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(54) **ORGANOMETALLIC COMPOUND, COMPOSITION CONTAINING THE ORGANOMETALLIC COMPOUND, AND ORGANIC LIGHT-EMITTING DEVICE INCLUDING THE ORGANOMETALLIC COMPOUND OR COMPOSITION**

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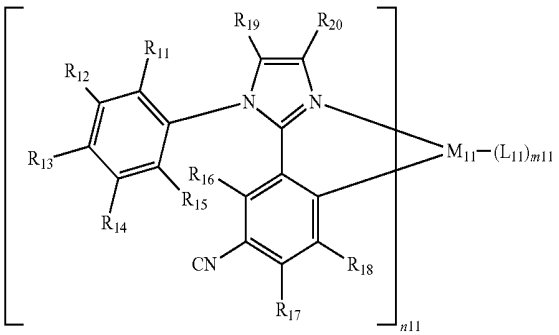
(57) **ABSTRACT**

An organometallic compound represented by Formula 1:

Formula 1



wherein, in Formula 1, groups an variables are the same as described in the specification.

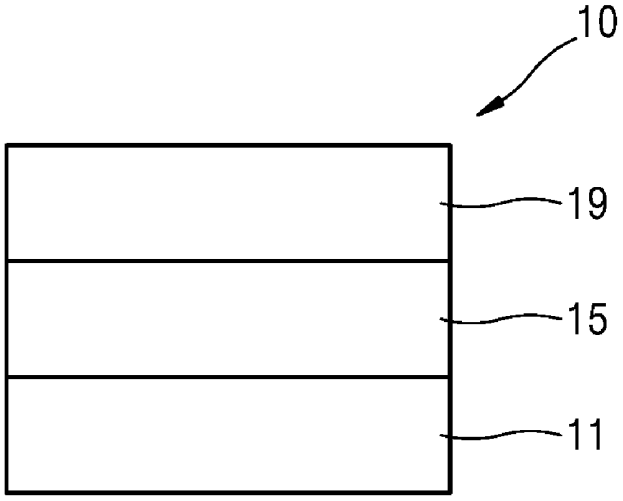


FIG. 1

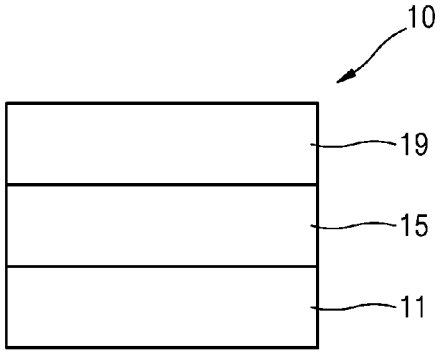
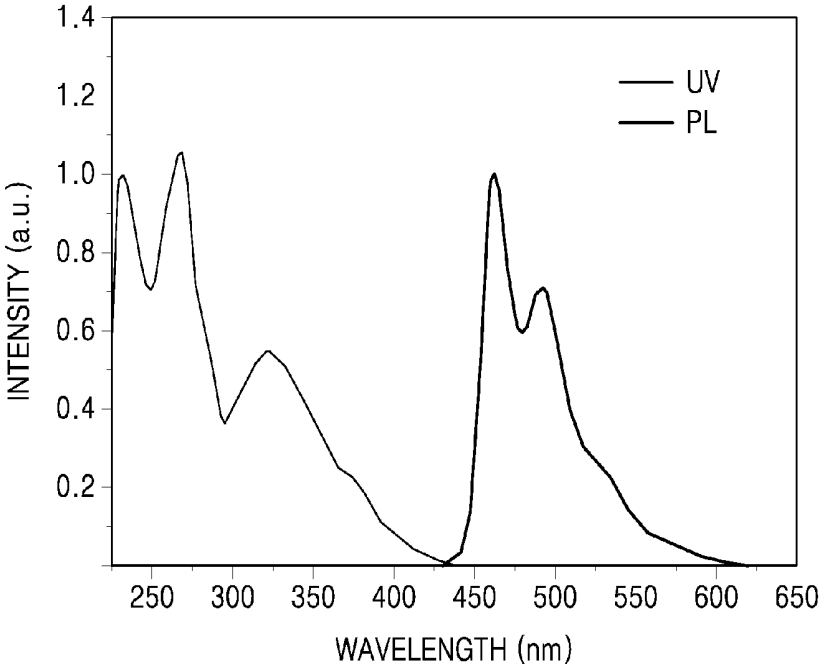

10
19
15
11

FIG. 2


1.4
1.2
1.0
0.8
0.6
0.4
0.2
INTENSITY (a.u.)
UV
PL
250
300
350
400
450
500
550
600
650
WAVELENGTH (nm)

ORGANOMETALLIC COMPOUND, COMPOSITION CONTAINING THE ORGANOMETALLIC COMPOUND, AND ORGANIC LIGHT-EMITTING DEVICE INCLUDING THE ORGANOMETALLIC COMPOUND OR COMPOSITION

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application claims priority to and the benefit of Korean Patent Application No. 10-2015-0018868, filed on Feb. 6, 2015, in the Korean Intellectual Property Office, and Korean Patent Application No. 10-2016-0011879, filed on Jan. 29, 2016, in the Korean Intellectual Property Office, the contents of which are incorporated herein in their entirety by reference.

BACKGROUND

[0002] 1. Field

[0003] The present disclosure relates to an organometallic compound, a composition containing the organometallic compound, and an organic light-emitting device including the organometallic compound or the composition.

[0004] 2. Description of the Related Art

[0005] Organic light-emitting devices (OLEDs) are self-emission devices that have wide viewing angles, high contrast ratios, and short response times. In addition, the OLEDs exhibit excellent luminance, driving voltage, and response speed characteristics, and produce full-color images.

[0006] A typical organic light-emitting device includes an anode, a cathode, and an organic layer that is disposed between the anode and the cathode and includes an emission layer. A hole transport region may be disposed between the anode and the emission layer, and an electron transport region may be disposed between the emission layer and the cathode. Holes provided from the anode may move toward the emission layer through the hole transport region, and electrons provided from the cathode may move toward the emission layer through the electron transport region. The holes and the electrons are recombined in the emission layer to produce excitons. These excitons change from an excited state to a ground state to thereby generate light.

[0007] Different types of organic light emitting devices are known. However, there still remains a need in OLEDs having low driving voltage, high efficiency, high brightness, and long lifespan.

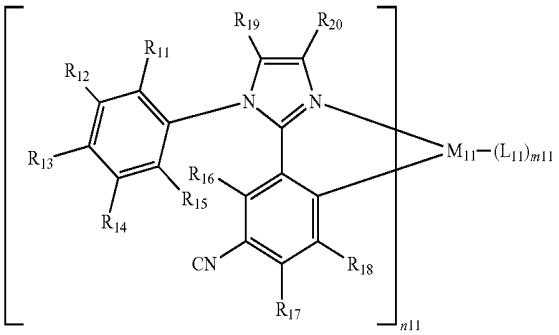
SUMMARY

[0008] Provided are a novel organometallic compound, a composition containing the novel organometallic compound, and an organic light-emitting devices including the organometallic compound or the composition.

[0009] Additional aspects will be set forth in part in the description which follows and, in part, will be apparent from the description, or may be learned by practice of the presented embodiments.

[0010] According to an aspect of the present invention, there is provided an organometallic compound represented by Formula 1:

Formula 1



[0011] wherein, in Formula 1,

[0012] M_{11} is selected from a first-row transition metal, a second-row ansition metal, and a third-row transition metal;

[0013] R_{11} to R_{18} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group; a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0014] optionally, adjacent two of R_{11} to R_{15} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

[0015] at least one of R_{11} to R_{15} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group; a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy

group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0016] R_{19} and R_{20} are each independently selected from a hydrogen, a deuterium, a C_1-C_{30} alkyl group, and a deuterium-substituted C_1-C_{30} alkyl group;

[0017] at least one of R_{11} to R_{23} is a deuterium-containing substituent;

[0018] n11 is selected from 1, 2, and 3;

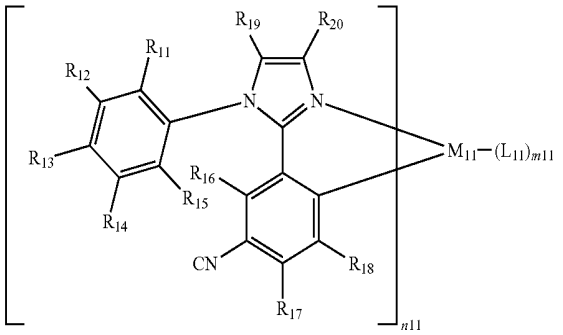
[0019] L_{11} is selected from a monodentate ligand and a bidentate ligand; and

[0020] m11 is selected from 0, 1, 2, 3, and 4.

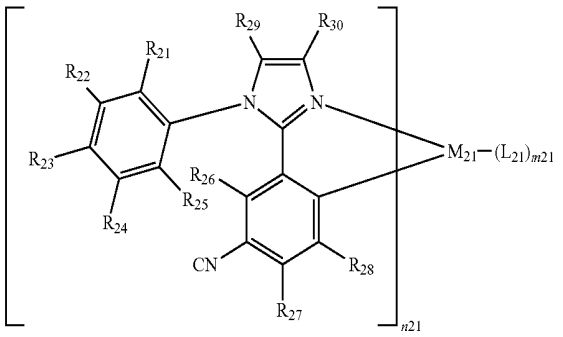
[0021] According to another aspect of the present invention, an organometallic compound-containing composition includes:

[0022] a first organometallic compound represented by Formula 1 and a second organometallic compound represented by Formula 2:

Formula 1



Formula 2



[0023] wherein, in Formulae 1 and 2,

[0024] R_{11} to R_{18} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0025] optionally, adjacent two of R_{11} to R_{15} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

[0026] at least one of R_{11} to R_{15} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0027] R_{19} and R_{20} are each independently selected from a hydrogen; a deuterium, a C_1-C_{30} alkyl group, and a deuterium-substituted C_1-C_{30} alkyl group;

[0028] at least one of R_{11} to R_{20} is a deuterium-containing substituent;

[0029] R_{21} to R_{28} are each independently selected from a hydrogen, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group; a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a

substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted alkylsilyl group;

[0030] optionally, adjacent two of R_{21} to R_{25} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

[0031] at least one of R_{21} to R_{25} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0032] R_{29} and R_{30} are each independently selected from a hydrogen and a C_1-C_{30} alkyl group;

[0033] R_{21} to R_{30} are a deuterium-non-containing substituent;

[0034] M_{11} and M_{21} are each independently selected from a first-row transition metal, a second-row transition metal, and a third-row transition metal;

[0035] n11 and n21 are each independently selected from 1, 2, and 3;

[0036] L_{11} and L_{21} are each independently selected from a monodentate ligand and a bidentate ligand; and

[0037] m11 and m21 are each independently selected from 0, 1, 2, 3, and 4.

[0038] According to another aspect of the present inventive concept, an organic light-emitting device includes:

[0039] a first electrode;

[0040] a second electrode; and

[0041] an organic layer disposed between the first electrode and the second electrode,

[0042] wherein the organic layer includes an emission layer and at least one organometallic compound of Formula 1, or

[0043] wherein the above-described organometallic compound-containing composition includes a first organometallic compound represented by Formula 1 described above and a second organometallic compound represented by Formula 2 described above.

[0044] The emission layer may include the organometallic compound or the organometallic compound-containing composition. The emission layer may further include a host, and the organometallic compound in the emission layer may serve as a dopant.

BRIEF DESCRIPTION OF THE DRAWINGS

[0045] These and/or other aspects will become apparent and more readily appreciated from the following description of the embodiments, taken in conjunction with the accompanying drawings in which:

[0046] FIG. **1** is a schematic cross-sectional view illustrating an organic light-emitting device according to an embodiment; and

[0047] FIG. **2** is a graph of intensity (arbitrary unit, a. u.) versus wavelength (nanometers, nm) illustrating photoluminescent (PL) spectra and ultraviolet (UV) absorption spectra of Compound BD040 according to an embodiment.

DETAILED DESCRIPTION

[0048] Reference will now be made in detail to embodiments, examples of which are illustrated in the accompanying drawings, wherein like reference numerals refer to like elements throughout. In this regard, the present embodiments may have different forms and should not be construed as being limited to the descriptions set forth herein. Accordingly, the embodiments are merely described below, by referring to the figures, to explain aspects of the present description. As used herein, the term "and/or" includes any and all combinations of one or more of the associated listed items. Expressions such as "at least one of," when preceding a list of elements, modify the entire list of elements and do not modify the individual elements of the list.

[0049] It will be understood that when an element is referred to as being "on" another element, it can be directly in contact with the other element or intervening elements may be present therebetween. In contrast, when an element is referred to as being "directly on" another element, there are no intervening elements present.

[0050] It will be understood that, although the terms first, second, third etc. may be used herein to describe various elements, components, regions, layers, and/or sections, these elements, components, regions, layers, and/or sections should not be limited by these terms. These terms are only used to distinguish one element, component, region, layer, or section from another element, component, region, layer, or section. Thus, a first element, component, region, layer, or section discussed below could be termed a second element, component, region, layer, or section without departing from the teachings of the present embodiments.

[0051] The terminology used herein is for the purpose of describing particular embodiments only and is not intended to be limiting. As used herein, the singular forms "a," "an," and "the" are intended to include the plural forms as well, unless the context clearly indicates otherwise.

[0052] The term "or" means "and/or." It will be further understood that the terms "comprises" and/or "comprising," or "includes" and/or "including" when used in this specification, specify the presence of stated features, regions, integers, steps, operations, elements, and/or components, but do not preclude the presence or addition of one or more other features, regions, integers, steps, operations, elements, components, and/or groups thereof.

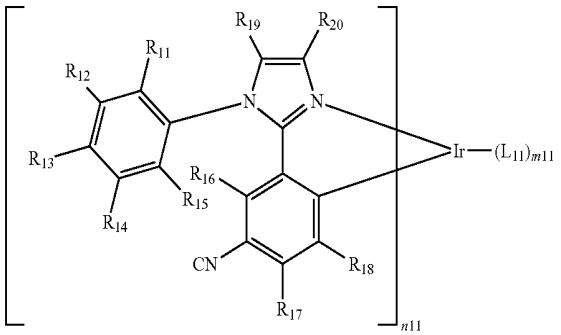
[0053] Unless otherwise defined, all terms (including technical and scientific terms) used herein have the same meaning as commonly understood by one of ordinary skill in the art to which this general inventive concept belongs. It will be further understood that terms, such as those defined in commonly used dictionaries, should be interpreted as having a meaning that is consistent with their meaning in the context of the relevant art and the present disclosure, and will not be interpreted in an idealized or overly formal sense unless expressly so defined herein.

[0054] Exemplary embodiments are described herein with reference to cross section illustrations that are schematic

illustrations of idealized embodiments. As such, variations from the shapes of the illustrations as a result, for example, of manufacturing techniques and/or tolerances, are to be expected. Thus, embodiments described herein should not be construed as limited to the particular shapes of regions as illustrated herein but are to include deviations in shapes that result, for example, from manufacturing. For example, a region illustrated or described as flat may, typically, have rough and/or nonlinear features. Moreover, sharp angles that are illustrated may be rounded. Thus, the regions illustrated in the figures are schematic in nature and their shapes are not intended to illustrate the precise shape of a region and are not intended to limit the scope of the present claims.

[0055] According to an aspect of the present disclosure, there is provided an organometallic compound represented by Formula 1:

Formula 1



[0056] In Formula 1, M_{11} may be selected from a first-row transition metal, a second-row transition metal, and a third-row transition metal.

[0057] For example, in Formula 1, M_{11} may be selected from iridium (Ir), platinum (Pt), osmium (Os), ruthenium (Ru), rhodium (Rh), palladium (Pd), copper (Cu), silver (Ag), gold (Au), titanium (Ti), zirconium (Zr), hafnium (Hf), europium (Eu), terbium (Tb), and thulium (Tm). However, embodiments are not limited thereto.

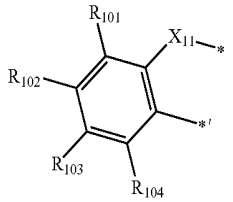
[0058] In some embodiments, in Formula 1, M_{11} may be selected from Ir, Pt, and Os, but is not limited thereto.

[0059] In some other embodiments, in Formula 1, M_{11} may be selected from Ir and Pt, but is not limited thereto.

[0060] In Formula 1, R_{11} to R_{18} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{1e} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, adjacent two of R_{11} to R_{15} may be linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring.

[0061] For example, in Formula 1, R_{11} to R_{18} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, adjacent two of R_{11} to R_{15} may be linked to form a substructure represented by Formula 10. However, embodiments are not limited thereto.

Formula 10



[0062] In Formula 10,

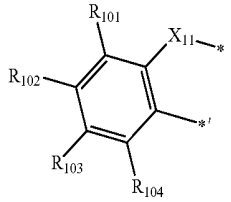
[0063] X_{11} may be selected from O, S, and $N(R_{105})$;

[0064] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group; and

[0065] * and *' may be each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

[0066] In some embodiments, in Formula 1, R_{11} to R_{18} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, adjacent two of R_{11} to R_{15} may be linked to form a substructure represented by Formula 10. However, embodiments are not limited thereto.

Formula 10



[0067] In Formula 10,

[0068] X_{11} may be selected from O, S, and $N(R_{105})$;

[0069] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0070] * and *' may be each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

[0071] In some embodiments, in Formula 1, R_{11} to R_{18} may be each independently selected from

[0072] a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, and $—Si(Q_1)(Q_2)(Q_3)$,

[0073] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

[0074] a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

[0075] $—Si(Q_4)(Q_5)(Q_6)$,

[0076] wherein Q_1 to Q_3 may be each independently selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group; and

[0077] Q_4 to Q_6 may be each independently selected from

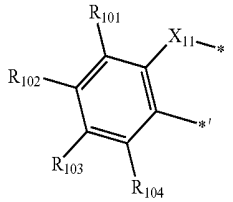
[0078] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

[0079] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I and a cyano group;

[0080] at least one of Q_4 to Q_6 may be selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group; and

[0081] optionally, adjacent two of R_{11} to R_{15} may be linked to form a substructure represented by Formula 10. However, embodiments are not limited thereto.

Formula 10



[0082] In Formula 10,

[0083] X_{11} may be selected from 0, 3, and $N(R_{105})$;

[0084] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

[0085] * and *' may be each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

[0086] In some embodiments, in Formula 1, R_{11} to R_{18} may be each independently selected from

[0087] a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and $—Si(Q_1)(Q_2)(Q_3)$,

[0088] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

[0089] a phenyl group and a biphenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, and

[0090] $—Si(Q_4)(Q_5)(Q_6)$;

[0091] Q_1 to Q_3 may be each independently selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group;

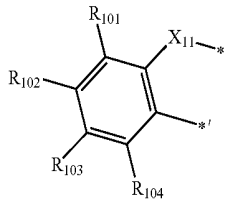
[0092] Q_4 to Q_6 may be each independently selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, and

[0093] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I and a cyano group;

[0094] at least one of Q_4 to Q_6 may be selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I and a cyano group; and

[0095] optionally, R_{12} and R_{13} may be linked to form a substructure represented by Formula 10. However, embodiments are not limited thereto,

Formula 10



[0096] In Formula 10,

[0097] X_{11} may be selected from O, S, and $N(R_{105})$:

[0098] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

[0099] * and *' may be each independently a carbon atom to which R_{12} and R_{13} are bound.

[0100] In some embodiments, in Formula 1, R_{11} to R_{19} may be each independently selected from

[0101] a hydrogen, a deuterium, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and $—Si(CH_3)_3$,

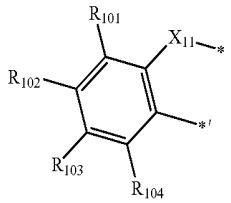
[0102] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group; and a neo-pentyl group, each substituted with a deuterium,

[0103] a phenyl group and a biphenyl group, each substituted with a deuterium, and

[0104] $—Si(CD_3)_3$; and

[0105] optionally, R_{12} and R_{13} may be linked to form a substructure represented by Formula 10. However, embodiments are not limited thereto.

Formula 10



[0106] In Formula 10,

[0107] X_{11} may be selected from O, S, and $N(R_{105})$:

[0108] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

[0109] * and *' may be each independently a carbon atom to which R_{12} and R_{13} are bound.

[0110] In some embodiments, in Formula 1, at least one of R_{11} to R_{15} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_5-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group.

[0111] For example, in Formula 1, at least one of R_{11} to R_{15} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, but is not limited thereto.

[0112] In some embodiments, in Formula 1, at least one of R_{11} to R_{15} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted

C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group. However, embodiments are not limited thereto.

[0113] In some other embodiments, in Formula 1, at least one of R_{11} to R_{15} may be selected from

[0114] an iso-propyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, and —$Si(Q_1)(Q_2)(Q_3)$,

[0115] an iso-propyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

[0116] a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

[0117] —$Si(Q_4)(Q_5)(Q_6)$,

[0118] wherein Q_1 to Q_3 may be each independently selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group;

[0119] Q_4 to Q_6 may be each independently selected from

[0120] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

[0121] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group; and

[0122] at least one of Q_4 to Q_6 may be selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group. However, embodiments are not limited thereto.

[0123] In some other embodiments, in Formula 1, at least one of R_{11} to R_{15} may be selected from

[0124] an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and —$Si(Q_1)(Q_2)(Q_3)$,

[0125] an iso-propyl group; an iso-butyl group; a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

[0126] a phenyl group and a biphenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group; and

[0127] —$Si(Q_4)(Q_5)(Q_6)$,

[0128] wherein Q_1 to Q_3 may be each independently a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group;

[0129] Q_4 to Q_6 may be each independently selected from

[0130] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, and

[0131] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I and a cyano group; and

[0132] at least one of Q_4 to Q_6 may be selected from a methyl group, an iso-propyl group, an iso-butyl group; a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group. However, embodiments are not limited thereto.

[0133] In some other embodiments, in Formula 1, at least one of R_{11} to R_{15} may be selected from

[0134] an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and —$Si(Q_1)(Q_2)(Q_3)$,

[0135] an iso-propyl group; an iso-butyl group; a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

[0136] a phenyl group and a biphenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, and

[0137] —$Si(Q_4)(Q_5)(Q_6)$;

[0138] Q_1 to Q_3 may be each independently selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group;

[0139] Q_4 to Q_6 may be each independently selected from

[0140] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, and

[0141] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I and a cyano group; and

[0142] at least one of Q_4 to Q_6 may be selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group. However, embodiments are not limited thereto.

[0143] In some other embodiments, in Formula 1, at least one of R_{11} to R_{15} may be selected from

[0144] an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and —$Si(CH_3)_3$,

[0145] an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with a deuterium,

[0146] a phenyl group, and a biphenyl group, each substituted with a deuterium, and —$Si(CD_3)_3$. However, embodiments are not limited thereto.

[0147] In some embodiments, in Formula 1, R_{11} and R_{12}, R_{12} and R_{13}, R_{13} and R_{14}, or R_{14} and R_{15} may be optionally linked to each other to form a condensed ring. However, embodiments are not limited thereto.

[0148] In some embodiments, in Formula 1, R_{15} and R_{15} may be optionally linked to each other via a single bond. However, embodiments are not limited thereto.

[0149] In Formula 1, R_{19} and R_{20} may be each independently selected from a hydrogen, a deuterium, a C_1-C_{30} alkyl group, and a deuterium-substituted C_1-C_{30} alkyl group.

[0150] For example, in Formula 1, R_{19} and R_{20} may be each independently selected from

[0151] a hydrogen;

[0152] a deuterium;

[0153] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group; an iso-butyl group, and a tert-butyl group; and

[0154] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, and a tert-butyl group, each substituted with a deuterium. However, embodiments are not limited thereto.

[0155] In some embodiments, in Formula 1, R_{19} and R_{20} may be each independently selected from a hydrogen and a deuterium. However, embodiments are not limited thereto.

[0156] In some embodiments, in Formula 1, R_{19} may be a deuterium, and R_{20} may be a hydrogen. However, embodiments are not limited thereto.

[0157] In some embodiments, in Formula 1, R_{19} may be a hydrogen, and R_{20} may be a deuterium. However, embodiments are not limited thereto,

[0158] In some embodiments, in Formula 1, R_{19} and R_{20} may be both a deuterium. However, embodiments are not limited thereto.

[0159] In Formula 1, at least one of R_{11} to R_{20} may be a deuterium-containing substituent.

[0160] As used herein, the term "deuterium-containing substituent" refers to a deuterium or a substituent that contains at least one deuterium. For example, a deuterium-containing substituent may refer to a substituent that is obtained by substituting at least one hydrogen atom in a substituent such as a C_1-C_{30} alkyl group, a C_6-C_{30} aryl group, or the like as described above with a deuterium atom.

[0161] For example, in Formula 1, the deuterium-containing substituent may be selected from

[0162] a deuterium, and

[0163] a C_1-C_{30} alkyl group, a C_3-C_{30} branched alkyl group; a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, a C_1-C_{30} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, and a C_1-C_{30} alkylsilyl group, each substituted with a deuterium. However, embodiments are not limited thereto.

[0164] In some embodiments, in Formula 1, the deuterium-containing substituent may be selected from

[0165] a deuterium,

[0166] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with a deuterium, and

[0167] —$Si(Q_4)(Q_5)(Q_6)$,

[0168] wherein Q_4 to Q_6 may be each independently selected from

[0169] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

[0170] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group, wherein at least one of Q_4 to Q_6 may be selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with a deuterium. However, embodiments are not limited thereto.

[0171] In some embodiments, in Formula 1, the deuterium-containing substituent may be selected from

[0172] a deuterium, and

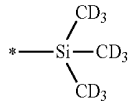
[0173] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with a deuterium. However, embodiments are not limited thereto.

[0174] In some embodiments, in Formula 1, the deuterium-containing substituent may be selected from

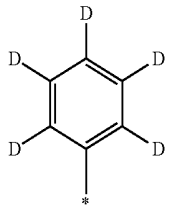
[0175] -D, —CH_2D, -CHD_2, -CD_3, —CH_2CH_2D, —CH_2CHD_2, —CH_2CD_3, -$CHDCH_3$, -$CHDCH_2D$, -$CHDCHD_2$, -$CHDCD_3$, -CD_2CH_3, -CD_2CH_2D, -CD_2CHD_2, -CD_2CD_3, —$CH_2CH_2CH_2D$, —$CH_2CH_2CHD_2$, —$CH_2CH_2CD_3$, —CH_2CHDCH_3, —CH_2CHDCH_2D, —$CH_2CHDCHD_2$, —CH_2CHDCD_3, —$CH_2CD_2CH_3$, —$CH_2CD_2CH_2D$, —$CH_2CD_2CHD_2$, —$CH_2CD_2CD_3$, -$CHDCH_2CH_2D$, -$CHDCH_2CHD_2$, -$CHDCH_2CD_3$, -$CHDCHDCH_3$, -$CHDCHDCH_2D$, -$CHDCHDCHD_2$, -$CHDCHDCD_3$, -$CHDCD_2CH_3$, -$CHDCD_2CH_2D$, -$CHDCD_2CHD_2$, -$CHDCD_2CD_3$, -$CD_2CH_2CH_2D$, -$CD_2CH_2CHD_2$, -$CD_2CH_2CD_3$, -CD_2CHDCH_3, -CD_2CHDCH_2D, -$CD_2CHDCHD_2$, -CD_2CHDCD_3, -$CD_2CD_2CH_3$, -$CD_2CD_2CH_2D$, -$CD_2CD_2CHD_2$, -$CD_2CD_2CD_3$, —$CH(CH_3)(CH_2D)$, —$CH(CH_3)(CHD_2)$, —$CH(CH_2D)(CH_2D)$, —$CH(CH_3)(CD_3)$, —$CH(CHD_2)(CHD_2)$, —$CH(CH_2D)(CD_3)$, —$CH(CHD_2)(CHD_2)$, —$CH(CHD_2)(CD_3)$, —$CH(CD_3)_2$, -$CD(CH_3)_2$, -$CD(CH_3)(CH_2D)$, -$CD(CH_3)(CHD_2)$,

-CD(CH_2D)(CH_2D), -CD(CH_3)(CD_3), -CD(CHD_2)(CHD_2), -CD(CH_2D)(CD_3), -CD(CHD_2)(CHD_2), -CD(CHD_2)(CD_3), -CD(CD_3)$_2$, -CD_2CD(CD_3)$_2$, —C(CD_3)$_3$, -CD_2C(CD_3)$_3$; and groups represented by Formulae 3-1 to 3-5. However, embodiments are not limited thereto.

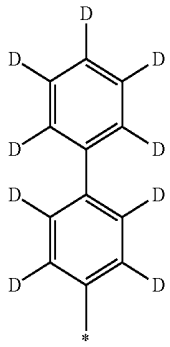
3-1



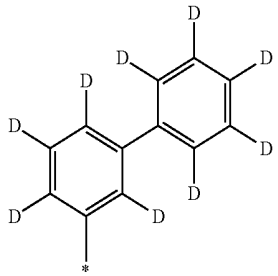
3-2



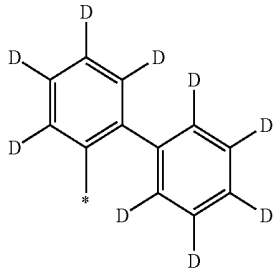
3-3



3-4



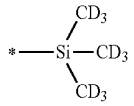
3-5



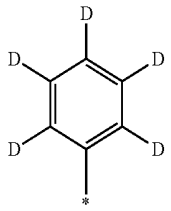
[0176] In Formulae 3-1 to 3-5, may be a binding site to an adjacent atom.

[0177] In some embodiments, in Formula 1, the deuterium-containing substituent may be selected from -D, —CH_2D, -CHD_2, -CD_3, —CH(CH_3)(CH_2D), —CH(CH_3)(CHD_2), —CH(CH_2D)$_2$, —CH(CH_3)(CD_3), —CH(CHD)(CHD_2), —CH(CH_2D)(CD_3), —CH(CHD_2)$_2$, —CH(CHD_2)(CD_3), —CH(CD_3)$_2$, -CD(CH_3)$_2$, -CD(CH_3)(CH_2D), -CD(CH_3)(CHD_2), -CD(CH_2D)(CH_2D), -CD(CH_3)(CD_3), -CD(CHD)(CHD_2), -CD(CH_2D)(CD_3), -CD(CHD_2)$_2$, -CD(CHD_2)(CD_3), -CD(CD_3)$_2$, -CD_2CD(CD_3)$_2$, —C(CD_3)$_3$, -CD_2C(CD_3)$_3$; and groups represented by Formulae 3-1 to 3-5. However, embodiments are not limited thereto:

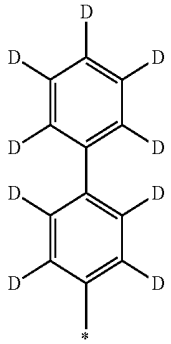
3-1



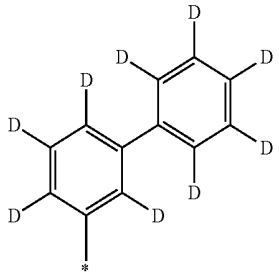
3-2



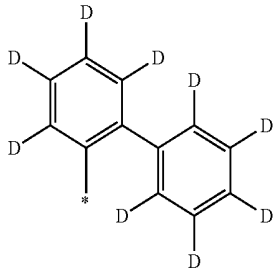
3-3



3-4



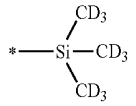
3-5



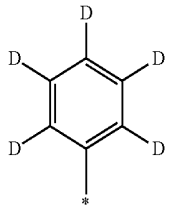
[0178] In Formulae 3-1 to 3-5, * may be a binding site to an adjacent atom.

[0179] In some other embodiments, in Formula 1, the deuterium-containing substituent may be selected from -D, —CH_2D, -CHD_2, -CD_3, -CD(CH_3)$_2$, -CD(CH_3)(CH_2D), -CD(CH_3)(CHD_2), -CD(CH_3)(CD_3), -CD(CH_2D)(CD_3), -CD(CHD_2)(CD_3), -CD(CD_3)$_2$, -CD_2CD(CD_3)$_2$, —C(CD_3)$_3$, -CD_2C(CD_3)$_3$, and groups represented by Formulae 3-1 to 3-5. However, embodiments are not limited thereto:

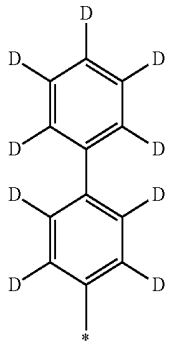
3-1



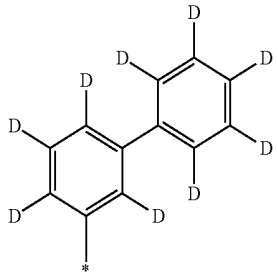
3-2



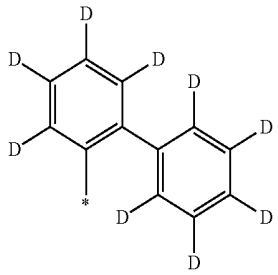
3-3



3-4

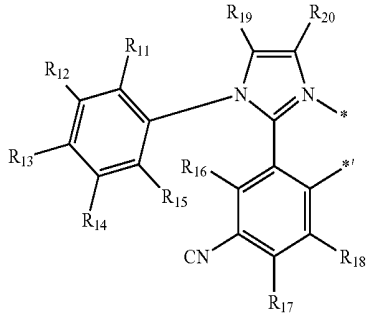


3-5



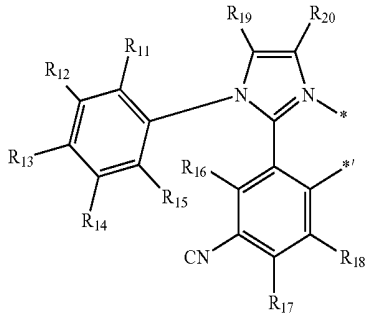
[0180] In Formulae 3-1 to 3-5, * may be a binding site to an adjacent atom.

