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(54) Title: ORGANIC ELECTROLUMINESCENT COMPOUND AND ORGANIC ELECTROLUMINESCENT DEVICE COMPRISING THE SAME

(57) Abstract: The present disclosure relates to an organic electroluminescent compound and an organic electroluminescent device comprising the same. The organic electroluminescent compound of the present disclosure can provide an organic electroluminescent device showing excellence in color purity, solubility, heat stability, driving voltage, current efficiency, and power efficiency, as well as remarkably improved lifespan.



Description

Title of Invention: ORGANIC ELECTROLUMINESCENT COMPOUND AND ORGANIC ELECTROLUMINESCENT DEVICE COMPRISING THE SAME

Technical Field

- [1] The present disclosure relates to an organic electroluminescent compound and an organic electroluminescent device comprising the same.

Background Art

- [2] An electroluminescent (EL) device is a self-light-emitting device which has advantages in that it provides a wider viewing angle, a greater contrast ratio, and a faster response time. An organic EL device was first developed by Eastman Kodak, by using small aromatic diamine molecules and aluminum complexes as materials to form a light-emitting layer [Appl. Phys. Lett. 51, 913, 1987].
- [3] Generally, the organic EL device has a structure comprising an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer of the organic EL device comprises a hole injection layer, a hole transport layer, an electron blocking layer, a light-emitting layer, a hole blocking layer, an electron transport layer, an electron injection layer, etc. When a voltage is applied to the organic EL device, holes and electrons are injected from an anode and a cathode, respectively, to the light-emitting layer. Excitons having high energy are formed by recombinations between the holes and the electrons. The energy of excitons puts the light-emitting organic compound in an excited state, and the decay of the excited state results in a relaxation of the energy level into a ground state, accompanied by light-emission. Therefore, the most important factor determining luminous efficiency in the organic EL device is light-emitting materials.
- [4] Depending on its function, the light-emitting materials can be classified as a host material and a dopant material. Generally, devices showing good electroluminescent characteristics comprise a light-emitting layer in which a dopant is doped into a host. The dopant/host system is provided to enhance luminous efficiency through energy transfer from a host to a dopant. In the dopant/host material system, the dopant and host materials highly affect efficiencies and lifespan of the device.
- [5] Iridium(III) complexes have been widely known as phosphorescent materials, including bis(2-(2'-benzothienyl)-pyridinato-N,C-3')iridium(acetylacetonate) ((acac)Ir(btp)₂), tris(2-phenylpyridine)iridium (Ir(ppy)₃) and bis(4,6-difluorophenylpyridinato-N,C2)picolate iridium (Firpic) as red-, green-, and blue-emitting materials, respectively.

- [6] However, considering EL characteristic requirements for a middle or large-sized panel of OLED, Iridium(III) complex-based dopant compounds showing better characteristics, i.e., long lifespan, high efficiency, and high color purity must be urgently developed.
- [7] Particularly, for a full-color display, pixels which show particular colors called as a “saturated” color are required, and especially, saturated red, green, and blue pixels are required, which can be measured by a CIE coordinate known in this field. In order to display more various colors, each of red, green, and blue should have high color purity. In the case of red, color purity becomes higher, as it approaches a deep-red coordinate around 0.680 of x-axis of CIE. A dopant compound which meets such requirements is desired.
- [8] Korean Patent No. 0662381, Korean Patent Application Laying-Open No. 2011-0086021, WO 2008/109824, and WO 2010/033550 disclose iridium complexes having 2-phenylquinoline-based ligand, as a dopant compound of an organic electroluminescent device. However, said prior arts fail to specifically disclose an iridium complex having a ligand in which quinoline of 2-phenylquinoline is substituted with alkyl at 4-position and is substituted with phenyl at 6-position.

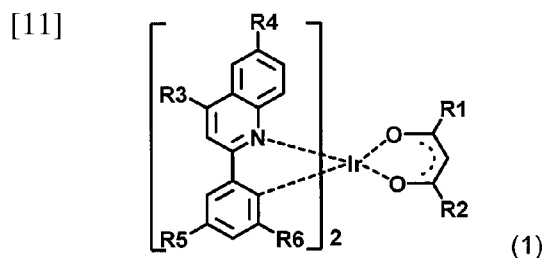
Disclosure of Invention

Technical Problem

- [9] The object of the present disclosure is to provide a compound which can be used to prepare an organic electroluminescent device showing good color purity and long lifespan, and to provide an organic electroluminescent device comprising the compound.

Solution to Problem

- [10] The present inventors found that the above object can be achieved by a compound represented by the following formula 1.



- [12] wherein
- [13] R_1 and R_2 , each independently, represent a (C1-C5)alkyl,
- [14] R_3 represents a (C3-C5)alkyl unsubstituted or substituted with deuterium,
- [15] R_4 represents phenyl unsubstituted or substituted with a (C1-C5)alkyl unsubstituted or substituted with deuterium, and

- [16] R_5 and R_6 , each independently, represent methyl unsubstituted or substituted with deuterium.

Advantageous Effects of Invention

- [17] The compound of the present disclosure can provide an organic electroluminescent device showing remarkably improved color purity and lifespan.
- [18] An electron-donating property and an electron-withdrawing property between two materials exchanging electrons are not absolutely determined, but relatively determined depending on relation between the materials. Phenyl is generally an electron-donating group, but in the present disclosure, is used as an electron-withdrawing group. In formula 1, phenyl is introduced as an electron-withdrawing group at R_4 position of quinoline which affects LUMO energy level of the molecule, thereby reducing electron density and lowering LUMO energy level. Due to the lowered LUMO energy level, an energy gap between HOMO energy level and LUMO energy level becomes smaller. As a result, color purity of a red-emitting organic electroluminescent device is improved.

Mode for the Invention

- [19] Hereinafter, the present disclosure will be described in detail. However, the following description is intended to explain the invention, and is not meant in any way to restrict the scope of the invention.
- [20] The present disclosure provides the compound of formula 1 above, an organic electroluminescent material comprising the compound, and an organic electroluminescent device comprising the compound.
- [21] The details of the compound of formula 1 are as follows.
- [22] Herein, a "(C1-C5)alkyl" indicates a linear or branched alkyl having 1 to 5 carbon atoms. Specifically, a (C1-C5)alkyl includes methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl, sec-butyl, tert-butyl, n-pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, and 1-ethylpropyl.
- [23] In formula 1, R_1 and R_2 , each independently, represent a (C1-C5)alkyl. Specifically, R_1 and R_2 , each independently, may be selected from methyl, ethyl, and a branched (C3-C5)alkyl. Preferably, R_1 and R_2 may be the same.
- [24] In formula 1, R_3 represents a (C3-C5)alkyl unsubstituted or substituted with deuterium. Specifically, R_3 may be selected from isopropyl, isobutyl, sec-butyl, tert-butyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, and 1-ethylpropyl. More specifically, R_3 may be selected from isopropyl, isobutyl, sec-butyl, tert-butyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl,

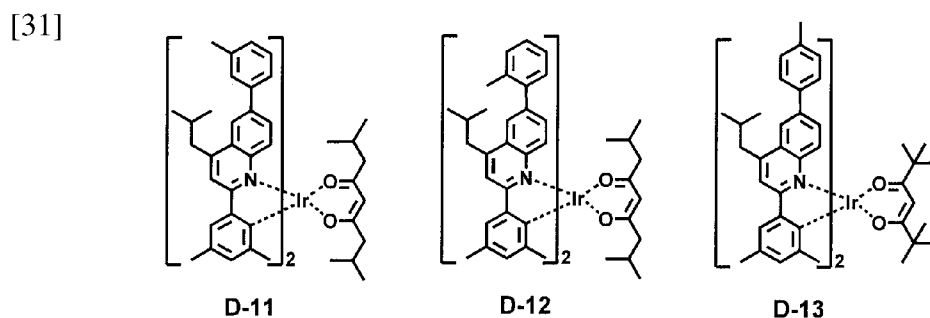
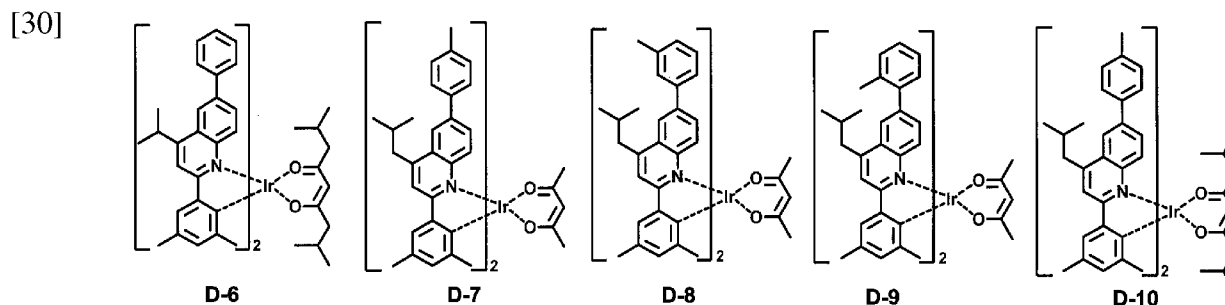
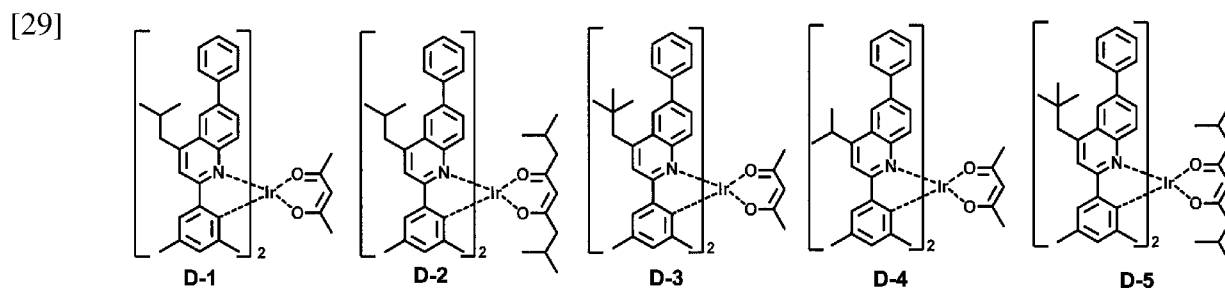
2,2-dimethylpropyl, and 1-ethylpropyl.

[25] In formula 1, R_4 represents phenyl unsubstituted or substituted with a (C1-C5)alkyl unsubstituted or substituted with deuterium. Specifically, R_4 may be phenyl unsubstituted or substituted with a (C1-C3)alkyl. More specifically, R_4 may be selected from phenyl, phenyl substituted with methyl, phenyl substituted with deuterium-substituted methyl, phenyl substituted with isopropyl, phenyl substituted with isobutyl, phenyl substituted with tert-butyl, and phenyl substituted with 2,2-dimethylpropyl.

