at least 60% deuterated, at least 70% deuterated, at least 80% deuterated, at least 90% deuterated, at least 95% deuterated, at least 99% deuterated, or 100% deuterated. As used herein, percent deuteration has its ordinary meaning and includes the percent of all possible hydrogen atoms in the compound (e.g., positions that are hydrogen or deuterium) that are occupied by deuterium atoms. In some embodiments, carbon atoms comprised the ring coordinated to the metal M are fully or partially

deuterated. In some embodiments, carbon atoms comprised by a polycyclic ring system coordinated to the metal M are fully or partially deuterated. In some embodiments, a substituent attached to a monocyclic or fused polycyclic ring system coordinated to the metal M is fully or partially deuterated.

[0254] In some embodiments, the compound of formula I has an emission at room temperature with a full width at half maximum (FWHM) of equal to or less than 50, 45, 40, 35, 30, 25, 20, 15, 10, or 5 nm. Narrower FWHM means better color purity for the OLED display application.

[0255] In some embodiments of heteroleptic compound having the formula of $M(L_{sub}A)_{sub}p(L_{sub}B)_{sub}q(L_{sub}C)_{sub}r$ as defined above, the ligand $L_{sub}A$ has a first substituent $R_{sup}I$, where the first substituent $R_{sup}I$ has a first atom $a-I$ that is the farthest away from the metal M among all atoms in the ligand $L_{sub}A$. Additionally, the ligand $L_{sub}B$, if present, has a second substituent $R_{sup}II$, where the second substituent $R_{sup}II$ has a first atom $a-II$ that is the farthest away from the metal M among all atoms in the ligand $L_{sub}B$. Furthermore, the ligand $L_{sub}C$, if present, has a third substituent $R_{sup}III$, where the third substituent $R_{sup}III$ has a first atom $a-III$ that is the farthest away from the metal M among all atoms in the ligand $L_{sub}C$.

[0256] In such heteroleptic compounds, vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ can be defined as follows. $V_{sub}D1$ represents the direction from the metal M to the first atom $a-I$ and the vector $V_{sub}D1$ has a value $D_{sup}1$ that represents the straight line distance between the metal M and the first atom $a-I$ in the first substituent $R_{sup}I$. $V_{sub}D2$ represents the direction from the metal M to the first atom $a-II$ and the vector $V_{sub}D2$ has a value $D_{sup}2$ that represents the straight line distance between the metal M and the first atom $a-II$ in the second substituent $R_{sup}II$.

$V_{sub}D3$ represents the direction from the metal M to the first atom $a-III$ and the vector $V_{sub}D3$ has a value $D_{sup}3$ that represents the straight line distance between the metal M and the first atom $a-III$ in the third substituent $R_{sup}III$.

[0257] In such heteroleptic compounds, a sphere having a radius r is defined whose center is the metal M and the radius r is the smallest radius that will allow the sphere to enclose all atoms in the compound that are not part of the substituents $R_{sup}I$, $R_{sup}II$ and $R_{sup}III$; and where at least one of $D_{sup}1$, $D_{sup}2$, and $D_{sup}3$ is greater than the radius r by at least 1.5 Å. In some embodiments, at least one of $D_{sup}1$, $D_{sup}2$, and $D_{sup}3$ is greater than the radius r by at least 2.9, 3.0, 4.3, 4.4, 5.2, 5.9, 7.3, 8.8, 10.3, 13.1, 17.6, or 19.1 Å. In some embodiments, at least two of $D_{sup}1$, $D_{sup}2$, and $D_{sup}3$ is greater than the radius r by at least 1.5, 2.9, 3.0, 4.3, 4.4, 5.2, 5.9, 7.3, 8.8, 10.3, 13.1, 17.6, or 19.1 Å.

[0258] In some embodiments of such heteroleptic compound, the compound has a transition dipole moment axis and angles are defined between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$, where at least one of the angles between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ is less than 40°. In some embodiments, at least one of the angles between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ is less than 30°, 20°, 15°, or 10°. In some embodiments, at least two of the angles between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ are less than 20°. In some embodiments, at least two of the angles between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ are less than 15° or 10°.

[0259] In some embodiments, all three angles between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ are less than 20°. In some embodiments, all three angles between the transition dipole moment axis and the vectors $V_{sub}D1$, $V_{sub}D2$, and $V_{sub}D3$ are less than 15° or 10°.

[0260] In some embodiments of such heteroleptic compounds, the compound has a vertical dipole ratio (VDR) of 0.33 or less. In some embodiments of such heteroleptic compounds, the compound has a VDR of 0.30, 0.25, 0.20, or 0.15 or less.

[0261] One of ordinary skill in the art would readily understand the meaning of the terms transition dipole moment axis of a compound and vertical dipole ratio of a compound. Nevertheless, the meaning of these terms can be found in U.S. Pat. No. 10,672,997 whose disclosure is incorporated herein by reference in its entirety. In U.S. Pat. No. 10,672,997, horizontal dipole ratio (HDR) of a compound, rather than VDR, is discussed. However, one skilled in the art readily understands that $VDR=1-HDR$.

[0262] In some embodiments, the compound can be an emissive dopant. In some embodiments, the compound can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, triplet-triplet annihilation, or combinations of these processes. In some embodiments, the emissive dopant can be a racemic mixture, or can be enriched in one enantiomer. In some embodiments, the present compounds can have different stereoisomers, such as fac and mer. The current compound relates both to individual isomers and to mixtures of various isomers in any mixing ratio. In some embodiments, the compound can be homoleptic (each ligand is the same). In some embodiments, the compound can be heteroleptic (at least one ligand is different from others). When there are more than one ligand coordinated to a metal, the ligands can all be the same in some embodiments. In some other embodiments, at least one ligand is different from the other ligands. In some embodiments, every ligand can be different from every other ligand. This is also true in embodiments where a ligand being coordinated to a metal can be linked with other ligands being coordinated to that metal to form a tridentate, tetradentate, pentadentate, or hexadentate ligands. Thus, where the coordinating ligands are being linked together, all of the ligands can be the same in some embodiments, and at least one of the ligands being linked can be different from the other ligand(s) in some other embodiments.

[0263] In yet another aspect of the present disclosure, a formulation that comprises the novel compound disclosed herein is described. The formulation can include one or more components selected from the group consisting of a solvent, an emitter, a host, a hole injection material, hole transport material, electron blocking material, hole blocking material, and an electron transport material, disclosed herein.

[0264] The present disclosure encompasses any chemical structure comprising the novel compound of the present disclosure, or a monovalent or polyvalent variant thereof. In other words, the inventive compound, or a monovalent or polyvalent variant thereof, can be a part of a larger chemical structure. Such chemical structure can be selected from the group consisting of a monomer, a polymer, a macromolecule, and a supramolecule (also known as supermolecule). As used herein, a “monovalent variant of a compound” refers to a moiety that is identical to the compound except that one hydrogen has been removed and replaced with a bond to the rest of the chemical structure. As used herein, a “polyvalent variant of a compound” refers to a moiety that is identical to the compound except that more than one hydrogen has been removed and replaced with a bond or bonds to the rest of the chemical structure. In the instance of a supramolecule, the inventive compound can also be incorporated into the supramolecule complex without covalent bonds. As used in this context, the description that a structure A comprises a moiety B means that the structure A includes the structure of moiety B not including the H or D atoms that can be attached to the moiety B. This is because at least one H or D on a given moiety structure has to be replaced to become a substituent so that the moiety B can be part of the structure A, and one or more of the H or D on a given moiety B structure can be further substituted once it becomes a part of structure A.

C. The OLEDs and the Devices of the Present Disclosure

[0265] In another aspect, the present disclosure also provides an OLED device comprising a first organic layer that contains a compound as disclosed in the above compounds section of the present disclosure.

[0266] In some embodiments, the OLED comprises: an anode; a cathode; and an organic layer disposed between the anode and the cathode, where the organic layer comprises a compound

having a first ligand L.sub.A comprising a structure of Formula I.

[0267] In some embodiments, the organic layer is selected from the group consisting of HIL, HTL, EBL, EML, HBL, ETL, and EIL. In some embodiments, the organic layer may be an emissive layer and the compound as described herein may be an emissive dopant or a non-emissive dopant.

[0268] In some embodiments, the organic layer may further comprise a host, wherein host comprises at least one chemical group selected from the group consisting of triphenylene, carbazole, indolocarbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, 5λ.sup.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-5λ.sup.2-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, and aza-(5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene).

[0269] In some embodiments, the host can be selected from the group consisting of the structures of the following HOST Group 1:

##STR00893## ##STR00894## ##STR00895## ##STR00896## ##STR00897## ##STR00898##
##STR00899## ##STR00900## ##STR00901## ##STR00902## ##STR00903## ##STR00904##
##STR00905## ##STR00906## ##STR00907##

##STR00908## ##STR00909## [0270] wherein: [0271] each of J.sub.1 to J.sub.6 is independently C or N; [0272] L' is a direct bond or an organic linker; [0273] each Y.sup.AA, Y.sup.BB, Y.sub.CC, and Y.sup.DD is independently selected from the group consisting of absent a bond, direct bond, O, S, Se, CRR', SiRR', GeRR', NR, BR, BRR'; [0274] each of R.sup.A', R.sup.B', R.sup.C', R.sup.D', R.sup.E', R.sup.F', and R.sup.G' independently represents mono, up to the maximum substitutions, or no substitutions; [0275] each R, R', R.sup.A', R.sup.B', R.sup.C', R.sup.D', R.sup.E', R.sup.F', and R.sup.G' is independently a hydrogen or a substituent selected from the group consisting of the General Substituents as defined herein; any two substituents can be joined or fused to form a ring; [0276] and where possible, each unsubstituted aromatic carbon atom is optionally replaced with one or more N to form an aza-substituted ring.

[0277] In some embodiments at least one of J.sub.1 to J.sub.3 is N. In some embodiments at least two of J.sub.1 to J.sub.3 are N. In some embodiments, all three of J.sub.1 to J.sub.3 are N. In some embodiments, each Y.sub.CC and Y.sub.DD is independently O, S, or SiRR', or more preferably O or S. In some embodiments, at least one unsubstituted aromatic carbon atom is replaced with N to form an aza-ring.

[0278] In some embodiments, the host is selected from the group consisting of EG1-MG1-EG1 to EG53-MG27-EG53 with a formula of EGa-MGb-EGc, or EG1-EG1 to EG53-EG53 with a formula of EGa-EGc when MGb is absent, wherein a is an integer from 1 to 53, b is an integer from 1 to 27, c is an integer from 1 to 53. The structure of EG1 to EG53 is shown below:

##STR00910## ##STR00911## ##STR00912## ##STR00913## ##STR00914## ##STR00915##
##STR00916##

[0279] The structures of MG1 to MG27 are shown below:

##STR00917## ##STR00918## ##STR00919##

In the MGb structures shown above, the two bonding positions in the asymmetric structures MG10, MG11, MG12, MG13, MG14, MG17, MG24, and MG25 are labeled with numbers for identification purposes.

[0280] In some embodiments, the host can be any of the aza-substituted variants thereof, fully or partially deuterated variants thereof, and combinations thereof. In some embodiments, the host has formula EGa-MGb-Egc and is selected from the group consisting of h1 to h112 defined in the following HOST Group 2 list, where each of MGb, EGa, and EGc are defined as follows:

TABLE-US-00007 h MGb EGa EGc h1 MG1 EG3 EG36 h2 MG1 EG8 EG12 h3 MG1 EG13 EG14 h4 MG1 EG13 EG18 h5 MG1 EG13 EG25 h6 MG1 EG13 EG36 h7 MG1 EG22 EG36 h8 MG1 EG25 EG46 h9 MG1 EG27 EG46 h10 MG1 EG27 EG48 h11 MG1 EG32 EG50 h12 MG1 EG35 EG46 h13 MG1 EG36 EG45 h14 MG1 EG36 EG49 h15 MG1 EG40 EG45 h16 MG2 EG3 EG36 h17 MG2 EG25 EG31 h18 MG2 EG31 EG33 h19 MG2 EG36 EG45 h20 MG2 EG36 EG46 h21 MG3 EG4 EG36 h22 MG3 EG34 EG45 h23 MG4 EG13 EG17 h24 MG5 EG13 EG45 h25 MG5 EG17 EG36 h26 MG5 EG18 EG36 h27 MG6 EG17 EG17 h28 MG7 EG43 EG45 h29 MG8 EG1 EG28 h30 MG8 EG6 EG7 h31 MG8 EG7 EG7 h32 MG8 EG7 EG11 h33 MG9 EG1 EG43 h34 MG10 4-EG1 2-EG37 h35 MG10 4-EG1 2-EG38 h36 MG10 EG1 EG42 h37 MG11 4-EG1 2-EG39 h38 MG12 1-EG17 9-EG31 h39 MG13 3-EG17 9-EG4 h40 MG13 3-EG17 9-EG13 h41 MG13 3-EG17 9-EG31 h42 MG13 3-EG17 9-EG45 h43 MG13 3-EG17 9-EG46 h44 MG13 3-EG17 9-EG48 h45 MG13 3-EG17 9-EG49 h46 MG13 3-EG32 9-EG31 h47 MG13 3-EG44 9-EG3 h48 MG14 3-EG13 5-EG45 h49 MG14 3-EG23 5-EG45 h50 MG15 EG3 EG48 h51 MG15 EG17 EG31 h52 MG15 EG31 EG36 h53 MG16 EG17 EG17 h54 MG17 EG17 EG17 h55 MG18 EG16 EG24 h56 MG18 EG16 EG30 h57 MG18 EG20 EG41 h58 MG19 EG16 EG29 h59 MG20 EG1 EG31 h60 MG20 EG17 EG18 h61 MG21 EG23 EG23 h62 MG22 EG1 EG45 h63 MG22 EG1 EG46 h64 MG22 EG3 EG46 h65 MG22 EG4 EG46 h66 MG22 EG4 EG47 h67 MG22 EG9 EG45 h68 MG23 EG1 EG3 h69 MG23 EG1 EG6 h70 MG23 EG1 EG14 h71 MG23 EG1 EG18 h72 MG23 EG1 EG19 h73 MG23 EG1 EG23 h74 MG23 EG1 EG51 h75 MG23 EG2 EG18 h76 MG23 EG3 EG3 h77 MG23 EG3 EG4 h78 MG23 EG3 EG5 h79 MG23 EG4 EG4 h80 MG23 EG4 EG5 h81 MG24 2-EG1 10-EG33 h82 MG24 2-EG4 10-EG36 h83 MG24 2-EG21 10-EG36 h84 MG24 2-EG23 10-EG36 h85 MG25 2-EG1 9-EG33 h86 MG25 2-EG3 9-EG36 h87 MG25 2-EG4 9-EG36 h88 MG25 2-EG17 9-EG27 h89 MG25 2-EG17 9-EG36 h90 MG25 2-EG21 9-EG36 h91 MG25 2-EG23 9-EG27 h92 MG25 2-EG23 9-EG36 h93 MG26 EG1 EG9 h94 MG26 EG1 EG10 h95 MG26 EG1 EG21 h96 MG26 EG1 EG23 h97 MG26 EG1 EG26 h98 MG26 EG3 EG3 h99 MG26 EG3 EG9 h100 MG26 EG3 EG23 h101 MG26 EG3 EG26 h102 MG26 EG4 EG10 h103 MG26 EG5 EG10 h104 MG26 EG6 EG10 h105 MG26 EG10 EG10 h106 MG26 EG10 EG14 h107 MG26 EG10 EG15 h108 MG27 EG52 EG53 h109 — EG13 EG18 h110 — EG17 EG31 h111 — EG17 EG50 h112 — EG40 EG45

In the table above, the EGa and EGc structures at are bonded to one of the asymmetric structures MG10, MG11, MG12, MG13, MG14, MG17, MG24, and MG25, are noted with a numeric prefix identifying their bonding position in the MGb structure.

