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

ORGANOMETALLISCHE VERBINDUNG, ZUSAMMENSETZUNG MIT DER ORGANOMETALLISCHEN VERBINDUNG UND ORGANISCHE LICHTEMITTIERENDE VORRICHTUNG MIT DER ORGANOMETALLISCHEN VERBINDUNG

COMPOSÉ ORGANOMÉTALLIQUE, COMPOSITION CONTENANT LE COMPOSÉ ORGANOMÉTALLIQUE ET DISPOSITIF ÉLECTROLUMINESCENT ORGANIQUE COMPRENANT LE COMPOSÉ ORGANOMÉTALLIQUE

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EP-A1- 3 053 986 **JP-A- 2014 111 549**

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Description

FIELD OF THE INVENTION

[0001] One or more embodiments relate to an organometallic compound, a composition containing the organometallic compound, and an organic light-emitting device including the organometallic compound.

BACKGROUND OF THE INVENTION

[0002] Organic light-emitting devices (OLEDs) are self-emission devices that produce full-color images, and also have wide viewing angles, high contrast ratios, short response times, and excellent characteristics in terms of brightness, driving voltage, and response speed, compared to devices in the art.

[0003] A typical organic light-emitting device includes an anode, a cathode, and an organic layer disposed between the anode and the cathode, wherein the organic layer 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 recombine in the emission layer to produce excitons. These excitons transition from an excited state to a ground state, thereby generating light.

[0004] Various 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.

[0005] JP 2014 111549 discloses an iridium complex and an organic electroluminescent element which uses the iridium complex as an organic electroluminescent element material.

[0006] EP 3 053 986 discloses an organometallic compound, a composition containing the organometallic compound and organic light-emitting device including the organometallic compound or composition.

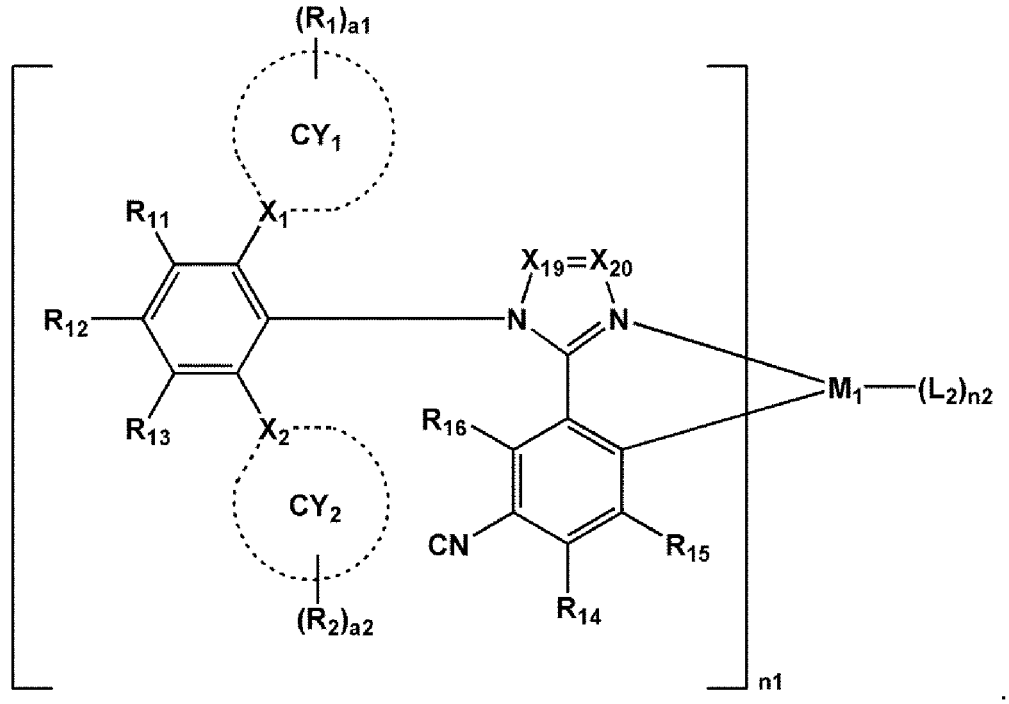
SUMMARY OF THE INVENTION

[0007] One or more embodiments include a novel organometallic compound, a composition containing the organometallic compound, and an organic light-emitting device including the organometallic compound.

[0008] 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.

[0009] According to one or more embodiments, an organometallic compound is represented by Formula 1:

Formula 1



In Formula 1,

M_1 may be selected from a first-row transition metal of the Periodic Table of Elements, a second-row transition metal of the Periodic Table of Elements, and a third-row transition metal of the Periodic Table of Elements,
n1 may be 1, 2, or 3,
L_2 is a mono- or bidentate ligand of formulae 3A, 3B, 3C, 3E or 3F as defined in the claims;
n2 may be 0, 1, 2, 3, or 4, wherein, when n2 is two or more, two or more groups L_2 may be identical to or different from each other,
X_1 and X_2 may each independently be carbon or nitrogen,
CY_1 and CY_2 may each independently be a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group,
X_{19} may be N or C(R_{19}), and X_{20} may be N or C(R_{20}), provided that at least one of X_{19} and X_{20} is N,
R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} may each independently be selected from hydrogen, deuterium, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and $-P(=O)(Q_8)(Q_9)$,
two or more neighboring groups selected from R_1, R_2, R_{11} to R_{13}, CY_1, and CY_2 may optionally be linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a1 and a2 may each independently be an integer from 0 to 5,
at least one substituent of the substituted C_5-C_{30} carbocyclic group, the substituted C_2-C_{30} heterocyclic group, the substituted C_1-C_{60} alkyl group, the substituted C_2-C_{60} alkenyl group, the substituted C_2-C_{60} alkynyl group, the substituted C_1-C_{60} 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_{60} aryl group, the substituted C_6-C_{60} aryloxy group, the substituted C_6-C_{60} arylthio group, the substituted C_7-C_{60} arylalkyl group, the substituted C_1-C_{60} heteroaryl group, the substituted C_1-C_{60} heteroaryloxy group, the substituted

C_1-C_{60} heteroarylthio group, the substituted C_2-C_{60} heteroarylalkyl group, the substituted monovalent non-aromatic condensed polycyclic group, and the substituted monovalent non-aromatic condensed heteropolycyclic group may be selected from:

deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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, and a C_1-C_{60} alkoxy group;

a C_1-C_{60} alkyl group, a C_2-C_{60} alkenyl group, a C_2-C_{60} alkynyl group, and a C_1-C_{60} alkoxy group, each substituted with at least one selected from deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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_{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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_{11})(Q_{12})$, $-Si(Q_{13})(Q_{14})(Q_{15})$, $-B(Q_{16})(Q_{17})$, and-$P(=O)(Q_{18})(Q_{19})$;

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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group;

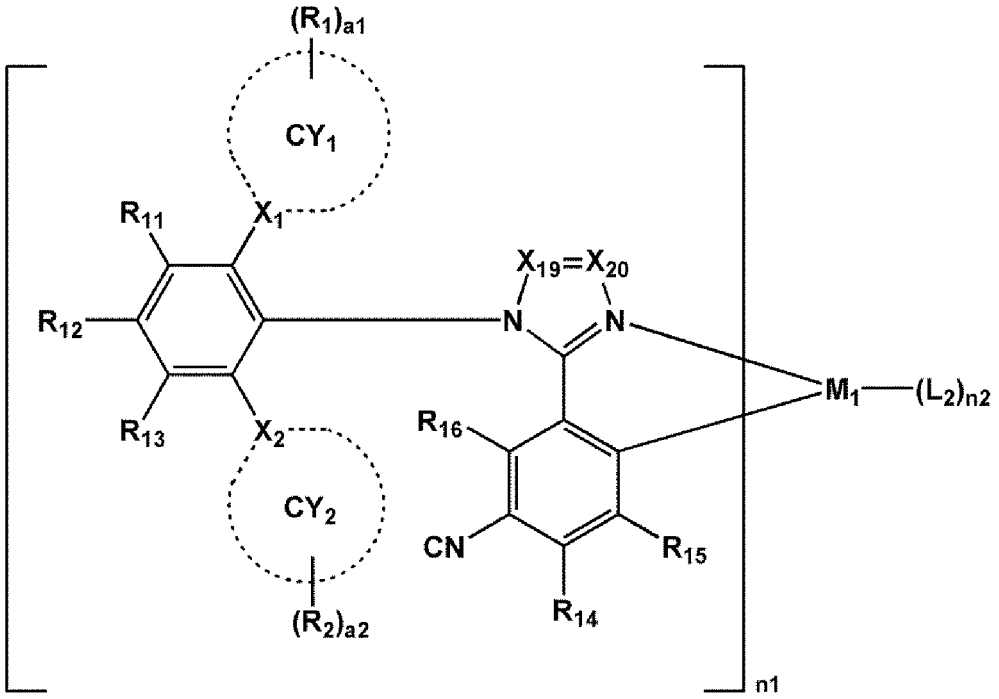
a C_3-C_{10} cycloalkyl group, a C_1-C_{10} heterocycloalkyl group, a C_3-C_{10} cycloalkenyl group, a C_1-C_{10} heterocycloalkenyl group, a C_6-C_{60} aryl group, a C_6-C_{60} aryloxy group, a C_6-C_{60} arylthio group, a C_7-C_{60} arylalkyl group, a C_1-C_{60} heteroaryl group, a C_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group, each substituted with at least one selected from deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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_1-C_{60} heteroaryl group, a C_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group,$-N(Q_{21})(Q_{22})$, $-Si(Q_{23})(Q_{24})(Q_{25})$, $-B(Q_{26})(Q_{27})$, and $-P(=O)(Q_{28})(Q_{29})$; and

$-N(Q_{31})(Q_{32})$, $-Si(Q_{33})(Q_{34})(Q_{35})$, $-B(Q_{36})(Q_{37})$, and $-P(=O)(Q_{38})(Q_{39})$, and

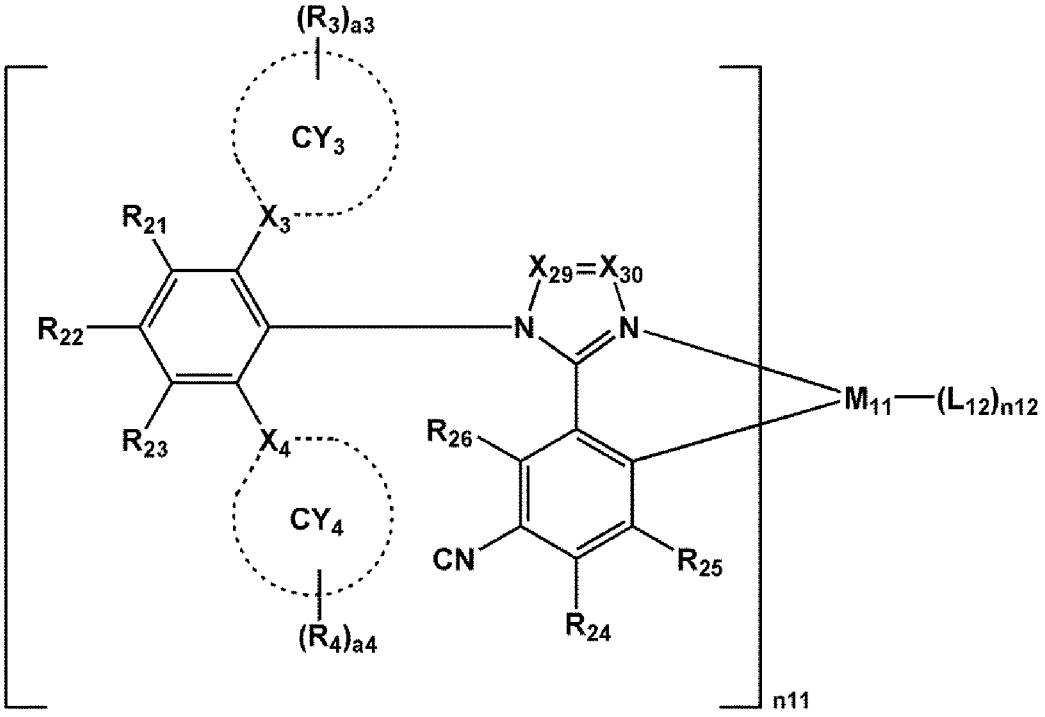
Q_1 to Q_9, Q_{11} to Q_{19}, Q_{21} to Q_{29}, and Q_{31} to Q_{39} may each independently be selected from hydrogen, deuterium, -F, -CI, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt 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} aryl group substituted with at least one selected from a C_1-C_{60} alkyl group and 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group.

[0010] According to one or more embodiments, a composition containing the organometallic compound includes a first organometallic compound represented by Formula 1 and including at least one deuterium and a second organometallic compound represented by Formula 2:

Formula 1



Formula 2



In Formulae 1 and 2,

M_1 and M_{11} may each independently be selected from a first-row transition metal of the Periodic Table of Elements, a second-row transition metal of the Periodic Table of Elements, and a third-row transition metal of the Periodic Table of Elements,

n1 and n11 may each independently be 1, 2, or 3,
L_2 and L_{12} are mono- or bidentate ligands as defined in the claims;
n2 and n12 may each independently be 0, 1, 2, 3, or 4, wherein, when n2 is two or more, two or more groups L_2 may be identical to or different from each other, and when n12 is two or more, two or more groups L_{12} may be identical to or different from each other,
X_1 to X_4 may each independently be carbon or nitrogen,
CY_1 to CY_4 may each independently be a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group,
X_{19} may be N or $C(R_{19})$, and X_{20} may be N or $C(R_{20})$, provided that at least one of X_{19} and X_{20} is N,
X_{29} may be N or $C(R_{29})$, and X_{30} may be N or $C(R_{30})$, provided that at least one of X_{29} and X_{30} is N,
R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} may each independently be selected from hydrogen, deuterium, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and-$P(=O)(Q_8)(Q_9)$,
two or more neighboring groups selected from R_1, R_2, R_{11} to R_{13}, CY_1, and CY_2 may optionally be linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a1 and a2 may each independently be an integer from 0 to 5,
i) X_{19} may be $C(R_{19})$, X_{20} may be N, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{19} may be a deuterium-containing substituent; ii) X_{19} may be N, X_{20} may be $C(R_{20})$, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{20} may be a deuterium-containing substituent; or iii) X_{19} and X_{20} may each be N, and at least one of R_1, R_2, and R_{11} to R_{16} may be a deuterium-containing substituent,
R_3, R_4, R_{21} to R_{26}, R_{29}, and R_{30} may each independently be selected from hydrogen, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and-$P(=O)(Q_8)(Q_9)$,
two or more neighboring groups selected from R_3, R_4, R_{21} to R_{23}, CY_3, and CY_4 may optionally be linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a3 and a4 may each independently be an integer from 0 to 5, and
R_3, R_4, R_{21} to R_{26}, R_{29}, and R_{30} may each be a deuterium-free substituent.

According to one or more embodiments, an organic light-emitting device includes:

a first electrode;
a second electrode; and
an organic layer disposed between the first electrode and the second electrode, wherein the organic layer includes an emission layer, and wherein the organic layer includes at least one organometallic compound or a composition containing the organometallic compound.

The organometallic compound may act as dopant in the organic layer.

BRIEF DESCRIPTION OF THE DRAWING

[0011] These and/or other aspects will become apparent and more readily appreciated from the following description of the embodiments, taken in conjunction with the FIGURE, which is a schematic view of an organic light-emitting device according to an embodiment.

DETAILED DESCRIPTION OF THE EMBODIMENTS

[0012] 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.

[0013] 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.

[0014] 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.

[0015] 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.

[0016] 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.

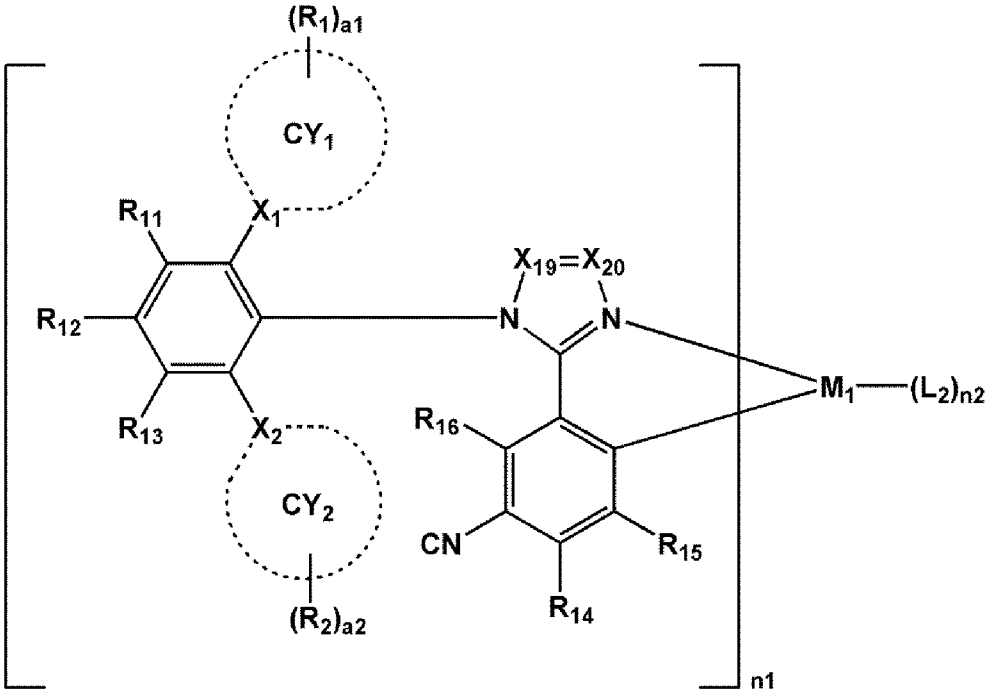
[0017] Unless otherwise defined, all terms (including technical and scientific terms) used herein have the same meaning as commonly understood by one of ordinary skill in the art to which this general inventive concept belongs. It will be further understood that terms, such as those defined in commonly 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.

[0018] 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.

[0019] "About" or "approximately" as used herein is inclusive of the stated value and means within an acceptable range of deviation for the particular value as determined by one of ordinary skill in the art, considering the measurement in question and the error associated with measurement of the particular quantity (i.e., the limitations of the measurement system). For example, "about" can mean within one or more standard deviations, or within ± 30%, 20%, 10%, 5% of the stated value.

[0020] An organometallic compound according to an embodiment is represented by Formula 1 below:

Formula 1

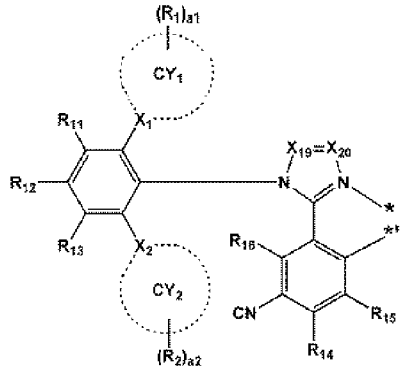


[0021] M_1 in Formula 1 may be selected from a first-row transition metal of the Periodic Table of Elements, a second-row transition metal of the Periodic Table of Elements, and a third-row transition metal of the Periodic Table of Elements.

[0022] For example, M_1 may be selected from iridium (Ir), platinum (Pt), osmium (Os), titanium (Ti), zirconium (Zr), hafnium (Hf), europium (Eu), terbium (Tb), thulium (Tm), and rhodium (Rh).

[0023] In an embodiment, M_1 may be iridium, but embodiments of the present disclosure are not limited thereto.

[0024] n1 in Formula 1 may be 1, 2, or 3, wherein, when n1 is two or more, two or more ligands represented by

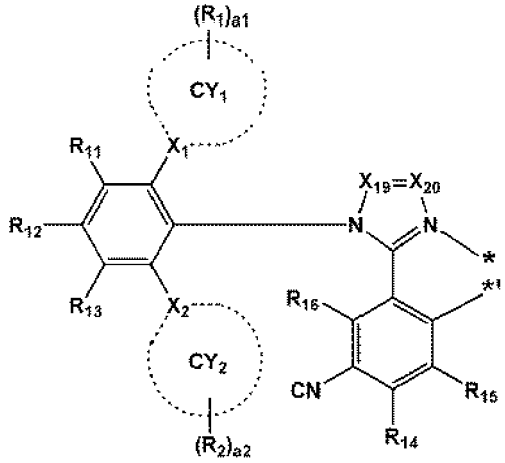


in Formula 1 (wherein * and *' each indicate a binding site to M_1 in Formula 1) may be identical to or different from each other, L_2 is a mono- or bidentate ligand as defined in the claims, and n2 may be 0, 1, 2, 3, or 4, wherein, when n2 is two or more, two or more groups L_2 may be identical to or different from each other. L_2 is the same as described below.

[0025] In an embodiment, in Formula 1, M_1 may be Ir or Os, and the sum of n1 and n2 may be 3 or 4; or M_1 may be Pt, and the sum of n1 and n2 may be 2.

[0026] In an embodiment, in Formula 1, M_1 may be Ir, n1 may be 3, and n2 may be 0, but embodiments of the present disclosure are not limited thereto.

[0027] In an embodiment, in Formula 1, M_1 may be Ir, n1 may be 3, n2 may be 0, and three ligands represented by



may be identical to or different from one another.

[0028] X_1 and X_2 in Formula 1 may each independently be carbon or nitrogen.

[0029] In an embodiment, X_1 and X_2 may each be carbon, but embodiments of the present disclosure are not limited thereto.

[0030] CY_1 and CY_2 in Formula 1 may each independently be a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group.

[0031] For example, CY_1 and CY_2 may each independently be selected from a cyclopentene group, a cyclohexene group, a benzene group, a pyridine group, a pyrimidine group, a pyridazine group, a pyrazine group, a triazine group, a pyrrole group, a pyrazole group, an imidazole group, a triazole group, an oxazole group, an isoxazole group, an oxadiazole group, a thiazole group, an isothiazole group, and a thiadiazole group.

[0032] In an embodiment, CY_1 and CY_2 may each independently be a benzene group, a pyridine group, or a pyrimidine group.

[0033] In one or more embodiments, CY_1 and CY_2 may each be a benzene group, but embodiments of the present disclosure are not limited thereto.

[0034] In Formula 1, X_{19} may be N or C(R_{19}), and X_{20} may be N or C(R_{20}), provided that at least one of X_{19} and X_{20} is N.

[0035] In an embodiment, one of X_{19} and X_{20} may be N.

[0036] In one or more embodiments, both X_{19} and X_{20} may be N at the same time.

[0037] For example, in Formula 1, X_{19} may be C(R_{19}), and X_{20} may be N.

[0038] In an embodiment, in Formula 1, X_{19} may be N, and X_{20} may be C(R_{20}).

[0039] R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} in Formula 1 may each independently be selected from hydrogen, deuterium, -F, -Cl, -Br, -I, -SF_5, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, -$N(Q_1)(Q_2)$, -$Si(Q_3)(Q_4)(Q_5)$, -$B(Q_6)(Q_7)$, and-$P(=O)(Q_8)(Q_9)$. Q_1 to Q_9 are each independently the same as described herein.

[0040] For example, R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} may each independently be selected from:

hydrogen, 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, -SF_5, a C_1-C20 alkyl group, and a C_1-C_{20} alkoxy group;

a C_1-C_{20} alkyl group and a C_1-C_{20} alkoxy group, each substituted with at least one selected from deuterium, -F, -Cl, -Br, -I, -CD_3, -CD_2H, -CDH_2,-CF_3, -CF_2H, -CFH_2, 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, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl

group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, and a pyrimidinyl group;

a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl 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 benzimidazolyl 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;

a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl 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 benzimidazolyl 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 deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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 cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl 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 benzimidazolyl 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

$-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and $-P(=O)(Q_8)(Q_9)$, and

Q_1 to Q_9 may each independently be selected from:

$-CH_3$, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CH_2CH_3$, $-CH_2CD_3$, $-CH_2CD_2H$,$-CH_2CDH_2$, $-CHDCH_3$, $-CHDCD_2H$, $-CHDCDH_2$, $-CHDCD_3$, $-CD_2CD_3$,$-CD_2CD_2H$, and $-CD_2CDH_2$;

an n-propyl group, an iso-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, a phenyl group, and a naphthyl group; and

an n-propyl group, an iso-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, a phenyl group, and a naphthyl group, each substituted with at least one selected from deuterium, a C_1-C_{10} alkyl group, and a phenyl group,

but embodiments of the present disclosure are not limited thereto.

[0041] In an embodiment, R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} may each independently be selected from:

hydrogen, deuterium, -F, a cyano group, a nitro group, $-SF_5$, a methyl group, an ethyl group, an n-propyl group, an

iso-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-decyl group, an iso-decyl group, a sec-decyl group, a tert-decyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group;

a methyl group, an ethyl group, an n-propyl group, an iso-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-decyl group, an iso-decyl group, a sec-decyl group, a tert-decyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group, each substituted with at least one selected from deuterium, -F, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, a cyano group, a nitro group, a C_1-C_{10} alkyl group, a C_1-C_{10} alkoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group; and

$-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and $-P(=O)(Q_8)(Q_9)$, and

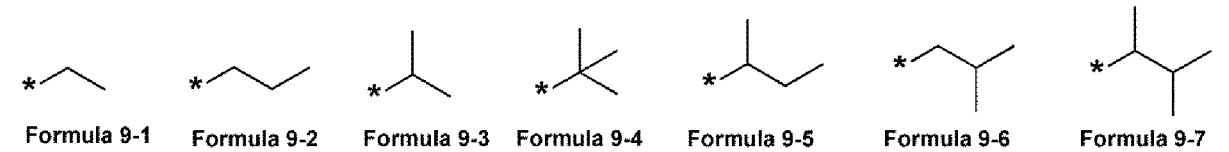
Q_1 to Q_9 are each independently the same as described herein.

[0042] In Formula 1, two or more neighboring groups selected from R_1, R_2, R_{11} to R_{13}, CY_1, and CY_2 may optionally be linked to form a C_5-C_{30} carbocyclic group unsubstituted or substituted with at least one R_{101} (for example, a 5-membered or 6-membered carbocyclic group unsubstituted or substituted with at least one R_{101}) or a C_2-C_{30} heterocyclic group unsubstituted or substituted with at least one R_{101} (for example, a 5-membered or 6-membered heterocyclic group unsubstituted or substituted with at least one R_{101}). R_{101} is the same as described in connection with R_1.

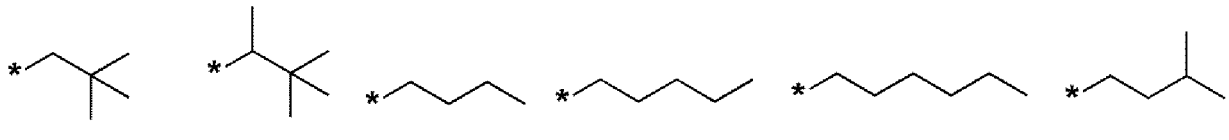
[0043] a1 and a2 in Formula 1 respectively indicate the number of groups R_1 and the number of groups R_2 and may each independently be an integer from 0 to 5.

[0044] For example, a1 and a2 may each independently be 0, 1, or 2, but embodiments of the present disclosure are not limited thereto.

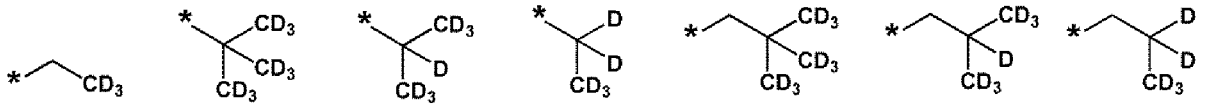
[0045] In an embodiment, R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} in Formula 1 may each independently be selected from hydrogen, deuterium, $-CH_3$, $-CD_3$, $-CD_2H$, $-CDH_2$,$-CH_2CH_3$, $-CH_2CD_3$, $-CH_2CD_2H$, $-CH_2CDH_2$, $-CHDCH_3$, $-CHDCD_2H$, $-CHDCDH_2$,$-CHDCD_3$, $-CD_2CD_3$, $-CD_2CD_2H$, $-CD_2CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, groups represented by Formulae 9-1 to 9-24, groups represented by Formulae 10-1 to 10-62, and-$Si(Q_3)(Q_4)(Q_5)$, but embodiments of the present disclosure are not limited thereto:



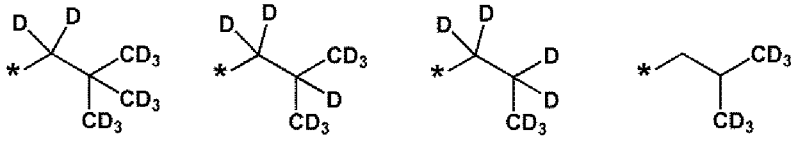
Formula 9-1 Formula 9-2 Formula 9-3 Formula 9-4 Formula 9-5 Formula 9-6 Formula 9-7



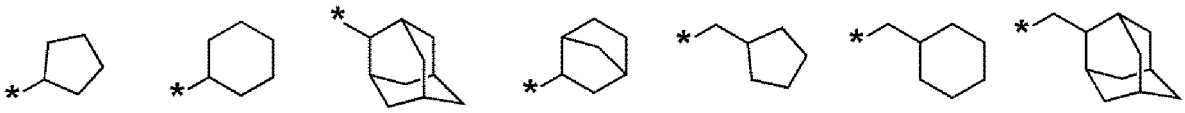
Formula 9-8 Formula 9-9 Formula 9-10 Formula 9-11 Formula 9-12 Formula 9-13



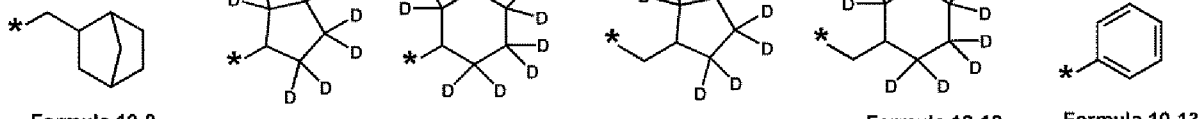
Formula 9-14 Formula 9-15 Formula 9-16 Formula 9-17 Formula 9-18 Formula 9-19 Formula 9-20



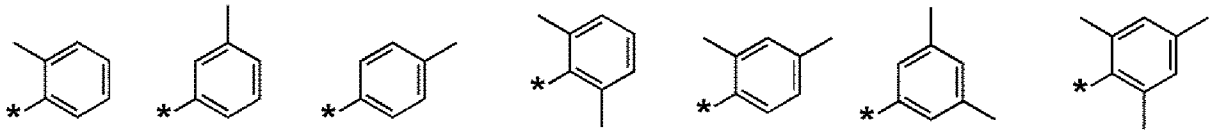
Formula 9-21 Formula 9-22 Formula 9-23 Formula 9-24



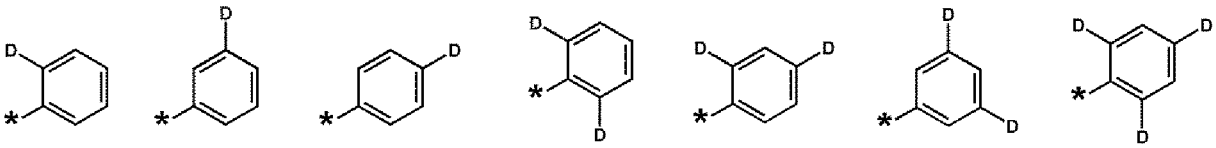
Formula 10-1 Formula 10-2 Formula 10-3 Formula 10-4 Formula 10-5 Formula10-6 Formula 10-7



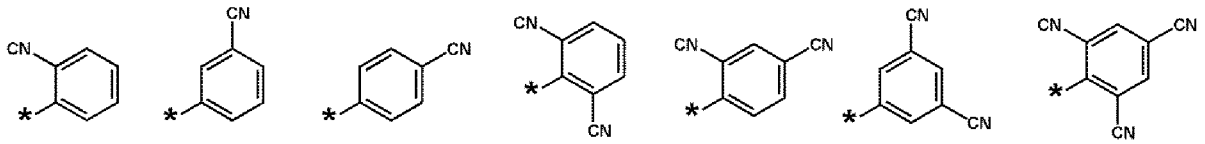
Formula 10-8 Formula 10-9 Formula 10-10 Formula 10-11 Formula 10-12 Formula 10-13



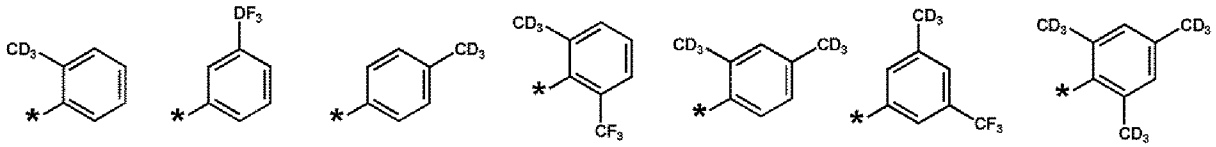
Formula 10-14 Formula 10-15 Formula 10-16 Formula 10-17 Formula 10-18 Formula 10-19 Formula 10-20



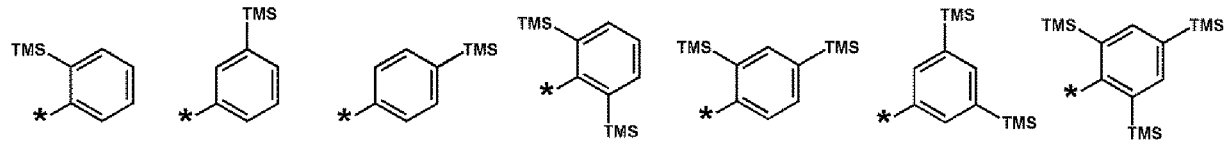
Formula 10-21 Formula 10-22 Formula 10-23 Formula 10-24 Formula 10-25 Formula 10-26 Formula 10-27



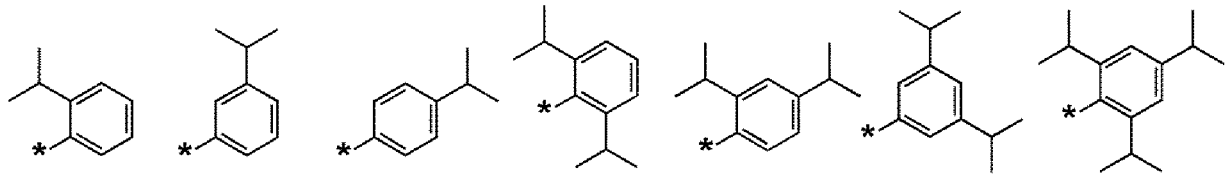
Formula 10-28 Formula 10-29 Formula 10-30 Formula 10-31 Formula 10-32 Formula 10-33 Formula 10-34



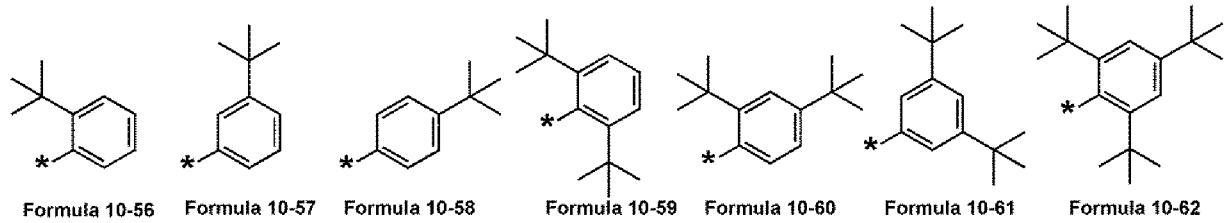
Formula 10-35 Formula 10-36 Formula 10-37 Formula 10-38 Formula 10-39 Formula 10-40 Formula 10-41



Formula 10-42 Formula 10-43 Formula 10-44 Formula 10-45 Formula 10-46 Formula 10-47 Formula 10-48



Formula 10-49 Formula 10-50 Formula 10-51 Formula 10-52 Formula 10-53 Formula 10-54 Formula 10-55



Formula 10-56 Formula 10-57 Formula 10-58 Formula 10-59 Formula 10-60 Formula 10-61 Formula 10-62

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* in Formulae 9-1 to 9-24 and 10-1 to 10-62 indicates a binding site to a neighboring atom.
In an embodiment, in Formula 1,

i) X_{19} may be $C(R_{19})$, X_{20} may be N, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{19} may be a deuterium-containing substituent;
ii) X_{19} may be N, X_{20} may be $C(R_{20})$, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{20} may be a deuterium-containing substituent; or
iii) X_{19} and X_{20} may each be N, and at least one of R_1, R_2, and R_{11} to R_{16} may be a deuterium-containing substituent, and

the deuterium-containing substituent may be selected from:

deuterium; and
a C_1-C_{20} alkyl group, a C_1-C_{20} alkoxy group, and a phenyl group, each substituted with at least one deuterium.

For example, the deuterium-containing substituent may be selected from:

deuterium; 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 deuterium.

In an embodiment, the deuterium-containing substituent may be selected from:

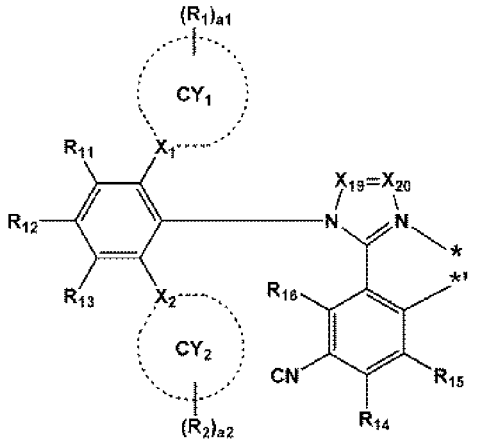
deuterium; and
a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, and a tert-butyl group, each substituted with at least one deuterium, but embodiments of the present disclosure are not limited thereto.

In an embodiment, the deuterium-containing substituent may be selected from:
-D, $-CH_2D$, $-CHD_2$, $-CD_3$, $-CH_2CH_2D$, $-CH_2CHD_2$, $-CH_2CD_3$, $-CHDCH_3$,$-CHDCH_2D$, $-CHDCHD_2$, $-CHDCD_3$, $-CD_2CH_3$, $-CD_2CH_2D$, $-CD_2CHD_2$,$-CD_2CD_3$, $-CH_2CH_2CH_2D$, $-CH_2CH_2CHD_2$, $-CH_2CH_2CD_3$, $-CH_2CHDCH_3$,$-CH_2CHDCH_2D$, $-CH_2CHDCHD_2$, $-CH_2CHDCD_3$, $-CH_2CD_2CH_3$,$-CH_2CD_2CH_2D$, $-CH_2CD_2CHD_2$, $-CH_2CD_2CD_3$,

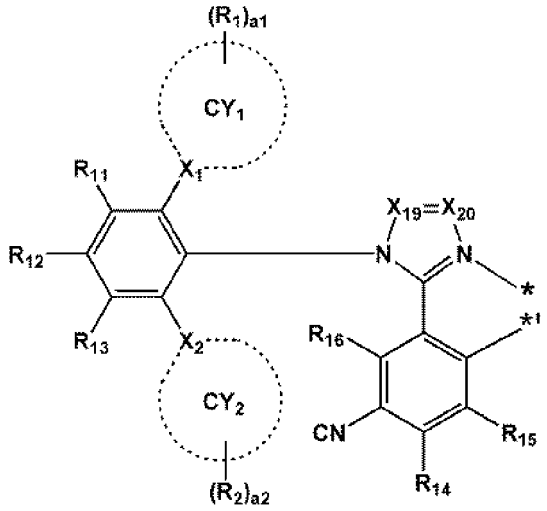
$-CHDCH_2CH_2D$,$-CHDCH_2CHD_2$, $-CHDCH_2CD_3$, $-CHDCHDCH_3$, $-CHDCHDCH_2D$,$-CHDCHDCHD_2$, $-CHDCHDCD_3$, $-CHDCD_2CH_3$, $-CHDCD_2CH_2D$,$-CHDCD_2CHD_2$, $-CHDCD_2CD_3$, $-CD_2CH_2CH_2D$, $-CD_2CH_2CHD_2$, $-CD_2CH_2CD_3$, $-CD_2CHDCH_3$, $-CD_2CHDCH_2D$, $-CD_2CHDCHD_2$, $-CD_2CHDCD_3$, $-CD_2CD_2CH_3$, $-CD_2CD_2CH_2D$, $-CD_2CD_2CHD_2$, $-CD_2CD_2CD_3$, $-CH(CH_3)(CH_2D)$,$-CH(CH_3)(CHD_2)$, $-CH(CH_2D)(CH_2D)$, $-CH(CH_3)(CD_3)$, $-CH(CHD_2)(CHD_2)$,$-CH(CH_2D)(CD_3)$, $-CH(CHD_2)(CD_3)$, $-CH(CD_3)_2$, $-CD(CH_3)_2$, $-CD(CH_3)(CH_2D)$, $-CD(CH_3)(CHD_2)$, $-CD(CH_2D)(CH_2D)$, $-CD(CH_3)(CD_3)$, $-CD(CHD_2)(CHD_2)$,$-CD(CH_2D)(CD_3)$, $-CD(CHD_2)(CD_3)$, $-CD(CD_3)_2$, and $-C(CD_3)_3$, but embodiments of the present disclosure are not limited thereto.

[0046] In an embodiment, the deuterium-containing substituent may be selected from deuterium, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CH_2CD_3$, $-CH_2CD_2H$, $-CH_2CDH_2$, $-CHDCH_3$,$-CHDCD_2H$, $-CHDCDH_2$, $-CHDCD_3$, $-CD_2CD_3$, $-CD_2CD_2H$, $-CD_2CDH_2$, and groups represented by Formulae 9-14 to 9-24, but embodiments of the present disclosure are not limited thereto.

[0047] In an embodiment, a ligand represented by



in Formula 1 (wherein * and *' each indicate a binding site to M_1 in Formula 1) may include at least one deuterium. Whether the ligand represented by



includes deuterium may be confirmed by analyzing the organometallic compound represented by Formula 1 through a ^1H NMR spectrum or analyzing a molecular weight of the organometallic compound by using a molecular weight measurement apparatus such as matrix-assisted laser desorption/ionization (MALDI) apparatus.

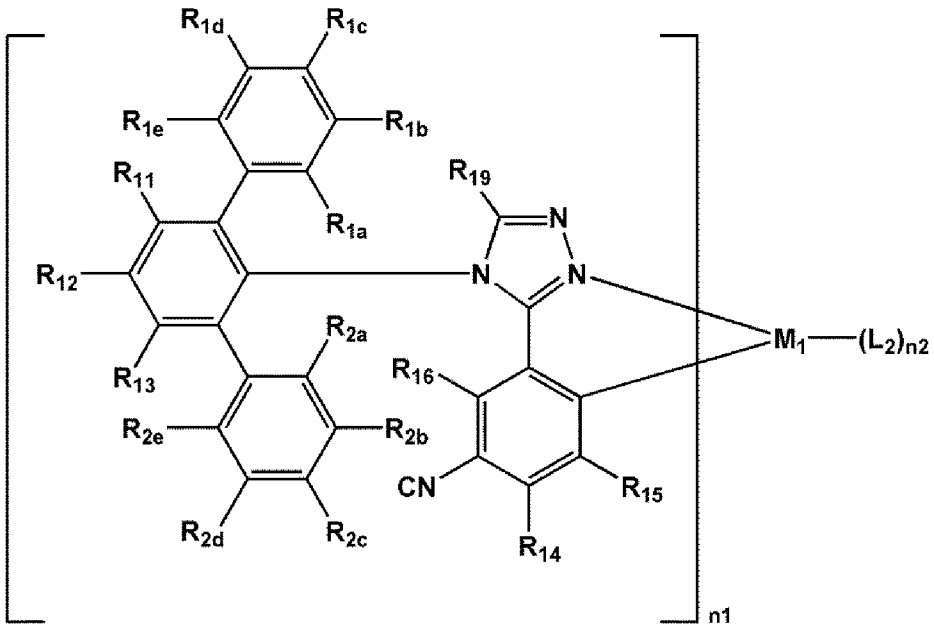
[0048] A compound, which has the same backbone as the organometallic compound represented by Formula 1 but does not include deuterium (hereinafter, referred to as a "first standard compound"), is prepared. A ^1H NMR spectrum of the first standard compound and a ^1H NMR spectrum of the organometallic compound represented by Formula 1 are obtained. Then, the number of hydrogens that are substituted with deuterium among hydrogens bonded at a specific position (specific carbon) of the organometallic compound represented by Formula 1 may be calculated by comparing integral values of signals of specific chemical shift (parts per million, ppm) selected from the measured spectrum.