[0181] In Formula 1, a moiety represented by



(wherein * and *' may be each a binding site to M_{11} in Formula 1) may include at least one deuterium.

[0182] Whether the moiety represented by



includes a deuterium or not may be identified by analyzing the ^{1}H NMR spectrum or molecular weight measured using a molecular weight measurement device such as a matrix-assisted laser desorption-ionization-time-of-flight mass spectrometer.

[0183] For example, a compound (hereinafter referred to as a "first reference compound") having a backbone that is identical to that of the organometallic compound represented by Formula 1 but including no deuterium atom may be prepared. The ^{1}H NMR spectra of the first reference compound and the organometallic compound represented by Formula 1 may be measured. Then, by comparing integral values of signals at a certain ppm in the measured spectra of the first reference compound and the organometallic compound with each other, the number of hydrogen atoms at certain positions (i.e., hydrogen atoms bound to certain carbons) in the organometallic compound represented by Formula 1 that are substituted with deuterium may be determined.

[0184] Alternatively, a compound (hereinafter referred to as a "second reference compound") having a backbone that is identical to that of the organometallic compound represented by Formula 1 and of which all hydrogen atoms are substituted with deuterium may be assumed. By comparing the calculated molecular weight of the second reference compound with the molecular weight of the organometallic compound represented by Formula 1, the number of hydrogen atoms in the organometallic compound represented by Formula 1 that are substituted with deuterium may be determined.

[0185] In some embodiments, the organometallic compound represented by Formula 1 may have a deuteration rate, which is determined by Equation 1 of 50% or more, but embodiments are not limited thereto:

$$\text{Deuteration rate (\%)} = n_{D1}/(n_{H1}+n_{D1})\times 100 \qquad \text{Equation 1}$$

[0186] In Equation 1,

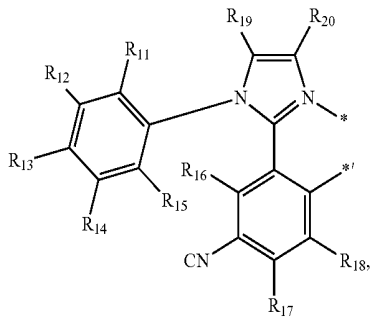
[0187] n_{H1} indicates a total number of hydrogens included in the deuterium-containing substituents; and

[0188] n_{D1} indicates a total number of deuterium atoms included in the deuterium-containing substituents.

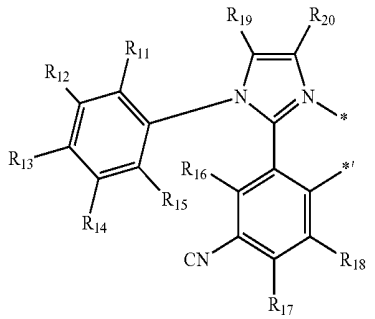
[0189] In some embodiments, a deuteration rate represented by Equation 1 of the organometallic compound represented by Formula 1 may be 70% or more, but embodiments are not limited thereto.

[0190] In some embodiments, a deuteration rate represented by Equation 1 of the organometallic compound represented by Formula 1 may be 90% or more, but embodiments are not limited thereto.

[0191] In Formula 1, n11 indicates the number of ligands represented by



and n11 may be selected from 1, 2, and 3. When n11 is 2 or more, the ligands represented by



may be identical to or different from each other.

[0192] In some embodiments, in Formula 1, M_{11} may be Ir; and n11 may be selected from 2 and 3. However, embodiments are not limited thereto.

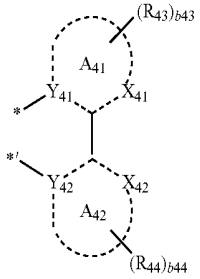
[0193] In some other embodiments, in Formula 1, M_{11} may be Pt; and n11 may be selected from 1 and 2. However, embodiments are not limited thereto.

[0194] In Formula 1, L_{11} may be selected from a monodentate ligand and a bidentate ligand.

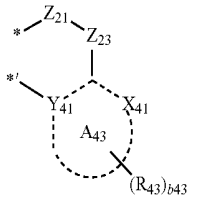
[0195] In some embodiments, in Formula 1, L_{11} may be selected from monodentate ligands. For example, L_{11} may be selected from I^-, Br^-, Cl^-, a sulfide, a nitrate, an azide, a hydroxide, a cyanate, an isocyanate, a thiocyanate, water, acetonitrile, a pyridine, ammonia, carbon monoxide, $P(Ph)_3$, $P(Ph)_2CH_3$, $PPh(CH_3)_2$, and $P(CH_3)_3$, but embodiments are not limited thereto.

[0196] In some embodiments, in Formula 1, L_{11} may be selected from bidentate ligands. For example, L_{11} may be selected from an oxalate, an acetylacetonate, a picolinic acid, a 1,2-bis(diphenylphosphino)ethane, a 1,1-bis(diphenylphosphino)methane, a glycinate, an ethylenediamine, and ligands represented by Formulae 4-1 to 4-4, but embodiments are not limited thereto:

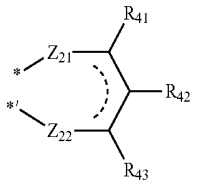
4-1



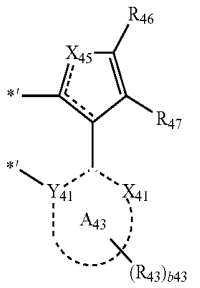
4-2



4-3



4-4



[0197] In Formulae 4-1 to 4-4,

[0198] X_{41} may be CR_{41} or a nitrogen atom (N);

[0199] X_{42} may be CR_{42} or N;

[0200] X_{45} may be O, S, or $N(R_{45})$;

[0201] Y_{41} and Y_{42} may be each independently a carbon (C) atom or N;

[0202] Z_{21} and Z_{22} may be each independently N, O, $N(R_{48})$, $P(R_{48})(R_{49})$, or $As(R_{48})(R_{49})$:

[0203] Z_{23} may be CO or CH_2;

[0204] A_{41} to A_{43} may be each independently selected from a C_3-C_{10} cycloalkane, a C_1-C_{10} heterocycloalkane, a C_3-C_{10} cycloalkene, a C_1-C_{10} heterocycloalkene, a C_6-C_{10} arena, a C_1-C_{10} heteroarene, a non-aromatic condensed polycycle, and a non-aromatic condensed heteropolycycle;

[0205] R_{41} to R_{49} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group

or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{60} alkyl group, a substituted or unsubstituted C_2-C_{60} alkenyl group, a substituted or unsubstituted C_2-C_{60} alkynyl group, a substituted or unsubstituted C_1-C_{60} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{60} aryl group, a substituted or unsubstituted C_6-C_{60} aryloxy group, a substituted or unsubstituted C_6-C_{60} arylthio group, a substituted or unsubstituted C_7-C_{60} arylalkyl group, a substituted or unsubstituted C_1-C_{60} heteroaryl group, a substituted or unsubstituted C_2-C_{60} heteroaryloxy group, a substituted or unsubstituted C_2-C_{60} heteroarylthio group, a substituted or unsubstituted C_3-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and —$Si(Q_{41})(Q_{42})(Q_{43})$;

[0206] optionally, adjacent two of R_{41} to R_{44} are linked to form a substituted or unsubstituted saturated ring or a substituted or unsubstituted unsaturated ring;

[0207] optionally, R_{46} and R_{47} are linked to form a substituted or unsubstituted saturated ring or a substituted or unsubstituted unsaturated ring;

[0208] b43 and b44 may be each independently an integer selected from 1 to 5;

[0209] Q_{41} to Q_{43} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{60} alkyl group, a C_2-C_{60} alkenyl group, a C_2-C_{60} alkynyl group, a C_1-C_{60} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{60} aryl group, a C_6-C_{60} aryloxy group, a C_6-C_{60} arylthio group, a C_7-C_{60} arylalkyl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_1-C_{60} heteroaryl group, a C_2-C_{60} heteroaryloxy group, a C_2-C_{60} heteroarylthio group, a C_3-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group; and

[0210] * and *' each independently indicate a binding site to M_{11} in Formula 1

[0211] In some embodiments, in Formula 1, L_{11} may be represented by one of Formulae 4-1 to 4-4;

[0212] A_{41} to A_{43} may be each independently selected from a benzene, a naphthalene, a fluorene, a spiro-fluorene, an indene, a furan, a thiophene, a carbazole, a benzofuran, a benzothiophene, a dibenzofuran, a dibenzothiophene, a pyrrole, an imidazole, a pyrazole, a thiazole, an isothiazole, an oxazole, an isoxazole, a triazole, a pyridine, a pyrazine, a pyrimidine, a quinoline, an isoquinoline, a benzoquinoline, a quinoxaline, a quinazoline, a naphthyridine, a benzoimidazole, a benzoxazole, an isobenzoxazole, an oxadiazole, and a triazine;

[0213] R_{41} to R_{47} may be each independently selected from

[0214] a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{20} alkyl group, and a C_1-C_{20} alkoxy group,

[0215] a C_1-C_{23} alkyl group, and a C_1-C_{60} alkoxy group, each substituted with at least one selected from a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a phenyl group, a naphthyl group, a pyridinyl group, and a pyrimidinyl group,

[0216] a phenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzoimidazolyl group, a benzofuranyl group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, an isobenzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, and an imidazopyrimidinyl group,

[0217] a phenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzoimidazolyl group, a benzofuranyl group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, an isobenzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, and an imidazopyrimidinyl group, each substituted with at least one selected from a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid or a salt thereof, a sulfonic acid or a salt thereof, a phosphoric acid or a salt thereof, a C_1-C_{20} alkyl group, a C_1-C_{20} alkoxy group, a phenyl group, a naphthyl group, a fluorenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a pyrrolyl group, a thiophenyl group, a furanyl group, an imidazolyl group, a pyrazolyl group, a thiazolyl group, an isothiazolyl group, an oxazolyl group, an isoxazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a quinoxalinyl group, a quinazolinyl group,

a cinnolinyl group, a carbazolyl group, a phenanthrolinyl group, a benzoimidazolyl group, a benzofuranyl group, a benzothiophenyl group, an isobenzothiazolyl group, a benzoxazolyl group, an isobenzoxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyridinyl group, and an imidazopyrimidinyl group, and

[0218] —$Si(Q_{41})(Q_{42})(Q_{43})$;

[0219] b43 and b44 may be each independently an integer selected from 1 to 3;

[0220] Q_{41} to Q_{43} may be each independently selected from a C_1-C_{10} alkyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, and a triazinyl group;

[0221] optionally, adjacent two of R_{41} to R_{44} may be linked to form a substituted or unsubstituted saturated ring or a substituted or unsubstituted unsaturated ring;

[0222] optionally, R_{48} and R_{47} may be linked to form a substituted or unsubstituted saturated ring or a substituted or unsubstituted unsaturated ring. However, embodiments are not limited thereto.

[0223] In some embodiments, in Formula 1, L_{11} may be represented by one of Formulae 4-1 to 4-4;

[0224] A_{41} may be selected from a pyridine, an imidazole, a pyrazole, a triazole, and a tetrazole,

[0225] A_{42} may be selected from a benzene, a pyridine, a pyrazine, a pyrimidine, and a triazine,

[0226] A_{43} may be selected from a benzene and a pyridine;

[0227] R_{41} to R_{44} may be each independently selected from

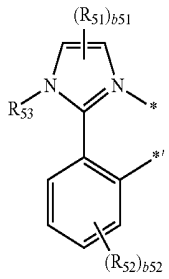
[0228] a hydrogen, —F, a cyano group, a nitro group, a methyl group, an ethyl group, a propyl group, an n-butyl group, an iso-butyl group, a sec-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a sec-pentyl group, a tert-pentyl group, an n-hexyl group, an iso-hexyl group, a sec-hexyl group, a tert-hexyl group, an n-heptyl group, an iso-heptyl group, a sec-heptyl group, a tert-heptyl group, an n-octyl group, an iso-octyl group, a sec-octyl group, a tert-octyl group, an n-nonyl group, an iso-nonyl group, a sec-nonyl group, a tert-nonyl group, an n-decanyl group, an iso-decanyl group, a sec-decanyl group, a tert-decanyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a triazinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group, and

[0229] a methyl group, an ethyl group, a propyl group, an n-butyl group, an iso-butyl group, a sec-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a sec-pentyl group, a tert-pentyl group, an n-hexyl group, an iso-hexyl group, a sec-hexyl group, a tert-hexyl group, an n-heptyl group, an iso-heptyl group, a sec-heptyl group, a tert-heptyl group, an n-octyl group, an iso-octyl group, a sec-octyl group, a tert-octyl group, an n-nonyl group, an iso-nonyl group, a sec-nonyl group, a tert-nonyl group, an n-decanyl group, an iso-decanyl group, a sec-decanyl group, a tert-decanyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a triazinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group, each substituted with at least one selected from —F, a cyano group, a nitro group, and a methyl group; and

[0230] b43 and b44 may be each independently an integer selected from 1 to 3. However, embodiments are not limited thereto.

[0231] In some embodiments, L_{11} in Formula 1 may be represented by one of Formulae 5-1 to 5-122. However, embodiments are not limited thereto

5-1



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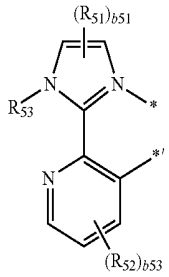

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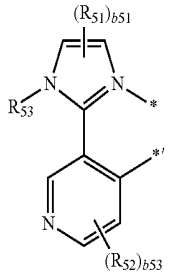

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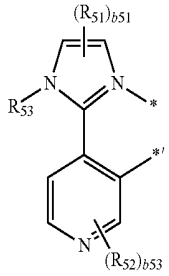

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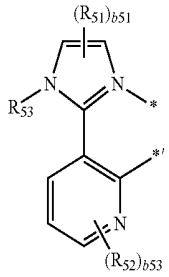

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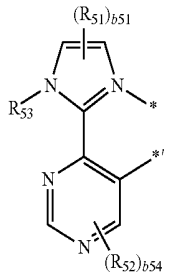

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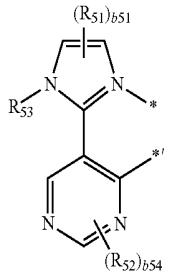

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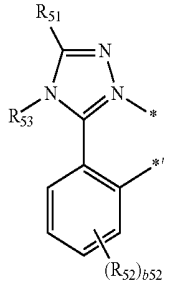

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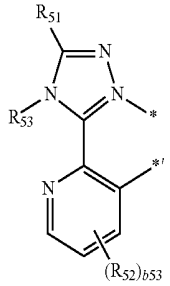

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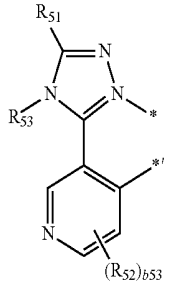

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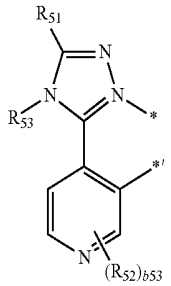

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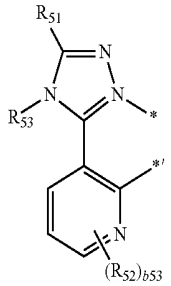

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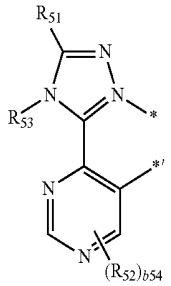

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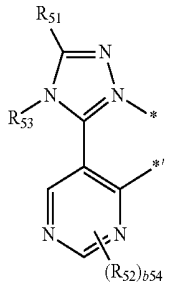

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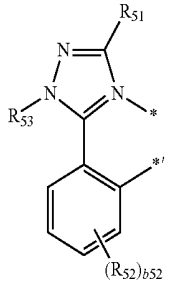

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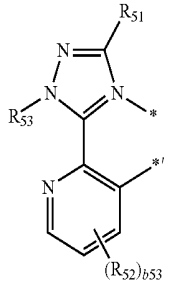

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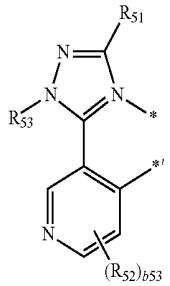

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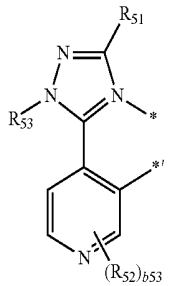

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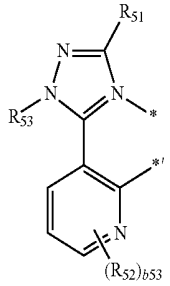

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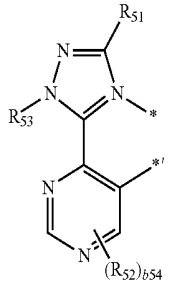

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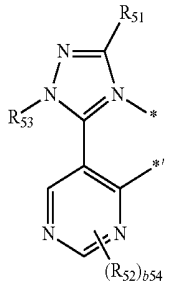

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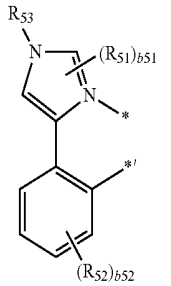

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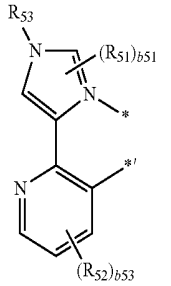

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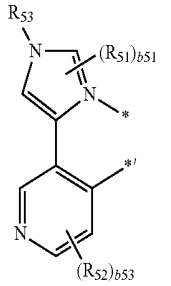

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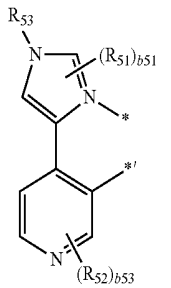

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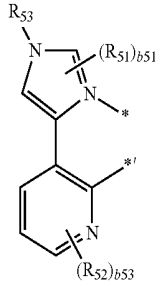

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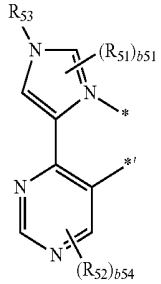

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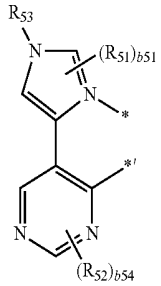

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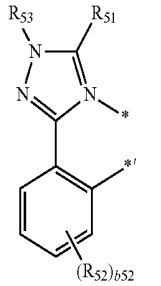

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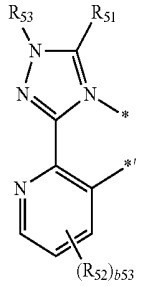

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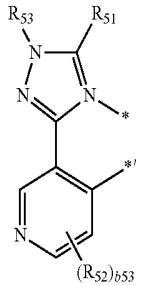

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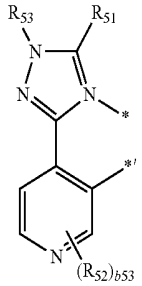

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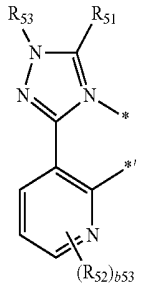

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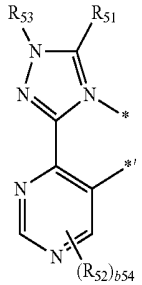

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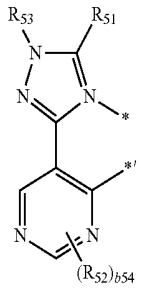

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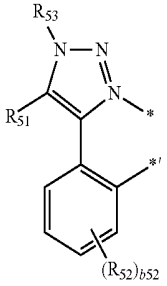

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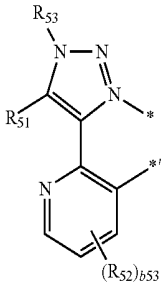

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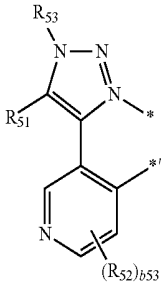

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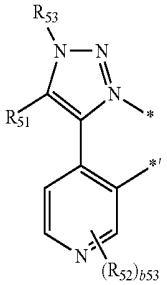

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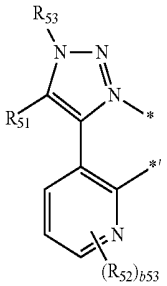

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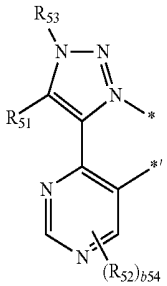

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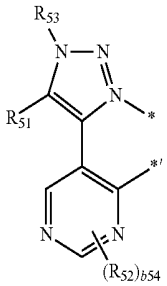

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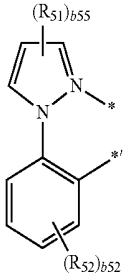

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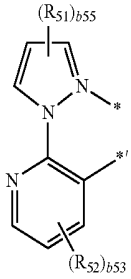

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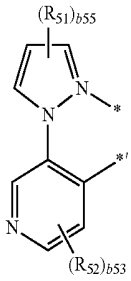

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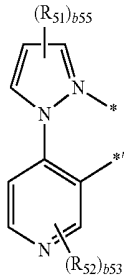

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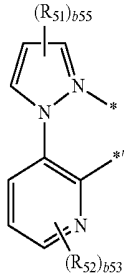

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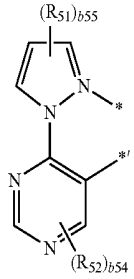

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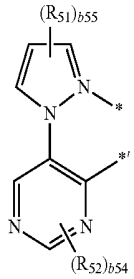

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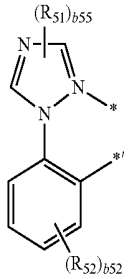

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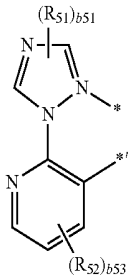

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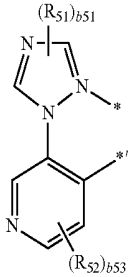

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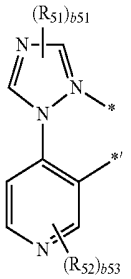

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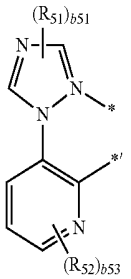

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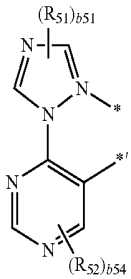

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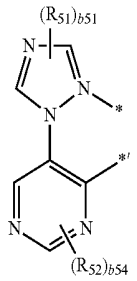

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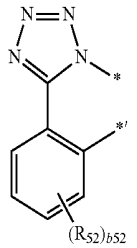

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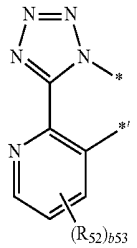

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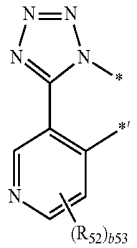

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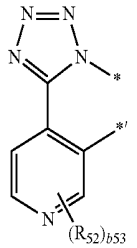

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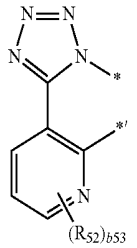

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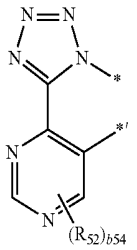

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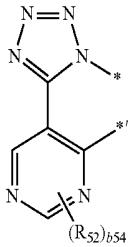

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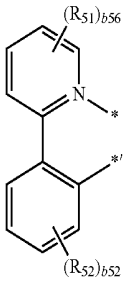

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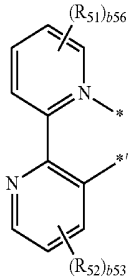

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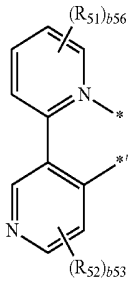

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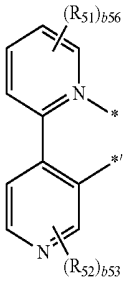

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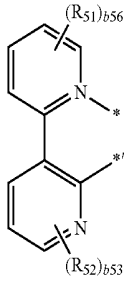

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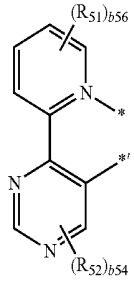

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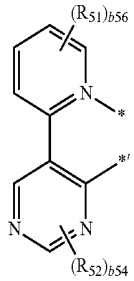

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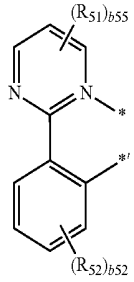

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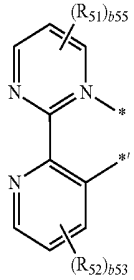

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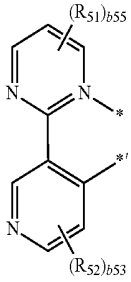

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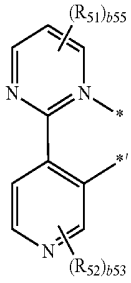

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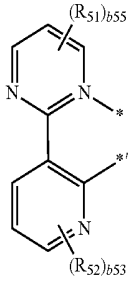

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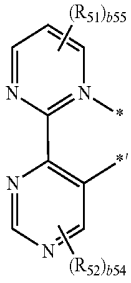

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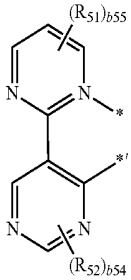

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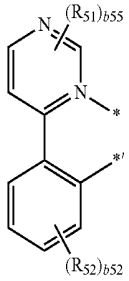

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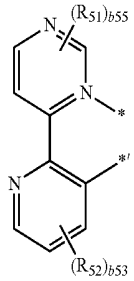

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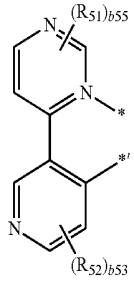

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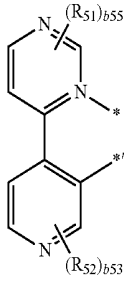

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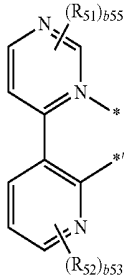

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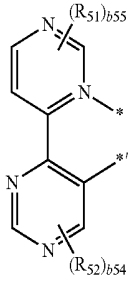

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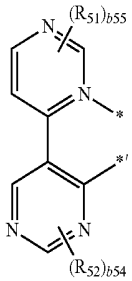

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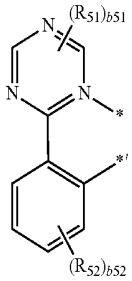

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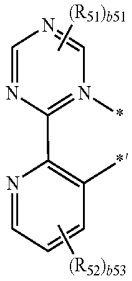

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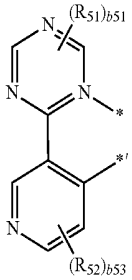

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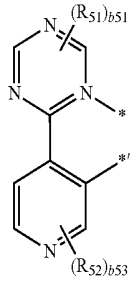

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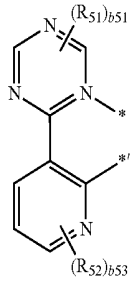

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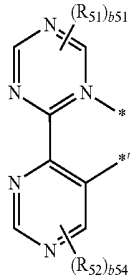

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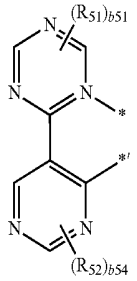

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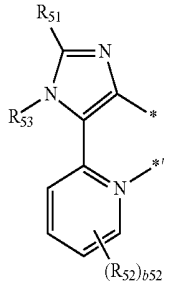

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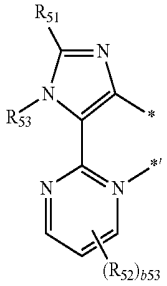

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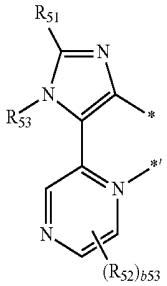

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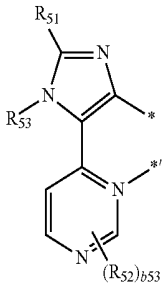

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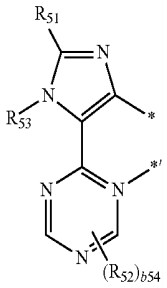

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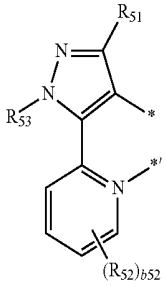

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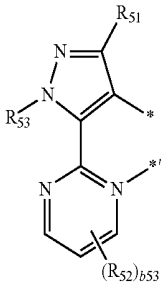

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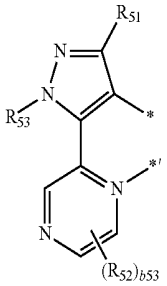

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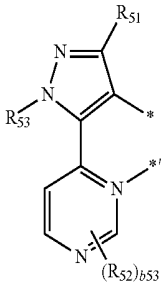

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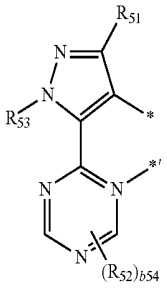

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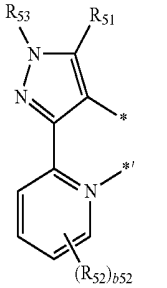

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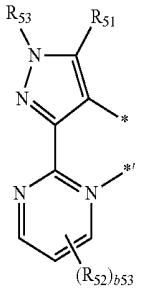

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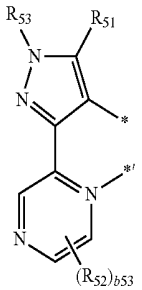

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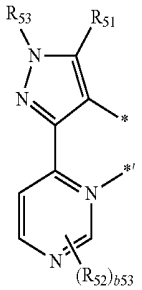

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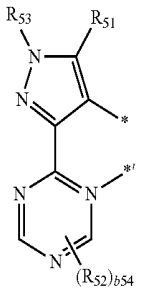

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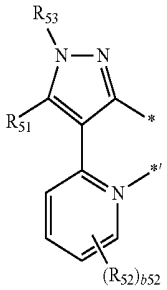

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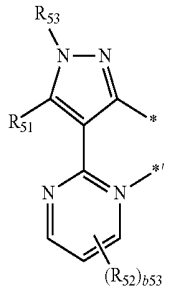

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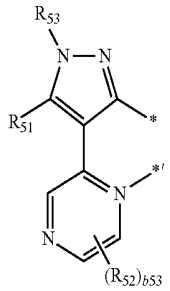

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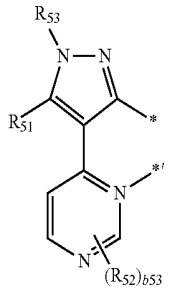

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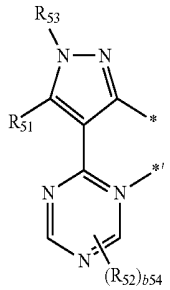

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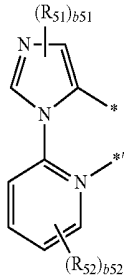

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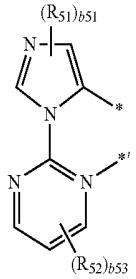

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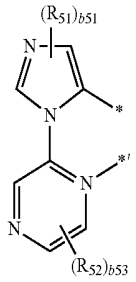

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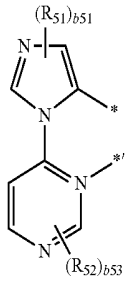

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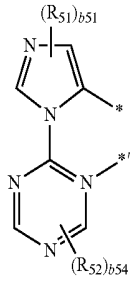

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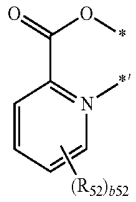

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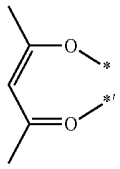

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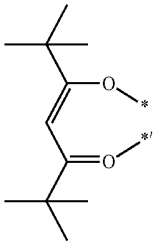


[0232] In Formulae 5-1 to 5-122,

[0233] R_{51} to R_{57} may be each independently selected from

[0234] a hydrogen, —F, a cyano group, a nitro group, a methyl group, an ethyl group, a propyl group, an n-butyl group, an iso-butyl group, a sec-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a sec-pentyl group, a tert-pentyl group, an n-hexyl group, an iso-hexyl group, a sec-hexyl group; a tert-hexyl group, an n-heptyl group, an iso-heptyl group, a sec-heptyl group, a tert-heptyl group, an n-octyl group, an iso-octyl group, a sec-octyl group; a tert-octyl group, an n-nonyl group, an iso-nonyl group, a sec-nonyl group, a tert-nonyl group, an n-decanyl group, an iso-decanyl group, a sec-decanyl group, a tert-decanyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a triazinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group, and

[0235] a methyl group, an ethyl group, a propyl group, an n-butyl group, an iso-butyl group, a sec-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a sec-pentyl group, a tert-pentyl group, an n-hexyl group, an iso-hexyl group, a sec-hexyl group, a tert-hexyl group, an n-heptyl group, an iso-heptyl group, a sec-heptyl group, a tert-heptyl group, an n-octyl group, an iso-octyl group, a sec-octyl group, a tert-octyl group, an n-nonyl group, an iso-nonyl group, a sec-nonyl group, a tert-nonyl group, an n-decanyl group, an iso-decanyl group, a sec-decanyl group, a tert-decanyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a phenyl group; a naphthyl group, a pyridinyl group, a pyrimidinyl group, a triazinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group, each substituted with at least one selected from —F, a cyano group, a nitro group, and a methyl group;

[0236] b51 and b54 may be each independently selected from 1 and 2;

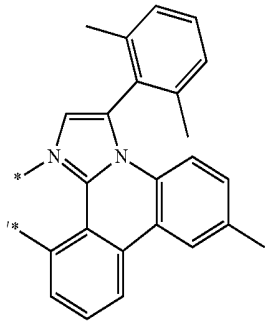
[0237] b53 and b55 may be each independently an integer selected from 1 to 3;

[0238] b52 may be an integer selected from 1 to 4; and

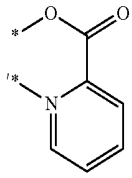
[0239] * and *' may be each independently a binding site to M_{11} in Formula 1.