[0281] In some embodiments, the organic layer may further comprise a host, wherein the host comprises a metal complex.

[0282] In some embodiments, the emissive layer can comprise two hosts, a first host and a second host. In some embodiments, the first host is a hole transporting host, and the second host is an electron transporting host. In some embodiments, the first host is a hole transporting host, and the second host is a bipolar host. In some embodiments, the first host is an electron transporting host, and the second host is a bipolar host. In some embodiments, the first host and the second host can form an exciplex. In some embodiments, the emissive layer can comprise a third host. In some embodiments, the third host is selected from the group consisting of an insulating host (wide band gap host), a hole transporting host, and an electron transporting host. In some embodiments, the third host forms an exciplex with one of the first host and the second host, or with both the first host and the second host. In some embodiments, the emissive layer can comprise a fourth host. In some embodiments, the fourth host is selected from the group consisting of an insulating host (wide band gap host), a hole transporting host, and an electron transporting host. In some embodiments, the fourth host forms an exciplex with one of the first host, the second host, and the third host, with two of the first host, the second host, and the third host, or with each of the first host, the second host, and the third host. In some embodiments, the electron transporting host has a LUMO less than -2.4 eV, less than -2.5 eV, less than -2.6 eV, or less than -2.7 eV. In some

embodiments, the hole transporting host has a HOMO higher than -5.6 eV, higher than -5.5 eV, higher than -5.4 eV, or higher than -5.35 eV. The HOMO and LUMO values can be determined using solution electrochemistry. Solution cyclic voltammetry and differential pulsed voltammetry can be performed using a CH Instruments model 6201B potentiostat using anhydrous dimethylformamide (DMF) solvent and tetrabutylammonium hexafluorophosphate as the supporting electrolyte. Glassy carbon, platinum wire, and silver wire were used as the working, counter and reference electrodes, respectively. Electrochemical potentials can be referenced to an internal ferrocene-ferroconium redox couple (Fc/Fc⁺) by measuring the peak potential differences from differential pulsed voltammetry. The corresponding highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies can be determined by referencing the cationic and anionic redox potentials to ferrocene (4.8 eV vs. vacuum) according to literature ((a) Fink, R.; Heischkel, Y.; Thelakkat, M.; Schmidt, H.-W. *Chem. Mater.* 1998, 10, 3620-3625. (b) Pommerehne, J.; Vestweber, H.; Guss, W.; Mahrt, R. F.; Bassler, H.; Porsch, M.; Daub, J. *Adv. Mater.* 1995, 7, 551).

[0283] In some embodiments, the compound as described herein may be a sensitizer or a component of a sensitizer; wherein the device may further comprise an acceptor that receives the energy from the sensitizer. In some embodiments, the acceptor is an emitter in the device. In some embodiments, the acceptor may be a fluorescent material. In some embodiments, the compound described herein can be used as a phosphorescent sensitizer in an OLED where one or multiple layers in the OLED contain an acceptor in the form of one or more non-delayed fluorescent and/or delayed fluorescence material. In some embodiments, the compound described herein can be used as one component of an exciplex to be used as a sensitizer. As a phosphorescent sensitizer, the compound must be capable of energy transfer to the acceptor and the acceptor will emit the energy or further transfer energy to a final emitter. The acceptor concentrations can range from 0.001% to 99.9%. The acceptor could be in either the same layer as the phosphorescent sensitizer or in one or more different layers. In some embodiments, the acceptor is a thermally activated delayed fluorescence (TADF) material. In some embodiments, the acceptor is a non-delayed fluorescent material. In some embodiments, the emission can arise from any or all of the sensitizer, acceptor, and final emitter. In some embodiments, the acceptor has an emission at room temperature with a full width at half maximum (FWHM) of equal to or less than 50, 45, 40, 35, 30, 25, 20, 15, 10, or 5 nm. Narrower FWHM means better color purity for the OLED display application.

[0284] As used herein, phosphorescence generally refers to emission of a photon with a change in electron spin quantum number, i.e., the initial and final states of the emission have different electron spin quantum numbers, such as from T₁ to S₀ state. Most of the Ir and Pt complexes currently used in OLED are phosphorescent emitters. In some embodiments, if an exciplex formation involves a triplet emitter, such exciplex can also emit phosphorescent light. On the other hand, fluorescent emitters generally refer to emission of a photon without a change in electron spin quantum number, such as from S₁ to S₀ state, or from D₁ to D₀ state. Fluorescent emitters can be delayed fluorescent or non-delayed fluorescent emitters. Depending on the spin state, fluorescent emitter can be a singlet emitter or a doublet emitter, or other multiplet emitter. It is believed that the internal quantum efficiency (IQE) of fluorescent OLEDs can exceed the 25% spin statistics limit through delayed fluorescence. There are two types of delayed fluorescence, i.e. P-type and E-type delayed fluorescence. P-type delayed fluorescence is generated from triplet-triplet annihilation (TTA). On the other hand, E-type delayed fluorescence does not rely on the collision of two triplets, but rather on the thermal population between the triplet states and the singlet excited states. Thermal energy can activate the transition from the triplet state back to the singlet state. This type of delayed fluorescence is also known as TADF. E-type delayed fluorescence characteristics can be found in an exciplex system or in a single compound. Without being bound by theory, it is believed that TADF emissions require a compound or an exciplex having a small singlet-triplet energy gap ($\Delta E_{\text{sub.S-T}}$) less than or equal to 400, 350, 300, 250, 200, 150, 100, or 50 meV. There are two

major types of TADF emitters, one is called donor-acceptor type TADF, the other one is called multiple resonance (MR) TADF. Often, single compound donor-acceptor TADF compounds are constructed by connecting an electron donor moiety such as amino- or carbazole-derivatives and an electron acceptor moiety such as N-containing six-membered aromatic rings or cyano-substituted aromatic rings. Donor-acceptor exciplexes can be formed between a hole transporting compound and an electron transporting compound. Examples of MR-TADF materials include highly conjugated fused ring systems. In some embodiments, MR-TADF materials comprises boron, carbon, and nitrogen atoms. Such materials may comprise other atoms, such as oxygen, as well. In some embodiments, the reverse intersystem crossing time from T1 to S1 of the delayed fluorescent emission at 293K is less than or equal to 10 microseconds. In some embodiments, such time can be greater than 10 microseconds and less than 100 microseconds.

[0285] In some embodiments, the OLED may comprise an additional compound selected from the group consisting of a non-delayed fluorescence material, a delayed fluorescence material, a phosphorescent material, and combination thereof.

[0286] In some embodiments, the inventive compound described herein is a phosphorescent material.

[0287] In some embodiments, the phosphorescent material is an emitter which emits light within the OLED. In some embodiments, the phosphorescent material does not emit light within the OLED. In some embodiments, the phosphorescent material energy transfers its excited state to another material within the OLED. In some embodiments, the phosphorescent material participates in charge transport within the OLED. In some embodiments, the phosphorescent material is a sensitizer or a component of a sensitizer, and the OLED further comprises an acceptor. In some embodiments, the phosphorescent material forms an exciplex with another material within the OLED, for example a host material, an emitter material.

[0288] In some embodiments, the non-delayed fluorescence material or the delayed fluorescence material is an emitter which emits light within the OLED. In some embodiments, the non-delayed fluorescence material or the delayed fluorescence material does not emit light within the OLED. In some embodiments, the non-delayed fluorescence material or the delayed fluorescence material energy transfers its excited state to another material within the OLED. In some embodiments, the non-delayed fluorescence material or the delayed fluorescence material participates in charge transport within the OLED. In some embodiments, the non-delayed fluorescence material or the delayed fluorescence material is an acceptor, and the OLED further comprises a sensitizer.

[0289] In some embodiments of the OLED, the delayed fluorescence material comprises at least one donor group and at least one acceptor group. In some embodiments, the delayed fluorescence material is a metal complex. In some embodiments, the delayed fluorescence material is a non-metal complex. In some embodiments, the delayed fluorescence material is a Pt, Pd, Zn, Cu, Ag, or Au complex (some of them are also called metal-assisted (MA) TADF). In some embodiments, the metal-assisted delayed fluorescence material comprises a metal-carbene bond. In some embodiments, the non-delayed fluorescence material or delayed fluorescence material comprises at least one chemical group selected from the group consisting of aryl-amine, aryloxy, arylthio, triphenylene, carbazole, indolocarbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, 5 λ .sup.2-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene, 5 λ .sup.2,9 λ .sup.2-diaza-13b-boranaphtho[2,3,4-de]anthracene, 5-oxa-9 λ .sup.2-aza-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, amino, silyl, aza-variants thereof, and combinations thereof. In some embodiments, non-delayed the fluorescence material or delayed fluorescence material comprises a tri(aryl/heteroaryl)borane with one or more pairs of the substituents from the aryl/heteroaryl being

joined to form a ring. In some embodiments, the fluorescence material comprises at least one chemical group selected from the group consisting of naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene.

[0290] In yet another aspect, the OLED of the present disclosure may also comprise an emissive region containing a compound or a formulation of the compound as disclosed in the above compounds section of the present disclosure. In some embodiments, the emissive region can comprise a compound or a formulation of the compound having a first ligand L.sub.A comprising a structure of Formula I disclosed herein. In some embodiments, the emissive region consists of one or more organic layers, wherein at least one of the one or more organic layers has a minimum thickness selected from the group consisting of 350, 400, 450, 500, 550, 600, 650 and 700 Å. In some embodiments, the at least one of the one or more organic layers are formed from an Emissive System that has a figure of merit (FOM) value equal to or larger than the number selected from the group consisting of 2.50, 2.55, 2.60, 2.65, 2.70, 2.75, 2.80, 2.85, 2.90, 2.95, 3.00, 5.00, 10.0, 15.0, and 20.0. The definition of FOM is available in U.S. patent Application Publication No. 2023/0292605, and its entire contents are incorporated herein by reference. In some embodiments, the at least one of the one or more organic layers comprises a compound or a formulation of the compound as disclosed in Sections A and D of the present disclosure.

[0291] In some embodiments, the OLED or the emissive region comprising the inventive compound disclosed herein can be incorporated into a full-color pixel arrangement of a device. The full-color pixel arrangement of such a device comprises at least one pixel, wherein the at least one pixel comprises a first subpixel and a second subpixel. The first subpixel includes a first OLED comprising a first emissive region. The second subpixel includes a second OLED comprising a second emissive region. In some embodiments, the first and/or second OLED, the first and/or second emissive region can be the same or different and each can independently have the various device characteristics and the various embodiments of the inventive compounds included therein, and various combinations and subcombinations of the various device characteristics and the various embodiments of the inventive compounds included therein, as disclosed herein.

[0292] In some embodiments, the first emissive region is configured to emit a light having a peak wavelength $\lambda_{\text{sub.max1}}$; the second emissive region is configured to emit a light having a peak wavelength $\lambda_{\text{sub.max2}}$. In some embodiments, the difference between the peak wavelengths $\lambda_{\text{sub.max1}}$ and $\lambda_{\text{sub.max2}}$ is at least 4 nm but within the same color. For example, a light blue and a deep blue light as described above. In some embodiments, a first emissive region is configured to emit a light having a peak wavelength $\lambda_{\text{sub.max1}}$ in one region of the visible spectrum of 400-500 nm, 500-600 nm, 600-700 nm; and a second emissive region is configured to emit light having a peak wavelength $\lambda_{\text{sub.max2}}$ in one of the remaining regions of the visible spectrum of 400-500 nm, 500-600 nm, 600-700 nm. In some embodiments, the first emissive region comprises a first number of emissive layers that are deposited one over the other if more than one; and the second emissive region comprises a second number of emissive layers that is deposited one over the other if more than one; and the first number is different from the second number. In some embodiments, both the first emissive region and the second emissive region comprise a phosphorescent material, which may be the same or different. In some embodiments, the first emissive region comprises a phosphorescent material, while the second emissive region comprises a fluorescent material. In some embodiments, both the first emissive region and the second emissive region comprise a fluorescent material, which may be the same or different.

[0293] In some embodiments, the at least one pixel of the OLED or emissive regions includes a total of N subpixels; wherein the N subpixels comprises the first subpixel and the second subpixel; wherein each of the N subpixels comprises an emissive region; wherein the total number of the emissive regions within the at least one pixel is equal to or less than N-1. In some embodiments, the second emissive region is exactly the same as the first emissive region; and each subpixel of the at least one pixel comprises the same one emissive region as the first emissive region. In some

embodiments, the full-color pixel arrangements can have a plurality of pixels comprising a first pixel region and a second pixel region; wherein at least one display characteristic in the first pixel region is different from the corresponding display characteristic of the second pixel region, and wherein the at least one display characteristic is selected from the group consisting of resolution, cavity mode, color, outcoupling, and color filter.

[0294] In some embodiments, the OLED is a stacked OLED comprising one or more charge generation layers (CGLs). In some embodiments, the OLED comprises a first electrode, a first emissive region disposed over the first electrode, a first CGL disposed over the first emissive region, a second emissive region disposed over the first CGL, and a second electrode disposed over the second emissive region. In some embodiments, the first and/or the second emissive regions can have the various device characteristics as described above for the pixelated device. In some embodiments, the stacked OLED is configured to emit white color. In some embodiments, one or more of the emissive regions in a pixelated or in a stacked OLED comprises a sensitizer and an acceptor with the various sensitizing device characteristics and the various embodiments of the inventive compounds disclosed herein. For example, the first emissive region is comprised in a sensitizing device, while the second emissive region is not comprised in a sensitizing device; in some instances, both the first and the second emissive regions are comprised in sensitizing devices.