[0049] Alternatively, a compound, which has the same backbone as the organometallic compound represented by Formula 1 and in which all hydrogens of the organometallic compound represented by Formula 1 are substituted with deuterium (hereinafter, referred to as a "second standard compound"), is assumed. The number of hydrogens that are substituted with deuterium among hydrogens of the organometallic compound represented by Formula 1 may be calculated by comparing a calculated molecular weight of the second standard compound with a molecular weight of the organometallic compound represented by Formula 1.

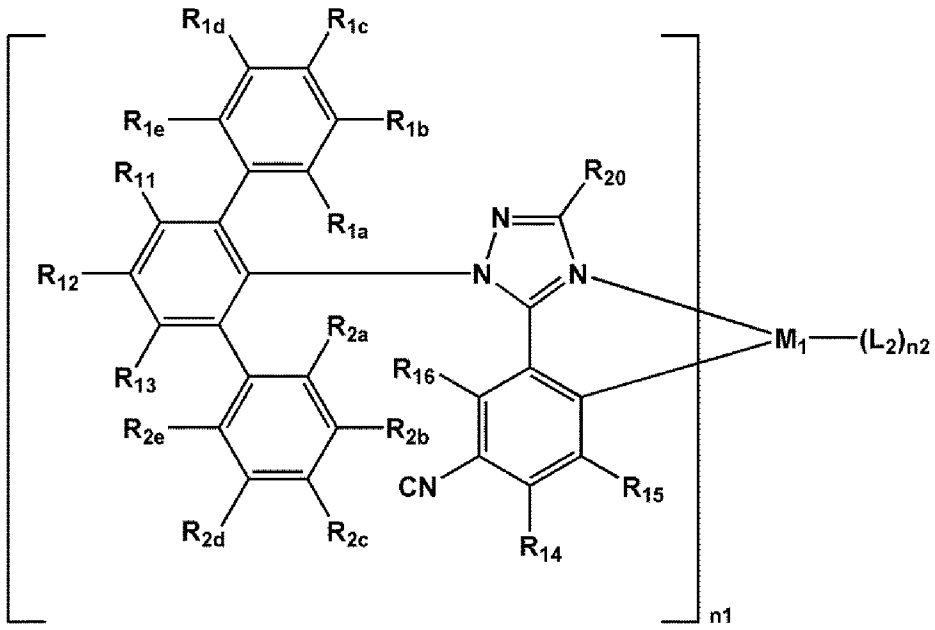
[0050] In one or more embodiments, in Formula 1, i) X_{19} may be $C(R_{19})$, X_{20} may be N, and at least one of R_{12}, R_{14}, and R_{19} may be a deuterium-containing substituent; ii) X_{19} may be N, X_{20} may be $C(R_{20})$, and at least one of R_{12}, R_{14}, and R_{20} may be a deuterium-containing substituent; or iii) X_{19} and X_{20} may each be N, and at least one of R_{12} and R_{14} may be a deuterium-containing substituent, wherein the deuterium-containing substituent is the same as described herein.

[0051] In an embodiment, the organometallic compound represented by Formula 1 may be represented by one of Formulae 1-1 to 1-3:

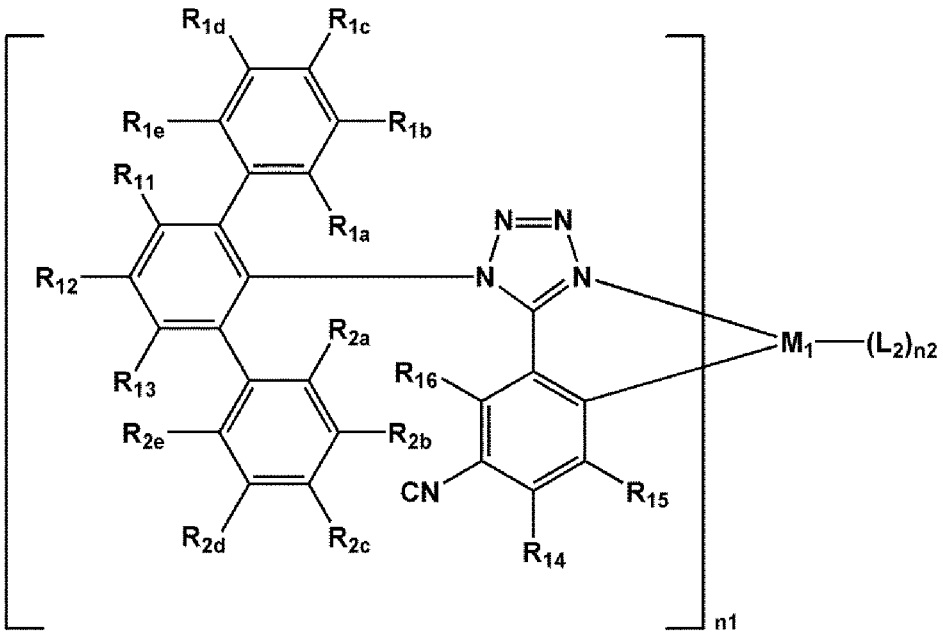
Formula 1-1



Formula 1-2



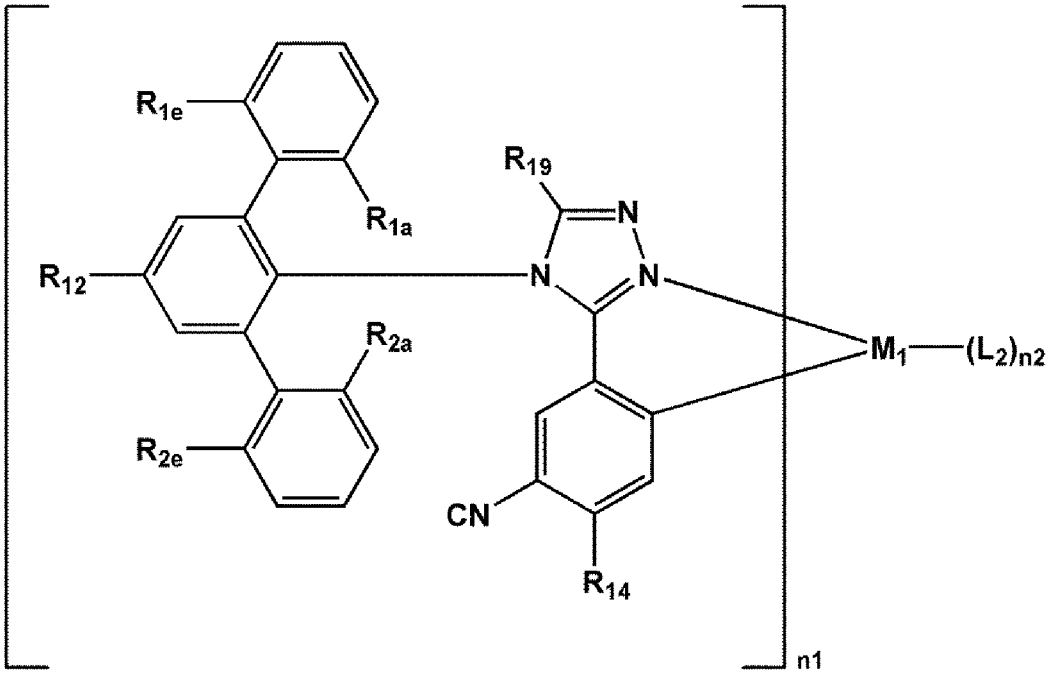
Formula 1-3



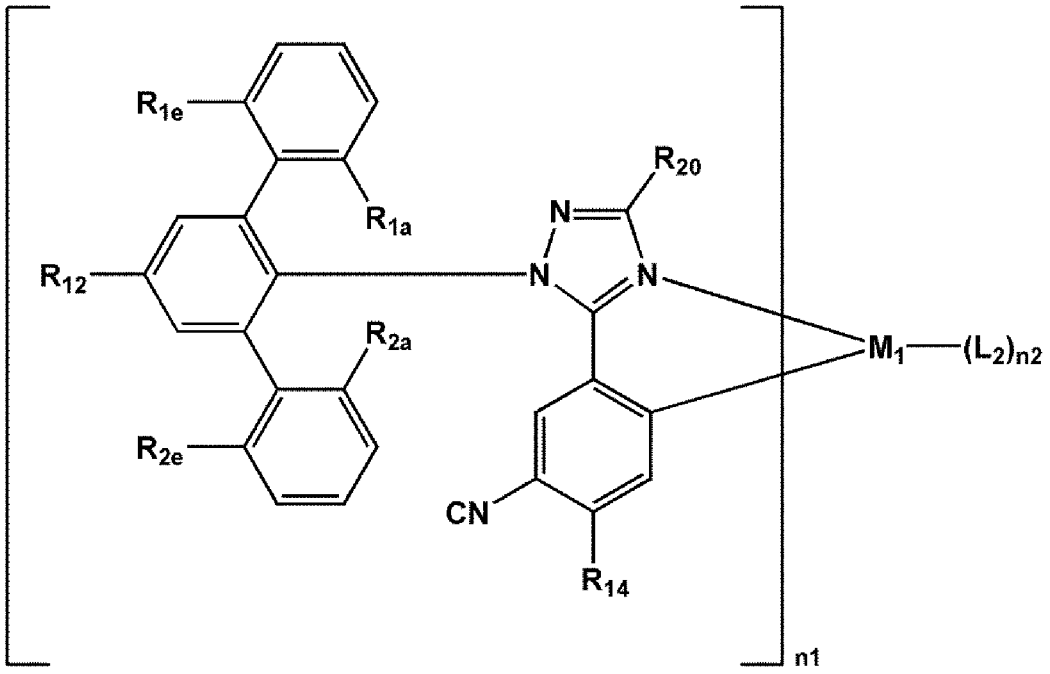
[0052] In Formulae 1-1 to 1-3, M_1, n1, L_2, n2, R_{11} to R_{16}, R_{19}, and R_{20} are each independently the same as described herein, R_{1a} to R_{1e} are each independently the same as described in connection with R_1, and R_{2a} to R_{2e} are each independently the same as described in connection with R_2.

[0053] In an embodiment, the organometallic compound represented by Formula 1 may be represented by one of Formulae 1(1) to 1(3):

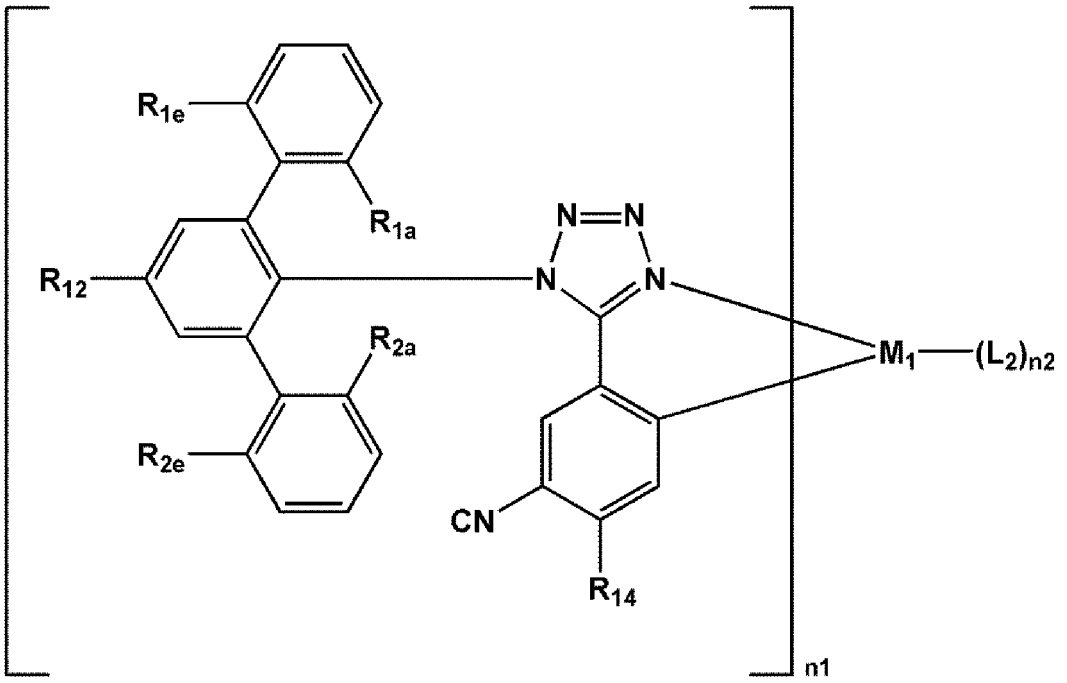
Formula 1(1)



Formula 1(2)



Formula 1(3)



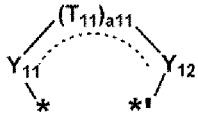
[0054] In Formulae 1(1) to 1(3), M_1, n1, L_2, n2, R_{12}, R_{14}, R_{19}, and R_{20} are each independently the same as described herein, R_{1a} and R_{1e} are each independently the same as described in connection with R_1, and R_{2a} and R_{2e} are each independently the same as described in connection with R_2.

[0055] L_2 in Formula 1 may be a monodentate ligand or a bidentate ligand.

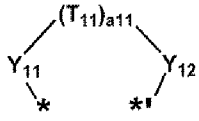
[0056] For example, in Formula 1, L_2 may be a monodentate ligand, and L_2 may be selected from I^-, Br^-, Cl^-, sulfide, nitrate, azide, hydroxide, cyanate, isocyanate, thiocyanate, water, acetonitrile, pyridine, ammonia, carbon monoxide, $P(Ph)_3$, $P(Ph)_2CH_3$, $PPh(CH_3)_2$, and $P(CH_3)_3$, but embodiments of the present disclosure are not limited thereto.

[0057] In an embodiment, in Formula 1, L_2 may be a bidentate ligand, and L_2 may be selected from oxalate, acetylacetonate, a picolinic acid, 1,2-bis(diphenylphosphino)ethane, 1,1-bis(diphenylphosphino)methane, glycinate, and ethylenediamine, but embodiments of the present disclosure are not limited thereto.

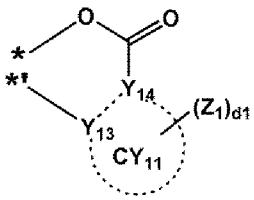
[0058] In an embodiment, L_2 in Formula 1 may be selected from ligands represented by Formulae 3A to 3F:



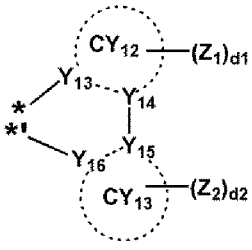
Formula 3A



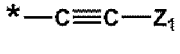
Formula 3B



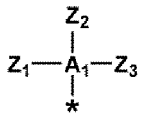
Formula 3C



Formula 3D



Formula 3E



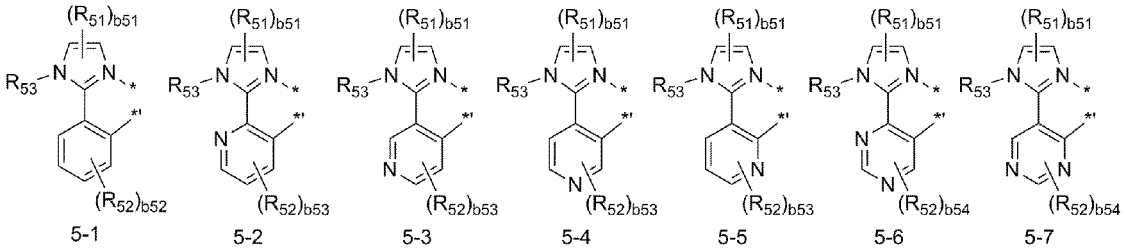
Formula 3F

In Formulae 3A to 3F,

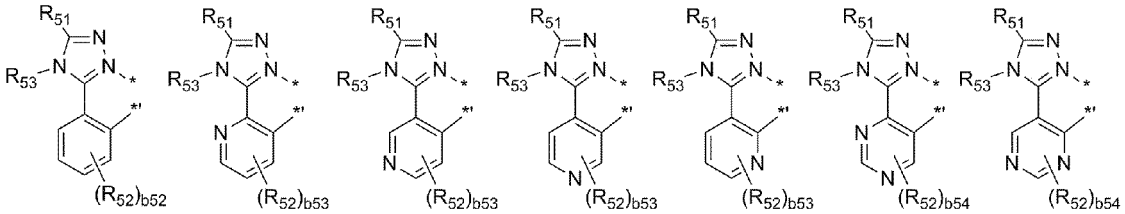
Y_{11} may be selected from O, N, $N(Z_1)$, $P(Z_1)(Z_2)$, and $As(Z_1)(Z_2)$,
Y_{12} may be selected from O, N, $N(Z_3)$, $P(Z_3)(Z_4)$, and $As(Z_3)(Z_4)$,
CY_{11} may be a C_2-C_{30} heterocyclic group (for example, a pyridine group, a pyrimidine group, a quinoline group, an isoquinoline group, a quinoxaline group, a carbazole group, or the like),
T_{11} may each independently be selected from a single bond, a double bond, *-$C(Z_{11})(Z_{12})$-*', *-$C(Z_{11})$=$C(Z_{12})$-*', *=$C(Z_{11})$-*', *-$C(Z_{11})$=*', *=$C(Z_{11})$-$C(Z_{12})$=$C(Z_{13})$-*', *-$C(Z_{11})$=$C(Z_{12})$-$C(Z_{13})$=*', *-$N(Z_{11})$-*', and a substituted or unsubstituted C_5-C_{30} carbocyclic group,
a11 may be an integer from 1 to 10,
Y_{13} to Y_{16} may each independently be carbon (C) or nitrogen (N), Y_{13} and Y_{14} may be linked via a single bond or a double bond, and Y_{15} and Y_{16} may be linked via a single bond or a double bond,
CY_{12} and CY_{13} may each independently be a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group (for example, a benzene group, a naphthalene group, a fluorene group, a dibenzofuran group, a dibenzothiophene group, a pyrazole group, an imidazole group, a triazole group, a tetrazole group, a pyridine group, a pyrimidine group, a quinoline group, an isoquinoline group, a quinoxaline group, a carbazole group, or the like),
A_1 may be P or As,
Z_1 to Z_4 and Z_{11} to Z_{13} may each independently be selected from hydrogen, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, -$N(Q_1)(Q_2)$, -$Si(Q_3)(Q_4)(Q_5)$, -$B(Q_6)(Q_7)$, and-$P(=O)(Q_8)(Q_9)$,
Q_1 to Q_9 may each be independently selected from hydrogen, 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} aryl group substituted with at least one selected from a C_1-C_{60} alkyl group and 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group,

d1 and d2 may each independently be an integer from 0 to 10, and
* and *' each indicate a binding site to M_1 in Formula 1.

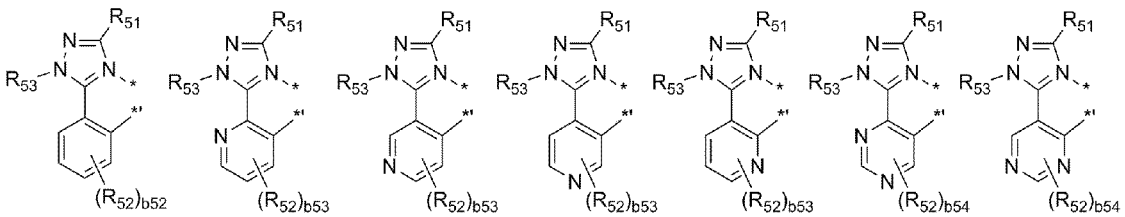
[0059] In an embodiment, L_2 in Formula 1 may be represented by one of Formulae 5-1 to 5-119, but embodiments of the present disclosure are not limited thereto:



5-1 5-2 5-3 5-4 5-5 5-6 5-7



5-8 5-9 5-10 5-11 5-12 5-13 5-14



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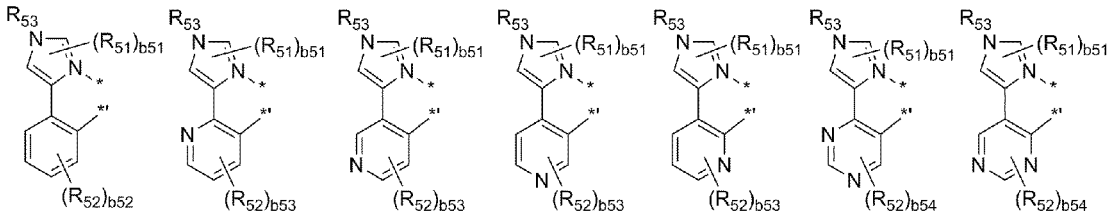

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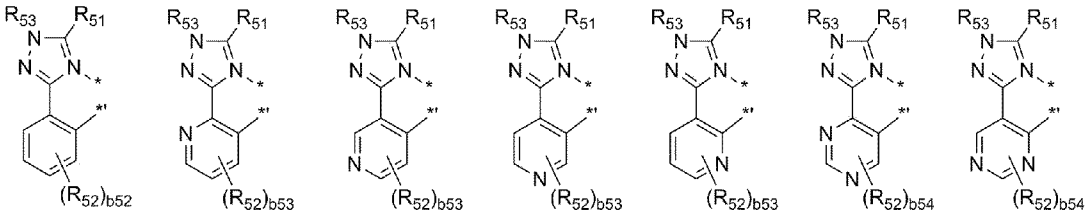

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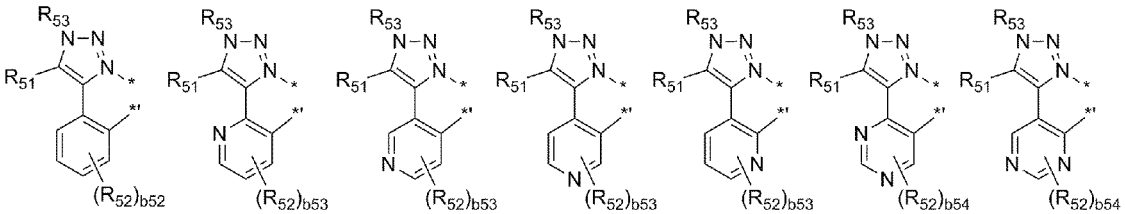

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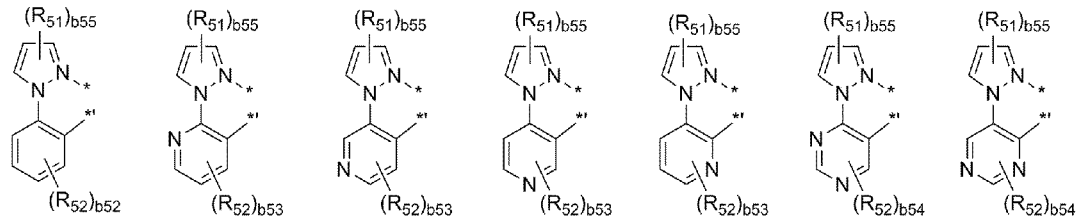

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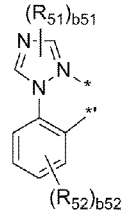
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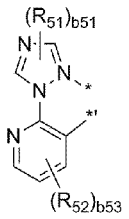
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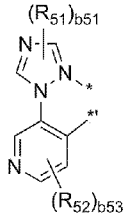
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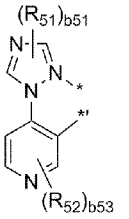
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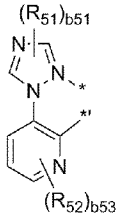
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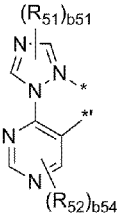
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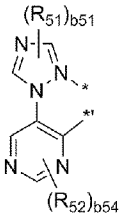
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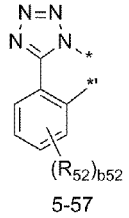
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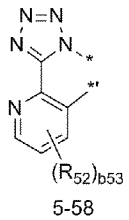
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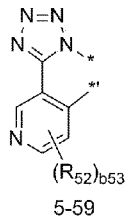
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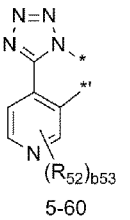
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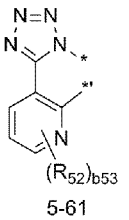
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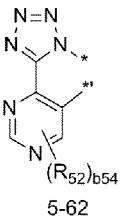
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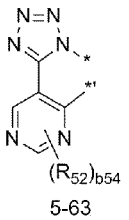
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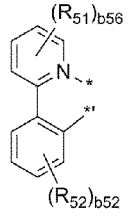
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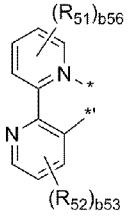
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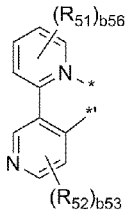
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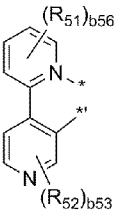
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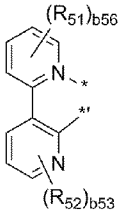
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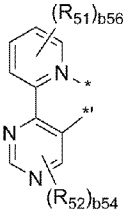
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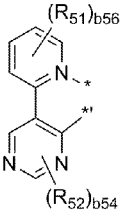
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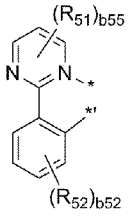
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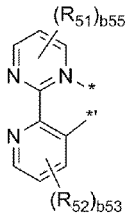
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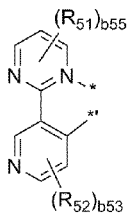
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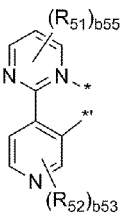
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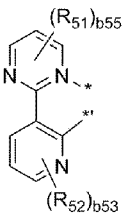
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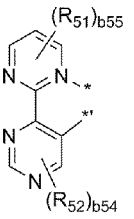
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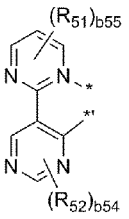
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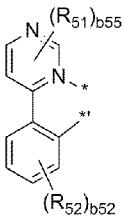
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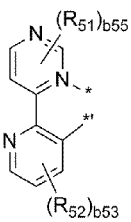
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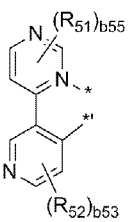
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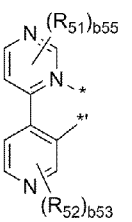
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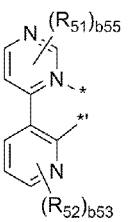
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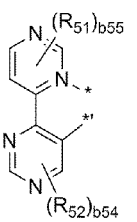
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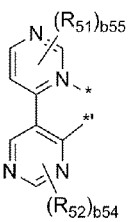
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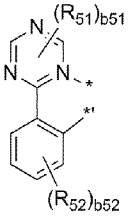
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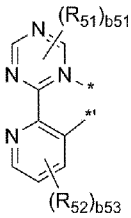
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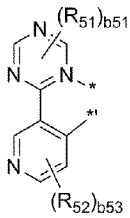
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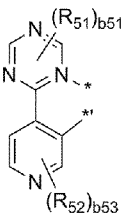
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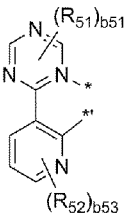
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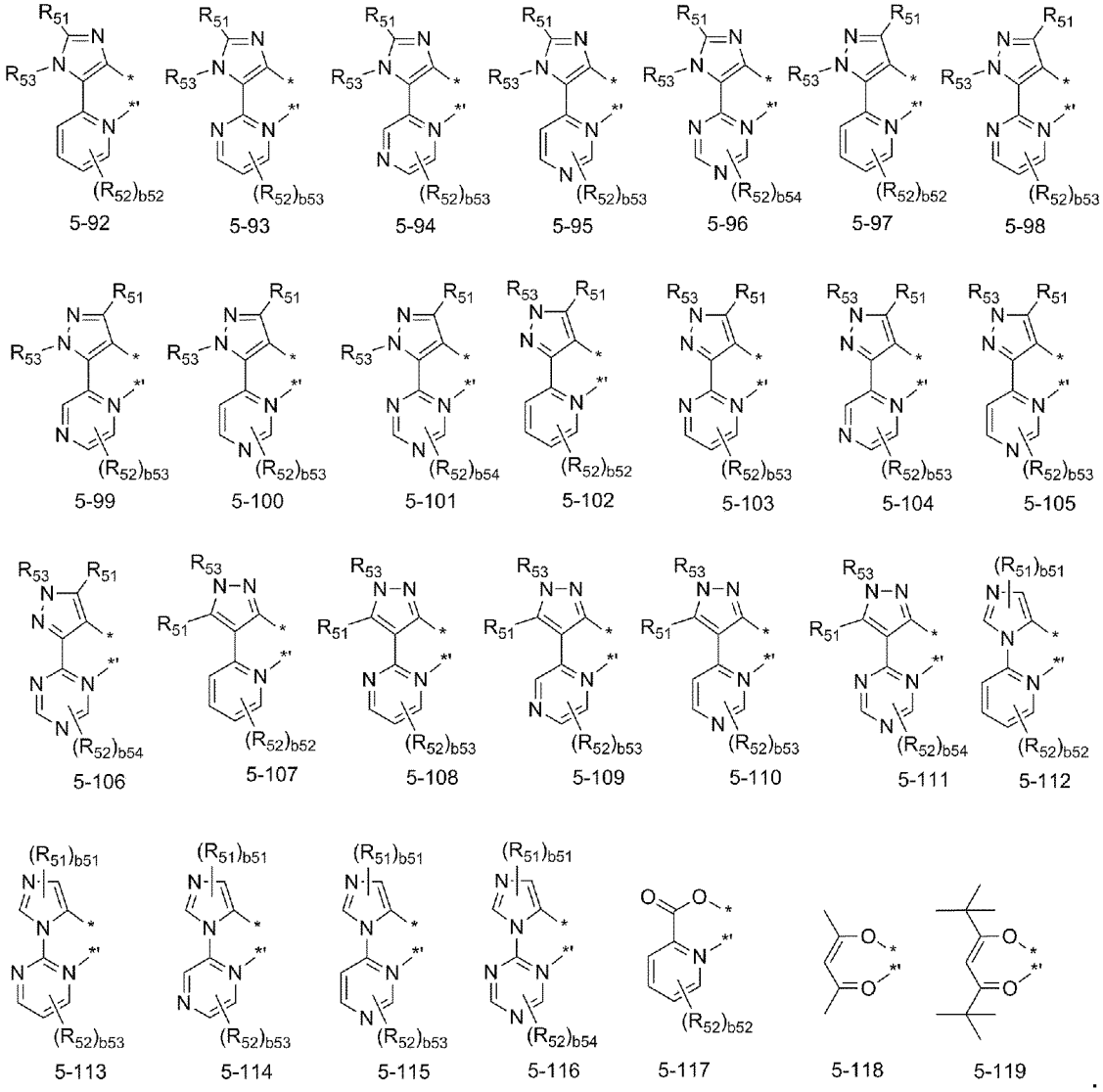


In Formulae 5-1 to 5-119,

R_{51} to R_{53} may each independently be selected from:

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

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, and a nitro group,

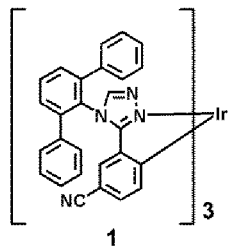
b51 and b54 may each independently be 1 or 2,

b53 and b55 may each independently be an integer from 1 to 3,

b52 may be an integer from 1 to 4, and
* and *' each indicate a binding site to M_1 in Formula 1.

[0060] The organometallic compound represented by Formula 1 is neutral and may not have a salt form including an anion and a cation.

[0061] The organometallic compound represented by Formula 1 may be selected from Compounds 1 to 10, but embodiments of the present disclosure are not limited thereto:



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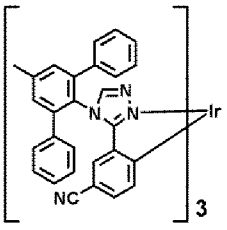

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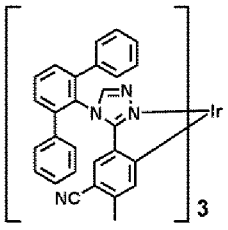

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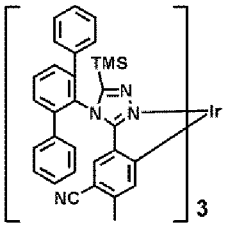

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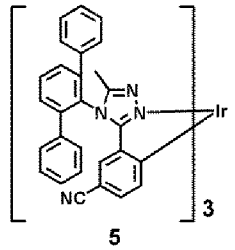

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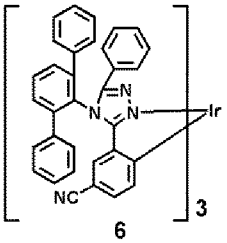

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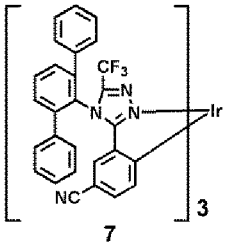

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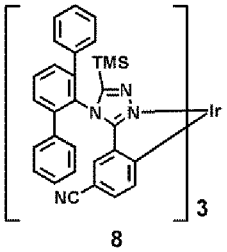

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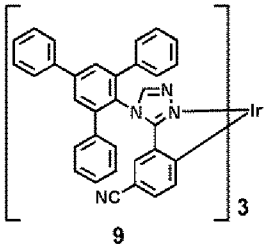

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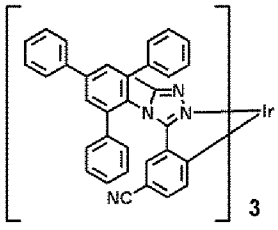


10

.

[0062] A maximum emission wavelength (experimental value) of the organometallic compound may be in a range of about 440 nanometers (nm) to about 465 nm, for example, about 440 nm to about 460 nm. When the maximum emission wavelength is in a range of about 440 nm to about 465 nm, an organic light-emitting device emitting deep blue light may be provided.

[0063] The organometallic compound represented by Formula 1 essentially includes CY_1 and CY_2 at positions defined herein.

[0064] Thus, the organometallic compound may have a natural population analysis (NPA) charge value of about 0.6 or less, for example, about 0.4 to about 0.55. The NPA charge value is evaluated by a density functional theory (DFT) method using a Gaussian program that is structurally optimized at a level of B3LYP/6-31G(d,p), and NPA charge values of Compounds 1 to 10 are shown in Table 1:

Table 1

Compound No.	NPA charge value
1	0.48
2	0.45
3	0.47

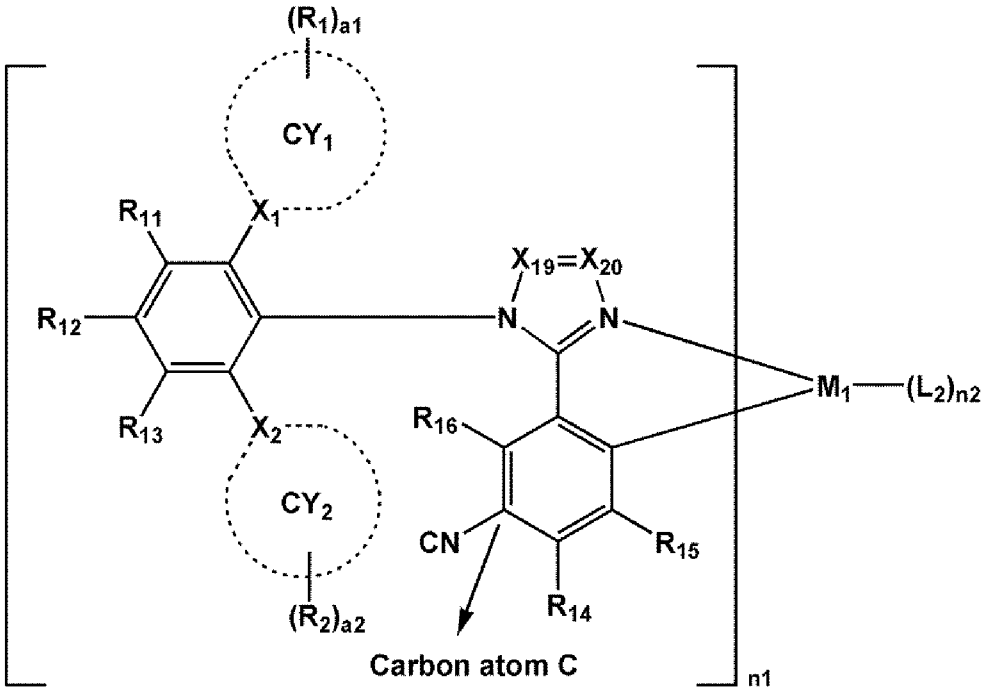
(continued)

Compound No.	NPA charge value
4	0.51
5	0.47
6	0.47
7	0.48
8	0.51
9	0.46
10	0.47

[0065] Since the organometallic compound having the NPA charge value in the above-described range has excellent heat resistance and/or decomposition resistance, an electronic device, for example, an organic light-emitting device, which includes the organometallic compound, may have a long lifespan.

[0066] On the other hand, a "carbon atom C" in Formula 1 is essentially bonded to a cyano group (see Formula 1'). Thus, since the organometallic compound represented by Formula 1 has a deep highest occupied molecular orbital (HOMO) energy level (that is, a low HOMO energy level or a large absolute value of a HOMO energy level), the organometallic compound may have a high triplet energy level. Therefore, the use of the organometallic compound represented by Formula 1 may make it possible to emit deep blue light having excellent color purity.

Formula 1'



[0067] Also, in one or more embodiments, the organometallic compound represented by Formula 1 may include at least one deuterium. Compared with a single bond between carbon and hydrogen, a single bond between carbon and deuterium has a stronger bond strength and a shorter bond length. Thus, the deuterium-containing organometallic compound may have higher thermal stability than the deuterium-free organometallic compound. Therefore, radicalization of the organometallic compound represented by Formula 1 slowly progresses due to heat and/or electric field generated when the organic light-emitting device is kept and/or driven, and thus, an organic light-emitting device including the organometallic compound may have a longer lifespan.

[0068] Furthermore, in one or more embodiments, R_{14} in Formula 1 may not be hydrogen, or may be, for example, a

deuterium-containing substituent. The organometallic compound represented by Formula 1 may have a high lowest unoccupied molecular orbital (LUMO) energy level and a high triplet (T_1) energy level. Thus, the use of the organometallic compound represented by Formula 1 may make it possible to emit blue light having excellent color purity.

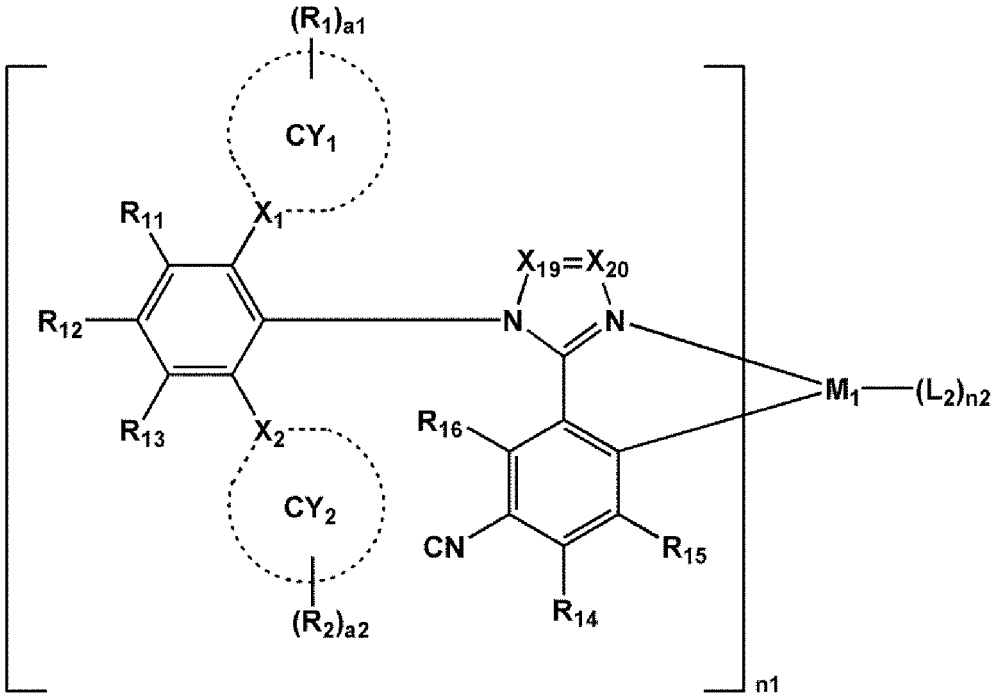
[0069] HOMO energy levels, LUMO energy levels, T_1 energy levels, emission wavelengths and maximum emission wavelengths (λ_{max}) of some of the organometallic compounds represented by Formula 1 were evaluated by using a Gaussian 09 program for optimizing a molecular structure through DFT based on B3LYP. Evaluation results thereof are shown in Table 2.

Table 2

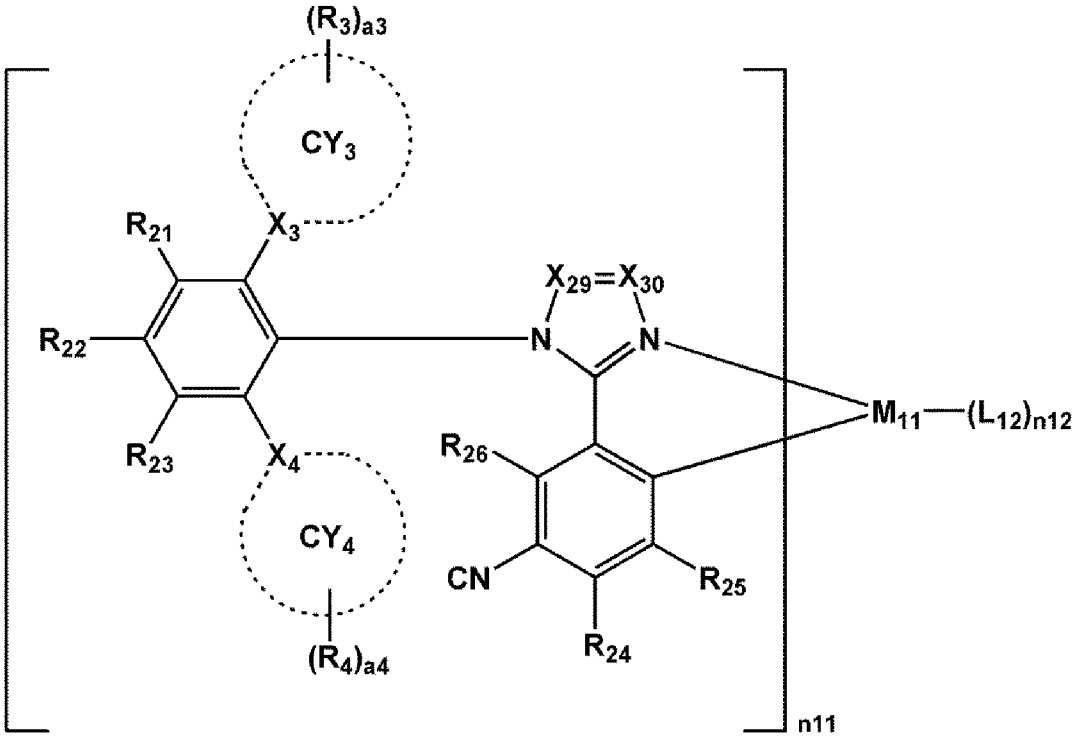
Compound No.	HOMO (e V)	LUMO (eV)	T_1 (eV)	emission wavelength(s) (nm)
1	-5.40	-1.40	2.73	467(λ_{max}), 492
2	-5.35	-1.31	2.74	465(λ_{max}), 492
3	-5.30	-1.31	2.77	460(λ_{max}), 484
4	-5.28	-1.25	2.78	453(λ_{max}), 480
5	-5.28	-1.33	2.70	470(λ_{max}), 497
6	-5.36	-1.52	2.63	478(λ_{max}), 509
7	-5.81	-1.77	2.75	458(λ_{max})
8	-5.38	-1.34	2.75	457(λ_{max}), 486
9	-5.37	-1.50	2.73	468(λ_{max}), 492
10	-5.25	-1.45	2.70	471(λ_{max}), 497

[0070] On the other hand, in synthesizing an organometallic compound that is represented by Formula 1 but includes at least one deuterium, if at least one of the organometallic compound is deuterated, an organometallic compound in which hydrogen is not substituted with deuterium (that is, an organometallic compound represented by Formula 2 as follows) may also be synthesized, simultaneously. Thus, a composition containing the organometallic compound, which includes organometallic compound represented by Formula 1 and includes at least one deuterium (hereinafter, a "first organometallic compound") and further includes an organometallic compound represented by Formula 2 (hereinafter, a "second organometallic compound"), may be provided:

Formula 1



Formula 2



In Formulae 1 and 2,

M_1 and M_{11} may each independently be selected from a first-row transition metal of the Periodic Table of Elements, a second-row transition metal of the Periodic Table of Elements, and a third-row transition metal of the Periodic Table of Elements,
n1 and n11 may each independently be 1, 2, or 3,
L_2 and L_{12} may each independently be a monodentate ligand or a bidentate ligand as defined in the claims,
n2 and n12 may each independently be 0, 1, 2, 3, or 4, wherein, when n2 is two or more, two or more groups L_2 may be identical to or different from each other, and when n12 is two or more, two or more groups L_{12} may be identical to or different from each other,
X_1 to X_4 may each independently be carbon or nitrogen,
CY_1 to CY_4 may each independently be a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group,
X_{19} may be N or C(R_{19}), and X_{20} may be N or C(R_{20}), provided that at least one of X_{19} and X_{20} is N,
X_{29} may be N or C(R_{29}), and X_{30} may be N or C(R_{30}), provided that at least one of X_{29} and X_{30} is N,
R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} may each independently be selected from hydrogen, deuterium, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, -N(Q_1)(Q_2), -Si(Q_3)(Q_4)(Q_5), -B(Q_6)(Q_7), and-P(=O)(Q_8)(Q_9),
two or more neighboring groups selected from R_1, R_2, R_{11} to R_{13}, CY_1, and CY_2 may optionally be linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a1 and a2 may each independently be an integer from 0 to 5,
i) X_{19} may be C(R_{19}), X_{20} may be N, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{19} may be a deuterium-containing substituent; ii) X_{19} may be N, X_{20} may be C(R_{20}), and at least one of R_1, R_2, R_{11} to R_{16}, and R_{20} may be a deuterium-containing substituent; or iii) X_{19} and X_{20} may each be N, and at least one of R_1, R_2, and R_{11} to R_{16} may be a deuterium-containing substituent,
R_3, R_4, R_{21} to R_{26}, R_{29}, and R_{30} may each independently be selected from hydrogen, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, -N(Q_1)(Q_2), -Si(Q_3)(Q_4)(Q_5), -B(Q_6)(Q_7), and-P(=O)(Q_8)(Q_9),
two or more neighboring groups selected from R_3, R_4, R_{21} to R_{23}, CY_3, and CY_4 may optionally be linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a3 and a4 may each independently be an integer from 0 to 5, and
R_3, R_4, R_{21} to R_{26}, R_{29}, and R_{30} may each be a deuterium-free substituent.