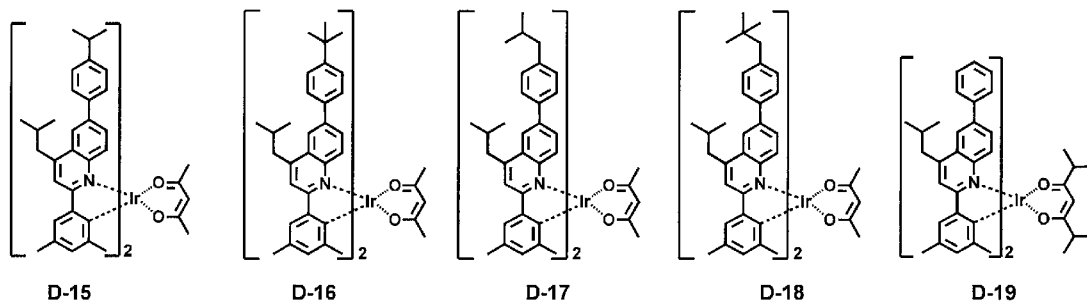
[26] According to one embodiment of the present disclosure, in formula 1, R_4 may be phenyl unsubstituted or substituted with a (C1-C4)alkyl.

[27] According to another embodiment of the present disclosure, in formula 1, R_3 may be selected from a branched (C3-C5)alkyl unsubstituted or substituted with deuterium, and R_4 may be phenyl unsubstituted or substituted with methyl unsubstituted or substituted with deuterium.

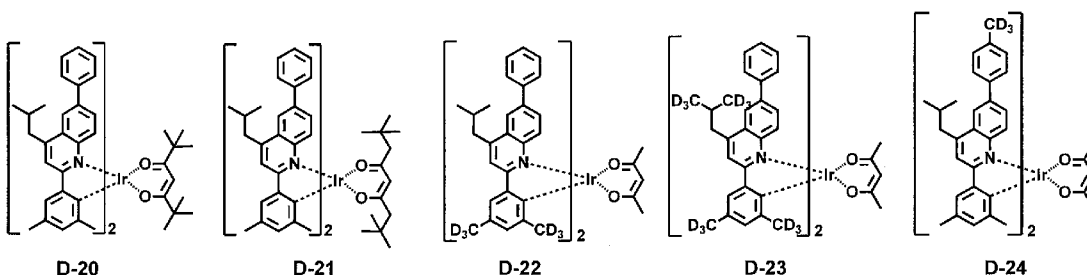
[28] More specifically, the compound of formula 1 includes the following, but is not limited thereto.



[32]

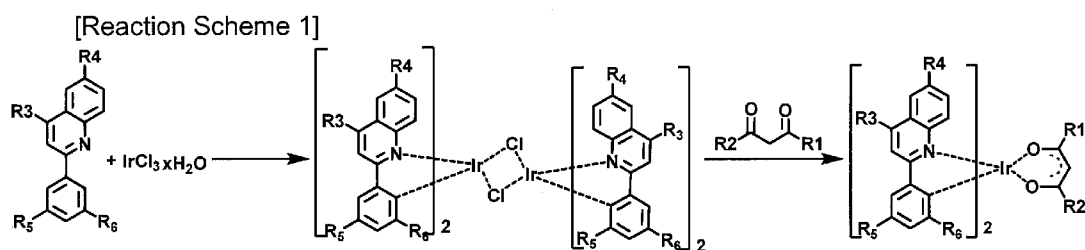


[33]



[34] The compound of the present disclosure can be prepared by a synthetic method known to one skilled in the art. For example, it can be prepared according to the following reaction scheme 1.

[35]



[36] In reaction scheme 1, R₁ to R₆ are as defined in formula 1.

[37] In addition, the present disclosure provides an organic electroluminescent material comprising the compound of formula 1, and an organic electroluminescent device comprising the material.

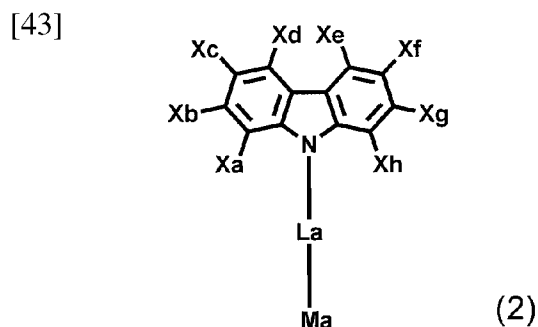
[38] The material may consist of the compound of the present disclosure. Otherwise, the material may further comprise a conventional compound(s) which has been comprised for an organic electroluminescent material.

[39] The organic electroluminescent device of the present disclosure may comprise a first electrode, a second electrode, and at least one organic layer disposed between the first and second electrodes. The organic layer may comprise at least one compound of formula 1.

[40] One of the first and second electrodes may be an anode, and the other may be a cathode. The organic layer may comprise a light-emitting layer, and may further comprise at least one layer selected from a hole injection layer, a hole transport layer, an electron transport layer, an electron injection layer, an interlayer, a hole blocking layer, an electron blocking layer, and an electron buffer layer.

[41] The compound of formula 1 of the present disclosure may be comprised as a dopant material in the light-emitting layer. The light-emitting layer may further comprise at least one host material.

[42] A host material which may be used to be comprised with the compound of the present disclosure includes the compound of formula 2:



[44] wherein

[45] Ma represents a substituted or unsubstituted nitrogen-containing 5- to 11-membered heteroaryl;

[46] La represents a single bond, or a substituted or unsubstituted (C6-C30)arylene;

[47] Xa to Xh, each independently, represent hydrogen, deuterium, a halogen, a cyano, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C6-C60)aryl, a substituted or unsubstituted 3- to 30-membered heteroaryl, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyl(C6-C30)aryl amino, or a substituted or unsubstituted mono- or di-(C6-C30)aryl amino; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur; and the heteroaryl contains at least one hetero atom selected from B, N, O, S, Si, and P.

[48] In formula 2, the substituent for the substituted alkyl, the substituted alkenyl, the substituted alkynyl, the substituted cycloalkyl, the substituted aryl, the substituted heteroaryl, the substituted trialkylsilyl, the substituted triarylsilyl, the substituted dialkylarylsilyl, the substituted alkyldiarylsilyl, the substituted alkylaryl amino, the substituted monoaryl amino, the substituted diaryl amino, or the substituted mono- or polycyclic, alicyclic or aromatic ring, each independently, may be at least one selected from the group consisting of deuterium; a halogen; a cyano; a carboxyl; a nitro; a

hydroxy; a (C1-C30)alkyl; a halo(C1-C30)alkyl; a (C2-C30)alkenyl; a (C2-C30)alkynyl; a (C1-C30)alkoxy; a (C1-C30)alkylthio; a (C3-C30)cycloalkyl; a (C3-C30)cycloalkenyl; a 3- to 7-membered heterocycloalkyl; a (C6-C30)aryloxy; a (C6-C30)arylthio; a 3- to 30-membered heteroaryl unsubstituted or substituted with a tri(C6-C30)arylsilyl, a (C6-C30)aryl, a (C1-C30)alkyl(C6-C30)aryl, or a tri(C6-C30)arylsilyl(C6-C30)aryl; a (C6-C30)aryl unsubstituted or substituted with a (C1-C30)alkyl, a halogen, a (C6-C30)aryl, or a 3- to 30-membered heteroaryl; a tri(C1-C30)alkylsilyl; a tri(C6-C30)arylsilyl; a di(C1-C30)alkyl(C6-C30)arylsilyl; a (C1-C30)alkyldi(C6-C30)arylsilyl; an amino; a mono- or di-(C1-C30)alkylamino; a mono- or di-(C6-C30)arylamino; a (C1-C30)alkyl(C6-C30)arylamino; a (C1-C30)alkylcarbonyl; a (C1-C30)alkoxycarbonyl; a (C6-C30)arylcarbonyl; a di(C6-C30)arylboronyl; a di(C1-C30)alkylboronyl; a (C1-C30)alkyl(C6-C30)arylboronyl; a (C6-C30)aryl(C1-C30)alkyl; and a (C1-C30)alkyl(C6-C30)aryl.

[49] In formula 2, preferably, La may be a single bond, or a substituted or unsubstituted (C6-C12)arylene. More preferably, La may be a single bond, or a (C6-C12)arylene unsubstituted or substituted with a tri(C6-C10)arylsilyl. Specifically, La may be a single bond, a substituted or unsubstituted phenylene, a substituted or unsubstituted naphthylene, or a substituted or unsubstituted biphenylene.

[50] In formula 2, preferably, Ma may be a substituted or unsubstituted nitrogen-containing 5- to 11-membered heteroaryl. More preferably, Ma may be a nitrogen-containing 6- to 11-membered heteroaryl unsubstituted or substituted with a cyano, a (C1-C6)alkyl, a tri(C6-C12)arylsilyl, a (C6-C18)aryl, or a 5- to 15-membered heteroaryl.

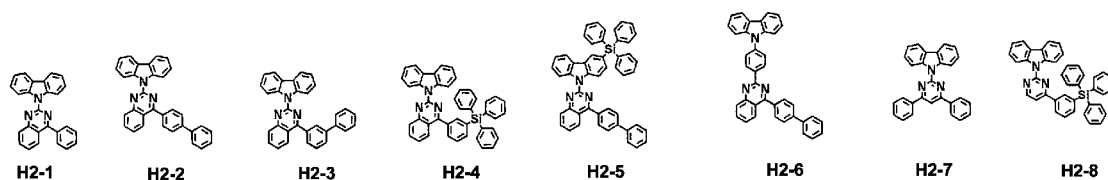
[51] Specifically, Ma may be a substituted or unsubstituted pyrrolyl, a substituted or unsubstituted imidazolyl, a substituted or unsubstituted pyrazolyl, a substituted or unsubstituted triazinyl, a substituted or unsubstituted tetrazinyl, a substituted or unsubstituted triazolyl, a substituted or unsubstituted tetrazolyl, a substituted or unsubstituted pyridyl, a substituted or unsubstituted pyrazinyl, a substituted or unsubstituted pyrimidinyl, a substituted or unsubstituted pyridazinyl, a substituted or unsubstituted benzimidazolyl, a substituted or unsubstituted isoindolyl, a substituted or unsubstituted indolyl, a substituted or unsubstituted indazolyl, a substituted or unsubstituted benzothiadiazolyl, a substituted or unsubstituted quinolyl, a substituted or unsubstituted isoquinolyl, a substituted or unsubstituted cinnolinyl, a substituted or unsubstituted quinazolinyl, a substituted or unsubstituted naphthylidiny, or a substituted or unsubstituted quinoxalinyl. More specifically, Ma may be a substituted or unsubstituted triazinyl, a substituted or unsubstituted pyrimidinyl, a substituted or unsubstituted pyridyl, a substituted or unsubstituted quinolyl, a substituted or unsubstituted iso-

quinolyl, a substituted or unsubstituted quinazolinyl, a substituted or unsubstituted naphthylidiny, or a substituted or unsubstituted quinoxaliny.