[0295] In some embodiments, the OLED can emit light having at least 1%, 5%, 10, 30%, 50%, 70%, 80%, 90%, 95%, 99%, or 100% from the plasmonic mode. In some embodiments, at least one of the anode, the cathode, or a new layer disposed over the organic emissive layer functions as an enhancement layer. The enhancement layer comprises a plasmonic material exhibiting surface plasmon resonance that non-radiatively couples to the emitter material and transfers excited state energy from the emitter material to non-radiative mode of surface plasmon polariton. In some embodiments, the enhancement layer is provided no more than a threshold distance away from the organic emissive layer, wherein the emitter material has a total non-radiative decay rate constant and a total radiative decay rate constant due to the presence of the enhancement layer. A threshold distance is where the total non-radiative decay rate constant is equal to the total radiative decay rate constant. Another threshold distance is the distance at which the total radiative decay rate constant divided by the sum of the total non-radiative decay rate constant and total radiative decay rate constant is equal to the photoluminescent yield of the emissive material without the enhancement layer present.

[0296] In some embodiments, the OLED further comprises an outcoupling layer. In some embodiments, the outcoupling layer is disposed over the enhancement layer on a side opposite the organic emissive layer. The outcoupling layer scatters the energy from the surface plasmon polaritons. In some embodiments this energy is scattered as photons to free space. In other embodiments, the energy is scattered from the surface plasmon mode into other modes of the device such as but not limited to the organic waveguide mode, the substrate mode, or another waveguiding mode. In some embodiments, one or more intervening layer can be disposed between the enhancement layer and the outcoupling layer. The examples for intervening layer(s) can be dielectric materials, including organic, inorganic, perovskites, oxides, and may include stacks and/or mixtures of these materials.

[0297] The enhancement layer modifies the effective properties of the medium in which the emitter material resides resulting in any or all of the following: a decreased rate of emission, a modification of emission line-shape, a change in emission intensity with angle, a change in the stability of the emitter material, a change in the efficiency of the OLED, and a reduced efficiency roll-off of the OLED device. Placement of the enhancement layer on the cathode side, anode side, or on both sides, or the enhancement layer itself being as the CGL, results in OLED devices which take advantage of any of the above-mentioned effects. In addition to the specific functional layers mentioned herein and illustrated in the various OLED examples shown in the figures, the OLEDs according to the present disclosure may include any of the other functional layers often found in

OLEDs.

[0298] In some embodiments, the enhancement layer can be comprised of plasmonic materials, optically active metamaterials, or hyperbolic metamaterials. In some embodiments, the plasmonic material includes at least one metal. In such embodiments the metal may include at least one of Ag, Al, Au, Ir, Pt, Ni, Cu, W, Ta, Fe, Cr, Mg, Ga, Rh, Ti, Ru, Pd, In, Bi, or Ca, alloys or mixtures of these materials, and stacks of these materials. In some embodiments, the enhancement layer is provided as a planar layer. In other embodiments, the enhancement layer has wavelength-sized features that are arranged periodically, quasi-periodically, or randomly, or sub-wavelength-sized features that are arranged periodically, quasi-periodically, or randomly.

[0299] In some embodiments, the outcoupling layer has wavelength-sized or sub-wavelength sized features that are arranged periodically, quasi-periodically, or randomly. In some embodiments, the outcoupling layer may be composed of a plurality of nanoparticles. In some embodiments, the outcoupling layer is composed of a plurality of nanoparticles disposed over a material. In these embodiments the outcoupling layer may be tunable by at least one of: varying a size of the plurality of nanoparticles, varying a shape of the plurality of nanoparticles, changing a material of the plurality of nanoparticles, adjusting a thickness of the material, changing the refractive index of the material, adding an additional layer disposed on the plurality of nanoparticles, varying a thickness of the enhancement layer, or varying the material of the enhancement layer. The plurality of nanoparticles of the device may be formed from at least one of metal, dielectric material, semiconductor materials, an alloy of metal, a mixture of dielectric materials, a stack or layering of one or more materials, and/or a core of one type of material and that is coated with a shell of a different type of material. In some embodiments, the outcoupling layer is composed of at least metal nanoparticles wherein the metal is selected from the group consisting of Ag, Al, Au, Ir, Pt, Ni, Cu, W, Ta, Fe, Cr, Mg, Ga, Rh, Ti, Ru, Pd, In, Bi, and Ca, alloys or mixtures of these materials, and stacks of these materials. In some embodiments the outcoupling layer is formed by lithography.

[0300] In some embodiments of a plasmonic device, the emitter, and/or host compounds used in the emissive layer has a vertical dipole ratio (VDR) of 0.33 or more. In some such embodiments, the emitter, and/or host compounds have a VDR of 0.40, 0.50, 0.60, 0.70, or more.

[0301] In yet another aspect, the present disclosure also provides a consumer product comprising an organic light-emitting device (OLED) having an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer may comprise a compound or a formulation of the compound as disclosed in the above compounds section of the present disclosure.

[0302] In some embodiments, the consumer product comprises an OLED having an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer may comprise a compound having a first ligand L.sub.A comprising a structure of Formula I disclosed herein.

[0303] Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, and an “exciton,” which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized as an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

[0304] FIG. 1 shows an organic light emitting device **100**. The figures are not necessarily drawn to scale. Device **100** may include a substrate **110**, an anode **115**, a hole injection layer (HIL) **120**, a hole transport layer (HTL) **125**, an electron blocking layer (EBL) **130**, an emissive layer (EML) **135**, a hole blocking layer (HBL) **140**, an electron transport layer (ETL) **145**, an electron injection layer (EIL) **150**, a protective layer **155**, a cathode **160**, and a barrier layer **170**. Cathode **160** is a

compound cathode having a first conductive layer **162** and a second conductive layer **164**. Device **100** may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

[0305] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with Fa-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

[0306] FIG. 2 shows an inverted OLED **200**. The device includes a substrate **210**, a cathode **215**, an emissive layer **220**, a hole transport layer **225**, and an anode **230**. Device **200** may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device **200** has cathode **215** disposed under anode **230**, device **200** may be referred to as an “inverted” OLED. Materials similar to those described with respect to device **100** may be used in the corresponding layers of device **200**. FIG. 2 provides one example of how some layers may be omitted from the structure of device **100**.

[0307] The simple layered structure illustrated in FIGS. 1 and 2 is provided by way of non-limiting example, and it is understood that embodiments of the present disclosure may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device **200**, hole transport layer **225** transports holes and injects holes into emissive layer **220**, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an “organic layer” disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.

[0308] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED

structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties. [0309] Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP, also referred to as organic vapor jet deposition (OVJD)), such as described in U.S. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation, sputtering, chemical vapor deposition, atomic layer deposition, and electron beam deposition. Preferred patterning methods include deposition through a mask, photolithography, and cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and organic vapor jet printing (OVJP). Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons are a preferred range. Materials with asymmetric structures may have better solution processability than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

[0310] Devices fabricated in accordance with embodiments of the present disclosure may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a plurality of alternative layers of polymeric material and non-polymeric material; organic material and inorganic material; or a mixture of a polymeric material and a non-polymeric material as one example described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties.

[0311] Devices fabricated in accordance with embodiments of the present disclosure can be incorporated into a wide variety of electronic component modules (or units) that can be incorporated into a variety of electronic products or intermediate components. Examples of such electronic products or intermediate components include display screens, lighting devices such as discrete light source devices or lighting panels, etc. that can be utilized by the end-user product manufacturers. Such electronic component modules can optionally include the driving electronics and/or power source(s). Devices fabricated in accordance with embodiments of the present disclosure can be incorporated into a wide variety of consumer products that have one or more of the electronic component modules (or units) incorporated therein. A consumer product comprising an OLED that includes the compound of the present disclosure in the organic layer in the OLED is

disclosed. Such consumer products would include any kind of products that include one or more light source(s) and/or one or more of some type of visual displays. Some examples of such consumer products include flat panel displays, curved displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads-up displays, fully or partially transparent displays, flexible displays, rollable displays, foldable displays, stretchable displays, laser printers, telephones, mobile phones, tablets, phablets, personal digital assistants (PDAs), wearable devices, laptop computers, digital cameras, camcorders, viewfinders, micro-displays (displays that are less than 2 inches diagonal), 3-D displays, virtual reality or augmented reality displays, vehicles, video walls comprising multiple displays tiled together, theater or stadium screen, a light therapy device, and a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present disclosure, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25° C.), but could be used outside this temperature range, for example, from -40 degree C. to +80° C.

[0312] More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

[0313] The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

[0314] In some embodiments, the OLED has one or more characteristics selected from the group consisting of being flexible, being rollable, being foldable, being stretchable, and being curved. In some embodiments, the OLED is transparent or semi-transparent. In some embodiments, the OLED further comprises a layer comprising carbon nanotubes. In some embodiments, the OLED further comprises one or more quantum dots. Such quantum dots can be in the emissive layer, or in other functional layers, such as a down conversion layer.

[0315] In some embodiments, the OLED comprises a RGB pixel arrangement or white plus color filter pixel arrangement. In some embodiments, the OLED is a mobile device, a handheld device, or a wearable device. In some embodiments, the OLED is a display panel having less than 10 inch diagonal or 50 square inch area. In some embodiments, the OLED is a display panel having at least 10 inch diagonal or 50 square inch area. In some embodiments, the OLED is a lighting panel.

D. Other Materials Used in the OLED

[0316] The materials described herein are as various examples useful for a particular layer in an OLED. They may also be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used by themselves in the EML, or in conjunction with a wide variety of other emitters, hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds and the devices disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

a) Conductivity Dopants:

[0317] A charge transport layer can be doped with conductivity dopants to substantially alter its density of charge carriers, which will in turn alter its conductivity. The conductivity is increased by generating charge carriers in the matrix material, and depending on the type of dopant, a change in the Fermi level of the semiconductor may also be achieved. Hole-transporting layer can be doped by p-type conductivity dopants and n-type conductivity dopants are used in the electron-transporting layer. In some embodiments, conductivity dopants comprise at least one chemical moiety selected from the group consisting of cyano, fluorinated aryl or heteroaryl, fluorinated alkyl or cycloalkyl, alkylene, heteroaryl, amide, benzodithiophene, and highly conjugated heteroaryl

groups extended by non-rings double bonds.

b) HIL/HTL:

[0318] A hole injecting/transporting material to be used in the present disclosure is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but are not limited to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as MoO₃; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-

Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

[0319] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:

##STR00920##

[0320] Each of Ar^{sup.1} to Ar^{sup.9} is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and the group consisting of 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Each of Ar^{sup.1} to Ar^{sup.9} may be unsubstituted or may be substituted by a general substituent as described above, any two substituents can be joined or fused into a ring.

[0321] In some embodiments, each Ar^{sup.1} to Ar^{sup.9} independently comprises a moiety selected from the group consisting of:

##STR00921## [0322] wherein k is an integer from 1 to 20; X^{sup.101} to X^{sup.108} is C or N; Z^{sup.101} is C, N, O, or S.

[0323] Examples of metal complexes used in HIL or HTL include, but are not limited to the following general formula:

##STR00922## [0324] wherein Met is a metal, which can have an atomic weight greater than 40; (Y^{sup.101}-Y^{sup.102}) is a bidentate ligand, the coordinating atoms of Y^{sup.101} and Y^{sup.102} are independently selected from C, N, O, P, and S; L^{sup.101} is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k'' is the maximum number of ligands that may be attached to the metal.

[0325] In some embodiments, (Y^{sup.101}-Y^{sup.102}) is a 2-phenylpyridine or 2-phenylimidazole derivative. In some embodiments, (Y^{sup.101}-Y^{sup.102}) is a carbene ligand. In some embodiments, Met is selected from Ir, Pt, Pd, Os, Cu, and Zn. In some embodiments, the metal complex has a smallest oxidation potential in solution vs. Fc^{sup.+}/Fc couple less than about 0.6 V.

[0326] In some embodiments, the HIL/HTL material is selected from the group consisting of phthalocyanine and porphyrin compounds, starburst triarylamine, CF_x fluorohydrocarbon polymer, conducting polymers (e.g., PEDOT:PSS, polyaniline, polythiophene), phosphonic acid

and silane SAMs, triarylamine or polythiophene polymers with conductivity dopants, Organic compounds with conductive inorganic compounds (such as molybdenum and tungsten oxides), n-type semiconducting organic complexes, metal organometallic complexes, cross-linkable compounds, polythiophene based polymers and copolymers, triarylamine, triarylamine with spirofluorene core, arylamine carbazole compounds, triarylamine with (di)benzothiophene/(di)benzofuran, indolocarbazoles, isoindole compounds, and metal carbene complexes.

c) EBL:

[0327] An electron blocking layer (EBL) may be used to reduce the number of electrons and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies, and/or longer lifetime, as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and/or higher triplet energy than one or more emitters closest to the EBL interface. In some embodiments, the compound used in EBL contains at least one carbazole group and/or at least one arylamine group. In some embodiments the HOMO level of the compound used in the EBL is shallower than the HOMO level of one or more of the hosts in the EML. In some embodiments, the compound used in EBL contains the same molecule or the same functional groups used as one of the hosts described herein.

d) Hosts:

[0328] The light emitting layer of the organic EL device of the present disclosure preferably contains at least a light emitting material as the dopant, and a host material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the host won't fully quench the emission of the dopant.

[0329] Examples of metal complexes used as host are preferred to have the following general formula:

##STR00923## [0330] wherein Met is a metal; (Y.sup.103-Y.sup.104) is a bidentate ligand, the coordinating atoms of Y.sup.103 and Y.sup.104 are independently selected from C, N, O, P, and S; L.sup.101 is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k'' is the maximum number of ligands that may be attached to the metal.

[0331] In some embodiments, the metal complexes are:

##STR00924## [0332] wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

[0333] In some embodiments, Met is selected from Ir and Pt. In a further embodiment, (Y.sup.103-Y.sup.104) is a carbene ligand.