[0071] Descriptions for the first organometallic compound are the same as described in Formula 1, except that at least one deuterium is included therein and descriptions for the second organometallic compound are the same as described in Formula 1, except that deuterium is not included therein.

[0072] A deuteration rate of the composition containing the organometallic compound may be about 50% or more. The deuteration rate may be calculated by using Equation 2:

Equation 2

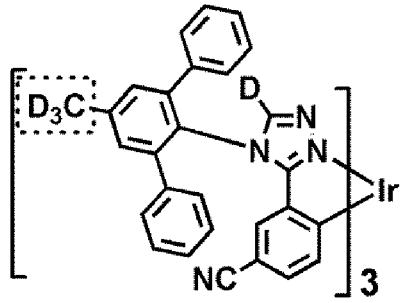
$$\text{deuteration rate (\%)} = n_{D2}/(n_{H2} + n_{D2}) \times 100.$$

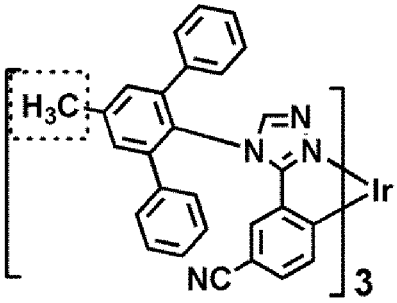
In Equation 2,

n_{H2} represents the sum of a total number of hydrogens included in the deuterium-containing substituents in the first organometallic compound and a total number of hydrogens included in the deuterium-free substituent of the second organometallic compound corresponding to the deuterium-containing substituent in the first organometallic compound, and

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

[0073] When a substituent indicated by a dashed box in the left compound of the following compounds is a deuterium-containing substituent, a deuterium-free substituent corresponding to the deuterium-containing substituent in the right compound may mean a substituent indicated by a dashed box in the right compound. That is, in the present disclosure, substituents bonded to carbon at the same position in two compounds that differ from each other only in terms of the presence or absence of isotope are defined as "corresponding" substituents.





[0074] For example, if the first organometallic compound includes two deuterium-containing substituents, n_{D2} means the total number of deuterium atoms included in the two deuterium-containing substituents. Also, n_{H2} means the sum of the number of hydrogens included in the two deuterium-containing substituents and the number of hydrogens included in the deuterium-free substituent of the second organometallic compound corresponding to the two deuterium-containing substituents.

[0075] In an embodiment, the deuteration rate may be about 70% or more, about 90% or more, about 95% or more, about 96% or more, about 97% or more, about 98% or more, or about 99% or more, but embodiments of the present disclosure are not limited thereto.

[0076] Synthesis methods of the organometallic compound represented by Formula 1 may be recognizable by one of ordinary skill in the art by referring to Synthesis Examples provided below.

[0077] The composition containing the organometallic compound including the first organometallic compound and the second organometallic compound may be obtained by an incomplete deuteration in synthesizing the first organometallic compound, not by mixing the first organometallic compound and the second organometallic compound.

[0078] Synthesis methods of the organometallic compound represented by Formula 1 may be recognizable by one of ordinary skill in the art by referring to Synthesis Examples provided below.

[0079] The organometallic compound represented by Formula 1 or a composition including the organometallic compound may be suitable for use in an organic layer of an organic light-emitting device, for example, for use as a dopant in an emission layer of the organic layer. Thus, another aspect of the present description provides an organic light-emitting device that includes:

a first electrode;
a second electrode; and
an organic layer disposed between the first electrode and the second electrode, wherein the organic layer includes an emission layer and at least one of the organometallic compound represented by Formula 1.

[0080] The organic light-emitting device may have, due to the inclusion of an organic layer including the organometallic compound represented by Formula 1 or the composition including the organometallic compound, high efficiency, a long

lifespan, and a high color purity.

[0081] The organometallic compound of Formula 1 or the composition including the organometallic compound may be used between a pair of electrodes of an organic light-emitting device. For example, the organometallic compound represented by Formula 1 or the composition including the organometallic compound may be included in the emission layer. In this embodiment, the organometallic compound or the composition including the organometallic compound may act as a dopant, and the emission layer may further include a host (that is, an amount of the organometallic compound represented by Formula 1 or the composition including the organometallic compound is smaller than an amount of the host). In this embodiment, the dopant may emit blue light.

[0082] The expression "(an organic layer) includes at least one of organometallic compounds" as used herein may include an embodiment in which "(an organic layer) includes identical organometallic compounds represented by Formula 1" and an embodiment in which "(an organic layer) includes two or more different organometallic compounds represented by Formula 1."

[0083] For example, the organic layer may include, as the organometallic compound, only Compound 1. In this regard, Compound 1 may be included in an emission layer of the organic light-emitting device. In one or more embodiments, the organic layer may include, as the organometallic compound, Compound 1 and Compound 2. In this embodiment, Compound 1 and Compound 2 may be included in an identical layer (for example, Compound 1 and Compound 2 may both be included in an emission layer).

[0084] The first electrode may be an anode, which is a hole injection electrode, and the second electrode may be a cathode, which is an electron injection electrode; or the first electrode may be a cathode, which is an electron injection electrode, and the second electrode may be an anode, which is a hole injection electrode.

[0085] In an embodiment, in the organic light-emitting device, the first electrode is an anode, and the second electrode is a cathode, and the organic layer further includes a hole transport region disposed between the first electrode and the emission layer and an electron transport region disposed between the emission layer and the second electrode, and the hole transport region includes a hole injection layer, a hole transport layer, an electron blocking layer, a buffer layer or any combination thereof and the electron transport region includes a hole blocking layer, an electron transport layer, an electron injection layer or any combination thereof.

[0086] The term "organic layer" as used herein refers to a single layer and/or a plurality of layers disposed between the first electrode and the second electrode of the organic light-emitting device. The "organic layer" may include, in addition to an organic compound, an organometallic complex including metal.

[0087] The FIGURE is a schematic view of an organic light-emitting device 10 according to an embodiment. Hereinafter, the structure of an organic light-emitting device according to an embodiment and a method of manufacturing an organic light-emitting device according to an embodiment will be described in connection with the FIGURE. The organic light-emitting device 10 includes a first electrode 11, an organic layer 15, and a second electrode 19, which are sequentially stacked.

[0088] A substrate may be additionally disposed under the first electrode 11 or above the second electrode 19. For use as the substrate, any substrate that is used in general organic light-emitting devices may be used, and the substrate may be a glass substrate or a transparent plastic substrate, each having excellent mechanical strength, thermal stability, transparency, surface smoothness, ease of handling, and water resistance.

[0089] The first electrode 11 may be formed by depositing or sputtering a material for forming the first electrode 11 on the substrate. The first electrode 11 may be an anode. The material for forming the first electrode 11 may be selected from materials with a high work function to facilitate hole injection. The first electrode 11 may be a reflective electrode, a semi-transmissive electrode, or a transmissive electrode. The material for forming the first electrode may be, for example, indium tin oxide (ITO), indium zinc oxide (IZO), tin oxide (SnO_2), and zinc oxide (ZnO). In one or more embodiments, magnesium (Mg), aluminum (Al), aluminum-lithium (Al-Li), calcium (Ca), magnesium-indium (Mg-In), or magnesium-silver (Mg-Ag) may be used as the material for forming the first electrode.

[0090] The first electrode 11 may have a single-layered structure or a multi-layered structure including two or more layers. For example, the first electrode 11 may have a three-layered structure of ITO/Ag/ITO, but the structure of the first electrode 110 is not limited thereto.

[0091] The organic layer 15 is disposed on the first electrode 11.

[0092] The organic layer 15 may include a hole transport region, an emission layer, and an electron transport region.

[0093] The hole transport region may be disposed between the first electrode 11 and the emission layer.

[0094] The hole transport region may include at least one selected from a hole injection layer, a hole transport layer, an electron blocking layer, and a buffer layer.

[0095] The hole transport region may include only either a hole injection layer or a hole transport layer. In one or more embodiments, the hole transport region may have a hole injection layer/hole transport layer structure or a hole injection layer/hole transport layer/electron blocking layer structure, which are sequentially stacked in this stated order from the first electrode 11.

[0096] A hole injection layer may be formed on the first electrode 11 by using one or more suitable methods selected

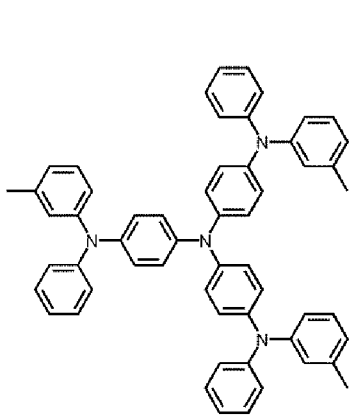
from vacuum deposition, spin coating, casting, or Langmuir-Blodgett (LB) deposition.

[0097] When a hole injection layer is formed by vacuum deposition, the deposition conditions may vary according to a compound that is used to form the hole injection layer, and the structure and thermal characteristics of the hole injection layer. For example, the deposition conditions may include a deposition temperature of about 100°C to about 500°C, a vacuum pressure of about 1.33×10^{-6} Pa (10^{-8} torr) to about 0.13 Pa (10^{-3} torr), and a deposition rate of about 0.01 Å/sec to about 100 Å/sec. However, the deposition conditions are not limited thereto.

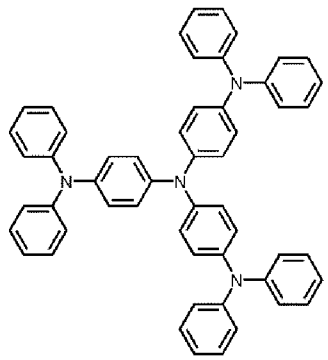
[0098] When the hole injection layer is formed using spin coating, coating conditions may vary according to the material used to form the hole injection layer, and the structure and thermal properties of the hole injection layer. For example, a coating speed may be from about 2,000 revolutions per minute (rpm) to about 5,000 rpm, and a temperature at which a heat treatment is performed to remove a solvent after coating may be from about 80°C to about 200°C. However, the coating conditions are not limited thereto.

[0099] Conditions for forming a hole transport layer and an electron blocking layer may be understood by referring to conditions for forming the hole injection layer.

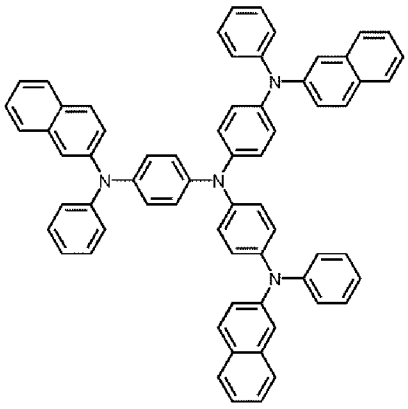
[0100] The hole transport region may include at least one selected from m-MTDATA, TDATA, 2-TNATA, NPB, β-NPB, TPD, Spiro-TPD, Spiro-NPB, methylated-NPB, TAPC, HMTPD, 4,4',4"-tris(N-carbazolyl)triphenylamine (TCTA), polyaniline/dodecylbenzene sulfonic acid (PANI/DBSA), poly(3,4-ethylenedioxythiophene)/poly(4-styrene sulfonate) (PEDOT/PSS), polyaniline/camphor sulfonic acid (PANI/CSA), polyaniline/poly(4-styrene sulfonate) (PANI/PSS), a compound represented by Formula 201 below, and a compound represented by Formula 202 below:



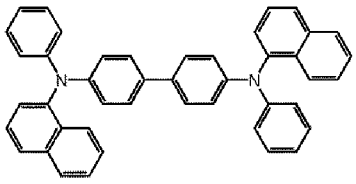
m-MTDATA



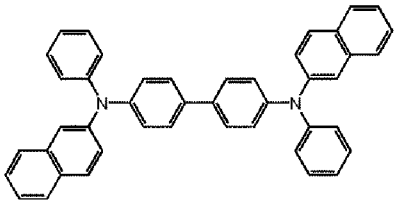
TDATA



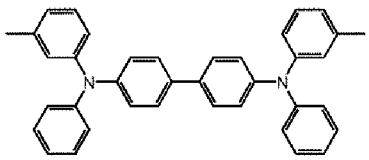
2-TNATA



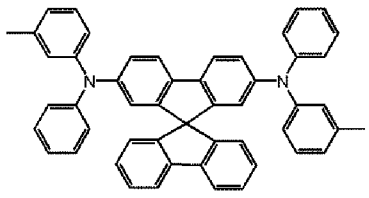
NPB



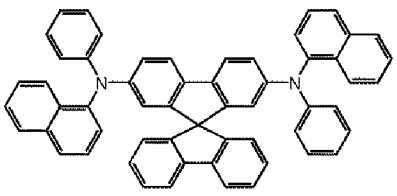
β-NPB



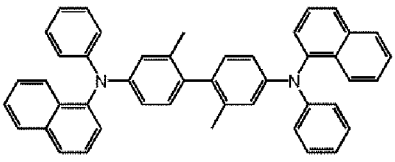
TPD



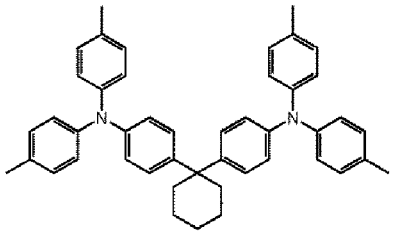
Spiro-TPD



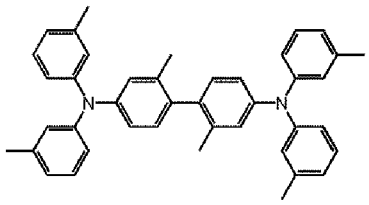
Spiro-NPB



methylated NPB

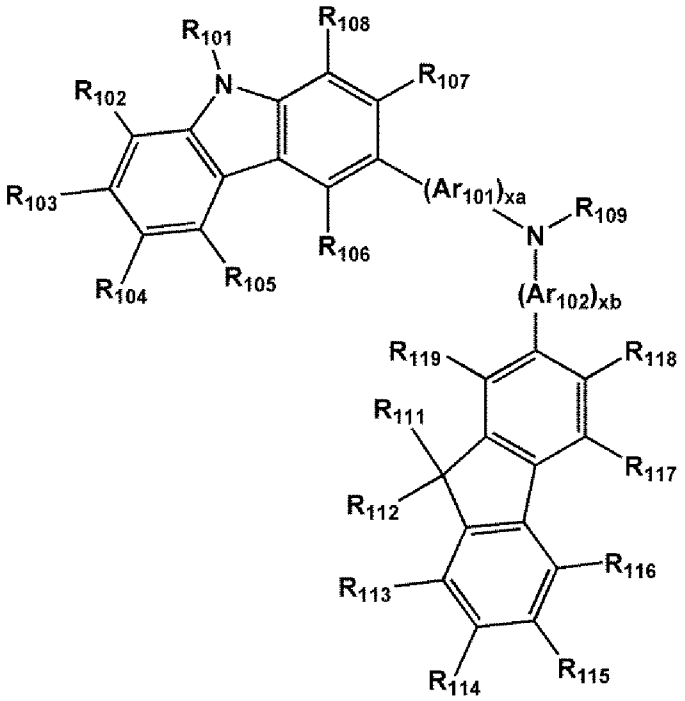


TAPC

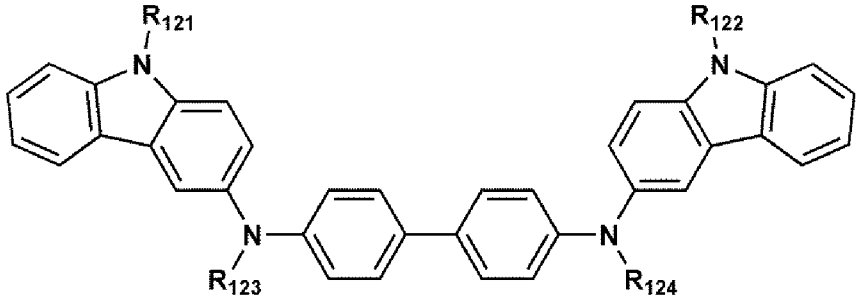


HMTPD

Formula 201



Formula 202



Ar_{101} and Ar_{102} in Formula 201 may each independently be 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 chrysenylenylene group, a naphthacenylene group, a picenylene group, a perylenylene group, and a pentacenylene group; and

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 chrysenylenylene group, a naphthacenylene group, a picenylene group, a perylenylene group, and a pentacenylene group, each substituted with at least one selected from 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_1-C_{10} heterocycloalkyl 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group.

[0101] In Formula 201, xa and xb may each independently be an integer from 0 to 5, or 0, 1, or 2. For example, xa may be 1, and xb may be 0, but embodiments of the present disclosure are not limited thereto.

[0102] In Formulae 201 and 202, R_{101} to R_{108}, R_{111} to R_{119}, and R_{121} to R_{124} may each independently be selected from:

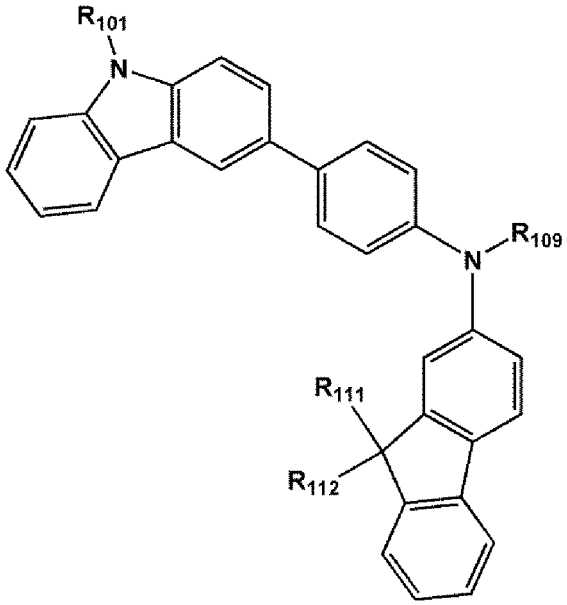
hydrogen, deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt thereof, a sulfonic acid group or a salt thereof, a phosphoric acid group or a salt thereof, a C_1-C_{10} alkyl group (for example, a methyl group, an ethyl group, a propyl group, a butyl group, pentyl group, and a hexyl group), and C_1-C_{10} alkoxy group (for example, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, and a pentoxy group);
a C_1-C_{10} alkyl group and a C_1-C_{10} alkoxy group, each substituted with at least one selected from 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;
a phenyl group, a naphthyl group, an anthracenyl group, a fluorenyl group, and a pyrenyl group; and
a phenyl group, a naphthyl group, an anthracenyl group, a fluorenyl group, and a pyrenyl group, each substituted with at least one selected from 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, but embodiments of the present disclosure are not limited thereto.

In Formula 201, R_{109} may be selected from:

a phenyl group, a naphthyl group, an anthracenyl group, and a pyridinyl group; and
a phenyl group, a naphthyl group, an anthracenyl group, and a pyridinyl group, each substituted with at least one selected from 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.

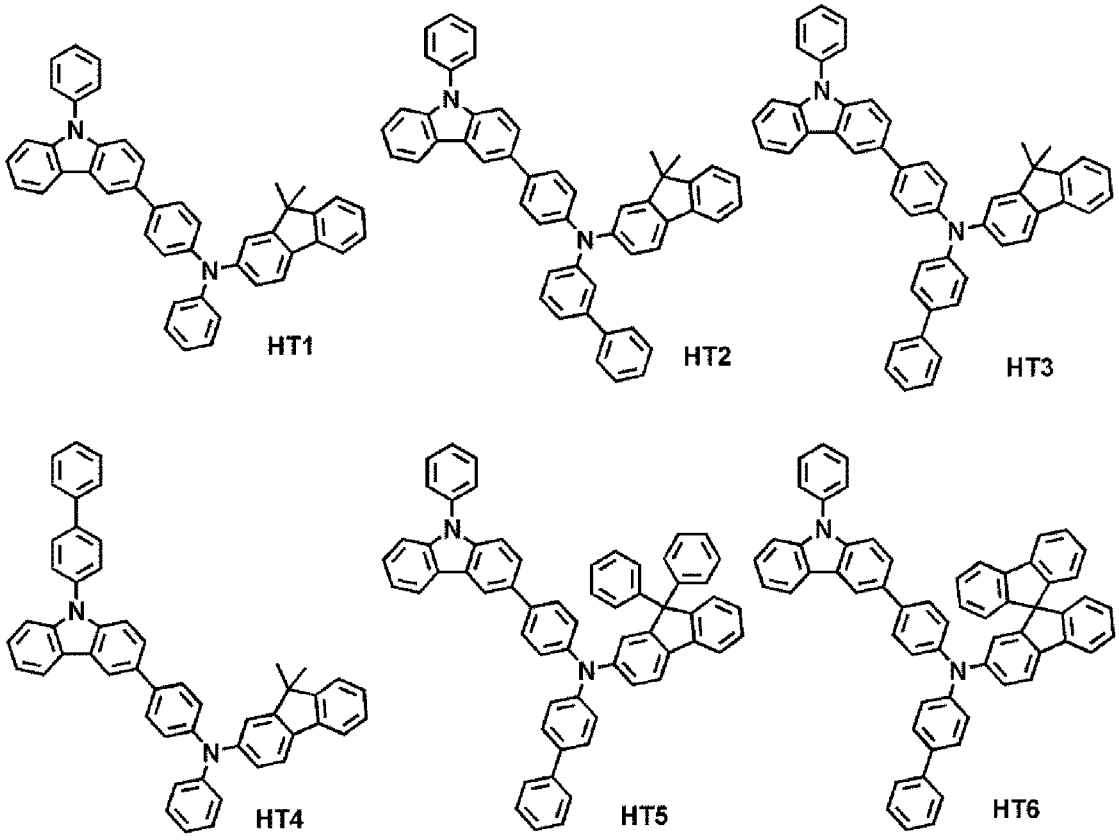
[0103] According to an embodiment, the compound represented by Formula 201 may be represented by Formula 201A, but embodiments of the present disclosure are not limited thereto:

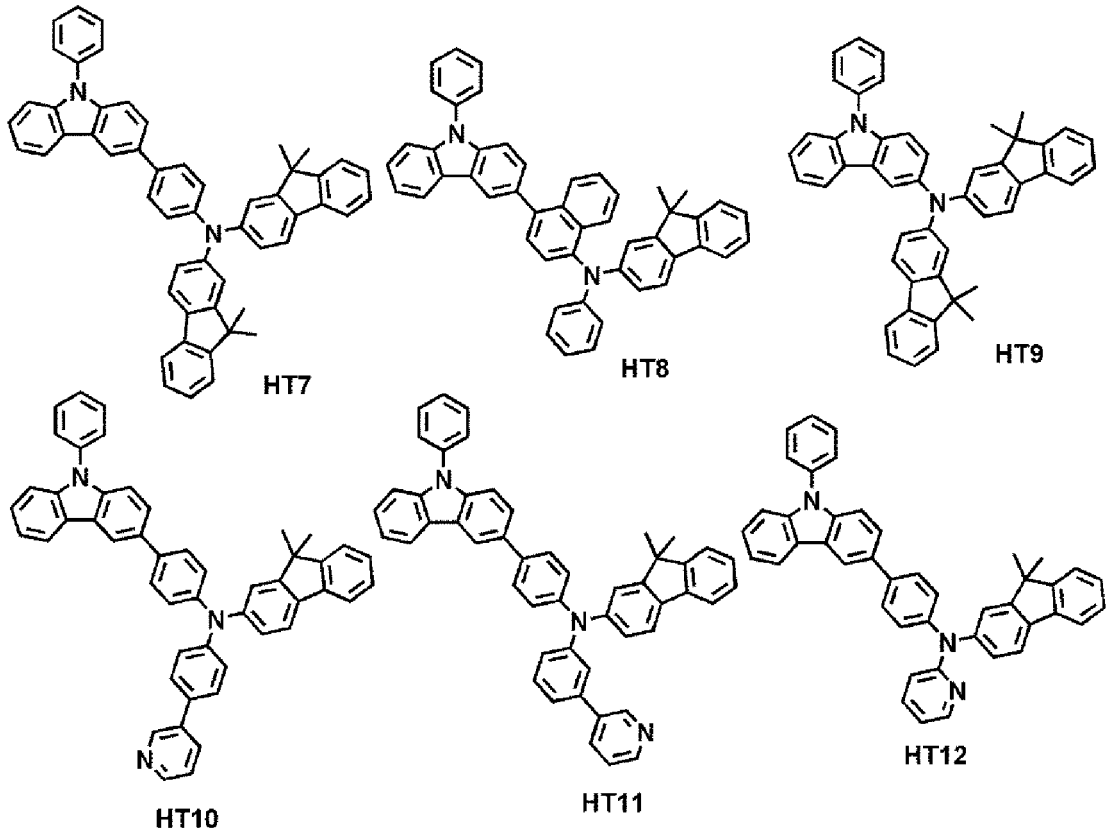
Formula 201A

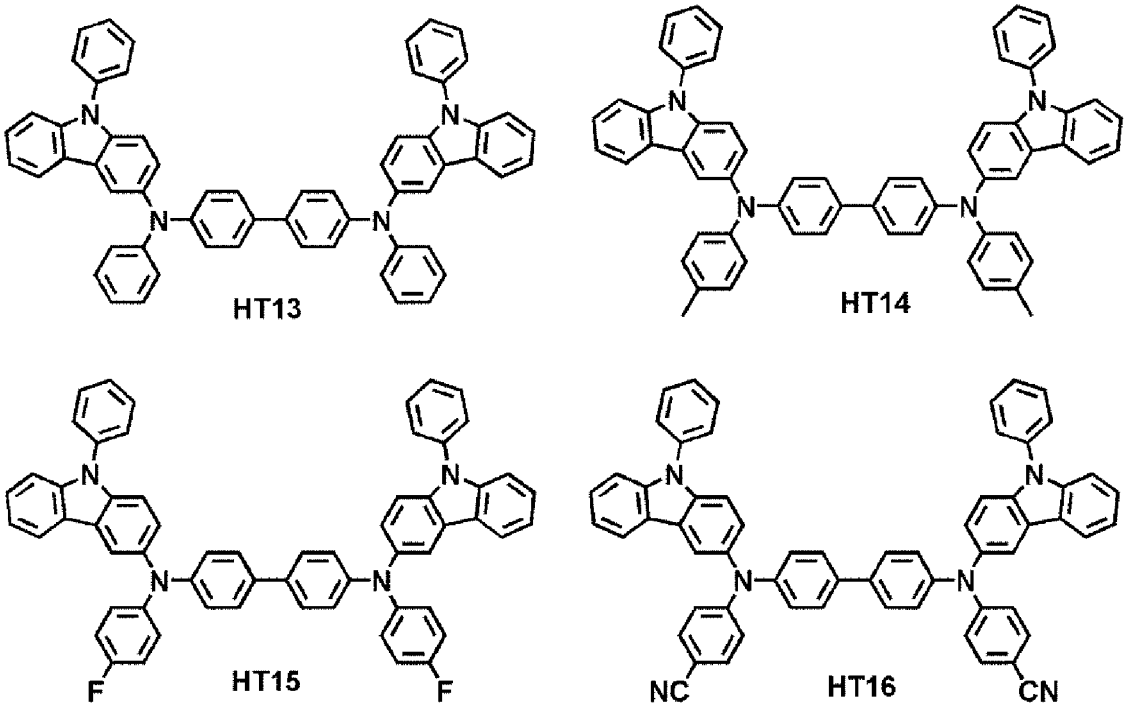


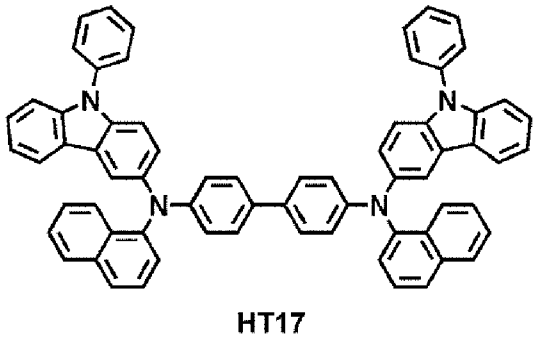
[0104] R_{101}, R_{111}, R_{112}, and R_{109} in Formula 201A may be understood by referring to the description provided herein.

[0105] For example, the compound represented by Formula 201, and the compound represented by Formula 202 may include compounds HT1 to HT20 illustrated below, but are not limited thereto.

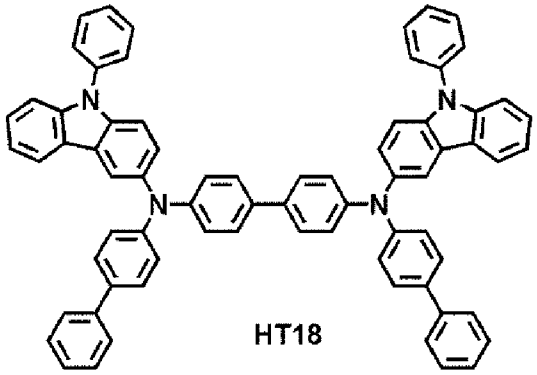



HT7
HT8
HT9
HT10
HT11
HT12

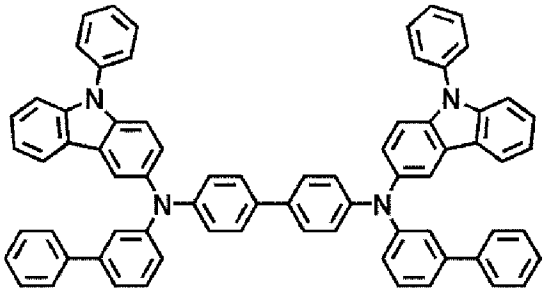

HT13
HT14
F
F
HT15
NC
CN
HT16



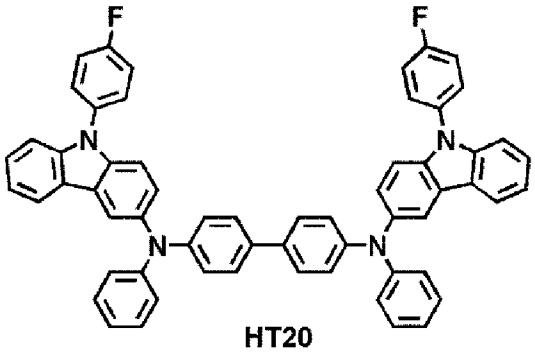
HT17



HT18



HT19

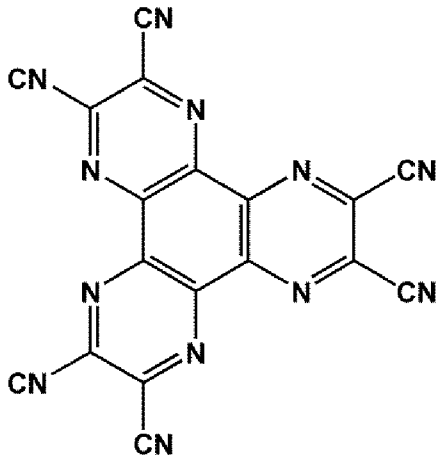


HT20

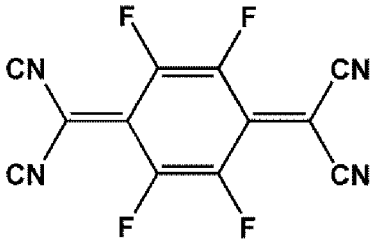
[0106] A thickness of the hole transport region may be in a range of about 100 Å to about 10,000 Å, for example, about 100 Å to about 1,000 Å. When the hole transport region includes a hole injection layer and a hole transport layer, the thickness of the hole injection layer may be in a range of about 100 Å to about 10,000 Å, and for example, about 100 Å to about 1,000 Å, and the thickness of the hole transport layer may be in a range of about 50 Å to about 2,000 Å, and for example, about 100 Å to about 1,500 Å. While not wishing to be bound by theory, it is understood that when the thicknesses of the hole transport region, the hole injection layer, and the hole transport layer are within these ranges, satisfactory hole transporting characteristics may be obtained without a substantial increase in driving voltage.

[0107] The hole transport region may further include, in addition to these materials, a charge-generation material for the improvement of conductive properties. The charge-generation material may be homogeneously or non-homogeneously dispersed in the hole transport region.

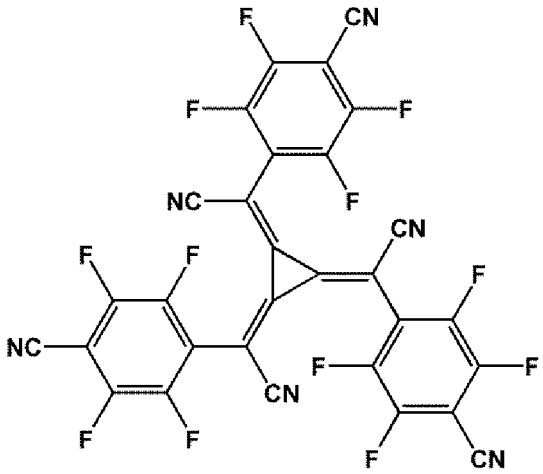
[0108] The charge-generation material may be, for example, a p-dopant. The p-dopant may be one selected from a quinone derivative, a metal oxide, and a cyano group-containing compound, but embodiments of the present disclosure are not limited thereto. Non-limiting examples of the p-dopant are a quinone derivative, such as tetracyanoquinonedimethane (TCNQ) or 2,3,5,6-tetrafluoro-tetracyano-1,4-benzoquinonedimethane (F4-TCNQ); a metal oxide, such as a tungsten oxide or a molybdenium oxide; and a cyano group-containing compound, such as Compound HT-D1 or Compound HT-D2 below, but are not limited thereto.



HT-D1



F4-TCNQ



HT-D2

[0109] The hole transport region may include a buffer layer.

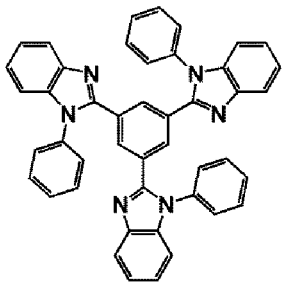
[0110] Also, the buffer layer may compensate for an optical resonance distance according to a wavelength of light emitted from the emission layer, and thus, efficiency of a formed organic light-emitting device may be improved.

[0111] Then, an emission layer may be formed on the hole transport region by vacuum deposition, spin coating, casting, LB deposition, or the like. When the emission layer is formed by vacuum deposition or spin coating, the deposition or coating conditions may be similar to those applied in forming the hole injection layer although the deposition or coating conditions may vary according to a compound that is used to form the emission layer.

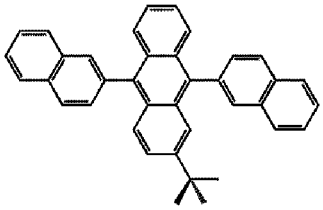
[0112] Meanwhile, when the hole transport region includes an electron blocking layer, a material for the electron blocking layer may be selected from materials for the hole transport region described above and materials for a host to be explained later. However, the material for the electron blocking layer is not limited thereto. For example, when the hole transport region includes an electron blocking layer, a material for the electron blocking layer may be mCP, which will be explained later.

[0113] The emission layer may include a host and a dopant, and the dopant may include the organometallic compound represented by Formula 1 or a composition containing the organometallic compound.

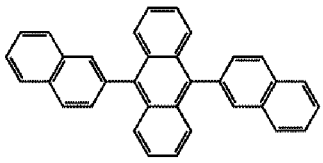
[0114] The host may include at least one selected from TPBi, TBADN, ADN (also referred to as "DNA"), CBP, CDBP, TCP, mCP, Compound H50, Compound H51 and Compound 52:



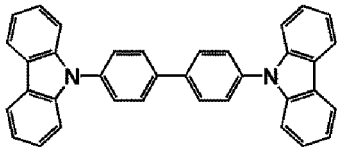
TPBi



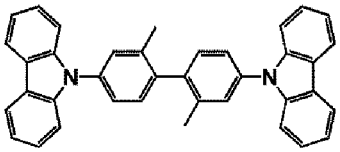
TBADN



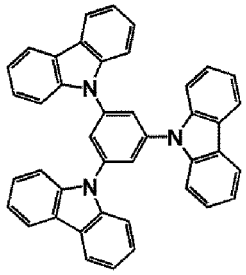
ADN



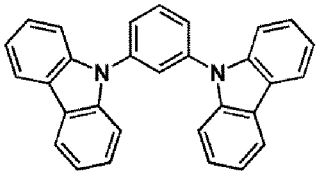
CBP



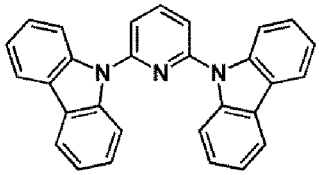
CDBP



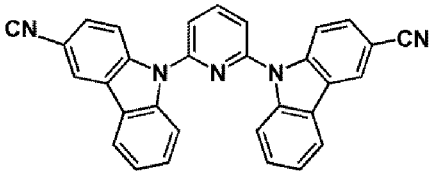
TCP



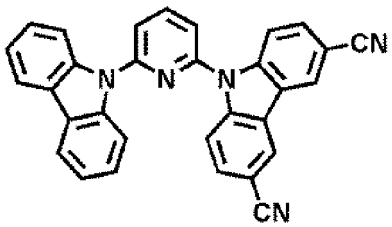
mCP



H50



H51



H52

[0115] 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 one or more embodiments, due to a stacked structure including a red emission layer, a green emission layer, and/or a blue emission layer, the emission layer may emit white light.

[0116] When the emission layer includes a host and a dopant, an amount of the dopant may be in a range of about 0.01 parts by weight to about 15 parts by weight based on 100 parts by weight of the host, but embodiments of the present disclosure are not limited thereto.

[0117] The dopant may include at least one of organometallic compounds represented by Formula 1 or the composition containing the organometallic compound described above.

[0118] A thickness of the emission layer may be in a range of about 100 Å to about 1,000 Å, for example, about 200 Å to about 600 Å. While not wishing to be bound by theory, it is understood that when the thickness of the emission layer is within this range, excellent light-emission characteristics may be obtained without a substantial increase in driving voltage.

[0119] Then, an electron transport region may be disposed on the emission layer.

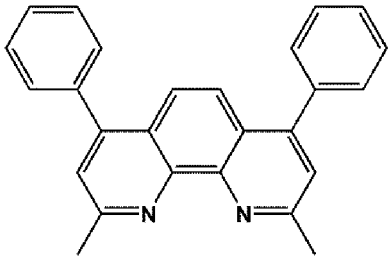
[0120] The electron transport region may include at least one selected from a hole blocking layer, an electron transport

layer, and an electron injection layer.

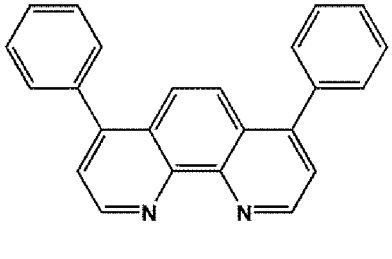
[0121] For example, the electron transport region may have a hole blocking layer/electron transport layer/electron injection layer structure or an electron transport layer/electron injection layer structure, but the structure of the electron transport region is not limited thereto. The electron transport layer may have a single-layered structure or a multi-layered structure including two or more different materials.

[0122] Conditions for forming the hole blocking layer, the electron transport layer, and the electron injection layer which constitute the electron transport region may be understood by referring to the conditions for forming the hole injection layer.

[0123] When the electron transport region includes a hole blocking layer, the hole blocking layer may include, for example, at least one of BCP, Bphen, and BAlq but embodiments of the present disclosure are not limited thereto.



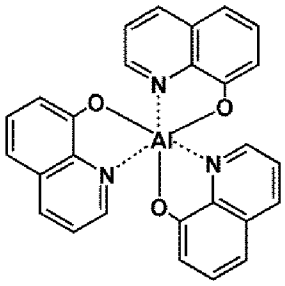
BCP



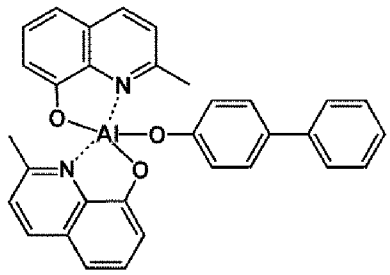
Bphen

[0124] A thickness of the hole blocking layer may be in a range of about 20 Å to about 1,000 Å, for example, about 30 Å to about 300 Å. While not wishing to be bound by theory, it is understood that when the thickness of the hole blocking layer is within these ranges, the hole blocking layer may have improved hole blocking ability without a substantial increase in driving voltage.

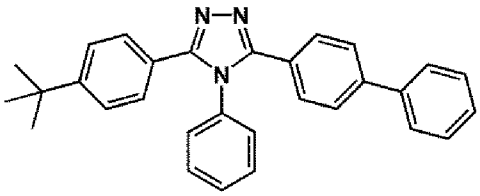
[0125] The electron transport layer may include at least one selected from BCP, Bphen, Alq_3, BAlq, TAZ, and NTAZ.