[0240] In some embodiments, in Formula 1, L_{11} may be selected from ligands represented by Formulae AN1 to AN5. However, embodiments are not limited thereto;

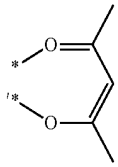
AN1



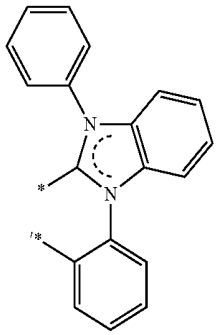
AN2



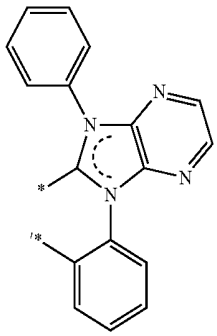
AN3



AN4



AN5



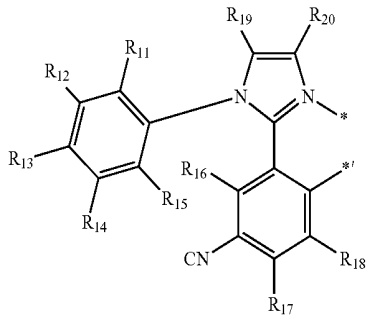
[0241] In Formulae AN1 to AN5, * and *' may be each independently a binding site to M_{11} in Formula 1.

[0242] In Formula 1, m11 indicates the number of groups L_{11}, and m11 may be selected from 0, 1, 2, 3, and 4. When m11 is 2 or more, a plurality of groups L_{11} may be identical to or different from each other. In some embodiments, in Formula 1, m11 may be selected from 0 and 1. However, embodiments are not limited thereto.

[0243] In Formula 1, n11 and m11 may be properly controlled based on the coordination number of Ir. For example,

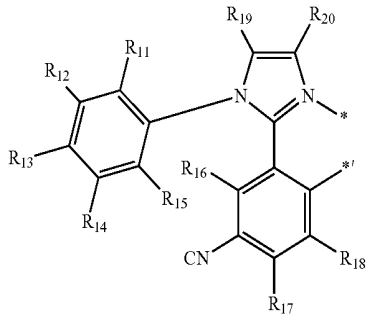
when n11 is 3, m11 may be 0. In some embodiments, when L_{11} is a bidentate ligand with n11 being 2, m11 may be 1. In some embodiments, when L_{11} is a bidentate ligand with n11 being 1, m11 may be 2.

[0244] In some embodiments, the moiety represented by

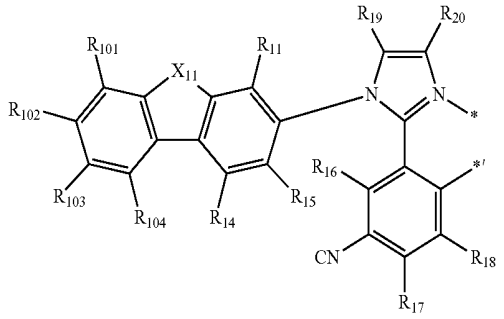


may be represented by one of Formulae 1-1 to 1-3. However, embodiments are not limited thereto:

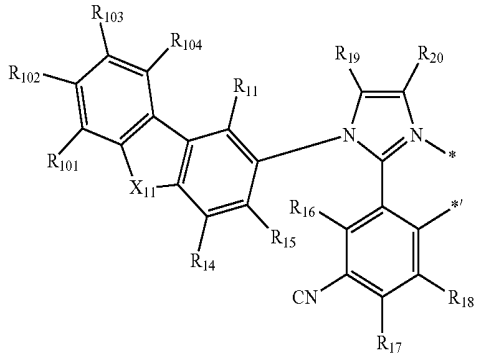
1-1



1-2



1-3



[0245] In Formulae 1-1 to 1-3,

[0246] X_{11} may be selected from O, S, and $N(R_{105})$;

[0247] R_{11} to R_{18} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0248] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0249] at least one of R_{11} to R_{15} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_5-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

[0250] R_{19} and R_{20} may be each independently selected from a hydrogen, a deuterium, C_1-C_{30} alkyl group, and a deuterium substituted C_1-C_{30} alkyl group; and

[0251] at least one of R_{11} to R_{20} may be a deuterium-containing substituent.

[0252] For example, substituents in Formula 1-1 may be defined as in Table 1. However, embodiments are not limited thereto.

TABLE 1

Formula 1-1										
Ligand name	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
LM1	X1	H	X3	H	X1	H	H	H	H	D
LM2	X1	H	X3	H	X1	H	H	H	D	H
LM3	X1	H	X3	H	X1	H	H	H	D	D
LM4	Y1	H	X3	H	Y1	H	H	H	D	D
LM5	Y2	H	X3	H	Y2	H	H	H	D	D
LM6	Y3	H	X3	H	Y3	H	H	H	D	D
LM7	Y3	D	X3	D	Y3	H	H	H	D	D
LM8	Y3	D	X3	D	Y3	D	H	H	D	D
LM9	Y3	D	X3	D	Y3	D	D	H	D	D
LM10	Y3	D	X3	D	Y3	D	D	D	D	D
LM11	Y3	D	Y11	D	Y3	D	D	D	D	D
LM12	Y3	D	Y11	D	Y3	H	X1	H	D	D
LM13	Y3	D	Y11	D	Y3	D	Y3	D	D	D
LM14	Y3	D	Y11	D	Y3	H	X4	H	D	D
LM15	Y3	D	Y11	D	Y3	D	Y12	D	D	D
LM16	X2	H	X3	H	X2	H	H	H	H	D
LM17	X2	H	X3	H	X2	H	H	H	D	H
LM18	X2	H	X3	H	X2	H	H	H	D	D
LM19	Y4	H	X3	H	Y4	H	H	H	D	D
LM20	Y5	H	X3	H	Y5	H	H	H	D	D
LM21	Y6	H	X3	H	Y6	H	H	H	D	D
LM22	Y7	H	X3	H	Y7	H	H	H	D	D
LM23	Y8	H	X3	H	Y8	H	H	H	D	D
LM24	Y9	H	X3	H	Y9	H	H	H	D	D
LM25	Y10	H	X3	H	Y10	H	H	H	D	D
LM26	Y10	D	X3	D	Y10	H	H	H	D	D
LM27	Y10	D	X3	D	Y10	D	H	H	D	D
LM28	Y10	D	X3	D	Y10	D	D	H	D	D
LM29	Y10	D	X3	D	Y10	D	D	D	D	D
LM30	Y10	D	Y11	D	Y10	D	D	D	D	D
LM31	Y10	D	Y11	D	Y10	H	X1	H	D	D
LM32	Y10	D	Y11	D	Y10	D	Y3	D	D	D
LM33	Y10	D	Y11	D	Y10	H	X4	H	D	D
LM34	Y10	D	Y11	D	Y10	D	Y12	D	D	D
LM35	X1	H	X4	H	X1	H	H	H	H	D
LM36	X1	H	X4	H	X1	H	H	H	D	H
LM37	X1	H	X4	H	X1	H	H	H	D	D
LM38	Y1	H	X4	H	Y1	H	H	H	D	D
LM39	Y2	H	X4	H	Y2	H	H	H	D	D
LM40	Y3	H	X4	H	Y3	H	H	H	D	D
LM41	Y3	D	X4	D	Y3	H	H	H	D	D
LM42	Y3	D	X4	D	Y3	D	H	H	D	D
LM43	Y3	D	X4	D	Y3	D	D	H	D	D
LM44	Y3	D	X4	D	Y3	D	D	D	D	D
LM45	Y3	D	Y12	D	Y3	D	D	D	D	D
LM46	Y3	D	Y12	D	Y3	H	X1	H	D	D
LM47	Y3	D	Y12	D	Y3	D	Y3	D	D	D
LM48	Y3	D	Y12	D	Y3	H	X4	H	D	D
LM49	Y3	D	Y12	D	Y3	D	Y12	D	D	D
LM50	X2	H	X4	H	X2	H	H	H	H	D
LM51	X2	H	X4	H	X2	H	H	H	D	H
LM52	X2	H	X4	H	X2	H	H	H	D	D
LM53	Y4	H	X4	H	Y4	H	H	H	D	D
LM54	Y5	H	X4	H	Y5	H	H	H	D	D
LM55	Y6	H	X4	H	Y8	H	H	H	D	D
LM56	Y7	H	X4	H	Y7	H	H	H	D	D
LM57	Y8	H	X4	H	Y8	H	H	H	D	D
LM58	Y9	H	X4	H	Y9	H	H	H	D	D
LM59	Y10	H	X4	H	Y10	H	H	H	D	D
LM60	Y10	D	X4	D	Y10	H	H	H	D	D
LM61	Y10	D	X4	D	Y10	D	H	H	D	D

TABLE 1-continued

Formula 1-1										
Ligand name	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
LM62	Y10	D	X4	D	Y10	D	D	H	D	D
LM63	Y10	D	X4	D	Y10	D	D	D	D	D
LM64	Y10	D	Y12	D	Y10	D	D	D	D	D
LM65	Y10	D	Y12	D	Y10	H	X1	H	D	D
LM66	Y10	D	Y12	D	Y10	D	Y3	D	D	D
LM67	Y10	D	Y12	D	Y10	H	X4	H	D	D
LM68	Y10	D	Y12	D	Y10	D	Y12	D	D	D
LM69	X1	H	X5	H	X1	H	H	H	H	D
LM70	X1	H	X5	H	X1	H	H	H	D	H
LM71	X1	H	X5	H	X1	H	H	H	D	D
LM72	Y1	H	X5	H	Y1	H	H	H	D	D
LM73	Y2	H	X5	H	Y2	H	H	H	D	D
LM74	Y3	H	X5	H	Y3	H	H	H	D	D
LM75	Y3	D	X5	D	Y3	H	H	H	D	D
LM76	Y3	D	X5	D	Y3	D	H	H	D	D
LM77	Y3	D	X5	D	Y3	D	D	H	D	D
LM78	Y3	D	X5	D	Y3	D	D	D	D	D
LM79	Y3	D	Y13	D	Y3	D	D	D	D	D
LM80	Y3	D	Y13	D	Y3	H	X1	H	D	D
LM81	Y3	D	Y13	D	Y3	D	Y3	D	D	D
LM82	Y3	D	Y13	D	Y3	H	X4	H	D	D
LM83	Y3	D	Y13	D	Y3	D	Y12	D	D	D
LM84	X2	H	X5	H	X2	H	H	H	H	D
LM85	X2	H	X5	H	X2	H	H	H	D	H
LM86	X2	H	X5	H	X2	H	H	H	D	D
LM87	Y4	H	X5	H	Y4	H	H	H	D	D
LM88	Y5	H	X5	H	Y5	H	H	H	D	D
LM89	Y6	H	X5	H	Y6	H	H	H	D	D
LM90	Y7	H	X5	H	Y7	H	H	H	D	D
LM91	Y8	H	X5	H	Y8	H	H	H	D	D
LM92	Y9	H	X5	H	Y9	H	H	H	D	D
LM93	Y10	H	X5	H	Y10	H	H	H	D	D
LM94	Y10	D	X5	D	Y10	H	H	H	D	D
LM95	Y10	D	X5	D	Y10	D	H	H	D	D
LM96	Y10	D	X5	D	Y10	D	D	H	D	D
LM97	Y10	D	X5	D	Y10	D	D	D	D	D
LM98	Y10	D	Y13	D	Y10	D	D	D	D	D
LM99	Y10	D	Y13	D	Y10	H	X1	H	D	D
LM100	Y10	D	Y13	D	Y10	D	Y3	D	D	D
LM101	Y10	D	Y13	D	Y10	H	X4	H	D	D
LM102	Y10	D	Y13	D	Y10	D	Y12	D	D	D
LM103	X1	H	X6	H	X1	H	H	H	H	D
LM104	X1	H	X6	H	X1	H	H	H	D	H
LM105	X1	H	X6	H	X1	H	H	H	D	D
LM106	Y1	H	X6	H	Y1	H	H	H	D	D
LM107	Y2	H	X6	H	Y2	H	H	H	D	D
LM108	Y3	H	X6	H	Y3	H	H	H	D	D
LM109	Y3	D	X6	D	Y3	H	H	H	D	D
LM110	Y3	D	X6	D	Y3	D	H	H	D	D
LM111	Y3	D	X6	D	Y3	D	D	H	D	D
LM112	Y3	D	X6	D	Y3	D	D	D	D	D
LM113	Y3	D	Y14	D	Y3	D	D	D	D	D
LM114	Y3	D	Y14	D	Y3	H	X1	H	D	D
LM115	Y3	D	Y14	D	Y3	D	Y3	D	D	D
LM116	Y3	D	Y14	D	Y3	H	X4	H	D	D
LM117	Y3	D	Y14	D	Y3	D	Y12	D	D	D
LM118	X2	H	X6	H	X2	H	H	H	H	D
LM119	X2	H	X6	H	X2	H	H	H	D	H
LM120	X2	H	X6	H	X2	H	H	H	D	D
LM121	Y4	H	X6	H	Y4	H	H	H	D	D
LM122	Y5	H	X6	H	Y5	H	H	H	D	D
LM123	Y6	H	X6	H	Y6	H	H	H	D	D
LM124	Y7	H	X6	H	Y7	H	H	H	D	D
LM125	Y8	H	X6	H	Y8	H	H	H	D	D
LM126	Y9	H	X6	H	Y9	H	H	H	D	D
LM127	Y10	H	X6	H	Y10	H	H	H	D	D
LM128	Y10	D	X6	D	Y10	H	H	H	D	D
LM129	Y10	D	X6	D	Y10	D	H	H	D	D
LM130	Y10	D	X6	D	Y10	D	D	H	D	D
LM131	Y10	D	X6	D	Y10	D	D	D	D	D
LM132	Y10	D	Y14	D	Y10	D	D	D	D	D
LM133	Y10	D	Y14	D	Y10	H	X1	H	D	D

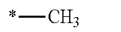
TABLE 1-continued

Formula 1-1										
Ligand name	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
LM134	Y10	D	Y14	D	Y10	D	Y3	D	D	D
LM135	Y10	D	Y14	D	Y10	H	X4	H	D	D
LM136	Y10	D	Y14	D	Y10	D	Y12	D	D	D
LM137	X1	H	X7	H	X1	H	H	H	H	D
LM138	X1	H	X7	H	X1	H	H	H	D	H
LM139	X1	H	X7	H	X1	H	H	H	D	D
LM140	Y1	H	X7	H	Y1	H	H	H	D	D
LM141	Y2	H	X7	H	Y2	H	H	H	D	D
LM142	Y3	H	X7	H	Y3	H	H	H	D	D
LM143	Y3	D	X7	D	Y3	H	H	H	D	D
LM144	Y3	D	X7	D	Y3	D	H	H	D	D
LM145	Y3	D	X7	D	Y3	D	D	H	D	D
LM146	Y3	D	X7	D	Y3	D	D	D	D	D
LM147	Y3	D	X8	D	Y3	D	D	D	D	D
LM148	Y3	D	Y16	D	Y3	D	D	D	D	D
LM149	Y3	D	Y17	D	Y3	D	D	D	D	D
LM150	Y3	D	Y18	D	Y3	D	D	D	D	D
LM151	Y3	D	Y15	D	Y3	D	D	D	D	D
LM152	Y3	D	Y15	D	Y3	H	X1	H	D	D
LM153	Y3	D	Y15	D	Y3	D	Y3	D	D	D
LM154	Y3	D	Y16	D	Y3	D	Y3	D	D	D
LM155	Y3	D	Y17	D	Y3	D	Y3	D	D	D
LM156	Y3	D	Y18	D	Y3	D	Y3	D	D	D
LM157	Y3	D	Y15	D	Y3	H	X4	H	D	D
LM158	Y3	D	Y15	D	Y3	D	Y12	D	D	D
LM159	Y3	D	Y16	D	Y3	D	Y12	D	D	D
LM160	Y3	D	Y17	D	Y3	D	Y12	D	D	D
LM161	Y3	D	Y18	D	Y3	D	Y12	D	D	D
LM162	X2	H	X7	H	X2	H	H	H	H	D
LM163	X2	H	X7	H	X2	H	H	H	D	H
LM164	X2	H	X7	H	X2	H	H	H	D	D
LM165	Y4	H	X7	H	Y4	H	H	H	D	D
LM166	Y5	H	X7	H	Y5	H	H	H	D	D
LM167	Y6	H	X7	H	Y6	H	H	H	D	D
LM168	Y7	H	X7	H	Y7	H	H	H	D	D
LM169	Y8	H	X7	H	Y8	H	H	H	D	D
LM170	Y9	H	X7	H	Y9	H	H	H	D	D
LM171	Y10	H	X7	H	Y10	H	H	H	D	D
LM172	Y10	D	X7	D	Y10	H	H	H	D	D
LM173	Y10	D	X7	D	Y10	D	H	H	D	D
LM174	Y10	D	X7	D	Y10	D	D	H	D	D
LM175	Y10	D	X7	D	Y10	D	D	D	D	D
LM176	Y10	D	X8	D	Y10	D	D	D	D	D
LM177	Y10	D	Y16	D	Y10	D	D	D	D	D
LM178	Y10	D	Y17	D	Y10	D	D	D	D	D
LM179	Y10	D	Y18	D	Y10	D	D	D	D	D
LM180	Y10	D	Y15	D	Y10	D	D	D	D	D
LM181	Y10	D	Y15	D	Y10	H	X1	H	D	D
LM182	Y10	D	Y15	D	Y10	D	Y3	D	D	D
LM183	Y10	D	Y16	D	Y10	D	Y3	D	D	D
LM184	Y10	D	Y17	D	Y10	D	Y3	D	D	D
LM185	Y10	D	Y18	D	Y10	D	Y3	D	D	D
LM186	Y10	D	Y15	D	Y10	H	X4	H	D	D
LM187	Y10	D	Y15	D	Y10	D	Y12	D	D	D
LM188	Y10	D	Y16	D	Y10	D	Y12	D	D	D
LM189	Y10	D	Y17	D	Y10	D	Y12	D	D	D
LM190	Y10	D	Y18	D	Y10	D	Y12	D	D	D
LM191	X1	X7	H	H	X1	H	H	H	H	D
LM192	X1	X7	H	H	X1	H	H	H	D	H
LM193	X1	X7	H	H	X1	H	H	H	D	D
LM194	Y1	X7	H	H	Y1	H	H	H	D	D
LM195	Y2	X7	H	H	Y2	H	H	H	D	D
LM196	Y3	X7	H	H	Y3	H	H	H	D	D
LM197	Y3	X7	D	D	Y3	H	H	H	D	D
LM198	Y3	X7	D	D	Y3	D	H	H	D	D
LM199	Y3	X7	D	D	Y3	D	D	H	D	D
LM200	Y3	X7	D	D	Y3	D	D	D	D	D
LM201	Y3	Y15	D	D	Y3	D	D	D	D	D
LM202	Y3	Y16	D	D	Y3	D	D	D	D	D
LM203	Y3	Y17	D	D	Y3	D	D	D	D	D
LM204	Y3	Y18	D	D	Y3	D	D	D	D	D
LM205	Y3	Y15	D	D	Y3	H	X1	H	D	D

TABLE 1-continued

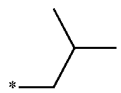
Formula 1-1										
Ligand name	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
LM206	Y3	Y15	D	D	Y3	D	Y3	D	D	D
LM207	Y3	Y16	D	D	Y3	D	Y3	D	D	D
LM208	Y3	Y17	D	D	Y3	D	Y3	D	D	D
LM209	Y3	Y18	D	D	Y3	D	Y3	D	D	D
LM210	Y3	Y15	D	D	Y3	H	X4	H	D	D
LM211	Y3	Y15	D	D	Y3	D	Y12	D	D	D
LM212	Y3	Y16	D	D	Y3	D	Y12	D	D	D
LM213	Y3	Y17	D	D	Y3	D	Y12	D	D	D
LM214	Y3	Y18	D	D	Y3	D	Y12	D	D	D
LM215	X2	X7	H	H	X2	H	H	H	H	D
LM216	X2	X7	H	H	X2	H	H	H	D	H
LM217	X2	X7	H	H	X2	H	H	H	D	D
LM218	Y4	X7	H	H	Y4	H	H	H	D	D
LM219	Y5	X7	H	H	Y5	H	H	H	D	D
LM220	Y6	X7	H	H	Y6	H	H	H	D	D
LM221	Y7	X7	H	H	Y7	H	H	H	D	D
LM222	Y8	X7	H	H	Y8	H	H	H	D	D
LM223	Y9	X7	H	H	Y9	H	H	H	D	D
LM224	Y10	X7	H	H	Y10	H	H	H	D	D
LM225	Y10	X7	D	D	Y10	H	H	H	D	D
LM226	Y10	X7	D	D	Y10	D	H	H	D	D
LM227	Y10	X7	D	D	Y10	D	D	H	D	D
LM228	Y10	X7	D	D	Y10	D	D	D	D	D
LM229	Y10	X8	D	D	Y10	D	D	D	D	D
LM230	Y10	Y16	D	D	Y10	D	D	D	D	D
LM231	Y10	Y17	D	D	Y10	D	D	D	D	D
LM232	Y10	Y18	D	D	Y10	D	D	D	D	D
LM233	Y10	Y15	D	D	Y10	D	D	D	D	D
LM234	Y10	Y15	D	D	Y10	H	X1	H	D	D
LM235	Y10	Y15	D	D	Y10	D	Y3	D	D	D
LM236	Y10	Y16	D	D	Y10	D	Y3	D	D	D
LM237	Y10	Y17	D	D	Y10	D	Y3	D	D	D
LM238	Y10	Y18	D	D	Y10	D	Y3	D	D	D
LM239	Y10	Y15	D	D	Y10	H	X4	H	D	D
LM240	Y10	Y15	D	D	Y10	D	Y12	D	D	D
LM241	Y10	Y16	D	D	Y10	D	Y12	D	D	D
LM242	Y10	Y17	D	D	Y10	D	Y12	D	D	D
LM243	Y10	Y18	D	D	Y10	D	Y12	D	D	D

[0253] In Table 1, X1 to 10 and Y1 to Y18 may be represented by the following formulae.



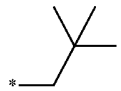
X1

X2



X3

X4

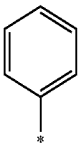


X5

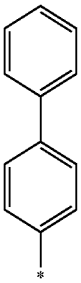
-continued

X6

X7

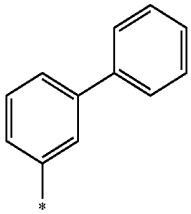


X8

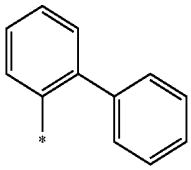


-continued

X9



X10

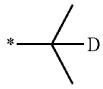


Y1 *—CH_2D

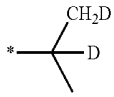
Y2 *—CHD_2

Y3 *—CD_3

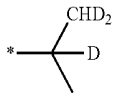
Y4



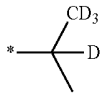
Y5



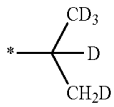
Y6



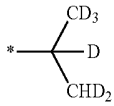
Y7



Y8



Y9



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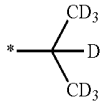

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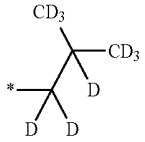

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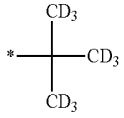

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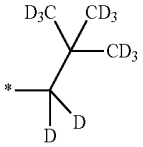

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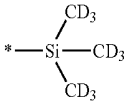

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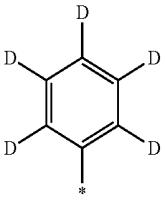

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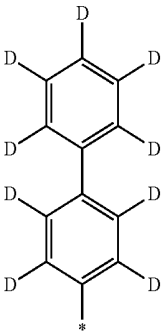

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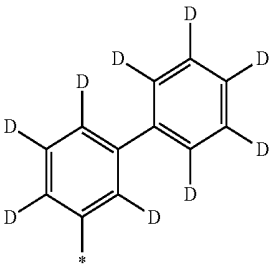

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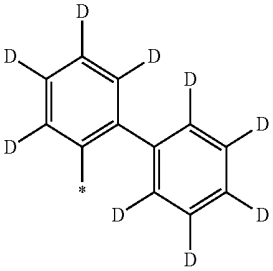


[0254] For example, substituents in Formula 1-2 may be defined as in Table 2. However, embodiments are not limited thereto.

TABLE 2

Formula 1-2													
Ligand name	R_{11}	X_{11}	R_{101}	R_{102}	R_{103}	R_{104}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
LFM1	Y10	N—Ph	D	D	D	D	D	Y10	D	D	D	D	D
LFM2	Y10	S	D	D	D	D	D	Y10	D	D	D	D	D
LFM3	Y10	O	D	D	D	D	D	Y10	D	D	D	D	D
LFM4	Y3	O	D	D	D	D	D	Y3	D	D	D	D	D
LFM5	Y10	O	D	D	D	D	D	Y10	D	D	D	D	D
LFM6	Y10	O	D	D	D	D	D	Y10	D	Y3	D	D	D
LFM7	Y10	O	D	D	D	D	D	Y10	D	Y12	D	D	D

[0255] In Table 2, "Ph" indicates a phenyl group, and X1 to X10 and Y1 to Y18 may be the same as those represented above in connection with Table 1.

[0256] For example, substituents in Formula 1-3 may be defined as in Table 3. However, embodiments are not limited thereto.

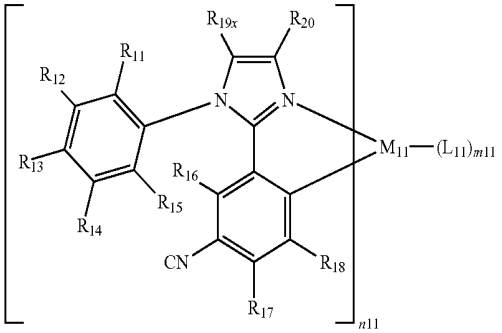
TABLE 3

Formula 1-3													
Ligand name	R_{11}	X_{11}	R_{101}	R_{102}	R_{103}	R_{104}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
LFP1	Y10	N—Ph	D	D	D	D	D	Y10	D	D	D	D	D
LFP2	Y10	S	D	D	D	D	D	Y10	D	D	D	D	D
LFP3	Y10	O	D	D	D	D	D	Y10	D	D	D	D	D
LFP4	Y3	O	D	D	D	D	D	Y3	D	D	D	D	D
LFP5	Y10	O	D	D	D	D	D	Y10	D	D	D	D	D
LFP6	Y10	O	D	D	D	D	D	Y10	D	Y3	D	D	D
LFP7	Y10	O	D	D	D	D	D	Y10	D	Y12	D	D	D

[0257] In Table 3, "Ph" indicates a phenyl group, and X1 to X10 and Y1 to Y18 may be the same as those represented above in connection with Table 1.

[0258] In some other embodiments, the organometallic compound of Formula 1 may be represented by one of Formulae 1-11 to 1-22. However, embodiments are not limited thereto.

1-11



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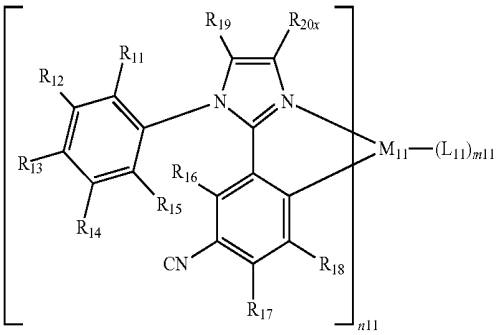

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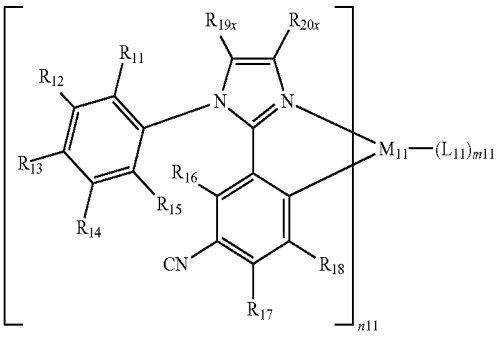

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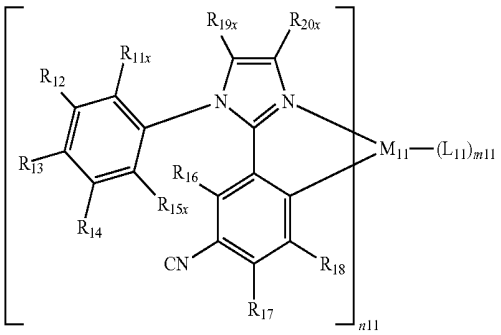

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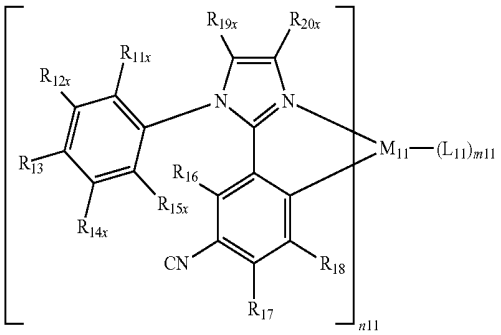

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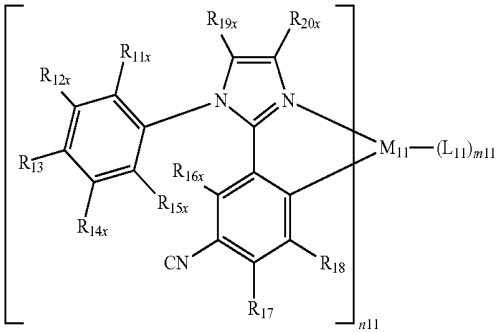

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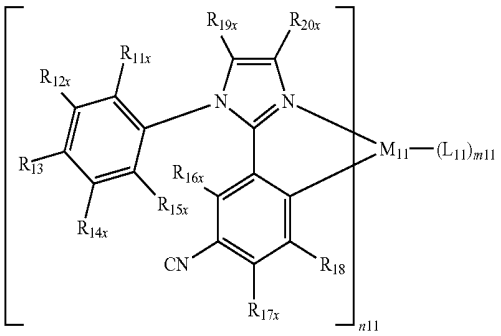

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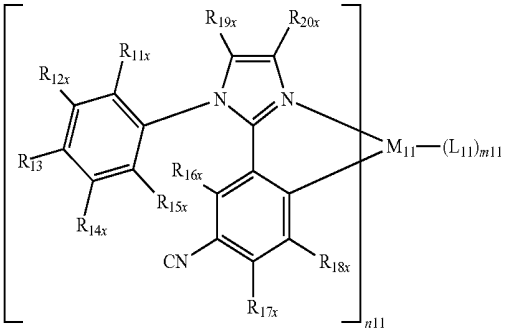

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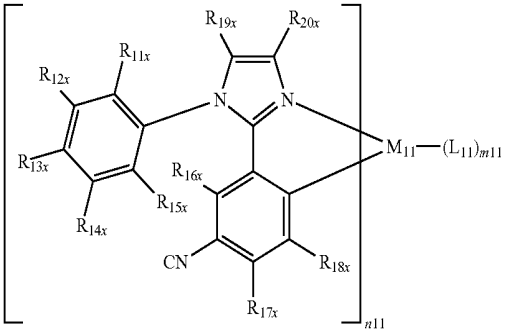

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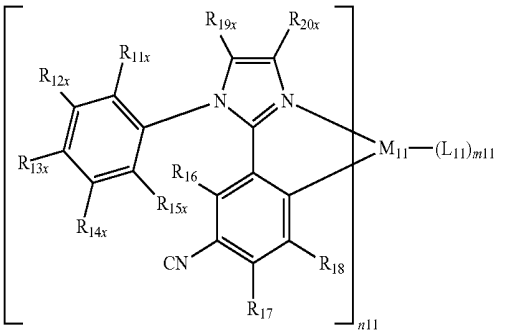

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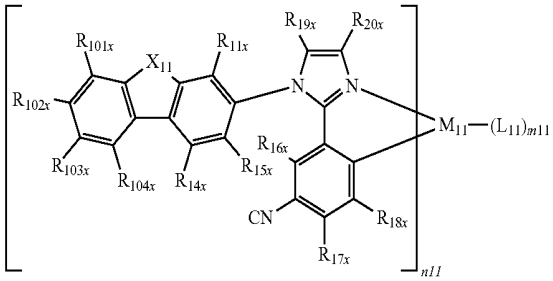

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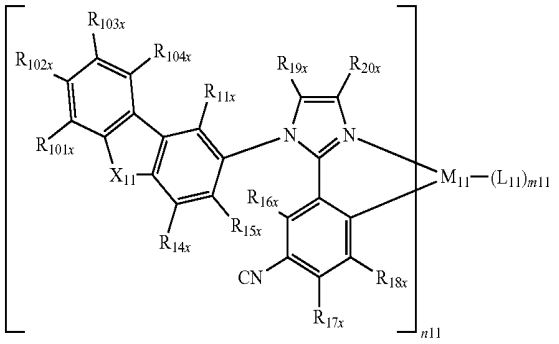

[0259] In Formulae 1-11 to 1-22,

[0260] M_{11}, R_{11} to R_{20}, n11, L_{11}, and m11 may be defined the same as those of Formula 1;

[0261] X_{11} may be selected from O, S, and $N(R_{105})$;

[0262] R_{101} to R_{105} may be each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group; and

[0263] R_{11x}, R_{12x}, R_{13x}, R_{14x}, R_{15x}, R_{16x}, R_{17x}, R_{18x}, R_{19x}, R_{20x}, R_{101x}, R_{102x}, R_{103x}, and R_{104x} may be each independently a deuterium-containing substituent.