[0334] In some embodiments, the host compound contains at least one of the following groups selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, aza-dibenzothiophene, aza-dibenzofuran, aza-dibenzoselenophene, aza-carbazole, aza-indolocarbazole, aza-triphenylene, aza-tetraphenylene, 5λ.sup.2-benzo[d]benzo[4,5]imidazo[3,2-a]imidazole, 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene; and the group consisting of 2 to 10 cyclic structural

units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Each option within each group may be unsubstituted or may be substituted by the General Substituents as described herein or may be further fused.

[0335] In some embodiments, the host compound comprises at least one of the moieties selected from the group consisting of:

##STR00925## ##STR00926##

wherein k is an integer from 0 to 20 or 1 to 20. X¹⁰¹ to X¹⁰⁸ are independently selected from C or N. Z¹⁰¹ and Z¹⁰² are independently selected from C, N, O, or S.

[0336] In some embodiments, the host material is selected from the group consisting of arylcarbazoles, metal 8-hydroxyquinolates, (e.g., alq₃, balq), metal phenoxybenzothiazole compounds, conjugated oligomers and polymers (e.g., polyfluorene), aromatic fused rings, zinc complexes, chrysene based compounds, aryltriphenylene compounds, poly-fused heteroaryl compounds, donor acceptor type molecules, dibenzofuran/dibenzothiophene compounds, polymers (e.g., pvk), spirofluorene compounds, spirofluorene-carbazole compounds, indolocbazoles, 5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole), tetraphenylene complexes, metal phenoxypyridine compounds, metal coordination complexes (e.g., Zn, Al with N{circumflex over ()}N ligands), dibenzothiophene/dibenzofuran-carbazole compounds, silicon/germanium aryl compounds, aryl benzoyl esters, carbazole linked by non-conjugated groups, aza-carbazole/dibenzofuran/dibenzothiophene compounds, and high triplet metal organometallic complexes (e.g., metal-carbene complexes).

e) Emitter Materials in EML:

[0337] One or more emitter materials may be used in conjunction with the compound or device of the present disclosure. The emitter material can be emissive or non-emissive in the current device as described herein. Examples of the emitter materials are not particularly limited, and any compounds may be used as long as the compounds are capable of producing emissions in a regular OLED device. Examples of suitable emitter materials include, but are not limited to, compounds which are capable of producing emissions via phosphorescence, non-delayed fluorescence, delayed fluorescence, especially the thermally activated delayed fluorescence, i.e., TADF (also referred to as E-type delayed fluorescence), triplet-triplet annihilation, or combinations of these processes.

[0338] In some embodiments, the emitter material has the formula of M(L¹)_x

(L²)_y(L³)_z; [0339] wherein L¹, L², and L³ can be the same or

different; [0340] wherein x is 1, 2, or 3; [0341] wherein y is 0, 1, or 2; [0342] wherein z is 0, 1, or

2; [0343] wherein x+y+z is the oxidation state of the metal M; [0344] wherein L¹ is selected

from the group consisting of the structures of LIGAND LIST:

##STR00927## ##STR00928## ##STR00929## ##STR00930## ##STR00931## [0345] wherein

each L² and L³ are independently selected from the group consisting of

##STR00932##

and the structures of LIGAND LIST; wherein: [0346] M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt, Pd, Zn, Au, Ag, and Cu; [0347] T is selected from the group consisting of B, Al, Ga, and In; [0348] K^{1'} is a direct bond or is selected from the group consisting of NR_e, PR_e, O, S, and Se; [0349] each Y¹ to Y¹⁵ are independently selected from the group consisting of carbon and nitrogen; [0350] Y' is selected from the group consisting of BR_e, NR_e, PR_e, O, S, Se, C=O, S=O, SO₂, CR_e, SiR_e, and GeR_e; [0351] each R_a, R_b, R_c, and R_d can independently represent from mono to the maximum possible number of substitutions, or no substitution; [0352] each R_{a1}, R_{b1}, R_{c1}, R_{d1}, R_a, R_b, R_c, R_d, R_e, and R_f is independently a hydrogen or a substituent selected from the group consisting of the General

Substituents as defined herein; and

wherein any two substituents can be fused or joined to form a ring or form a multidentate ligand.

[0353] In some embodiments, the emitter material is selected from the group consisting of the following Dopant Group 1:

##STR00933## ##STR00934## ##STR00935## ##STR00936## [0354] wherein [0355] each of X.sup.96 to X.sup.99 is independently C or N; [0356] each Y.sup.100 is independently selected from the group consisting of a NR'', O, S, and Se; [0357] each of R.sup.10a, R.sup.20a, R.sup.30a, R.sup.40a, and R.sup.50a independently represents mono substitution, up to the maximum substitutions, or no substitution; [0358] each of R, R', R'', R.sup.10a, R.sup.11a, R.sup.12a, R.sup.13a, R.sup.20a, R.sup.30a, R.sup.40a, R.sup.50a, R.sup.60a, R.sup.70a, R.sup.97, R.sup.98, and R.sup.99 is independently a hydrogen or a substituent selected from the group consisting of the General Substituents as defined herein; any two substituents can be joined or fused to form a ring. [0359] In some embodiments, the emitter material is selected from the group consisting of the following Dopant Group 2:

##STR00937## ##STR00938## ##STR00939## ##STR00940## ##STR00941## ##STR00942## ##STR00943## ##STR00944## ##STR00945## ##STR00946## ##STR00947## ##STR00948## ##STR00949## ##STR00950## ##STR00951## ##STR00952## ##STR00953## ##STR00954## [0360] wherein: [0361] each Y.sup.100 is independently selected from the group consisting of a NR'', O, S, and Se; [0362] L is independently selected from the group consisting of a direct bond, BR'', BR''R'', NR'', PR'', O, S, Se, C=O, C=S, C=Se, C=NR'', C=CR''R'', S=O, SO.sub.2, CR'', CR''R'', SiR''R'', GeR''R'', alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof; [0363] X.sup.100 and X.sup.200 for each occurrence is selected from the group consisting of O, S, Se, NR'', and CR''R''; [0364] each R.sup.A'', R.sup.B'', R.sup.C'', R.sup.D'', R.sup.E'', and R.sup.F'' independently represents mono-, up to the maximum substitutions, or no substitutions; [0365] each of R, R', R'', R''', R.sup.A1', R.sup.A2', R.sup.A'', R.sup.B'', R.sup.C'', R.sup.D'', R.sup.E'', R.sup.F'', R.sup.G'', R.sup.H'', R.sup.I'', R.sup.J'', R.sup.K'', R.sup.L'', R.sup.M'', and R.sup.N'' is independently a hydrogen or a substituent selected from the group consisting of the General Substituents as defined herein; and any two substituents can be joined or fused to form a ring. [0366] In some embodiments of the above Dopant Groups 1 and 2, each unsubstituted aromatic carbon atom can be replaced with N to form an aza-ring. In some embodiments, the maximum number of N atom in one ring is 1 or 2. In some embodiments of the above Dopant Groups 2, Pt atom in each formula can be replaced by Pd atom.

[0367] In some embodiments of the OLED, the delayed fluorescence material comprises at least one donor group and at least one acceptor group. In some embodiments, the delayed fluorescence material is a metal complex. In some embodiments, the delayed fluorescence material is a non-metal complex. In some embodiments, the delayed fluorescence material is a Zn, Cu, Ag, or Au complex.

[0368] In some embodiments of the OLED, the delayed fluorescence material has the formula of M(L.sup.5)(L.sup.6), wherein M is Cu, Ag, or Au, L.sup.5 and L.sup.6 are different, and L.sup.5 and L.sup.6 are independently selected from the group consisting of:

##STR00955## [0369] wherein A.sup.1-A.sup.9 are each independently selected from C or N; [0370] each R.sup.P, R.sup.Q, and R.sup.U independently represents mono-, up to the maximum substitutions, or no substitutions; [0371] wherein each R.sup.P, R.sup.P, R.sup.U, R.sup.SA, R.sup.SB, R.sup.RA, R.sup.RB, R.sup.RC, R.sup.RD, R.sup.RE, and R.sup.RF is independently a hydrogen or a substituent selected from the group consisting of the General Substituents as defined herein; any two substituents can be joined or fused to form a ring.

[0372] In some embodiments of the OLED, the delayed fluorescence material comprises at least one of the donor moieties selected from the group consisting of:

##STR00956## ##STR00957## ##STR00958##

wherein Y.sup.T, Y.sup.U, Y.sup.V, and Y.sup.W are each independently selected from the group

consisting of B, C, Si, Ge, N, P, O, S, Se, C=O, S=O, and SO.sub.2.

[0373] In some of the above embodiments, any carbon ring atoms up to maximum of a total number of three, together with their substituents, in each phenyl ring of any of above structures can be replaced with N.

[0374] In some embodiments, the delayed fluorescence material comprises at least one of the acceptor moieties selected from the group consisting of nitrile, isonitrile, borane, fluoride, pyridine, pyrimidine, pyrazine, triazine, aza-carbazole, aza-dibenzothiophene, aza-dibenzofuran, aza-dibenzoselenophene, aza-triphenylene, imidazole, pyrazole, oxazole, thiazole, isoxazole, isothiazole, triazole, thiadiazole, and oxadiazole. In some embodiments, the acceptor moieties and the donor moieties as described herein can be connected directly, through a conjugated linker, or a non-conjugated linker, such as a sp³ carbon or silicon atom.

[0375] In some embodiments, the fluorescent material comprises at least one of the chemical moieties selected from the group consisting of:

##STR00959## ##STR00960## ##STR00961## ##STR00962## ##STR00963## ##STR00964##

##STR00965## [0376] wherein Y^{sup}.F, Y^{sup}.G, Y^{sup}.H, and Y^{sup}.I are each independently selected from the group consisting of B, C, Si, Ge, N, P, O, S, Se, C=O, S=O, and SO.sub.2;

[0377] wherein X^{sup}.F and X^{sup}.G are each independently selected from the group consisting of C and N.

[0378] In some of the above embodiments, any carbon ring atoms up to maximum of a total number of three, together with their substituents, in each phenyl ring of any of above structures can be replaced with N.

f) HBL:

[0379] A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies and/or longer lifetime as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the HBL material has a lower HOMO (further away from the vacuum level) and/or higher triplet energy than one or more of the emitters closest to the HBL interface.

[0380] In some embodiments, a compound used in the HBL contains the same molecule or the same functional groups used as host described above.

[0381] In some embodiments, a compound used in the HBL comprises at least one of the following moieties selected from the group consisting of:

##STR00966## [0382] wherein k is an integer from 1 to 20; L^{sup}.101 is another ligand, k' is an integer from 1 to 3.

g) ETL:

[0383] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

[0384] In some embodiments, compound used in ETL comprises at least one of the following moieties in the molecule:

##STR00967##

and fullerenes; wherein k is an integer from 1 to 20, X^{sup}.101 to X^{sup}.108 is selected from C or N; Z^{sup}.101 is selected from the group consisting of C, N, O, and S.

[0385] In some embodiments, the metal complexes used in ETL contains, but not limit to the following general formula:

##STR00968## [0386] wherein (O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L^{sup}.101 is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

[0387] In some embodiments, the ETL material is selected from the group consisting of anthracene-benzimidazole compounds, aza triphenylene derivatives, anthracene-benzothiazole compounds, metal 8-hydroxyquinolates, metal hydroxybenzoquinolates, bathocuprine compounds, 5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzimidazole), silole compounds, arylborane compounds, fluorinated aromatic compounds, fullerene (e.g., C60), triazine complexes, and Zn (N{circumflex over ()})N complexes.

h) Charge Generation Layer (CGL)

[0388] In tandem or stacked OLEDs, the CGL plays an essential role in the performance, which is composed of an n-doped layer and a p-doped layer for injection of electrons and holes, respectively. Electrons and holes are supplied from the CGL and electrodes. The consumed electrons and holes in the CGL are refilled by the electrons and holes injected from the cathode and anode, respectively; then, the bipolar currents reach a steady state gradually. Typical CGL materials include n and p conductivity dopants used in the transport layers.

[0389] In any compounds disclosed herein, the hydrogen atoms can be partially or fully deuterated. The minimum amount of hydrogen of the compound being deuterated is selected from the group consisting of 30%, 40%, 50%, 60%, 70%, 80%, 90%, 95%, 99%, and 100%. As used herein, percent deuteration has its ordinary meaning and includes the percent of all possible hydrogen and deuterium atoms that are replaced by deuterium atoms. In some embodiments, the deuterium atoms are attached to an aromatic ring. In some embodiments, the deuterium atoms are attached to a saturated carbon atom, such as an alkyl or cycloalkyl carbon atom. In some other embodiments, the deuterium atoms are attached to a heteroatom, such as Si, or Ge atom.

[0390] It is understood that the various embodiments described herein are by way of example only and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

E. Experimental Data

##STR00969##

Synthesis of 3-Chloro-2,6-difluoro-N,N-bis(2-methoxyphenyl)aniline

[0391] 1-Iodo-2-methoxybenzene (25.8 g, 14.3 mL, 3 Eq, 110 mmol), 3-chloro-2,6-difluoroaniline (6.00 g, 1 Eq, 36.7 mmol), potassium carbonate (30.4 g, 6 Eq, 220 mmol) and 18-crown-6 (1.94 g, 0.2 Eq, 7.34 mmol) were suspended in dry o-dichlorobenzene (100 mL) under nitrogen and degassed for 15 min. Copper (6.99 g, 3 Eq, 110 mmol) was added and the reaction mixture was stirred at 180° C. overnight then at 200° C. overnight. The mixture was cooled to room temperature, the copper solids filtered off, the solids washed with EtOAc and the combined filtrates concentrated. The residue was purified by silica chromatography eluting with an isohexanes:EtOAc gradient. The desired fractions were collected and concentrated under reduced pressure. The resulting solid was suspended in hexanes and stirred at room temperature for 5 h. The solids were filtered off and dried in vacuo to 2.12 g of product.

##STR00970##

Synthesis of 2,2'-((3-Chloro-2,6-difluorophenyl)azanediyl)diphenol

[0392] 3-Chloro-2,6-difluoro-N,N-bis(2-methoxyphenyl)aniline (9.32 g, 1 Eq, 24.3 mmol) was dissolved in dry DCM (150 mL) under nitrogen at cooled to 5° C. BBr₃ (1M in DCM) (15 g, 60 mL, 1.00 molar, 2.5 Eq, 60 mmol) was added portion wise over 10 min and the reaction allowed to warm slowly to RT over 18 h. The reaction mixture was quenched portion wise into ice-cold MeOH (400 mL) over 10 min and the resulting mixture stirred in an icebath for 5 hours. The resulting thin suspension was concentrated in vacuo to give a solid. This was suspended in water (100 mL) and stirred at room temperature for 4 hours. The solids were filtered off, dried in vacuo,

then azeotropically with MeCN then hexane to afford 8.91 g of 2,2'-((3-chloro-2,6-difluorophenyl)azanediyl)diphenol.