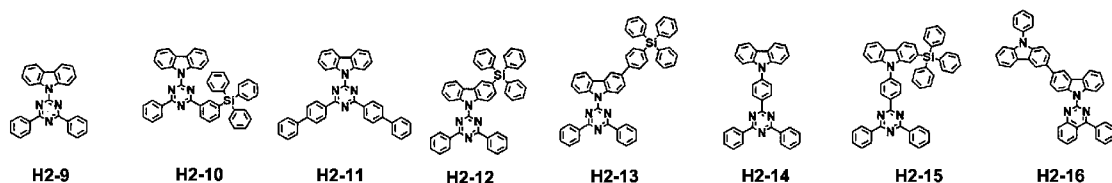
- [52] In formula 2, preferably, Xa to Xh, each independently, may be hydrogen, a cyano, a substituted or unsubstituted (C6-C15)aryl, a substituted or unsubstituted 6- to 20-membered heteroaryl, or a substituted or unsubstituted tri(C6-C15)arylsilyl; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted 6- to 20-membered, mono- or polycyclic aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur. More preferably, Xa to Xh, each independently, may be hydrogen; a cyano; a (C6-C15)aryl unsubstituted or substituted with a tri(C6-C10)arylsilyl; or a 10- to 20-membered heteroaryl unsubstituted or substituted with a (C6-C12)aryl; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted benzene, a substituted or unsubstituted indole, a substituted or unsubstituted benzindole, a substituted or unsubstituted indene, a substituted or unsubstituted benzofuran, or a substituted or unsubstituted benzothiophene. Specifically, at least one of Xa to Xh, for example, Xb, Xc, Xf, or Xg, may be a substituted or unsubstituted dibenzothiophene; a substituted or unsubstituted dibenzofuran; a substituted or unsubstituted carbazole; a substituted or unsubstituted benzocarbazole; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted benzene, a substituted or unsubstituted indole, a substituted or unsubstituted benzindole, a substituted or unsubstituted indene, a substituted or unsubstituted benzofuran, or a substituted or unsubstituted benzothiophene.

- [53] More specifically, the compound of formula 2 includes the following, but is not limited thereto:

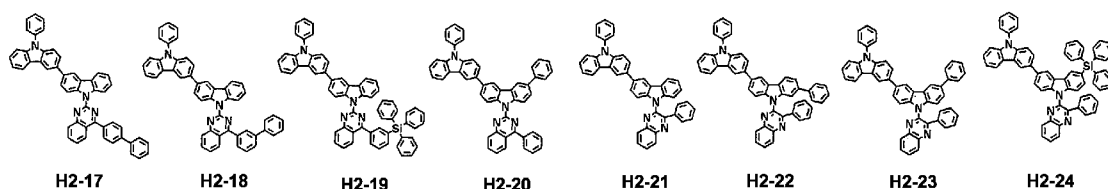
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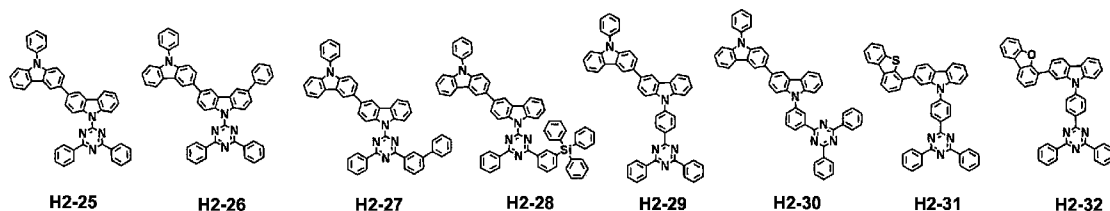
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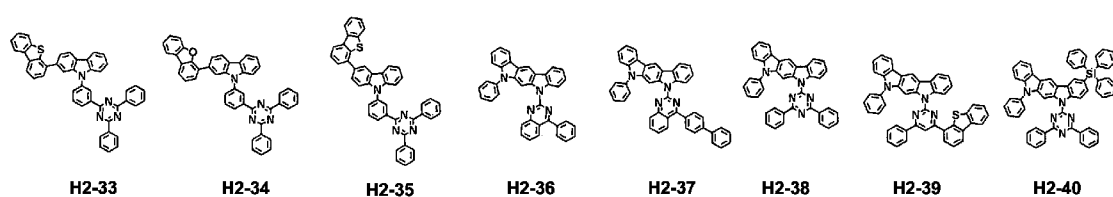
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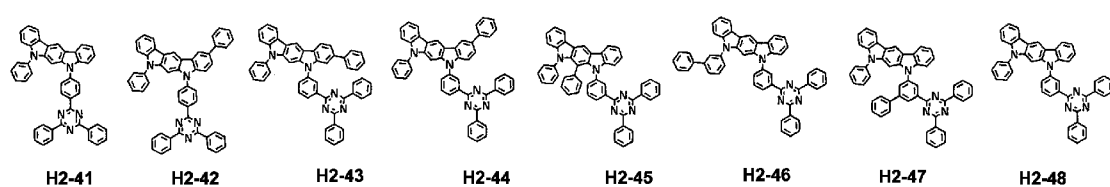
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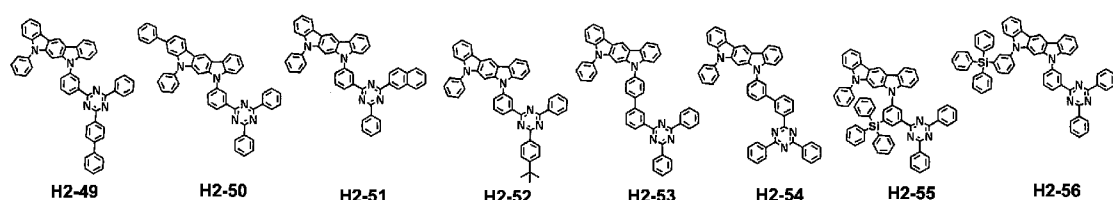
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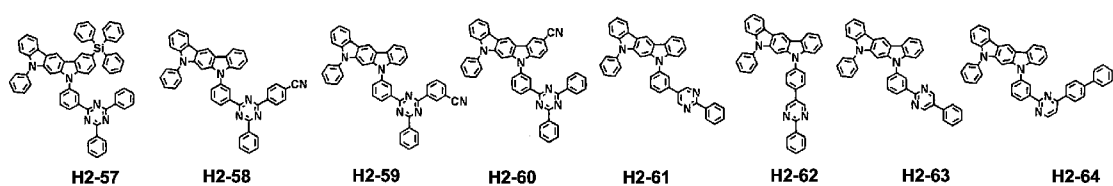
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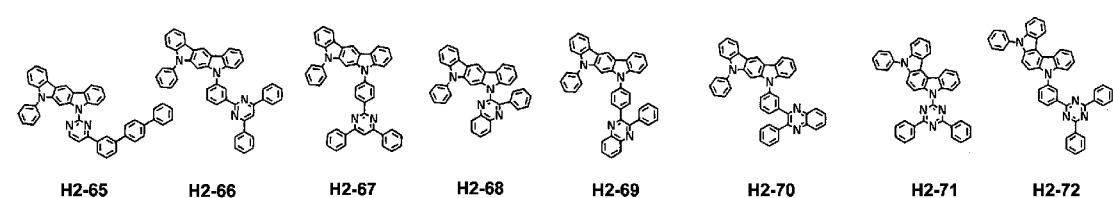
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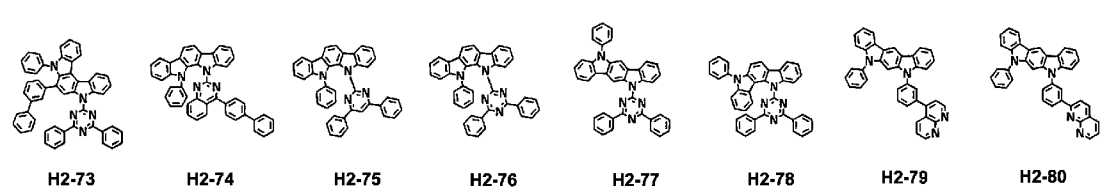
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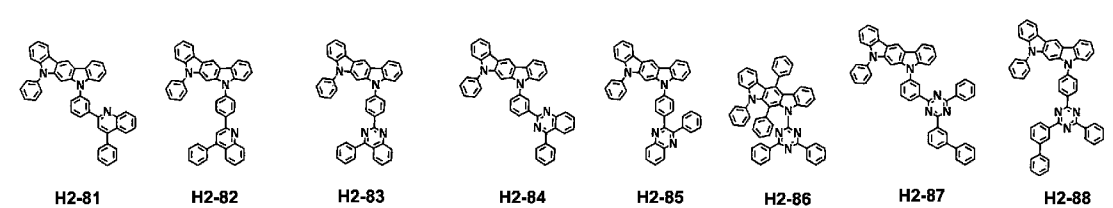
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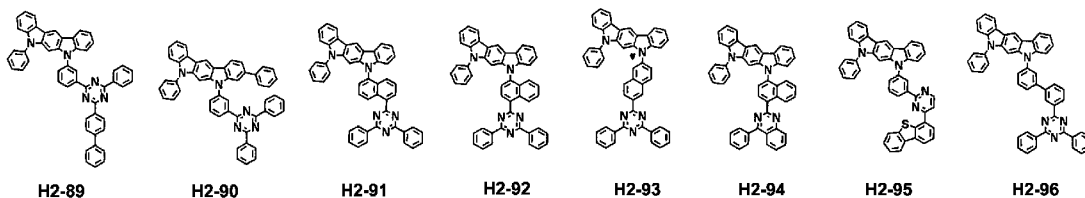
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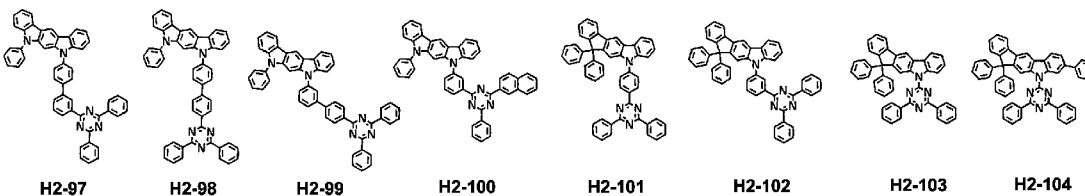
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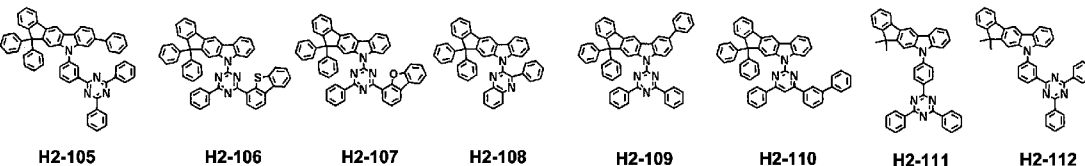
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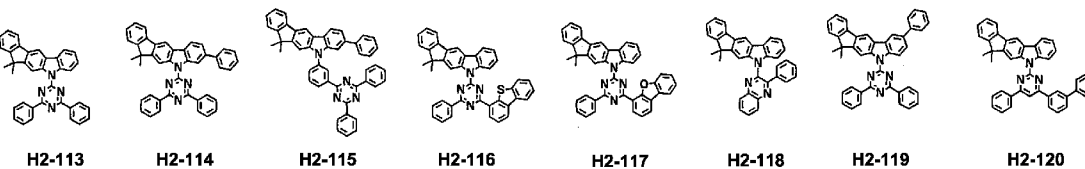
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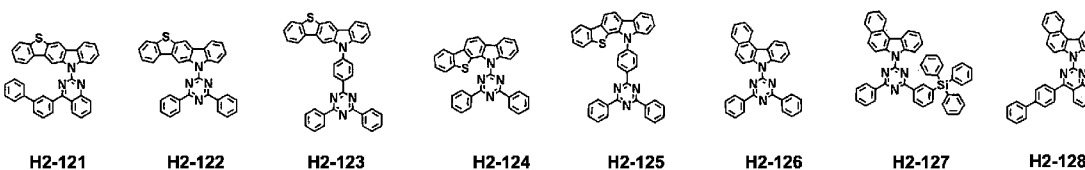
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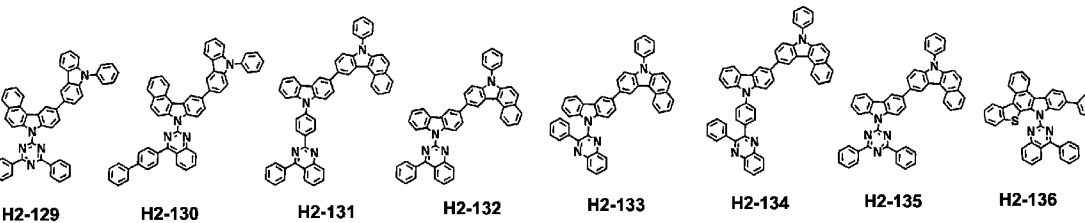
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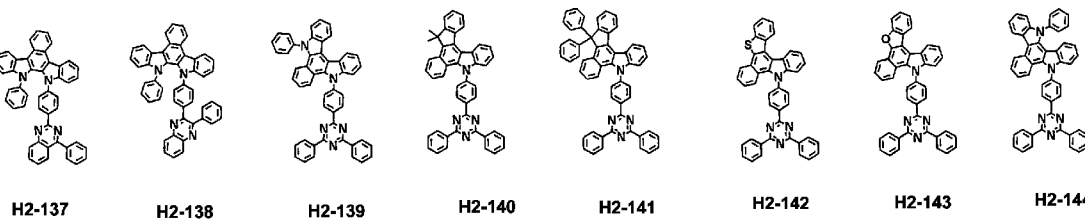
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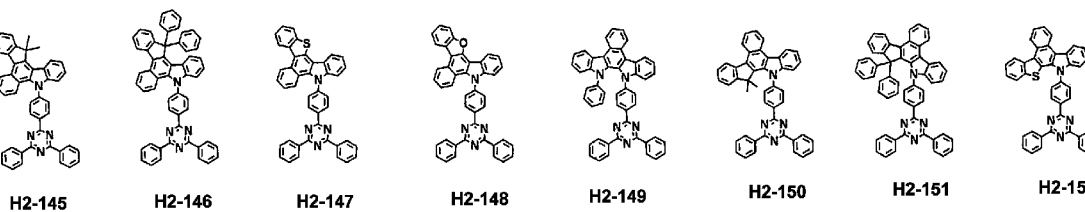
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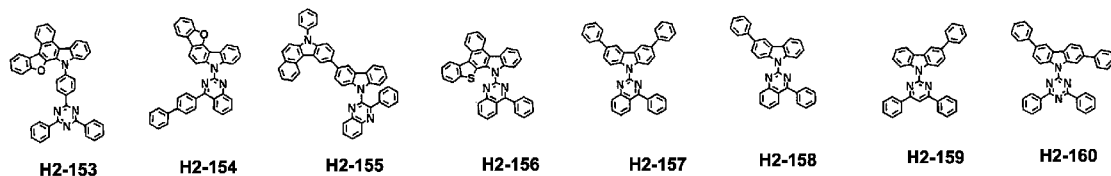
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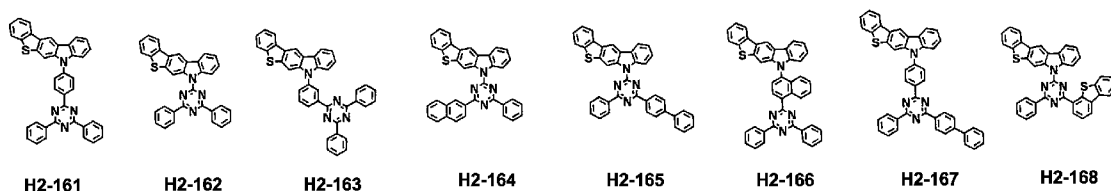
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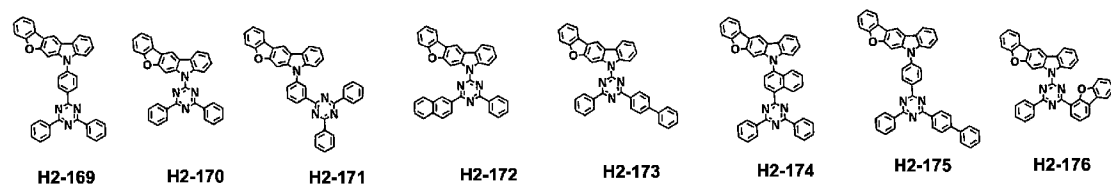