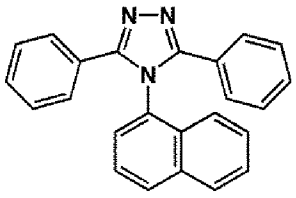
Alq_3



BAlq

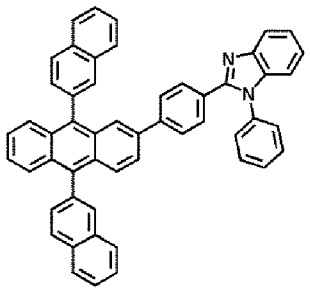


TAZ

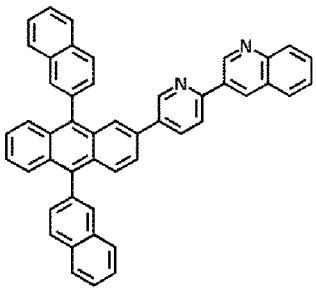


NTAZ

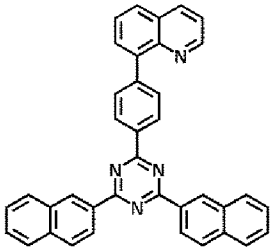
[0126] In one or more embodiments, the electron transport layer may include at least one of ET1 to ET25, but are not limited thereto:



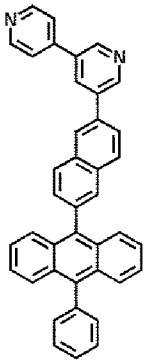
ET1



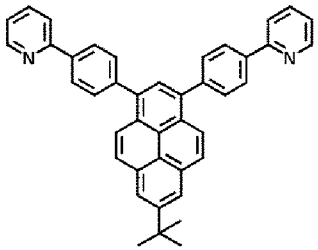
ET2



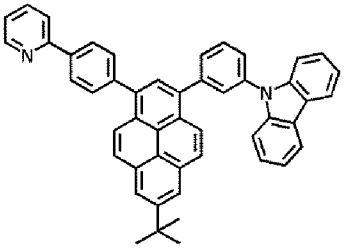
ET3



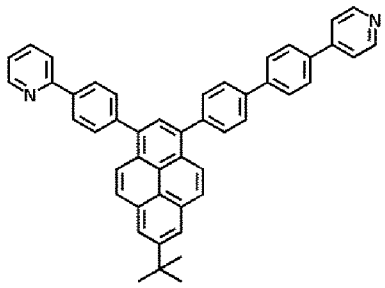
ET4



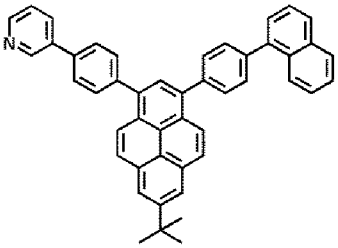
ET5



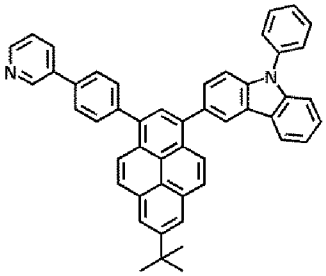
ET6



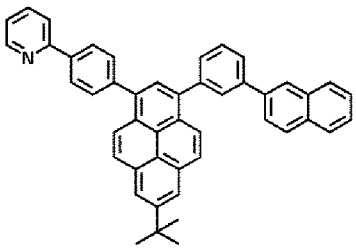
ET7



ET8



ET9



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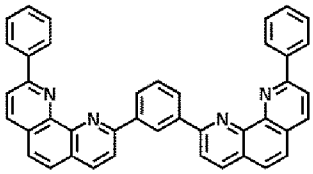

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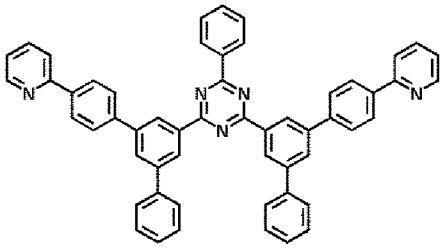
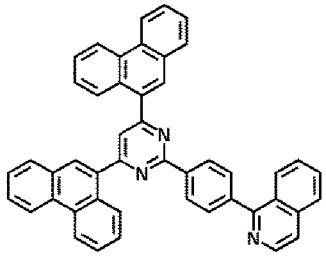
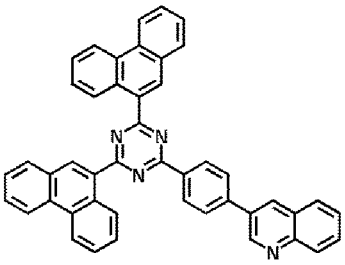


ET12



ET13



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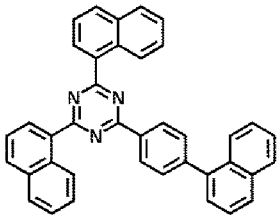

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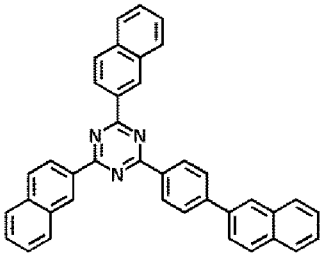

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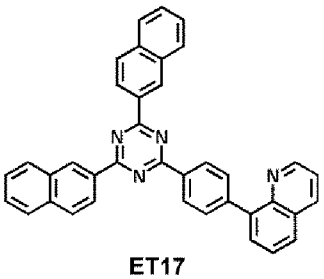
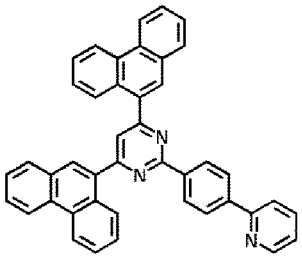
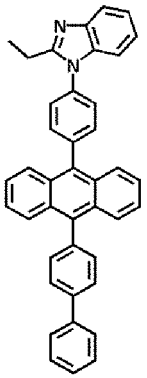


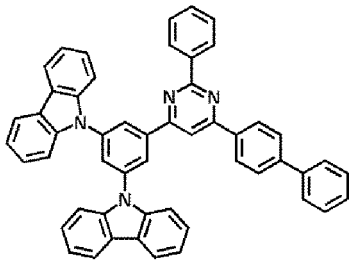
ET17



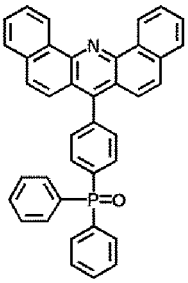
ET18



ET19



ET20



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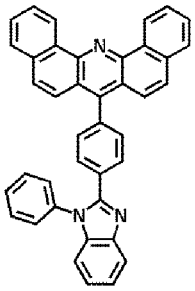

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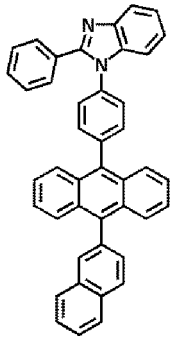

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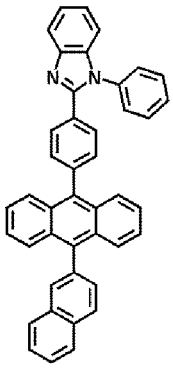
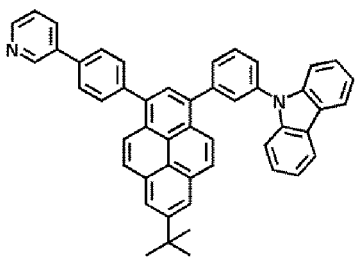


ET24

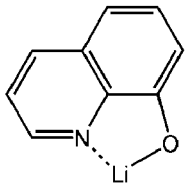


ET25

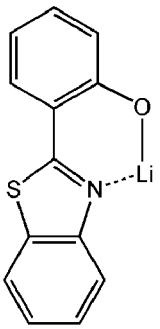
[0127] A thickness of the electron transport layer may be in a range of about 100 Å to about 1,000 Å, for example, about 150 Å to about 500 Å. While not wishing to be bound by theory, it is understood that when the thickness of the electron transport layer is within the range described above, the electron transport layer may have satisfactory electron transport characteristics without a substantial increase in driving voltage.

[0128] Also, the electron transport layer may further include, in addition to the materials described above, a metal-containing material.

[0129] The metal-containing material may include a Li complex. The Li complex may include, for example, Compound ET-D1 (lithium 8-hydroxyquinolate, LiQ) or ET-D2.



ET-D1



ET-D2

[0130] The electron transport region may include an electron injection layer that promotes injection of electrons from the second electrode 19 thereinto.

[0131] The electron injection layer may include at least one selected from LiF, NaCl, CsF, Li_2O, and BaO.

[0132] A thickness of the electron injection layer may be in a range of about 1 Å to about 100 Å, for example, about 3 Å to about 90 Å. While not wishing to be bound by theory, it is understood that when the thickness of the electron injection layer is within the range described above, the electron injection layer may have satisfactory electron injection characteristics without a substantial increase in driving voltage.

[0133] The second electrode 19 is disposed on the organic layer 15. The second electrode 19 may be a cathode. A material for forming the second electrode 19 may be selected from metal, an alloy, an electrically conductive compound, and a combination thereof, which have a relatively low work function. For example, lithium (Li), magnesium (Mg), aluminum (Al), aluminum-lithium (Al-Li), calcium (Ca), magnesium-indium (Mg-In), or magnesium-silver (Mg-Ag) may be used as a material for forming the second electrode 19. In one or more embodiments, to manufacture a top-emission type light-emitting device, a transmissive electrode formed using ITO or IZO may be used as the second electrode 19.

[0134] Hereinbefore, the organic light-emitting device has been described with reference to the FIGURE, but embodiments of the present disclosure are not limited thereto.

[0135] The term "C_1-C_{60} alkyl group" as used herein refers to a linear or branched saturated aliphatic hydrocarbon monovalent group having 1 to 60 carbon atoms, and non-limiting examples thereof include a methyl group, an ethyl group, a propyl group, an iso-butyl group, a sec-butyl group, a tert-butyl group, a pentyl group, an iso-amyl group, and a hexyl group. The term "C_1-C_{60} alkylene group" as used herein refers to a divalent group having the same structure as the C_1-C_{60} alkyl group.

[0136] The term "C_1-C_{60} alkoxy group" as used herein refers to a monovalent group represented by $-OA_{101}$ (wherein A_{101} is the C_1-C_{60} alkyl group), and non-limiting examples thereof include a methoxy group, an ethoxy group, and an iso-propyloxy group.

[0137] The term "C_2-C_{60} alkenyl group" as used herein refers to a hydrocarbon group formed by including at least one carbon-carbon double bond in the middle or at the terminus of the C_2-C_{60} alkyl group, and examples thereof include an ethenyl group, a propenyl group, and a butenyl group. The term "C_2-C_{60} alkenylene group" as used herein refers to a divalent group having the same structure as the C_2-C_{60} alkenyl group.

[0138] The term "C_2-C_{60} alkynyl group" as used herein refers to a hydrocarbon group formed by including at least one carbon-carbon triple bond in the middle or at the terminus of the C_2-C_{60} alkyl group, and examples thereof include an ethynyl group, and a propynyl group. The term "C_2-C_{60} alkynylene group" as used herein refers to a divalent group having the same structure as the C_2-C_{60} alkynyl group.

[0139] The term "C_3-C_{10} cycloalkyl group" as used herein refers to a monovalent saturated hydrocarbon monocyclic group having 3 to 10 carbon atoms, and non-limiting examples thereof include a cyclopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, and a cycloheptyl group. The term "C_3-C_{10} cycloalkylene group" as used herein refers to a divalent group having the same structure as the C_3-C_{10} cycloalkyl group.

[0140] The term "C_1-C_{10} heterocycloalkyl group" as used herein refers to a monovalent saturated monocyclic group having at least one heteroatom selected from N, O, P, Si and S as a ring-forming atom and 1 to 10 carbon atoms, and non-limiting examples thereof include a tetrahydrofuranyl group, and a tetrahydrothiophenyl group. The term "C_1-C_{10} heterocycloalkylene group" as used herein refers to a divalent group having the same structure as the C_1-C_{10} heterocycloalkyl group.

[0141] The term "C_3-C_{10} cycloalkenyl group" as used herein refers to a monovalent monocyclic hydrocarbon group that has 3 to 10 carbon atoms and at least one carbon-carbon double bond in the ring thereof and that has no aromaticity,

and non-limiting examples thereof include a cyclopentenyl group, a cyclohexenyl group, and a cycloheptenyl group. The term "C_3-C_{10} cycloalkenylene group" as used herein refers to a divalent group having the same structure as the C_3-C_{10} cycloalkenyl group.

[0142] The term "C_1-C_{10} heterocycloalkenyl group" as used herein refers to a monovalent monocyclic group that has at least one heteroatom selected from N, O, P, Si, and S as a ring-forming atom, 1 to 10 carbon atoms, and at least one double bond in its ring. Examples of the C_1-C_{10} heterocycloalkenyl group are a 2,3-dihydrofuranyl group and a 2,3-dihydrothiophenyl group. The term "C_1-C_{10} heterocycloalkenylene group" as used herein refers to a divalent group having the same structure as the C_1-C_{10} heterocycloalkenyl group.

[0143] The term "C_6-C_{60} aryl group" as used herein refers to a monovalent group having a carbocyclic aromatic system having 6 to 60 carbon atoms, and a C_6-C_{60} arylene group as used herein refers to a divalent group having a carbocyclic aromatic system having 6 to 60 carbon atoms. Non-limiting examples of the C_6-C_{60} aryl group include 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 and the C_6-C_{60} arylene group each include two or more rings, the rings may be fused to each other.

[0144] The term "C_1-C_{60} heteroaryl group" as used herein refers to a monovalent group having a heterocyclic aromatic system that has at least one heteroatom selected from N, O, P, Si, and S as a ring-forming atom, and 1 to 60 carbon atoms. The term "C_1-C_{60} heteroarylene group," as used herein refers to a divalent group having a heterocyclic aromatic system that has at least one heteroatom selected from N, O, P, Si, and S as a ring-forming atom, and 1 to 60 carbon atoms. Non-limiting examples of the C_1-C_{60} heteroaryl group include a pyridinyl group, a pyrimidinyl group, a pyrazinyl group, a pyridazinyl group, a triazinyl group, a quinolinyl group, and an isoquinolinyl group. When the C_1-C_{60} heteroaryl group and the C_1-C_{60} heteroarylene group each include two or more rings, wherein the rings may be fused to each other.

[0145] The term "C_6-C_{60} aryloxy group" as used herein indicates -OA_{102} (wherein A_{102} is the C_6-C_{60} aryl group), the term "C_6-C_{60} arylthio group" as used herein indicates -SA_{103} (wherein A_{103} is the C_6-C_{60} aryl group), and the term "C_7-C_{60} arylalkyl group" as used herein indicates -$A_{104}A_{105}$ (wherein A_{104} is the C_6-C_{59} aryl group and A_{105} is the C_1-C_{53} alkyl group).

[0146] The term "C_2-C_{60} heteroaryloxy group" as used herein refers to -OA_{106} (wherein A_{106} is the C_2-C_{60} heteroaryl group), and the term "C_2-C_{60} heteroarylthio group" as used herein indicates -SA_{107} (wherein A_{107} is the C_2-C_{60} heteroaryl group).

[0147] The term "C_3-C_{60} heteroarylalkyl group" as used herein refers to -$A_{108}A_{109}$ (A_{109} is a C_2-C_{59} heteroaryl group, and A_{108} is a C_1-C_{58} alkylene group).

[0148] The term "monovalent non-aromatic condensed polycyclic group" as used herein refers to a monovalent group (for example, having 8 to 60 carbon atoms) having two or more rings condensed to each other, only carbon atoms as ring-forming atoms, and having no aromaticity in its entire molecular structure. Examples of the monovalent non-aromatic condensed polycyclic group include a fluorenyl group. The term "divalent non-aromatic condensed polycyclic group," as used herein, refers to a divalent group having the same structure as the monovalent non-aromatic condensed polycyclic group.

[0149] The term "monovalent non-aromatic condensed heteropolycyclic group" as used herein refers to a monovalent group (for example, having 2 to 60 carbon atoms) having two or more rings condensed to each other, a heteroatom selected from N, O, P, Si, and S, other than carbon atoms, as a ring-forming atom, and having no aromaticity in its entire molecular structure. Non-limiting examples of the monovalent non-aromatic condensed heteropolycyclic group include a carbazolyl group. The term "divalent non-aromatic condensed heteropolycyclic group" as used herein refers to a divalent group having the same structure as the monovalent non-aromatic condensed heteropolycyclic group.

[0150] The term "C_5-C_{30} carbocyclic group" as used herein refers to a saturated or unsaturated cyclic group having, as a ring-forming atom, 5 to 30 carbon atoms only. The term "C_5-C_{30} carbocyclic group" as used herein refers to a monocyclic group or a polycyclic group, and, according to its chemical structure, a monovalent, divalent, trivalent, tetravalent, pentavalent, or hexavalent group.

[0151] The term "C_2-C_{30} heterocyclic group" as used herein refers to a saturated or unsaturated cyclic group having, as a ring-forming atom, at least one heteroatom selected from N, O, Si, P, and S other than 2 to 30 carbon atoms. The term "C_2-C_{30} heterocyclic group" as used herein refers to a monocyclic group or a polycyclic group, and, according to its chemical structure, a monovalent, divalent, trivalent, tetravalent, pentavalent, or hexavalent group.

[0152] At least one substituent of the substituted C_5-C_{30} carbocyclic group, the substituted C_2-C_{30} heterocyclic group, the substituted C_1-C_{60} alkyl group, the substituted C_2-C_{60} alkenyl group, the substituted C_2-C_{60} alkynyl group, the substituted C_1-C_{60} 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_{60} aryl group, the substituted C_6-C_{60} aryloxy group, the substituted C_6-C_{60} arylthio group, the substituted C_7-C_{60} arylalkyl group, the substituted C_1-C_{60} heteroaryl group, the substituted C_1-C_{60} heteroaryloxy group, the substituted C_1-C_{60} heteroarylthio group, the substituted C_2-C_{60} heteroarylalkyl group, the substituted monovalent non-aromatic condensed polycyclic group, and the substituted monovalent non-aromatic condensed heteropolycyclic group may be selected from:

deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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, and a C_1-C_{60} alkoxy group;

a C_1-C_{60} alkyl group, a C_2-C_{60} alkenyl group, a C_2-C_{60} alkynyl group, and a C_1-C_{60} alkoxy group, each substituted with at least one selected from deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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_{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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_{11})(Q_{12})$, $-Si(Q_{13})(Q_{14})(Q_{15})$, $-B(Q_{16})(Q_{17})$, and-$P(=O)(Q_{18})(Q_{19})$;

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 C6-C60 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group, each substituted with at least one selected from deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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_1-C_{60} heteroaryl group, a C_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, - $N(Q_{21})(Q_{22})$, $-Si(Q_{23})(Q_{24})(Q_{25})$, $-B(Q_{26})(Q_{27})$, and $-P(=O)(Q_{28})(Q_{29})$; and

$-N(Q_{31})(Q_{32})$, $-Si(Q_{33})(Q_{34})(Q_{35})$, $-B(Q_{36})(Q_{37})$, and $-P(=O)(Q_{38})(Q_{39})$, and

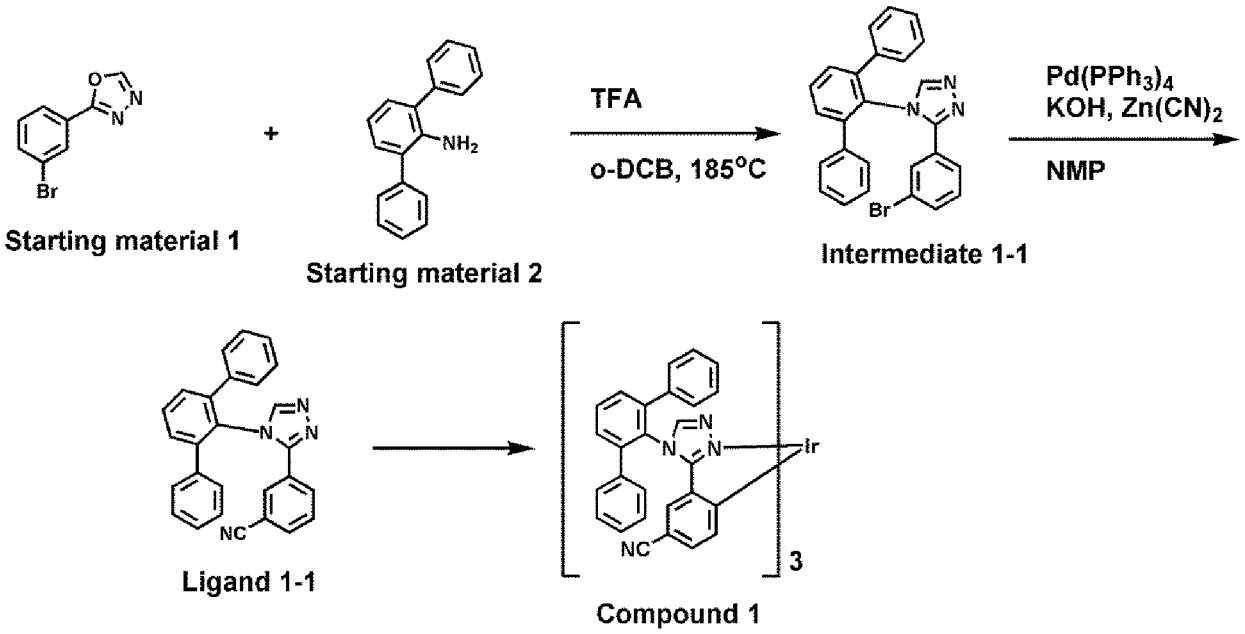
Q_1 to Q_9, Q_{11} to Q_{19}, Q_{21} to Q_{29}, and Q_{31} to Q_{39} may each independently be selected from hydrogen, deuterium, -F, -Cl, -Br, -I, a hydroxyl group, a cyano group, a nitro group, an amino group, an amidino group, a hydrazine group, a hydrazone group, a carboxylic acid group or a salt 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} aryl group substituted with at least one selected from a C_1-C_{60} alkyl group and 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group.

[0153] Hereinafter, a compound and an organic light-emitting device according to embodiments are described in detail with reference to Synthesis Example and Examples. However, the organic light-emitting device is not limited thereto. The wording "B was used instead of A" used in describing Synthesis Examples means that an amount of A used was identical to an amount of B used, in terms of molar equivalents.

Examples

Synthesis Example 1 : Synthesis of Compound 1

[0154]



Synthesis of Intermediate 1-1

[0155] 0.5 grams (g) (1.56 millimoles, mmol) of a starting material 1, 0.49 g (2.18 mmol) of a starting material 2, and 1.3 milliliters (mL) of o-dichlorobenzene (o-DCB) were mixed, and 0.25 g (2.18 mmol) of trifluoroacetic acid (TFA) were added thereto. The resultant mixture was heated and stirred at a temperature of 185°C overnight. The resultant mixture was then cooled to room temperature, and an excess amount of water was added thereto. The pH of the resultant mixture was adjusted to about 9 by using 10% Na_2CO_3 aqueous solution, and an organic layer was extracted by using ethyl acetate. The extracted organic layer was washed by using brine and dried by using anhydrous $MgSO_4$, and a solvent was removed therefrom under reduced pressure. The product obtained therefrom was purified by silica gel column chromatography to obtain 0.35 g (yield: 50%) of Intermediate 1-1.

Synthesis of Ligand 1-1

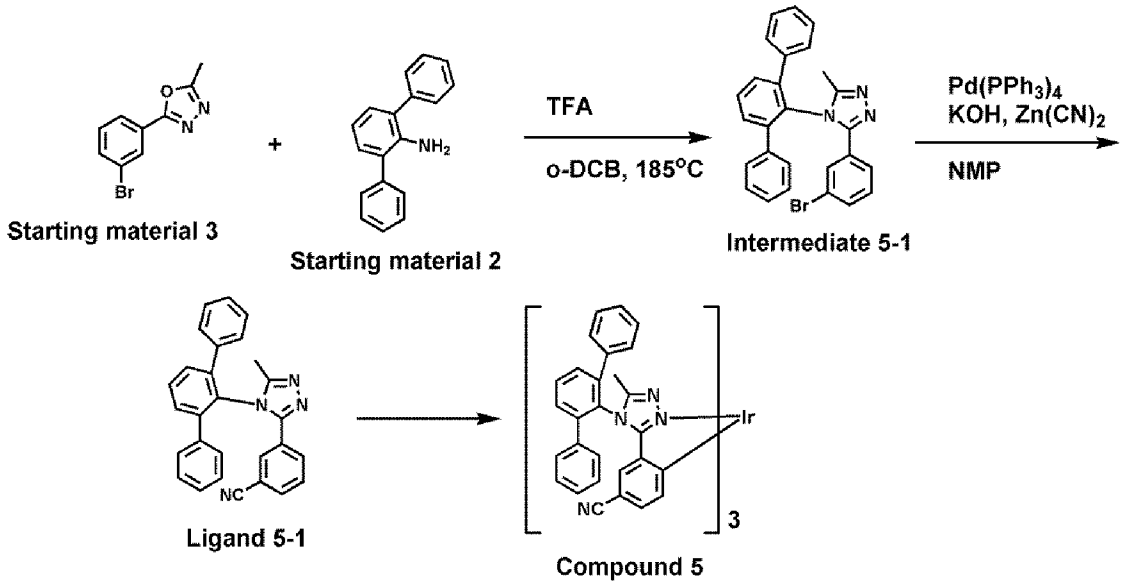
[0156] 0.9 g (2 mmol) of Intermediate 1-1 and 10 mL of N-methyl pyrrolidone (NMP) were mixed, and 0.29 g (2.5 mmol) of $Zn(CN)_2$, 0.19 g (3.4 mmol) of KOH, and 0.7 g (0.63 mmol) of $Pd(PPh_3)_4$ were added thereto. The resultant mixture was heated at a temperature of 100°C for 10 hours. The resultant obtained therefrom was cooled to room temperature, and water is added thereto. An organic layer was extracted by using $CHCl_3$ and washed by using 1 molar (M) NaOH aqueous solution and brine, dried by using anhydrous $MgSO_4$, and a solvent was removed therefrom. The product obtained therefrom was purified by silica gel column chromatography to obtain 0.56 g (yield: 70%) of Ligand 1-1.

Synthesis of Compound 1

[0157] 3.98 g (10 mmol) of Ligand 1-1 and 1.24 g (2.5 mmol) of $Ir(COD)_2BF_4$ were mixed with 40 mL of NMP, and the resultant mixture underwent a reaction at a temperature of 200°C for 48 hours. 200 mL of dichloromethane (DCM) was added thereto, and the resultant mixture was washed by using 200 mL of 10% NH_4OH aqueous solution, 200 mL of saturated $NaHCO_3$ aqueous solution, and 200 mL of brine (saturated NaCl aqueous solution). An organic layer obtained therefrom was dried by using anhydrous $MgSO_4$, filtered, and a solvent was removed therefrom under reduced pressure. The product was purified by silica gel column chromatography (DCM 100% - EtOAc (1% in DCM)) to obtain 0.17 g (0.125 mol, yield: 5%) of Compound 1.
M/Z 1384.264 ^1H NMR (CD_2Cl_2, 500 MHz) δ = 7.82 (t, 3H), 7.67 (dd, 3H), 7.64(dd, 3H), 7.58 (s, 3H), 7.10 (t, 6H), 7.05 (tt, 3H), 6.95-7.02 (m, 9H), 6.77-6.85 (m, 9H), 6.73-6.79 (m, 9H), 6.33 (d, 3H).

Synthesis Example 2 : Synthesis of Compound 5

[0158]



Synthesis of Intermediate 5-1

[0159] Intermediate 5-1 was synthesized in the same manner as Intermediate 1-1 in Synthesis Example 1, except that a starting material 3 was used instead of the starting material 1.

Synthesis of Ligand 5-1

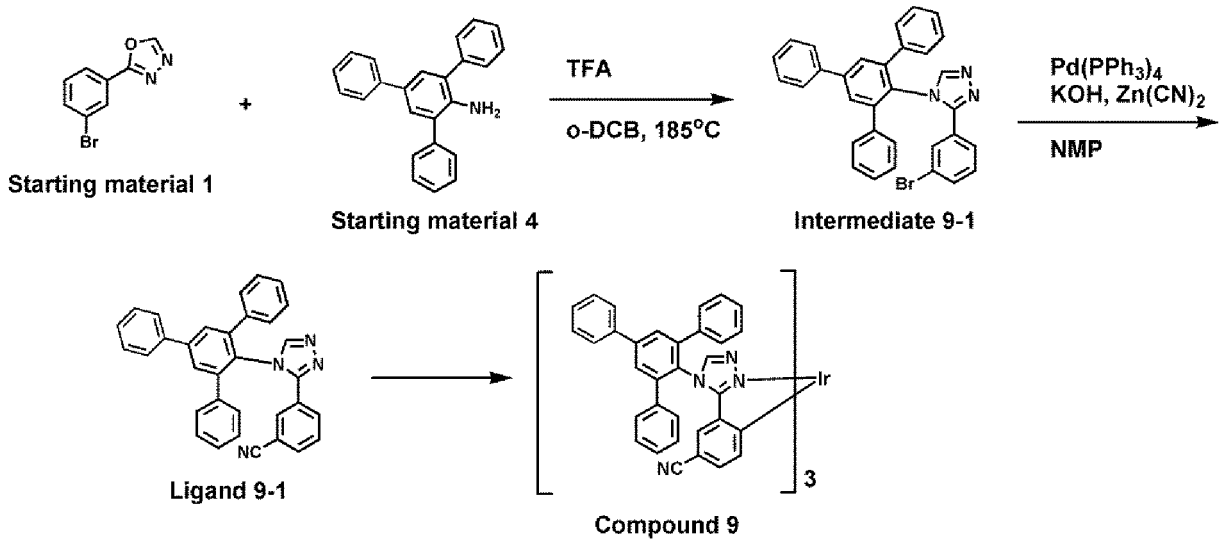
[0160] Ligand 5-1 was synthesized in the same manner as Ligand 1-1 in Synthesis Example 1, except that Intermediate 5-1 was used instead of Intermediate 1-1.

Synthesis of Compound 5

[0161] Compound 5 (yield: 7%) was synthesized in the same manner as in Synthesis Example 1, except that Ligand 5-1 was used instead of Ligand 1-1.
^{1}H NMR (CD_2Cl_2, 500 MHz) δ = 7.85 (t, 3H), 7.69 (td, 6H), 6.95-7.05 (m, 9H), 6.95(d, 6H), 6.91 (t, 3H), 6.85 (dd, 3H), 6.81 (d, 6H), 6.72 (t, 9H), 6.39 (d, 3H), 1.92 (s, 9H).

Synthesis Example 3 : Synthesis of Compound 9

[0162]



Synthesis of Intermediate 9-1

[0163] Intermediate 9-1 was synthesized in the same manner as Intermediate 1-1 in Synthesis Example 1, except that a starting material 4 was used instead of the starting material 2.

Synthesis of Ligand 9-1

[0164] Ligand 9-1 was synthesized in the same manner as Ligand 1-1 in Synthesis Example 1, except that Intermediate 9-1 was used instead of Intermediate 1-1.

Synthesis of Compound 9

[0165] Compound 9 (yield: 6%) was synthesized in the same manner as in Synthesis Example 1, except that Ligand 9-1 was used instead of Ligand 1-1.
M/Z 1613.872 NMR data (CD_2Cl_2, 300 MHz) δ = 7.9 (d, 6H), 7.82 (d, 6H), 7.62 (s, 3H), 7.4-7.6 (m, 9H), 7.0-7.2 (m, 18H), 6.98 (s, 3H), 6.76-6.94 (m, 15H), 6.38 (d, 3H).

Evaluation Example 1: Evaluation of HOMO, LUMO, and Triplet (T_1) Energy Levels

[0166] HOMO, LUMO, and T_1 energy levels of Compounds 1, 5, and 9 were evaluated by using the methods provided in Table 3. Results thereof are shown in Table 4.

Table 3

HOMO energy level evaluation method	A voltage-current (V-A) graph of each Compound was obtained by using a cyclic voltammetry (CV) (electrolyte: 0.1 M Bu_4NClO_4 / solvent: CH_2Cl_2 / electrode: 3-electrode system (working electrode: GC, reference electrode: Ag/AgCl, auxiliary electrode: Pt)), and then, a HOMO energy level of each Compound was calculated from an onset oxidation potential of the V-A graph.
LUMO energy level evaluation method	Each Compound was diluted at a concentration of $1x10^{-5}$ M in $CHCl_3$, an UV absorption spectrum thereof was measured at room temperature by using a Shimadzu UV-350 Spectrometer, and then, a LUMO energy level thereof was calculated by using an optical band gap (Eg) from an edge of the absorption spectrum.
T_1 energy level evaluation method	After a mixture of toluene and each Compound (1 milligram (mg) of each Compound was dissolved in 3 cubic centimeters (cc) of toluene) was added to a quartz cell and then added to liquid nitrogen (77 Kelvins, K), a photoluminescence spectrum was measured by using a photoluminescence measurement apparatus. The T_1 energy level was calculated by analyzing peaks observed only at a low temperature through comparison between the photoluminescence spectrum and a general room-temperature photoluminescence spectrum.

Table 4

Compound No.	HOMO (eV)	LUMO (eV)	T_1 (eV)
1	-5.49	-2.76	2.73
5	-5.43	-2.72	2.71
9	-5.49	-2.76	2.73

[0167] Referring to Table 4, it is confirmed that Compounds 1, 5, and 9 have electrical characteristics suitable for use as materials for an organic light-emitting device.

Evaluation Example 2: Evaluation of Thermal Characteristics

[0168] A thermal analysis (N_2 atmosphere, temperature range: room temperature to 600°C (10°C/min), pan type: Pt pan in disposable Al pan) was performed on Compounds 1, 5, and 9 by using thermo gravimetric analysis (TGA). Results thereof are shown in Table 5.

Table 5

Compound No.	Td(1%,°C)
1	310
5	230
9	245

[0169] Referring to Table 5, it has been determined that Compounds 1, 5, and 9 have excellent thermal stability.

[0170] Evaluation Example 3: Evaluation of Photoluminescence (PL) Spectrum Light emission characteristics of each Compound were evaluated by evaluating PL spectra of Compounds 1, 5, and 9. Compound 1 was diluted at a concentration of 10 millimolar (mM) in $CHCl_3$, and a PL spectrum was measured at room temperature by using an ICS PC1 Spectrofluorometer equipped with a xenon lamp. This process was repeated on Compounds 5 and 9.

[0171] Emission wavelengths and maximum emission wavelengths (λ_{max}) of the PL spectra of Compounds 1, 5, and 9 are shown in Table 6.

Table 6

Compound No.	Emission wavelengths(nm)
1	454(λ_{max}), 482
5	457(λ_{max}), 487
9	454(λ_{max}), 483

[0172] Referring to Table 6, it is confirmed that Compounds 1, 5, and 9 have PL emission characteristics suitable for deep blue light emission.

Example 1

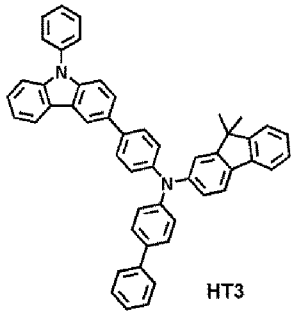
[0173] A glass substrate, on which an ITO electrode (first electrode, anode) having a thickness of 1,500 Å was formed, was sonicated with distilled water. After the sonicating with distilled water was completed, the glass substrate was ultrasonically cleaned by sequentially using iso-propyl alcohol, acetone, and methanol, was dried, and then transferred to a plasma cleaner. The glass substrate was cleaned for 5 minutes by using oxygen plasma and was provided to a vacuum deposition apparatus.

[0174] Compound HT3 was vacuum-deposited on the ITO electrode of the glass substrate to form a first hole injection layer having a thickness of 3,500 Å, Compound HT-D1 was vacuum-deposited on the first hole injection layer to form a second hole injection layer having a thickness of 300 Å, and TAPC was vacuum-deposited on the second hole injection layer to form an electron blocking layer having a thickness of 100 Å, thereby forming a hole transport region.

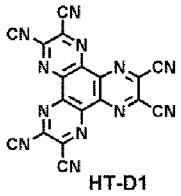
[0175] Compound H52 and Compound 1 (dopant, 10wt%) were co-deposited on the hole transport region to form an

emission layer having a thickness of 300 Å.

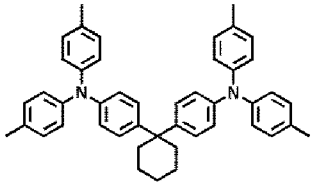
[0176] Compound ET3 was vacuum-deposited on the emission layer to form an electron transport layer having a thickness of 250 Å, ET-D1 (LiQ) was deposited on the electron transport layer to form an electron injection layer having a thickness of 5 Å, and Al was deposited on the electron injection layer to form a second electrode (cathode) having a thickness of 1,000 Å, thereby completing the manufacture of an organic light-emitting device.



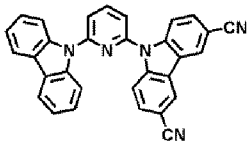
HT3



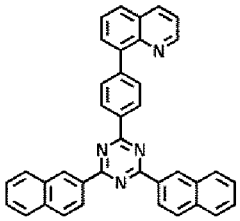
HT-D1



TAPC



H52



ET3

ET-D1

Examples 2 and 3

[0177] Organic light-emitting devices were manufactured in the same manner as in Example 1, except that Compounds shown in Table 7 were each used instead of Compound 1 as a dopant in forming an emission layer.

Evaluation Example 4: Evaluation of Characteristics of Organic Light-Emitting Device

[0178] An EL spectrum, a change in current density according to voltage, a change in luminance according to voltage, efficiency, conversion efficiency, external quantum emission efficiency, lifespan, and CIE color coordinates were measured with respect to the organic light-emitting devices manufactured according to Examples 1 to 3. Specific measurement methods are as follows, and results thereof are shown in Table 7.

(1) Measurement of EL spectrum

[0179] EL spectra of the manufactured organic light-emitting devices were measured by using a luminance meter (Minolta Cs-1000A) at a luminance of 500 candelas per square meter (cd/m^2).

(2) Measurement of Change in Current Density According to Voltage

[0180] A current value flowing through the manufactured organic light-emitting devices was measured by using a current-voltage meter (Keithley 2400) with respect to the manufactured organic light-emitting devices while increasing a voltage from 0 volts (V) to 10 V, and a current density was obtained by dividing the measured current value by an area.

(3) Measurement of Change in Luminance According to Voltage

[0181] Luminance was measured by using a luminance meter (Minolta Cs-1000A) with respect to the manufactured organic light-emitting devices while increasing a voltage from 0 V to 10 V, and results thereof were obtained.

(4) Measurement of Conversion Efficiency

[0182] Current efficiency (cd/A) of the same current density (10 milliamperes per square centimeter, mA/cm^2) was calculated by using the luminance and the current density measured from (2) and (3) and the voltage. Then, conversion efficiency was calculated by dividing the current efficiency by a y value of CIE color coordinates measured in (6).

(5) Measurement of Lifespan

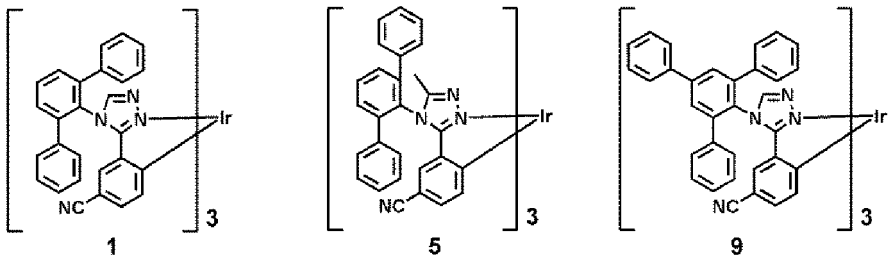
[0183] An amount of time (T_{95}) that lapsed when luminance measured from (3) was 95% of initial luminance (100%) was calculated.

(6) Measurement of CIE Color Coordinates

[0184] CIE color coordinates were obtained by measuring EL spectra of the manufactured organic light-emitting devices at a luminance of 500 cd/m^2 by using a luminance meter (Minolta Cs-1000A).

Table 7

Example	Dopant	Current density (mA/cm^2)	Luminance (cd/m^2)	Efficiency (cd/A)	Conversion Efficiency	EQE (%)	λ_{max} in EL spectrum (nm)	T_{95} (hr)	Color coordinates (x,y)
1	1	3.97	1000	25.24	110.1	14.6	455	3.03	0.166, 0.22 9
2	5	3.58	1000	28.09	108.2	15.0	458	0.96	0.171, 0.25 9
3	9	3.55	1000	28.23	120.4	16.2	457	2.85	0.169, 0.23 5



[0185] Referring to Table 7, it is confirmed that the organic light-emitting devices of Examples 1 to 3 have excellent efficiency, external quantum emission efficiency, and lifespan characteristics and can also emit deep blue light.

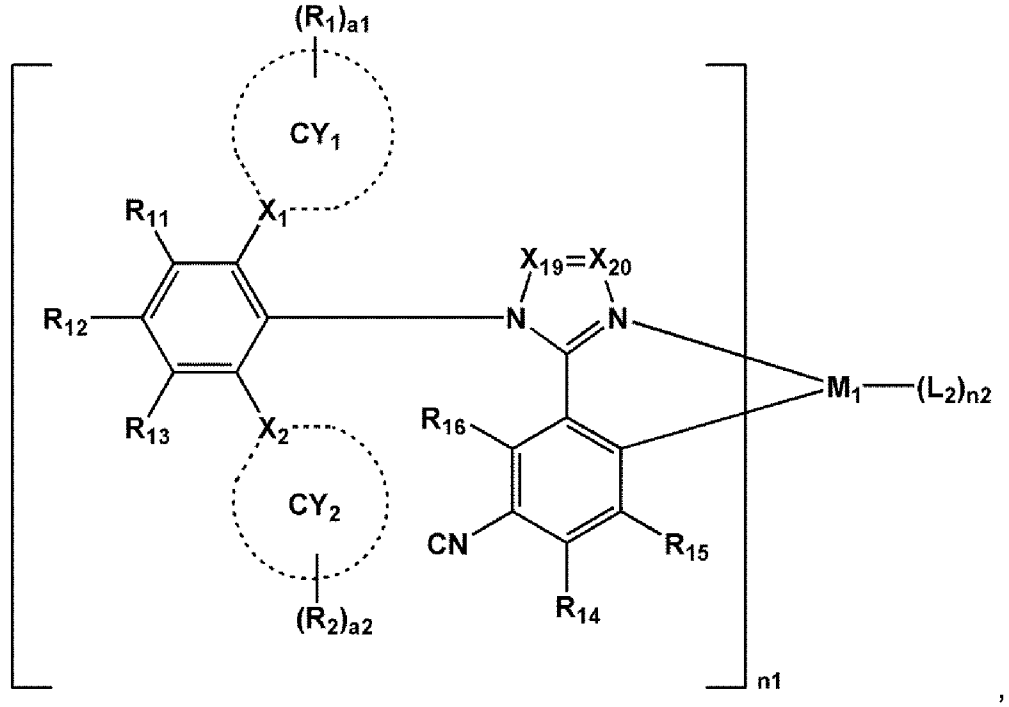
[0186] As described above, the organometallic compounds according to embodiments of the present disclosure have excellent electrical characteristics and thermal stability, and accordingly, organic light-emitting devices including such organometallic compounds may have excellent driving voltage, current density, efficiency, power, color purity, and lifespan characteristics.

[0187] It should be understood that embodiments described herein 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.