##STR00971##

Synthesis of 6-Chlorobenzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine

[0393] 2,2'-((3-Chloro-2,6-difluorophenyl)azanediyl)diphenol (8.91 g, 24.9 mmol) and potassium carbonate (10.3 g, 3 Eq, 74.6 mmol) were dissolved in dry DMF (150 mL) under nitrogen and heated to 100° C. for 5 hours. The reaction mixture was cooled to room temperature to form a tan suspension. Water (225 mL) was added and the mixture was stirred at room temperature for 40 min. The solids were filtered off, washed with water (3×50 mL) and dried in vacuo, then dried azeotropically with MeCN, then hexane to 7.49 g of 6-chlorobenzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine.

##STR00972##

Synthesis of 6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine

[0394] 6-Chlorobenzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (5.08 g, 1 Eq, 16.2 mmol) and bispin (4.93 g, 1.2 Eq, 19.4 mmol) were suspended in MeTHF (100 mL), potassium carbonate (4.92 g, 2.2 Eq, 35.6 mmol) and KEH (0.5 M in THF) (177 mg, 1.94 mL, 0.50 molar, 0.06 Eq, 971 µmol) were added. The reaction mixture was degassed with nitrogen for 15 min. XPhos (386 mg, 0.05 Eq, 809 µmol) and XPhosPd(crotyl)Cl (545 mg, 0.05 Eq, 809 µmol) were added and the reaction mixtures heated to 52° C. (baseplate) overnight. The reaction mixture was filtered and the solid washed with EtOAc (2×50 mL). The filtrate was concentrated in vacuo to give a brown solid, 8.74 g. This solid was triturated with MeOH (20 mL) and stirred for 5 min. The resulting solid was filtered off to give 7.75 g of product.

##STR00973##

Synthesis of 6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine

[0395] 6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (3.40 g, 1 Eq, 7.49 mmol), 2-chloro-4-(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridine (1.67 g, 1.1 Eq, 8.24 mmol) and XPhosPd(crotyl)Cl (252 mg, 0.05 Eq, 375 µmol) were placed in a round bottom flask and pump evacuated/nitrogen filled 5×. Dry MeTHF (135 mL) was added and the mixture sonicated to form a dark brown solution. A solution of potassium phosphate tribasic (4.77 g, 3 Eq, 22.5 mmol) in water (40 mL) was added to the reaction mixture while rapidly stirring and the reaction mixture was further degassed by pump evacuation/nitrogen filling 5 times. The reaction mixture was heated to 60° C. (baseplate T, pre-heated) for 30 min. The reaction mixture was cooled to room temperature, diluted with EtOAc (500 mL) and water (100 mL), the phases were separated, the resulting organics were dried over Na.sub.2SO.sub.4, filtered and concentrated in vacuo to give a dark brown oil. The crude product was purified by silica chromatography eluting with a DCM:EtOAc gradient then the desired fractions were concentrated and further purified by reverse-phase chromatography eluting with a gradient of MeCN:THF:water. The pure material was dissolved in DCM (80 mL), diluted with 2M NaOH (25 mL) and stirred for 10 min, the phases were separated, and the organics were dried over Na.sub.2SO.sub.4, filtered and concentrated in vacuo, then dried azeotropically with MtBE to give 855 mg of 6-(4-(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridin-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine.

##STR00974##

Synthesis Inventive Compound 1

[0396] (CD₃)₂ppy iridium (III) solvato complex (89 mg, 1 Eq, 0.11 mmol) and 6-(4-(2,2-dimethylpropyl-1,1-d₂)-5-(methyl-d₃)pyridin-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (0.050 g, 1 Eq, 0.11 mmol) were added to a Schlenk tube charge with a stir bar. The reaction vessel was sealed with a septum, evacuated and back-filled with N.sub.2 three times, then the reagents

were dissolved in 2-ethoxyethanol (0.93 mL). The reaction solution was purged with N.sub.2 for five minutes, treated with 2,6-dimethylpyridine (30 mg, 33 μ L, 2.5 Eq, 0.28 mmol) via syringe, then heated to 135° C. for 20 hours. The crude mixture was purified by silica chromatography eluting with a toluene:heptane gradient. The desired fractions were concentrated in vacuo to yield 0.024 g of the inventive compound.

##STR00975##

[0397] Photoluminescence (PL) spectra of the inventive example and comparative example were taken in PMMA. The Inventive Compound 1 showed narrower lineshape (FWHM=81 nm) compared to the Comparative Compound (FWHM=90 nm) (Table 1). This improvement in lineshape is believed to be due to the excited state centered on the fused, triangulane moiety in the Inventive Compound 1 versus the freely rotating naphthyl group of the Comparative Compound.

TABLE-US-00008

Compound	λ max (nm)	FWHM (nm)
Inventive Compound 1	544	81
Comparative Compound	546	96

##STR00976##

Synthesis of ((2-bromo-1,3-phenylene)bis(oxy))dibenzene

[0398] To a dry flask equipped with a mechanical stirrer, a thermowell and a reflux condenser, 1 eq. of phenol, 2.3 eq potassium carbonate and NMP were added and stirred, 0.45 eq. of 2-Bromo-1,3-difluorobenzene was added then the reaction mixture was heated to 120° C. overnight. After 16 hours, the temperature was raised to 150° C. After 72 hours, the reaction mixture was cooled to room temperature and added into ice cold water to obtain a suspension which was filtered and washed with water. The solid was isolated in air, washed with MeOH and dried to obtain the product.

##STR00977##

Synthesis of ((2-bromo-1,3-phenylene)bis(oxy))dibenzene

[0399] To a flask under nitrogen was added 1 eq. of ((2-bromo-1,3-phenylene)bis(oxy))dibenzene and m-xylene. The solution was cooled to -40° C. and 1.05 eq. of 2.3 M hexyllithium in hexane was added slowly. The reaction was removed from the cooling bath and warmed to room temperature. The reaction mixture was heated to 60° C. for 3 hours then cooled to -30° C. and 1.15 eq. tribromoborane (25.5 ml, 270 mmol) was added slowly. The reaction mixture was removed from the cooling bath and stirred as it warmed to room temperature overnight. After stirring for 18 hours the solution was cooled to 0° C. and 2.5 eq. N-ethyl-N-isopropylpropan-2-amine is added slowly. The reaction mixture was heated to 126° C. for 2 hours. The reaction mixture was cooled to 3° C. To the reaction mixture was added sat. NaOAc.sub.(aq and brine). The mixture was filtered and the filtrate was separated, concentrated, then triturated with heptane and filtered to yield the product.

##STR00978##

Synthesis of 8-bromo-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene

[0400] To a solution of 1 eq. Of 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene (27.0 g, 100 mmol) in DCM under nitrogen 0.9 eq. of N-bromosuccinimide is added and the reaction mixture was stirred at room temperature overnight. The reaction mixture was filtered and the solid obtained was washed with minimal DCM. The solid obtained upon air drying was triturated in MeOH then acetone to yield the desired product.

##STR00979##

Synthesis of 6-(4,4,5,5-tetramethyl-1,3,2-doxaborolan-2-yl)-5,9-doxa-13b-boranaphtho[3,2,1-de]anthracene

[0401] 1 eq. of 8-bromo-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene (5.08 g, 1 Eq, 16.2 mmol) and 1.2 eq. of bispin were suspended in MeTHF, 2.2 eq. of potassium carbonate and 0.06 KEH (0.5 M in THF) was added. The reaction mixture was degassed with nitrogen for 15 min then 0.05 eq. of XPhos and 0.05 eq. of XPhosPd(crotyl)Cl were added and the reaction mixture was heated to 52° C. overnight. The reaction mixture was filtered and the solid washed with EtOAc. The filtrate was

concentrated in vacuo then triturated with MeOH and stirred for 5 min. The resulting solid was filtered off to give the desired product.

##STR00980##

Synthesis of 2-(5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracen-yl)-4-(2,2-dimethylpropyl-1,1-d2)-5-(methyl-d3)pyridine

[0402] 1 eq. of 6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene, 1.1 eq. of 2-chloro-4-(2,2-dimethylpropyl-1,1-d2)-5-(methyl-d3) and 0.05 eq. of XPhosPd(crotyl)Cl were placed in a round bottom flask and pump evacuated/nitrogen filled. Dry MeTHF and a solution of 3 eq. of potassium phosphate tribasic in water were added to the stirring reaction. The mixture was further degassed by pump evacuation/nitrogen filling then heated to 60° C. for 30 min. The reaction mixture was cooled to room temperature then diluted with EtOAc and extracted with water. The organic phase was separated, dried over Na.sub.2SO.sub.4, filtered and concentrated in vacuo. The crude product was purified by silica chromatography eluting with a DCM:EtOAc gradient then the desired fractions were concentrated to yield the desired product.

##STR00981##

Synthesis Inventive Compound 2

[0403] 1 eq. of (CD.sub.3).sub.2 ppy iridium (III) solvato complex and 1 eq. of 2-(5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracen-6-yl)-4-(2,2-dimethylpropyl-1,1-d2)-5-(methyl-d3)pyridine are added to a Schlenk tube charged with a stir bar. The reaction vessel was sealed with a septum, evacuated and back-filled with N.sub.2 three times, then the reagents were dissolved in 2-ethoxyethanol. The reaction solution was purged with N.sub.2 for five minutes, treated with 2.5 eq. of 2,6-dimethylpyridine via syringe, then heated to 135° C. for 20 hours. The crude mixture was purified by silica chromatography eluting with a toluene:heptane gradient. The desired fractions were concentrated in vacuo to yield the inventive compound.

Claims

1. A compound having a first ligand L.sub.A comprising a structure of Formula I: ##STR00982## wherein 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 to 10-membered carbocyclic or heterocyclic ring; each of X.sup.1 to X.sup.12 and Z.sup.1 is independently C or N; Z is B or N; each of Y.sup.1, Y.sup.2, and Y.sup.3 is independently absent or selected from the group consisting of O, S, C=O, C=S, C=NR, CRR', and C=CRR', with at least one of them being present; each of K.sup.1 and K.sup.2 is independently selected from the group consisting of a direct bond, O, S, N(R.sup.α), P(R.sup.α), B(R.sup.α), C(R.sup.α)(R.sup.β), and Si(R.sup.α)(R.sup.β); each R.sup.A, R.sup.B, R.sup.C, and R.sup.D independently represents mono to the maximum allowable substitution, or no substitution; each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently a 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, selenyl, and combinations thereof; L.sub.A is coordinated to a metal M, having an atomic mass of at least 40; metal M can be coordinated to other ligands; any two substituents can be joined or fused to form a ring; and L.sub.A can join with other ligands to comprise a tridentate, tetradentate, pentadentate, or hexadentate ligand, with the proviso that if M is Ir, Y.sup.2 is present, and Y.sup.3 is absent, then moiety A is joined to X.sup.1 or X.sup.3, and K.sup.2 is joined to X.sup.2; and with the proviso that if M is Pt, then Z.sup.1 is not a carbene carbon.

2. The compound of claim 1, wherein each R, R', R.sup.α, R.sup.β, R.sup.A, R.sup.B, R.sup.C, and R.sup.D is independently 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 moiety A is independently selected from the group consisting of: 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, benzimidazole derived carbene, aza-benzimidazole derived carbene, carbazole, aza-carbazole, dibenzofuran, aza-dibenzofuran, dibenzothiophene, aza-dibenzothiophene, quinoxaline, phthalhine, phenanthrene, aza-phenanthrene, anthracene, aza-anthracene, phenanthridine, fluorene, and aza-fluorene.

4. The compound of claim 1, wherein Z^{sup.1} is N or carbene C; and/or wherein each of X^{sup.1} to X^{sup.12} is C or wherein at least one of X^{sup.1} to X^{sup.12} is N; and/or wherein Z is B or N; and/or wherein each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is independently O or S; and/or wherein each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} that is present is the same; and/or wherein K^{sup.1} is a direct bond, O, or S; and/or wherein K^{sup.2} is a direct bond, or S; and/or wherein metal M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt Pd, Ag, Au, and Cu.








5. The compound of claim 1, wherein each of Y^{sup.1}, Y^{sup.2}, and Y^{sup.3} is present; or wherein Y^{sup.1} and Y^{sup.2} are present, and Y^{sup.3} is absent; or wherein Y^{sup.1} is present, and Y^{sup.2} and Y^{sup.3} are absent.

6. The compound of claim 1, wherein at least one R^{sup.A} comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof; and/or wherein at least one R^{sup.B} comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof; and/or wherein at least one R^{sup.C} comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof; and/or wherein at least one R^{sup.D} comprises a substituent selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof; and/or wherein Formula I comprises an electron-withdrawing group selected from the group consisting of: F, CF₃, CN, COCH₃, CHO, COCF₃, COOMe, COOCF₃, NO₂, SF₃, SiF₃, PF₄, SF₅, OCF₃, SCF₃, SeCF₃, SOCF₃, SeOCF₃, SO₂F, SO₂CF₃, SeO₂CF₃, OSeO₂CF₃, OCN, SCN, SeCN, NC, ^{sup.+N(R^{sup.k2})₃, (R^{sup.k2})₂CCN, (R^{sup.k2})₂CCF₃, CNC(CF₃)₂, BR^{sup.k3}R^{sup.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, ##STR00983## ##STR00984## wherein each R^{sup.k1} represents mono to the maximum allowable substitution, or no substitutions; wherein Y^{sup.G} is selected from the group consisting of BR_e, NR_e, PR_e, O, S, Se, C=O, S=O, SO₂, CR_eR_f, SiR_eR_f, and GeR_eR_f; and wherein each of R^{sup.k1}, R^{sup.k2}, R^{sup.k3}, R_e, and R_f is independently a 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, selenyl, sulfinyl, sulfonyl, phosphino, and combinations}

thereof.

7. The compound of claim 1, wherein two R.sup.B are joined or fused to form moiety B1, wherein moiety B1 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 to 10-membered carbocyclic or heterocyclic ring; and/or wherein two R.sup.C are joined or fused to form moiety C1, wherein moiety C1 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 to 10-membered carbocyclic or heterocyclic ring.