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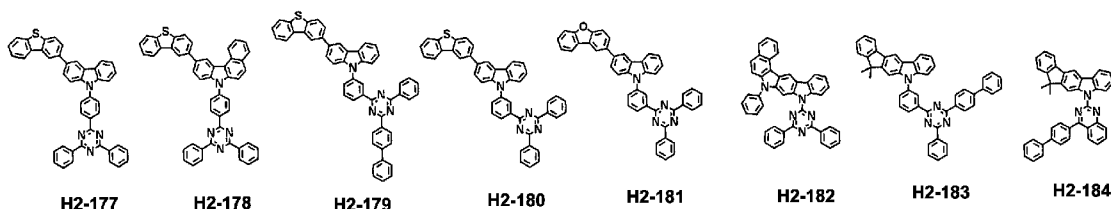
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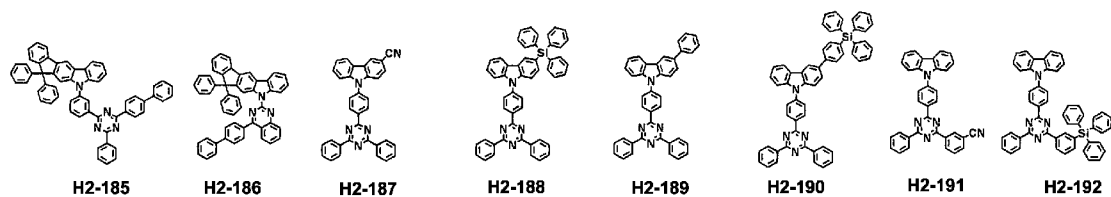
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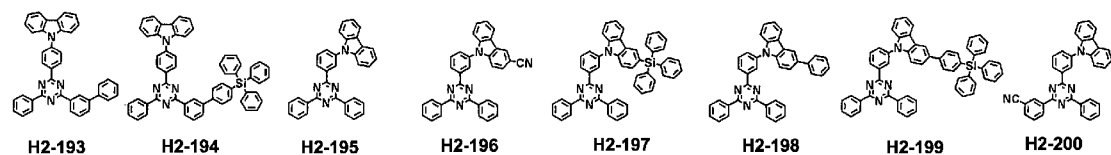
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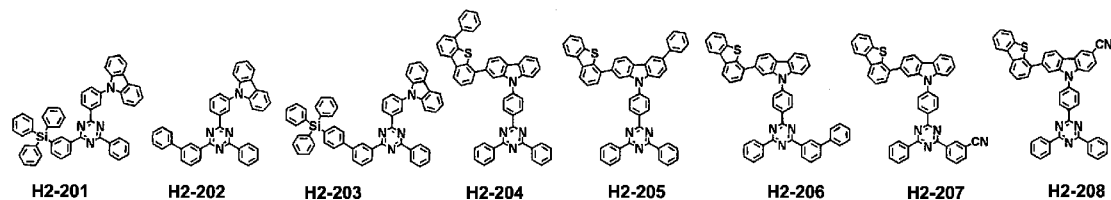
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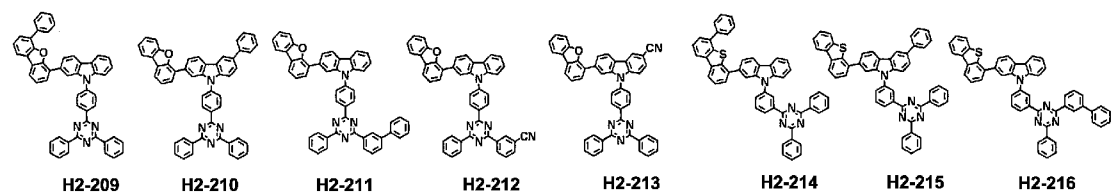
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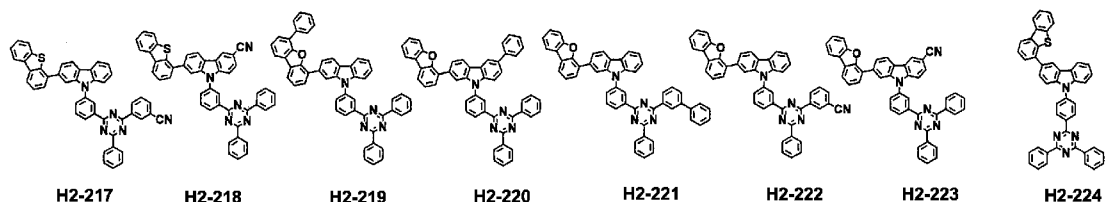
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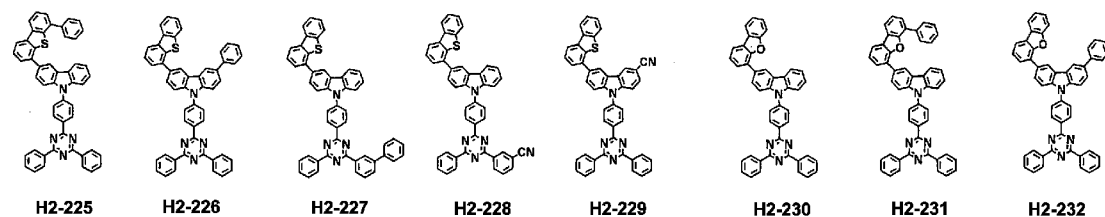
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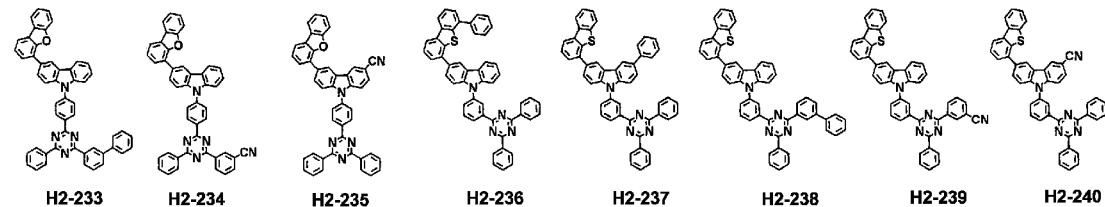
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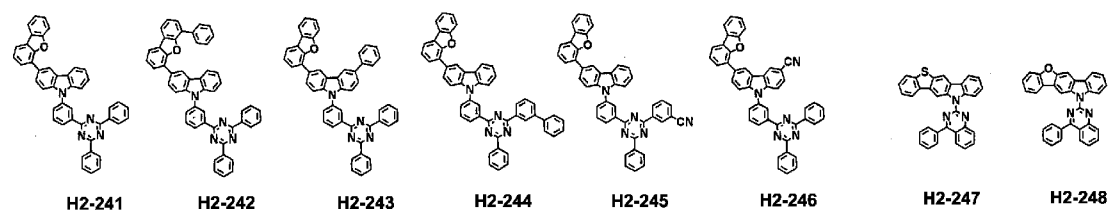
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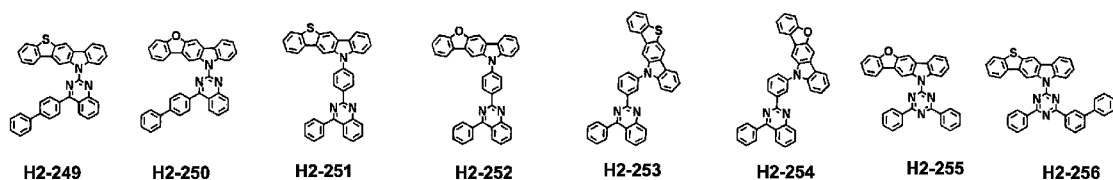
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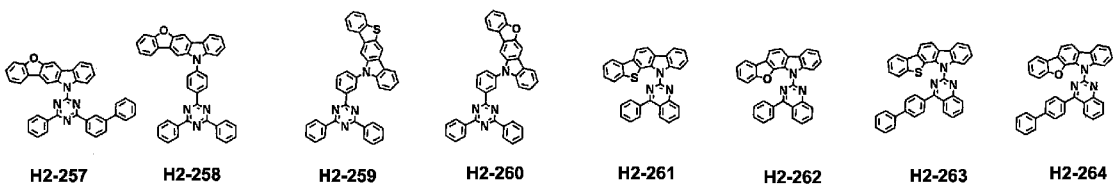
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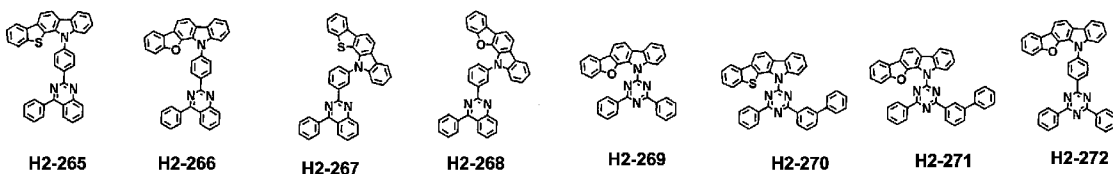
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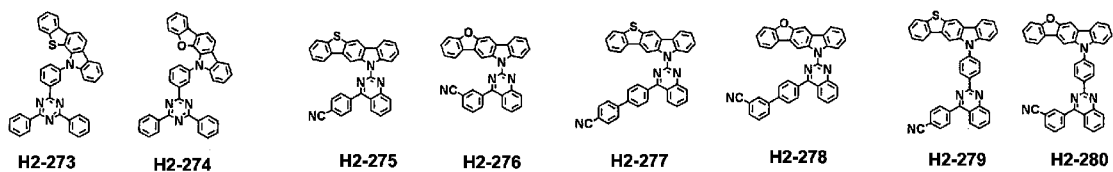
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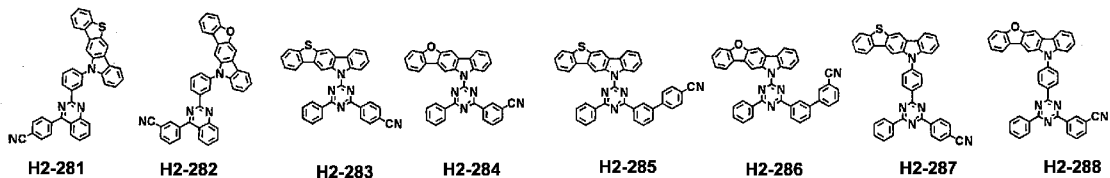
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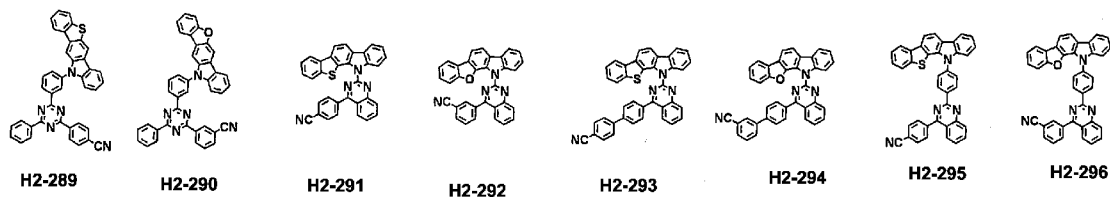
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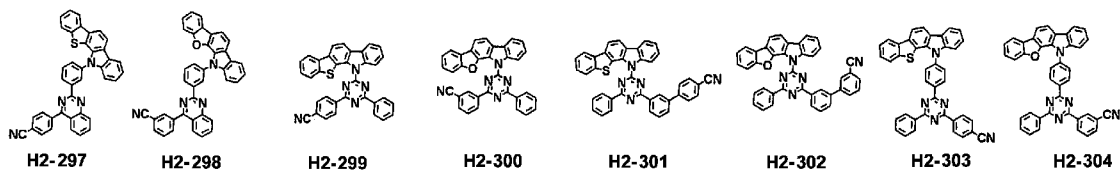
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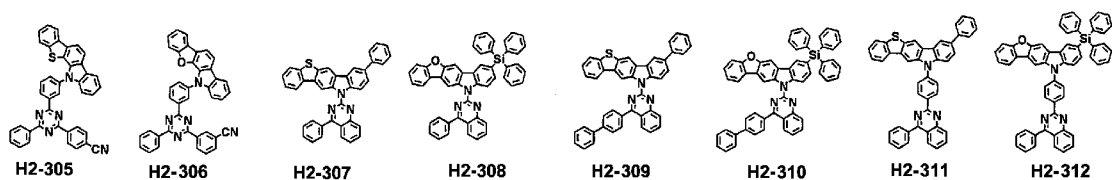
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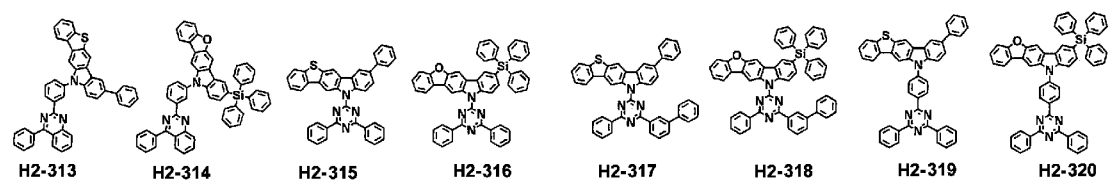
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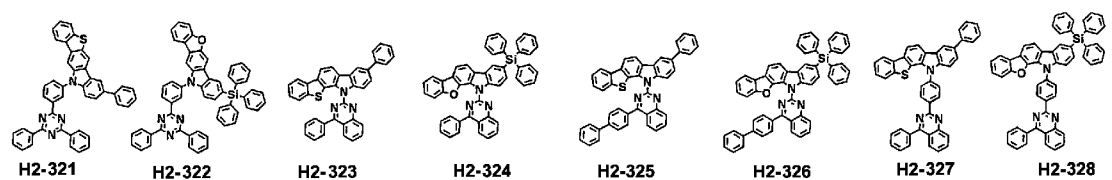
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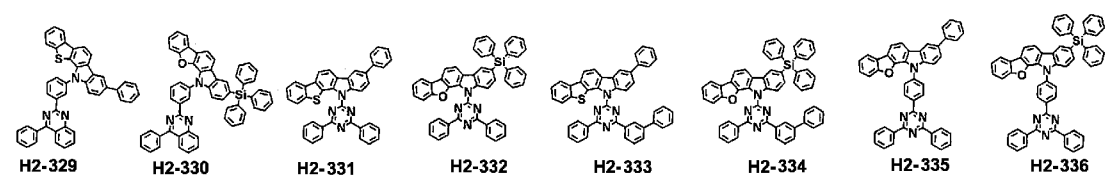