[0264] In some embodiments, the organometallic compound of Formula 1 may be represented by Formula 101. However, embodiments are not limited thereto.

$$(L_{101})_{n101}\text{-}M_{101}\text{-}(L_{102})_{m101} \qquad \text{Formula 101}$$

[0265] In Formula 101, L_{101}, n101, M_{101}, L_{102}, and m101 may be defined as shown in Tables 4 to 6.

TABLE 4

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD001	LM1	3	Ir	—	0
BD002	LM2	3	Ir	—	0
BD003	LM3	3	Ir	—	0
BD004	LM4	3	Ir	—	0
BD005	LM5	3	Ir	—	0
BD006	LM6	3	Ir	—	0
BD007	LM7	3	Ir	—	0
BD008	LM8	3	Ir	—	0
BD009	LM9	3	Ir	—	0
BD010	LM10	3	Ir	—	0
BD011	LM11	3	Ir	—	0
BD012	LM12	3	Ir	—	0
BD013	LM13	3	Ir	—	0
BD014	LM14	3	Ir	—	0

TABLE 4-continued

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD015	LM15	3	Ir	—	0
BD016	LM16	3	Ir	—	0
BD017	LM17	3	Ir	—	0
BD018	LM18	3	Ir	—	0
BD019	LM19	3	Ir	—	0
BD020	LM20	3	Ir	—	0
BD021	LM21	3	Ir	—	0
BD022	LM22	3	Ir	—	0
BD023	LM23	3	Ir	—	0
BD024	LM24	3	Ir	—	0
BD025	LM25	3	Ir	—	0
BD026	LM26	3	Ir	—	0
BD027	LM27	3	Ir	—	0
BD028	LM28	3	Ir	—	0
BD029	LM29	3	Ir	—	0
BD030	LM30	3	Ir	—	0
BD031	LM31	3	Ir	—	0
BD032	LM32	3	Ir	—	0
BD033	LM33	3	Ir	—	0
BD034	LM34	3	Ir	—	0
BD035	LM35	3	Ir	—	0
BD036	LM36	3	Ir	—	0
BD037	LM37	3	Ir	—	0
BD038	LM38	3	Ir	—	0
BD039	LM39	3	Ir	—	0
BD040	LM40	3	Ir	—	0
BD041	LM41	3	Ir	—	0
BD042	LM42	3	Ir	—	0
BD043	LM43	3	Ir	—	0
BD044	LM44	3	Ir	—	0
BD045	LM45	3	Ir	—	0
BD046	LM46	3	Ir	—	0
BD047	LM47	3	Ir	—	0
BD048	LM48	3	Ir	—	0
BD049	LM49	3	Ir	—	0
BD050	LM50	3	Ir	—	0
BD051	LM51	3	Ir	—	0
BD052	LM52	3	Ir	—	0
BD053	LM53	3	Ir	—	0
BD054	LM54	3	Ir	—	0
BD055	LM55	3	Ir	—	0
BD056	LM56	3	Ir	—	0
BD057	LM57	3	Ir	—	0
BD058	LM58	3	Ir	—	0
BD059	LM59	3	Ir	—	0
BD060	LM60	3	Ir	—	0
BD061	LM61	3	Ir	—	0
BD062	LM62	3	Ir	—	0
BD063	LM63	3	Ir	—	0
BD064	LM64	3	Ir	—	0
BD065	LM65	3	Ir	—	0
BD066	LM66	3	Ir	—	0
BD067	LM67	3	Ir	—	0
BD068	LM68	3	Ir	—	0
BD069	LM69	3	Ir	—	0
BD070	LM70	3	Ir	—	0
BD071	LM71	3	Ir	—	0
BD072	LM72	3	Ir	—	0
BD073	LM73	3	Ir	—	0
BD074	LM74	3	Ir	—	0
BD075	LM75	3	Ir	—	0
BD076	LM76	3	Ir	—	0
BD077	LM77	3	Ir	—	0
BD078	LM78	3	Ir	—	0
BD079	LM79	3	Ir	—	0
BD080	LM80	3	Ir	—	0
BD081	LM81	3	Ir	—	0
BD082	LM82	3	Ir	—	0
BD083	LM83	3	Ir	—	0
BD084	LM84	3	Ir	—	0
BD085	LM85	3	Ir	—	0
BD086	LM86	3	Ir	—	0
BD087	LM87	3	Ir	—	0
BD088	LM88	3	Ir	—	0

TABLE 4-continued

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD089	LM89	3	Ir	—	0
BD090	LM90	3	Ir	—	0
BD091	LM91	3	Ir	—	0
BD092	LM92	3	Ir	—	0
BD093	LM93	3	Ir	—	0
BD094	LM94	3	Ir	—	0
BD095	LM95	3	Ir	—	0
BD096	LM96	3	Ir	—	0
BD097	LM97	3	Ir	—	0
BD098	LM98	3	Ir	—	0
BD099	LM99	3	Ir	—	0
BD100	LM100	3	Ir	—	0

TABLE 5

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD101	LM101	3	Ir	—	0
BD102	LM102	3	Ir	—	0
BD103	LM103	3	Ir	—	0
BD104	LM104	3	Ir	—	0
BD105	LM105	3	Ir	—	0
BD106	LM106	3	Ir	—	0
BD107	LM107	3	Ir	—	0
BD108	LM108	3	Ir	—	0
BD109	LM109	3	Ir	—	0
BD110	LM110	3	Ir	—	0
BD111	LM111	3	Ir	—	0
BD112	LM112	3	Ir	—	0
BD113	LM113	3	Ir	—	0
BD114	LM114	3	Ir	—	0
BD115	LM115	3	Ir	—	0
BD116	LM116	3	Ir	—	0
BD117	LM117	3	Ir	—	0
BD118	LM118	3	Ir	—	0
BD119	LM119	3	Ir	—	0
BD120	LM120	3	Ir	—	0
BD121	LM121	3	Ir	—	0
BD122	LM122	3	Ir	—	0
BD123	LM123	3	Ir	—	0
BD124	LM124	3	Ir	—	0
BD125	LM125	3	Ir	—	0
BD126	LM126	3	Ir	—	0
BD127	LM127	3	Ir	—	0
BD128	LM128	3	Ir	—	0
BD129	LM129	3	Ir	—	0
BD130	LM130	3	Ir	—	0
BD131	LM131	3	Ir	—	0
BD132	LM132	3	Ir	—	0
BD133	LM133	3	Ir	—	0
BD134	LM134	3	Ir	—	0
BD135	LM135	3	Ir	—	0
BD136	LM136	3	Ir	—	0
BD137	LM137	3	Ir	—	0
BD138	LM138	3	Ir	—	0
BD139	LM139	3	Ir	—	0
BD140	LM140	3	Ir	—	0
BD141	LM141	3	Ir	—	0
BD142	LM142	3	Ir	—	0
BD143	LM143	3	Ir	—	0
BD144	LM144	3	Ir	—	0
BD145	LM145	3	Ir	—	0
BD146	LM146	3	Ir	—	0
BD147	LM147	3	Ir	—	0
BD148	LM148	3	Ir	—	0
BD149	LM149	3	Ir	—	0
BD150	LM150	3	Ir	—	0
BD151	LM151	3	Ir	—	0
BD152	LM152	3	Ir	—	0
BD153	LM153	3	Ir	—	0

TABLE 5-continued

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD154	LM154	3	Ir	—	0
BD155	LM155	3	Ir	—	0
BD156	LM156	3	Ir	—	0
BD157	LM157	3	Ir	—	0
BD158	LM158	3	Ir	—	0
BD159	LM159	3	Ir	—	0
BD160	LM160	3	Ir	—	0
BD161	LM161	3	Ir	—	0
BD162	LM162	3	Ir	—	0
BD163	LM163	3	Ir	—	0
BD164	LM164	3	Ir	—	0
BD165	LM165	3	Ir	—	0
BD166	LM166	3	Ir	—	0
BD167	LM167	3	Ir	—	0
BD168	LM168	3	Ir	—	0
BD169	LM169	3	Ir	—	0
BD170	LM170	3	Ir	—	0
BD171	LM171	3	Ir	—	0
BD172	LM172	3	Ir	—	0
BD173	LM173	3	Ir	—	0
BD174	LM174	3	Ir	—	0
BD175	LM175	3	Ir	—	0
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BD189	LM189	3	Ir	—	0
BD190	LM190	3	Ir	—	0
BD191	LM191	3	Ir	—	0
BD192	LM192	3	Ir	—	0
BD193	LM193	3	Ir	—	0
BD194	LM194	3	Ir	—	0
BD195	LM195	3	Ir	—	0
BD196	LM196	3	Ir	—	0
BD197	LM197	3	Ir	—	0
BD198	LM198	3	Ir	—	0
BD199	LM199	3	Ir	—	0
BD200	LM200	3	Ir	—	0

TABLE 6

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD201	LM201	3	Ir	—	0
BD202	LM202	3	Ir	—	0
BD203	LM203	3	Ir	—	0
BD204	LM204	3	Ir	—	0
BD205	LM205	3	Ir	—	0
BD206	LM206	3	Ir	—	0
BD207	LM207	3	Ir	—	0
BD208	LM208	3	Ir	—	0
BD209	LM209	3	Ir	—	0
BD210	LM210	3	Ir	—	0
BD211	LM211	3	Ir	—	0
BD212	LM212	3	Ir	—	0
BD213	LM213	3	Ir	—	0
BD214	LM214	3	Ir	—	0
BD215	LM215	3	Ir	—	0
BD216	LM216	3	Ir	—	0
BD217	LM217	3	Ir	—	0
BD218	LM218	3	Ir	—	0

TABLE 6-continued

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD219	LM219	3	Ir	—	0
BD220	LM220	3	Ir	—	0
BD221	LM221	3	Ir	—	0
BD222	LM222	3	Ir	—	0
BD223	LM223	3	Ir	—	0
BD224	LM224	3	Ir	—	0
BD225	LM225	3	Ir	—	0
BD226	LM226	3	Ir	—	0
BD227	LM227	3	Ir	—	0
BD228	LM228	3	Ir	—	0
BD229	LM229	3	Ir	—	0
BD230	LM230	3	Ir	—	0
BD231	LM231	3	Ir	—	0
BD232	LM232	3	Ir	—	0
BD233	LM233	3	Ir	—	0
BD234	LM234	3	Ir	—	0
BD235	LM235	3	Ir	—	0
BD236	LM236	3	Ir	—	0
BD237	LM237	3	Ir	—	0
BD238	LM238	3	Ir	—	0
BD239	LM239	3	Ir	—	0
BD240	LM240	3	Ir	—	0
BD241	LM241	3	Ir	—	0
BD242	LM242	3	Ir	—	0
BD243	LM243	3	Ir	—	0
BD244	LFM1	3	Ir	—	0
BD245	LFM2	3	Ir	—	0
BD246	LFM3	3	Ir	—	0
BD247	LFM4	3	Ir	—	0
BD248	LFM5	3	Ir	—	0
BD249	LFM8	3	Ir	—	0
BD250	LFM7	3	Ir	—	0
BD251	LFP1	3	Ir	—	0
BD252	LFP2	3	Ir	—	0
BD253	LFP3	3	Ir	—	0
BD254	LFP4	3	Ir	—	0
BD255	LFP5	3	Ir	—	0
BD256	LFP6	3	Ir	—	0
BD257	LFP7	3	Ir	—	0
BD258	LM47	2	Ir	AN1	1
BD259	LM47	2	Ir	AN2	1
BD260	LM47	2	Ir	AN3	1
BD261	LM47	2	Ir	AN4	1
BD262	LM47	2	Ir	AN5	1
BD263	LM11	2	Pt	—	0
BD264	LM13	2	Pt	—	0
BD265	LM15	2	Pt	—	0
BD266	LM45	2	Pt	—	0
BD267	LM47	2	Pt	—	0
BD268	LM49	2	Pt	—	0
BD269	LM98	2	Pt	—	0
BD270	LM100	2	Pt	—	0
BD271	LM102	2	Pt	—	0
BD272	LM132	2	Pt	—	0
BD273	LM134	2	Pt	—	0
BD274	LM136	2	Pt	—	0
BD275	LM151	2	Pt	—	0
BD276	LM153	2	Pt	—	0
BD277	LM158	2	Pt	—	0
BD278	LM180	2	Pt	—	0
BD279	LM182	2	Pt	—	0
BD280	LM187	2	Pt	—	0
BD281	LM201	2	Pt	—	0
BD282	LM206	2	Pt	—	0
BD283	LM211	2	Pt	—	0
BD284	LM233	2	Pt	—	0
BD285	LM235	2	Pt	—	0
BD286	LM240	2	Pt	—	0
BD287	LFM5	2	Pt	—	0
BD288	LFM6	2	Pt	—	0
BD289	LFM7	2	Pt	—	0
BD290	LFP5	2	Pt	—	0
BD291	LFP6	2	Pt	—	0
BD292	LFP7	2	Pt	—	0

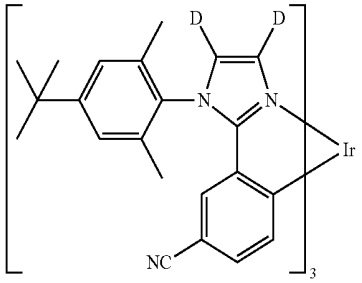
TABLE 6-continued

Compound name	L_{101}	n101	M_{101}	L_{102}	m101
BD293	LM47	1	Pt	AN1	1
BD294	LM47	1	Pt	AN2	1
BD295	LM47	1	Pt	AN3	1
BD296	LM47	1	Pt	AN4	1
BD297	LM47	1	Pt	AN5	1

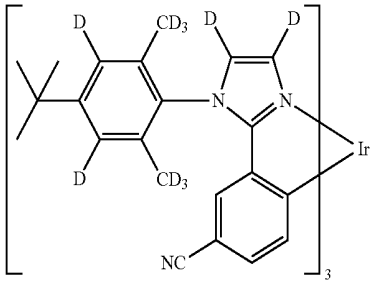
[0266] In Tables 4 to 6, LM1 to LM243, LFM1 to LFM7, LFP1 to LFP7, and AN1 to AN5 may be understood based on those described above.

[0267] For example, some of compounds BD001 to BD297 may be represented as follows.

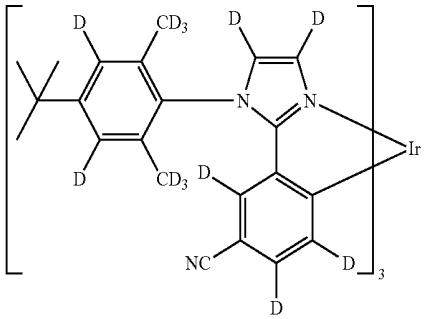
BD037



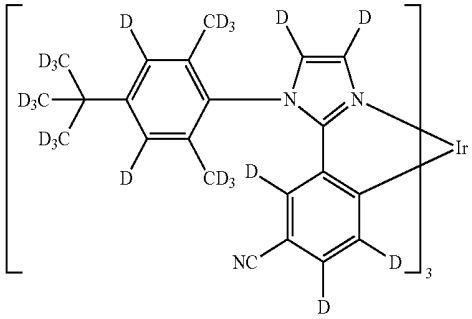
BD040



BD044



BD045



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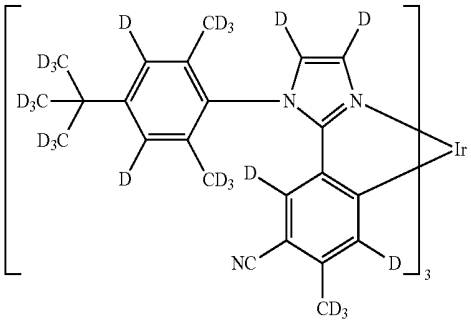
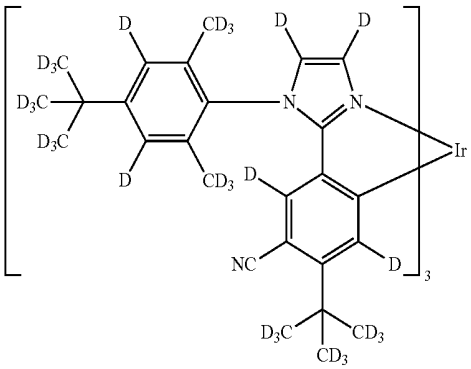
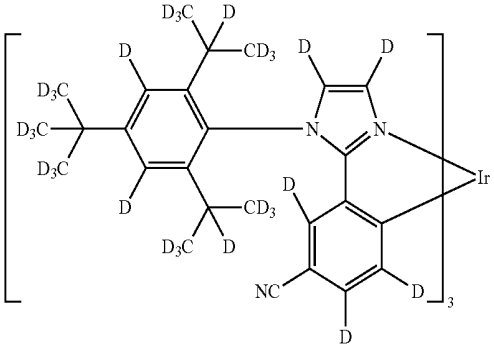
BD047



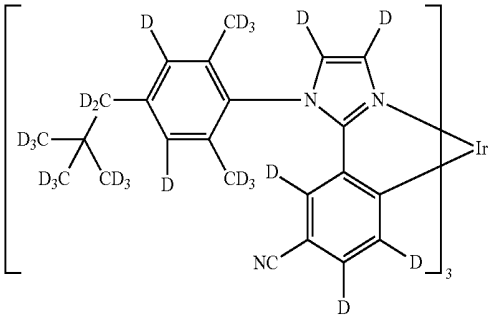
BD049



BD064



BD079



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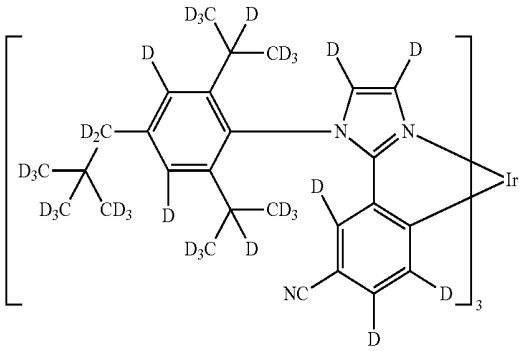
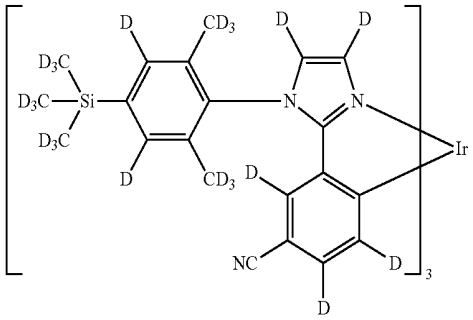
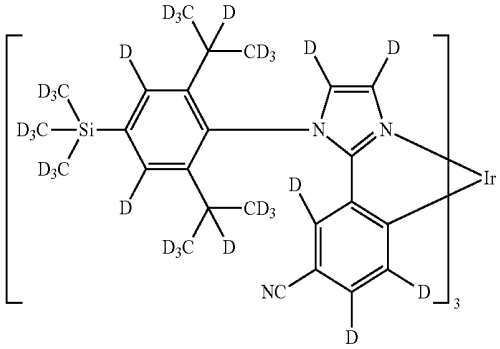
BD098



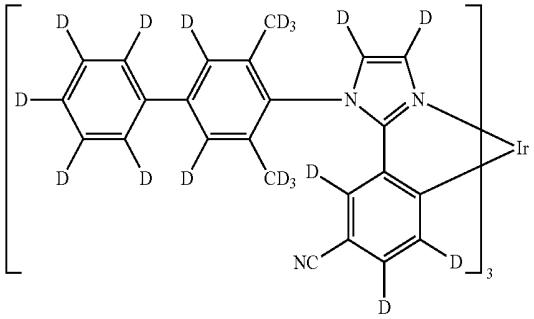
BD113



BD132



BD151



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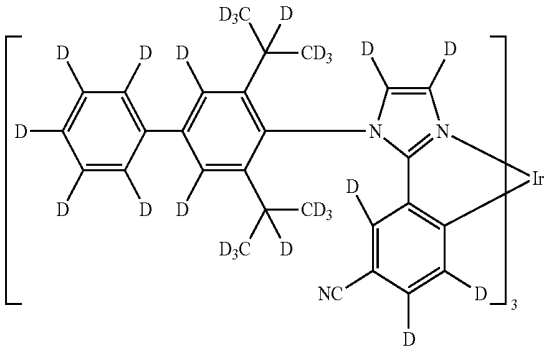
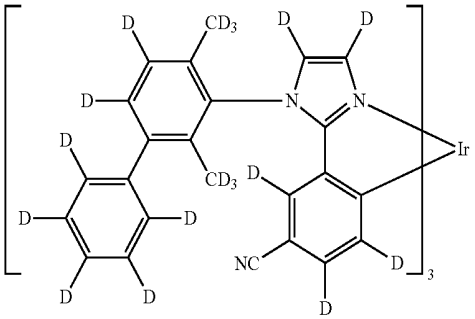
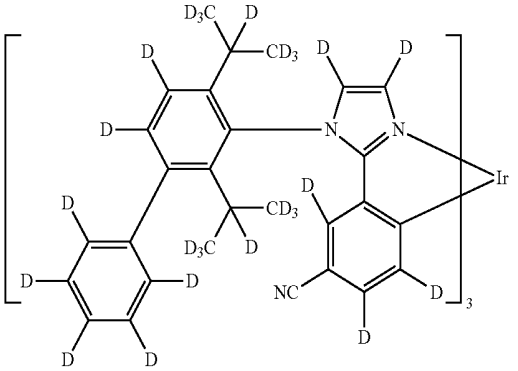
BD180



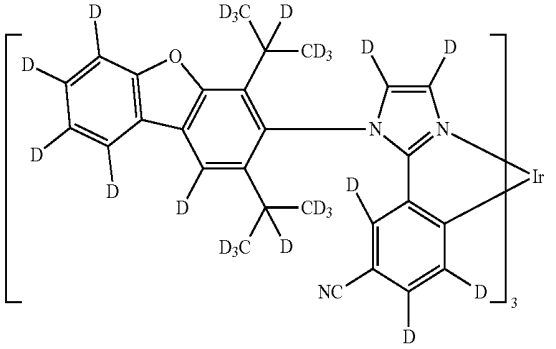
BD201



BD233



BD248



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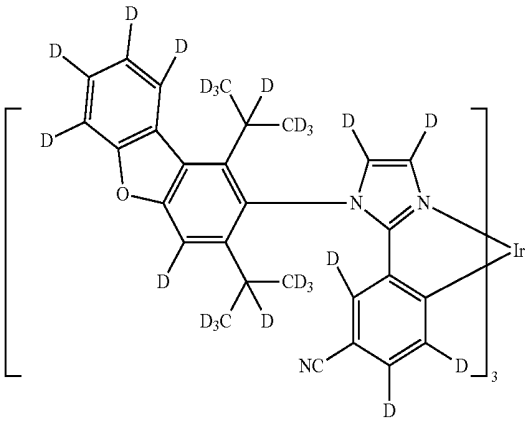
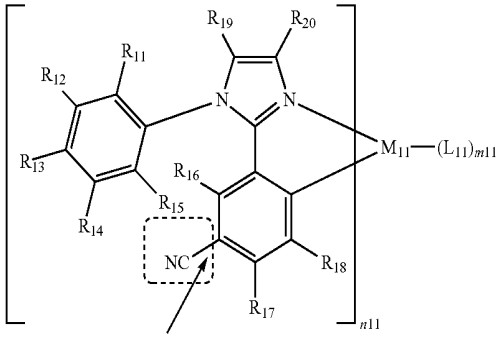
BD255



[0268] The organometallic compound of Formula 1 may have a maximum emission wavelength of about 420 nanometers (nm) to about 480 nm or less, and in some embodiments, about 440 nm to about 465 nm. When the organometallic compound has a maximum emission wavelength of 480 nm or less, an organic light-emitting device including the organometallic compound may have blue emission color. For example, when the organometallic compound has a maximum emission wavelength of 465 nm or less, an organic light-emitting device including the organometallic compound may have deep blue emission color.

[0269] The organometallic compound of Formula 1 may provide deep blue emission color when it includes "a cyano group" at a "certain position".

Formula 1'



Para-position with respect to Ir-carbon bonding site

[0270] As shown in Formula 1', when a cyano group is at a para position with respect to a Ir—C binding site, the organometallic compound of Formula 1 may have a deep highest occupied molecular orbital (HOMO) energy level. Accordingly, the organometallic compound of Formula 1 may have a high triplet energy level due to an increased band gap, and thus provide deep blue emission color.

[0271] The organometallic compound of Formula 1 essentially includes "deuterium", and thus may have improved thermal stability. In particular, a carbon-deuterium single bond has a stronger bond strength than a carbon-hydrogen single bond, and thus the amount of byproducts that may be produced due to radicalization and/or oxidation-reduction by

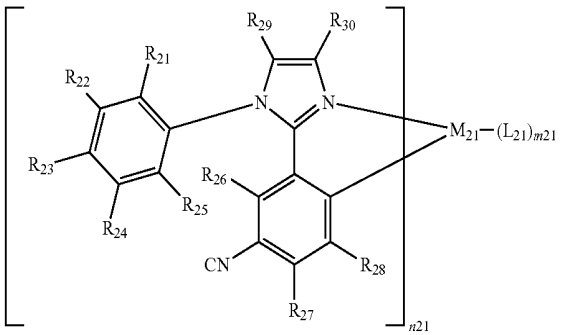
heat and/or an electric field applied during the synthesis of the organometallic compound of Formula 1, a sublimation purification process, deposition in the manufacturing of an organic light-emitting device, and/or storage and/or operation of an organic light-emitting device may be considerably reduced. The organometallic compound of Formula 1 may suppress the generation of byproducts that are fatal to the lifespan of an organic light-emitting device. Therefore, an organic light-emitting device including the organometallic compound of Formula 1 may have an improved lifespan.

[0272] The organometallic compound represented by Formula 1 essentially includes a "bulky unit" such as a branched alkyl group, an aryl group, or the like, so that aggregation of the organometallic compound may be suppressed during deposition, and the organometallic compound may be deposited in a uniform ratio with respect to a host in an emission layer. Therefore, an organic light-emitting device including the organometallic compound of Formula 1 may prevent exciton quenching caused by aggregation, and thus may have improved efficiency and an improved lifespan.

[0273] In synthesizing the organometallic compound of Formula 1, when 100% deuteration does not occur in the organometallic compound, an organometallic compound that includes a hydrogen not substituted with deuterium may also be synthesized together with the organometallic compound of Formula 1.

[0274] In this regard, according to another aspect of the present disclosure, there is provided an organometallic compound-containing composition that includes the organometallic compound (also referred to as a "first organometallic compound") represented by Formula 1 and an organometallic compound (also referred to as a "second organometallic compound") represented by Formula 2,

Formula 2



[0275] In Formula 2, M_{21} may be selected from a first-row transition metal, a second-row transition metal, and a third-row transition metal.

[0276] For example, in Formula 2, M_{21} may be selected from iridium (Ir), platinum (Pt), osmium (Os), ruthenium (Ru), rhodium (Rh), palladium (Pd), copper (Cu), silver (Ag), gold (Au), titanium (Ti), zirconium (Zr), hafnium (Hf), europium (Eu), terbium (Tb), and thulium (Tm). However, embodiments are not limited thereto.

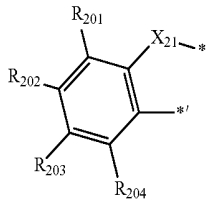
[0277] In some embodiments, in Formula 2, M_{21} may be selected from Ir, Pt, and Os. However, embodiments are not limited thereto.

[0278] In some other embodiments, in Formula 2, M_{21} may be selected from Ir and Pt. However, embodiments are not limited thereto.

[0279] In Formula 2, R_{21} to R_{28} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, at least two of R_{21} to R_{25} may be linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring.

[0280] For example, in Formula 2, R_{21} to R_{28} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, adjacent two of R_{21} to R_{25} may be linked to form a substructure represented by Formula 20. However, embodiments are not limited thereto.

Formula 20



[0281] In Formula 20,

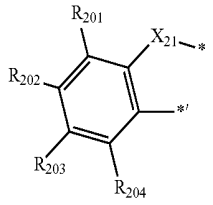
[0282] X_{21} may be selected from O, S, and $N(R_{205})$;

[0283] R_{201} to R_{205} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group; and

[0284] * and *' may be each independently a carbon atom to which adjacent two of R_{21} to R_{25} are bound.

[0285] In some embodiments, in Formula 2, R_{21} to R_{28} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a cyano group, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, adjacent two of R_{21} to R_{25} may be linked to form a substructure represented by Formula 20. However, embodiments are not limited thereto.

Formula 20



[0286] In Formula 20,

[0287] X_{21} may be selected from O, S, and $N(R_{205})$;

[0288] R_{201} to R_{205} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a cyano group, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group; and

[0289] * and *' may be each independently a carbon atom to which adjacent two of R_{21} to R_{25} are bound,

[0290] In some embodiments, in Formula 2, R_{21} to R_{28} may be each independently selected from

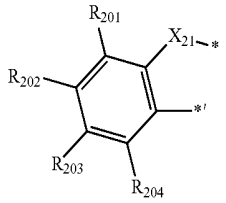
[0291] a hydrogen, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, and $—Si(Q_1)(Q_2)(Q_3)$,

[0292] a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of —F, —Cl, —Br, —I, and a cyano group, and

[0293] a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with at least one of —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group,

[0294] wherein Q_1 to Q_3 may be each independently selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, wherein optionally, adjacent two of R_{21} to R_{25} may be linked to form a substructure represented by Formula 20. However, embodiments are not limited thereto.

Formula 20



[0295] In Formula 20,

[0296] X_{21} may be selected from O, S, and $N(R_{205})$;

[0297] R_{201} to R_{205} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

[0298] * and *' may be each independently a carbon atom to which adjacent two of R_{21} to R_{25} are bound.

[0299] In some embodiments, in Formula 2, R_{21} to R_{28} may be each independently selected from

[0300] a hydrogen, —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and $—Si(Q_1)(Q_2)(Q_3)$,

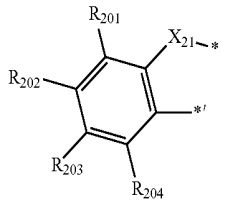
[0301] a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of —F, —Cl, —Br, —I, and a cyano group, and

[0302] a phenyl group and a biphenyl group, each substituted with at least one of —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group;

[0303] Q_1 to Q_3 may be each independently selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group; and

[0304] optionally, R_{22} and R_{23} are linked to form a substructure represented by Formula 20. However; embodiments are not limited thereto:

Formula 20



[0305] In Formula 20,

[0306] X_{21} may be selected from O, S, and $N(R_{205})$;

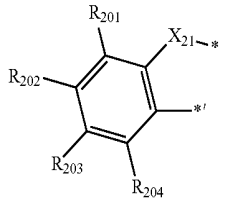
[0307] R_{201} to R_{205} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group; a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group; a phenanthrenyl group, an anthracenyl group; a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

[0308] * and *' may be each independently a carbon atom to which R_{22} and R_{23} are bound.

[0309] In some other embodiments; in Formula 2; R_{21} to R_{28} may be each independently selected from a hydrogen, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group; a biphenyl group, and $—Si(CH_3)_3$; and

[0310] optionally, R_{22} and R_{23} may be linked to form a substructure represented by Formula 20. However, embodiments are not limited thereto.

Formula 20



[0311] In Formula 20,

[0312] X_{21} may be selected from O, S, and $N(R_{205})$

[0313] R_{201} to R_{235} may be each independently selected from a hydrogen, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

[0314] * and *' may be each independently a carbon atom to which R_{22} to R_{23} are bound.

[0315] In some embodiments, in Formula 2, at least one of R_{21} to R_{25} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group.

[0316] For example, in Formula 2, at least one of R_{21} to R_{25} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group. However, embodiments are not limited thereto.

[0317] In some other embodiments, in Formula 2, at least one of R_{21} to R_{25} may be selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group. However, embodiments are not limited thereto.

[0318] In some other embodiments, in Formula 2, at least one of R_{21} to R_{25} may be selected from

[0319] an iso-propyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, and $—Si(Q_1)(Q_2)(Q_3)$,

[0320] an iso-propyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of —F, —Cl, —Br, —I, and a cyano group, and

[0321] a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with at least one of —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group,

[0322] wherein Q_1 to Q_3 may be each independently selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group. However, embodiments are not limited thereto.

[0323] In some embodiments, in Formula 2, at least one of R_{21} to R_{25} may be selected from

[0324] an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and —$Si(Q_1)(Q_2)(Q_3)$,

[0325] an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of —F, —Cl, —Br, —I, and a cyano group, and

[0326] a phenyl group, and a biphenyl group, each substituted with at least one of —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group,

[0327] wherein Q_1 to Q_3 may be each independently selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group. However, embodiments are not limited thereto.

[0328] In some embodiments, in Formula 2, at least one of R_{21} to R_{25} may be selected from

[0329] an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and —$Si(Q_1)(Q_2)(Q_3)$,

[0330] an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with at least one of —F, —Cl, —Br, —I, and a cyano group, and

[0331] a phenyl group and a biphenyl group, each substituted with at least one of —F, —Cl, —Br, —I, a cyano group, a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group,

[0332] wherein Q_1 to Q_3 may be each independently selected from a methyl group, an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group. However, embodiments are not limited thereto.

[0333] In some other embodiments, in Formula 2, at least one of R_{21} to R_{25} may be selected from an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and —$Si(CH_3)_3$. However, embodiments are not limited thereto.

[0334] In some embodiments, in Formula 2, R_{21} and R_{22}, R_{22} and R_{23}, R_{23} and R_{24}, or R_{24} and R_{25} may be optionally linked to each other to form a condensed ring, but embodiments are not limited thereto.

[0335] In some embodiments, in Formula 2, R_{25} and R_{26} may be optionally linked to each other via a single bond, but embodiments are not limited thereto.

[0336] In Formula 2, R_{29} and R_{30} may be each independently selected from a hydrogen and a C_1-C_{30} alkyl group.