8. The compound of claim 1, wherein the ligand L.sub.A is selected from the group consisting of: ##STR00985## ##STR00986## ##STR00987## ##STR00988## ##STR00989## ##STR00990## ##STR00991## ##STR00992## ##STR00993## wherein X.sub.15 to X.sub.19 are each independently C or N; each of Y.sub.4, Y.sub.5, and Y.sub.6 is independently absent or selected from the group consisting of O, S, C=O, C=S, C=NR, CRR', and C=CRR'; K.sup.1 and K.sup.2 are each independently selected from the group consisting of a direct bond, O, S, N(R.sup.α), P(R.sup.α), B(R.sup.α), C(R.sup.α)(R.sup.β), and Si(R.sup.α)(R.sup.β); each R.sup.AA, R.sup.BB, R.sup.CC, and R.sup.DD independently represents mono to the maximum allowable substitution, or no substitution; each R, R', R'', R.sup.AA, R.sup.BB, R.sup.CC, and R.sup.DD is independently a 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, selenyl, and combinations thereof; and any two substituents can be fused or joined to form a ring.

9. The compound of claim 1, wherein ligand L.sub.A is selected from L.sub.Aw-(Ri)(Rj)(Rk)(Rl).sub.Q(Ym)(Yn)(Yo).sub.V, wherein w is an integer from 1 to 37; Q is 1 when w is 1, 3, 4, 5, 6, 7, 10, 11, 12, 13, or 14, otherwise Q is 0; v is 1 when w is 5, 7, 9, 12, 17, 19, 21, 24, 28, 30, 37, or 38, otherwise v is 0; each of Ri, Rj, Rk, and R.sup.I is independently selected from the group consisting of R1 to R468; and each of Ym and Yn is independently selected from the group consisting of Y1 to Y3; wherein each of L.sub.A1-(R1)(R1)(R1)(R1)(Y1)(Y1) to L.sub.A38-(R468)(R468)(R468)(Y3)(Y3)(Y3) is defined as follows: TABLE-US-00009 L.sub.A Structure of L.sub.A L.sub.A1- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A1- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A1- (R468)(R468)(R468) (R468)(Y3)(Y3), have the structure  embedded image L.sub.A2- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A2- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A2- (R468)(R468) (R468) (Y3)(Y3), have the structure  embedded image L.sub.A3- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A3- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A3- (R468)(R468)(R468) (R468)(Y3) (Y3), have the structure  embedded image L.sub.A4- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A4- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A4- (R468)(R468)(R468) (R468)(Y3)(Y3), have the structure  embedded image L.sub.A5- (Ri)(Rj)(Rk)(Rl) (Ym)(Yn)(Yo), wherein L.sub.A5- (R1)(R1)(R1)(R1) (Y1)(Y1)(Y1) to L.sub.A5- (R468)(R468)(R468) (R468)(Y3)(Y3)(Y3), have the structure  embedded image L.sub.A6- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A6- (R1) (R1)(R1) (Y1)(Y1) to L.sub.A6- (R468)(R468)(R468) (R468)(Y3)(Y3), have the structure  embedded image L.sub.A7- (Ri)(Rj)(Rk)(Rl) (Ym)(Yn)(Yo), wherein L.sub.A7- (R1)(R1)(R1) (R1) (Y1)(Y1)(Y1) to L.sub.A7- (R468)(R468)(R468) (R468)(Y3)(Y3)(Y3), have the structure  embedded image L.sub.A8- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A8- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A8- (R468)(R468)(R468) (Y3)(Y3), have the structure  embedded image L.sub.A9- (Ri) (Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A9- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A9- (R468)(R468) (R468) (Y3)(Y3)(Y3), have the structure  embedded image L.sub.A10- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A10- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A10- (R468)(R468)(R468) (R468) (Y3)(Y3), have the structure  embedded image L.sub.A11- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A11- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A11- (R468)(R468)(R468) (R468)(Y3)(Y3), have the structure  embedded image L.sub.A12- (Ri)(Rj)(Rk)(Rl) (Ym)(Yn)(Yo), wherein L.sub.A12-

(R1)(R1)(R1)(R1) (Y1)(Y1)(Y1) to L.sub.A12- (R468)(R468)(R468) (R468)(Y3)(Y3)(Y3), have the structure  L.sub.A13- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A13- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A13- (R468)(R468)(R468) (R468)(Y3)(Y3), have the structure  L.sub.A14- (Ri)(Rj)(Rk)(Rl)(Ym) (Yn), wherein L.sub.A14- (R1)(R1)(R1)(R1) (Y1)(Y1) to L.sub.A14- (R468)(R468)(R468) (R468)(Y3)(Y3), have the structure  L.sub.A15- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A15- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A15- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A16- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A16- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A16- (R468)(R468) (R468) (Y3)(Y3), have the structure  L.sub.A17- (Ri)(Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A17- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A17- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A18- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A18- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A18- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A19- (Ri)(Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A19- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A19- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A20- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A20- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A20- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A21- (Ri)(Rj)(Rk) (Ym)(Yn)(Yo), wherein L.sub.A21- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A21- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A22- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A22- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A22- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A23- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A23- (R1)(R1)(R1) (Y1)(Y1) to L.sub.A23- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A24- (Ri)(Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A24- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A24- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A25- (Ri)(Rj) (Rk)(Ym)(Yn), wherein L.sub.A25- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A25- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A26- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A26- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A26- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A27- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A27- (R1)(R1)(R1) (Y1)(Y1) to L.sub.A27- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A28- (Ri)(Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A28- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A28- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A29- (Ri)(Rj) (Rk)(Ym)(Yn), wherein L.sub.A29- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A29- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A30- (Ri)(Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A30- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A30- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A31- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A31- (R1)(R1)(R1) (Y1)(Y1) to L.sub.A31- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A32- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A32- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A32- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A33- (Ri)(Rj)(Rk) (Ym)(Yn), wherein L.sub.A33- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A33- (R468)(R468)(R468) (Y3) (Y3), have the structure  L.sub.A34- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A34- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A34- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A35- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A35- (R1)(R1)(R1) (Y1)(Y1) to L.sub.A35- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A36- (Ri)(Rj)(Rk)(Ym)(Yn), wherein L.sub.A36- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A36- (R468)(R468)(R468) (Y3)(Y3), have the structure  L.sub.A37- (Ri)(Rj)(Rk) (Ym)(Yn)(Yo), wherein L.sub.A37- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A37- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  L.sub.A38- (Ri)(Rj)(Rk)(Ym)(Yn)(Yo), wherein L.sub.A38- (R1)(R1)(R1)(Y1)(Y1) to L.sub.A38- (R468)(R468)(R468) (Y3)(Y3)(Y3), have the structure  wherein Y.sup.1 is ##STR01032## wherein R1 to R468 have the structures defined as follows: TABLE-US-00010 Structure  R1  R2  R3  R4  R5

 R6  R7  R8  R9
 R10  R11  R12  R13
 R14  R15  R16  R17
 R18  R19  R20  R21
 R22  R23  R24  R25
 R26  R27  R28  R29
 R30  R31  R32  R33
 R34  R35  R36  R37
 R38  R39  R40  R41
 R42  R43  R44  R45
 R46  R47  R48  R49
 R50  R51  R52  R53
 R54  R55  R56  R57
 R58  R59  R60  R61
 R62  R63  R64  R65
 R66  R67  R68  R69
 R70  R71  R72  R73
 R74  R75  R76  R77
 R78  R79  R80  R81
 R82  R83  R84  R85
 R86  R87  R88  R89
 R90  R91  R92  R93
 R94  R95  R96  R97
 R98  R99  R100 
R101  R102  R103  R104
 R105  R106  R107 
R108  R109  R110  R111
 R112  R113  R114 
R115  R116  R117  R118
 R119  R120  R121 
R122  R123  R124  R125
 R126  R127  R128 
R129  R130  R131  R132
 R133  R134  R135 
R136  R137  R138  R139
 R140  R141  R142 
R143  R144  R145  R146
 R147  R148  R149 
R150  R151  R152  R153
 R154  R155  R156 
R157  R158  R159  R160
 R161  R162  R163 
R164  R165  R166  R167
 R168  R169  R170 
R171  R172  R173  R174
 R175  R176  R177 
R178  R179  R180  R181
 R182  R183  R184 
R185  R186  R187  R188
 R189  R190  R191 

R192  R193  R194  R195 
R196  R197  R198  R199 
R200  R201  R202 
R203  R204  R205  R206 
R207  R208  R209 
R210  R211  R212  R213 
R214  R215  R216 
R217  R218  R219  R220 
R221  R222  R223 
R224  R225  R226  R227 
R228  R229  R230 
R231  R232  R233  R234 
R235  R236  R237 
R238  R239  R240  R241 
R242  R243  R244 
R245  R246  R247  R248 
R249  R250  R251 
R252  R253  R254  R255 
R256  R257  R258 
R259  R260  R261  R262 
R263  R264  R265 
R266  R267  R268  R269 
R270  R271  R272 
R273  R274  R275  R276 
R277  R278  R279 
R280  R281  R282  R283 
R284  R285  R286 
R287  R288  R289  R290 
R291  R292  R293 
R294  R295  R296  R297 
R298  R299  R300 
R301  R302  R303  R304 
R305  R306  R307 
R308  R309  R310  R311 
R312  R313  R314 
R315  R316  R317  R318 
R319  R320  R321 
R322  R323  R324  R325 
R326  R327  R328 
R329  R330  R331  R332 
R333  R334  R335 
R336  R337  R338  R339 
R340  R341  R342 
R343  R344  R345  R346 
R347  R348  R349 
R350  R351  R352  R353 
R354  R355  R356 
R357  R358  R359  R360 
R361  R362  R363 
R364  R365  R366 

R367  R368  R369  R370 
 R371  R372  R373 
R374  R375  R376  R377
 R378  R379  R380 
R381  R382  R383  R384
 R385  R386  R387 
R388  R389  R390  R391
 R392  R393  R394 
R395  R396  R397  R398
 R399  R400  R401 
R402  R403  R404  R405
 R406  R407  R408 
R409  R410  R411  R412
 R413  R414  R415 
R416  R417  R418  R419
 R420  R421  R422 
R423  R424  R425  R426
 R427  R428  R429 
R430  R431  R432  R433
 R434  R435  R436 
R437  R438  R439  R440
 R441  R442  R443 
R444  R445  R446  R447
 R448  R449  R450 
R451  R452  R453  R454
 R455  R456  R457 
R458  R459  R460  R461
 R462  R463  R464 
R465  R466  R467  R468

10. The compound of claim 1, wherein the compound has a formula of $M(L.sub.A).sub.p(L.sub.B).sub.q(L.sub.C)$ wherein L.sub.B and L.sub.C are each a bidentate ligand; and wherein p is 1, 2, or 3; q is 0, 1, or 2; r is 0, 1, or 2; and $p+q+r$ is the oxidation state of the metal M.

11. The compound of claim 10, wherein the compound has a formula selected from the group consisting of $Ir(L.sub.A).sub.3$, $Ir(L.sub.A)(L.sub.B).sub.2$, $Ir(L.sub.A).sub.2(L.sub.B)$, $Ir(L.sub.A).sub.2(L.sub.C)$, and $Ir(L.sub.A)(L.sub.B)(L.sub.C)$; and wherein L.sub.A, L.sub.B, and L.sub.C are different from each other, or a formula of $Pt(L.sub.A)(L.sub.B)$; and wherein L.sub.A and L.sub.B can be same or different.

12. The compound of claim 10, wherein L.sub.B and L.sub.C are each independently selected from the group consisting of: ##STR01501## ##STR01502## ##STR01503## ##STR01504## ##STR01505## wherein: T is selected from the group consisting of B, Al, Ga, and In; K.sup.1' is selected from the group consisting of a single bond, O, S, NR.sub.e, PR.sub.e, BR.sub.e, CR.sub.eR.sub.f, and SiR.sub.eR.sub.f; each of Y.sup.1 to Y.sup.13 is independently selected from the group consisting of C and N; Y' is selected from the group consisting of BR.sub.e, BR.sub.eR.sub.f, NR.sub.e, PR.sub.e, P(O)R.sub.e, O, S, Se, C=O, C=S, C=Se, C=NR.sub.e, C=CR.sub.eR.sub.f, S=O, SO.sub.2, CR.sub.eR.sub.f, SiR.sub.eR.sub.f, and GeR.sub.eR.sub.f; R.sub.e and R.sub.f can be fused or joined to form a ring; each R.sub.a, R.sub.b, R.sub.c, and R.sub.d independently represents from mono to the maximum allowed number of substitutions, or no substitution; each R.sub.a1, R.sub.b1, R.sub.c1, R.sub.d1, R.sub.a, R.sub.b, R.sub.c, R.sub.d, R.sub.e, and R.sub.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, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, selenyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and any two substituents of R.sub.a1, R.sub.b1, R.sub.c1, R.sub.d1, R.sub.a, R.sub.b, R.sub.c, and R.sub.d can be fused or joined to form a ring or form a multidentate ligand.