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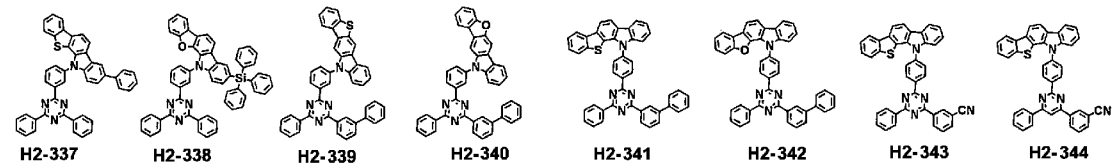
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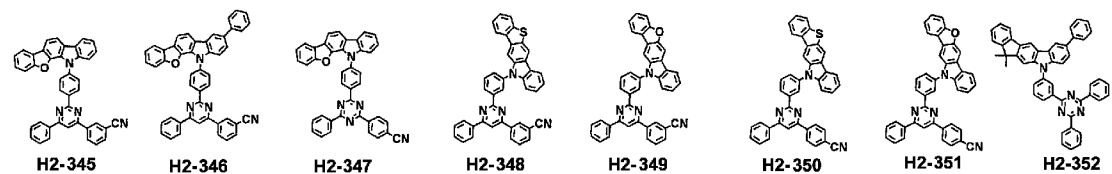
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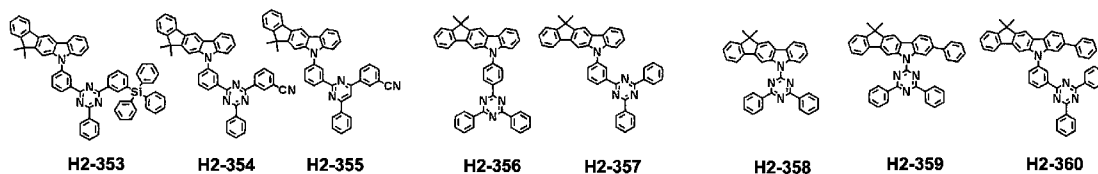
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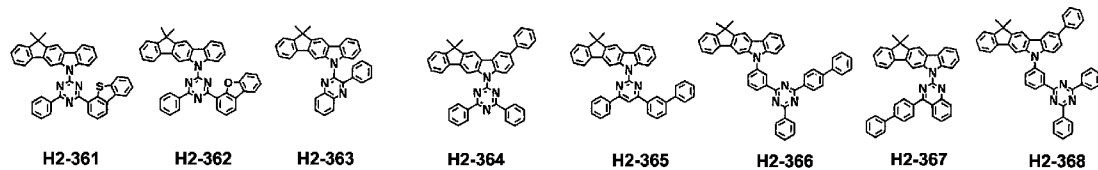
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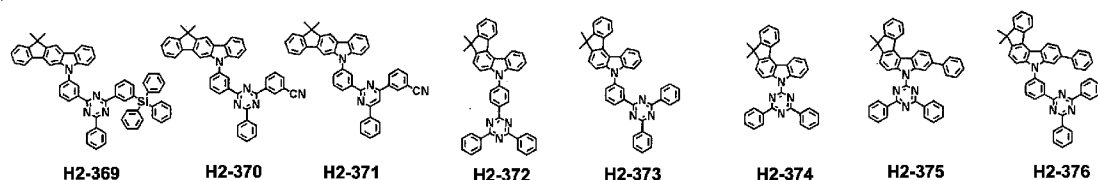
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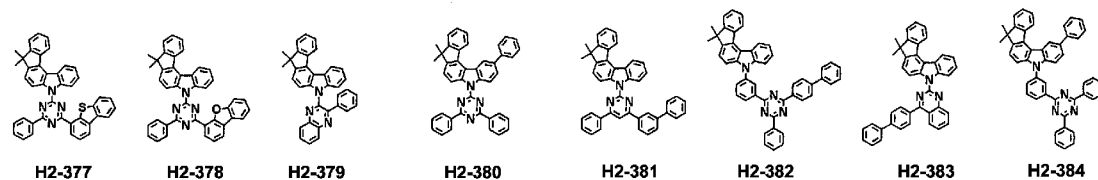
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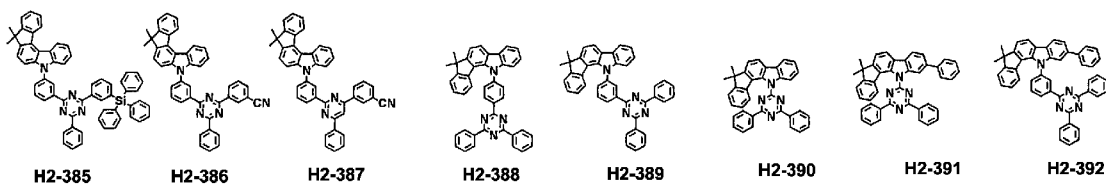
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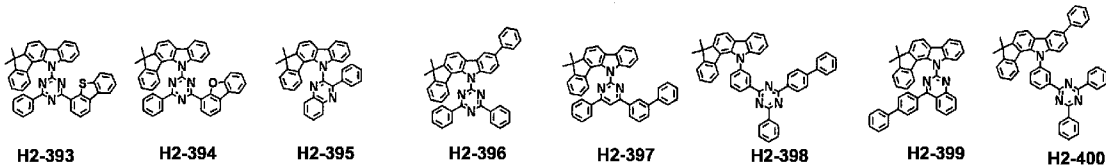
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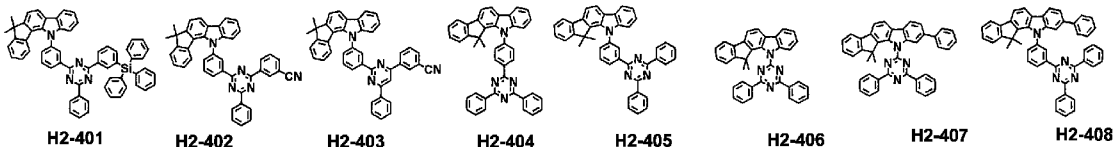
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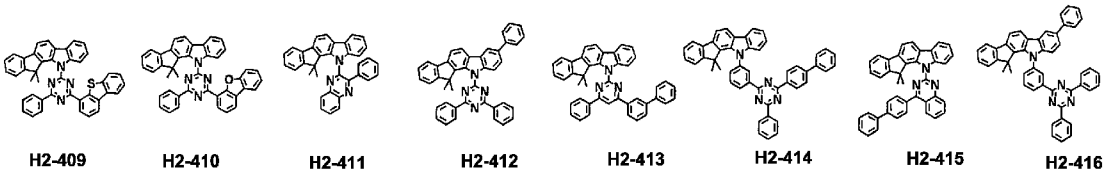
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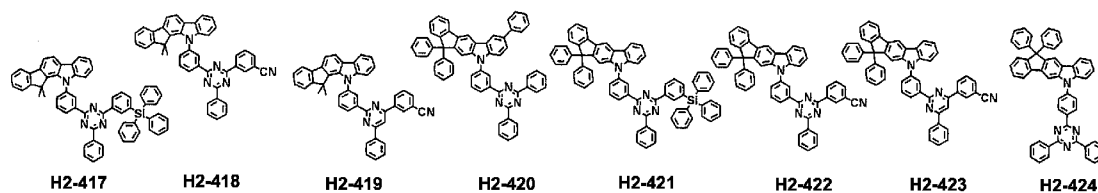
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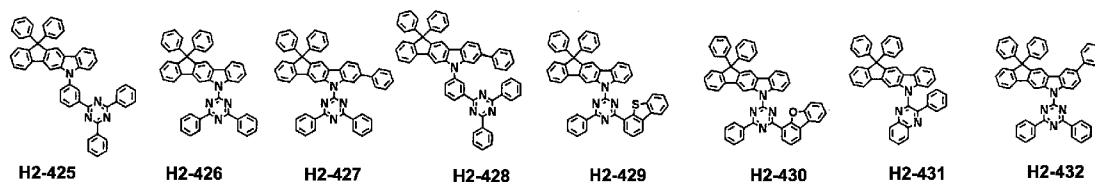
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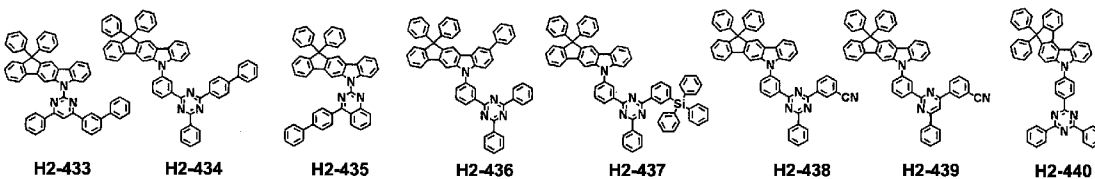
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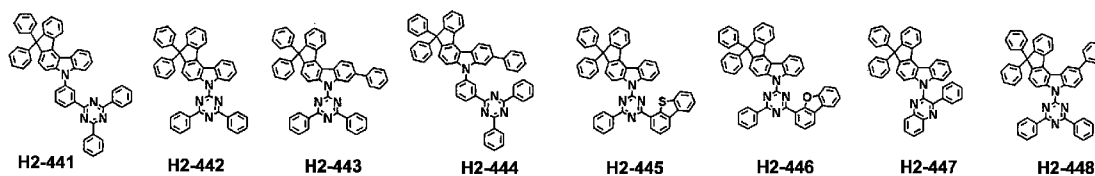
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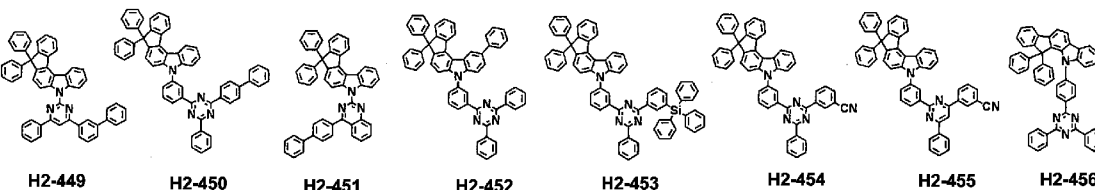
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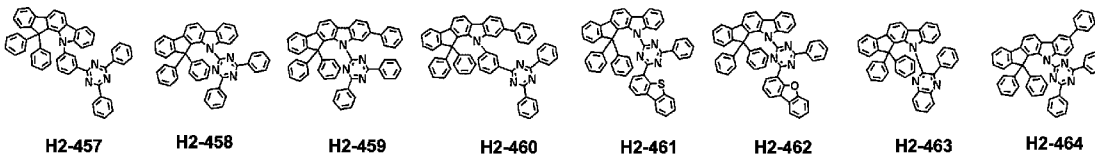
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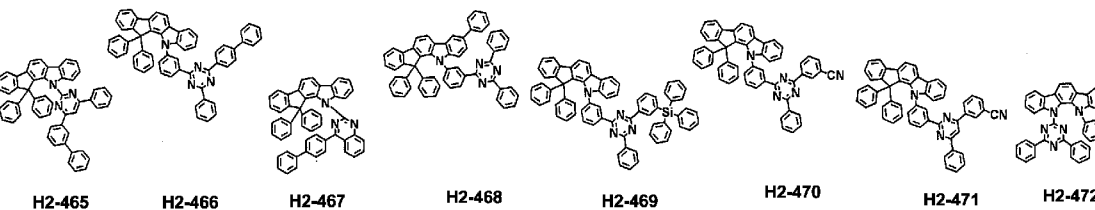
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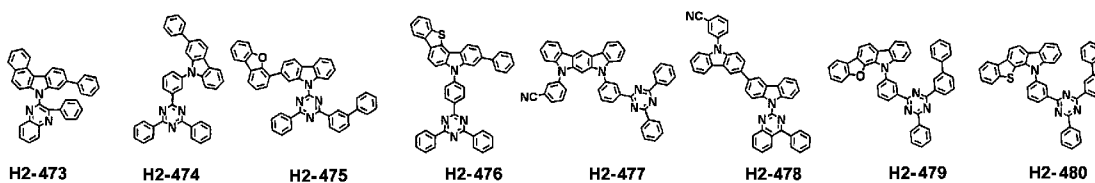
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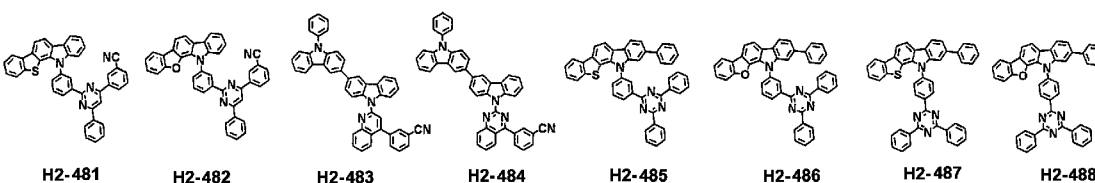
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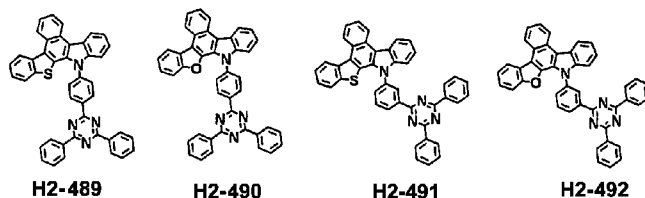
[113]