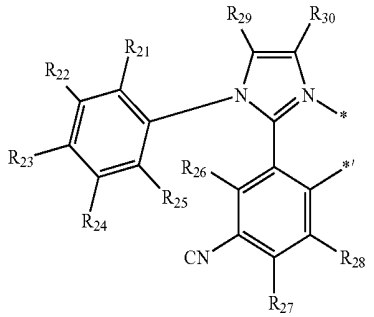
[0337] In some embodiments, in Formula 2, R_{29} and R_{30} may be each independently selected from a hydrogen, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, and a tert-butyl group, but embodiments are not limited thereto.

[0338] In some embodiments, in Formula 2, R_{29} and R_{30} may be both a hydrogen, but embodiments are not limited thereto.

[0339] In Formula 2, R_{21} to R_{30} may be each independently a deuterium-non-containing substituent.

[0340] As used herein, the term "deuterium-non-containing substituent" may refer to a substituent no hydrogen is substituted with deuterium.

[0341] In Formula 2, a moiety represented by



(wherein * and *' each indicate a binding site to M_{21} in Formula 2) may not include a deuterium. For example, the organometallic compound-containing composition that includes the first organometallic compound and the second organometallic compound may have a deuteration rate, which is represented by Equation 2, of 50% or more, but embodiments are not limited thereto:

$$\text{Deuteration rate (\%)} = n_{D2}/(n_{H2}+n_{D2}) \times 100 \qquad \text{Equation 2}$$

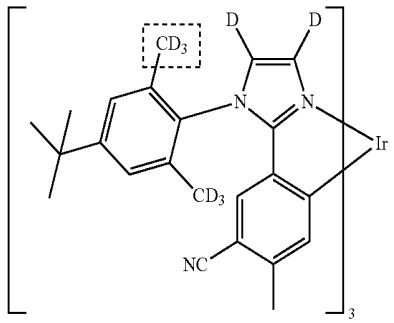
[0342] In Equation 2,

[0343] n_{H2} represents a sum of a total number of hydrogens in the deuterium-containing substituents and a total number of hydrogens in substituents that are equivalent to the deuterium-containing substituents; and

[0344] n_{D2} represents a total number of deuterium atoms in the deuterium-containing substituents.

[0345] If a substituent in the dashed region in Compound 1' is a deuterium-containing substituent, the "substituents that are equivalent to the deuterium-containing substituents" used herein may include a substituent in the dashed region in Compound 1". That is, substituents bound at the same carbon location in two compounds that are the same except for having or not having an isotope thereof are defined as "equivalent" substituents.

1'



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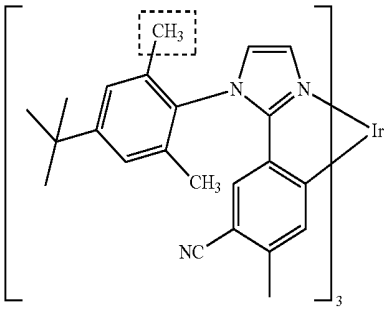
1″



[0346] For example, when the first organometallic compound includes two deuterium-containing substituents, n_{D2} indicates the total number of deuterium atoms included in the two deuterium-containing substituents. In addition, n_{H2} indicates the total number of hydrogens included in the two deuterium-containing substituents and the total number of hydrogens included in substituents corresponding to the two deuterium-containing substituents.

[0347] In some embodiments, the deuteration rate may be 70% or more, 90% or more, 95% or more, 96% or more, 97% or more, 98% or more, or 99% or more, but embodiments are not limited thereto.

[0348] A method of synthesizing the organometallic compound represented by Formula 1 may be obvious to one of ordinary skill in the art by referring to Synthesis Examples used herein. The organometallic compound-containing composition may be obtained as a result of imperfect deuteration during the synthesis of the organometallic compound represented by Formula 1, not by further adding at least one second organometallic compound,

[0349] The organometallic compound of Formula 1 or the organometallic compound-containing composition may be appropriate for use as a material for an organic layer of an organic light-emitting device, for example, as a dopant of an EML.

[0350] According to another aspect of the present disclosure, an organic light-emitting device includes:

[0351] a first electrode,

[0352] a second electrode, and

[0353] an organic layer that is disposed between the first electrode and the second electrode,

[0354] wherein the organic layer includes an EML and an organometallic compound of Formula 1 or an organometallic compound-containing composition according to any of the above-described embodiments.

[0355] Due to the inclusion of the organic layer that includes an organometallic compound of Formula 1 or an organometallic compound-containing composition according to any of the above-described embodiments, the organic light-emitting device may have improved efficiency, lifespan, and color purity characteristics.

[0356] The organometallic compound of Formula 1 or the organometallic compound-containing composition may be used between a pair of electrodes of an organic light-emitting device. For example, the organometallic compound of Formula 1 or the organometallic compound-containing composition may be included in the EML. In this regard, the organometallic compound of Formula 1 may serve as a dopant in the EML, and the EML may further include a host. The EML may emit red light, green light, or blue light.

[0357] As used herein, "(for example, the organic layer) including an organometallic compound" means that "(the organic layer) including an organometallic compound of Formula 1 above, or at least two different organometallic compounds of Formula 1 above".

[0358] For example, the organic layer of the organic light-emitting device may include only Compound 1 as the organometallic compound. For example, Compound 1 may be included in the EML of the organic light-emitting device. In some embodiments, the organic layer of the organic light-emitting device may include Compounds 1 and 2 as the organometallic compound. For example, Compounds 1 and 2 may be included both in the EML.

[0359] The first electrode may be an anode as a hole injection electrode, and the second electrode may be a cathode as an electron injection electrode. In some embodiments, the first electrode may be a cathode as an electron injection electrode, and the second electrode may be an anode as a hole injection electrode.

[0360] For example, the first electrode may be an anode, the second electrode may be a cathode, and the organic layer may include:

[0361] i) a hole transport region disposed between the first electrode and the emission layer, wherein the hole transport region includes at least one of a hole injection layer, a hole transport layer, and an electron blocking layer; and

[0362] ii) an electron transport region disposed between the emission layer and the second electrode, wherein the electron transport region includes at least one of a hole blocking layer, an electron transport layer, and an electron injection layer.

[0363] The term "organic layer" as used herein refers to a single layer and/or a plurality of layers disposed between the first and second electrodes of the organic light-emitting device. The "organic layer" may include, for example, an organic compound or an organometallic complex including a metal.

[0364] FIG. **1** is a schematic view of an organic light-emitting device **10** according to an embodiment of the present disclosure. Hereinafter, a structure of an organic light-emitting device according to an embodiment of the present disclosure and a method of manufacturing the same will now be described with reference to FIG. **1**. Referring to FIG. **1**, the organic light-emitting device **10** has a structure in which a first electrode **11**, an organic layer **15**, and a second electrode **19** are sequentially stacked in this order on a substrate (not shown).

[0365] The substrate (not shown) may be disposed under the first electrode **11** or on the second electrode **190** in FIG. **1**. The substrate may be any substrate that is used in conventional organic light-emitting devices. In some embodiments the substrate may be a glass substrate or a transparent plastic substrate with strong mechanical strength, thermal stability, transparency, surface smoothness, ease of handling, and water resistance.

[0366] The first electrode **11** may be formed by depositing or sputtering a first electrode-forming material on the substrate. The first electrode **11** may be an anode. A material having a high work function may be selected as a material for the first electrode **11** to facilitate hole injection. The first electrode **11** may be a reflective electrode, a semi-transmissive electrode, or a transmissive electrode. For example, the material for the first electrode **11** may be indium tin oxide (ITO), indium zinc oxide (IZO), tin oxide (SnO_2), or zinc oxide (ZnO). In some embodiments, the material for the first electrode **11** may be metals, for example, magnesium (Mg), aluminum (Al), aluminum-lithium (Al—Li), calcium (Ca), magnesium-indium (Mg—In), magnesium-silver (Mg—Ag), or the like.

[0367] The first electrode **11** may have a single-layer structure or a multi-layer structure including at least two layers. For example, the first electrode **11** may have, but not limited to, a three-layered structure including ITO, Ag, and ITO layers.

[0368] The organic layer **15** may be disposed on the first electrode **11**.

[0369] The organic layer **15** may include at least one a hole transport region; an EML, and an electron transport region.

[0370] The hole transport region may be disposed between the first electrode **11** and the EML.

[0371] The hole transport region may include at least one of a hole injection layer (HIL), a hole transport layer (HTL), an electron blocking layer (EBL), and a buffer layer.

[0372] The hole transport region may only include the HIL or the HTL. In some embodiments, the electron transport region may have a structure including a HIL/HTL or a HIL/HTL/EBL, wherein the layers forming the structure of the electron transport region may be sequentially stacked on the first electrode **10** in the stated order.

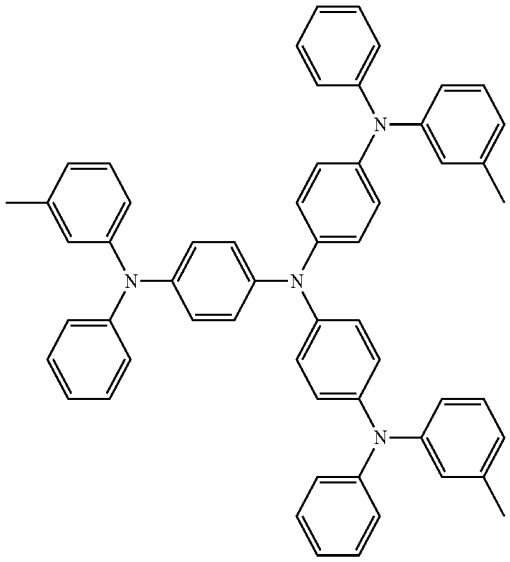
[0373] When the hole transport region includes the HIL, the HIL may be formed on the first electrode **11** by any of a variety of methods, for example, vacuum deposition, spin coating, casting, Langmuir-Blodgett (LB) deposition, or the like.

[0374] When the HIL is formed using vacuum deposition, vacuum deposition conditions may vary depending on the material that is used to form the HIL, and the desired structure and thermal properties of the HIL to be formed. For example, vacuum deposition may be performed at a temperature of about 100 t to about 500° C., a pressure of about 10^{-8} torr to about 10^{-3} torr, and a deposition rate of about 0.01 to about 100 Angstroms per second (Å/sec). However, the deposition conditions are not limited thereto.

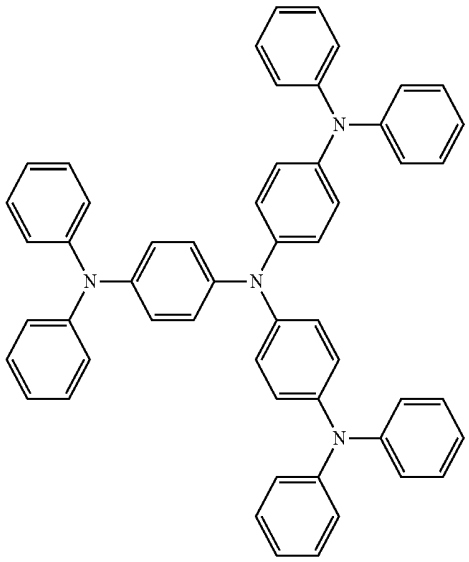
[0375] When the HIL is formed using spin coating, the coating conditions may vary depending on the material that is used to form the HIL, and the desired structure and thermal properties of the HIL to be formed. For example, the coating rate may be in the range of about 2,000 revolutions per minute (rpm) to about 5,000 rpm, and a temperature at which heat treatment is performed to remove a solvent after coating may be in a range of about 80° C. to about 200° C. However, the coating conditions are not limited thereto.

[0376] Conditions for forming the HTL and the EBL may be the same as those for the HIL described above.

[0377] In some embodiments, the hole transport region may include at least one of m-MTDATA, TDATA, 2-TNATA, methylated NPB, β-NPB, TPD, Spiro-TPD, Spiro-NPB, α-NPB, TAPC, HMTPD, 4,4',4"-tris(N-carbazolyl)triphenylamine (TCTA), polyaniline/dodecylbenzene sulfonic acid (Pani/DBSA), poly(3,4-ethylenedioxythiophene)/poly(4-styrenesulfonate)(PEDOTIPSS), polyaniline/camphor sulfonic acid (Pani/CSA), polyaniline/poly(4-styrenesulfonate) (PANUPSS), a compound represented by Formula 201, and a compound represented by Formula 202.



m-MTDATA



TDATA

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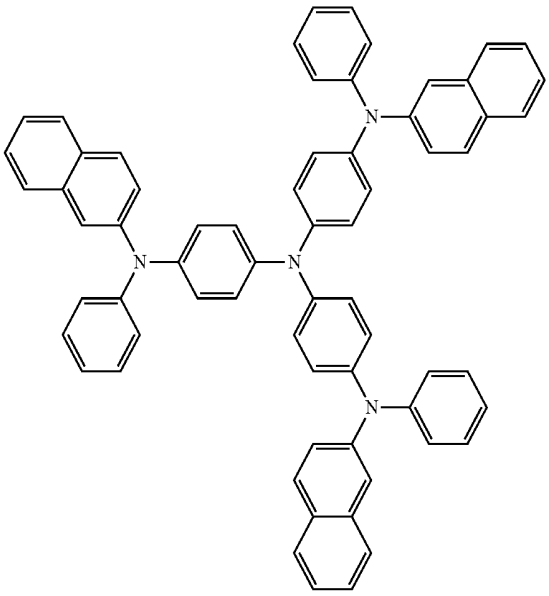
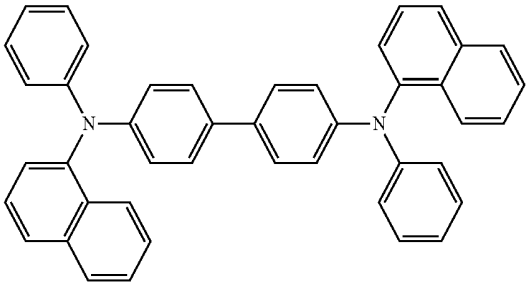
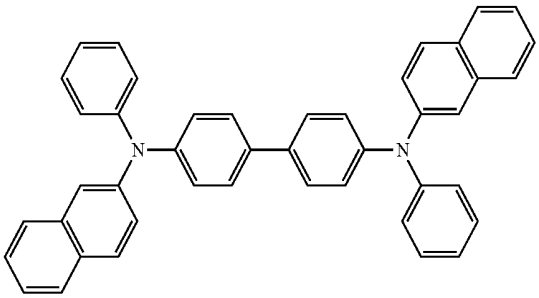


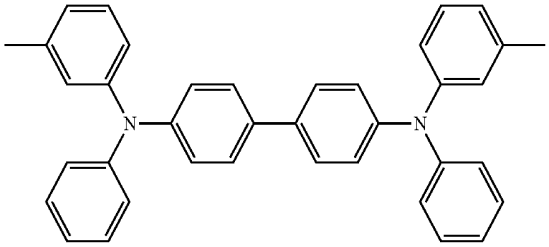
2-TNATA



NPB



β-NPB



TPD

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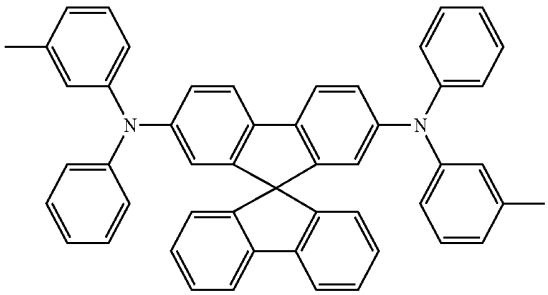
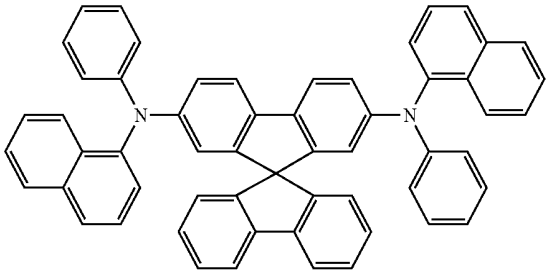
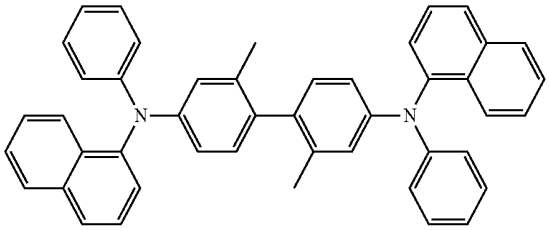


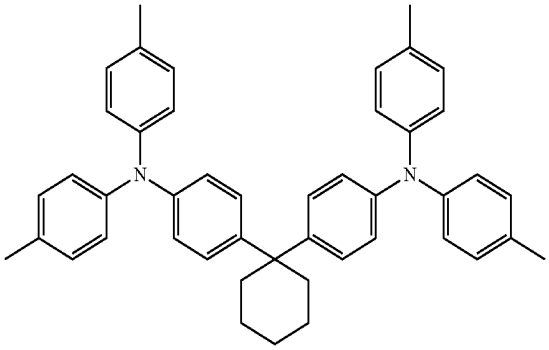
Spiro-TPD



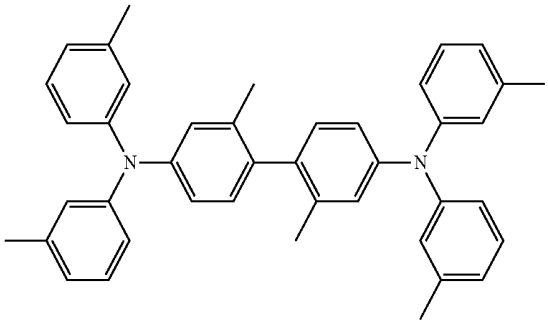
Spiro-NPB



methylated NPB



TAPC



HMTPD

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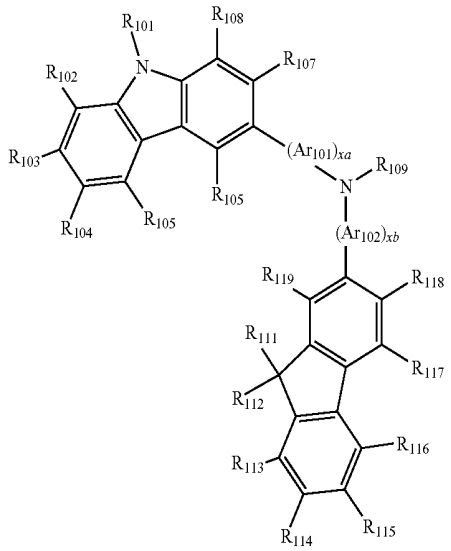
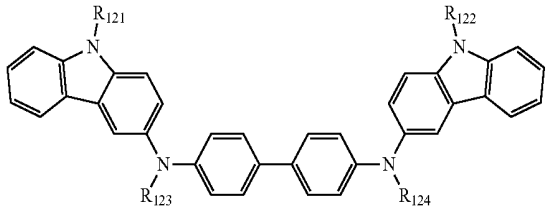
Formula 201



Formula 202



[0378] In Formula 201 Ar_{101} and Ar_{102} may be each independently selected from a phenylene group, a pentalenylene group, an indenylene group, a naphthylene group, an azulenylene group, a heptalenylene group, an acenaphthylene group, a fluorenylene group, a phenalenylene group, a phenanthrenylene group, an anthracenylene group, a fluoranthenylene group, a triphenylenylene group, a pyrenylene group, a chrysenylene group, a naphthacenylene group, a picenylene group, a perylenylene group, and a pentacenylene group, and

[0379] a phenylene group, a pentalenylene group, an indenylene group, a naphthylene group, an azulenylene group, a heptalenylene group, an acenaphthylene group, a fluorenylene group, a phenalenylene group, a phenanthrenylene group, an anthracenylene group, a fluoranthenylene group, a triphenylenylene group, a pyrenylene group, a chrysenylene group, a naphthacenylene group, a picenylene group, a perylenylene group, and a pentacenylene group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{60} alkyl group, a C_2-C_{60} alkenyl group, a C_2-C_{60} alkynyl group, a C_1-C_{60} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_2-C_{10} heterocycloalkyl group, a C_2-C_{10} heterocycloalkenyl group, a C_6-C_{60} aryl group, a C_6-C_{60} aryloxy group, a C_6-C_{60} arylthio group, a C_7-C_{60} arylalkyl group, a C_2-C_{60} heteroaryl group, a C_2-C_{60} heteroaryloxy group, a C_2-C_{60} heteroarylthio group, a C_3-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group.

[0380] In Formula 201, xa and xb may be each independently an integer from 0 to 5, for example, may be 0, 1, or 2. For example, xa may be 1, and xb may be 0, but are not limited thereto.

[0381] In Formulae 201 and 202, R_{101} to R_{108}, R_{111} to R_{119}, and R_{121} to R_{124} may be each independently selected from

[0382] a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{10} alkyl group (for example, a methyl group, an ethyl group, a propyl group, a butyl group, a pentyl group, a hexyl group, or the like), and a C_1-C_{10} alkoxy group (for example, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, or the like),

[0383] a C_1-C_{10} alkyl group, and a C_1-C_{10} alkoxy group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, and a phosphoric acid group or a salt thereof,

[0384] a phenyl group, a naphthyl group, an anthracenyl group, a fluorenyl group, and a pyrenyl group, and

[0385] a phenyl group, a naphthyl group, an anthracenyl group, a fluorenyl group, and a pyrenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{10} alkyl group, and a C_1-C_{10} alkoxy group. However, embodiments of the present disclosure are not limited thereto.

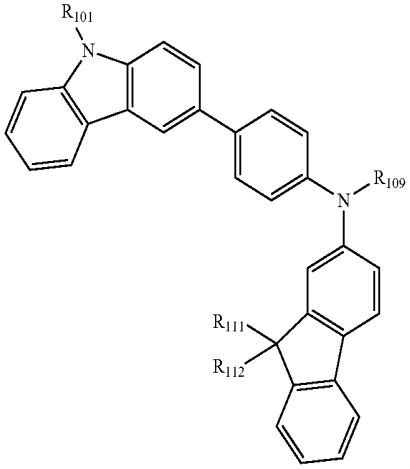
[0386] In Formula 201 above, R_{109} may be selected from

[0387] a phenyl group, a naphthyl group, an anthracenyl group, and a pyridinyl group, or

[0388] a phenyl group, a naphthyl group, an anthracenyl group, and a pyridinyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{20} alkyl group, a C_1-C_{20} alkoxy group, a phenyl group, a naphthyl group, an anthracenyl group, and a pyridinyl group,

[0389] In some embodiments, the compound of Formula 201 may be a compound represented by Formula 201A, but is not limited thereto:

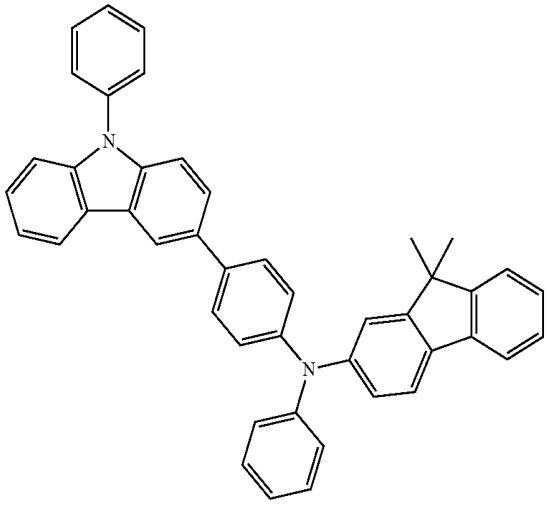
Formula 201A



[0390] In Formula 201A, R_{101}, R_{111}, R_{112}, and R_{109} may be defined the same as described above,

[0391] For example, the compound of Formula 201 and the compound of Formula 202 may be Compounds HT1 to HT20, but are not limited thereto:

HT1



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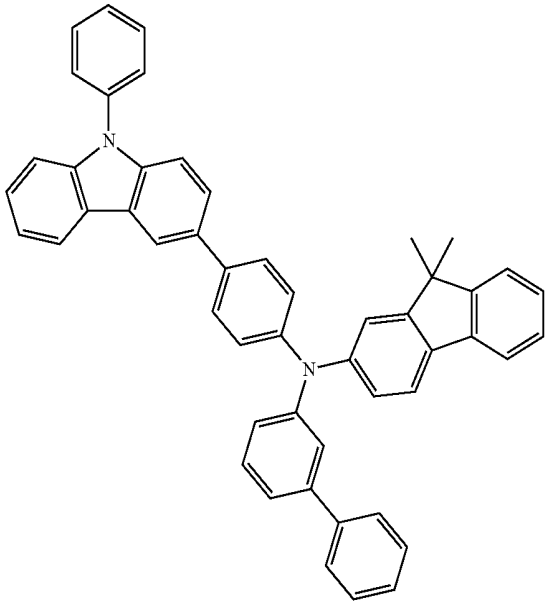
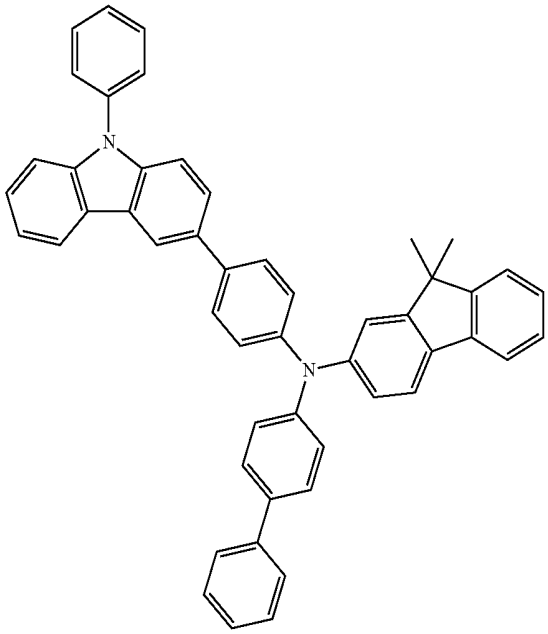
HT2



HT3



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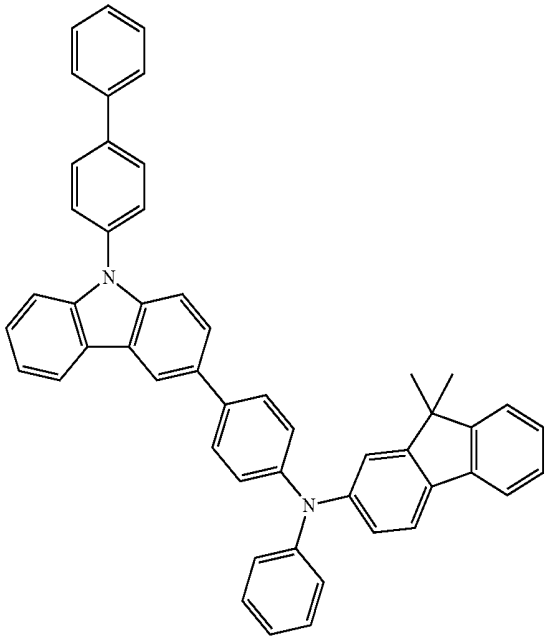
HT4



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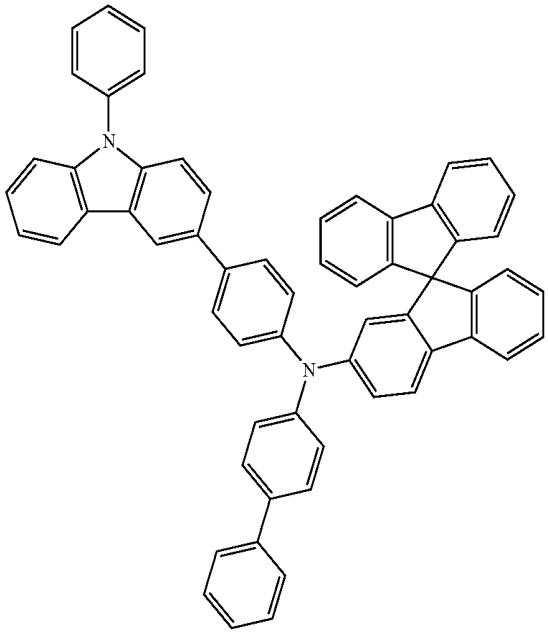
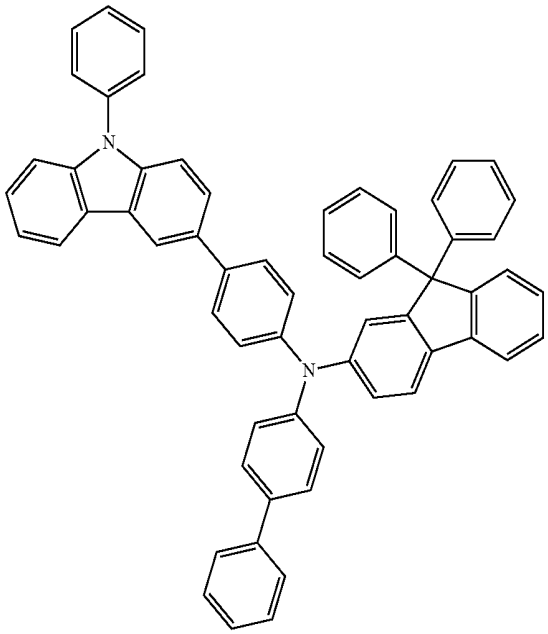
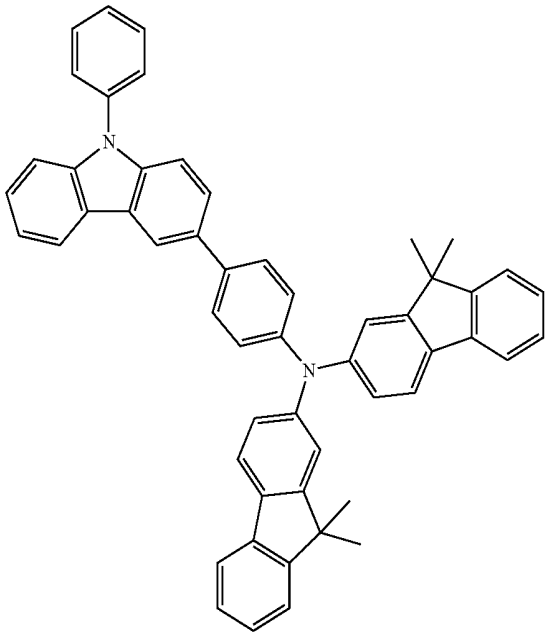
HT6



HT5



HT7



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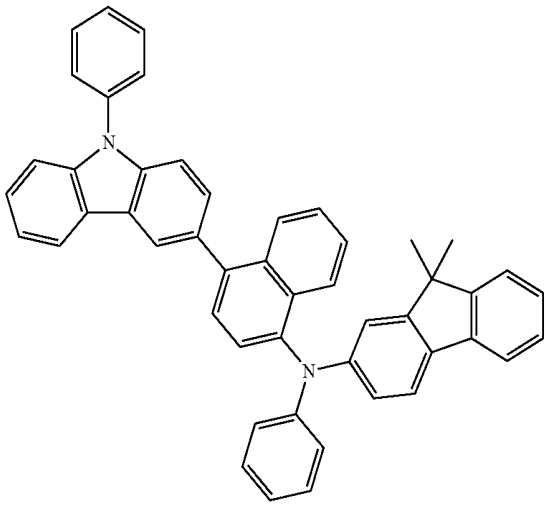
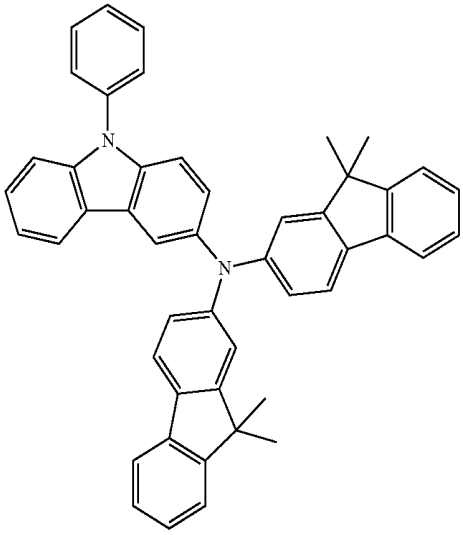
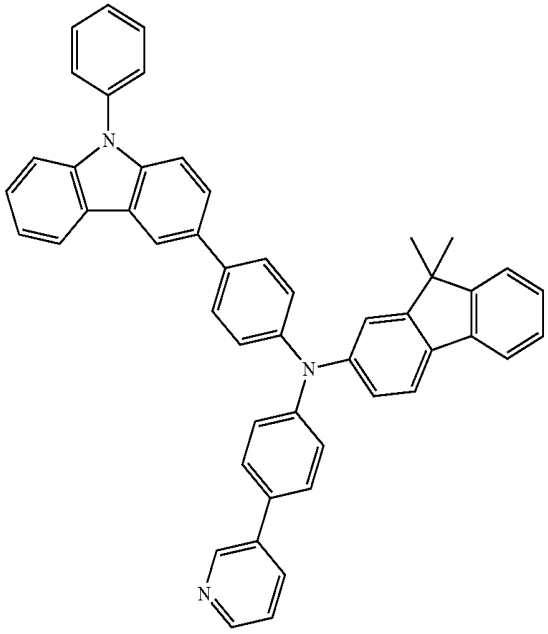
HT8