13. The compound of claim 10, wherein the compound has formula Ir(L.sub.A).sub.3, formula Ir(L.sub.A)(L.sub.bk).sub.2, formula Ir(L.sub.A).sub.2(L.sub.bk), formula Ir(L.sub.A).sub.2(L.sub.Cj-I), or Ir(L.sub.A).sub.2(L.sub.Cj-II); wherein L.sub.A is according to Formula I; wherein k is an integer from 1 to 836, and each L.sub.Bk has the structure defined as follows: ##STR01506## ##STR01507## ##STR01508## ##STR01509## ##STR01510## ##STR01511## ##STR01512## ##STR01513## ##STR01514## ##STR01515## ##STR01516## ##STR01517## ##STR01518## ##STR01519## ##STR01520## ##STR01521## ##STR01522## ##STR01523## ##STR01524## ##STR01525## ##STR01526## ##STR01527## ##STR01528## ##STR01529## ##STR01530## ##STR01531## ##STR01532## ##STR01533## ##STR01534## ##STR01535## ##STR01536## ##STR01537## ##STR01538## ##STR01539## ##STR01540## ##STR01541## ##STR01542## ##STR01543## ##STR01544## ##STR01545## ##STR01546## ##STR01547## ##STR01548## ##STR01549## ##STR01550## ##STR01551## ##STR01552## ##STR01553## ##STR01554## ##STR01555## ##STR01556## ##STR01557## ##STR01558## ##STR01559## ##STR01560## ##STR01561## ##STR01562## ##STR01563## ##STR01564## ##STR01565## ##STR01566## ##STR01567## ##STR01568## ##STR01569## ##STR01570## ##STR01571## ##STR01572## ##STR01573## ##STR01574## ##STR01575## ##STR01576## ##STR01577## ##STR01578## ##STR01579## ##STR01580## ##STR01581## ##STR01582## ##STR01583## ##STR01584## ##STR01585## ##STR01586## ##STR01587## ##STR01588## ##STR01589## ##STR01590## ##STR01591## ##STR01592## ##STR01593## ##STR01594## ##STR01595## ##STR01596## ##STR01597## ##STR01598## ##STR01599## ##STR01600## ##STR01601## ##STR01602## ##STR01603## ##STR01604## ##STR01605## ##STR01606## ##STR01607## ##STR01608## ##STR01609## ##STR01610## ##STR01611## ##STR01612## ##STR01613## ##STR01614## ##STR01615## ##STR01616## ##STR01617## ##STR01618## ##STR01619## ##STR01620## ##STR01621## ##STR01622## ##STR01623## ##STR01624## ##STR01625## ##STR01626## ##STR01627## ##STR01628## ##STR01629## ##STR01630## ##STR01631## ##STR01632## ##STR01633## ##STR01634## ##STR01635## ##STR01636## ##STR01637## ##STR01638## ##STR01639## ##STR01640## ##STR01641## ##STR01642## ##STR01643## ##STR01644## ##STR01645## ##STR01646## ##STR01647## ##STR01648## ##STR01649## ##STR01650## ##STR01651## ##STR01652## ##STR01653## ##STR01654## ##STR01655## ##STR01656## ##STR01657## ##STR01658## ##STR01659## ##STR01660## ##STR01661## ##STR01662## ##STR01663## ##STR01664## ##STR01665## ##STR01666## ##STR01667## ##STR01668## ##STR01669## ##STR01670## ##STR01671## ##STR01672## ##STR01673## ##STR01674## ##STR01675## ##STR01676## ##STR01677## ##STR01678## ##STR01679## ##STR01680## ##STR01681## ##STR01682## ##STR01683## wherein each L.sub.Cj-I has a structure based on formula ##STR01684## and each L.sub.Cj-II has a structure based on formula ##STR01685## wherein for each L.sub.Cj in L.sub.Cj-I and L.sub.Cj-II, R.sup.201 and R.sup.202 are defined as follows: TABLE-US-00011 L.sub.Cj R.sup.201 R.sup.202 L.sub.Cj R.sup.201 R.sup.202 L.sub.Cj R.sup.201 R.sup.202 L.sub.C1 R.sup.D1 R.sup.D1 L.sub.C193 R.sup.D1 R.sup.D3 L.sub.C385 R.sup.D17 R.sup.D40 L.sub.C577 R.sup.D143 R.sup.D120 L.sub.C2 R.sup.D2 R.sup.D2 L.sub.C194 R.sup.D1 R.sup.D4 L.sub.C386 R.sup.D17 R.sup.D41 L.sub.C578 R.sup.D143 R.sup.D133 L.sub.C3 R.sup.D3 R.sup.D3 L.sub.C195 R.sup.D1 R.sup.D5 L.sub.C387 R.sup.D17 R.sup.D42 L.sub.C579 R.sup.D143 R.sup.D134 L.sub.C4 R.sup.D4 R.sup.D4 L.sub.C196 R.sup.D1 R.sup.D9 L.sub.C388 R.sup.D17 R.sup.D43 L.sub.C580 R.sup.D143 R.sup.D135 L.sub.C5 R.sup.D5 R.sup.D5 L.sub.C197 R.sup.D1 R.sup.D10 L.sub.C389 R.sup.D17 R.sup.D48 L.sub.C581 R.sup.D143

R.sup.D136 L.sub.D6 R.sup.D6 R.sup.D6 L.sub.C198 R.sup.D1 R.sup.D17 L.sub.C390 R.sup.D17
R.sup.D49 L.sub.C582 R.sup.D143 R.sup.D144 L.sub.C7 R.sup.D7 R.sup.D7 L.sub.C199
R.sup.D1 R.sup.D18 L.sub.C391 R.sup.D17 R.sup.D50 L.sub.C583 R.sup.D143 R.sup.D145
L.sub.C8 R.sup.D8 R.sup.D8 L.sub.C200 R.sup.D1 R.sup.D20 L.sub.C392 R.sup.D17 R.sup.D54
L.sub.C584 R.sup.D143 R.sup.D146 L.sub.C9 R.sup.D9 R.sup.D9 L.sub.C201 R.sup.D1
R.sup.D22 L.sub.C393 R.sup.D17 R.sup.D55 L.sub.C585 R.sup.D143 R.sup.D147 L.sub.C10
R.sup.D10 R.sup.D10 L.sub.C202 R.sup.D1 R.sup.D37 L.sub.C394 R.sup.D17 R.sup.D58
L.sub.C586 R.sup.D143 R.sup.D149 L.sub.C11 R.sup.D11 R.sup.D11 L.sub.C203 R.sup.D1
R.sup.D40 L.sub.C395 R.sup.D17 R.sup.D59 L.sub.C587 R.sup.D143 R.sup.D151 L.sub.C12
R.sup.D12 R.sup.D12 L.sub.C204 R.sup.D1 R.sup.D41 L.sub.C396 R.sup.D17 R.sup.D78
L.sub.C588 R.sup.D143 R.sup.D154 L.sub.C13 R.sup.D13 R.sup.D13 L.sub.C205 R.sup.D1
R.sup.D42 L.sub.C397 R.sup.D17 R.sup.D79 L.sub.C589 R.sup.D143 R.sup.D155 L.sub.C14
R.sup.D14 R.sup.D14 L.sub.C206 R.sup.D1 R.sup.D43 L.sub.C398 R.sup.D17 R.sup.D81
L.sub.C590 R.sup.D143 R.sup.D161 L.sub.C15 R.sup.D15 R.sup.D15 L.sub.C207 R.sup.D1
R.sup.D48 L.sub.C399 R.sup.D17 R.sup.D87 L.sub.C591 R.sup.D143 R.sup.D175 L.sub.C16
R.sup.D16 R.sup.D16 L.sub.C208 R.sup.D1 R.sup.D49 L.sub.C400 R.sup.D17 R.sup.D88
L.sub.C592 R.sup.D144 R.sup.D3 L.sub.C17 R.sup.D17 R.sup.D17 L.sub.C209 R.sup.D1
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R.sup.D18 R.sup.D18 L.sub.C210 R.sup.D1 R.sup.D54 L.sub.C402 R.sup.D17 R.sup.D93
L.sub.C594 R.sup.D144 R.sup.D17 L.sub.C19 R.sup.D19 R.sup.D19 L.sub.C211 R.sup.D1
R.sup.D55 L.sub.C403 R.sup.D17 R.sup.D116 L.sub.C595 R.sup.D144 R.sup.D18 L.sub.C20
R.sup.D20 R.sup.D20 L.sub.C212 R.sup.D1 R.sup.D58 L.sub.C404 R.sup.D17 R.sup.D117
L.sub.C596 R.sup.D144 R.sup.D20 L.sub.C21 R.sup.D21 R.sup.D21 L.sub.C213 R.sup.D1
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L.sub.C598 R.sup.D144 R.sup.D37 L.sub.C23 R.sup.D23 R.sup.D23 L.sub.C215 R.sup.D1
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R.sup.D24 R.sup.D24 L.sub.C216 R.sup.D1 R.sup.D81 L.sub.C408 R.sup.D17 R.sup.D133
L.sub.C600 R.sup.D144 R.sup.D41 L.sub.C25 R.sup.D25 R.sup.D25 L.sub.C217 R.sup.D1
R.sup.D87 L.sub.C409 R.sup.D17 R.sup.D134 L.sub.C601 R.sup.D144 R.sup.D42 L.sub.C26
R.sup.D26 R.sup.D26 L.sub.C218 R.sup.D1 R.sup.D88 L.sub.C410 R.sup.D17 R.sup.D135
L.sub.C602 R.sup.D144 R.sup.D43 L.sub.C27 R.sup.D27 R.sup.D27 L.sub.C219 R.sup.D1
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L.sub.C604 R.sup.D144 R.sup.D49 L.sub.C29 R.sup.D29 R.sup.D29 L.sub.C221 R.sup.D1
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L.sub.C606 R.sup.D144 R.sup.D58 L.sub.C31 R.sup.D31 R.sup.D31 L.sub.C223 R.sup.D1
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L.sub.C608 R.sup.D144 R.sup.D78 L.sub.C33 R.sup.D33 R.sup.D33 L.sub.C225 R.sup.D1
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R.sup.D36 R.sup.D36 L.sub.C228 R.sup.D1 R.sup.D135 L.sub.C420 R.sup.D17 R.sup.D155
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L.sub.C616 R.sup.D144 R.sup.D117 L.sub.C41 R.sup.D41 R.sup.D41 L.sub.C233 R.sup.D1
R.sup.D146 L.sub.C425 R.sup.D50 R.sup.D18 L.sub.C617 R.sup.D144 R.sup.D118 L.sub.C42
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L.sub.C638 R.sup.D145 R.sup.D22 L.sub.C63 R.sup.D63 R.sup.D63 L.sub.C255 R.sup.D4
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R.sup.D20 L.sub.C485 R.sup.D55 R.sup.D88 L.sub.C677 R.sup.D146 R.sup.D20 L.sub.C102
R.sup.D102 R.sup.D102 L.sub.C294 R.sup.D9 R.sup.D22 L.sub.C486 R.sup.D55 R.sup.D89
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R.sup.D37 L.sub.C487 R.sup.D55 R.sup.D93 L.sub.C679 R.sup.D146 R.sup.D37 L.sub.C104
R.sup.D104 R.sup.D104 L.sub.C296 R.sup.D9 R.sup.D40 L.sub.C488 R.sup.D55 R.sup.D116
L.sub.C680 R.sup.D146 R.sup.D40 L.sub.C105 R.sup.D105 R.sup.D105 L.sub.C297 R.sup.D9
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R.sup.D106 R.sup.D106 L.sub.C298 R.sup.D9 R.sup.D42 L.sub.C490 R.sup.D55 R.sup.D118
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L.sub.C684 R.sup.D146 R.sup.D48 L.sub.C109 R.sup.D109 R.sup.D109 L.sub.C301 R.sup.D9
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R.sup.D116 R.sup.D116 L.sub.C308 R.sup.D9 R.sup.D79 L.sub.C500 R.sup.D55 R.sup.D146
L.sub.C692 R.sup.D146 R.sup.D87 L.sub.C117 R.sup.D117 R.sup.D117 L.sub.C309 R.sup.D9
R.sup.D81 L.sub.C501 R.sup.D55 R.sup.D147 L.sub.C693 R.sup.D146 R.sup.D88 L.sub.C118
R.sup.D118 R.sup.D118 L.sub.C310 R.sup.D9 R.sup.D87 L.sub.C502 R.sup.D55 R.sup.D149
L.sub.C694 R.sup.D146 R.sup.D89 L.sub.C119 R.sup.D119 R.sup.D119 L.sub.C311 R.sup.D9
R.sup.D88 L.sub.C503 R.sup.D55 R.sup.D151 L.sub.C695 R.sup.D146 R.sup.D93 L.sub.C120
R.sup.D120 R.sup.D120 L.sub.C312 R.sup.D9 R.sup.D89 L.sub.C504 R.sup.D55 R.sup.D154
L.sub.C696 R.sup.D146 R.sup.D117 L.sub.C121 R.sup.D121 R.sup.D121 L.sub.C313 R.sup.D9
R.sup.D93 L.sub.C505 R.sup.D55 R.sup.D155 L.sub.C697 R.sup.D146 R.sup.D118 L.sub.C122
R.sup.D122 R.sup.D122 L.sub.C314 R.sup.D9 R.sup.D116 L.sub.C506 R.sup.D55 R.sup.D161
L.sub.C698 R.sup.D146 R.sup.D119 L.sub.C123 R.sup.D123 R.sup.D123 L.sub.C315 R.sup.D9
R.sup.D117 L.sub.C507 R.sup.D55 R.sup.D175 L.sub.C699 R.sup.D146 R.sup.D120 L.sub.C124
R.sup.D124 R.sup.D124 L.sub.C316 R.sup.D9 R.sup.D118 L.sub.C508 R.sup.D116 R.sup.D3
L.sub.C700 R.sup.D146 R.sup.D133 L.sub.C125 R.sup.D125 R.sup.D125 L.sub.C317 R.sup.D9
R.sup.D119 L.sub.C509 R.sup.D116 R.sup.D5 L.sub.C701 R.sup.D146 R.sup.D134 L.sub.C126
R.sup.D126 R.sup.D126 L.sub.C318 R.sup.D9 R.sup.D120 L.sub.C510 R.sup.D116 R.sup.D17
L.sub.C702 R.sup.D146 R.sup.D135 L.sub.C127 R.sup.D127 R.sup.D127 L.sub.C319 R.sup.D9
R.sup.D133 L.sub.C511 R.sup.D116 R.sup.D18 L.sub.C703 R.sup.D146 R.sup.D136 L.sub.C128
R.sup.D128 R.sup.D128 L.sub.C320 R.sup.D9 R.sup.D134 L.sub.C512 R.sup.D116 R.sup.D20
L.sub.C704 R.sup.D146 R.sup.D146 L.sub.C129 R.sup.D129 R.sup.D129 L.sub.C321 R.sup.D9
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R.sup.D130 R.sup.D130 L.sub.C322 R.sup.D9 R.sup.D136 L.sub.C514 R.sup.D116 R.sup.D37
L.sub.C706 R.sup.D146 R.sup.D149 L.sub.C131 R.sup.D131 R.sup.D131 L.sub.C323 R.sup.D9
R.sup.D143 L.sub.C515 R.sup.D116 R.sup.D40 L.sub.C707 R.sup.D146 R.sup.D151 L.sub.C132
R.sup.D132 R.sup.D132 L.sub.C324 R.sup.D9 R.sup.D144 L.sub.C516 R.sup.D116 R.sup.D41
L.sub.C708 R.sup.D146 R.sup.D154 L.sub.C133 R.sup.D133 R.sup.D133 L.sub.C325 R.sup.D9
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L.sub.C710 R.sup.D146 R.sup.D161 L.sub.C135 R.sup.D135 R.sup.D135 L.sub.C327 R.sup.D9
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R.sup.D136 R.sup.D136 L.sub.C328 R.sup.D9 R.sup.D149 L.sub.C520 R.sup.D116 R.sup.D49
L.sub.C712 R.sup.D133 R.sup.D3 L.sub.C137 R.sup.D137 R.sup.D137 L.sub.C329 R.sup.D9
R.sup.D151 L.sub.C521 R.sup.D116 R.sup.D54 L.sub.C713 R.sup.D133 R.sup.D5 L.sub.C138
R.sup.D138 R.sup.D138 L.sub.C330 R.sup.D9 R.sup.D154 L.sub.C522 R.sup.D116 R.sup.D58
L.sub.C714 R.sup.D133 R.sup.D3 L.sub.C139 R.sup.D139 R.sup.D139 L.sub.C331 R.sup.D9