[114]



[115]



[116] According to an additional aspect of the present disclosure, a combination of the compound of formula 1 and the compound of formula 2, and an organic electroluminescent device comprising the combination are provided.

[117] According to an additional aspect of the present disclosure, a mixture or composition for preparing an organic electroluminescent device is provided. The mixture or composition comprises the compound of formula 1. The mixture or composition may be the one for preparing a light-emitting layer of an organic electroluminescent device. The mixture or composition may further comprise the host compound of formula 2, in addition to a compound of the present disclosure. The mixture or composition may comprise the compound of formula 1 to be combined with the host compound of formula 2. The mixture or composition may further comprise a conventional material which has been used to prepare an organic electroluminescent device.

[118] The organic electroluminescent device of the present disclosure may further comprise, in addition to the compound of formula 1, at least one compound selected from the group consisting of arylamine-based compounds and styrylarylamine-based compounds.

[119] In the organic electroluminescent device of the present disclosure, the organic layer may further comprise, in addition to the compound of formula 1, at least one metal selected from the group consisting of metals of Group 1, metals of Group 2, transition metals of the 4th period, transition metals of the 5th period, lanthanides and organic metals of the d-transition elements of the Periodic Table, or at least one complex compound comprising the metal. The organic layer may further comprise a light-emitting layer and a charge generating layer.

[120] In addition, the organic electroluminescent device of the present disclosure may emit white light by further comprising at least one light-emitting layer, which comprises a blue electroluminescent compound, a red electroluminescent compound or a green electroluminescent compound known in the art, besides the compound of the present disclosure. If necessary, it may further comprise an orange light-emitting layer or a yellow light-emitting layer.

[121] In the organic electroluminescent device of the present disclosure, preferably, at least one layer (hereinafter, "a surface layer") may be placed on an inner surface(s) of one or both electrode(s), selected from a chalcogenide layer, a metal halide layer, and a metal oxide layer. Specifically, a chalcogenide (includes oxides) layer of silicon or aluminum

is preferably placed on an anode surface of an electroluminescent medium layer, and a metal halide layer or a metal oxide layer is preferably placed on a cathode surface of an electroluminescent medium layer. Such a surface layer provides operation stability for the organic electroluminescent device. Preferably, the chalcogenide includes SiO_x ($1 \leq x \leq 2$), AlO_x ($1 \leq x \leq 1.5$), SiON , SiAlON , etc.; the metal halide includes LiF , MgF_2 , CaF_2 , a rare earth metal fluoride, etc.; and the metal oxide includes Cs_2O , Li_2O , MgO , SrO , BaO , CaO , etc.

[122] In the organic electroluminescent device of the present disclosure, a mixed region of an electron transport compound and a reductive dopant, or a mixed region of a hole transport compound and an oxidative dopant may be placed on at least one surface of a pair of electrodes. In this case, the electron transport compound is reduced to an anion, and thus it becomes easier to inject and transport electrons from the mixed region to an electroluminescent medium. Furthermore, the hole transport compound is oxidized to a cation, and thus it becomes easier to inject and transport holes from the mixed region to the electroluminescent medium. Preferably, the oxidative dopant includes various Lewis acids and acceptor compounds, and the reductive dopant includes alkali metals, alkali metal compounds, alkaline earth metals, rare-earth metals, and mixtures thereof. A reductive dopant layer may be employed as a charge generating layer to prepare an electroluminescent device having two or more light-emitting layers and emitting white light.

[123] In order to form each layer of the organic electroluminescent device of the present disclosure, dry film-forming methods such as vacuum evaporation, sputtering, plasma and ion plating methods, or wet film-forming methods such as ink jet printing, nozzle printing, slot coating, spin coating, dip coating, and flow coating methods can be used.

[124] When using a wet film-forming method, a thin film can be formed by dissolving or diffusing materials forming each layer into any suitable solvent such as ethanol, chloroform, tetrahydrofuran, dioxane, etc. The solvent can be any solvent where the materials forming each layer can be dissolved or diffused, and where there are no problems in film-formation capability.

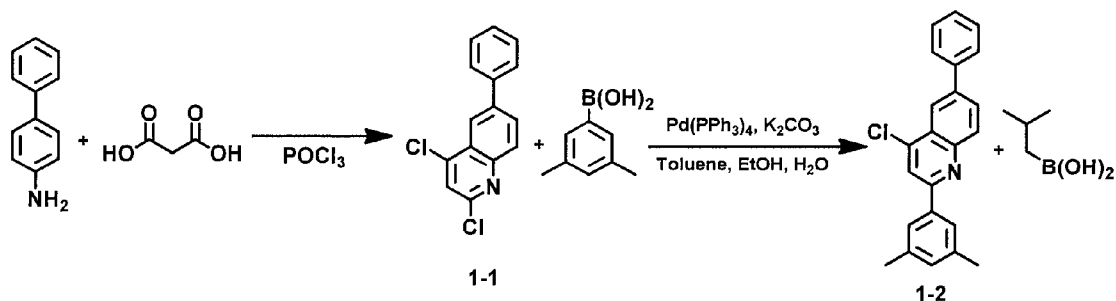
[125] Hereinafter, the compound of the present disclosure, the preparation method of the compound, and the luminescent properties of the device will be explained in detail with reference to the following examples.

[126]

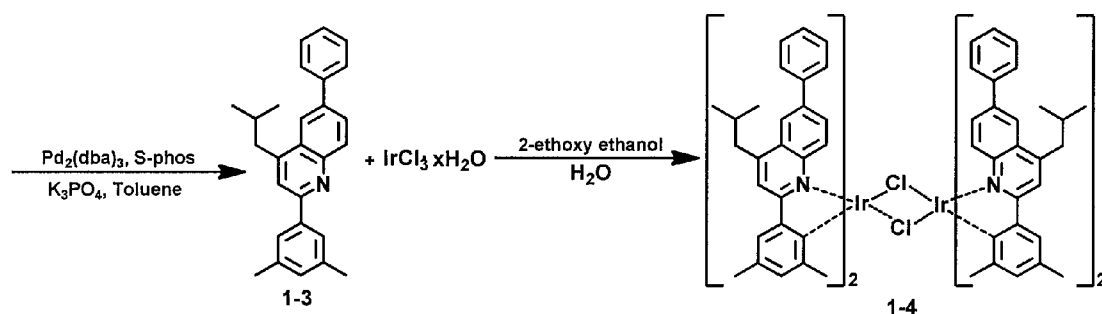
[127] **Example 1: Preparation of compound D-1**

[128]

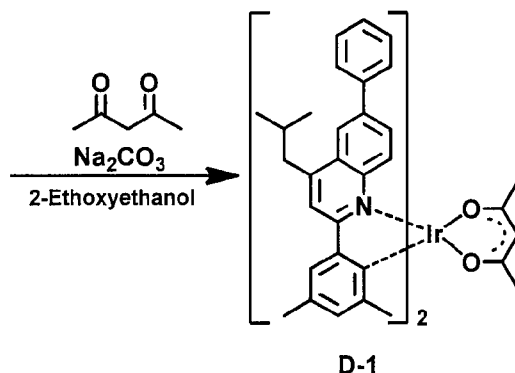
[129]



[130]



[131]

[132] Preparation of compound 1-1

[133] After introducing malonic acid (23g, 222mmol) and POCl₃ (161mL, 1729mmol) into a reaction vessel, the mixture was stirred at room temperature for 10 minutes. [1,1'-biphenyl]-4-amine (25g, 148mmol) was slowly added dropwise to the mixture. Afterward, the mixture was stirred at 150°C. After slowly adding H₂O dropwise to the mixture, the mixture was extracted with methylene chloride (MC), and a solvent was removed therefrom. The obtained substance was subjected to column chromatography to obtain compound 1-1 (20g, 50%).

[134] Preparation of compound 1-2

[135] After introducing compound 1-1 (19.5g, 92mmol), (3,5-dimethylphenyl)boronic acid (13.8g, 92mmol), Pd(PPh₃)₄ (3.2g, 3mmol), K₂CO₃ (38g, 276mmol), toluene (383mL), and H₂O (128mL) into a reaction vessel, the mixture was under reflux at 120°C, cooled to room temperature, and then extracted with ethyl acetate and H₂O. The extracted organic layer was subjected to column chromatography to obtain compound 1-2 (15g, 47%).

[136] Preparation of compound 1-3

[137] After introducing compound 1-2 (14.5g, 42mmol), isobutyl boronic acid (8.6g, 84mmol), S-Phos (1.38g, 3.37mmol), K_3PO_4 (43.86g, 207mmol), $Pd_2(dba)_3$ (1.55g, 1.7mmol), and toluene (280mL), the mixture was stirred for 12 hours. The mixture was cooled to room temperature, and extracted with ethyl acetate and H_2O . The extracted organic layer was subjected to column chromatography to obtain compound 1-3 (6.5g, 42%).

[138] Preparation of compound 1-4

[139] After introducing compound 1-3 (6.5g, 18mmol), $IrCl_3 \cdot xH_2O$ (2.4g, 8mmol), 2-ethoxyethanol (136mL), and H_2O (68mL) into a reaction vessel, the mixture was under reflux at $130^\circ C$ for 24 hours. The mixture was cooled to room temperature, and H_2O was added thereto. The mixture was stirred for 30 minutes, and filtered to obtain a solid, compound 1-4 (4.8g, 63%).

[140] Preparation of compound D-1

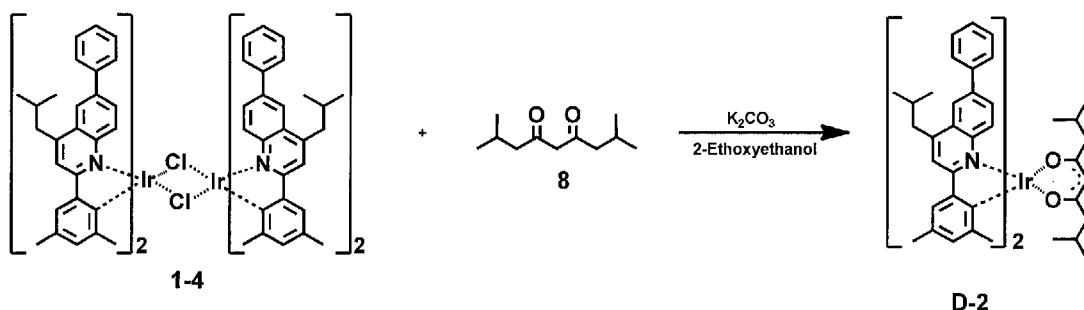
[141] After introducing compound 1-4 (4.8g, 2.5mmol), pentan-2,4-dione (2.6mL, 25mmol), Na_2CO_3 (0.83g, 7.8mmol), and 2-ethoxyethanol (10mL) into a reaction vessel, the mixture was reacted at room temperature overnight. The mixture was filtered, and the obtained solid was subjected to column chromatography to obtain compound D-1 (2g, 39%).

[142]

	Molecular Weight	UV (nm)	PL (nm)	Melting Point (MP) ($^\circ C$)
D-1	1020.33	228	613	322

[143] Example 2: Preparation of compound D-2

[144]



[145] After introducing compound 1-4 (8.0g, 4.2mmol), compound 8 (7.9mL, 41.8mmol), K_2CO_3 (5.78g, 41.8mmol), and 2-ethoxyethanol (50mL) into a reaction vessel, the mixture was reacted at room temperature for 24 hours. The mixture was filtered, and the obtained solid was subjected to column chromatography to obtain compound D-2 (1.6g, 35%).