HT9



HT10



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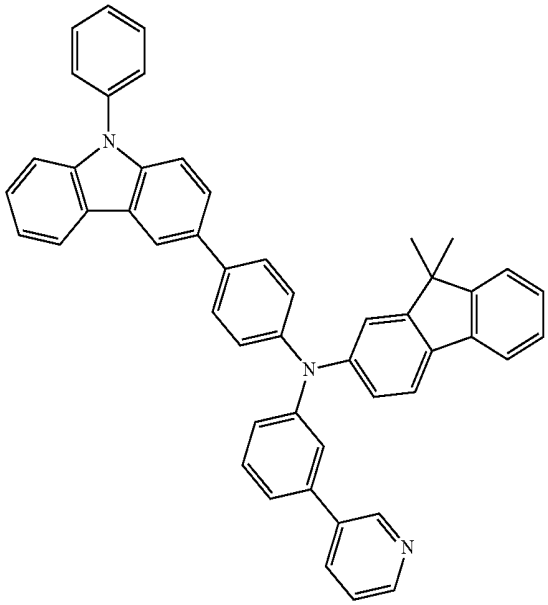
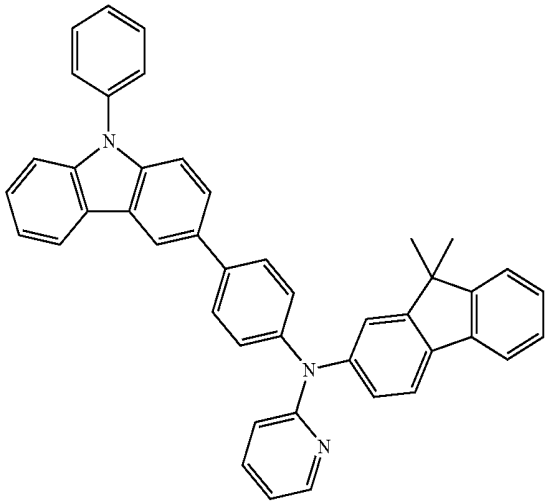
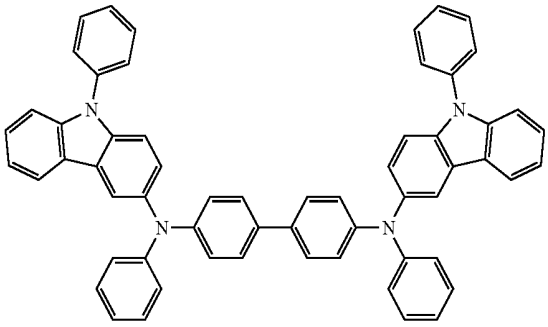
HT11



HT12



HT13



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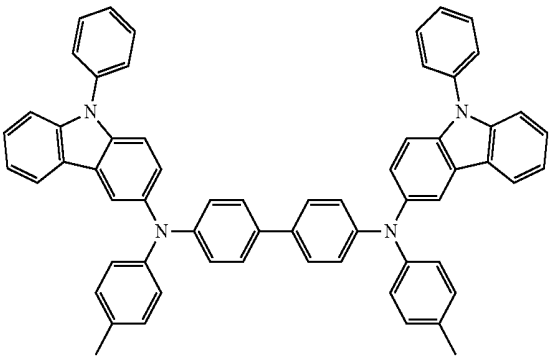
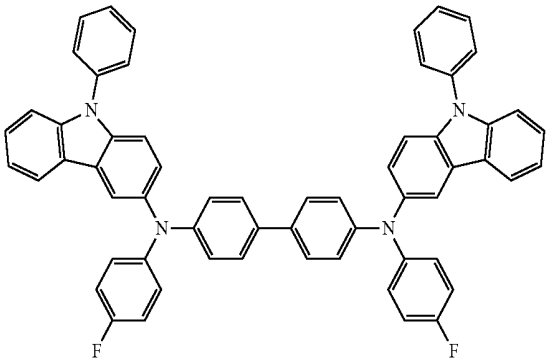
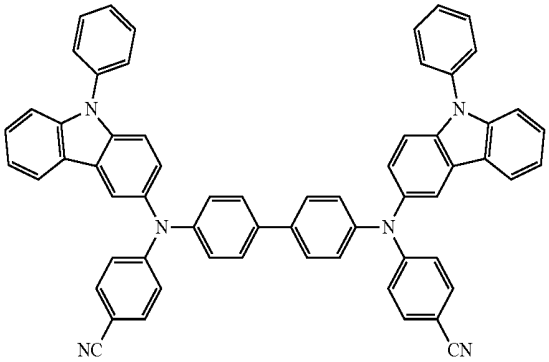
HT14



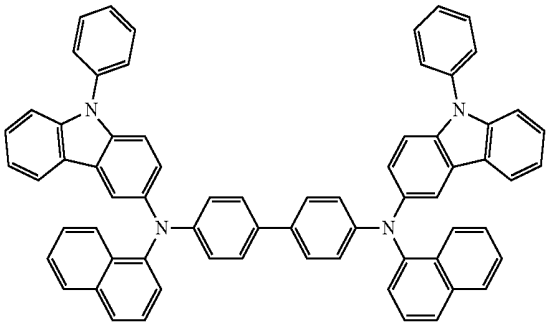
HT15



HT16



HT17



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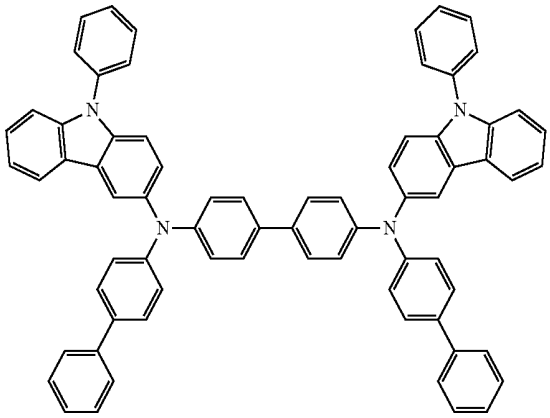
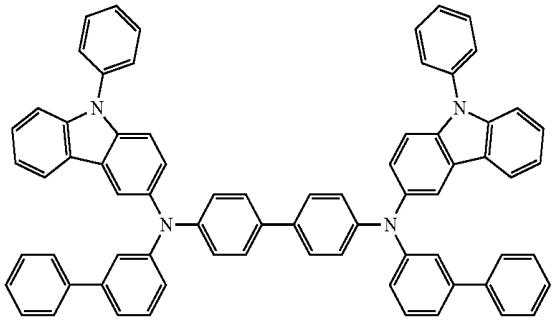
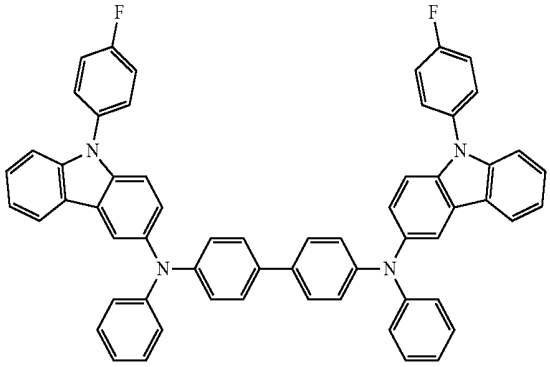
HT18



HT19



HT20

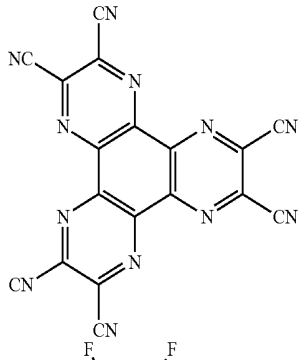


[0392] The thickness of the hole transport region may be from about 100 Angstroms (Å) to about 10,000 Å, and in some embodiments, from about 100 Å to about 1,000 Å. When the hole transport region includes a HIL and a HTL, a thickness of the NIL may be from about 100 Å to about 10,000 Å, and in some embodiments, from about 100 Å to about 1,000 Å, and the thickness of the HTL may be from about 50 Å to about 2,000 Å, and in some embodiments, from about 100 Å to about 1,500 Å. While not wishing to be bound by theory, it is believed that when the thicknesses of the hole transport region, the HIL, and the HTL are within these ranges, satisfactory hole transport characteristics may be obtained without a substantial increase in driving voltage.

[0393] The hole transport region may further include a charge-generating material to improve conductivity, in addition to the materials described above. The charge-generating material may be homogeneously or non-homogeneously dispersed in the hole transport region.

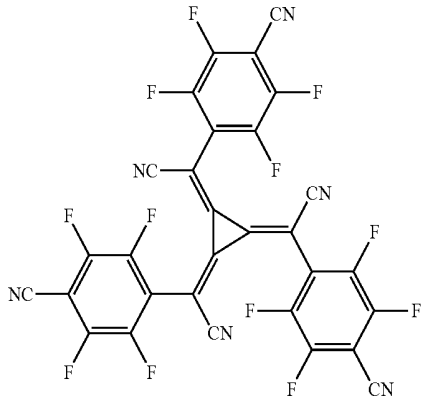
[0394] The charge-generating material may be, for example, a p-dopant. The p-dopant may be one of a quinine derivative, a metal oxide, and a cyano group-containing compound, but is not limited thereto. Non-limiting examples of the p-dopant are quinone derivatives such as tetracyanoquinonedimethane (TCNQ), 2,3,5,6-tetrafluoro-tetracyano-1,4-benzoquinonedimethane (F4-TCNQ), and the like; metal oxides such as tungsten oxide, molybdenum oxide, and the like; and cyano-containing compounds such as Compound HT-D1, Compound HT-D2, and the like.

Compound HT-D1



F4-TCNQ

Compound HT-D2



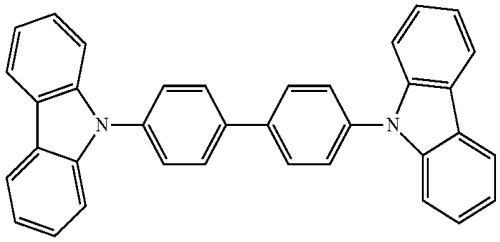
[0395] The hole transport region may further include a buffer layer.

[0396] The buffer layer may compensate for an optical resonance distance of light according to a wavelength of the light emitted from the EML, and thus may increase efficiency.

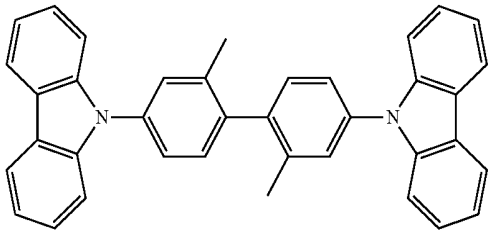
[0397] The EML may be formed on the hole transport region by using vacuum deposition, spin coating, casting, LB deposition, or the like. When the EML is formed using vacuum deposition or spin coating, the conditions for deposition and coating may be similar to those for the formation of the HIL, though the conditions for the deposition and coating may vary depending on the material that is used to form the EML.

[0398] The EML may include a host and a dopant.

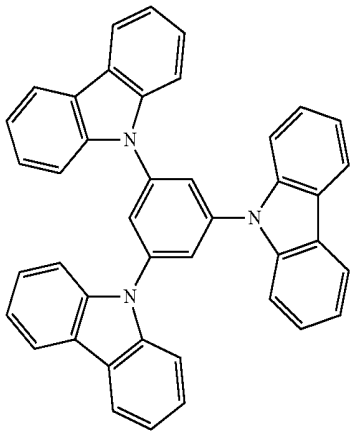
[0399] The host may include at least one of CBP, CDBP, TCP, and mCP.



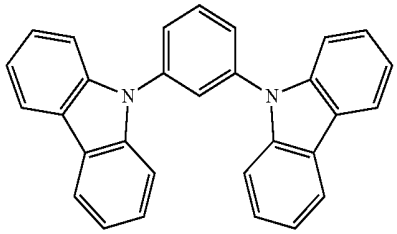
CBP



CDBP



TCP



mCP

[0400] When the organic light-emitting device is a full color organic light-emitting device, the emission layer may be patterned into a red emission layer, a green emission layer, and a blue emission layer. In some embodiments, the EML may have a stack structure including a red emission layer, a green emission layer, and/or a blue emission layer that are stacked upon one another to emit white light, but is not limited thereto.

[0401] The EML may include the organometallic compound of Formula 1 as a dopant.

[0402] When the EML includes both a host and a dopant, the amount of the dopant may be from about 0.01 to about 20

parts by weight based on 100 parts by weight of the host. However, the amount of the dopant is not limited to this range.

[0403] The thickness of the EML may be about 100 Å to about 1000 Å, and in some embodiments, may be from about 200 Å to about 600 Å. When the thickness of the EML is within these ranges, the EML may have improved light-emitting ability without a substantial increase in driving voltage.

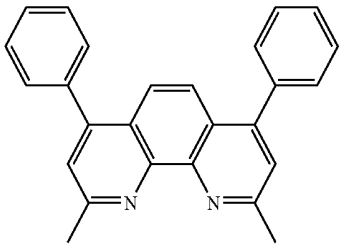
[0404] Next, the electron transport region may be formed on the EML.

[0405] The electron transport region may include at least one of a HBL, an ETL, and an EIL.

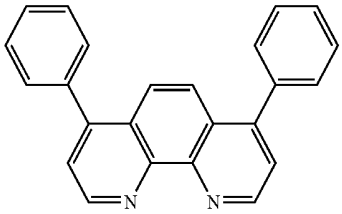
[0406] In some embodiments, the electron transport region may have a structure including a HBL/ETL/EIL, or an ETL/EIL, wherein the layers forming the structure of the electron transport region may be sequentially stacked on the EML in the stated order. However, embodiments of the present disclosure are not limited thereto. The ETL may have a single-layer structure or a multi-layer structure including at least two different materials.

[0407] Conditions for forming the HBL, ETL, and EIL of the electron transport region may be the same as those for the NIL described above.

[0408] When the electron transport region includes the HBL, the HBL may include at least one of BCP and Bphen. However, embodiments of the present disclosure are not limited thereto.



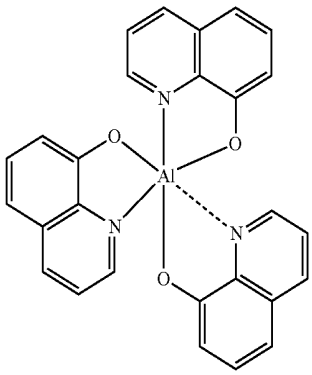
BCP



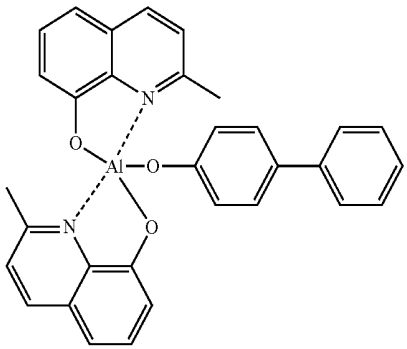
Bphen

[0409] The thickness of the HBL may be from about 20 Å to about 1,000 Å, and in some embodiments, from about 30 Å to about 300 Å. While not wishing to be bound by theory, it is believed that when the thickness of the HBL is within these ranges, the HBL may have improved hole blocking ability without a substantial increase in driving voltage.

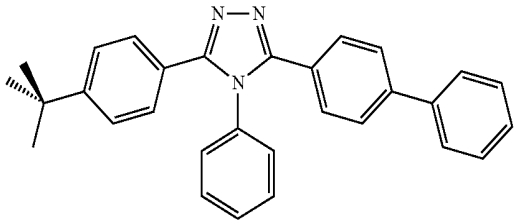
[0410] The ETL may further include at least one of Alq_3, Balq, TAZ, and NTAZ, in addition to BCP and Bphen described above.



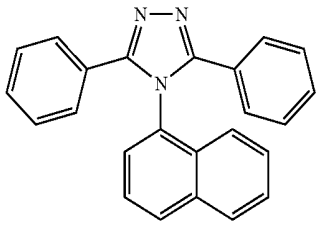
Alq_3



BAlq



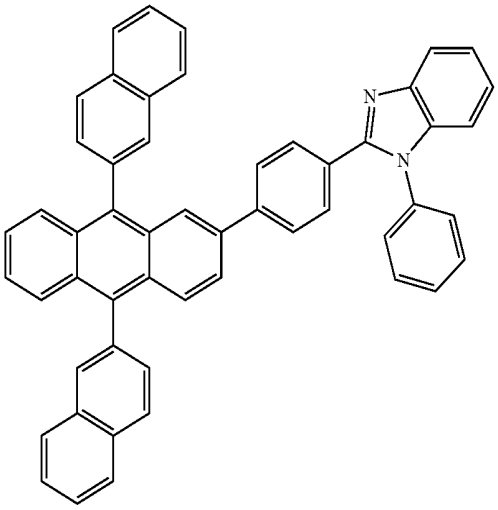
TAZ



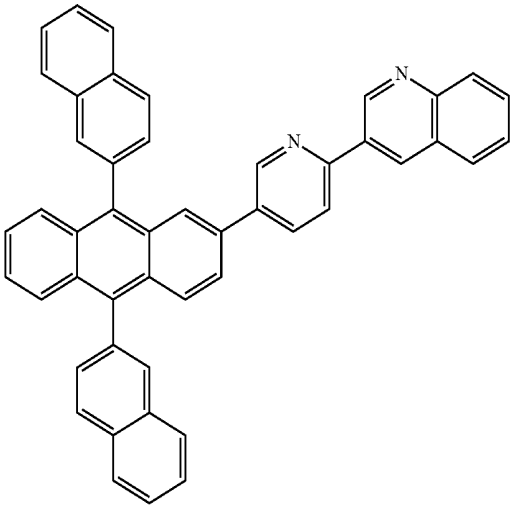
NTAZ

[0411] In some embodiments, the ETL may include at least one of Compounds ET1 to ET19, but is not limited thereto.

ET1



ET2



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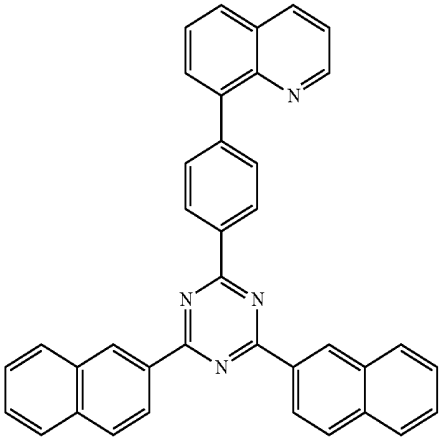

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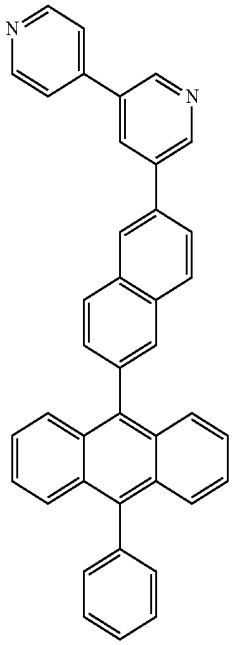

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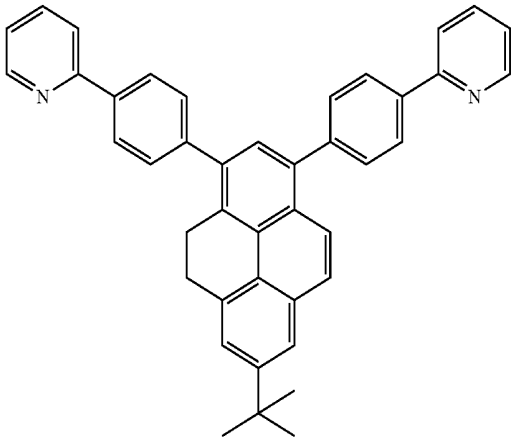

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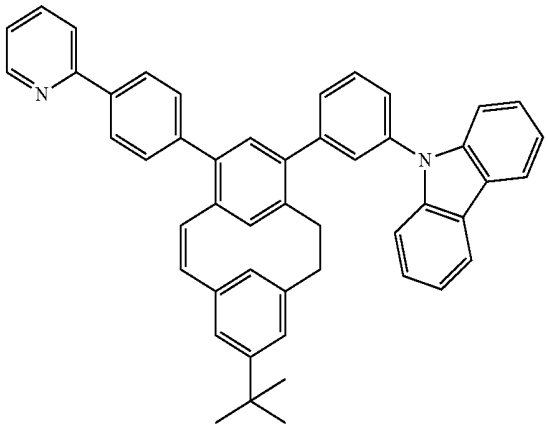

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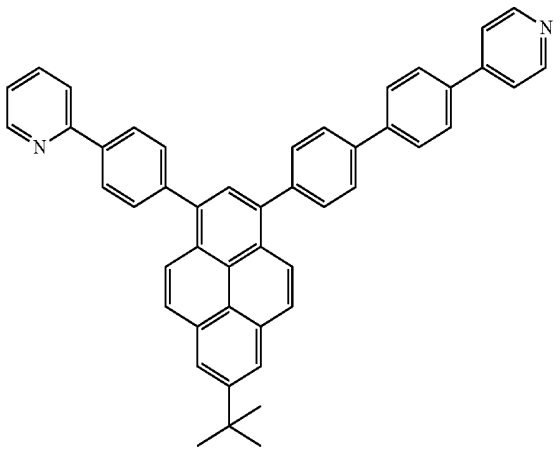

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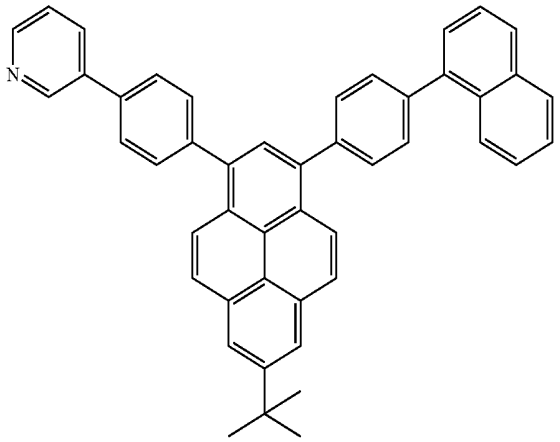

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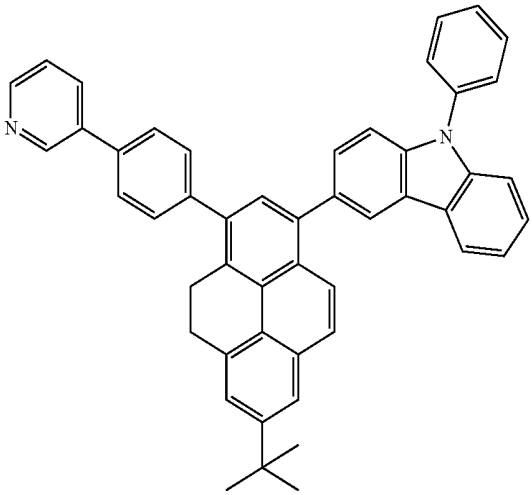

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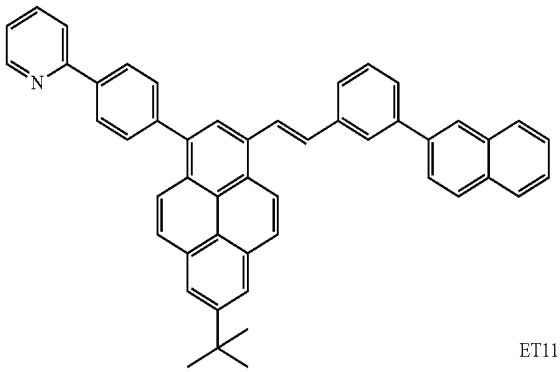

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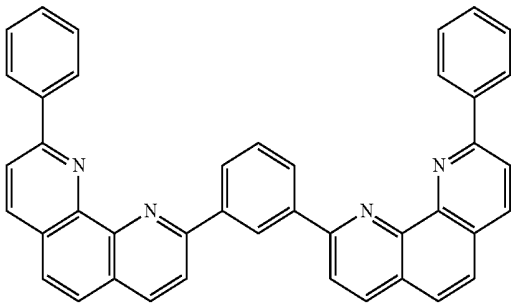

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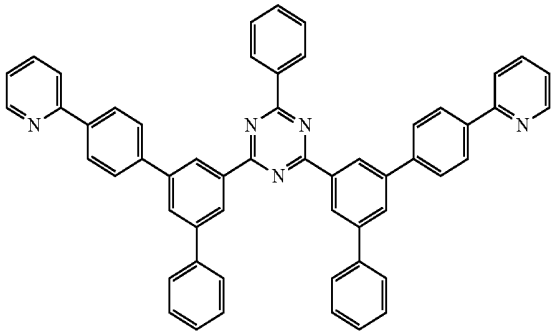

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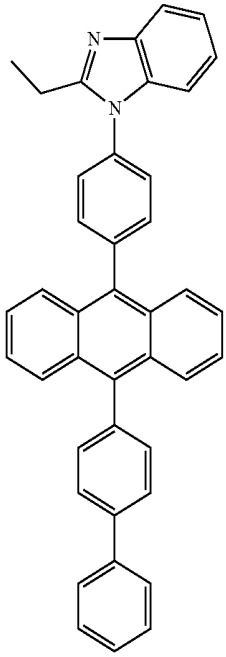

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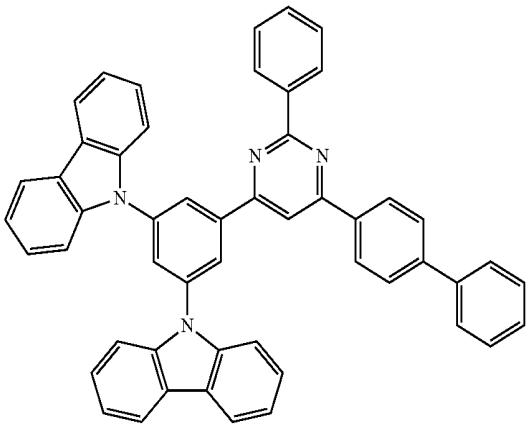

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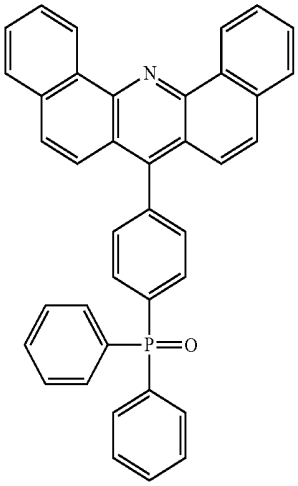

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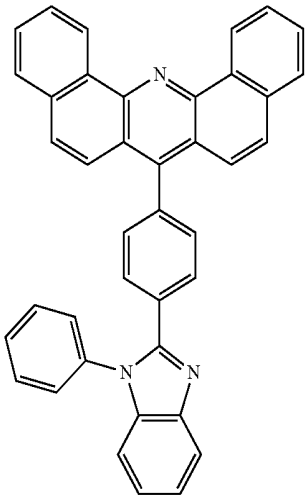

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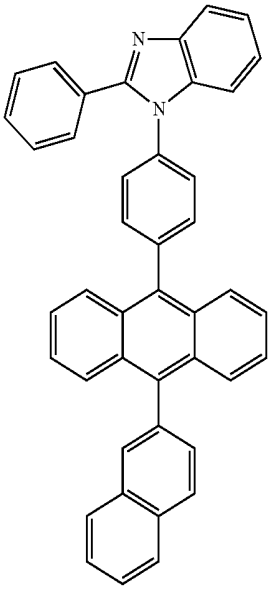
ET17



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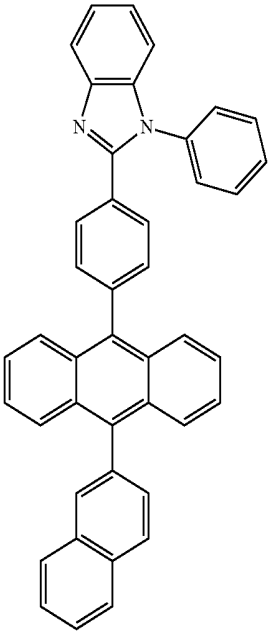

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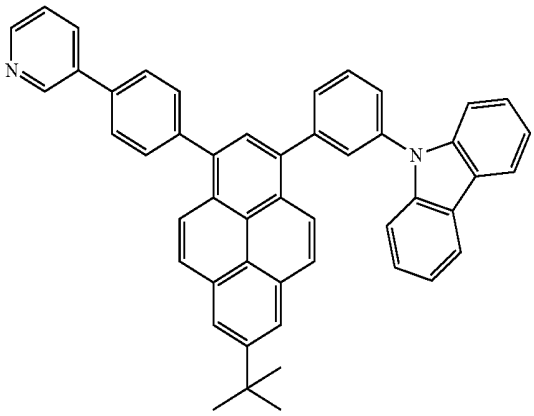
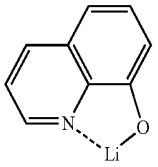


[0412] The thickness of the ETL may be from about 100 Å to about 1,000 Å, and in some embodiments, from about 150 Å to about 500 Å. When the thickness of the ETL is within these ranges, the ETL may have satisfactory electron transporting ability without a substantial increase in driving voltage,

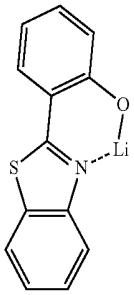
[0413] In some embodiments the ETL may further include a metal-containing material, in addition to the above-described materials.

[0414] The metal-containing material may include a lithium (Li) complex. Non-limiting examples of the Li complex are compound ET-D1 (lithium quinolate (LiQ)), or compound ET-D2.

ET-D1



ET-D2



[0415] The electron transport region may include an EIL that may facilitate injection of electrons from the second electrode **19**. The EIL may include at least one selected from LiF, NaCl, CsF, Li_2O, and BaO. The thickness of the EIL may be from about 1 Angstrom (Å) to about 100 Å and in some embodiments, from about 3 Å to about 90 Å. When the thickness of the EIL is within these ranges, the EIL may have satisfactory electron injection ability without a substantial increase in driving voltage.

[0416] The second electrode **19** is disposed on the organic layer **15**. The second electrode **19** may be a cathode. A material for the second electrode **19** may be a metal, an alloy, or an electrically conductive compound that has a low work function, or a combination thereof. Non-limiting examples of the material for the second electrode **19** are lithium (Li), magnesium (Mg), aluminum (Al), aluminum (Al)-lithium (Li), calcium (Ca), magnesium (Mg)-indium (In), magnesium (Mg)-silver (Ag), or the like. In some embodiments, to manufacture a top-emission light-emitting device, the second electrode **19** may be formed as a transmissive electrode from, for example, indium tin oxide (ITO) or indium zinc oxide (IZO).

[0417] Although the organic light-emitting device **10** of FIG. **1** is described above, embodiments of the present disclosure are not limited thereto,

[0418] As used herein, a C_1-C_{30} alkyl group refers to a linear or branched aliphatic hydrocarbon monovalent group having 1 to 30 carbon atoms. Non-limiting examples of the C_1-C_{60} alkyl group are a methyl group, an ethyl group, a propyl group, an isobutyl group, a sec-butyl group, a tert-butyl group, a pentyl group, an iso-amyl group, and a hexyl group.

[0419] As used herein, a C_1-C_{30} alkoxy group refers to a monovalent group represented by $-OA_{101}$ (where A_{101} is a C_1-C_{30} alkyl group as described above). Non-limiting examples of the C_1-C_{30} alkoxy group are a methoxy group, an ethoxy group, and an isopropyloxy group.

[0420] As used herein, a C_2-C_{30} alkenyl group refers to a structure including at least one carbon double bond in the middle or terminal of the C_2-C_{30} alkyl group. Non-limiting examples of the C_2-C_{30} alkenyl group are an ethenyl group, a propenyl group, and a butenyl group.

[0421] As used herein, a C_2-C_{30} alkynyl group refers to a structure including at least one carbon triple bond in the middle or terminal of the C_2-C_{30} alkyl group. Non-limiting examples of the C_2-C_{30} alkynyl group are an ethynyl group, and a propynyl group.

[0422] As used herein, a C_3-C_{10} cycloalkyl group refers to a monovalent monocyclic hydrocarbon group having 3 to 10 carbon atoms. Non-limiting examples of the C_3-C_{10} cycloalkyl group are a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, and a cycloheptyl group.

[0423] As used herein, a C_1-C_{10} heterocycloalkyl group refers to a monovalent monocyclic group having 1 to 10 carbon atoms in which at least one heteroatom selected from N, O, P, and S is included as a ring-forming atom. Non-limiting examples of the C_1-C_{10} heterocycloalkyl group are a tetrahydrofuranyl group, and a tetrahydrothiophenyl group.

[0424] As used herein, a C_3-C_{10} cycloalkenyl group refers to a monovalent monocyclic group having 3 to 10 carbon atoms that includes at least one double bond in the ring but does not have aromaticity. Non-limiting examples of the C_3-C_{10} cycloalkenyl group are a cyclopentenyl group, a cyclohexenyl group, and a cycloheptenyl group.

[0425] As used herein, a C_1-C_{10} heterocycloalkenyl group used herein refers to a monovalent monocyclic group having 1 to 10 carbon atoms that includes at least one double bond in the ring and in which at least one heteroatom selected from N, O, P, and S is included as a ring-forming atom. Non-limiting examples of the C_1-C_{10} heterocycloalkenyl group are a 2,3-dihydrofuranyl group, and a 2,3-dihydrothiophenyl group.

[0426] As used herein, a C_6-C_{30} aryl group refers to a monovalent, aromatic carbocyclic aromatic group having 6 to 30 carbon atoms. Non-limiting examples of the C_6-C_{30} aryl group are a phenyl group, a naphthyl group, an anthracenyl group, a phenanthrenyl group, a pyrenyl group, and a chrysenyl group. When the C_6-C_{60} aryl group includes at least two rings, the rings may be fused to each other.

[0427] As used herein, a C_1-C_{30} heteroaryl group refers to a monovalent, aromatic carbocyclic aromatic group having 1 to 30 carbon atoms in which at least one heteroatom selected from N, O, P, and S is included as a ring-forming atom. Non-limiting examples of the C_1-C_{30} heteroaryl group are a pyridinyl group, a pyrimidinyl group, a pyrazinyl group, a pyridazinyl group, a triazinyl group, a quinolinyl group, and an isoquinolinyl group. When a C_1-C_{30} heteroaryl group has at least two rings, the rings may be fused to each other.