R.sup.D155 L.sub.C523 R.sup.D156 R.sup.D59 L.sub.C715 R.sup.D133 R.sup.D18 L.sub.C140
R.sup.D140 R.sup.D140 L.sub.C332 R.sup.D9 R.sup.D161 L.sub.C524 R.sup.D116 R.sup.D78
L.sub.C716 R.sup.D133 R.sup.D20 L.sub.C141 R.sup.D141 R.sup.D141 L.sub.C333 R.sup.D9
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L.sub.C724 R.sup.D133 R.sup.D49 L.sub.C149 R.sup.D149 R.sup.D149 L.sub.C341 R.sup.D10
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L.sub.C728 R.sup.D133 R.sup.D78 L.sub.C153 R.sup.D153 R.sup.D153 L.sub.C345 R.sup.D10
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L.sub.C748 R.sup.D133 R.sup.D155 L.sub.C173 R.sup.D173 L.sub.C365 R.sup.D10
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R.sup.D18 L.sub.C573 R.sup.D143 R.sup.D116 L.sub.C765 R.sup.D175 R.sup.D59 L.sub.C190
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R.sup.D197 L.sub.C989 R.sup.D4 R.sup.D197 L.sub.C1097 R.sup.D9 R.sup.D197 L.sub.C774
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L.sub.C1098 R.sup.D9 R.sup.D198 L.sub.C775 R.sup.D199 R.sup.D199 L.sub.C883 R.sup.D1
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L.sub.C1118 R.sup.D9 R.sup.D218 L.sub.C795 R.sup.D219 R.sup.D219 L.sub.C903 R.sup.D1
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R.sup.D224 R.sup.D224 L.sub.C908 R.sup.D1 R.sup.D224 L.sub.C1016 R.sup.D4 R.sup.D224
L.sub.C1124 R.sup.D9 R.sup.D224 L.sub.C801 R.sup.D225 R.sup.D225 L.sub.C909 R.sup.D1
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R.sup.D226 R.sup.D226 L.sub.C910 R.sup.D1 R.sup.D226 L.sub.C1018 R.sup.D4 R.sup.D226
L.sub.C1126 R.sup.D9 R.sup.D226 L.sub.C803 R.sup.D227 R.sup.D227 L.sub.C911 R.sup.D1
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L.sub.C1279 R.sup.D55 R.sup.D217 L.sub.C1333 R.sup.D37 R.sup.D217 L.sub.C1387
R.sup.D143 R.sup.D217 L.sub.C1226 R.sup.D10 R.sup.D218 L.sub.C1280 R.sup.D55 R.sup.D218
L.sub.C1334 R.sup.D37 R.sup.D218 L.sub.C1388 R.sup.D143 R.sup.D218 L.sub.C1227
R.sup.D10 R.sup.D219 L.sub.C1281 R.sup.D55 R.sup.D219 L.sub.C1335 R.sup.D37 R.sup.D219
L.sub.C1389 R.sup.D143 R.sup.D219 L.sub.C1228 R.sup.D10 R.sup.D220 L.sub.C1282
R.sup.D55 R.sup.D220 L.sub.C1336 R.sup.D37 R.sup.D220 L.sub.C1390 R.sup.D143 R.sup.D220
L.sub.C1229 R.sup.D10 R.sup.D221 L.sub.C1283 R.sup.D55 R.sup.D221 L.sub.C1337 R.sup.D37
R.sup.D221 L.sub.C1391 R.sup.D143 R.sup.D221 L.sub.C1230 R.sup.D10 R.sup.D222
L.sub.C1284 R.sup.D55 R.sup.D222 L.sub.C1338 R.sup.D37 R.sup.D222 L.sub.C1392
R.sup.D143 R.sup.D222 L.sub.C1231 R.sup.D10 R.sup.D223 L.sub.C1285 R.sup.D55 R.sup.D223
L.sub.C1339 R.sup.D37 R.sup.D223 L.sub.C1393 R.sup.D143 R.sup.D223 L.sub.C1232
R.sup.D10 R.sup.D224 L.sub.C1286 R.sup.D55 R.sup.D224 L.sub.C1340 R.sup.D37 R.sup.D224
L.sub.C1394 R.sup.D143 R.sup.D224 L.sub.C1233 R.sup.D10 R.sup.D225 L.sub.C1287
R.sup.D55 R.sup.D225 L.sub.C1341 R.sup.D37 R.sup.D225 L.sub.C1395 R.sup.D143 R.sup.D225
L.sub.C1234 R.sup.D10 R.sup.D226 L.sub.C1288 R.sup.D55 R.sup.D226 L.sub.C1342 R.sup.D37

R.sup.D226 L.sub.C1296 R.sup.D143 R.sup.D226 L.sub.C1235 R.sup.D10 R.sup.D227
L.sub.C1289 R.sup.D55 R.sup.D227 L.sub.C1343 R.sup.D37 R.sup.D227 L.sub.C1397
R.sup.D143 R.sup.D227 L.sub.C1236 R.sup.D10 R.sup.D228 L.sub.C1290 R.sup.D55 R.sup.D228
L.sub.C1344 R.sup.D37 R.sup.D228 L.sub.C1398 R.sup.D143 R.sup.D228 L.sub.C1237
R.sup.D10 R.sup.D229 L.sub.C1291 R.sup.D55 R.sup.D229 L.sub.C1345 R.sup.D37 R.sup.D229
L.sub.C1399 R.sup.D143 R.sup.D229 L.sub.C1238 R.sup.D10 R.sup.D230 L.sub.C1292
R.sup.D55 R.sup.D230 L.sub.C1346 R.sup.D37 R.sup.D230 L.sub.C1400 R.sup.D143 R.sup.D230
L.sub.C1239 R.sup.D10 R.sup.D231 L.sub.C1293 R.sup.D55 R.sup.D231 L.sub.C1347 R.sup.D37
R.sup.D231 L.sub.C1401 R.sup.D143 R.sup.D231 L.sub.C1240 R.sup.D10 R.sup.D232
L.sub.C1294 R.sup.D55 R.sup.D232 L.sub.C1348 R.sup.D37 R.sup.D232 L.sub.C1402
R.sup.D143 R.sup.D232 L.sub.C1241 R.sup.D10 R.sup.D233 L.sub.C1295 R.sup.D55 R.sup.D233
L.sub.C1349 R.sup.D37 R.sup.D233 L.sub.C1403 R.sup.D143 R.sup.D233 L.sub.C1242
R.sup.D10 R.sup.D234 L.sub.C1296 R.sup.D55 R.sup.D234 L.sub.C1350 R.sup.D37 R.sup.D234
L.sub.C1404 R.sup.D143 R.sup.D234 L.sub.C1243 R.sup.D10 R.sup.D235 L.sub.C1297
R.sup.D55 R.sup.D235 L.sub.C1351 R.sup.D37 R.sup.D235 L.sub.C1405 R.sup.D143 R.sup.D235
L.sub.C1244 R.sup.D10 R.sup.D236 L.sub.C1298 R.sup.D55 R.sup.D236 L.sub.C1352 R.sup.D37
R.sup.D236 L.sub.C1406 R.sup.D143 R.sup.D236 L.sub.C1245 R.sup.D10 R.sup.D237
L.sub.C1299 R.sup.D55 R.sup.D237 L.sub.C1353 R.sup.D37 R.sup.D237 L.sub.C1407
R.sup.D143 R.sup.D237 L.sub.C1246 R.sup.D10 R.sup.D238 L.sub.C1300 R.sup.D55 R.sup.D238
L.sub.C1354 R.sup.D37 R.sup.D238 L.sub.C1408 R.sup.D143 R.sup.D238 L.sub.C1247
R.sup.D10 R.sup.D239 L.sub.C1301 R.sup.D55 R.sup.D239 L.sub.C1355 R.sup.D37 R.sup.D239
L.sub.C1409 R.sup.D143 R.sup.D239 L.sub.C1248 R.sup.D10 R.sup.D240 L.sub.C1302
R.sup.D55 R.sup.D240 L.sub.C1356 R.sup.D37 R.sup.D240 L.sub.C1410 R.sup.D143 R.sup.D240
L.sub.C1249 R.sup.D10 R.sup.D241 L.sub.C1303 R.sup.D55 R.sup.D241 L.sub.C1357 R.sup.D37
R.sup.D241 L.sub.C1411 R.sup.D143 R.sup.D241 L.sub.C1250 R.sup.D10 R.sup.D242
L.sub.C1304 R.sup.D55 R.sup.D242 L.sub.C1358 R.sup.D37 R.sup.D242 L.sub.C1412
R.sup.D143 R.sup.D242 L.sub.C1251 R.sup.D10 R.sup.D243 L.sub.C1305 R.sup.D55 R.sup.D243
L.sub.C1359 R.sup.D37 R.sup.D243 L.sub.C1413 R.sup.D143 R.sup.D243 L.sub.C1252
R.sup.D10 R.sup.D244 L.sub.C1306 R.sup.D55 R.sup.D244 L.sub.C1360 R.sup.D37 R.sup.D244
L.sub.C1414 R.sup.D143 R.sup.D244 L.sub.C1253 R.sup.D10 R.sup.D245 L.sub.C1307
R.sup.D55 R.sup.D245 L.sub.C1361 R.sup.D37 R.sup.D245 L.sub.C1415 R.sup.D143 R.sup.D245
L.sub.C1254 R.sup.D10 R.sup.D246 L.sub.C1308 R.sup.D55 R.sup.D246 L.sub.C1362 R.sup.D37
R.sup.D246 L.sub.C1416 R.sup.D143 R.sup.D246 wherein R.sup.D1 to R.sup.D246 have the
following structures: ##STR01686## ##STR01687## ##STR01688## ##STR01689##
##STR01690## ##STR01691## ##STR01692## ##STR01693## ##STR01694## ##STR01695##
##STR01696## ##STR01697## ##STR01698## ##STR01699## ##STR01700## ##STR01701##
##STR01702## ##STR01703## ##STR01704## ##STR01705## ##STR01706## ##STR01707##
##STR01708## ##STR01709##

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

##STR01710## ##STR01711## ##STR01712## ##STR01713## ##STR01714## ##STR01715##
##STR01716## ##STR01717## ##STR01718## ##STR01719## ##STR01720## ##STR01721##
##STR01722## ##STR01723## ##STR01724## ##STR01725## ##STR01726## ##STR01727##

15. The compound of claim 10, wherein the compound has a structure of Formula II:

##STR01728## wherein M.sup.1 is Pd or Pt; moieties E and F are each independently monocyclic or polycyclic ring structure, 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; Z.sup.3 and Z.sup.4 are each independently C or N; K.sup.1, K.sup.2, K.sup.3, and K.sup.4 are each independently selected from the group consisting of a direct bond, O, and S, wherein at least two of them are direct bonds; L.sup.1, L.sup.2, and L.sup.3 are each independently absent or selected from the group consisting of a direct bond, BR, BRR', NR, PR, P(O)R, O, S, Se, C=O, C=S, C=Se,

C=NR, C=CRR', S=O, SO.sub.2, CRR', SiRR', GeRR', alkylene, cycloalkyl, aryl, cycloalkylene, arylene, heteroarylene, and combinations thereof, wherein at least one of L.sup.1 and L.sup.2 is present; R.sup.E and R.sup.F each independently represents zero, mono, or up to a maximum allowed number of substitutions; each of R, R', R.sup.E, and R.sup.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, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, selenyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and two adjacent R.sup.A, R.sup.B, R.sup.C, R.sup.E, and R.sup.F can be joined or fused together to form a ring where chemically feasible.

16. The compound of claim 15, wherein the compound is selected from the group consisting of compounds having the formula of Pt(L.sub.A')(Ly): ##STR01729## wherein L.sub.A' is selected from the group consisting of: ##STR01730## ##STR01731## ##STR01732## ##STR01733## ##STR01734## wherein L.sub.y is selected from the group consisting of: ##STR01735## ##STR01736## ##STR01737## ##STR01738## wherein Z' is B or N; each of Y.sup.1', Y.sup.2', and Y.sup.3' is independently absent or selected from the group consisting of BR, BRR', NR, PR, P(O)R, O, S, Se, C=O, C=S, C=Se, C=NR, C=CRR', S=O, SO.sub.2, CRR', SiRR', and GeRR'; each of L.sub.Z and L.sub.Z' is independently a direct bond, O, or S; R.sup.AA, R.sup.BB, R.sup.CC, and R.sup.G each independently represents zero, mono, or up to a maximum allowed number of substitutions; each of R.sup.AA, R.sup.BB, R.sup.CC, R.sup.G, R.sup.N, R.sup.X, and R.sup.Y 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, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, selenyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, and any two substituents can be joined or fused to form a ring.

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 according to claim 1.

18. The OLED of claim 17, wherein the organic layer further comprises a host, wherein the host is selected from the group consisting of: ##STR01739## ##STR01740## ##STR01741## ##STR01742## ##STR01743## ##STR01744## ##STR01745## wherein each of J.sub.1 to J.sub.6 is independently C or N; L' is a direct bond or an organic linker, each Y.sup.AA, Y.sup.BB, Y.sup.CC, and Y.sup.DD is independently selected from the group consisting of absent a bond, direct bond, O, S, Se, CRR', SiRR', GeRR', NR, BR, BRR'; each of R.sup.A', R.sup.B', R.sup.C', R.sup.D', R.sup.E', R.sup.F', and R.sup.G' independently represents mono, up to the maximum substitutions, or no substitutions; each R, R', R.sup.A', R.sup.B', R.sup.C', R.sup.D', R.sup.E', R.sup.F', and R.sup.G' is independently a 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, selenyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; any two substituents can be joined or fused to form a ring; and where possible, each unsubstituted aromatic carbon atom is optionally replaced with one or more N to form an aza-substituted ring.

19. The OLED of claim 17, wherein the compound is a sensitizer, and the OLED further comprises an acceptor selected from the group consisting of a fluorescent emitter, a delayed fluorescence emitter, and combination thereof.

20. A consumer product comprising an organic light-emitting device comprising: an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer comprises a compound according to claim 1.