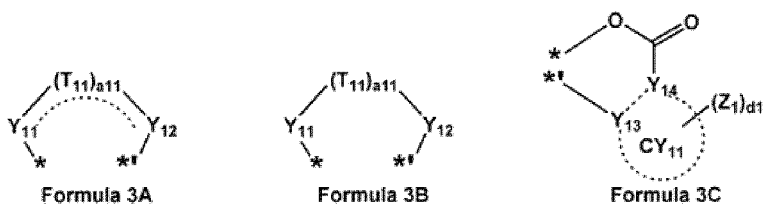
Claims

1. An organometallic compound represented by Formula 1:

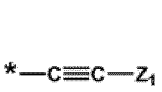
Formula 1



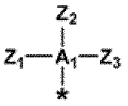
,



Formula 3A Formula 3B Formula 3C



Formula 3E



Formula 3F

wherein,

M_1 in Formula 1 is selected from a first-row transition metal of the Periodic Table of Elements, a second-row transition metal of the Periodic Table of Elements, and a third-row transition metal of the Periodic Table of Elements,
n1 in Formula 1 is 1, 2, or 3,
L_2 in Formula 1 is selected from ligands represented by Formulae 3A to 3C, 3E and 3F,
n2 in Formula 1 is 0, 1, 2, 3, or 4, wherein, when n2 is two or more, two or more groups L_2 are identical to or different from each other,
X_1 and X_2 in Formula 1 are each independently carbon or nitrogen,
CY_1 and CY_2 in Formula 1 are each independently a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group,
X_{19} in Formula 1 is N or $C(R_{19})$, and X_{20} is N or $C(R_{20})$, provided that at least one of X_{19} and X_{20} is N,
Y_{11} in Formula 3A is selected from O, N, $N(Z_1)$, $P(Z_1)(Z_2)$, and $As(Z_1)(Z_2)$,
Y_{12} in Formula 3A is selected from O, N, $N(Z_3)$, $P(Z_3)(Z_4)$, and $As(Z_3)(Z_4)$,
CY_{11} in Formula 3C is a C_2-C_{30} heterocyclic group,
T_{11} in Formula 3A is selected from a single bond, a double bond, *-$C(Z_{11})(Z_{12})$-*', *-$C(Z_{11})$=$C(Z_{12})$-*', *=$C(Z_{11})$-*', *-$C(Z_{11})$=*,, -$C(Z_{11})$-$C(Z_{12})$=$C(Z_{13})$-*', *-$C(Z_{11})$=$C(Z_{12})$-$C(Z_{13})$=*', *-$N(Z_{11})$-*', and a substituted or unsubstituted C_5-C_{30} carbocyclic group,
a11 in Formula 3A is an integer from 1 to 10,
Y_{13} and Y_{14} in Formula 3C are each independently carbon (C) or nitrogen (N), Y_{13} and Y_{14} are linked via a single bond or a double bond,
A_1 in Formula 3F is P or As,
d1 in Formula 2C is an integer from 0 to 10,
* and *' in Formulae 3A to 3C, 3E and 3F each indicate a binding site to M_1 in Formula 1,
R_1, R_2, R_{11} to R_{16}, R_{19}, R_{20}, Z_1 to Z_4 and Z_{11} to Z_{13} are each independently selected from hydrogen, deuterium, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and-$P(=O)(Q_8)(Q_9)$,
two or more neighboring groups selected from R_1, R_2, R_{11} to R_{13}, CY_1, and CY_2 are optionally linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a1 and a2 are each independently an integer from 0 to 5,
at least one substituent of the substituted C_5-C_{30} carbocyclic group, the substituted C_2-C_{30} heterocyclic group, the substituted C_1-C_{60} alkyl group, the substituted C_2-C_{60} alkenyl group, the substituted C_2-C_{60} alkynyl group, the substituted C_1-C_{60} 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_{60} aryl group, the substituted C_6-C_{60} aryloxy group, the substituted C_6-C_{60} arylthio group, the substituted C_7-C_{60} arylalkyl group, the substituted C_1-C_{60} heteroaryl group, the substituted C_1-C_{60} heteroaryloxy group, the substituted C_1-C_{60} heteroarylthio group, the substituted C_2-C_{60} heteroarylalkyl group, the substituted monovalent non-aromatic condensed polycyclic group, and the substituted monovalent non-aromatic condensed heteropolycyclic group is selected from:

deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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, and a C_1-C_{60} alkoxy group;

a C_1-C_{60} alkyl group, a C_2-C_{60} alkenyl group, a C_2-C_{60} alkynyl group, and a C_1-C_{60} alkoxy group, each substituted with at least one selected from deuterium, -F,-Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, 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_{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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_{11})(Q_{12})$, $-Si(Q_{13})(Q_{14})(Q_{15})$, $-B(Q_{16})(Q_{17})$, and $-P(=O)(Q_{18})(Q_{19})$;

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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group, each substituted with at least one selected from deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$,$-CF_2H$, $-CFH_2$, 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_1-C_{60} heteroaryl group, a C_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, a monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_{21})(Q_{22})$,$-Si(Q_{23})(Q_{24})(Q_{25})$, $-B(Q_{26})(Q_{27})$, and $-P(=O)(Q_{28})(Q_{29})$; and
$-N(Q_{31})(Q_{32})$, $-Si(Q_{33})(Q_{34})(Q_{35})$, $-B(Q_{36})(Q_{37})$, and $-P(=O)(Q_{38})(Q_{39})$, and

Q_1 to Q_9, Q_{11} to Q_{19}, Q_{21} to Q_{29}, and Q_{31} to Q_{39} are each independently selected from hydrogen, 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} aryl group substituted with at least one selected from a C_1-C_{60} alkyl group and 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_1-C_{60} heteroaryloxy group, a C_1-C_{60} heteroarylthio group, a C_2-C_{60} heteroarylalkyl group, a monovalent non-aromatic condensed polycyclic group, and a monovalent non-aromatic condensed heteropolycyclic group.

2. The organometallic compound of claim 1, wherein
M_1 is Ir or Os, and the sum of n1 and n2 is 3 or 4; or
M_1 is Pt, and the sum of n1 and n2 is 2.

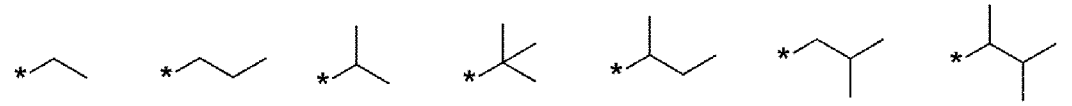
3. The organometallic compound of claims 1 or 2, wherein
CY_1 and CY_2 are each independently selected from a cyclopentene group, a cyclohexene group, a benzene group, a pyridine group, a pyrimidine group, a pyridazine group, a pyrazine group, a triazine group, a pyrrole group, a pyrazole group, an imidazole group, a triazole group, an oxazole group, an isoxazole group, an oxadiazole group, a thiazole group, an isothiazole group, and a thiadiazole group; and/or
wherein
X_{19} is $C(R_{19})$, and X_{20} is N, or
X_{19} is N, and X_{20} is $C(R_{20})$.

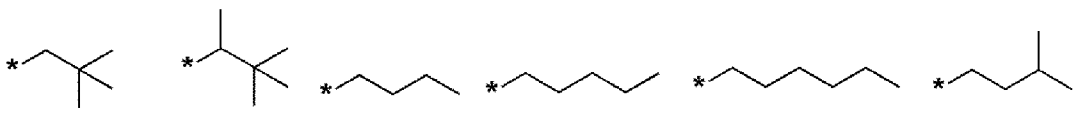
4. The organometallic compound of any of claims 1-3, wherein
R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} are each independently selected from:

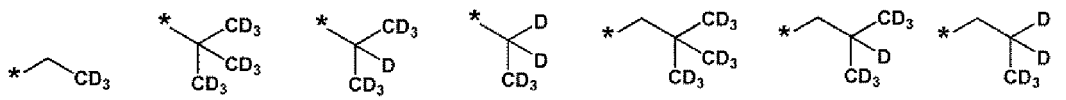
hydrogen, deuterium, -F, a cyano group, a nitro group, $-SF_5$, a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, an iso-butyl group, a sec-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a sec-pentyl group, a tert-pentyl group, an n-hexyl 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-decyl group, an iso-decyl group, a sec-decyl group, a tert-decyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group;
a methyl group, an ethyl group, an n-propyl group, an iso-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-decyl group, an iso-decyl group, a sec-decyl group, a tert-decyl group, a methoxy group, an ethoxy group, a propoxy group, a butoxy group, a pentoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group, each substituted with at least one selected from deuterium, -F, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, a cyano group, a nitro group, a C_1-C_{10} alkyl group, a C_1-C_{10} alkoxy group, a cyclopentyl group, a cyclohexyl group, a cycloheptyl group, a cyclooctyl group, an adamantanyl group, a norbornanyl group, a norbornenyl group, a cyclopentenyl group, a cyclohexenyl group, a cycloheptenyl group, a phenyl group, a naphthyl group, a pyridinyl group, a pyrimidinyl group, a dibenzofuranyl group, and a dibenzothiophenyl group; and
$-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and $-P(=O)(Q_8)(Q_9)$, and
Q_1 to Q_9 are each independently selected from:

$-CH_3$, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CH_2CH_3$, $-CH_2CD_3$, $-CH_2CD_2H$, $-CH_2CDH_2$,$-CHDCH_3$, $-CHDCD_2H$, $-CHDCDH_2$, $-CHDCD_3$, $-CD_2CD_3$, $-CD_2CD_2H$, and $-CD_2CDH_2$;
an n-propyl group, an iso-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, a phenyl group, and a naphthyl group; and
an n-propyl group, an iso-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, a phenyl group, and a naphthyl group, each substituted with at least one selected from deuterium, a C_1-C_{10} alkyl group, and a phenyl group.

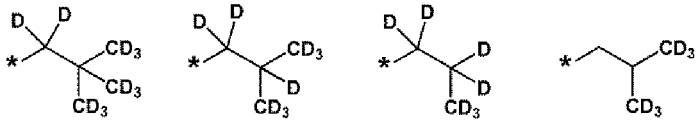
5. The organometallic compound of any of claims 1-4, wherein
R_1, R_2, R_{11} to R_{16}, R_{19}, and R_{20} are each independently selected from hydrogen, deuterium, $-CH_3$, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CH_2CH_3$, $-CH_2CD_3$, $-CH_2CD_2H$,$-CH_2CDH_2$, $-CHDCH_3$, $-CHDCD_2H$, $-CHDCDH_2$, $-CHDCD_3$, $-CD_2CD_3$, $-CD_2CD_2H$,$-CD_2CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, groups represented by Formulae 9-1 to 9-24, groups represented by Formulae 10-1 to 10-62, and $-Si(Q_3)(Q_4)(Q_5)$:


Formula 9-1 Formula 9-2 Formula 9-3 Formula 9-4 Formula 9-5 Formula 9-6 Formula 9-7

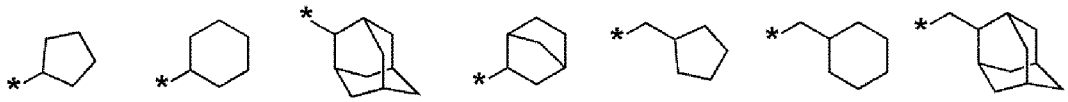

Formula 9-8 Formula 9-9 Formula 9-10 Formula 9-11 Formula 9-12 Formula 9-13



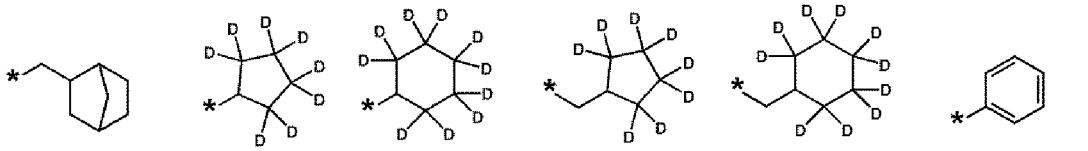
Formula 9-14 Formula 9-15 Formula 9-16 Formula 9-17 Formula 9-18 Formula 9-19 Formula 9-20



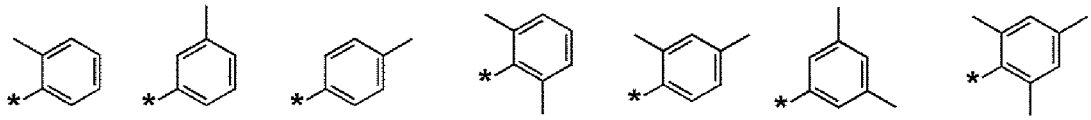
Formula 9-21 Formula 9-22 Formula 9-23 Formula 9-24



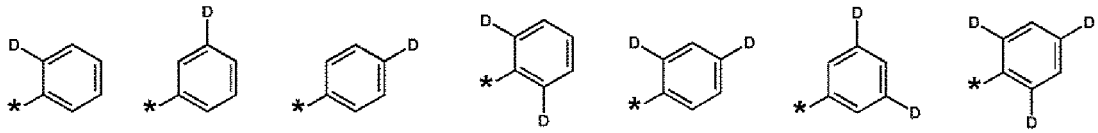
Formula 10-1 Formula 10-2 Formula 10-3 Formula 10-4 Formula 10-5 Formula10-6 Formula 10-7



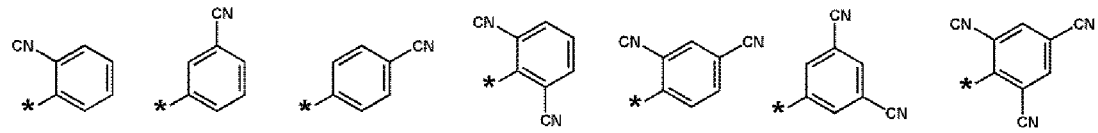
Formula 10-8 Formula 10-9 Formula 10-10 Formula 10-11 Formula 10-12 Formula 10-13



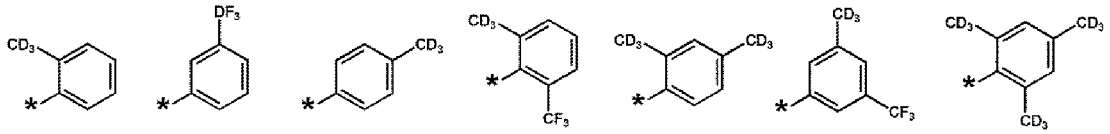
Formula 10-14 Formula 10-15 Formula 10-16 Formula 10-17 Formula 10-18 Formula 10-19 Formula 10-20



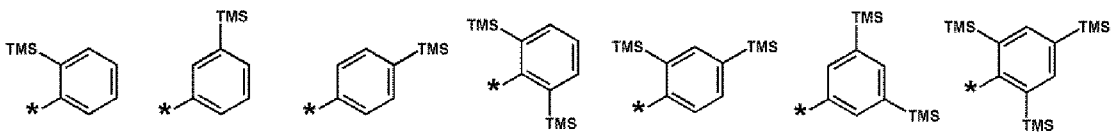
Formula 10-21 Formula 10-22 Formula 10-23 Formula 10-24 Formula 10-25 Formula 10-26 Formula 10-27



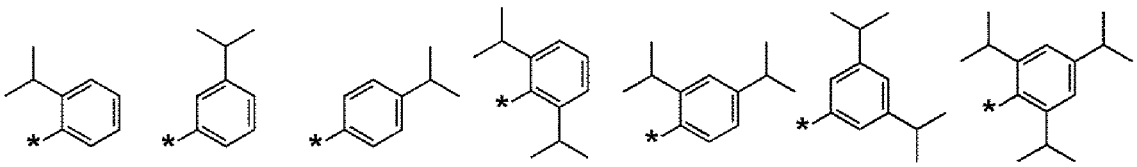
Formula 10-28 Formula 10-29 Formula 10-30 Formula 10-31 Formula 10-32 Formula 10-33 Formula 10-34



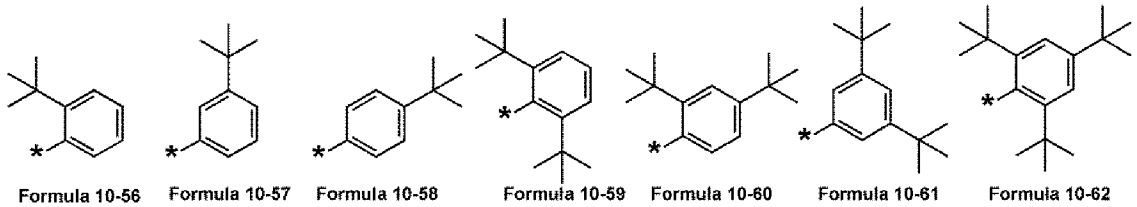
Formula 10-35 Formula 10-36 Formula 10-37 Formula 10-38 Formula 10-39 Formula 10-40 Formula 10-41



Formula 10-42 Formula 10-43 Formula 10-44 Formula 10-45 Formula 10-46 Formula 10-47 Formula 10-48



Formula 10-49 Formula 10-50 Formula 10-51 Formula 10-52 Formula 10-53 Formula 10-54 Formula 10-55



Formula 10-56 Formula 10-57 Formula 10-58 Formula 10-59 Formula 10-60 Formula 10-61 Formula 10-62

, wherein * in Formulae 9-1 to 9-24 and 10-1 to 10-62 indicates a binding site to a neighboring atom.

6. The organometallic compound of any of claims 1-5, wherein

i) X_{19} is $C(R_{19})$, X_{20} is N, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{19} is a deuterium-containing substituent;
ii) X_{19} is N, X_{20} is $C(R_{20})$, and at least one of R_1, R_2, R_{11} to R_{16}, and R_{20} is a deuterium-containing substituent; or
iii) X_{19} and X_{20} are each N, and at least one of R_1, R_2, and R_{11} to R_{16} is a deuterium-containing substituent, and

the deuterium-containing substituent is selected from:

deuterium; and
a C_1-C_{20} alkyl group, a C_1-C_{20} alkoxy group, and a phenyl group, each substituted with at least one deuterium;
preferably wherein
the deuterium-containing substituent is selected from:

deuterium; 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 neopentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one deuterium.

7. The organometallic compound of any of claims 1-6, wherein

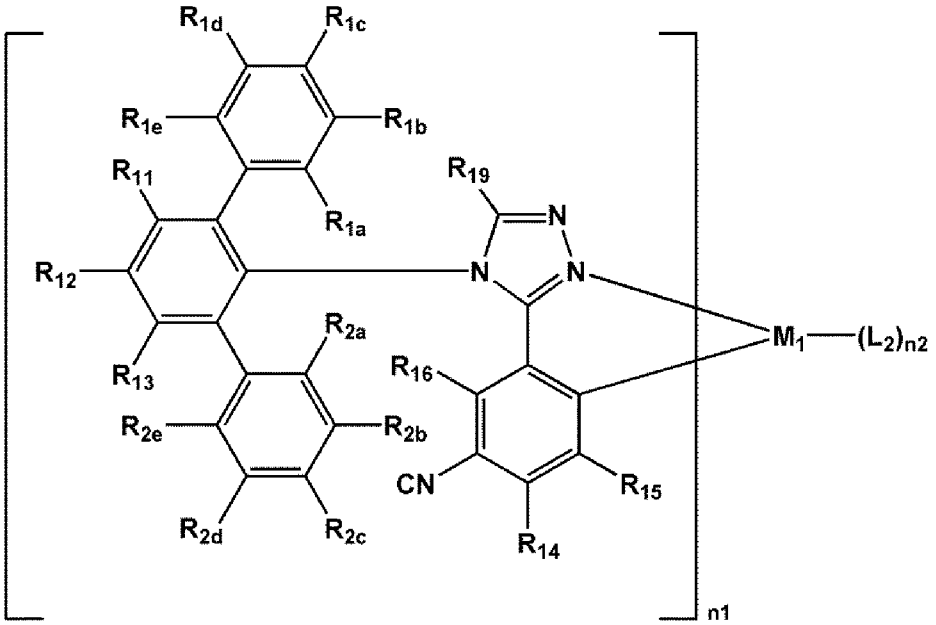
i) X_{19} is $C(R_{19})$, X_{20} is N, and at least one of R_{12}, R_{14}, and R_{19} is a deuterium-containing substituent;
ii) X_{19} is N, X_{20} is $C(R_{20})$, and at least one of R_{12}, R_{14}, and R_{20} is a deuterium-containing substituent; or
iii) X_{19} and X_{20} are each N, and at least one of R_{12} and R_{14} is a deuterium-containing substituent, and

the deuterium-containing substituent is selected from:

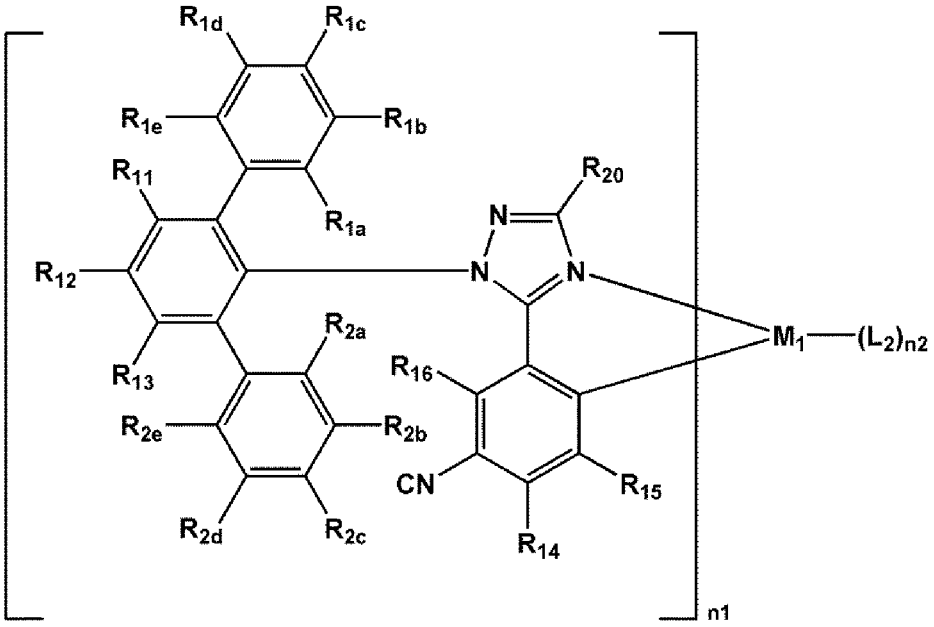
deuterium; and
a methyl group, an ethyl group, an n-propyl group, an iso-propyl group, an n-butyl group, a sec-butyl group, an iso-butyl group, a tert-butyl group, an n-pentyl group, an iso-pentyl group, a 1-methylbutyl group, a 2-methylbutyl group, a neopentyl group, a 1,2-dimethylpropyl group, and a tert-pentyl group, each substituted with at least one deuterium.

8. The organometallic compound of any of claims 1-7, wherein
the organometallic compound is represented by one of Formulae 1-1 to 1-3:

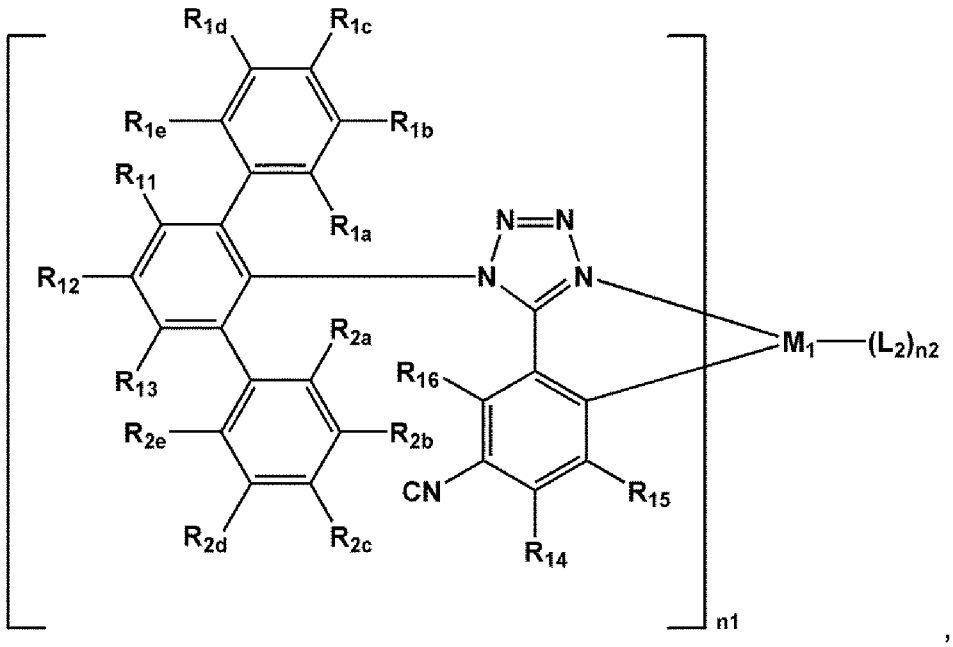
Formula 1-1



Formula 1-2



Formula 1-3

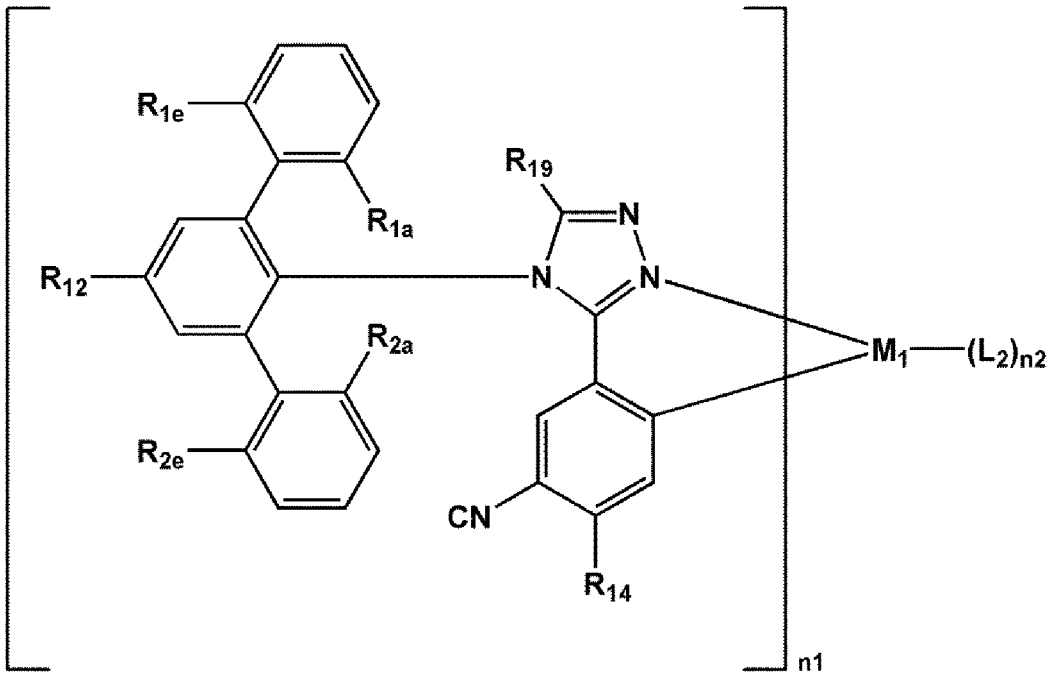


,

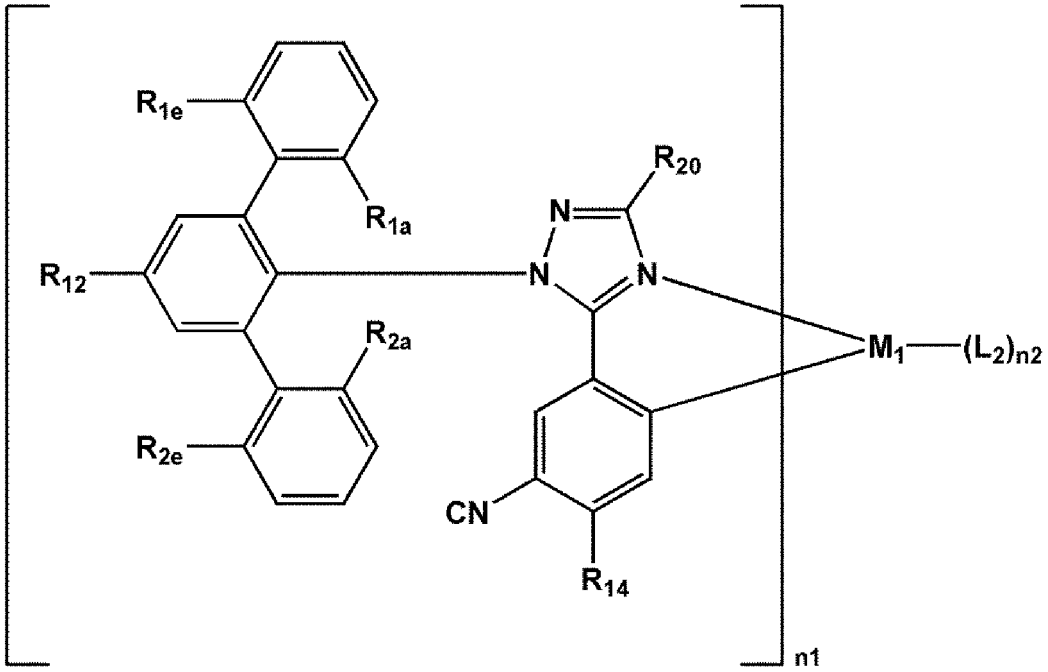
wherein, in Formulae 1-1 to 1-3, M_1, n1, L_2, n2, R_{11} to R_{16}, R_{19}, and R_{20} are each independently the same as described in claim 1, R_{1a} to R_{1e} are each independently the same as described in connection with R_1 in claim 1, and R_{2a} to R_{2e} are each independently the same as described in connection with R_2 in claim 1.

9. The organometallic compound of any of claims 1-8, wherein
the organometallic compound is represented by one of Formulae 1(1) to 1 (3):

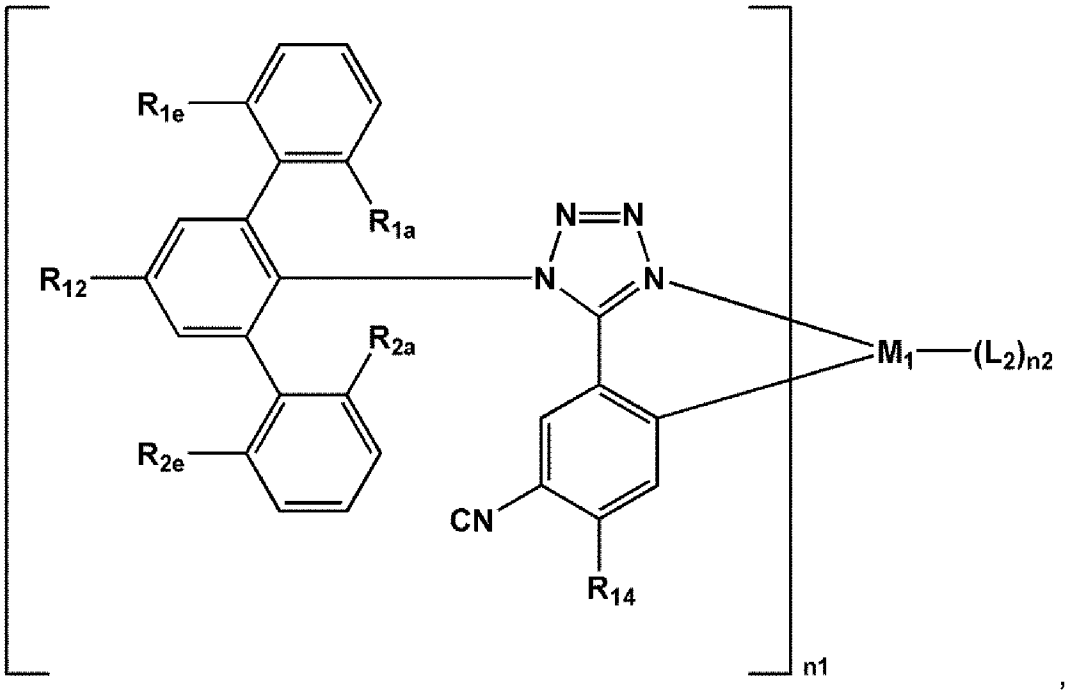
Formula 1(1)



Formula 1(2)



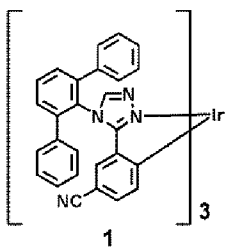
Formula 1(3)



,

wherein, in Formulae 1(1) to 1(3), M_1, n1, L_2, n2, R_{12}, R_{14}, R_{19}, and R_{20} are each independently the same as described in claim 1, R_{1a} and R_{1e} are each independently the same as described in connection with R_1 in claim 1, and R_{2a} and R_{2e} are each independently the same as described in connection with R_2 in claim 1.

10. The organometallic compound of any of claims 1-9, wherein the organometallic compound is one of Compounds 1 to 10: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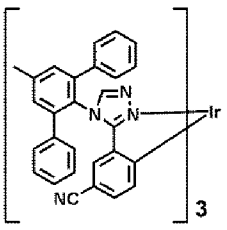
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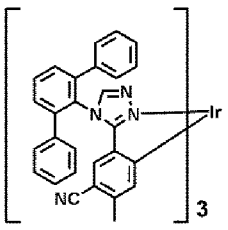
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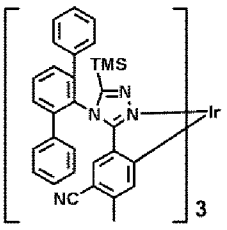
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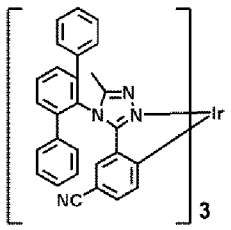
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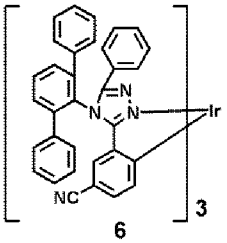
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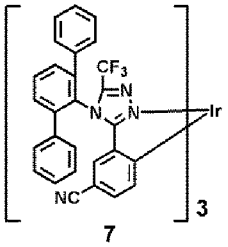
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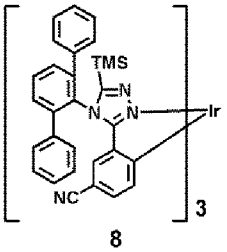
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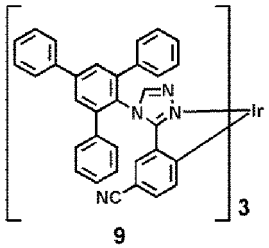
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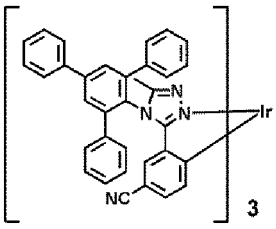
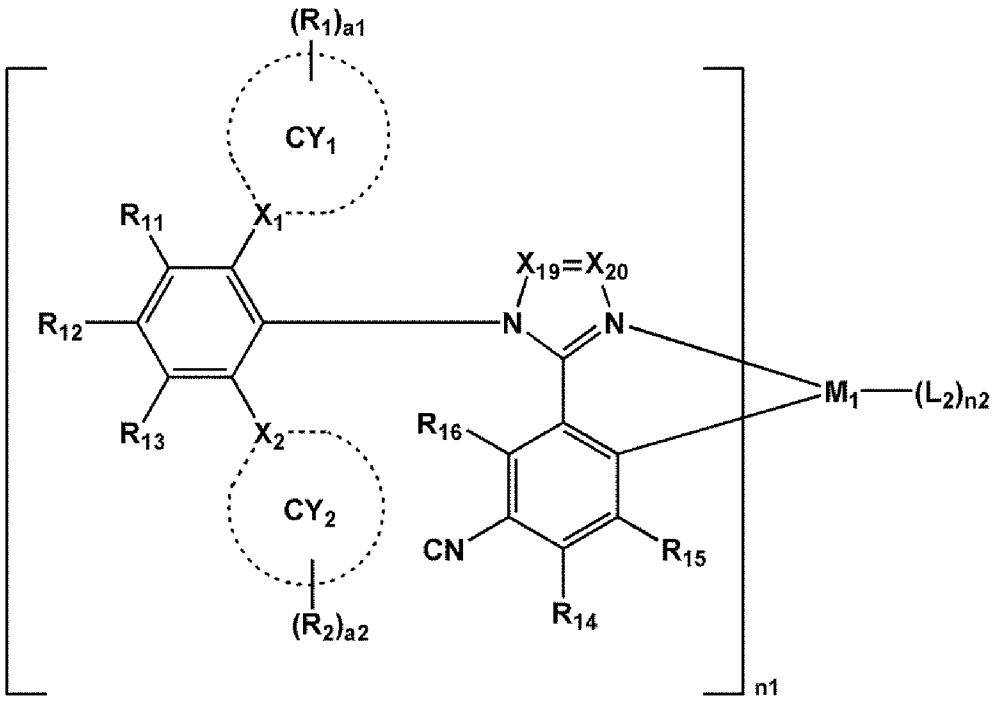

10

.

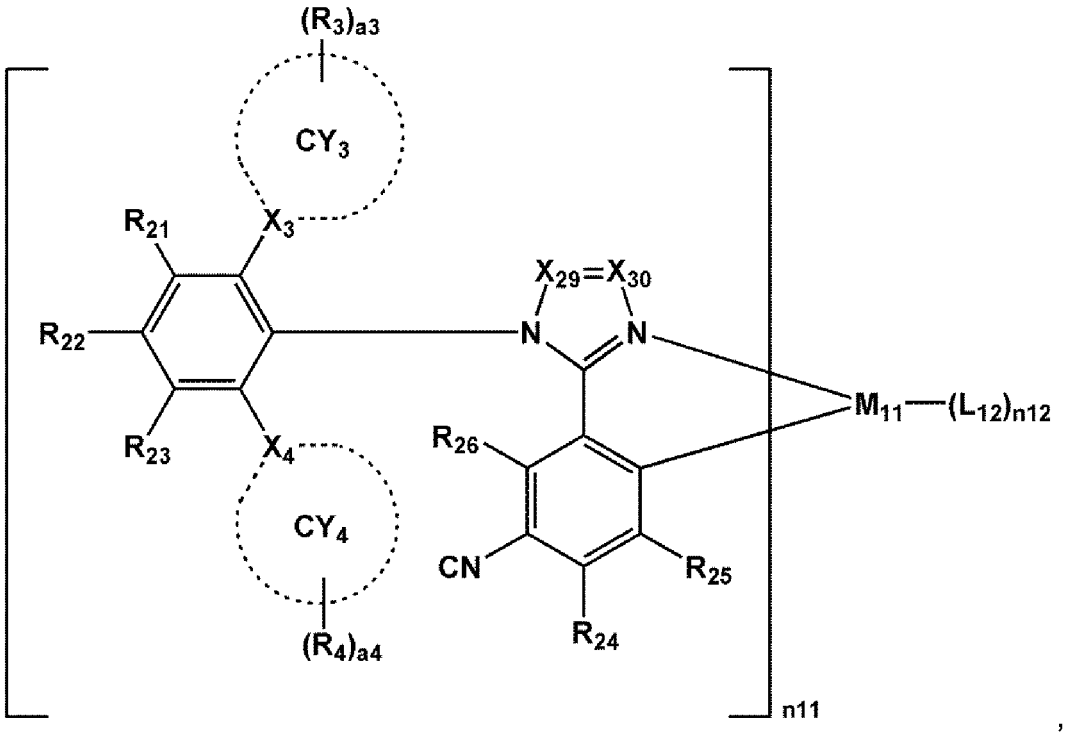
11. A composition containing an organometallic compound, the composition comprising:

a first organometallic compound represented by Formula 1 according to any of claims 1-10 and comprising at least one deuterium; and
a second organometallic compound represented by Formula 2:

Formula 1



Formula 2



,

wherein, in Formulae 1 and 2,

M_{11} is selected from a first-row transition metal of the Periodic Table of Elements, a second-row transition metal of the Periodic Table of Elements, and a third-row transition metal of the Periodic Table of Elements,
n11 is 1, 2, or 3,
L_{12} is a monodentate ligand or a bidentate ligand,
n12 is 0, 1, 2, 3, or 4, wherein, when n12 is two or more, two or more groups L_{12} are identical to or different

from each other,
X_3 and X_4 are each independently carbon or nitrogen,
CY_3 and CY_4 are each independently a C_5-C_{30} carbocyclic group or a C_2-C_{30} heterocyclic group,
X_{29} is N or $C(R_{29})$, and X_{30} is N or $C(R_{30})$, provided that at least one of X_{29} and X_{30} is N,
R_3, R_4, R_{21} to R_{26}, R_{29}, and R_{30} are each independently selected from hydrogen, -F, -Cl, -Br, -I, $-SF_5$, 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_1-C_{60} heteroaryloxy group, a substituted or unsubstituted C_1-C_{60} heteroarylthio group, a substituted or unsubstituted C_2-C_{60} heteroarylalkyl group, a substituted or unsubstituted monovalent non-aromatic condensed polycyclic group, a substituted or unsubstituted monovalent non-aromatic condensed heteropolycyclic group, $-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$, and-$P(=O)(Q_8)(Q_9)$,
two or more neighboring groups selected from R_3, R_4, R_{21} to R_{23}, CY_3, and CY_4 are optionally linked to form a substituted or unsubstituted C_5-C_{30} carbocyclic group or a substituted or unsubstituted C_2-C_{30} heterocyclic group,
a3 and a4 are each independently an integer from 0 to 5, and
R_3, R_4, R_{21} to R_{26}, R_{29}, and R_{30} are each a deuterium-free substituent; preferably wherein
a deuteration rate represented by Equation 2 is 50% or more:

Equation 2

$$\text{deuteration rate (\%)} = n_{D2}/(n_{H2} + n_{D2}) \times 100,$$

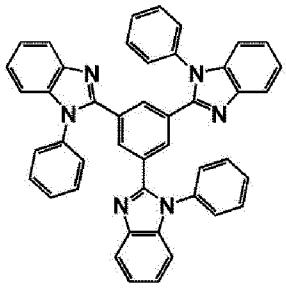
wherein, in Equation 2,

n_{H2} represents the sum of a total number of hydrogens included in deuterium-containing substituents in the first organometallic compound and a total number of hydrogens included in a deuterium-free substituent of the second organometallic compound corresponding to the deuterium-containing substituent in the first organometallic compound, and
n_{D2} represents a total number of deuterium atoms included in the deuterium-containing substituents in the first organometallic compound.

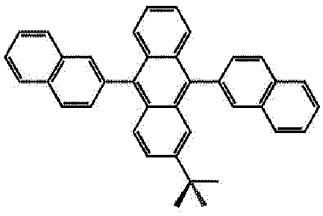
12. An organic light-emitting device comprising:

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,
wherein the organic layer comprises at least one of the organometallic compound of any of claims 1-10 or the composition of claim 11;
preferably wherein
the emission layer comprises the organometallic compound or the composition.