[0428] A C_6-C_{30} aryloxy group as used herein indicates $-OA_{102}$ (wherein A_{102} is the C_6-C_{30} aryl group), a C_6-C_{30} arylthio group as used herein indicates $-SA_{103}$ (wherein A_{103} is the C_6-C_{30} aryl group), and a C_7-C_{30} arylalkyl group as

used herein indicates $-A_{104}A_{105}$ (wherein A_{104} is the C_6-C_{30} aryl group and A_{105} is the C_1-C_{30} alkyl group).

[0429] A C_2-C_{30} heteroaryloxy group as used herein indicates $-OA_{106}$ (wherein A_{106} is the C_2-C_{30} heteroaryl group), a C_2-C_{30} heteroarylthio group as used herein indicates $-SA_{107}$ (wherein A_{107} is the C_2-C_{30} heteroaryl group), and a C_3-C_{30} heteroarylalkyl group as used herein indicates $-A_{108}A_{109}$ (wherein A_{108} is the C_2-C_{30} heteroaryl group and A_{109} is the C_1-C_{30} alkyl group).

[0430] As used herein, a monovalent non-aromatic condensed polycyclic group refers to a monovalent group having at least two rings condensed to each other, in which only carbon atoms are exclusively included as ring-forming atoms and the entire molecule has non-aromaticity. A non-limiting example of the monovalent non-aromatic condensed polycyclic group is a fluorenyl group.

[0431] As used herein, a monovalent non-aromatic condensed heteropolycyclic group refers to a monovalent group having at least two rings condensed to each other, in which carbon atoms and a heteroatom selected from N, O, P, and S are included as ring-forming atoms and the entire molecule has non-aromaticity. A non-limiting example of the monovalent non-aromatic condensed heteropolycyclic group is a carbazolyl group.

[0432] As used herein, a C_1-C_{30} alkylsilyl group refers to $—Si(A_{102})(A_{103})(A_{104})$ (where A_{102} to A_{104} may be each independently a C_1-C_{30} alkyl group as described above).

[0433] As used herein, at least one substituent of the substituted C_1-C_{30} alkyl group, the substituted C_3-C_{30} branched alkyl group, the substituted C_2-C_{30} alkenyl group, the substituted C_2-C_{30} alkynyl group, the substituted C_1-C_{30} alkoxy group, the substituted C_3-C_{10} cycloalkyl group, the substituted C_1-C_{10} heterocycloalkyl group, the substituted C_3-C_{10} cycloalkenyl group, the substituted C_1-C_{10} heterocycloalkenyl group, the substituted C_6-C_{30} aryl group, the substituted C_6-C_{30} aryloxy group, the substituted C_6-C_{30} arylthio group, the substituted C_7-C_{30} arylalkyl group, the substituted C_1-C_{30} heteroaryl group, the substituted C_2-C_{30} heteroaryloxy group, the substituted C_2-C_{30} heteroarylthio group, the substituted C_3-C_{30} heteroarylalkyl group, the substituted monovalent non-aromatic condensed polycyclic group, the substituted monovalent non-aromatic condensed heteropolycyclic group, and the substituted C_1-C_{30} alkylsilyl group may be selected from

[0434] a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, and a C_1-C_{30} alkoxy group,

[0435] a C_1-C_{60} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, and a C_1-C_{30} alkoxy group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, $—N(Q_{11})(Q_{12})$, $—Si(Q_{13})(Q_{14})(Q_{15})$, and $—B(Q_{16})(Q_{17})$,

[0436] a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_{3-10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group,

[0437] a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, and a C_1-C_{30} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, $—N(Q_{21})(Q_{22})$, $—Si(Q_{23})(Q_{24})(Q_{25})$ and $—B(Q_{26})(Q_{27})$, and

[0438] $—N(Q_{31})(Q_{32})$, $—Si(Q_{33})(Q_{34})(Q_{35})$, and $—B(Q_{36})(Q_{37})$.

[0439] In some embodiments, Q_{11} to Q_{17} and Q_{31} to Q_{37} herein may be each independently selected from a hydrogen, a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, a C_1-C_{30} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group.

[0440] For example, at least one substituent of the substituted C_1-C_{60} alkylene group, the substituted C_2-C_{30} alkenylene group, the substituted C_2-C_{30} alkynylene group, the substituted C_3-C_{10} cycloalkylene group, the substituted C_1-C_{10} heterocycloalkylene group, the substituted C_3-C_{10} cycloalkenylene group, the substituted C_1-C_{10} heterocycloalkenylene group, the substituted C_6-C_{30} arylene group, the substituted C_1-C_{30} heteroarylene group, the substituted divalent non-aromatic condensed polycyclic group, the substituted divalent non-aromatic condensed heteropolycyclic group, the substituted C_1-C_{30} alkyl group, the substituted C_2-C_{30} alkenyl group, the substituted C_2-C_{30} alkynyl group, the substituted C_3-C_{10} cycloalkyl group, the substituted

C_1-C_{10} heterocycloalkyl group, the substituted C_3-C_{11} cycloalkenyl group, the substituted C_1-C_{10} heterocycloalkenyl group, the substituted C_6-C_{30} aryl group, the substituted C_6-C_{30} aryloxy group, the substituted C_6-C_{30} arylthio group, the substituted C_7-C_{30} arylalkyl group, the substituted C_1-C_{30} heteroaryl group, the substituted C_2-C_{30} heteroaryloxy group, the substituted C_2-C_{30} heteroarylthio group, the substituted C_3-C_{30} heteroarylalkyl group, the substituted monovalent non-aromatic condensed polycyclic group, and the substituted monovalent non-aromatic condensed heteropolycyclic group may be selected from

[0441] a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, and a C_1-C_{30} alkoxy group,

[0442] a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, and a C_1-C_{30} alkoxy group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_3© heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, —$N(Q_{11})(Q_{12})$, —$Si(Q_{13})(Q_{14})(Q_{15})$, and —$B(Q_{16})(Q_{17})$,

[0443] a phenyl group, a pentalenyl group, an indenyl group, a naphthyl group, an azulenyl group, a heptalenyl group, an indacenyl group, an acenaphthyl group, a fluorenyl group, a spiro-fluorenyl group, a phenalenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthrenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a naphthacenyl group, a picenyl group, a perylenyl group, a pentaphenyl group, a hexacenyl group, a pyrrolyl group, an imidazolyl group, a pyrazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a phthalazinyl group, a naphthyridinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthridinyl group, an acridinyl group, a phenanthrolinyl group, a phenazinyl group, a benzoxazolyl group, a benzoimidazolyl group, a furanyl group, a benzofuranyl group, a thiophenyl group, a benzothiophenyl group, a thiazolyl group, an isothiazolyl group, a benzothiazolyl group, an isoxazolyl group, an oxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyrimidinyl group, and an imidazopyridinyl group, each substituted with at least one of a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, an anthracenyl group, a pyrenyl group, a phenanthrenyl group, a fluorenyl group, a carbazolyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, a pyridinyl group, a pyrimidinyl group, a pyrazinyl group, a pyridazinyl group, a triazinyl group, a quinolinyl group, an isoquinolinyl group, a phthalazinyl group, a quinoxalinyl group, a cinnolinyl group, and a quinazolinyl group,

[0444] a phenyl group, a pentalenyl group, an indenyl group, a naphthyl group, an azulenyl group, a heptalenyl group, an indacenyl group, an acenaphthyl group, a fluorenyl group, a spiro-fluorenyl group, a phenalenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthrenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a naphthacenyl group, a picenyl group, a perylenyl group, a pentaphenyl group, a hexacenyl group, a pyrrolyl group, an imidazolyl group, a pyrazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a phthalazinyl group, a naphthyridinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthridinyl group, an acridinyl group, a phenanthrolinyl group, a phenazinyl group, a benzoxazolyl group, a benzoimidazolyl group, a furanyl group, a benzofuranyl group, a thiophenyl group, a benzothiophenyl group, a thiazolyl group, an isothiazolyl group, a benzothiazolyl group, an isoxazolyl group, an oxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyrimidinyl group, and an imidazopyridinyl group, each substituted with at least one of a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, an anthracenyl group, a pyrenyl group, a phenanthrenyl group, a fluorenyl group, a carbazolyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, a pyridinyl group, a pyrimidinyl group, a pyrazinyl group, a pyridazinyl group, a triazinyl group, a quinolinyl group, an isoquinolinyl group, a phthalazinyl group, a quinoxalinyl group, a cinnolinyl group, and a quinazolinyl group that are each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a

[0445] salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, and a C_1-C_{30} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{11} heterocycloalkyl group, a C_s—C cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, —$N(Q_{21})(Q_{22})$, —$Si(Q_{23})(Q_{24})(Q_{25})$, and —$B(Q_{26})(Q_{27})$, and

[0446] —$N(Q_{31})(Q_{32})$, —$Si(Q_{33})(Q_{34})(Q_{35})$, and —$B(Q_{36})(Q_{37})$,

[0447] wherein Q_{11} to Q_{17} and Q_{31} to Q_{37} may be each independently selected from a phenyl group, a pentalenyl group, an indenyl group, a naphthyl group, an azulenyl group, a heptalenyl group, an indacenyl group, an acenaphthyl group, a fluorenyl group, a spiro-fluorenyl group, a phenalenyl group, a phenanthrenyl group, an anthracenyl group, a fluoranthrenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, a naphthacenyl group, a picenyl group, a perylenyl group, a pentaphenyl group, a hexacenyl group, a pyrrolyl group, an imidazolyl group, a pyrazolyl group, a pyridinyl group, a pyrazinyl group, a pyrimidinyl group, a pyridazinyl group, an isoindolyl group, an indolyl group, an indazolyl group, a purinyl group, a quinolinyl group, an isoquinolinyl group, a benzoquinolinyl group, a phthalazinyl group, a naphthyridinyl group, a quinoxalinyl group, a quinazolinyl group, a cinnolinyl group, a carbazolyl group, a phenanthridinyl group, an acridinyl group, a phenanthrolinyl group, a phenazinyl group, a benzoxazolyl group, a benzoimidazolyl group, a furanyl group, a benzofuranyl group, a thiophenyl group, a benzothiophenyl group, a thiazolyl group, an isothiazolyl group, a benzothiazolyl group, an isoxazolyl group, an oxazolyl group, a triazolyl group, a tetrazolyl group, an oxadiazolyl group, a triazinyl group, a dibenzofuranyl group, a dibenzothiophenyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, an imidazopyrimidinyl group, and an imidazopyridinyl group, each substituted with at least one of a hydrogen, a C_1-C_{30} alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, a C_1-C_{30} alkoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, an anthracenyl group, a pyrenyl group, a phenanthrenyl group, a fluorenyl group, a carbazolyl group, a benzocarbazolyl group, a dibenzocarbazolyl group, a pyridinyl group, a pyrimidinyl group, a pyrazinyl group, a pyridazinyl group, a triazinyl group, a quinolinyl group, an isoquinolinyl group, a phthalazinyl group, a quinoxalinyl group, a cinnolinyl group, and a quinazolinyl group. However, embodiments are not limited thereto.

[0448] When a group containing a specified number of carbon atoms is substituted with any of the groups listed in the preceding paragraph, the number of carbon atoms in the resulting "substituted" group is defined as the sum of the carbon atoms contained in the original (unsubstituted) group and the carbon atoms (if any) contained in the substituent. For example, when the term "substituted C_1-C_{10} alkyl" refers to a C_1-C_{30} alkyl group substituted with C_6-C_{60} aryl group, the total number of carbon atoms in the resulting aryl substituted alkyl group is C_7-C_{90}.

[0449] Hereinafter, the present inventive concept will be described in detail with reference to the following synthesis examples and other examples of compounds and organic light-emitting devices. However, these examples are for illustrative purposes only and are not intended to limit the scope of the present inventive concept. In the following synthesis examples, the expression that "'B' instead of 'A' was used" means that the amounts of 'B' and 'A' were the same in equivalent amounts.

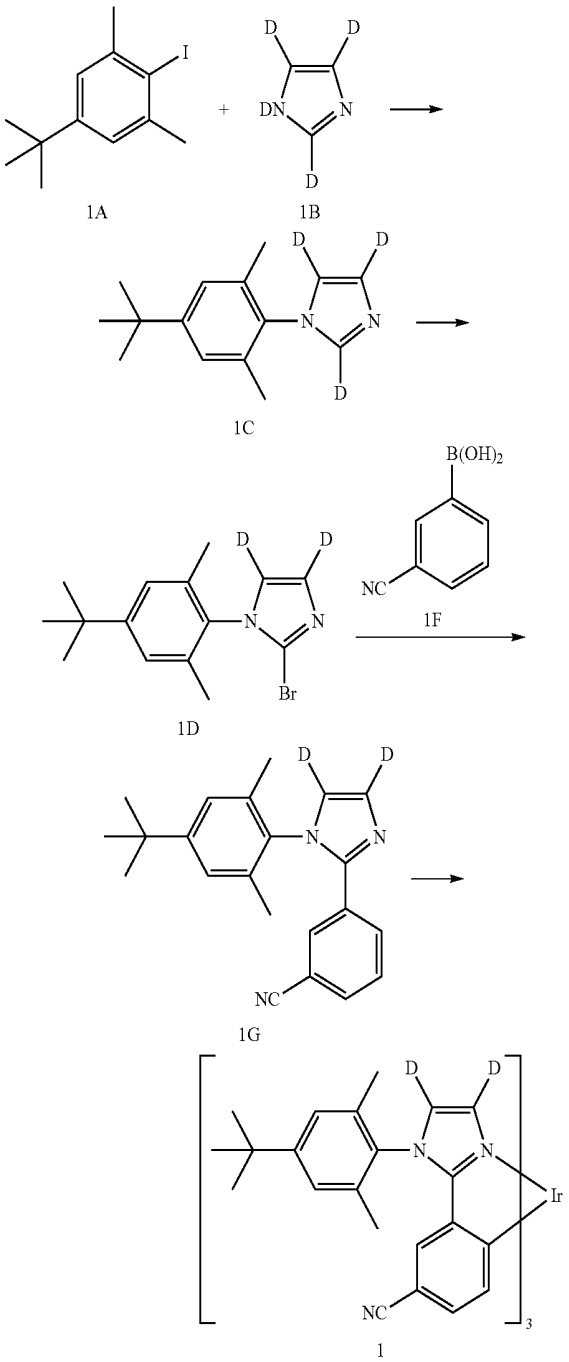
EXAMPLES

Synthesis Example 1

Synthesis of Compound 1

[0450]

Reaction Scheme 1



(1) Synthesis of Intermediate 37C

[0451] 34.70 millimoles (mmol) of Compound 37A, 41.64 mmol of Compound B, mmol of K_2CO_3, 1.74 mmol of CuI,

3.47 mmol of 1,10-phenanthroline, and 500 milliliters (mL) of dimethylformamide (DMF) were placed into a 1 liter (L)-reaction container, and refluxed under a nitrogen atmosphere for about 12 hours. After the reaction finished, the resulting reaction product was cooled down to room temperature, dichloromethane and distilled water were added thereto, and the organic phase was separated therefrom. After the separated organic phase was washed with distilled water twice and dried using $MgSO_4$, the solvent was removed to obtain a crude product. The crude product was purified by silica gel column chromatography (using ethyl acetate and n-hexane as an eluent) to thereby obtain 26.37 mmol of Intermediate 37C. This intermediate 37C was identified by liquid chromatography-mass spectroscopy (LC-MS).

[0452] LC-MS (m/z): 232.47 [M+1]

(2) Synthesis of Intermediate 37D

[0453] 26.37 mmol of Compound 37C and tetrahydrofuran (THF) were placed into a reaction container, and cooled to about −78° C. under a nitrogen atmosphere. 27.69 mmol of 2.5 molar (M) n-BuLi (in n-hexane) was slowly added thereto at the same temperature and stirred for about 1 hour, and 52.74 mmol of Br_2 was slowly added thereto at the same temperature. After 30 minutes, the cooling by the cooler was stopped to allow a natural temperature to rise to room temperature, at which the resulting product was then stirred for about 6 hours. After the reaction finished, dichloromethane and distilled water were added thereto, and the organic phase was separated therefrom. After the separated organic phase was washed with distilled water twice and dried using $MgSO_4$, the solvent was removed to obtain a crude product. The crude product was purified by silica gel column chromatography (using ethyl acetate and n-hexane as an eluent) to thereby obtain 18.72 mmol of Intermediate 37D. This intermediate 37D was identified by LC-MS.

[0454] LC-MS (m/z): 310.18 [M+1]

(3) Synthesis of Intermediate LM037

[0455] 18.72 mmol of Compound 37D, 28.08 mmol of Compound 1E, 1.87 mmol of $Pd(PPh_3)_4$, 210.63 mmol of K_2CO_3, and a mixture of THF and distilled water (2:1) were placed into a reaction container and refluxed under a nitrogen atmosphere for about 12 hours. After the reaction finished, the resulting reaction product was cooled down to room temperature, dichloromethane and distilled water were added thereto, and the organic phase was separated therefrom. After the separated organic phase was washed with distilled water twice and dried using $MgSO_4$, the solvent was removed to obtain a crude product. The crude product was purified by silica gel column chromatography (using ethyl acetate and n-hexane as an eluent) to thereby obtain 16.47 mmol of Intermediate LM037. This intermediate LM037 was identified by LC-MS.

[0456] LC-MS (m/z): 332.58 [M+1]

(4) Synthesis of Compound BD037

[0457] 3.29 mmol of $Ir(acac)_3$, 16.47 mmol of Compound LM037, and glycerol were placed into a reaction container together and refluxed under a nitrogen atmosphere for about 12 hours. After the reaction finished, the resulting reaction product was cooled down to room temperature, dichloromethane and distilled water were added thereto, and the organic phase was separated therefrom. After the separated organic phase was washed with distilled water twice and dried using $MgSO_4$, the solvent was removed to obtain a crude product. The crude product was purified by silica gel column chromatography (using ethyl acetate and n-hexane as an eluent) to thereby obtain 0.49 mmol of Compound BD037. This Compound BD037 was identified by matrix assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS)

[0458] MALDI-TOF(m/z): 1183.57 [M]+

Synthesis Example 2

Synthesis of Compound BD040

[0459] Compound BD040 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediate 40A represented by a formula below, instead of Compound 37A used in the synthesis of Compound BD037 according to Reaction Scheme 1, was used.

[0460] MALDI-TOF(m/z): 1201.66 [M]+

Synthesis Example 3

Synthesis of Compound BD044

[0461] Compound BD044 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 44A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD044 was identified by MALDI-TOF.

[0462] MALDI-TOF(m/z): 1216.71 [M]+

Synthesis Example 4

Synthesis of Compound BD045

[0463] Compound BD045 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 45A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD045 was identified by MALDI-TOF.

[0464] MALDI-TOF(m/z): 1243.88 [M]+

Synthesis Example 5

Synthesis of Compound BD047

[0465] Compound BD047 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 45A and 3E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD047 was identified by MALDI-TOF.

[0466] MALDI-TOF(m/z): 1292.05 [M]+

Synthesis Example 6

Synthesis of Compound BD049

[0467] Compound BD049 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 45A and 4E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD049 was identified by MALDI-TOF.

[0468] MALDI-TOF(m/z): 1436.22 [M]+

Synthesis Example 7

Synthesis of Compound BD064

[0469] Compound BD064 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 64A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD046 was identified by MALDI-TOF.

[0470] MALDI-TOF(m/z): 1446.28 [M]+

Synthesis Example 8

Synthesis of Compound BD079

[0471] Compound BD079 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 79A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD079 was identified by MALDI-TOF.

[0472] MALDI-TOF(m/z): 1292.01 [M]+

Synthesis Example 9

Synthesis of Compound BD079

[0473] Compound BD098 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 98A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD079 was identified by MALDI-TOF.

[0474] MALDI-TOF(m/z): 1484.26 [M]+

Synthesis Example 10

Synthesis of Compound BD113

[0475] Compound BD113 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 113A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD113 was identified by MALDI-TOF.

[0476] MALDI-TOF(m/z): 1291.82 [M]+

Synthesis Example 11

Synthesis of Compound BD132

[0477] Compound BD132 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 132A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD132 according to Reaction Scheme 1, were used. This Compound BD132 was identified by MALDI-TOF.

[0478] MALDI-TOF(m/z): 1484.11 [M]+

Synthesis Example 12

Synthesis of Compound BD151

[0479] Compound BD151 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 151A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD151 was identified by MALDI-TOF.

[0480] MALDI-TOF(m/z): 1291.61 [M]+

Synthesis Example 13

Synthesis of Compound BD180

[0481] Compound BD180 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 180A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD180 was identified by MALDI-TOF.

[0482] MALDI-TOF(m/z): 1484.05 [M]+

Synthesis Example 14

Synthesis of Compound BD201

[0483] Compound BD201 was synthesized in the same manner as in Reaction Scheme 1 except that Intermediates 201A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD201 was identified by MALDI-TOF.

[0484] MALDI-TOF(m/z): 1291.65 [M]+

Synthesis Example 15

Synthesis of Compound BD233

[0485] Compound BD233 was synthesized in the same manner as in Reaction Scheme 1 except that Intermediates 233A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD233 was identified by MALDI-TOF.

[0486] MALDI-TOF(m/z): 1484.05 [M]+

Synthesis Example 16

Synthesis of Compound BD248

[0487] Compound BD248 was synthesized in the same manner as in Reaction Scheme 1 except that Intermediates 248A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD248 was identified by MALDI-TOF.

[0488] MALDI-TOF(m/z): 1519.95 [M]+

Synthesis Example 17

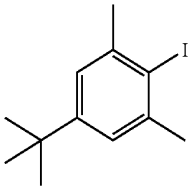
Synthesis of Compound BD255

[0489] Compound BD255 was synthesized in the same manner as in Reaction Scheme 1, except that Intermediates 255A and 2E represented by formulae below, instead of Compounds 37A and 1E used in the synthesis of Compound BD037 according to Reaction Scheme 1, were used. This Compound BD255 was identified by MALDI-TOF.

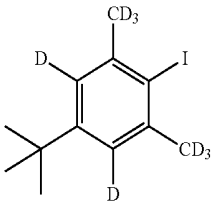
[0490] MALDI-TOF(m/z): 1519.93 [M]+

[0491] Formulae of Intermediates

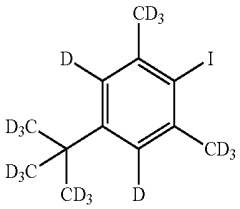
37A



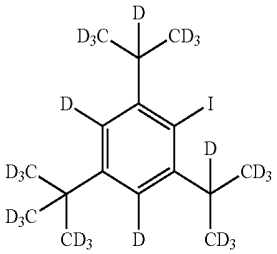
40A



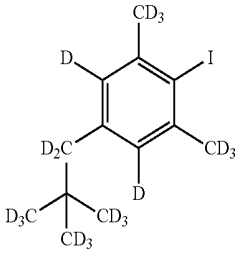
45A



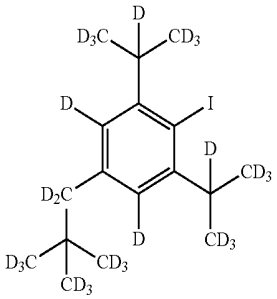
64A



79A



98A



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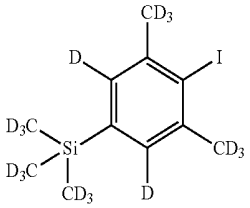
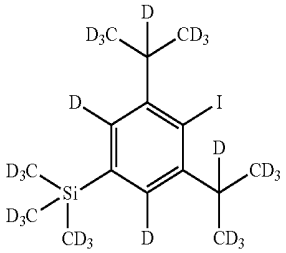
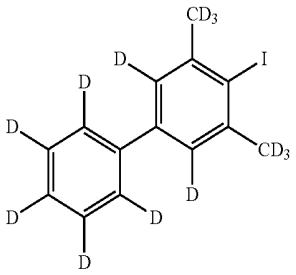
113A



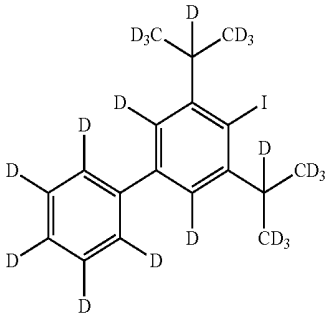
132A



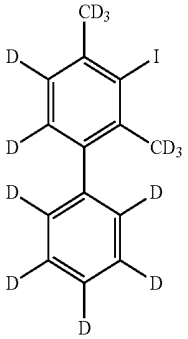
151A



180A



201A



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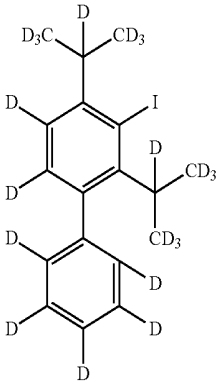
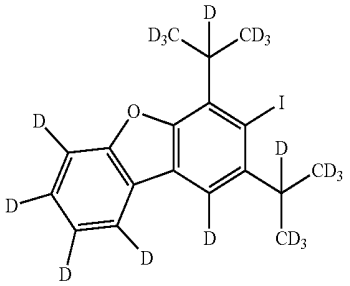
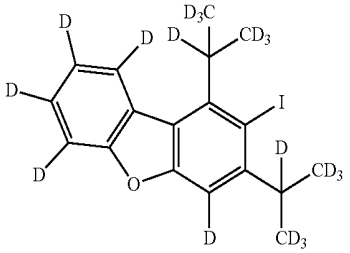
233A



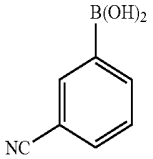
248A



255A



1E



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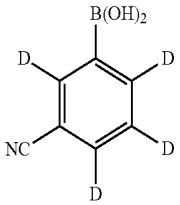
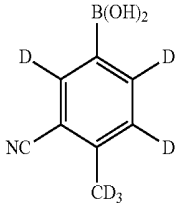
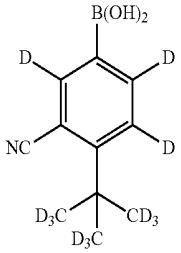


-continued

3E



4E



Evaluation Example 1

Evaluation on HOMO, LUMO, and Triplet (T1) Energy Levels

[0492] Highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), triplet (T1) energy levels, and λ_{max} of Compounds BD037, BD040, BD044, BD045, BD047, BD049, BD064, BD079, BD098, BD113, BD132, BD151, BD180, BD201, BD233, BD248, BD255, and A were evaluated according to the methods described in Table 7. The results are shown in Table 8,

A

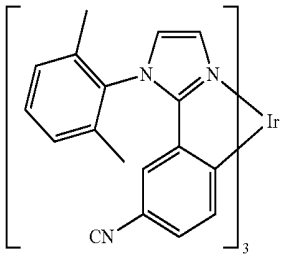


TABLE 7

HOMO energy level evaluation method	A potential (V)-current (A) graph of each compound was obtained by using cyclic voltammetry (CV) (electrolyte: 0.1M Bu_4NClO_4/solvent: CH_2Cl_2/electrode: 3 electrode system (working electrode: GC, reference electrode: Ag/AgCl, auxiliary electrode: Pt)). Then, from reduction onset of the graph, a HOMO energy level of a compound was calculated.
LUMO energy level evaluation method	Each compound was diluted at a concentration of 1×10^{-5}M in $CHCl_3$, and a UV absorption spectrum thereof was measured at room temperature by using a Shimadzu UV-350 spectrometer. Then a LUMO energy level thereof was calculated by using an optical band gap (Eg) from an edge of the absorption spectrum.

TABLE 7-continued

T1 energy level and λ_{max} evaluation method	Each compound was diluted with CH_2Cl_2 to a concentration 10 millimolar (mM), and loaded into a ISC PC1 spectrofluorometer equipped with a xenon lamp to measure a photoluminescence (PL) spectrum at room temperature. The obtained maximum absorption peak (λ_{max}) was converted to energy in electron volts (eV).

TABLE 8

Compound	HOMO (eV)	LUMO (eV)	T1 (eV)	λ_{max} (nm)
A	−5.35	−2.43	2.68	461
BD037	−5.32	−2.41	2.68	461
BD040	−5.32	−2.41	2.68	461
BD044	−5.32	−2.41	2.68	461
BD045	−5.32	−2.41	2.68	461
BD047	−5.21	−2.24	2.72	456
BD049	−5.23	−2.25	2.72	456
BD064	−5.31	−2.41	2.68	461
BD079	−5.32	−2.40	2.68	461
BD098	−5.32	−2.40	2.68	461
BD113	−5.29	−2.38	2.68	461
BD132	−5.29	−2.38	2.68	461
BD151	−5.29	−2.44	2.67	463
BD180	−5.29	−2.43	2.68	462
BD201	−5.30	−2.36	2.67	463
BD233	−5.31	−2.37	2.68	462
BD248	−5.26	−2.18	2.68	461
BD255	−5.28	−2.22	2.68	461

[0493] Referring to Table 8, compounds BD037, BD040; BD044, BD045, BD047, BD049, BD064, BD079, BD098, BD113, BD132, BD151, BD180, BD201, BD233, BD248, and BD255 were found to have suitable electric characteristics for use as materials for organic light-emitting devices.

Evaluation Example 2

Purity Analysis of Compound after Deposition as Thin Film

[0494] Each of compounds BD037, BD040, BD044, BD045, BD047, BD049, BD064, BD079, BD098, BD113, BD132, BD151, BD180, BD201, BD233, BD248, BD255, and A was vacuum-deposited to form a thin film. Purities of the compounds before and after the vacuum deposition were analyzed by high-performance liquid chromatography (HPLC). The results are shown in Table 9.

TABLE 9

Compound	Before vacuum deposition (%)	After vacuum deposition (%)	Purity difference between before and after vacuum deposition (%)
BD037	98.57	97.70	−0.87
BD040	98.45	97.65	−0.80
BD044	99.05	98.36	−0.69
BD045	99.53	98.91	−0.62
BD047	99.28	98.06	−1.22
BD049	99.51	98.53	−0.98
BD064	99.68	99.50	−0.18
BD079	99.42	98.71	−0.71
BD098	99.35	99.01	−0.34
BD113	99.23	98.64	−0.59
BD132	99.42	99.06	−0.36
BD151	99.75	99.04	−0.71
BD180	99.88	99.47	−0.41
BD201	99.70	99.05	−0.65
BD233	99.73	99.35	−0.38
BD248	99.35	98.66	−0.69

TABLE 9-continued

Compound	Before vacuum deposition (%)	After vacuum deposition (%)	Purity difference between before and after vacuum deposition (%)
BD255	99.43	98.87	−0.56
A	99.57	95.75	−3.82

[0495] Referring to Table 9, compounds BD037, BD040, BD044, BD045, BD047, BD049, BD064, BD079, BD098, BD113, BD132, BD151, BD180, BD201, BD233, BD248, and BD255 were found to have less purity difference between before and after vacuum deposition, compared to Compound A. Based on the results in Table 9, the organometallic compound of Formula 1 is found to have good thermal stability due to the substitution with deuterium.

Example 1

[0496] A glass substrate with a 1,500 Angstrom (Å)-thick indium tin oxide (ITO) electrode (first electrode, anode) thereon was ultrasonically washed with distilled water and then with isopropyl alcohol, acetone, and methanol. After being dried, the glass substrate was cleaned using oxygen plasma in a plasma-cleaning system for about 5 minutes, and then mounted into a vacuum deposition device.

[0497] Compound HT3 was vacuum-deposited on the ITO anode of the glass substrate to form a first hole injection layer (HIL) having a thickness of 3,500 Å, and Compound HT-D1 was vacuum-deposited on the first HIL to form a second HIL having a thickness of about 300 Å. Subsequently, TAPC was vacuum-deposited on the second HIL to form an electron blocking layer (EBL) having a thickness of about 100 Å, thereby forming a hole transport region.

[0498] Next, mCP (as a host) and Compound BD037 (as a dopant, 7 percent by weight (wt %)) were co-deposited on the hole transport region to form an emission layer (EML) having a thickness of about 300 Å.

[0499] After Compound ET3 was vacuum-deposited on the EML to form an electron transport layer (ETL) having a thickness of about 250 Å, ET-D1 was deposited on the ETL to form an electron injection layer (EIL) having a thickness of about 5 Å, followed by forming an electron transport region.

[0500] An aluminum (Al) second electrode (cathode) having a thickness of about 1,000 Å was then formed on the electron transport region thereby manufacturing an organic light-emitting device.

Example 2

[0501] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD040, instead of Compound BD037, was used as a dopant in forming the EML.

Example 3

[0502] An organic light-emitting device was manufactured in the same manner as in Example 1 except that Compound BD044, instead of Compound BD037, was used as a dopant in forming the EML.

Example 4

[0503] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD045, instead of Compound BD037, was used as a dopant in forming the EML.

Example 5

[0504] An organic light-emitting device was manufactured in the same manner as in Example 1 except that Compound BD047, instead of Compound BD037, was used as a dopant in forming the EML.

Example 6

[0505] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD049, instead of Compound BD037, was used as a dopant in forming the EML.

Example 7

[0506] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD064, instead of Compound BD037, was used as a dopant in forming the EML.

Example 8

[0507] An organic light-emitting device was manufactured in the same manner as in Example 1 except that Compound BD079, instead of Compound BD037, was used as a dopant in forming the EML.

Example 9

[0508] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD098, instead of Compound BD037, was used as a dopant in forming the EML.

Example 10

[0509] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD113, instead of Compound BD037, was used as a dopant in forming the EML.

Example 11

[0510] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD132, instead of Compound BD037, was used as a dopant in forming the EML.

Example 12

[0511] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD151, instead of Compound BD037, was used as a dopant in forming the EML.

Example 1

[0512] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD180, instead of Compound BD037, was used as a dopant in forming the EML.