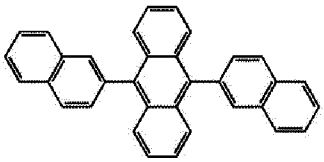
13. The organic light-emitting device of claim 12, wherein
the emission layer further comprises a host;
preferably wherein
the host is selected from the following compounds:



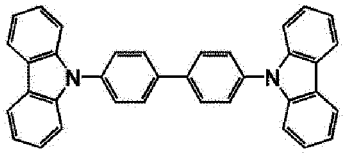
TPBi



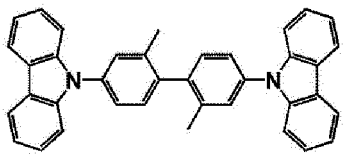
TBADN



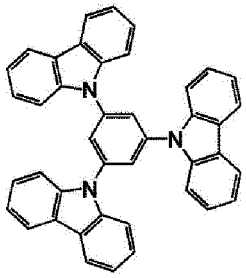
ADN



CBP



CDBP



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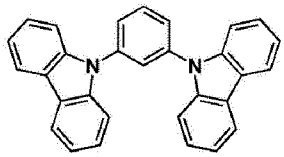

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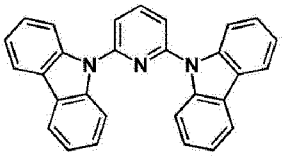

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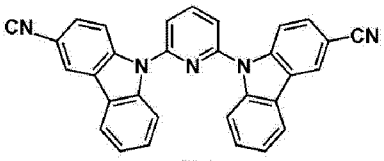
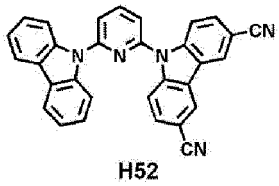


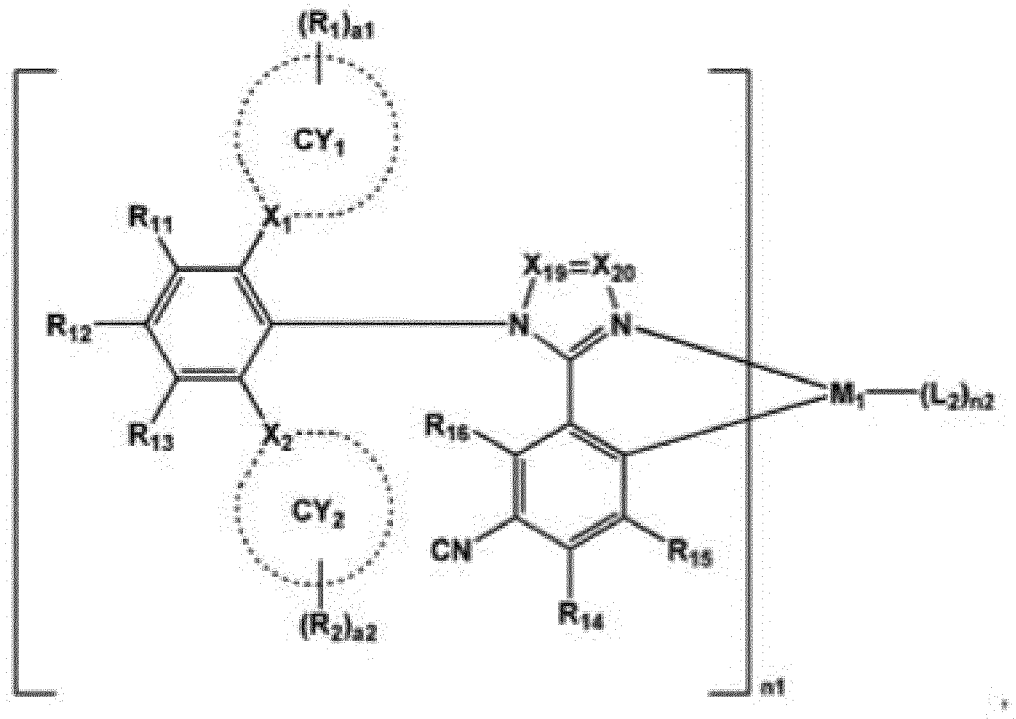
H51

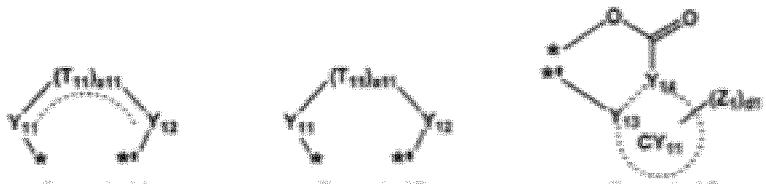


H52

Patentansprüche

1. Organometallische Verbindung, dargestellt durch Formel 1: Formel 1





Formel 3A Formel 3B Formel 3C

Formel 3E Formel 3F

wobei

M_1 in Formel 1 ausgewählt ist aus einem Übergangsmetall der ersten Reihe des Periodensystems, einem Übergangsmetall der zweiten Reihe des Periodensystems und einem Übergangsmetall der dritten Reihe des Periodensystems,
n1 in Formel 1 1, 2 oder 3 ist,
L_2 in Formel 1 ausgewählt ist aus Liganden, die durch die Formeln 3A bis 3C, 3E und 3F dargestellt sind,
n2 in Formel 1 0, 1, 2, 3 oder 4 ist, wobei, wenn n2 zwei oder mehr ist, zwei oder mehr Gruppen von L_2 miteinander identisch oder unterschiedlich sind,
X_1 und X_2 in Formel 1 jeweils unabhängig Kohlenstoff oder Stickstoff sind,
CY_1 und CY_2 in Formel 1 jeweils unabhängig eine C_5-C_{30} carbocyclische Gruppe oder eine C_2-C_{30} heterocyclische Gruppe sind,
X_{19} in Formel 1 N oder $C(R_{19})$ ist, und X_{20} N oder $C(R_{20})$ ist, vorausgesetzt, dass mindestens eines von X_{19} und X_{20} N ist,
Y_{11} in Formel 3A ausgewählt ist aus O, N, $N(Z_1)$, $P(Z_1)(Z_2)$ und $As(Z_1)(Z_2)$,
Y_{12} in Formel 3A ausgewählt ist aus O, N, $N(Z_3)$, $P(Z_3)(Z_4)$ und $As(Z_3)(Z_4)$,
CY_{11} in Formel 3C eine C_2-C_{30} heterocyclische Gruppe,

T_{11} in Formel 3A ausgewählt ist aus einer Einzelbindung, einer Doppelbindung, *-C(Z_{11})(Z_{12})-*', *-C(Z_{11})=C(Z_{12})-*', *=C(Z_{11})-*', *-C(Z_{11})=*', *=C(Z_{11})-C(Z_{12})=C(Z_{13})-*', *-C(Z_{11})=C(Z_{12})-C(Z_{13})=*', *-N(Z_{11})-*' und einer substituierten oder unsubstituierten C_5-C_{30} carbocyclischen Gruppe,
a11 in Formel 3A eine ganze Zahl von 1 bis 10 ist,
Y_{13} und Y_{14} in Formel 3C jeweils unabhängig Kohlenstoff (C) oder Stickstoff (N) sind, wobei Y_{13} und Y_{14} über eine Einzelbindung oder eine Doppelbindung verknüpft sind,
A_1 in Formel 3F P oder As ist,
d1 in Formel 2C eine ganze Zahl von 0 bis 10 ist,
* und *' in den Formeln 3A bis 3C, 3E und 3F jeweils eine Bindungsstelle an M_1 in Formel 1 anzeigen,
R_1, R_2, R_{11} bis R_{16}, R_{19}, R_{20}, Z_1 bis Z_4 und Z_{11} bis Z_{13} jeweils unabhängig ausgewählt sind aus Wasserstoff, Deuterium, -F, -Cl, -Br, -I, -SF_5, einer Hydroxylgruppe, einer Cyanogruppe, einer Nitrogruppe, einer Aminogruppe, einer Amidinogruppe, einer Hydrazingruppe, einer Hydrazongruppe, einer Carbonsäuregruppe oder einem Salz davon, einer Sulfonsäuregruppe oder einem Salz davon, einer Phosphorsäuregruppe oder einem Salz davon, einer substituierten oder unsubstituierten C_1-C_{60}-Alkylgruppe, einer substituierten oder unsubstituierten C_2-C_{60}-Alkenylgruppe, einer substituierten oder unsubstituierten C_2-C_{60}-Alkynylgruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Alkoxygruppe, einer substituierten oder unsubstituierten C_3-C_{10}-Cycloalkylgruppe, einer substituierten oder unsubstituierten C_1-C_{10}-Heterocycloalkylgruppe, einer substituierten oder unsubstituierten C_3-C_{10}-Cycloalkenylgruppe, einer substituierten oder unsubstituierten C_1-C_{10}-Heterocycloalkenylgruppe, einer substituierten oder unsubstituierten C_6-C_{60}-Arylgruppe, einer substituierten oder unsubstituierten C_6-C_{60}-Aryloxygruppe, einer substituierten oder unsubstituierten C_6-C_{60}-Arylthiogruppe, einer substituierten oder unsubstituierten C_7-C_{60}-Arylalkylgruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Heteroarylgruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Heteroaryloxygruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Heteroarylthiogruppe, einer substituierten oder unsubstituierten C_2-C_{60}-Heteroarylalkylgruppe, einer substituierten oder unsubstituierten monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer substituierten oder unsubstituierten monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe, -N(Q_1)(Q_2), -Si(Q_3)(Q_4)(Q_5), -B(Q_6)(Q_7) und -P(=O)(Q_8)(Q_9),
zwei oder mehr benachbarte Gruppen, die ausgewählt sind aus R_1, R_2, R_{11} bis R_{13}, CY_1 und CY_2, optional verknüpft sind, so dass sie eine substituierte oder unsubstituierte C_5-C_{30} carbocyclische Gruppe oder eine substituierte oder unsubstituierte C_2-C_{30} heterocyclische Gruppe bilden,
a1 und a2 jeweils unabhängig eine ganze Zahl von 0 bis 5 sind,
mindestens ein Substituent der substituierten C_5-C_{30} carbocyclischen Gruppe, der substituierten C_2-C_{30} heterocyclischen Gruppe, der substituierten C_1-C_{60}-Alkylgruppe, der substituierten C_2-C_{60}-Alkenylgruppe, der substituierten C_2-C_{60}-Alkynylgruppe, der substituierten C_1-C_{60}-Alkoxygruppe, der substituierten C_3-C_{10}-Cycloalkylgruppe, der substituierten C_1-C_{10}-Heterocycloalkylgruppe, der substituierten C_3-C_{10}-Cycloalkenylgruppe, der substituierten C_1-C_{10}-Heterocycloalkenylgruppe, der substituierten C_6-C_{60}-Arylgruppe, der substituierten C_6-C_{60}-Aryloxygruppe, der substituierten C_6-C_{60}-Arylthiogruppe, der substituierten C_7-C_{60}-Arylalkylgruppe, der substituierten C_1-C_{60}-Heteroarylgruppe, der substituierten C_1-C_{60}-Heteroaryloxygruppe, der substituierten C_1-C_{60}-Heteroarylthiogruppe, der substituierten C_2-C_{60}-Heteroarylalkylgruppe, der substituierten monovalenten nichtaromatischen kondensierten polycyclischen Gruppe und der substituierten monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe ausgewählt ist aus:

Deuterium, -F, -Cl, -Br, -I, -CD_3, -CD_2H, -CDH_2, -CF_3, -CF_2H, -CFH_2, einer Hydroxylgruppe, einer Cyanogruppe, einer Nitrogruppe, einer Aminogruppe, einer Amidinogruppe, einer Hydrazingruppe, einer Hydrazongruppe, einer Carbonsäuregruppe oder einem Salz davon, einer Sulfonsäuregruppe oder einem Salz davon, einer Phosphorsäuregruppe oder einem Salz davon, einer C_1-C_{60}-Alkylgruppe, einer C_2-C_{60}-Alkenylgruppe, einer C_2-C_{60}-Alkynylgruppe und einer C_1-C_{60}-Alkoxygruppe;
einer C_1-C_{60}-Alkylgruppe, einer C_2-C_{60}-Alkenylgruppe, einer C_2-C_{60}-Alkynylgruppe und einer C_1-C_{60}-Alkoxygruppe, jeweils substituiert mit mindestens einem, ausgewählt aus Deuterium, -F, -Cl, -Br, -I, -CD_3, -CD_2H, -CDH_2, -CF_3, -CF_2H,-CFH_2, einer Hydroxylgruppe, einer Cyanogruppe, einer Nitrogruppe, einer Aminogruppe, einer Amidinogruppe, einer Hydrazingruppe, einer Hydrazongruppe, einer Carbonsäuregruppe oder einem Salz davon, einer Sulfonsäuregruppe oder einem Salz davon, einer Phosphorsäuregruppe oder einem Salz davon, einer C_3-C_{10}-Cycloalkylgruppe, einer C_1-C_{10}-Heterocycloalkylgruppe, einer C_3-C_{10}-Cycloalkenylgruppe, einer C_1-C_{10}-Heterocycloalkenylgruppe, einer C_6-C_{60}-Arylgruppe, einer C_6-C_{60}-Aryloxygruppe, einer C_6-C_{60}-Arylthiogruppe, einer C_7-C_{60}-Arylalkylgruppe, einer C_1-C_{60}-Heteroarylgruppe, einer C_1-C_{60}-Heteroaryloxygruppe, einer C_1-C_{60}-Heteroarylthiogruppe, einer C_2-C_{60}-Heteroarylalkylgruppe, einer monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe, -N(Q_{11})(Q_{12}),-Si(Q_{13})(Q_{14})(Q_{15}), -B(Q_{16})(Q_{17}) und -P(=O)(Q_{18})(Q_{19});

einer C_3-C_{10}-Cycloalkylgruppe, einer C_1-C_{10}-Heterocycloalkylgruppe, einer C_3-C_{19}-Cycloalkenylgruppe, einer C_1-C_{10}-Heterocycloalkenylgruppe, einer C_6-C_{60}-Arylgruppe, einer C_6-C_{60}-Aryloxygruppe, einer C_6-C_{60}-Arylthiogruppe, einer C_7-C_{60}-Arylalkylgruppe, einer C_1-C_{60}-Heteroarylgruppe, einer C_1-C_{60}-Heteroaryloxygruppe, einer C_1-C_{60}-Heteroarylthiogruppe, einer C_2-C_{60}-Heteroarylalkylgruppe, einer monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe;
einer C_3-C_{10}-Cycloalkylgruppe, einer C_1-C_{10}-Heterocycloalkylgruppe, einer C_3-C_{19}-Cycloalkenylgruppe, einer C_1-C_{10}-Heterocycloalkenylgruppe, einer C_6-C_{60}-Arylgruppe, einer C_6-C_{60}-Aryloxygruppe, einer C_6-C_{60}-Arylthiogruppe, einer C_7-C_{60}-Arylalkylgruppe, einer C_1-C_{60}-Heteroarylgruppe, einer C_1-C_{60}-Heteroaryloxygruppe, einer C_1-C_{60}-Heteroarylthiogruppe, einer C_2-C_{60}-Heteroarylalkylgruppe, einer monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe, jeweils substituiert mit mindestens einem, ausgewählt aus Deuterium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, einer Hydroxylgruppe, einer Cyanogruppe, einer Nitrogruppe, einer Aminogruppe, einer Amidinogruppe, einer Hydrazingruppe, einer Hydrazongruppe, einer Carbonsäuregruppe oder einem Salz davon, einer Sulfonsäuregruppe oder einem Salz davon, einer Phosphorsäuregruppe oder einem Salz davon, einer C_1-C_{60}-Alkylgruppe, einer C_2-C_{60}-Alkenylgruppe, einer C_2-C_{60}-Alkynylgruppe, C_1-C_{60}-Alkoxygruppe, einer C_3-C_{10}-Cycloalkylgruppe, einer C_1-C_{10}-Heterocycloalkylgruppe, einer C_3-C_{10}-Cycloalkenylgruppe, einer C_1-C_{10}-Heterocycloalkenylgruppe, einer C_6-C_{60}-Arylgruppe, einer C_6-C_{60}-Aryloxygruppe, einer C_6-C_{60}-Arylthiogruppe, einer C_7-C_{60}-Arylalkylgruppe, einer C_1-C_{60}-Heteroarylgruppe, einer C_1-C_{60}-Heteroaryloxygruppe, einer C_1-C_{60}-Heteroarylthiogruppe, einer C_2-C_{60}-Heteroarylalkylgruppe, einer monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe, $-N(Q_{21})(Q_{22})$, $-Si(Q_{23})(Q_{24})(Q_{25})$, $-B(Q_{26})(Q_{27})$ und $-P(=O)(Q_{28})(Q_{29})$; und
$-N(Q_{31})(Q_{32})$, $-Si(Q_{33})(Q_{34})(Q_{35})$, $-B(Q_{36})(Q_{37})$ und $-P(=O)(Q_{38})(Q_{39})$; und
Q_1 bis Q_9, Q_{11} bis Q_{19}, Q_{21} bis Q_{29} und Q_{31} bis Q_{39} sind jeweils unabhängig ausgewählt aus Wasserstoff, Deuterium, -F, -Cl, -Br, -I, einer Hydroxylgruppe, einer Cyanogruppe, einer Nitrogruppe, einer Aminogruppe, einer Amidinogruppe, einer Hydrazingruppe, einer Hydrazongruppe, einer Carbonsäuregruppe oder einem Salz davon, einer Sulfonsäuregruppe oder einem Salz davon, einer Phosphorsäuregruppe oder einem Salz davon, einer C_1-C_{60}-Alkylgruppe, einer C_2-C_{60}-Alkenylgruppe, einer C_2-C_{60}-Alkynylgruppe, C_1-C_{60}-Alkoxygruppe, einer C_3-C_{10}-Cycloalkylgruppe, einer C_1-C_{10}-Heterocycloalkylgruppe, einer C_3-C_{10}-Cycloalkenylgruppe, einer C_1-C_{10}-Heterocycloalkenylgruppe, einer C_6-C_{60}-Arylgruppe, einer C_6-C_{60}-Aryloxygruppe, einer C_6-C_{60}-Arylthiogruppe, einer C_7-C_{60}-Arylalkylgruppe, einer C_1-C_{60}-Heteroarylgruppe, einer C_1-C_{60}-Heteroaryloxygruppe, einer C_1-C_{60}-Heteroarylthiogruppe, einer C_2-C_{60}-Heteroarylalkylgruppe, einer monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe.

2. Organometallische Verbindung nach Anspruch 1, wobei
M_1 Ir oder Os ist, und wobei die Summe aus n1 und n2 3 oder 4 ist; oder
M_1 Pt ist, und die Summe aus n1 und n2 2 ist.

3. Organometallische Verbindung nach Anspruch 1 oder 2, wobei
CY_1 und CY_2 jeweils unabhängig ausgewählt sind aus einer Cyclopentengruppe, einer Cyclohexengruppe, einer Benzolgruppe, einer Pyridingruppe, einer Pyrimidingruppe, einer Pyridazingruppe, einer Pyrazingruppe, einer Triazingruppe, einer Pyrrolgruppe, einer Pyrazolgruppe, einer Imidazolgruppe, einer Triazolgruppe, einer Oxazolgruppe, einer Isoxazolgruppe, einer Oxadiazolgruppe, einer Thiazolgruppe, einer Isothiazolgruppe und einer Thiadiazolgruppe;
und/oder
wobei

X_{19} $C(R_{19})$ ist und X_{20} N ist, oder
X_{19} N ist und X_{20} $C(R_{20})$ ist.

4. Organometallische Verbindung nach einem der Ansprüche 1 bis 3, wobei R_1, R_2, R_{11} bis R_{16}, R_{19} und R_{20} jeweils unabhängig ausgewählt sind aus:

Wasserstoff, Deuterium, -F, einer Cyanogruppe, einer Nitrogruppe, $-SF_5$, einer Methylgruppe, einer Ethylgruppe, einer n-Propylgruppe, einer Isopropylgruppe, einer n-Butylgruppe, einer Isobutylgruppe, einer sec-Butylgruppe, einer tert-Butylgruppe, einer n-Pentylgruppe, einer Isopentylgruppe, einer sec-Pentylgruppe, einer tert-Pentyl-

gruppe, einer n-Hexylgruppe, einer Isohexylgruppe, einer sec-Hexylgruppe, einer tert-Hexylgruppe, einer n-Heptylgruppe, einer Isoheptylgruppe, einer sec-Heptylgruppe, einer tert-Heptylgruppe, einer n-Octylgruppe, einer Isooctylgruppe, einer sec-Octylgruppe, einer tert-Octylgruppe, einer n-Nonylgruppe, einer Isononylgruppe, einer sec-Nonylgruppe, einer tert-Nonylgruppe, einer n-Decylgruppe, einer Isodecylgruppe, einer sec-Decylgruppe, einer tert-Decylgruppe, einer Methoxygruppe, einer Ethoxygruppe, einer Propoxygruppe, einer Butoxygruppe, einer Pentoxygruppe, einer Cyclopentylgruppe, einer Cyclohexylgruppe, einer Cycloheptylgruppe, einer Cyclooctylgruppe, einer Adamantanylgruppe, einer Norbornanylgruppe, einer Norbornenylgruppe, einer Cyclopentylgruppe, einer Cyclohexenylgruppe, einer Cycloheptenylgruppe, einer Phenylgruppe, einer Naphthylgruppe, einer Pyridinylgruppe, einer Pyrimidinylgruppe, einer Dibenzofuranylgruppe und einer Dibenzothiophenylgruppe;

einer Methylgruppe, einer Ethylgruppe, einer n-Propylgruppe, einer Isopropylgruppe, einer n-Butylgruppe, einer Isobutylgruppe, einer sec-Butylgruppe, einer tert-Butylgruppe, einer n-Pentylgruppe, einer Isopentylgruppe, einer sec-Pentylgruppe, einer tert-Pentylgruppe, einer n-Hexylgruppe, einer Isohexylgruppe, einer sec-Hexylgruppe, einer tert-Hexylgruppe, einer n-Heptylgruppe, einer Isoheptylgruppe, einer sec-Heptylgruppe, einer tert-Heptylgruppe, einer n-Octylgruppe, einer Isooctylgruppe, einer sec-Octylgruppe, einer tert-Octylgruppe, einer n-Nonylgruppe, einer Isononylgruppe, einer sec-Nonylgruppe, einer tert-Nonylgruppe, einer n-Decylgruppe, einer Isodecylgruppe, einer sec-Decylgruppe, einer tert-Decylgruppe, einer Methoxygruppe, einer Ethoxygruppe, einer Propoxygruppe, einer Butoxygruppe, einer Pentoxygruppe, einer Cyclopentylgruppe, einer Cyclohexylgruppe, einer Cycloheptylgruppe, einer Cyclooctylgruppe, einer Adamantanylgruppe, einer Norbornanylgruppe, einer Norbornenylgruppe, einer Cyclopentylgruppe, einer Cyclohexenylgruppe, einer Cycloheptenylgruppe, einer Phenylgruppe, einer Naphthylgruppe, einer Pyridinylgruppe, einer Pyrimidinylgruppe, einer Dibenzofuranylgruppe und einer Dibenzothiophenylgruppe, jeweils substituiert mit mindestens einem, ausgewählt aus Deuterium, -F, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$,$-CFH_2$, einer Cyanogruppe, einer Nitrogruppe, einer C_1-C_{10}-Alkylgruppe, einer C_1-C_{10}-Alkoxygruppe, einer Cyclopentylgruppe, einer Cyclohexylgruppe, einer Cycloheptylgruppe, einer Cyclooctylgruppe, einer Adamantanylgruppe, einer Norbornanylgruppe, einer Norbornenylgruppe, einer Cyclopentylgruppe, einer Cyclohexenylgruppe, einer Cycloheptenylgruppe, einer Phenylgruppe, einer Naphthylgruppe, einer Pyridinylgruppe, einer Pyrimidinylgruppe, einer Dibenzofuranylgruppe und einer Dibenzothiophenylgruppe; und

$-N(Q_1)(Q_2)$, $-Si(Q_3)(Q_4)(Q_5)$, $-B(Q_6)(Q_7)$ und $-P(=O)(Q_8)(Q_9)$, und

Q_1 bis Q_9 sind jeweils unabhängig ausgewählt aus:

$-CH_3$, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CH_2CH_3$, $-CH_2CD_3$, $-CH_2CD_2H$, $-CH_2CDH_2$,$-CHDCH_3$, $-CHDCD_2H$, $-CHDCDH_2$, $-CHDCD_3$, $-CD_2CD_3$, $-CD_2CD_2H$ und $-CD_2CDH_2$;

einer n-Propylgruppe, einer Isopropylgruppe, einer n-Butylgruppe, einer Isobutylgruppe, einer sec-Butylgruppe, einer tert-Butylgruppe, einer n-Pentylgruppe, einer Isopentylgruppe, einer sec-Pentylgruppe, einer tert-Pentylgruppe, einer Phenylgruppe und einer Naphthylgruppe; und

einer n-Propylgruppe, einer Isopropylgruppe, einer n-Butylgruppe, einer Isobutylgruppe, einer sec-Butylgruppe, einer tert-Butylgruppe, einer n-Pentylgruppe, einer Isopentylgruppe, einer sec-Pentylgruppe, einer tert-Pentylgruppe, einer Phenylgruppe und einer Naphthylgruppe, jeweils substituiert mit mindestens einem, ausgewählt aus Deuterium, einer C_1-C_{19}-Alkylgruppe und einer Phenylgruppe.

5. Organometallische Verbindung nach einem der Ansprüche 1 bis 4, wobei

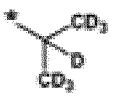
R_1, R_2, R_{11} bis R_{16}, R_{19} und R_{20} jeweils unabhängig ausgewählt sind aus Wasserstoff, Deuterium, $-CH_3$, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CH_2CH_3$, $-CH_2CD_3$, $-CH_2CD_2H$,$-CH_2CDH_2$, $-CHDCH_3$, $-CHDCD_2H$, $-CHDCDH_2$, $-CHDCD_3$, $-CD_2CD_3$, $-CD_2CD_2H$,$-CD_2CDH_2$, $-CF_3$, $-CF_2H$, $-CFH_2$, Gruppen, die durch die Formeln 9-1 bis 9-24 dargestellt sind, Gruppen, die durch die Formeln 10-1 bis 10-62 dargestellt sind, und-$Si(Q_3)(Q_4)(Q_5)$:

Formel 9-1 Formel 9-2 Formel 9-3 Formel 9-4 Formel 9-5 Formel 9-6 Formel 9-7

Formel 9-8 Formel 9-9 Formel 9-10 Formel 9-11 Formel 9-12 Formel 9-13

Formel 9-14

Formel 9-15



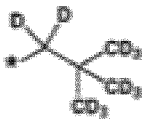
Formel 9-16

Formel 9-17

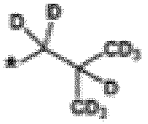
Formel 9-18

Formel 9-19

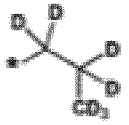
Formel 9-20



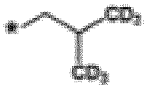
Formel 9-21



Formel 9-22



Formel 9-23



Formel 9-24

Formel 10-1

Formel 10-2

Formel 10-3

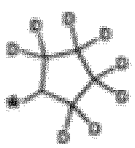
Formel 10-4

Formel 10-5

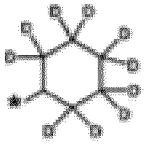
Formel 10-6

Formel 10-7

Formel 10-8



Formel 10-9



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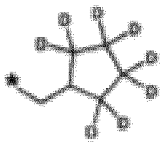
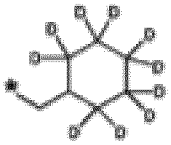


Formel 10-11

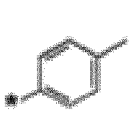


Formel 10-12

Formel 10-13

Formel 10-14

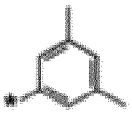
Formel 10-15



Formel 10-16

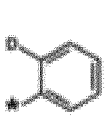
Formel 10-17

Formel 10-18

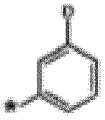


Formel 10-19

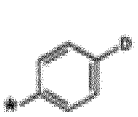
Formel 10-20



Formel 10-21



Formel 10-22



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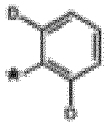
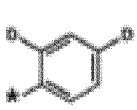
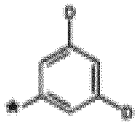


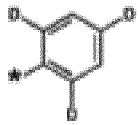
Formel 10-24



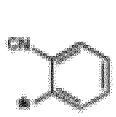
Formel 10-25



Formel 10-26



Formel 10-27



Formel 10-28

Formel 10-29

Formel 10-30

Formel 10-31

Formel 10-32

Formel 10-33

Formel 10-34

Formel 10-35

Formel 10-36

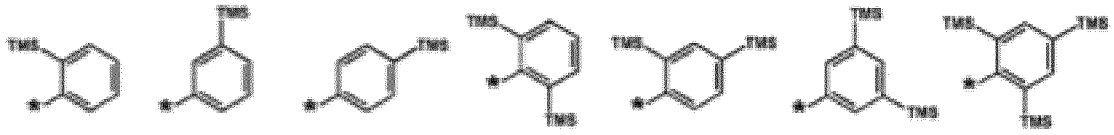
Formel 10-37

Formel 10-38

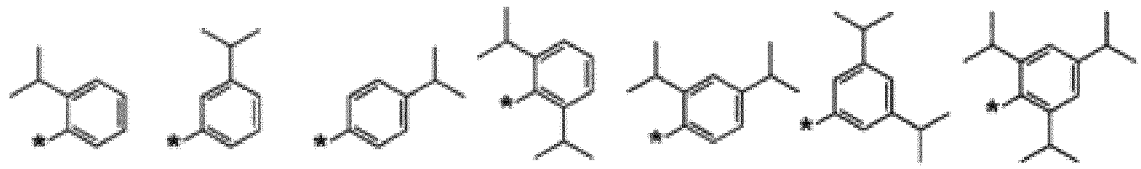
Formel 10-39

Formel 10-40

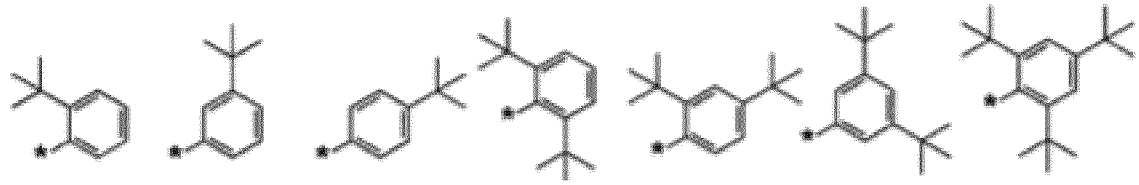
Formel 10-41



Formel 10-42 Formel 10-43 Formel 10-44 Formel 10-45 Formel 10-46 Formel 10-47 Formel 10-48



Formel 10-49 Formel 10-50 Formel 10-51 Formel 10-52 Formel 10-53 Formel 10-54 Formel 10-55



Formel 10-56 Formel 10-57 Formel 10-58 Formel 10-59 Formel 10-60 Formel 10-61 Formel 10-62,

wobei * in den Formeln 9-1 bis 9-24 und 10-1 bis 10-62 eine Bindungsstelle mit einem benachbarten Atom anzeigt.

6. Organometallische Verbindung nach einem der Ansprüche 1 bis 5, wobei

i) X_{19} $C(R_{19})$ ist, X_{20} N ist und mindestens eines von R_1, R_2, R_{11} bis R_{16} und R_{19} ein Deuterium enthaltender Substituent ist;
ii) X_{19} N ist, X_{20} $C(R_{20})$ ist und mindestens eines von R_1, R_2, R_{11} bis R_{16} und R_{20} ein Deuterium enthaltender Substituent ist;
iii) X_{19} und X_{20} jeweils N sind und mindestens eines von R_1, R_2 und R_{11} bis R_{16} ein Deuterium enthaltender Substituent ist, und wobei

der Deuterium enthaltende Substituent ausgewählt ist aus:

Deuterium; und
einer C_1-C_{29}-Alkylgruppe, einer C_1-C_{29}-Alkoxygruppe und einer Phenylgruppe, jeweils substituiert mit mindestens einem Deuterium;
wobei vorzugsweise
der Deuterium enthaltende Substituent ausgewählt ist aus:

Deuterium; und
einer Methylgruppe, einer Ethylgruppe, einer n-Propylgruppe, einer Isopropylgruppe, einer n-Butylgruppe, einer sec-Butylgruppe, einer Isobutylgruppe, einer tert-Butylgruppe, einer n-Pentylgruppe, einer Isopentylgruppe, einer 1-Methylbutylgruppe, einer 2-Methylbutylgruppe, einer Neopentylgruppe, einer 1,2-Dimethylpropylgruppe und einer tert-Pentylgruppe, jeweils substituiert mit mindestens einem Deuterium.

7. Organometallische Verbindung nach einem der Ansprüche 1 bis 6, wobei

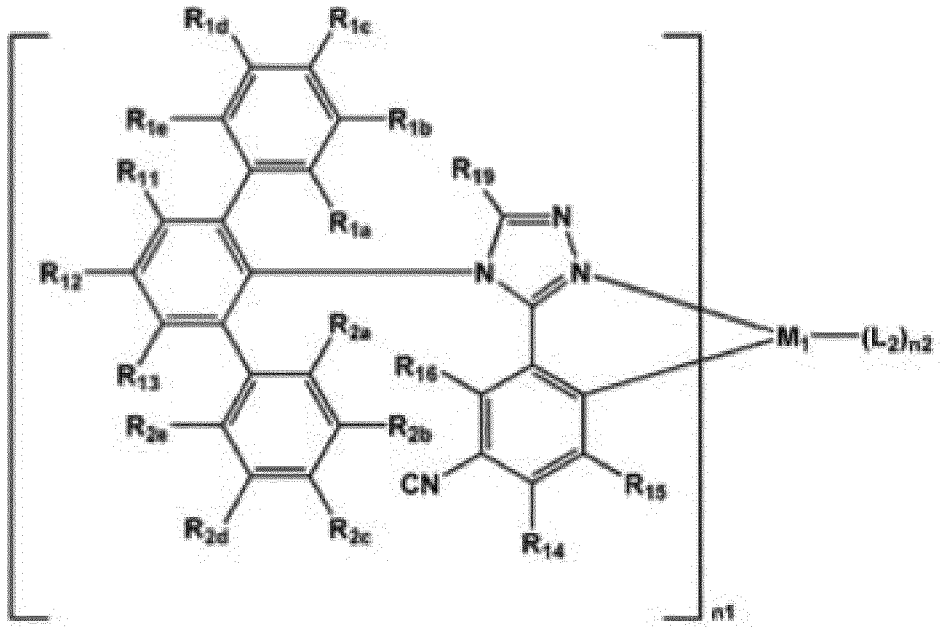
i) X_{19} $C(R_{19})$ ist, X_{20} N ist und mindestens eines von R_{12}, R_{14} und R_{19} ein Deuterium enthaltender Substituent ist;
ii) X_{19} N ist, X_{20} $C(R_{20})$ ist und mindestens eines von R_{12}, R_{14} und R_{20} ein Deuterium enthaltender Substituent ist;
iii) X_{19} und X_{20} jeweils N sind und mindestens eines von R_{12} und R_{14} ein Deuterium enthaltender Substituent ist, und wobei

der Deuterium enthaltende Substituent ausgewählt ist aus:

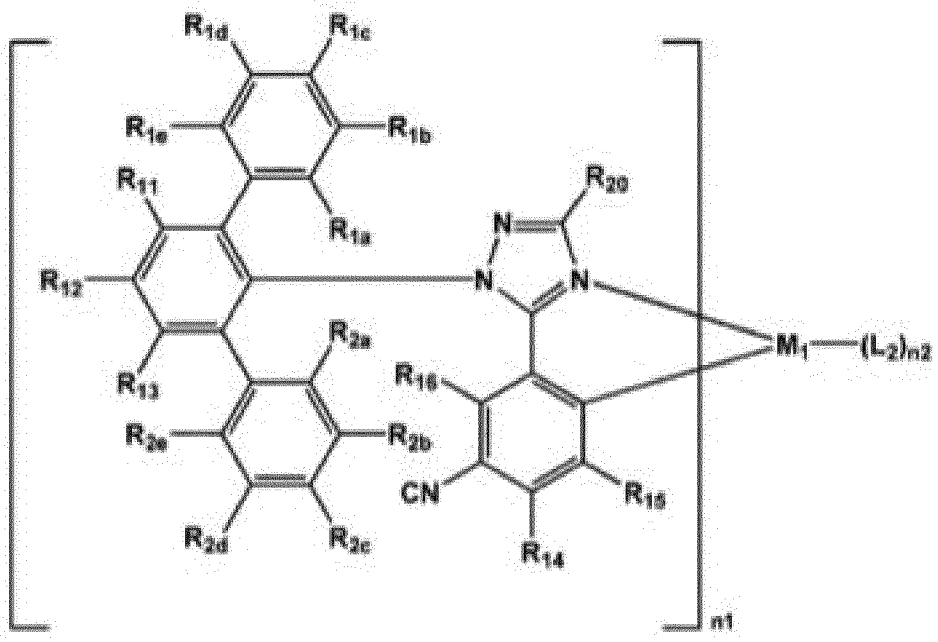
Deuterium; und
einer Methylgruppe, einer Ethylgruppe, einer n-Propylgruppe, einer Isopropylgruppe, einer n-Butylgruppe, einer sec-Butylgruppe, einer Isobutylgruppe, einer tert-Butylgruppe, einer n-Pentylgruppe, einer Isopentylgruppe, einer 1-Methylbutylgruppe, einer 2-Methylbutylgruppe, einer Neopentylgruppe, einer 1,2-Dimethylpropylgruppe und einer tert-Pentylgruppe, jeweils substituiert mit mindestens einem Deuterium.

8. Organometallische Verbindung nach einem der Ansprüche 1 bis 7, wobei
die organometallische Verbindung durch eine der Formeln 1-1 bis 1-3 dargestellt ist:

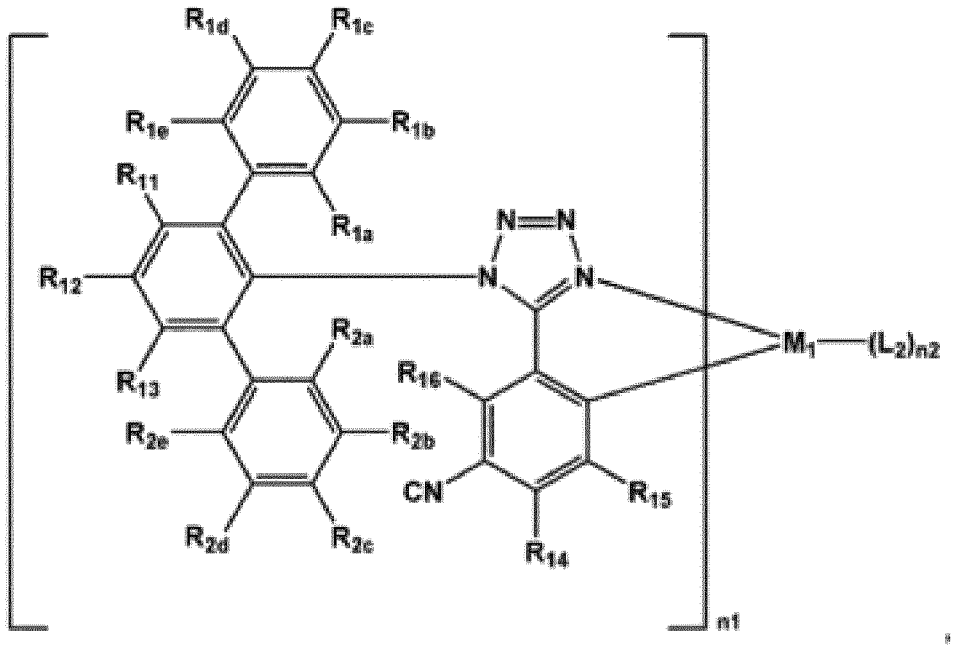
Formel 1-1



Formel 1-2



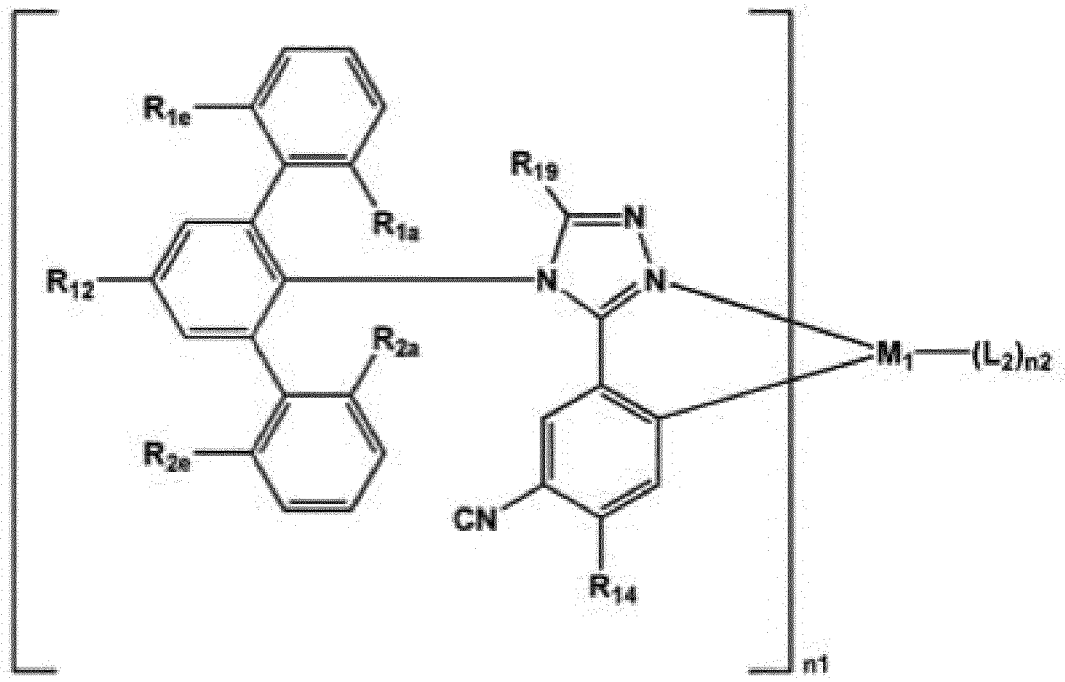
Formel 1-3



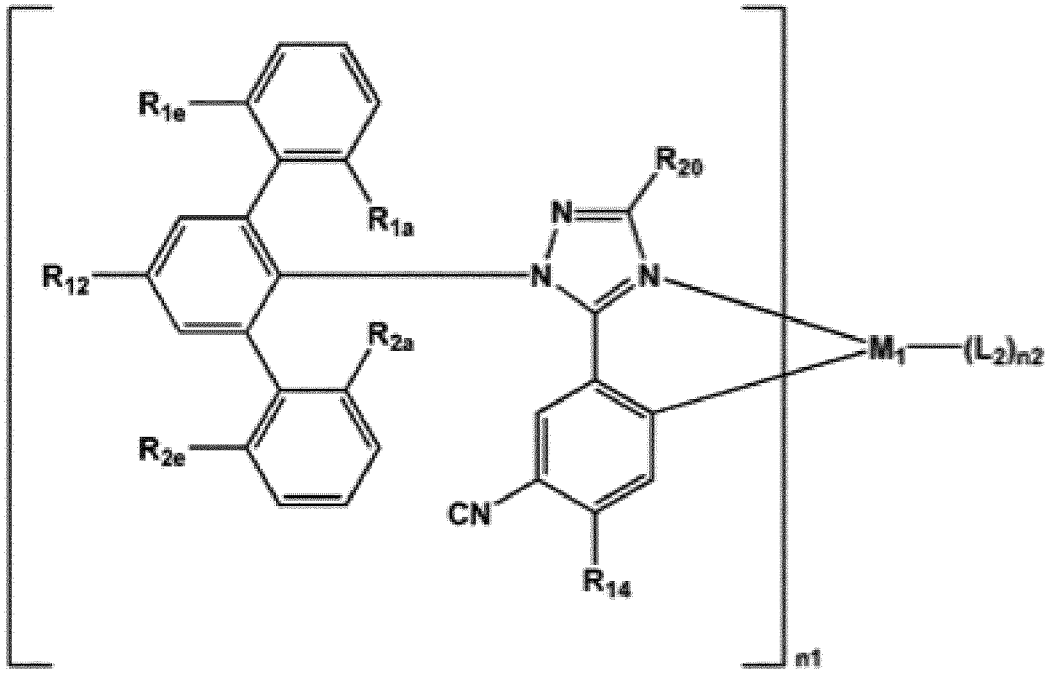
wobei in den Formeln 1-1 bis 1-3, M_1, n1, L_2, n2, R_{11} bis R_{16}, R_{19} und R_{20} jeweils unabhängig der Beschreibung aus Anspruch 1 entsprechen, R_{1a} bis R_{1e} jeweils unabhängig der Beschreibung in Bezug auf R_1 aus Anspruch 1 entsprechen, R_{2a} bis R_{2e} jeweils unabhängig der Beschreibung in Bezug auf R_2 aus Anspruch 1 entsprechen.