Example 14

[0513] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD201, instead of Compound BD037, was used as a dopant in forming the EML.

Example 15

[0514] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD233, instead of Compound BD037, was used as a dopant in forming the EML.

Example 16

[0515] An organic light-emitting device was manufactured in the same manner as in Example 1 except that Compound BD248, instead of Compound BD037, was used as a dopant in forming the EML.

Example 17

[0516] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound BD255, instead of Compound BD037, was used as a dopant in forming the EML.

Comparative Example 1

[0517] An organic light-emitting device was manufactured in the same manner as in Example 1, except that Compound A, instead of Compound BD037, was used as a dopant in forming the EML.

Evaluation Example 3

Evaluation of Characteristics of Organic Light-Emitting Devices

[0518] Current density values, luminance values, efficiency values, lifespan values and color coordinates of the organic light-emitting devices of Examples 1 to 17 and Comparative Example 1 were evaluated using the following methods. The results are shown in Table 10.

[0519] (1) Measurement of Current Density Changes with Respect to Voltage

[0520] While increasing a voltage applied to each of the organic light-emitting devices from 0 volts (V) to about 10 V, a current flowing through each organic light-emitting device was measured using a current voltmeter (Keithley 2400), followed by dividing the current value by the area of the organic light-emitting device to obtain a current density.

[0521] (2) Measurement of Luminance Changes with Respect to Voltage

[0522] While increasing a voltage applied to each of the organic light-emitting devices from about 0 V to about 10 V, luminances of the organic light-emitting devices were measured using a luminance meter (Minolta Cs-1000A).

[0523] (3) Measurement of Current Efficiencies

[0524] Current efficiencies (candelas per ampere, cd/A) of the organic light-emitting devices at the same current density of 10 milliamperes per square centimeter (mA/cm^2) were calculated based on the measured luminances, current densities, and voltages in Sections (1) and (2).

[0525] (4) Measurement of Lifespan

[0526] T_{50}, which indicates a period of time taken till an initial luminance (assumed as 100%) measured in Section (2) is reduced to 50%, was calculated. T_{50} in Table 10 is a relative lifetime T_{50} to that of the organic light-emitting device of Comparative Example 1.

[0527] (5) Measurement of CIE Color Coordinate

[0528] CIE color coordinates of the organic light-emitting devices at a luminance of about 500 candelas per square meter (cd/m^2) were measured using a luminance meter (Minolta Cs-1000A).

TABLE 10

Example	Host	Dopant	Driving voltage (V)	Current Efficiency (cd/A)	Luminance (cd/m^2)	T_{50} (as relative lifetime) (%)	Color coordinates CIE x	CIE y
Example 1	mCP	BD037	5.1	33.4	500	312	0.17	0.26
Example 2	mCP	BD040	5.1	33.7	500	326	0.17	0.26
Example 3	mCP	BD044	5.1	33.5	500	334	0.17	0.26
Example 4	mCP	BD045	5.1	34.8	500	350	0.17	0.26
Example 5	mCP	BD047	5.0	32.0	500	182	0.15	0.21
Example 6	mCP	BD049	5.1	32.4	500	220	0.15	0.21
Example 7	mCP	BD064	5.1	34.3	500	341	0.17	0.26
Example 8	mCP	BD079	5.1	34.1	500	325	0.17	0.26
Example 9	mCP	BD098	5.1	34.0	500	323	0.17	0.26
Example 10	mCP	BD113	5.2	34.6	500	339	0.17	0.26
Example 11	mCP	BD132	5.1	33.9	500	334	0.17	0.26
Example 12	mCP	BD151	5.1	36.5	500	440	0.17	0.28
Example 13	mCP	BD180	5.1	36.9	500	455	0.17	0.27
Example 14	mCP	BD201	5.1	36.7	500	445	0.17	0.27
Example 15	mCP	BD233	5.0	36.9	500	453	0.17	0.27
Example 16	mCP	BD248	5.2	35.2	500	378	0.17	0.27
Example 17	mCP	BD255	5.2	35.7	500	385	0.17	0.26
Comparative Example 1	mCP	A	5.2	31.1	500	100	0.17	0.26

[0529] Referring to Table 10, the organic light-emitting devices of Examples 1 to 17 were found to have similar color purity, lower driving voltage, higher current efficiency, and longer lifespans, compared to those of the organic light-emitting device of Comparative Example 1.

[0530] As described above, according to the one or more of the above embodiments of the present disclosure, an organometallic compound represented by Formula 1 may have improved optical characteristics, electrical characteristics, and thermal stability. Accordingly, an organic light-emitting device that includes the organometallic compound of Formula 1 or a composition containing the organometallic compound of Formula 1 may have a reduced driving voltage, and improved efficiency, lifespan, and color purity characteristics.

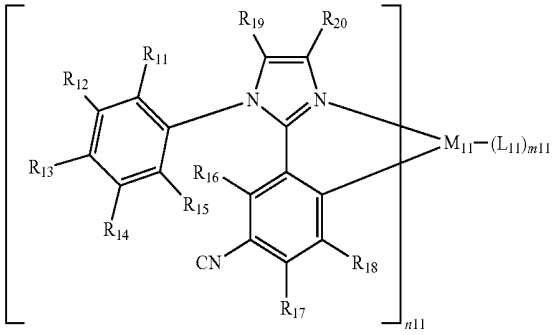
[0531] It should be understood that the exemplary embodiments described therein should be considered in a descriptive sense only and not for purposes of limitation. Descriptions of features or aspects within each embodiment should typically be considered as available for other similar features or aspects in other embodiments.

[0532] While one or more embodiments of the present inventive concept have been described with reference to the figures, it will be understood by those of ordinary skill in the art that various changes in form and details may be made therein without departing from the spirit and scope of the present inventive concept as defined by the following claims.

What is claimed is:

1. An organometallic compound represented by Formula 1:

Formula 1



wherein, in Formula 1,

M_{11} is selected from a first-row transition metal, a second-row transition metal, and a third-row transition metal;

R_{11} to R_{18} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substi-

tuted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

optionally, adjacent two of R_{11} to R_{15} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

at least one of R_{11} to R_{15} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group; a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

R_{19} and R_{20} are each independently selected from a hydrogen, a deuterium, C_1-C_{30} alkyl group, and a deuterium-substituted C_1-C_{30} alkyl group;

at least one of R_{11} to R_{20} is a deuterium-containing substituent;

n11 is selected from 1, 2, and 3;

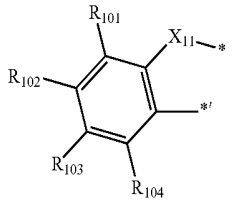
L_{11} is selected from a monodentate ligand and a bidentate ligand; and

m11 is selected from 0, 1, 2, 3, and 4.

2. The organometallic compound of claim **1**, wherein M_{11} is selected from Ir and Pt.

3. The organometallic compound of claim **1**, wherein R_{11} to R_{18} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, wherein optionally, adjacent two of R_{11} to R_{15} are linked to form a substructure represented by Formula 10:

Formula 10



wherein, in Formula 10,

X_{11} is selected from O, S, and $N(R_{105})$;

R_{101} to R_{105} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group; and

* and *' are each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

4. The organometallic compound of claim **1**, wherein R_{11} to R_{18} are each independently selected from

a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, and —$Si(Q_1)(Q_2)(Q_3)$,

a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

—$Si(Q_4)(Q_5)(Q_6)$,

wherein Q_1 to Q_3 are each independently selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group; and

Q_4 to Q_6 are each independently selected from

a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an

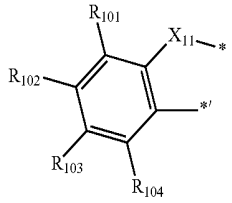
iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

wherein at least one of Q_4 to Q_6 is selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group; and

optionally, adjacent two of R_{11} to R_{15} are linked to form a substructure represented by Formula 10:

Formula 10



wherein, in Formula 10,

X_{11} is selected from O, S and $N(R_{105})$;

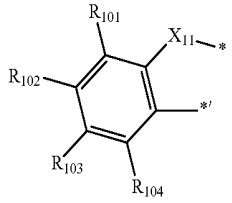
R_{101} to R_{105} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

* and *' are each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

5. The organometallic compound of claim **1**, wherein at least one of R_{11} to R_{15} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group, and

optionally, adjacent two of R_{11} to R_{15} are linked to form a substructure represented by Formula 10:

Formula 10



wherein, in Formula 10,

X_{11} is selected from O, S, and $N(R_{105})$;

R_{101} to R_{105} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidine group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

* and *' are each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

6. The organometallic compound of claim **1**, wherein at least one of R_{11} to R_{15} is selected from

an iso-propyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, a chrysenyl group, and $—Si(Q_1)(Q_2)(Q_3)$,

an iso-propyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group,

a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

$—Si(Q_4)(Q_5)(Q_6)$,

wherein Q_1 to Q_3 are each independently selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group; a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group;

Q_4 to Q_6 are each independently selected from

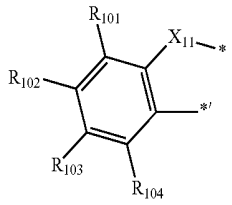
a methyl group; an ethyl group, an n-propyl group, an iso-propyl group; an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

a methyl group; an ethyl group, an n-propyl group, an iso-propyl group; an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br; —I, and a cyano group;

at least one of Q_4 to Q_6 is selected from a methyl group; an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I and a cyano group; and

optionally, adjacent two of R_{11} to R_{15} are linked to form a substructure represented by Formula 10:

Formula 10



wherein, in Formula 10,

X_{11} is selected from O, S, and $N(R_{105})$;

R_{101} to R_{105} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group;

* and *' are each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

7. The organometallic compound of claim **1**, wherein at least one of R_{11} to R_{15} is selected from

an iso-propyl group, an iso-butyl group, a tert-butyl group, a neo-pentyl group, a phenyl group, a biphenyl group, and $—Si(CH_3)_3$,

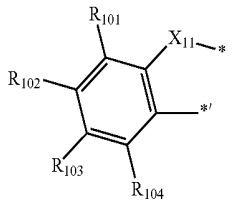
an iso-propyl group, an iso-butyl group, a tert-butyl group, and a neo-pentyl group, each substituted with a deuterium,

a phenyl group and a biphenyl group, each substituted with a deuterium, and

$—Si(CD_3)_3$, and

optionally, R_{12} and R_{13} are linked to form a substructure represented by Formula 10:

Formula 10



wherein, in Formula 10,

X_{11} is selected from O, S, and $N(R_{105})$;

R_{101} to R_{105} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a cyano group, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group; and

* and *' are each independently a carbon atom to which adjacent two of R_{11} to R_{15} are bound.

8. The organometallic compound of claim **1**, wherein R_{19} is a deuterium and R_{20} is a hydrogen; R_{19} is a hydrogen and R_{20} is a deuterium; or R_{19} and R_{20} are both deuterium.

9. The organometallic compound of claim **1**, wherein the deuterium-containing substituent is selected from

a deuterium, and

a C_1-C_{30} alkyl group, a C_3-C_{30} branched alkyl group, a C_2-C_{30} alkenyl group, a C_2-C_{30} alkynyl group, a C_1-C_{30} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{30} aryl group, a C_6-C_{30} aryloxy group, a C_6-C_{30} arylthio group, a C_7-C_{30} arylalkyl group, a C_1-C_{30} heteroaryl group, a C_2-C_{30} heteroaryloxy group, a C_2-C_{30} heteroarylthio group, a C_3-C_{30} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, and a C_1-C_{30} alkylsilyl group, each substituted with a deuterium.

10. The organometallic compound of claim **1**, wherein the deuterium-containing substituent is selected from

a deuterium,

a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, a tert-pentyl group, a phenyl group, a biphenyl group, a terphenyl group, a naphthyl group, a phenanthrenyl group, an anthracenyl group, a triphenylenyl group, a pyrenyl group, and a chrysenyl group, each substituted with a deuterium, and

$—Si(Q_4)(Q_5)(Q_6)$,

wherein Q_4 to Q_6 are each independently selected from

a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbu-

tyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, and

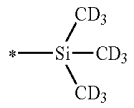
a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one of a deuterium, —F, —Cl, —Br, —I, and a cyano group; and

at least one of Q_4 to Q_6 is selected from a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neo-pentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with a deuterium.

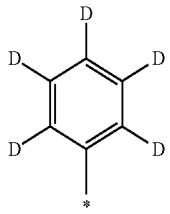
11. The organometallic compound of claim **1**, wherein the deuterium-containing substituent is selected from

-D, —CH_2D, -CHD_2, -CD_3, —CH_2CH_2D, —CH_2CHD_2, —CH_2CD_3, -$CHDCH_3$, -$CHDCH_2D$, -$CHDCHD_2$, -$CHDCD_3$, -CD_2CH_3, -CD_2CH_2D, -CD_2CHD_2, -CD_2CD_3, —$CH_2CH_2CH_2D$, —$CH_2CH_2CHD_2$, —$CH_2CH_2CD_3$, —CH_2CHDCH_3, —CH_2CHDCH_2D, —$CH_2CHDCHD_2$, —CH_2CHDCD_3, —$CH_2CD_2CH_3$, —$CH_2CD_2CH_2D$, —$CH_2CD_2CHD_2$, —$CH_2CD_2CD_3$, -$CHDCH_2CH_2D$, -$CHDCH_2CHD_2$, -$CHDCH_2CD_3$, -$CHDCHDCH_3$, -$CHDCHDCH_2D$, -$CHDCHDCHD_2$, -$CHDCHDCD_3$, -$CHDCD_2CH_3$, -$CHDCD_2CH_2D$, -$CHDCD_2CHD_2$, -$CHDCD_2CD_3$, -$CD_2CH_2CH_2D$, -$CD_2CH_2CHD_2$, -$CD_2CH_2CD_3$, -CD_2CHDCH_3, -CD_2CHDCH_2D, -$CD_2CHDCHD_2$, -CD_2CHDCD_3, -$CD_2CD_2CH_3$, -$CD_2CD_2CH_2D$, -$CD_2CD_2CHD_2$, -$CD_2CD_2CD_3$, —$CH(CH_3)(CH_2D)$, —$CH(CH_3)(CHD_2)$, $CH(CH_2D)_2$, —$CH(CH_3)(CD_3)$, —$CH(CHD)(CHD_2)$, —$CH(CH_2D)(CD_3)$, —$CH(CHD_2)_2$, —$CH(CHD_2)(CD_3)$, —$CH(CD_3)_2$, -$CD(CH_3)_2$, -$CD(CH_3)(CH_2D)$, -$CD(CH_3)(CHD_2)$, -$CD(CH_2D)(CH_2D)$, -$CD(CH_3)(CD_3)$, -$CD(CH_2D)(CHD_2)$, -$CD(CH_2D)(CD_3)$, -$CD(CHD_2)_2$, -$CD(CHD_2)(CD_3)$, -$CD(CD_3)_2$, -$CD_2CD(CD_3)_2$, —$C(CD_3)_3$, -$CD_2C(CD_3)_3$, and groups represented by Formulae 3-1 to 3-5:

3-1



3-2



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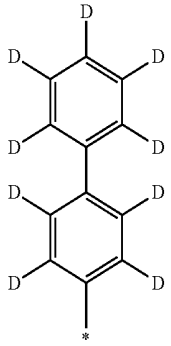
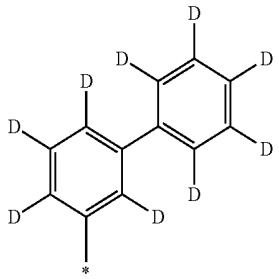
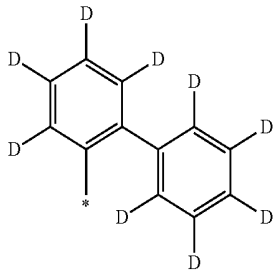
3-3



3-4



3-5

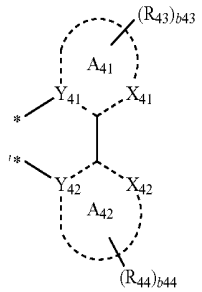


wherein, in Formulae 3-1 to 3-5, * is a binding site to an adjacent atom.

12. The organometallic compound of claim **1**, wherein L_{11} is selected from divalent organic ligands.

13. The organometallic compound of claim **1**, wherein L_{11} is represented by one of Formulae 4-1 to 4-4:

4-1



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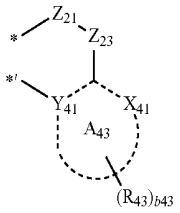
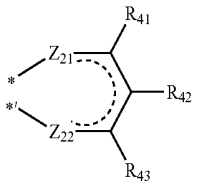
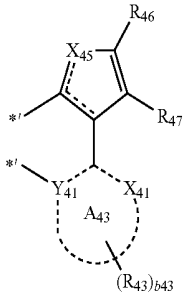
4-2



4-3



4-4



wherein, in Formulae 4-1 to 4-4,

X_{41} is CR_{41} or a nitrogen atom (N);

X_{42} is CR_{42} or N;

X_{45} is O, S, or $N(R_{45})$;

Y_{41} and Y_{42} are each independently C or N;

Z_{21} and Z_{22} are each independently N, O, $N(R_{48})$, $P(R_{48})(R_{49})$, or $As(R_{48})(R_{49})$;

Z_{23} is CO or CH_2,

A_{41} to A_{43} are each independently selected from a C_3-C_{10} cycloalkane, a C_1-C_{10} heterocycloalkane; a C_3-C_{10} cycloalkene, a C_1-C_{10} heterocycloalkene, a C_6-C_{10} arene, a C_1-C_{10} heteroarene, a non-aromatic condensed polycycle, and a non-aromatic condensed heteropolycycle;

R_{41} to R_{49} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{60} alkyl group, a substituted or unsubstituted C_2-C_{60} alkenyl group, a substituted or unsubstituted C_2-C_{60} alkynyl group, a substituted or unsubstituted C_1-C_{60} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{60} aryl group, a substituted or unsubstituted C_6-C_{60} aryloxy group, a substituted or unsubstituted C_6-C_{60} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{60} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group; a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and $—Si(Q_{41})(Q_{42})(Q_{43})$;

optionally, adjacent two of R_{41} to R_{44} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

optionally, R_{46} and R_{47} are linked to form a substituted or unsubstituted saturated ring or a substituted or unsubstituted unsaturated ring;

b43 and b44 are each independently selected from an integer of 1 to 5;

Q_{41} to Q_{43} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, C_1-C_{60} alkyl group, a C_2-C_{60} alkenyl group, a C_2-C_{60} alkynyl group, a C_1-C_{63} alkoxy group, a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{60} aryl group, a C_6-C_{60} aryloxy group, a C_6-C_{60} arylthio group, a C_7-C_{60} arylalkyl group, a C_1-C_{60} heteroaryl group, a C_2-C_{60} heteroaryloxy group, a C_2-C_{60} heteroarylthio group, a C_3-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group; and

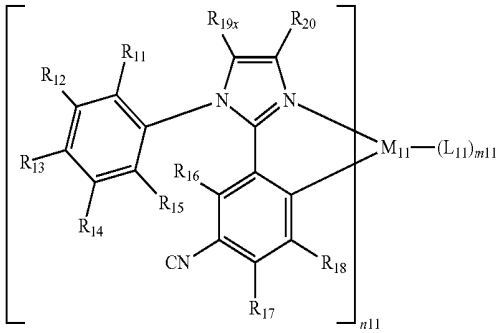
* and *' are each independently a binding site to M_{11} in Formula 1.

14. The organometallic compound of claim **1**, wherein M_{11} is iridium (Ir); and n11 is selected from 2 and 3.

15. The organometallic compound of claim **1**, wherein M_{11} is platinum (Pt); and n11 is selected from 1 and 2.

16. The organometallic compound of claim **1**, wherein the organometallic compound of Formula 1 is a compound represented by one of Formulae 1-11 to 1-22:

1-11



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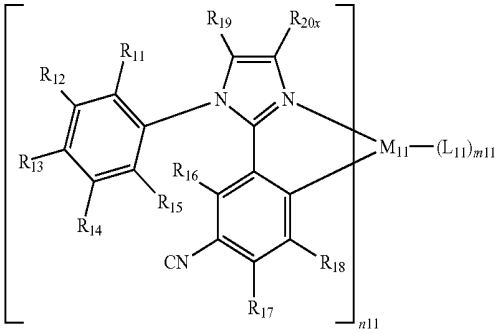
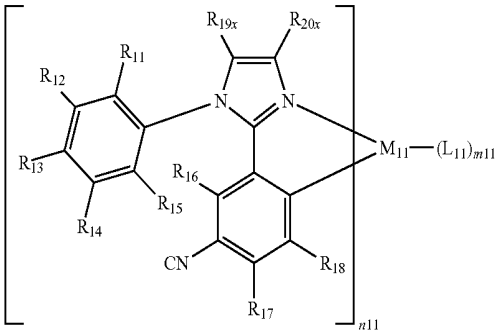
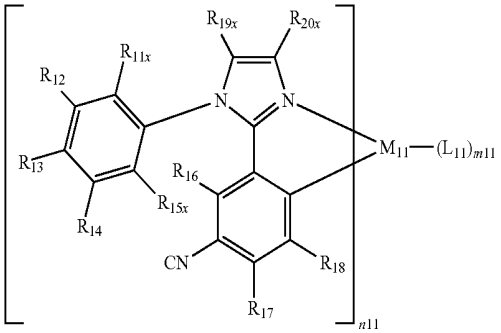
1-12



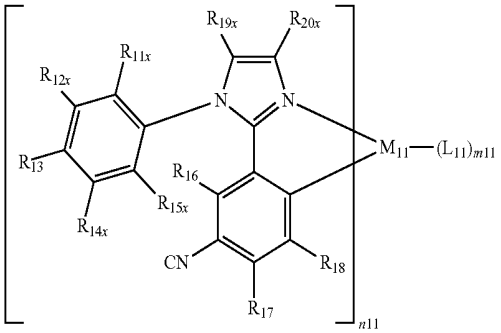
1-13



1-14



1-15



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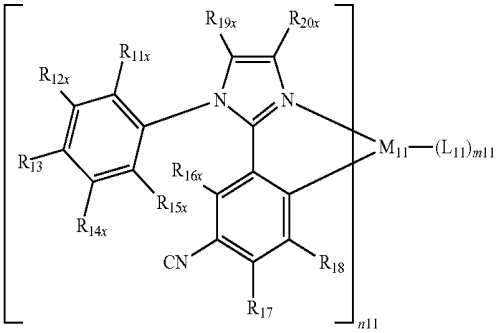
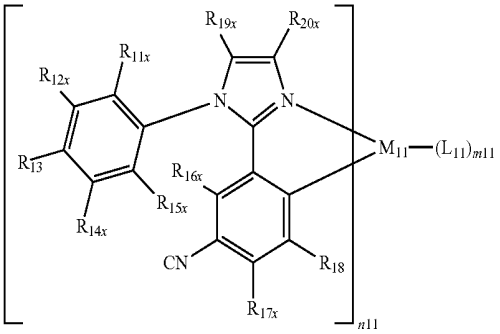
1-16



1-17



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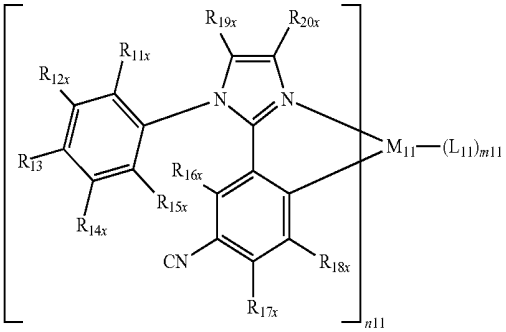

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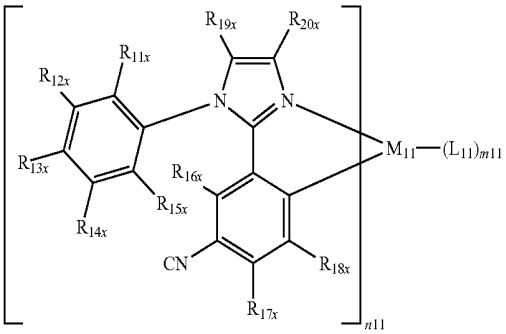

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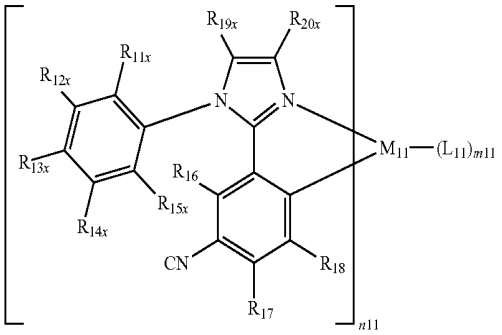
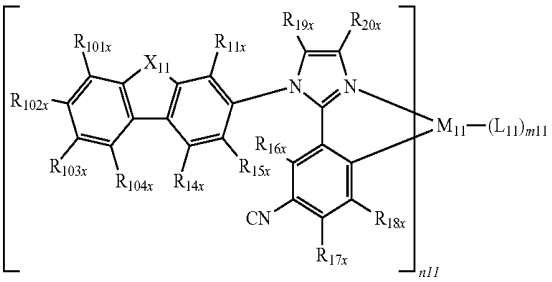
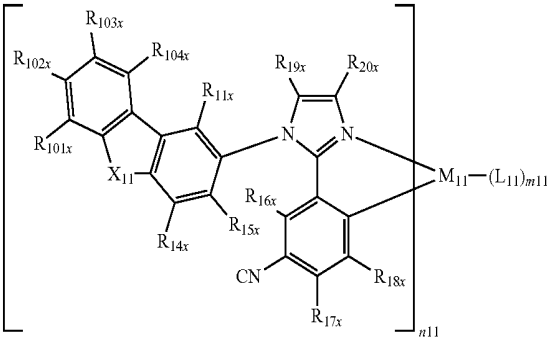
1-20



1-21



1-22



wherein, in Formulae 1-11 to 1-22,

M_{11}, R_{11} to R_{20}, n11, L_{11}, and m11 are defined the same as those in Formula 1;

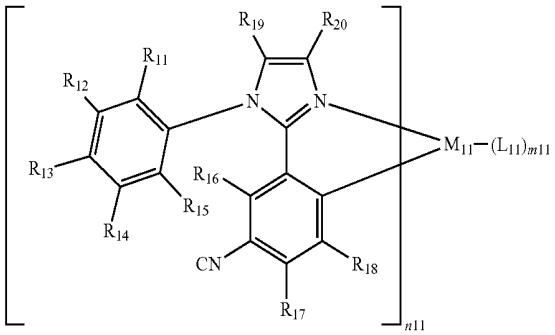
X_{11} is selected from O, S, and $N(R_{105})$;

R_{101} to R_{105} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group; a hydrazone group; a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{10} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group; and

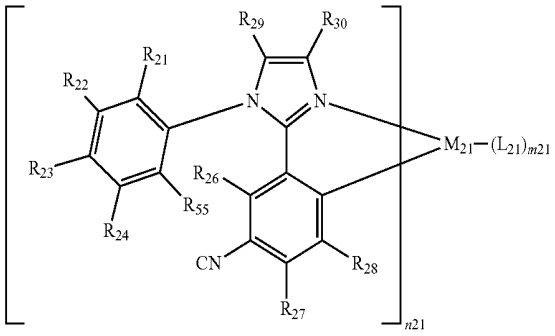
R_{11x}, R_{12x}, R_{13x}, R_{14x}, R_{15x}, R_{16x}, R_{17x}; R_{18x}, R_{19x}, R_{20x}, R_{101x}, R_{102x}, R_{103x}, and R_{104x}, are each independently a deuterium-containing substituent.

17. An organometallic compound-containing composition comprising a first organometallic compound represented by Formula 1 and a second organometallic compound represented by Formula 2:

Formula 1



Formula 2



wherein, in Formulae 1 and 2,

R_{11} to R_{18} are each independently selected from a hydrogen, a deuterium, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

optionally, adjacent two of R_{11} to R_{15} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

at least one of R_{11} to R_{15} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

R_{19} and R_{20} are each independently selected from a hydrogen, a deuterium, a C_1-C_{30} alkyl group, and a deuterium-substituted C_1-C_{30} alkyl group;

at least one of R_{11} to R_{20} is a deuterium-containing substituent;

R_{21} to R_{28} are each independently selected from a hydrogen, —F, —Cl, —Br, —I, a hydroxyl group, a cyano group, a nitro group, a carbonyl group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a substituted or unsubstituted C_1-C_{30} alkyl group, a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_2-C_{30} alkenyl group, a substituted or unsubstituted C_2-C_{30} alkynyl group, a substituted or unsubstituted C_1-C_{30} alkoxy group, a substituted or unsubstituted C_{3-10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

optionally, adjacent two of R_{21} to R_{25} are linked to form a substituted or unsubstituted saturated ring, or a substituted or unsubstituted unsaturated ring;

at least one of R_{21} to R_{25} is selected from a substituted or unsubstituted C_3-C_{30} branched alkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkyl group, a substituted or unsubstituted C_3-C_{10} cycloalkenyl group, a substituted or unsubstituted C_1-C_{10} heterocycloalkenyl group, a substituted or unsubstituted C_6-C_{30} aryl group, a substituted or unsubstituted C_6-C_{30} aryloxy group, a substituted or unsubstituted C_6-C_{30} arylthio group, a substituted or unsubstituted C_7-C_{30} arylalkyl group, a substituted or unsubstituted C_1-C_{30} heteroaryl group, a substituted or unsubstituted C_2-C_{30} heteroaryloxy group, a substituted or unsubstituted C_2-C_{30} heteroarylthio group, a substituted or unsubstituted C_3-C_{30} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, and a substituted or unsubstituted C_1-C_{30} alkylsilyl group;

R_{29} and R_{30} are each independently selected from a hydrogen and a C_1-C_{30} alkyl group;

R_{21} to R_{30} are a deuterium-non-containing substituent;

M_{11} and M_{21} are each independently selected from a first-row transition metal, a second-row transition metal, and a third-row transition metal;

n11 and n21 are each independently selected from 1, 2, and 3;

L_{11} and L_{21} are each independently selected from a monodentate ligand and a bidentate ligand; and

m11 and m21 are each independently selected from 0, 1, 2, 3, and 4.

18. The organometallic compound-containing composition of claim **17**, wherein the organometallic compound-containing composition has a deuteration rate of about 50% or more, wherein the deuteration rate is represented by Equation 2:

$$\text{Deuteration rate } (\%) = n_{D2}/(n_{H2}+n_{D2}) \times 100 \qquad \text{Equation 2}$$

wherein, in Equation 2,

n_{H2} represents a sum of a total number of hydrogens in the deuterium-containing substituents and a total number of hydrogens in substituents that are equivalent to the deuterium-containing substituents; and

n_{D2} represents a total number of deuterium atoms in the deuterium-containing substituents.

19. An organic light-emitting device comprising:

a first electrode;

a second electrode; and

an organic layer disposed between the first electrode and the second electrode,

wherein the organic layer comprises an emission layer and the organometallic compound of claim **1**, or the organometallic compound-containing composition of any one of claim **17**.

20. The organic light-emitting device of claim **19**, wherein the emission layer comprises the organometallic compound or the organometallic compound-containing composition,

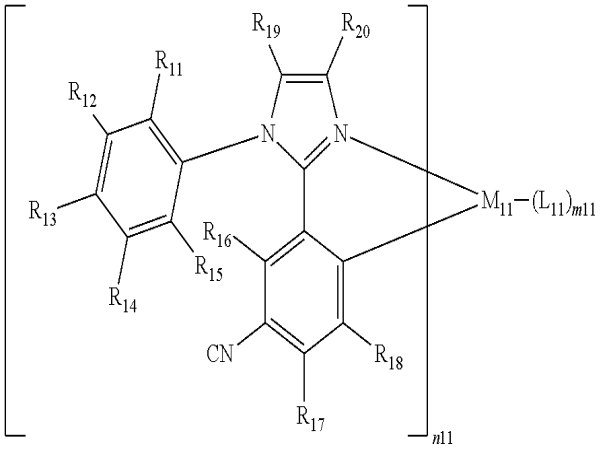
wherein the emission layer further comprises a host, and

wherein the organometallic compound in the emission layer is a dopant.

* * * * *

专利名称(译)	有机化合物，含有有机化合物的组合物，以及包括有机化合物或组合物的有机发光装置		
公开(公告)号	US20160233441A1	公开(公告)日	2016-08-11
申请号	US15/013404	申请日	2016-02-02
[标]申请(专利权)人(译)	三星电子株式会社		
申请(专利权)人(译)	SAMSUNG ELECTRONICS CO. , LTD. 三星SDI CO. , LTD.		
当前申请(专利权)人(译)	SAMSUNG ELECTRONICS CO. , LTD. 三星SDI CO. , LTD.		
[标]发明人	KIM WOOK NOH CHANGHO DAS RUPASREE RAGINI PARK YOUNGSEOK BAE HYEJIN CHAE MIYOUNG KRAVCHUK DMITRY		
发明人	KIM, WOOK NOH, CHANGHO DAS, RUPASREE RAGINI PARK, YOUNGSEOK BAE, HYEJIN CHAE, MIYOUNG KRAVCHUK, DMITRY		
IPC分类号	H01L51/00 C09K11/06 C09K11/02 C07F15/00		
CPC分类号	C09K11/06 H01L51/50 C09K2211/1007 C09K2211/1044 C09K2211/185 H01L51/0085 C07F15/0033 C09K2211/1088 C09K11/025 H01L2251/552 H01L51/5012 H01L51/5004 H01L51/0094 H01L51/0072 B32B2457/206 H01L51/006 H01L51/0067 H01L51/5016		
优先权	1020150018868 2015-02-06 KR 1020160011879 2016-01-29 KR		
其他公开文献	US10326086		
外部链接	Espacenet USPTO		

摘要(译)

由式1表示的有机金属化合物： 其中，在公式1中，组变量与规范中描述的相同。

Formula 1