9. Organometallische Verbindung nach einem der Ansprüche 1 bis 8, wobei
die organometallische Verbindung durch eine der Formeln 1(1) bis 1 (3) dargestellt ist:

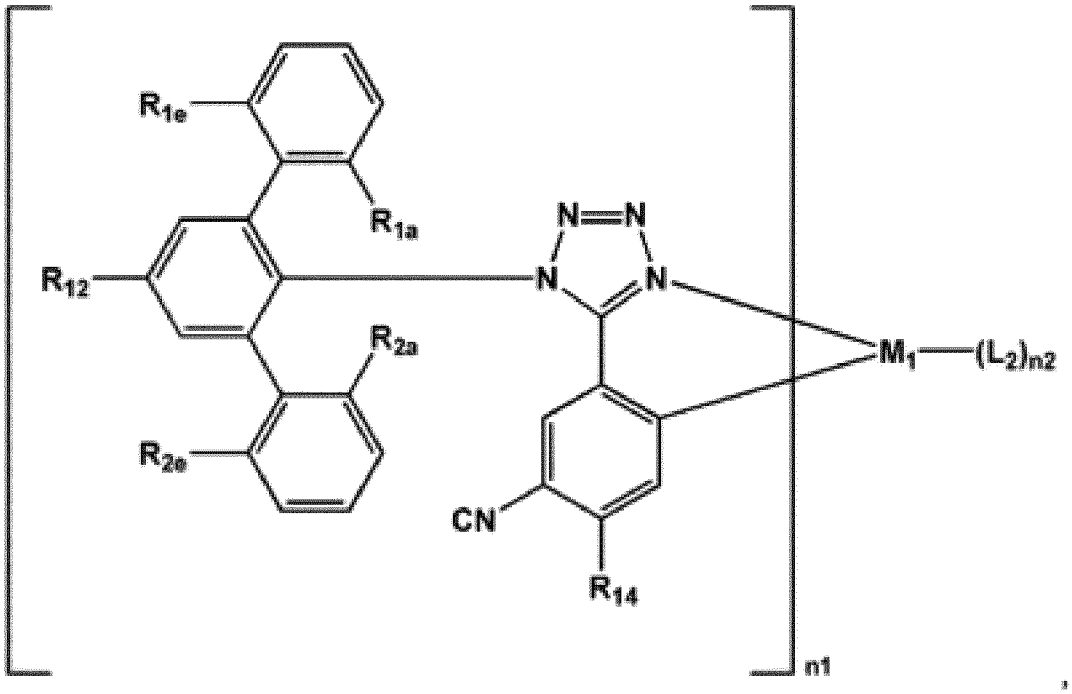
Formel 1(1)



Formel 1(2)

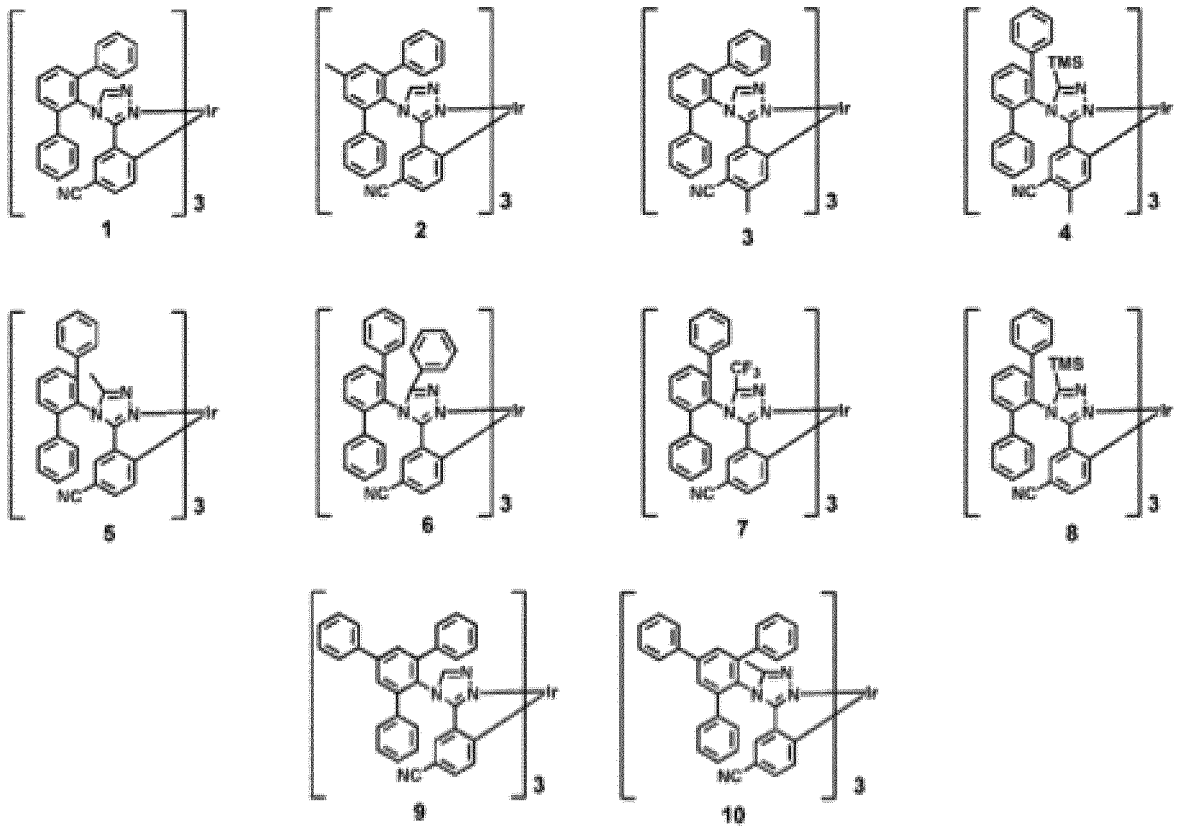


Formel 1(3)



wobei in den Formeln 1(1) bis 1(3), M_1, n1, L_2, n2, R_{12}, R_{14}, R_{19} und R_{20} jeweils unabhängig der Beschreibung aus Anspruch 1 entsprechen, R_{1a} bis R_{1e} jeweils unabhängig der Beschreibung in Bezug auf R_1 aus Anspruch 1 entsprechen, R_{2a} bis R_{2e} jeweils unabhängig der Beschreibung in Bezug auf R_2 aus Anspruch 1 entsprechen.

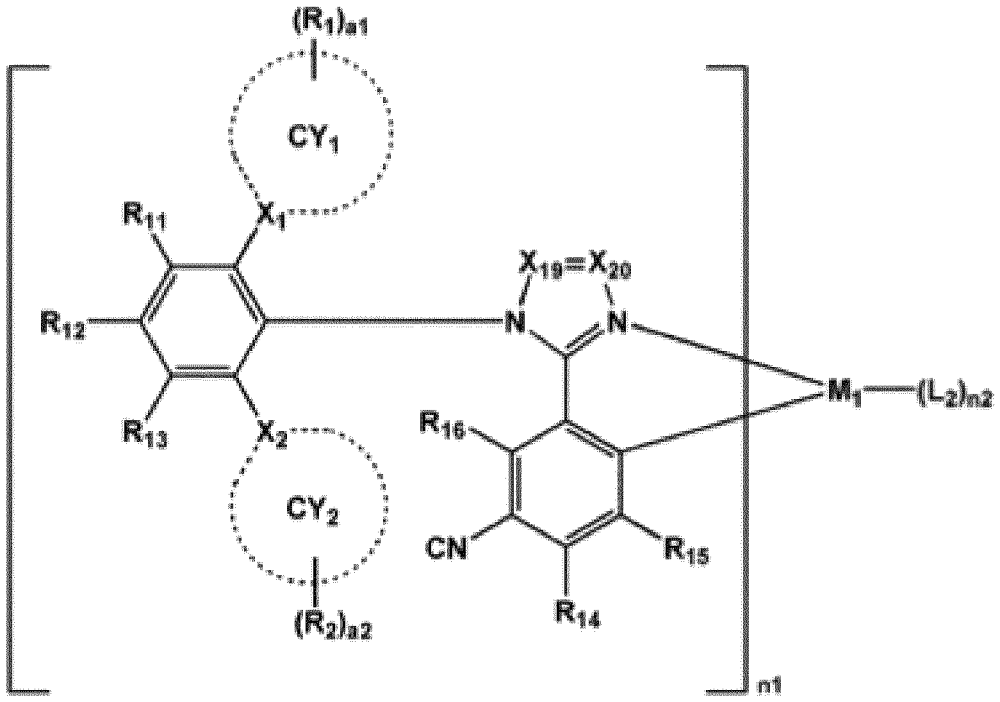
10. Organometallische Verbindung nach einem der Ansprüche 1 bis 9, wobei die organometallische Verbindung eine der Verbindungen 1 bis 10 ist:



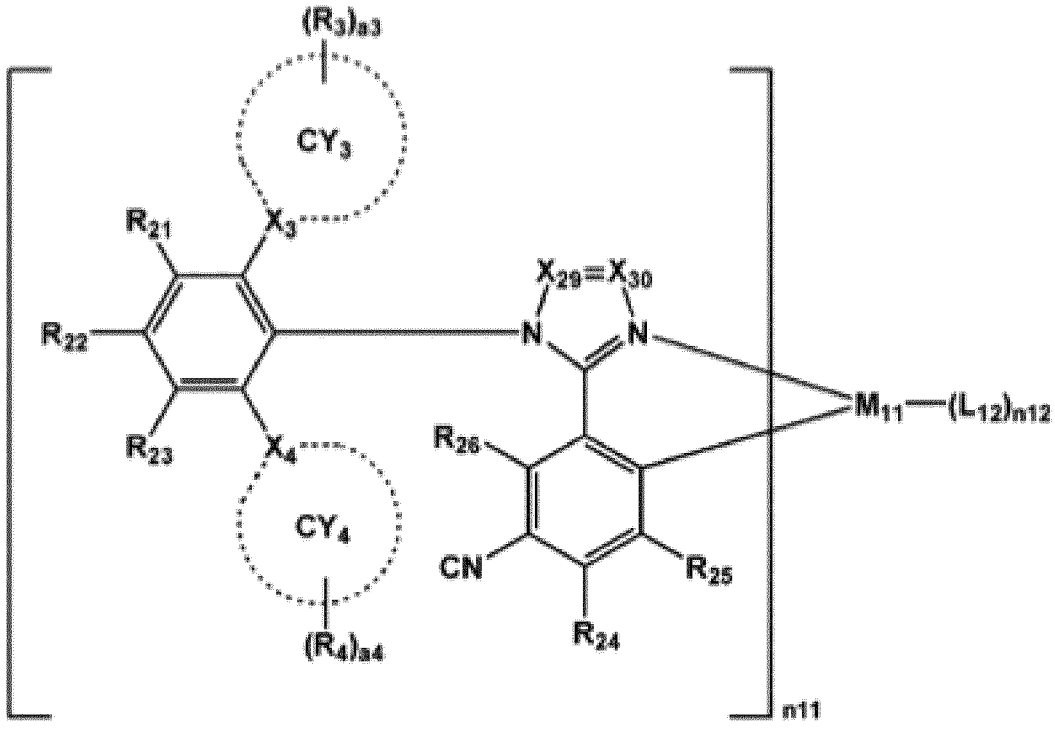
11. Zusammensetzung, die eine organometallische Verbindung enthält, wobei die Zusammensetzung folgendes umfasst:

eine erste organometallische Verbindung, dargestellt durch Formel 1 gemäß einem der Ansprüche 1 bis 10, und die mindestens ein Deuterium umfasst; und
eine zweite organometallische Verbindung, dargestellt durch Formel 2:

Formel 1



Formel 2



wobei in den Formeln 1 und 2:

M_{11} ausgewählt ist ausgewählt ist aus einem Übergangsmetall der ersten Reihe des Periodensystems, einem Übergangsmetall der zweiten Reihe des Periodensystems und einem Übergangsmetall der dritten Reihe des Periodensystems,
n11 1, 2 oder 3 ist,
L_{12} ein einzähniger Ligand oder ein zweizähniger Ligand ist,

n12 0, 1, 2, 3 oder 4 ist, wobei, wenn n12 zwei oder mehr ist, zwei oder mehr Gruppen von L_{12} miteinander identisch oder unterschiedlich sind,
X_3 und X_4 jeweils unabhängig Kohlenstoff oder Stickstoff sind,
CY_3 und CY_4 jeweils unabhängig eine C_5-C_{30} carbocyclische Gruppe oder eine C_2-C_{30} heterocyclische Gruppe sind,
X_{29} N oder C(R_{29}) ist, und X_{30} N oder C(R_{30}) ist, vorausgesetzt, dass mindestens eines von X_{29} und X_{30} N ist,
R_3, R_4, R_{21} bis R_{26}, R_{29} und R_{30} jeweils unabhängig ausgewählt sind aus Wasserstoff, -F, -Cl, -Br, -I, -SF_5, einer Hydroxylgruppe, einer Cyanogruppe, einer Nitrogruppe, einer Aminogruppe, einer Amidinogruppe, einer Hydrazingruppe, einer Hydrazongruppe, einer Carbonsäuregruppe oder einem Salz davon, einer Sulfonsäuregruppe oder einem Salz davon, einer Phosphorsäuregruppe oder einem Salz davon, einer substituierten oder unsubstituierten C_1-C_{60}-Alkylgruppe, einer substituierten oder unsubstituierten C_2-C_{60}-Alkenylgruppe, einer substituierten oder unsubstituierten C_2-C_{60}-Alkynylgruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Alkoxygruppe, einer substituierten oder unsubstituierten C_3-C_{10}-Cycloalkylgruppe, einer substituierten oder unsubstituierten C_1-C_{19}-Heterocycloalkylgruppe, einer substituierten oder unsubstituierten C_3-C_{10}-Cycloalkenylgruppe, einer substituierten oder unsubstituierten C_1-C_{19}-Heterocycloalkenylgruppe, einer substituierten oder unsubstituierten C_6-C_{60}-Arylgruppe, einer substituierten oder unsubstituierten C_6-C_{60}-Aryloxygruppe, einer substituierten oder unsubstituierten C_6-C_{60}-Arylthiogruppe, einer substituierten oder unsubstituierten C_7-C_{60}-Arylalkylgruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Heteroarylgruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Heteroaryloxygruppe, einer substituierten oder unsubstituierten C_1-C_{60}-Heteroarylthiogruppe, einer substituierten oder unsubstituierten C_2-C_{60}-Heteroarylalkylgruppe, einer substituierten oder unsubstituierten monovalenten nichtaromatischen kondensierten polycyclischen Gruppe, einer substituierten oder unsubstituierten monovalenten nichtaromatischen kondensierten heteropolycyclischen Gruppe, -$N(Q_1)(Q_2)$, -$Si(Q_3)(Q_4)(Q_5)$, -$B(Q_6)(Q_7)$ und -$P(=O)(Q_8)(Q_9)$,
zwei oder mehr benachbarte Gruppen, die ausgewählt sind aus R_3, R_4, R_{21} bis R_{23}, CY_3 und CY_4, optional verknüpft sind, so dass sie eine substituierte oder unsubstituierte C_5-C_{30} carbocyclische Gruppe oder eine substituierte oder unsubstituierte C_2-C_{30} heterocyclische Gruppe bilden,
a3 und a4 jeweils unabhängig eine ganze Zahl von 0 bis 5 sind, und
R_3, R_4, R_{21} bis R_{26}, R_{29} und R_{30} jeweils unabhängig ein Deuterium-freier Substituent sind;
wobei vorzugsweise
eine durch Gleichung 2 ausgedrückte Deuterierungsrate 50% oder mehr beträgt:

Gleichung 2
Deuterierungsrate (%) = $n_{D2}/(n_{H2} + n_{D2})$ X 100,
wobei in Gleichung 2 folgendes gilt:

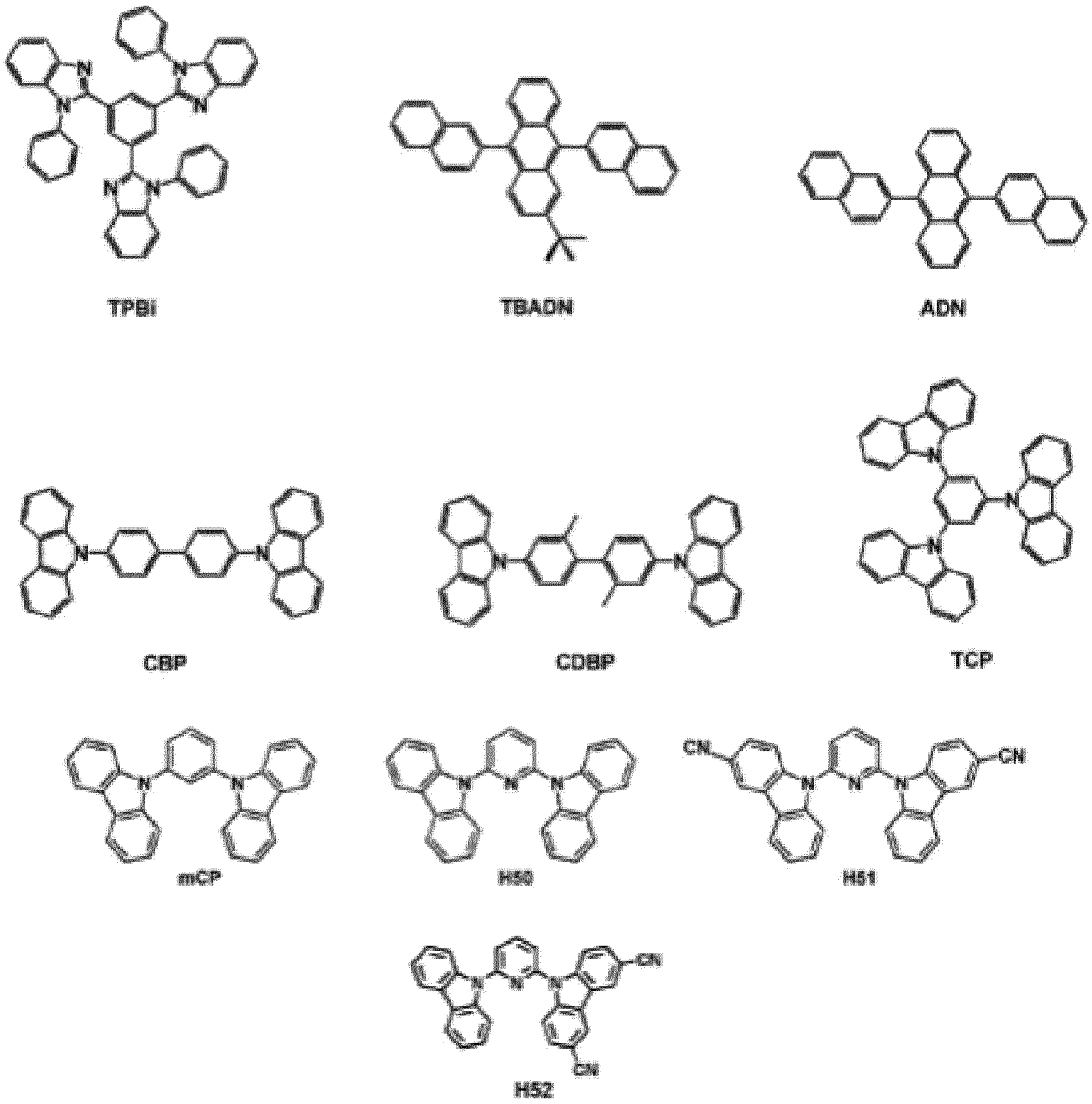
n_{H2} steht für die Summe einer Anzahl an Wasserstoffen insgesamt in den Deuterium enthaltenden Substituenten in der ersten organometallischen Verbindung und einer Anzahl an Wasserstoffen insgesamt in einem Deuterium-freien Substituenten der zweiten organometallischen Verbindung entsprechend dem Deuterium enthaltenden Substituenten in der ersten organometallischen Verbindung, und
n_{D2} steht für eine Anzahl an insgesamt in den Deuterium enthaltenden Substituenten in der ersten organometallischen Verbindung enthaltenen Deuteriumatomen.

12. Organische lichtemittierende Vorrichtung, umfassend:

eine erste Elektrode;
eine zweite Elektrode; und
eine organische Schicht, die sich zwischen der ersten Elektrode und der zweiten Elektrode befindet, wobei die organische Schicht eine Emissionsschicht umfasst,
wobei die organische Schicht mindestens eines der folgenden umfasst: eine organische Verbindung nach einem der Ansprüche 1 bis 10 und/oder die Zusammensetzung nach Anspruch 11;
wobei
die Emissionsschicht vorzugsweise die organometallische Verbindung oder die Zusammensetzung umfasst.

13. Organische lichtemittierende Vorrichtung nach Anspruch 12, wobei
die Emissionsschicht ferner einen Wirt umfasst;
wobei

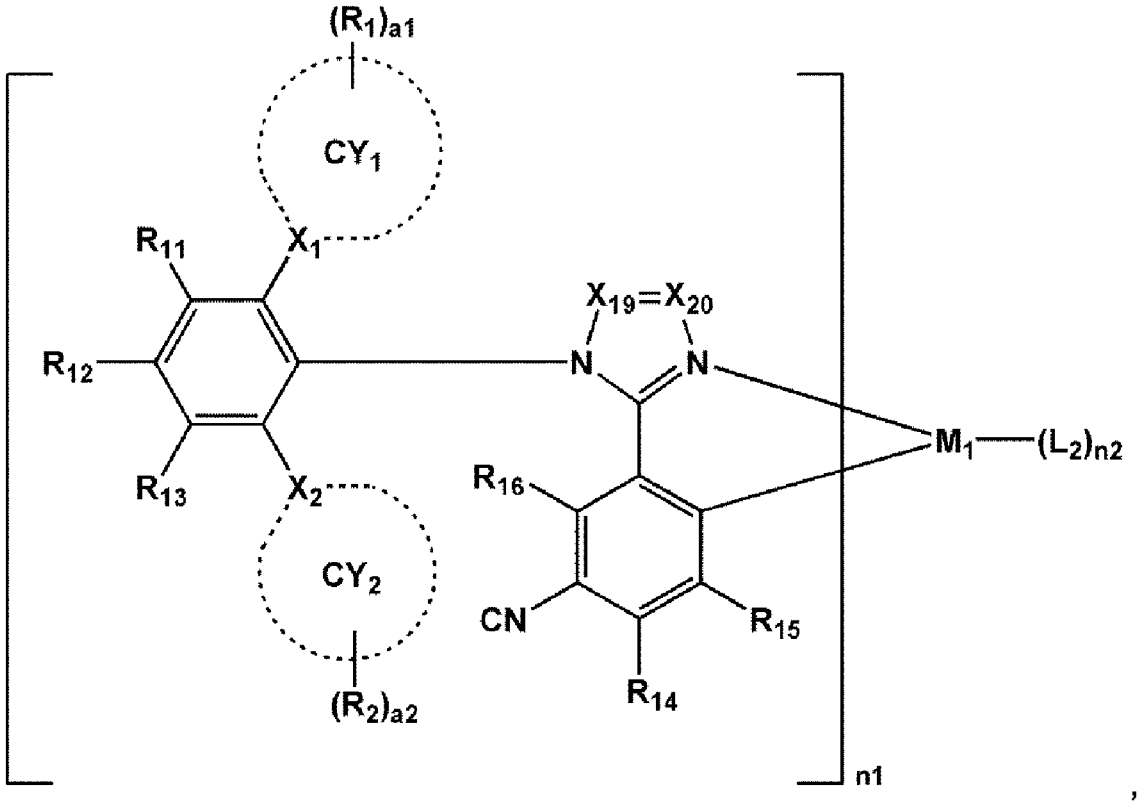
der Wirt vorzugsweise aus den folgenden Verbindungen ausgewählt ist:



Revendications

1. Composé organométallique représenté par la Formule 1 :

Formule 1



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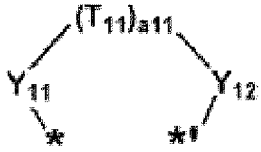
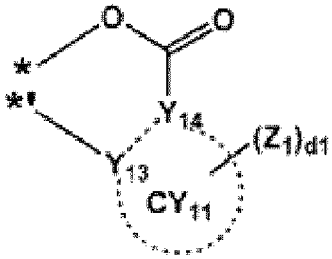
Formule 3A

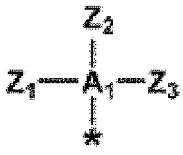


Formule 3B



Formule 3C

Formule 3E



Formule 3F

dans lequel

M_1 dans la Formule 1 est choisi parmi un métal de transition de la première rangée du Tableau Périodique des Éléments, un métal de transition de la deuxième rangée du Tableau Périodique des Éléments, et un métal de transition de la troisième rangée du Tableau Périodique des Éléments,
n1 dans la Formule 1 est 1, 2, ou 3,
L_2 dans la Formule 1 est choisi parmi les ligands représentés par les Formules 3A à 3C, 3E et 3F,
n2 dans la Formule 1 est 0, 1, 2, 3 ou 4, lorsque n2 vaut deux ou davantage, deux ou davantage de groupes

L_2 étant identiques ou différents les uns des autres,
X_1 et X_2 dans la Formule 1 sont chacun indépendamment carbone ou azote,
CY_1 et CY_2 dans la Formule 1 sont chacun indépendamment un groupe carbocyclique en C_5-C_{30} ou un groupe hétérocyclique en C_2-C_{30},
X_{19} dans la Formule 1 est N ou C(R_{19}), et X_{20} est N ou C(R_{20}), à condition qu'au moins un parmi X_{19} et X_{20} soit N,
Y_{11} dans la Formule 3A est choisi parmi O, N, N(Z_1), P(Z_1)(Z_2), et As(Z_1)(Z_2),
Y_{12} dans la Formule 3A est choisi parmi O, N, N(Z_3), P(Z_3)(Z_4), et As(Z_3)(Z_4),
CY_{11} dans la formule 3C est un groupe hétérocyclique en C_2-C_{30},
T_{11} dans la Formule 3A est choisi parmi une simple liaison, une double liaison, *-C(Z_{11})(Z_{12})-*', *-C(Z_{11})=C(Z_{12})-*', *=C(Z_{11})-*', *-C(Z_{11})=*', *=C(Z_{11})-C(Z_{12})=C(Z_{13})-*', *-C(Z_{11})=C(Z_{12})-C(Z_{13})=*', *-N(Z_{11})-*', et un groupe carbocyclique en C_5-C_{30} substitué ou non substitué,
a11 dans la Formule 3A est un entier de 1 à 10,
Y_{13} et Y_{14} dans la Formule 3C sont chacun indépendamment carbone (C) ou azote (N),
Y_{13} et Y_{14} sont reliés par une simple liaison ou une double liaison,
A_1 dans la Formule 3F est P ou As,
d1 dans la Formule 2C est un entier de 0 à 10,
* et *' dans les Formules 3A à 3C, 3E et 3F indiquent chacun un site de liaison à M_1 dans la Formule 1,
R_1, R_2, R_{11} à R_{16}, R_{19}, R_{20}, Z_1 à Z_4 et Z_{11} à Z_{13} sont chacun indépendamment choisis parmi hydrogène, deutérium, -F, -Cl, -Br, -I, -SF_5, un groupe hydroxyle, un groupe cyano, un groupe nitro, un groupe amino, un groupe amidino, un groupe hydrazine, un groupe hydrazone, un groupe acide carboxylique ou un sel de celui-ci, un groupe acide sulfonique ou un sel de celui-ci, un groupe acide phosphorique ou un sel de celui-ci, un groupe alkyle en C_1-C_{60} substitué ou non substitué, un groupe alcényle en C_2-C_{60} substitué ou non substitué, un groupe alcynyle en C_2-C_{60} substitué ou non substitué, un groupe alcoxy en C_1-C_{60} substitué ou non substitué, un groupe cycloalkyle en C_3-C_{19} substitué ou non substitué, un groupe hétérocycloalkyle en C_1-C_{10} substitué ou non substitué, un groupe cycloalcényle en C_3-C_{10} substitué ou non substitué, un groupe hétérocycloalcényle en C_1-C_{10} substitué ou non substitué, un groupe aryle en C_6-C_{60} substitué ou non substitué, un groupe aryloxy en C_6-C_{60} substitué ou non substitué, un groupe arylthio en C_6-C_{60} substitué ou non substitué, un groupe arylalkyle en C_7-C_{60} substitué ou non substitué, un groupe hétéroaryle en C_1-C_{60} substitué ou non substitué, un groupe hétéroaryloxy en C_1-C_{60} substitué ou non substitué, un groupe hétéroarylthio en C_1-C_{60} substitué ou non substitué, un groupe hétéroarylalkyle en C_2-C_{60} substitué ou non substitué, un groupe polycyclique condensé non aromatique monovalent substitué ou non substitué, un groupe hétéropolycyclique condensé non aromatique monovalent substitué ou non substitué, -N(Q_1)(Q_2), -Si(Q_3)(Q_4)(Q_5),-B(Q_6)(Q_7), et -P(=O)(Q_8)(Q_9), deux ou davantage de groupes voisins choisis parmi R_1, R_2, R_{11} à R_{13}, CY_1 et CY_2 sont éventuellement reliés pour former un groupe carbocyclique en C_5-C_{30} substitué ou non substitué ou un groupe hétérocyclique en C_2-C_{30} substitué ou non substitué,
a1 et a2 sont chacun indépendamment un entier de 0 à 5,
au moins un substituant du groupe carbocyclique en C_5-C_{30} substitué, du groupe hétérocyclique en C_2-C_{30} substitué, du groupe alkyle en C_1-C_{60} substitué, du groupe alcényle en C_2-C_{60} substitué, du groupe alcynyle en C_2-C_{60} substitué, du groupe alcoxy en C_1-C_{60} substitué, du groupe cycloalkyle en C_3-C_{19} substitué, du groupe hétérocycloalkyle en C_1-C_{10} substitué, du groupe cycloalcényle en C_3-C_{19} substitué, du groupe hétérocycloalcényle en C_1-C_{10} substitué, du groupe aryle en C_6-C_{60} substitué, du groupe aryloxy en C_6-C_{60} substitué, du groupe arylthio en C_6-C_{60} substitué, du groupe arylalkyle en C_7-C_{60} substitué, du groupe hétéroaryle en C_1-C_{60} substitué, du groupe hétéroaryloxy en C_1-C_{60} substitué, du groupe hétéroarylthio en C_1-C_{60} substitué, du groupe hétéroarylalkyle en C_2-C_{60} substitué, du groupe polycyclique condensé non aromatique monovalent substitué, et du groupe hétéropolycyclique condensé non aromatique monovalent substitué est choisi parmi :

deutérium, -F, -Cl, -Br, -I, -CD_3, -CD_2H, -CDH_2, -CF_3, -CF_2H, -CFH_2, un groupe hydroxyle, un groupe cyano, un groupe nitro, un groupe amino, un groupe amidino, un groupe hydrazine, un groupe hydrazone, un groupe acide carboxylique ou un sel de celui-ci, un groupe acide sulfonique ou un sel de celui-ci, un groupe acide phosphorique ou un sel de celui-ci, un groupe alkyle en C_1-C_{60}, un groupe alcényle en C_2-C_{60}, un groupe alcynyle en C_2-C_{60}, et un groupe alcoxy en C_1-C_{60} ;
un groupe alkyle en C_1-C_{60}, un groupe alcényle en C_2-C_{60}, un groupe alcynyle en C_2-C_{60}, et un groupe alcoxy en C_1-C_{60}, chacun substitués avec au moins un choisi parmi deutérium, -F, -Cl, -Br, -I, -CD_3, -CD_2H, -CDH_2, -CF_3, -CF_2H, -CFH_2, un groupe hydroxyle, un groupe cyano, un groupe nitro, un groupe amino, un groupe amidino, un groupe hydrazine, un groupe hydrazone, un groupe acide carboxylique ou un sel de celui-ci, un groupe acide sulfonique ou un sel de celui-ci, un groupe acide phosphorique ou un sel de celui-ci, un groupe cycloalkyle en C_3-C_{10}, un groupe hétérocycloalkyle en C_1-C_{10}, un groupe cycloalcényle en C_3-C_{10}, un groupe hétérocycloalcényle en C_1-C_{10}, un groupe aryle en C_6-C_{60}, un groupe aryloxy en C_6-C_{60},

un groupe arylthio en C_6-C_{60}, un groupe arylalkyle en C_7-C_{60}, un groupe hétéroaryle en C_1-C_{60}, un groupe hétéroaryloxy en C_1-C_{60}, un groupe hétéroarylthio en C_1-C_{60}, un groupe hétéroarylalkyle en C_2-C_{60}, un groupe polycyclique condensé non aromatique monovalent, un groupe hétéropolycyclique condensé non aromatique monovalent, $-N(Q_{11})(Q_{12})$,$-Si(Q_{13})(Q_{14})(Q_{15})$, $-B(Q_{16})(Q_{17})$, et $-P(=O)(Q_{18})(Q_{19})$;

un groupe cycloalkyle en C_3-C_{10}, un groupe hétérocycloalkyle en C_1-C_{10}, un groupe cycloalcényle en C_3-C_{10}, un groupe hétérocycloalcényle en C_1-C_{10}, un groupe aryle en C_6-C_{60}, un groupe aryloxy en C_6-C_{60}, un groupe arylthio en C_6-C_{60}, un groupe arylalkyle en C_7-C_{60}, un groupe hétéroaryle en C_1-C_{60}, un groupe hétéroaryloxy en C_1-C_{60}, un groupe hétéroarylthio en C_1-C_{60}, un groupe hétéroarylalkyle en C_2-C_{60}, un groupe polycyclique condensé non aromatique monovalent, et un groupe hétéropolycyclique condensé non aromatique monovalent ;

un groupe cycloalkyle en C_3-C_{10}, un groupe hétérocycloalkyle en C_1-C_{10}, un groupe cycloalcényle en C_3-C_{10}, un groupe hétérocycloalcényle en C_1-C_{10}, un groupe aryle en C_6-C_{60}, un groupe aryloxy en C_6-C_{60}, un groupe arylthio en C_6-C_{60}, un groupe arylalkyle en C_7-C_{60}, un groupe hétéroaryle en C_1-C_{60}, un groupe hétéroaryloxy en C_1-C_{60}, un groupe hétéroarylthio en C_1-C_{60}, un groupe hétéroarylalkyle en C_2-C_{60}, un groupe polycyclique condensé non aromatique monovalent, et un groupe hétéropolycyclique condensé non aromatique monovalent, chacun substitués avec au moins un choisi parmi deutérium, -F, -Cl, -Br, -I, $-CD_3$, $-CD_2H$, $-CDH_2$, $-CF_3$, $-CF_2H$,$-CFH_2$, un groupe hydroxyle, un groupe cyano, un groupe nitro, un groupe amino, un groupe amidino, un groupe hydrazine, un groupe hydrazone, un groupe acide carboxylique ou un sel de celui-ci, un groupe acide sulfonique ou un sel de celui-ci, un groupe acide phosphorique ou un sel de celui-ci, un groupe alkyle en C_1-C_{60}, un groupe alcényle en C_2-C_{60}, un groupe alcynyle en C_2-C_{60}, un groupe alcoxy en C_1-C_{60}, un groupe cycloalkyle en C_3-C_{10}, un groupe hétérocycloalkyle en C_1-C_{10}, un groupe cycloalcényle en C_3-C_{10}, un groupe hétérocycloalcényle en C_1-C_{10}, un groupe aryle en C_6-C_{60}, un groupe aryloxy en C_6-C_{60}, un groupe arylthio en C_6-C_{60}, un groupe arylalkyle en C_7-C_{60}, un groupe hétéroaryle en C_1-C_{60}, un groupe hétéroaryloxy en C_1-C_{60}, un groupe hétéroarylthio en C_1-C_{60}, un groupe hétéroarylalkyle en C_2-C_{60}, un groupe polycyclique condensé non aromatique monovalent, un groupe hétéropolycyclique condensé non aromatique monovalent, $-N(Q_{21})(Q_{22})$, $-Si(Q_{23})(Q_{24})(Q_{25})$, $-B(Q_{26})(Q_{27})$, et $-P(=O)(Q_{28})(Q_{29})$; et

$-N(Q_{31})(Q_{32})$, $-Si(Q_{33})(Q_{34})(Q_{35})$, $-B(Q_{36})(Q_{37})$, et $-P(=O)(Q_{38})(Q_{39})$, et

Q_1 à Q_9, Q_{11} à Q_{19}, Q_{21} à Q_{29}, et Q_{31} à Q_{39} sont chacun indépendamment choisis parmi hydrogène, deutérium, -F, -Cl, -Br, -I, un groupe hydroxyle, un groupe cyano, un groupe nitro, un groupe amino, un groupe amidino, un groupe hydrazine, un groupe hydrazone, un groupe acide carboxylique ou un sel de celui-ci, un groupe acide sulfonique ou un sel de celui-ci, un groupe acide phosphorique ou un sel de celui-ci, un groupe alkyle en C_1-C_{60}, un groupe alcényle en C_2-C_{60}, un groupe alcynyle en C_2-C_{60}, un groupe alcoxy en C_1-C_{60}, un groupe cycloalkyle en C_3-C_{10}, un groupe hétérocycloalkyle en C_1-C_{10}, un groupe cycloalcényle en C_3-C_{10}, un groupe hétérocycloalcényle en C_1-C_{10}, un groupe aryle en C_6-C_{60}, , un groupe aryle en C_6-C_{60} substitué avec au moins un choisi parmi un groupe alkyle en C_1-C_{60} et un groupe aryle en C_6-C_{60}, un groupe aryloxy en C_6-C_{60}, un groupe arylthio en C_6-C_{60}, un groupe arylalkyle en C_7-C_{60}, un groupe hétéroaryle en C_1-C_{60}, un groupe hétéroaryloxy en C_1-C_{60}, un groupe hétéroarylthio en C_1-C_{60}, un groupe hétéroarylalkyle en C_2-C_{60}, un groupe polycyclique condensé non aromatique monovalent, et un groupe hétéropolycyclique condensé non aromatique monovalent.

2. Composé organométallique de la revendication 1, dans lequel
M_1 est Ir ou Os, et la somme de n1 et n2 est 3 ou 4 ; ou
M_1 est Pt, et la somme de n1 et n2 est 2.

3. Composé organométallique des revendications 1 ou 2, dans lequel CY_1 et CY_2 sont chacun indépendamment choisis parmi un groupe cyclopentène, un groupe cyclohexène, un groupe benzène, un groupe pyridine, un groupe pyrimidine, un groupe pyridazine, un groupe pyrazine, un groupe triazine, un groupe pyrrole, un groupe pyrazole, un groupe imidazole, un groupe triazole, un groupe oxazole, un groupe isoxazole, un groupe oxadiazole, un groupe thiazole, un groupe isothiazole, et un groupe thiadiazole ;
et/ou
dans lequel
X_{19} est $C(R_{19})$, et X_{20} est N, ou
X_{19} est N, et X_{20} est $C(R_{20})$.

4. Composé organométallique de l'une quelconque des revendications 1 à 3, dans lequel
R_1, R_2, R_{11} à R_{16}, R_{19}, et R_{20} sont chacun indépendamment choisis parmi :
hydrogène, deutérium, -F, un groupe cyano, un groupe nitro, $-SF_5$, un groupe méthyle, un groupe éthyle, un groupe

n-propyle, un groupe iso-propyle, un groupe n-butyle, un groupe iso-butyle, un groupe sec-butyle, un groupe tert-butyle, un groupe n-pentyle, un groupe iso-pentyle, un groupe sec-pentyle, un groupe tert-pentyle, un groupe n-hexyle, un groupe iso-hexyle, un groupe sec-hexyle, un groupe tert-hexyle, un groupe n-heptyle, un groupe iso-heptyle, un groupe sec-heptyle, un groupe tert-heptyle, un groupe n-octyle, un groupe iso-octyle, un groupe sec-octyle, un groupe tert-octyle, un groupe n-nonyle, un groupe iso-nonyle, un groupe sec-nonyle, un groupe tert-nonyle, un groupe n-décyle, un groupe iso-décyle, un groupe sec-décyle, un groupe tert-décyle, un groupe méthoxy, un groupe éthoxy, un groupe propoxy, un groupe butoxy, un groupe pentoxy, un groupe cyclopentyle, un groupe cyclohexyle, un groupe cycloheptyle, un groupe cyclooctyle, un groupe adamantanyle, un groupe norbornanyle, un groupe norbornényle, un groupe cyclopenténylе, un groupe cyclohexénylе, un groupe cycloheptényle, un groupe phényle, un groupe naphtyle, un groupe pyridinyle, un groupe pyrimidinyle, un groupe dibenzofuranyle, et un groupe dibenzothiophényle ;

un groupe méthyle, un groupe éthyle, un groupe n-propyle, un groupe iso-propyle, un groupe n-butyle, un groupe iso-butyle, un groupe sec-butyle, un groupe tert-butyle, un groupe n-pentyle, un groupe iso-pentyle, un groupe sec-pentyle, un groupe tert-pentyle, un groupe n-hexyle, un groupe iso-hexyle, un groupe sec-hexyle, un groupe tert-hexyle, un groupe n-heptyle, un groupe iso-heptyle, un groupe sec-heptyle, un groupe tert-heptyle, un groupe n-octyle, un groupe iso-octyle, un groupe sec-octyle, un groupe tert-octyle, un groupe n-nonyle, un groupe iso-nonyle, un groupe sec-nonyle, un groupe tert-nonyle, un groupe n-décyle, un groupe iso-décyle, un groupe sec-décyle, un groupe tert-décyle, un groupe méthoxy, un groupe éthoxy, un groupe propoxy, un groupe butoxy, un groupe pentoxy, un groupe cyclopentyle, un groupe cyclohexyle, un groupe cycloheptyle, un groupe cyclooctyle, un groupe adamantanyle, un groupe norbornanyle, un groupe norbornényle, un groupe cyclopenténylе, un groupe cyclohexénylе, un groupe cycloheptényle, un groupe phényle, un groupe naphtyle, un groupe pyridinyle, un groupe pyrimidinyle, un groupe dibenzofuranyle, et un groupe dibenzothiophényle, chacun substitués avec au moins un choisi parmi deutérium, -F,-CD_3, -CD_2H, -CDH_2, -CF_3, -CF_2H, -CFH_2, un groupe cyano, un groupe nitro, un groupe alkyle en C_1-C_{10}, un groupe alcoxy en C_1-C_{10}, un groupe cyclopentyle, un groupe cyclohexyle, un groupe cycloheptyle, un groupe cyclooctyle, un groupe adamantanyle, un groupe norbornanyle, un groupe norbornényle, un groupe cyclopenténylе, un groupe cyclohexénylе, un groupe cycloheptényle, un groupe phényle, un groupe naphtyle, un groupe pyridinyle, un groupe pyrimidinyle, un groupe dibenzofuranyle, et un groupe dibenzothiophényle ; et

-$N(Q_1)(Q_2)$, -$Si(Q_3)(Q_4)(Q_5)$, -$B(Q_6)(Q_7)$, et -$P(=O)(Q_8)(Q_9)$, et

Q_1 à Q_9 sont chacun indépendamment choisis parmi :

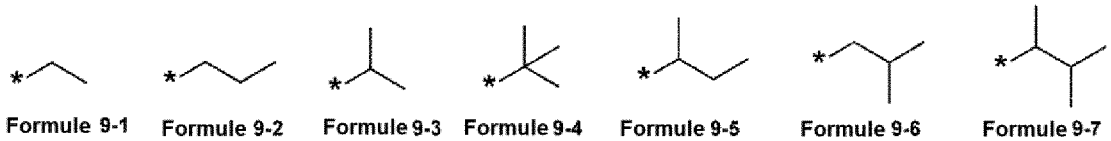
-CH_3, -CD_3, -CD_2H, -CDH_2, -CH_2CH_3, -CH_2CD_3, -CH_2CD_2H, -CH_2CDH_2,-$CHDCH_3$, -$CHDCD_2H$, -$CHDCDH_2$, -$CHDCD_3$, -CD_2CD_3, -CD_2CD_2H, et -CD_2CDH_2 ;

un groupe n-propyle, un groupe iso-propyle, un groupe n-butyle, un groupe iso-butyle, un groupe sec-butyle, un groupe tert-butyle, un groupe n-pentyle, un groupe iso-pentyle, un groupe sec- pentyle, un groupe tert-pentyle, un groupe phényle, et un groupe naphtyle ; et

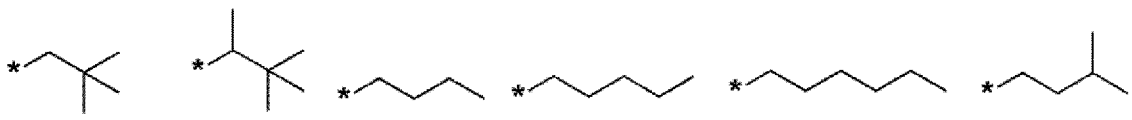
un groupe propyle, un groupe iso-propyle, un groupe n-butyle, un groupe iso-butyle, un groupe sec-butyle, un groupe tert-butyle, un groupe n-pentyle, un groupe iso-pentyle, un groupe sec-pentyle, un groupe tert-pentyle, un groupe phényle, et un groupe naphtyle, chacun substitués avec au moins un choisi parmi deutérium, un groupe alkyle en C_1-C_{10}, et un groupe phényle.

5. Composé organométallique de l'une quelconque des revendications 1 à 4, dans lequel

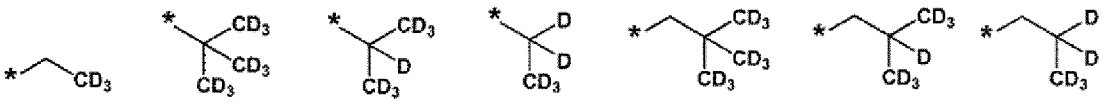
R_1, R_2, R_{11} à R_{16}, R_{19} et R_{20} sont chacun indépendamment choisis parmi hydrogène, deutérium, -CH_3, -CD_3, -CD_2H, -CDH_2, -CH_2CH_3, -CH_2CD_3, -CH_2CD_2H,-CH_2CDH_2, -$CHDCH_3$, -$CHDCD_2H$, -$CHDCDH_2$, -$CHDCD_3$, -CD_2CD_3, -CD_2CD_2H,-CD_2CDH_2, -CF_3, -CF_2H, -CFH_2, les groupes représentés par les Formules 9-1 à 9-24, les groupes représentés par les Formules 10-1 à 10-62, et $Si(Q_3)(Q_4)(Q_5)$:



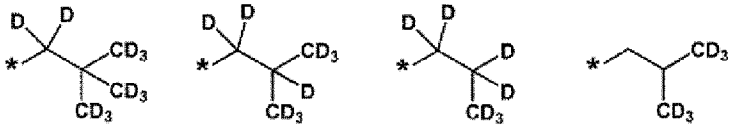
Formule 9-1 Formule 9-2 Formule 9-3 Formule 9-4 Formule 9-5 Formule 9-6 Formule 9-7



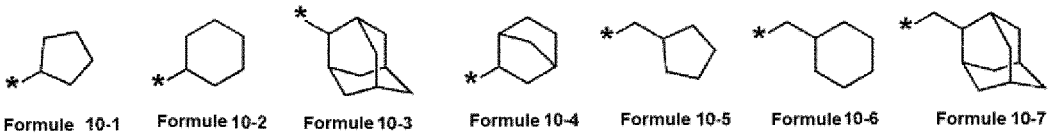
Formule 9-8 Formule 9-9 Formule 9-10 Formule 9-11 Formule 9-12 Formule 9-13



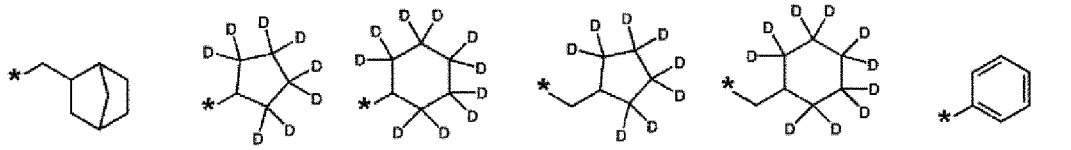
Formula 9-14 Formula 9-15 Formula 9-16 Formula 9-17 Formula 9-18 Formula 9-19 Formula 9-20



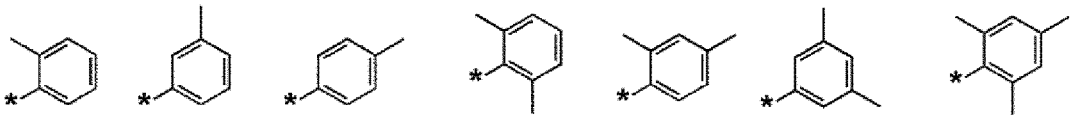
Formule 9-21 Formule 9-22 Formule 9-23 Formule 9-24



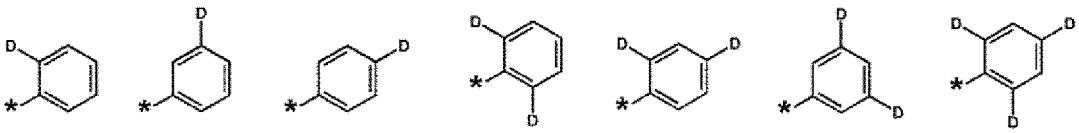
Formule 10-1 Formule 10-2 Formule 10-3 Formule 10-4 Formule 10-5 Formule 10-6 Formule 10-7



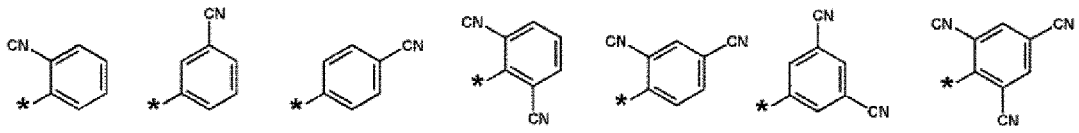
Formule 10-8 Formule 10-9 Formule 10-10 Formule 10-11 Formule 10-12 Formule 10-13



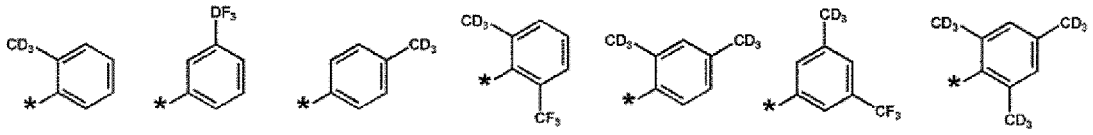
Formule 10-14 Formule 10-15 Formule 10-16 Formule 10-17 Formule 10-18 Formule 10-19 Formule 10-20



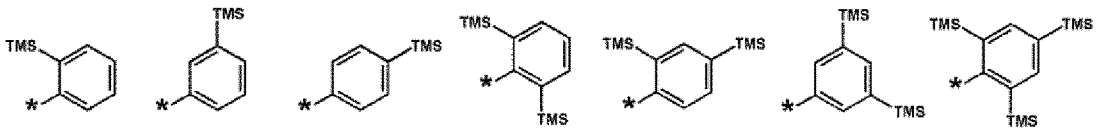
Formule 10-21 Formule 10-22 Formule 10-23 Formule 10-24 Formule 10-25 Formule 10-26 Formule 10-27



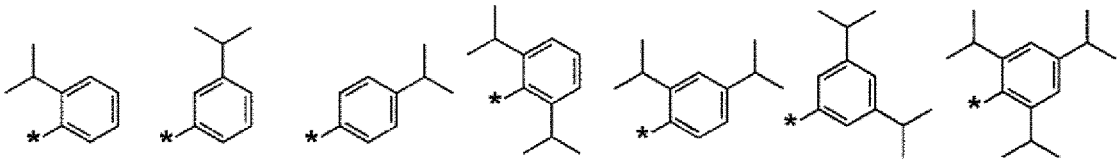
Formule 10-28 Formule 10-29 Formule 10-30 Formule 10-31 Formule 10-32 Formule 10-33 Formule 10-34



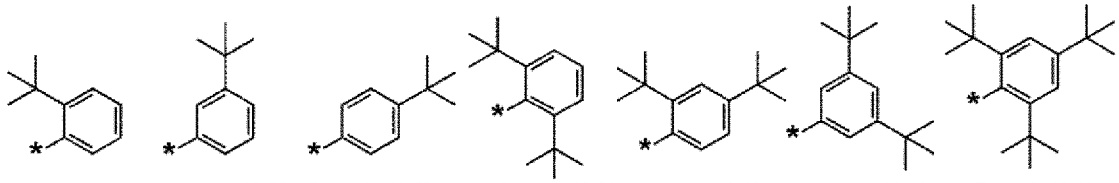
Formule 10-35 Formule 10-36 Formule 10-37 Formule 10-38 Formule 10-39 Formule 10-40 Formule 10-41



Formule 10-42 Formule 10-43 Formule 10-44 Formule 10-45 Formule 10-46 Formule 10-47 Formule 10-48



Formule 10-49 Formule 10-50 Formule 10-51 Formule 10-52 Formule 10-53 Formule 10-54 Formule 10-55



Formule 10-56 Formule 10-57 Formule 10-58 Formule 10-59 Formule 10-60 Formule 10-61 Formule 10-62

* dans les Formules 9-1 à 9-24 et 10-1 à 10-62 indiquant un site de liaison à un atome voisin.

6. Composé organométallique de l'une quelconque des revendications 1 à 5, dans lequel

i) X_{19} est $C(R_{19})$, X_{20} est N, et au moins un parmi R_1, R_2, R_{11} à R_{16}, et R_{19} est un substituant contenant du deutérium ;
ii) X_{19} est N, X_{20} est $C(R_{20})$, et au moins un parmi R_1, R_2, R_{11} à R_{16}, et R_{20} est un substituant contenant du deutérium ; ou
iii) X_{19} et X_{20} sont chacun N, et au moins un parmi R_1, R_2, et R_{11} à R_{16} est un substituant contenant du deutérium, et

le substituant contenant du deutérium est choisi parmi :

le deutérium ; et
un groupe alkyle en C_1-C_{29}, un groupe alcoxy en C_1-C_{29}, et un groupe phényle, chacun substitués avec au moins un deutérium ;
de préférence dans lequel
le substituant contenant du deutérium est choisi parmi :
le deutérium ; et
un groupe méthyle, un groupe éthyle, un groupe n-propyle, un groupe iso-propyle, un groupe n-butyle, un groupe sec-butyle, un groupe iso-butyle, un groupe tert-butyle, un groupe n-pentyle, un groupe iso-pentyle, un groupe 1-méthylbutyle, un groupe 2-méthylbutyle, un groupe néo-pentyle, un groupe 1,2-diméthylpropyle, et un groupe tert-pentyle, chacun substitués avec au moins un deutérium.

7. Composé organométallique de l'une quelconque des revendications 1 à 6, dans lequel

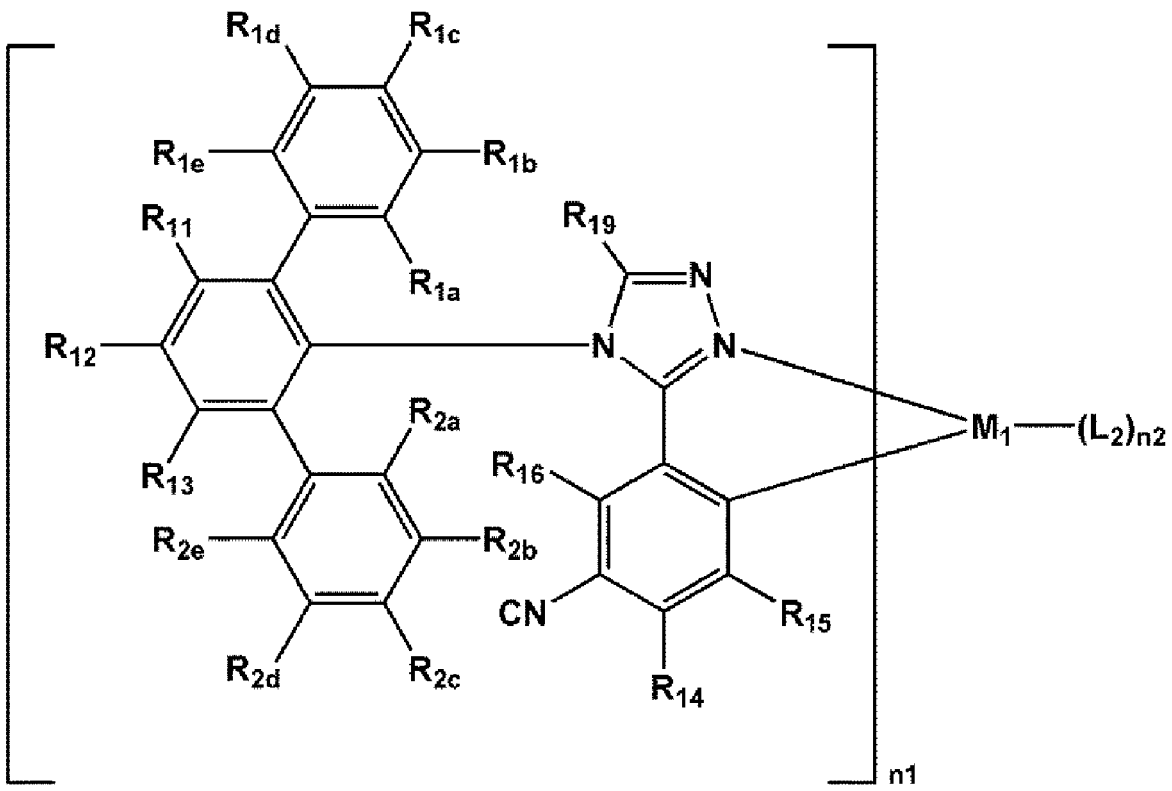
i) X_{19} est $C(R_{19})$, X_{20} est N, et au moins un parmi R_{12}, R_{14}, et R_{19} est un substituant contenant du deutérium ;
ii) X_{19} est N, X_{20} est $C(R_{20})$, et au moins un parmi R_{12}, R_{14}, et R_{20} est un substituant contenant du deutérium ; ou
iii) X_{19} et X_{20} sont chacun N, et au moins un parmi R_{12} et R_{14} est un substituant contenant du deutérium, et

le substituant contenant du deutérium est choisi parmi :

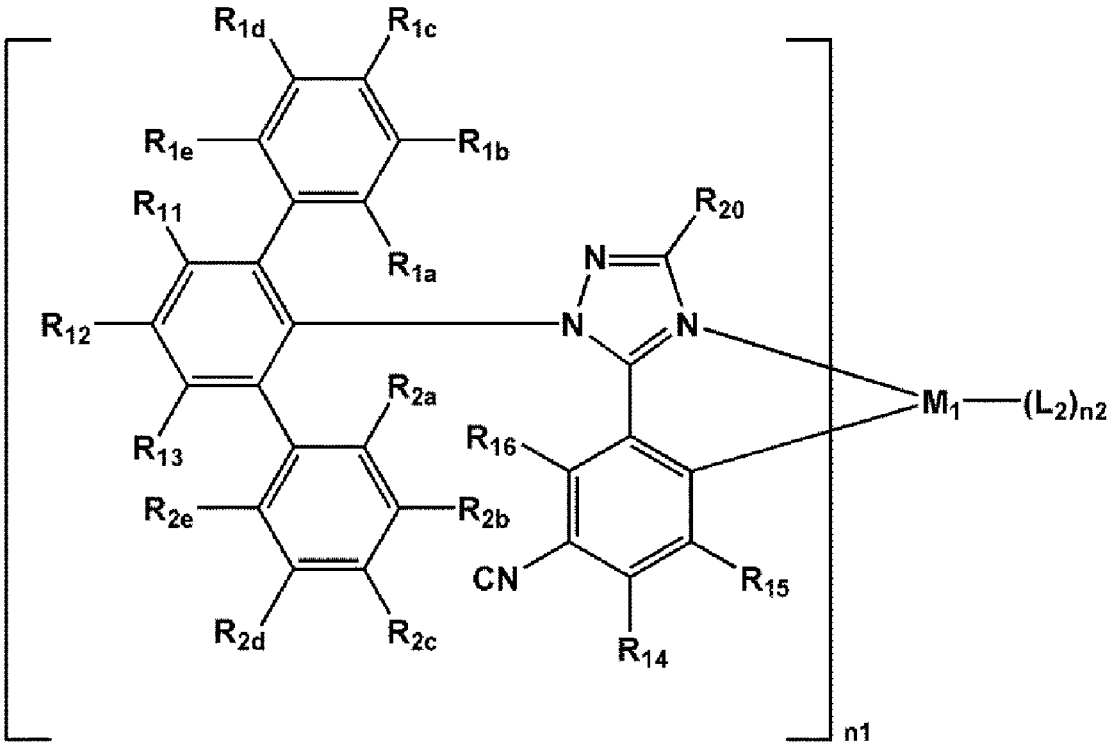
le deutérium ; et
un groupe méthyle, un groupe éthyle, un groupe n-propyle, un groupe iso-propyle, un groupe n-butyle, un groupe sec-butyle, un groupe iso-butyle, un groupe tert-butyle, un groupe n-pentyle, un groupe iso-pentyle, un groupe 1-méthylbutyle, un groupe 2-méthylbutyle, un groupe néo-pentyle, un groupe 1,2-diméthylpropyle, et un groupe tert-pentyle, chacun substitués avec au moins un deutérium.

8. Composé organométallique de l'une quelconque des revendications 1 à 7, dans lequel
le composé organométallique est représenté par une des Formules 1-1 à 1-3 :

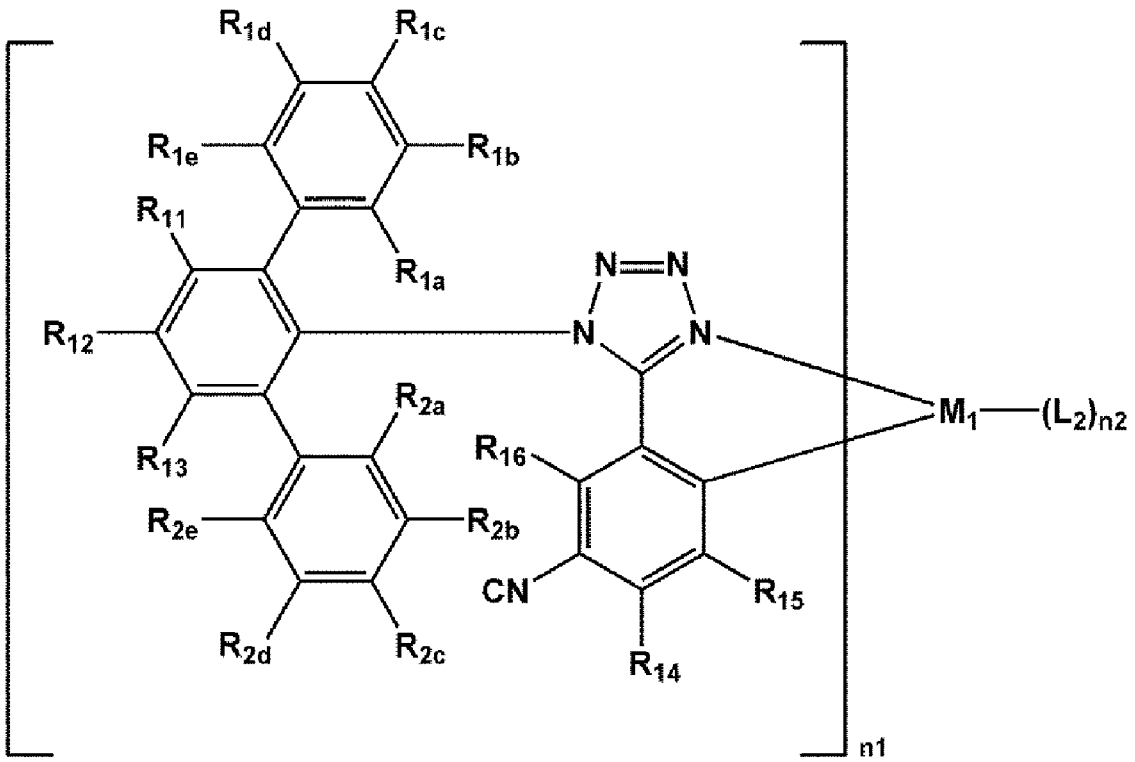
Formule 1-1



Formule 1-2



Formule 1-3

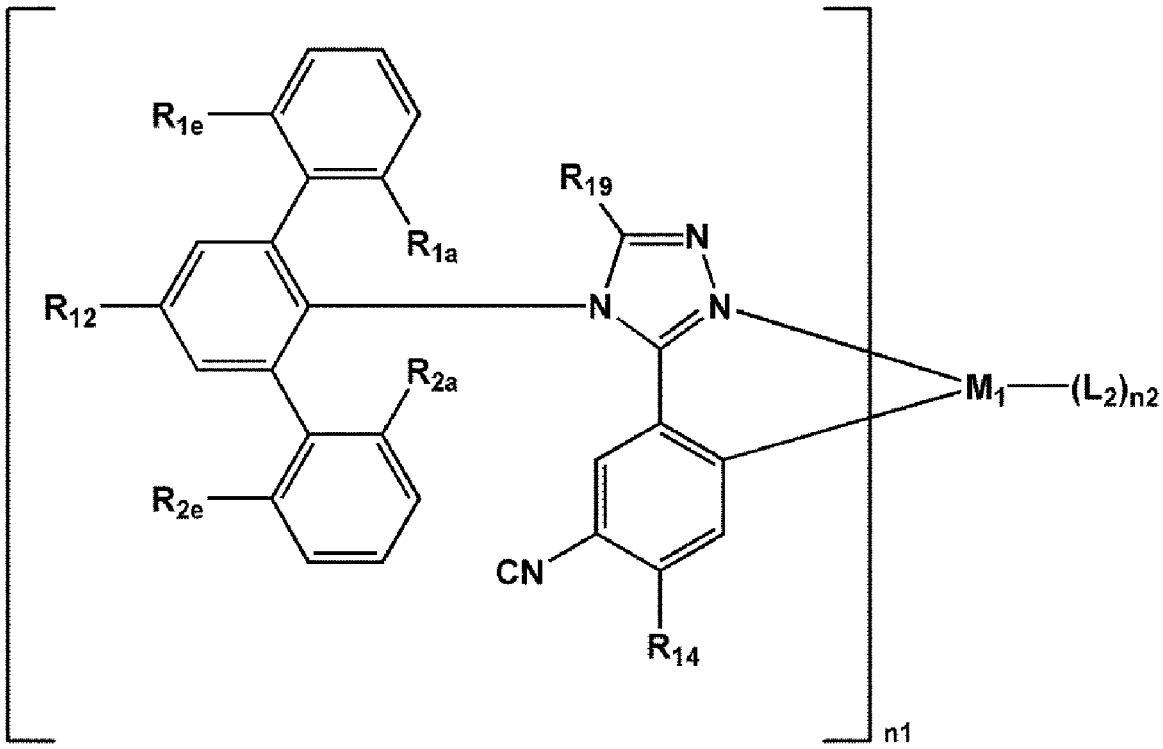


,

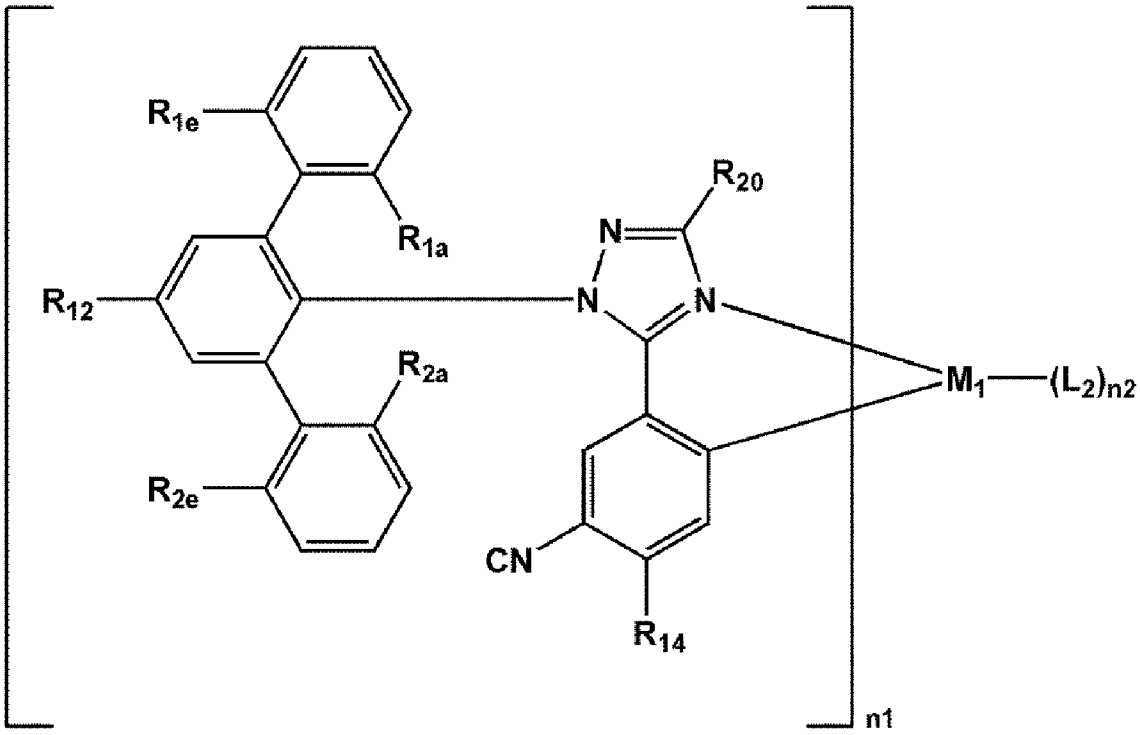
dans lequel, dans les Formules 1-1 à 1-3, M_1, n1, L_2, n2, R_{11} à R_{16}, R_{19}, et R_{20} sont chacun indépendamment les mêmes que décrits dans la revendication 1, R_{1a} à R_{1e} sont chacun indépendamment les mêmes que décrits en connexion avec R_1 dans la revendication 1, et R_{2a} à R_{2e} sont chacun indépendamment les mêmes que décrits en connexion avec R_2 dans la revendication 1.

9. Composé organométallique de l'une quelconque des revendications 1 à 8, dans lequel le composé organométallique est représenté par une des formule 1(1) à 1(3) :

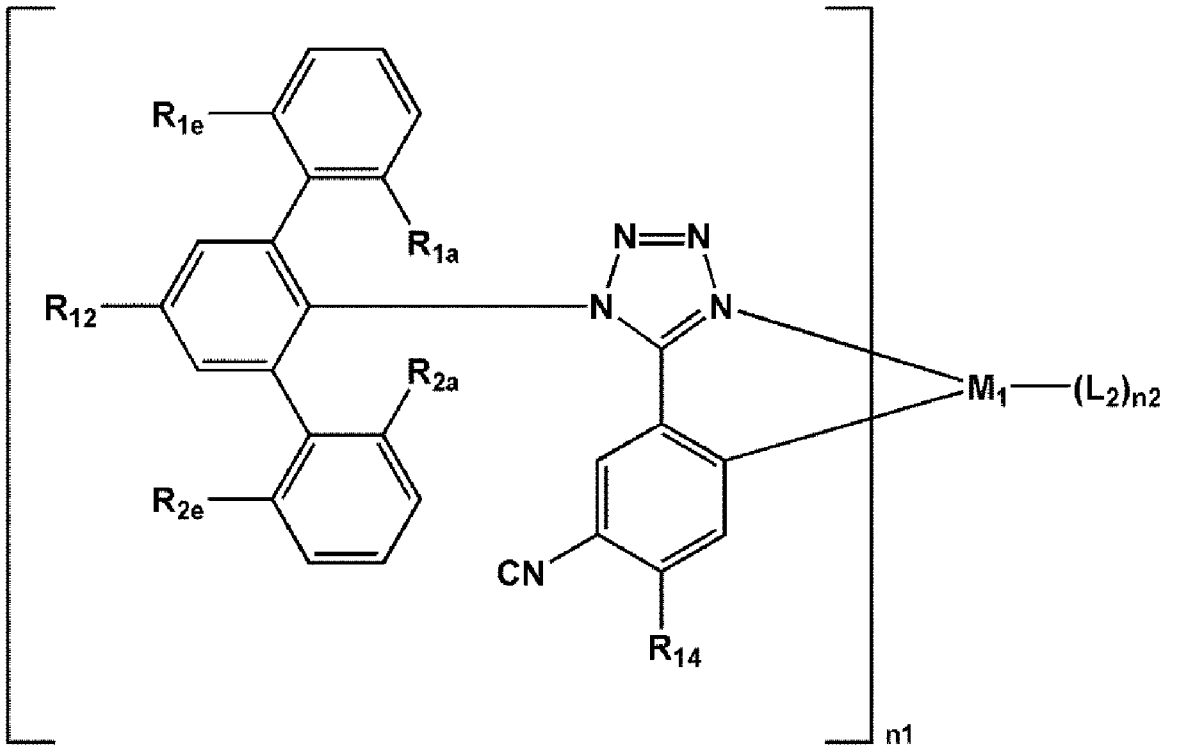
Formule 1(1)



Formule 1(2)



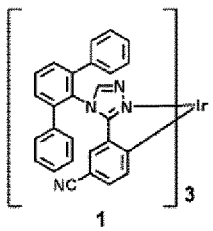
Formule 1(3)



,

dans lequel, dans les Formules 1(1) à 1(3), M_1, n1, L_2, n2, R_{12}, R_{14}, R_{19}, et R_{20} sont chacun indépendamment les mêmes que décrits dans la revendication 1, R_{1a} et R_{1e} sont chacun indépendamment les mêmes que décrits en connexion avec R_1 dans la revendication 1, et R_{2a} et R_{2e} sont chacun indépendamment les mêmes que décrits en connexion avec R_2 dans la revendication 1.

10. Composé organométallique de l'une quelconque des revendications 1 à 9, dans lequel le composé organométallique est un des Composés 1 à 10 :



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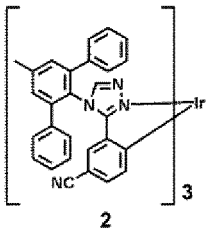

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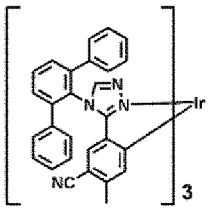

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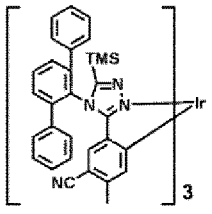

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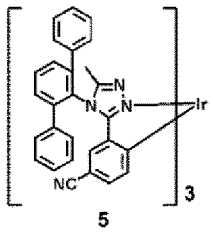

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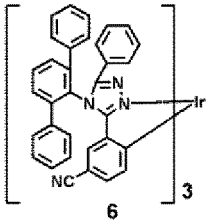

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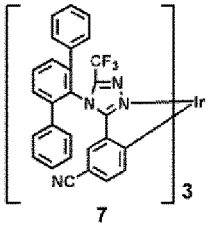

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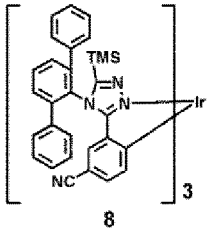

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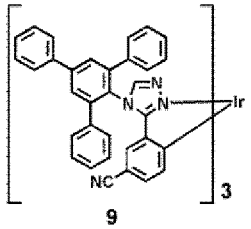

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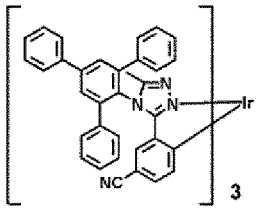
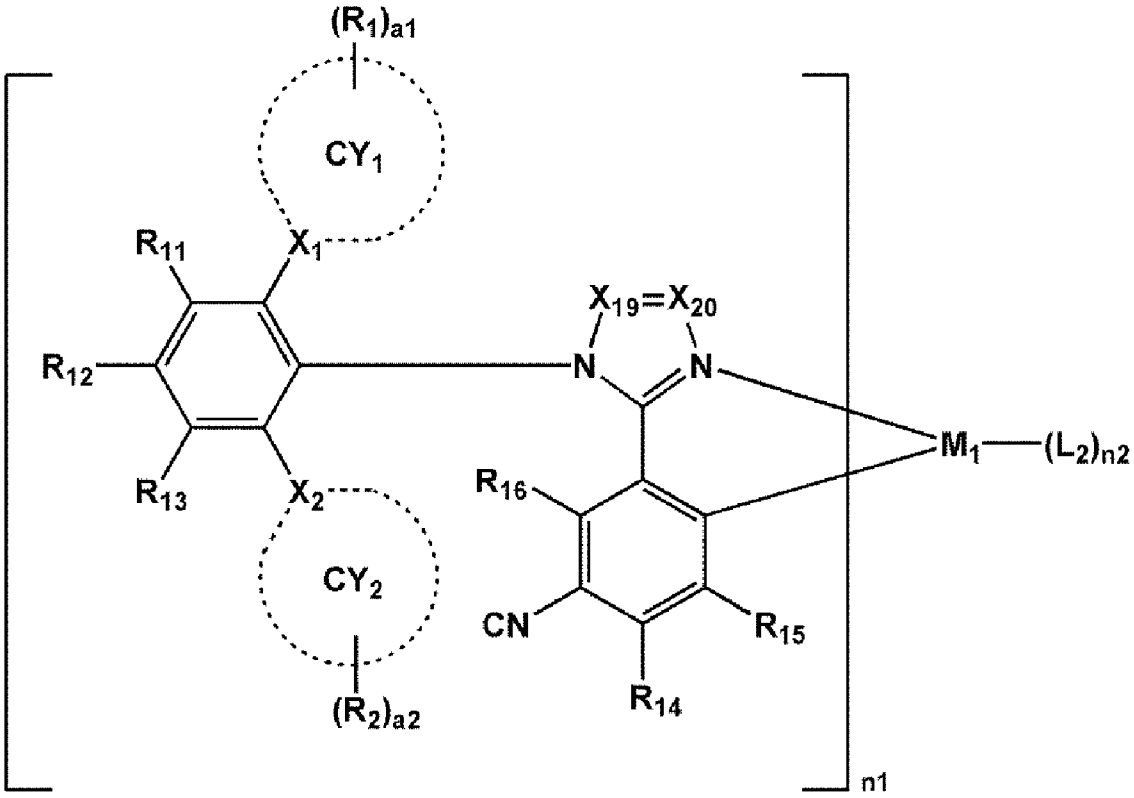


10

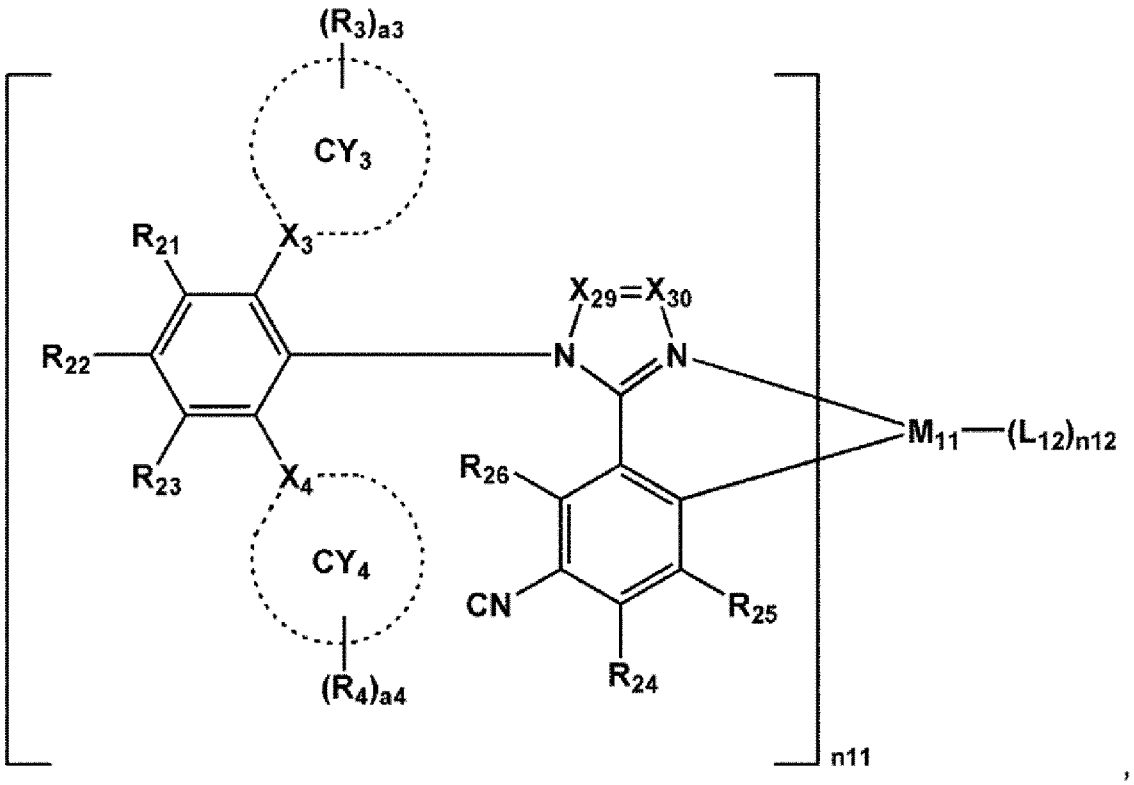
11. Composition contenant un composé organométallique, la composition comprenant :

un premier composé organométallique représenté par la Formule 1 selon l'une quelconque des revendications 1 à 10 et comprenant au moins un deutérium ; et
un deuxième composé organométallique représenté par la Formule 2 :

Formule 1



Formule 2



,

dans lequel, dans les Formules 1 et 2,

M_{11} est choisi parmi un métal de transition de la première rangée du Tableau Périodique des Éléments, un métal de transition de la deuxième rangée du Tableau Périodique des Éléments, et un métal de transition de la troisième rangée du Tableau Périodique des Éléments,
n11 est 1, 2 ou 3,
L_{12} est un ligand monodentate ou un ligand bidentate,
n12 est 0, 1, 2, 3 ou 4, lorsque n12 vaut deux ou davantage, deux ou davantage de groupes L_{12} étant identiques ou différents les uns des autres,
X_3 et X_4 sont chacun indépendamment carbone ou azote,
CY_3 et CY_4 sont chacun indépendamment un groupe carbocyclique en C_5-C_{30} ou un groupe hétérocyclique en C_2-C_{30},
X_{29} est N ou C(R_{29}), et X_{30} est N ou C(R_{30}), à condition qu'au moins un parmi X_{29} et X_{30} soit N,
R_3, R_4, R_{21} à R_{26}, R_{29}, et R_{30} sont chacun indépendamment choisis parmi hydrogène, -F, -Cl, -Br, -I, -SF_5, un groupe hydroxyle, un groupe cyano, un groupe nitro, un groupe amino, un groupe amidino, un groupe hydrazine, un groupe hydrazone, un groupe acide carboxylique ou un sel de celui-ci, un groupe acide sulfonique ou un sel de celui-ci, un groupe acide phosphorique ou un sel de celui-ci, un groupe alkyle en C_1-C_{60} substitué ou non substitué, un groupe alcényle en C_2-C_{60} substitué ou non substitué, un groupe alcynyle en C_2-C_{60} substitué ou non substitué, un groupe alcoxy en C_1-C_{60} substitué ou non substitué, un groupe cycloalkyle en C_3-C_{19} substitué ou non substitué, un groupe hétérocycloalkyle en C_1-C_{10} substitué ou non substitué, un groupe cycloalcényle en C_3-C_{19} substitué ou non substitué, un groupe hétérocycloalcényle en C_1-C_{10} substitué ou non substitué, un groupe aryle en C_6-C_{60} substitué ou non substitué, un groupe aryloxy en C_6-C_{60} substitué ou non substitué, un groupe arylthio en C_6-C_{60} substitué ou non substitué, un groupe arylalkyle en C_7-C_{60} substitué ou non substitué, un groupe hétéroaryle en C_1-C_{60} substitué ou non substitué, un groupe hétéroaryloxy en C_1-C_{60} substitué ou non substitué, un groupe hétéroarylthio en C_1-C_{60} substitué ou non substitué, un groupe hétéroarylalkyle en C_2-C_{60} substitué ou non substitué, un groupe polycyclique condensé non aromatique monovalent substitué ou non substitué, un groupe hétéropolycyclique condensé non aromatique monovalent substitué ou non substitué, -$N(Q_1)(Q_2)$, -$Si(Q_3)(Q_4)(Q_6)$,

$-B(Q_6)(Q_7)$, et $-P(=O)(Q_8)(Q_9)$,
deux ou davantage de groupes voisins choisis parmi R_3, R_4, R_{21} à R_{23}, CY_3 et CY_4 sont éventuellement reliés pour former un groupe carbocyclique en C_5-C_{30} substitué ou non substitué ou un groupe hétérocyclique en C_2-C_{30} substitué ou non substitué,
a3 et a4 sont chacun indépendamment un entier de 0 à 5, et
R_3, R_4, R_{21} à R_{26}, R_{29} et R_{30} sont chacun un substituant exempt de deutérium ; de préférence dans lequel un taux de deutération représenté par l'Équation 2 est de 50 % ou plus :

Équation 2

$$\text{taux de deutération (\%)} = n_{D2}/(n_{H2} + n_{D2}) \times 100,$$

dans lequel, dans l'Équation 2,

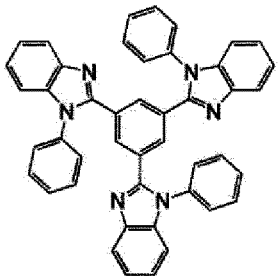
n_{H2} représente la somme d'un nombre total d'hydrogènes inclus dans les substituants contenant du deutérium dans le premier composé organométallique et d'un nombre total d'hydrogènes inclus dans un substituant exempt de deutérium du deuxième composé organométallique correspondant au substituant contenant du deutérium dans le premier composé organométallique, et
n_{D2} représente un nombre total d'atomes de deutérium inclus dans les substituants contenant du deutérium dans le premier composé organométallique.

12. Dispositif organique électroluminescent comprenant :

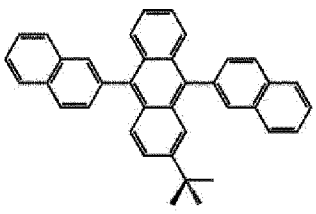
une première électrode ;
une deuxième électrode ; et
une couche organique disposée entre la première électrode et la deuxième électrode, la couche organique comprenant une couche d'émission,

dans lequel la couche organique comprend au moins un parmi le composé organométallique de l'une quelconque des revendications 1 à 10 ou la composition de la revendication 11 ;
de préférence dans lequel
la couche d'émission comprend le composé organométallique ou la composition.

13. Dispositif organique électroluminescent de la revendication 12, dans lequel
la couche d'émission comprend en outre un hôte ;
de préférence dans lequel
l'hôte est choisi parmi les composés suivants :



TPBi



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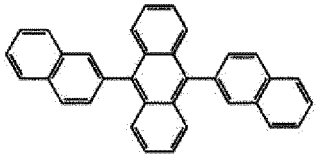
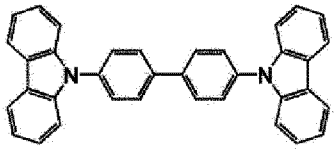
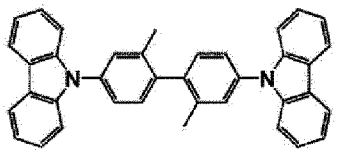


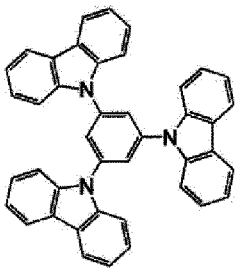
ADN



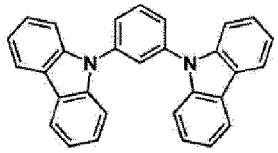
CBP



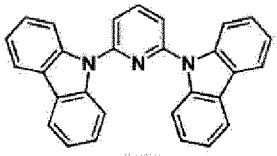
CDBP



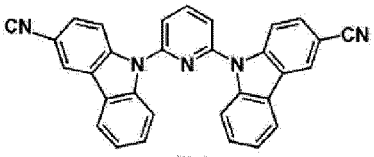
TCP



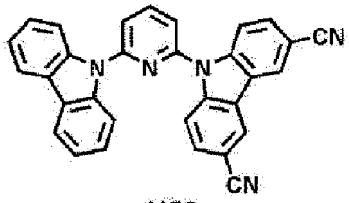
mCP



H50

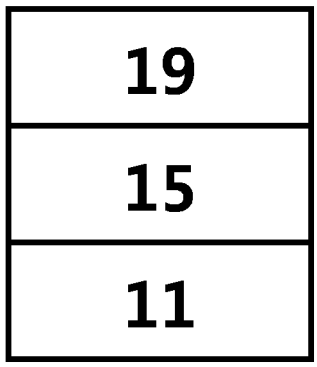


H51



H52

FIGURE



REFERENCES CITED IN THE DESCRIPTION

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Patent documents cited in the description

- JP 2014111549 A **[0005]**
- EP 3053986 A **[0006]**

专利名称(译)	有机化合物，包含有机化合物的组合物以及包含有机化合物的有机电致发光装置		
公开(公告)号	EP3372611B1	公开(公告)日	2020-06-24
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[标]申请(专利权)人(译)	三星电子株式会社 三星斯笛爱股份有限公司		
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	PARK SANGHO SOTOYAMA WATARU KIM WOOK KWON EUNSUK KIM SANGMO CHANG JAEJUN KRAVCHUK DMITRY BAE HYEJIN CHUNG YEONSOOK SON YOUNGMOK LEE NAMHEON CHWAE JUN KIM SUNGHAN		
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摘要(译)

由式1表示的有机金属化合物：其中，在式1中，基团和变量与说明书中描述的相同。