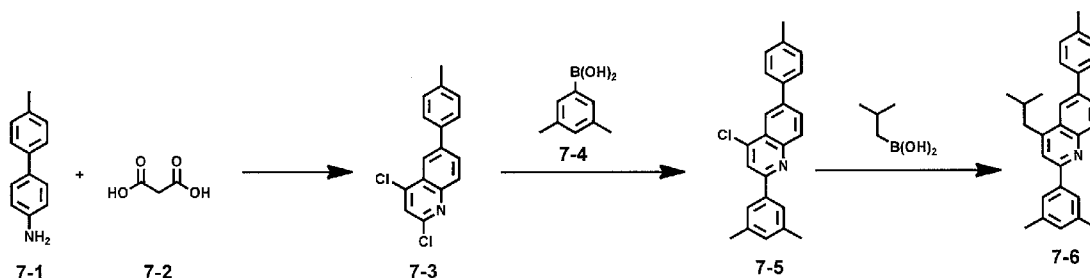
[146]

	Molecular weight	UV (nm)	PL (nm)	MP (°C)
D-2	1104.49	258	613	334

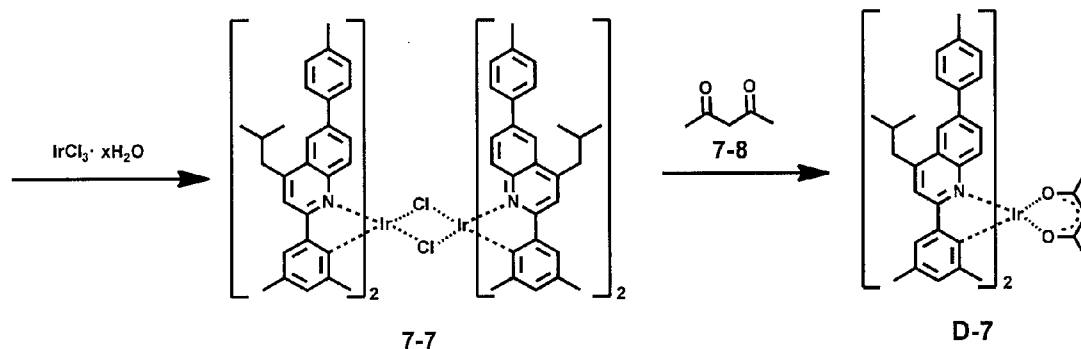
[147]

Example 3: Preparation of compound D-7

[148]



[149]

**Preparation of compound 7-3**

After introducing compound 7-2 (34g, 327mmol) and POCl₃ (218mL, 2342mmol) into a reaction vessel, the mixture was stirred at room temperature for 10 minutes. After slowly adding compound 7-1 (40g, 218mmol) dropwise to the mixture, the mixture was stirred at 150°C. After slowly adding H₂O dropwise, the mixture was extracted with MC, and the solvent was removed therefrom. The remaining substance was subjected to column chromatography to obtain compound 7-3 (34g, 44%).

Preparation of compound 7-5

After introducing compound 7-3 (33g, 116mmol), compound 7-4 (21g, 139mmol), Pd(PPh₃)₄ (4.01g, 3.47mmol), K₂CO₃ (48g, 347mmol), toluene (500mL), and H₂O (173mL) into a reaction vessel, the mixture was stirred under reflux at 120°C. The mixture was cooled to room temperature, extracted with ethyl acetate and H₂O, and subjected to column chromatography to obtain compound 7-5 (28g, 68%).

Preparation of compound 7-6

After introducing compound 7-5 (27g, 75.4 mmol), isobutyl boronic acid (15.4g, 150.9mmol), S-Phos (2.5g, 6mmol), K₃PO₄ (78.4g, 369mmol), Pd₂(dba)₃ (2.76g, 3mmol), and toluene (300mL) into a reaction vessel, the mixture was stirred for 5 hours. The mixture was cooled to room temperature, extracted with ethyl acetate and H

$_2\text{O}$, and subjected to column chromatography to obtain compound 7-6 (20g, 69%).

[156] Preparation of compound 7-7

[157] After introducing compound 7-6 (20g, 52.7mmol), $\text{IrCl}_3 \cdot x\text{H}_2\text{O}$ (7.2g, 23.9mmol), 2-ethoxyethanol (210mL), and H_2O (70mL) into a reaction vessel, the mixture was stirred under reflux at 130°C for 24 hours. The mixture was cooled to room temperature, and H_2O was added thereto. The mixture was stirred for 30 minutes, and filtered to obtain a solid, compound 7-7 (12g, 51%).

[158] Preparation of compound D-7

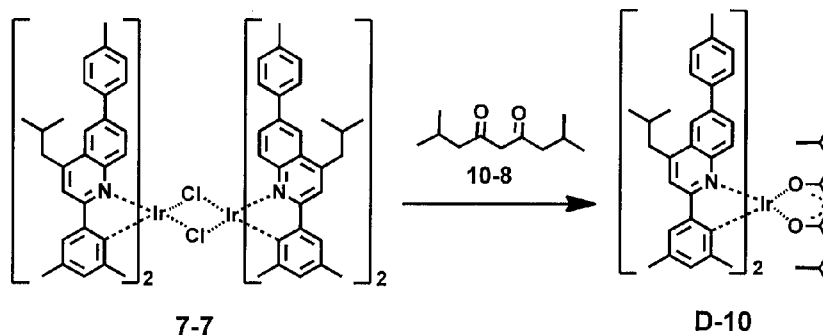
[159] After introducing compound 7-7 (6g, 3mmol), compound 7-8 (3.1mL, 30mmol), K_2CO_3 (4.1g, 30mmol), and 2-ethoxyethanol (50mL) into a reaction vessel, the mixture was reacted at room temperature for 24 hours. The mixture was filtered, and the obtained solid was subjected to column chromatography to obtain compound D-7 (1.5g, 23.8%).

[160]

	Molecular Weight	MP ($^\circ\text{C}$)	UV (nm)	PL (nm)
D-7	1048.38	270	344	616

[161] Example 4: Preparation of compound D-10

[162]



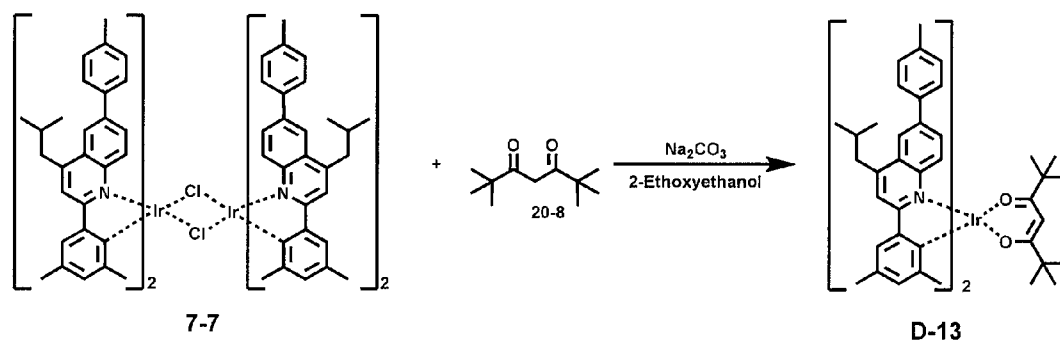
[163] After introducing compound 7-7 (6g, 3mmol), compound 10-8 (4mL, 17.3mmol), K_2CO_3 (4.8g, 30mmol), and 2-ethoxyethanol (60mL) into a reaction vessel, the mixture was reacted at room temperature for 24 hours. The mixture was filtered and subjected to column chromatography to obtain compound D-10 (1.8g, 23%).

[164]

	Molecular weight	MP ($^\circ\text{C}$)	UV (nm)	PL (nm)
D-10	1132.54	293	344	615

[165] Example 5: Preparation of compound D-13

[166]



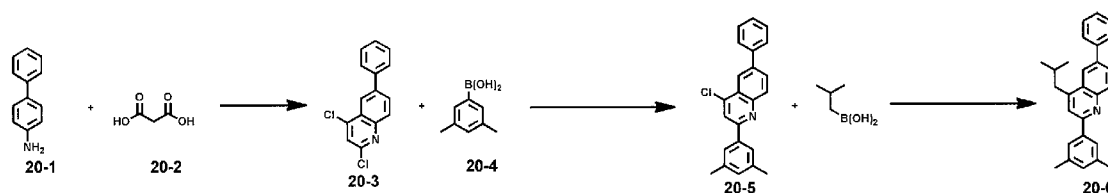
[167] After introducing compound 7-7 (9g, 4.6mmol), compound 20-8 (8.4g, 46mmol), Na_2CO_3 (4.9g, 46mmol), and 2-ethoxyethanol (57mL) into a reaction vessel, the mixture was reacted at room temperature overnight. The mixture was filtered, and the obtained solid was subjected to column chromatography to obtain compound D-13 (1g, 10%).

[168]

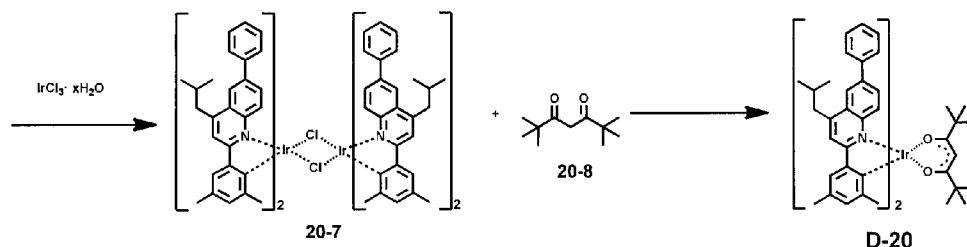
	Molecular Weight	MP (°C)	UV (nm)	PL (nm)
D-13	1132.54	306	278	615

[169] **Example 6: Preparation of compound D-20**

[170]



[171]



[172]

[173] **Preparation of compound 20-3**

[174] After introducing compound 20-2 (23g, 222mmol) and POCl_3 (161mL, 1729mmol) into a reaction vessel, the mixture was stirred at room temperature for 10 minutes. After slowly adding compound 20-1 (25g, 148mmol) dropwise, the mixture was stirred at 150°C . After slowly adding H_2O dropwise, the mixture was extracted with MC, and the solvent was removed therefrom. The remaining substance was subjected to column chromatography to obtain compound 20-3 (20g, 50%).

[175] **Preparation of compound 20-5**

[176] After introducing compound 20-3 (19.5g, 92mmol), compound 20-4 (13.8g,

92mmol), Pd(PPh₃)₄ (3.2g, 3mmol), K₂CO₃ (38g, 276mmol), toluene (383mL), and H₂O (128mL) into a reaction vessel, the mixture was under reflux at 120°C. The mixture was cooled to room temperature, extracted with ethyl acetate and H₂O, and subjected to column chromatography to obtain compound 20-5 (15g, 47%).

[177] Preparation of compound 20-6

[178] After introducing compound 20-5 (15g, 43mmol), isobutylboronic acid (8.9g, 87mmol), S-Phos (1.4g, 3.49mmol), K₃PO₄ (45g, 213mmol), Pd₂(dba)₃ (1.6g, 1.7mmol), and toluene (290mL) into a reaction vessel, the mixture was stirred for 12 hours. The mixture was cooled to room temperature, extracted with ethyl acetate and H₂O, and subjected to column chromatography to obtain compound 20-6 (12.2g, 77%).

[179] Preparation of compound 20-7

[180] After introducing compound 20-6 (12g, 33mmol), IrCl₃ · xH₂O (4.5g, 15mmol), 2-ethoxyethanol (115mL), and H₂O (55mL) into a reaction vessel, the mixture was under reflux at 130°C for 24 hours. The mixture was cooled to room temperature, and H₂O was added thereto. The mixture was stirred for 30 minutes, and filtered to obtain a solid, compound 20-7 (8g, 57%).

[181] Preparation of compound D-20

[182] After introducing compound 20-7 (8g, 4.2mmol), compound 20-8 (7.7g, 42mmol), Na₂CO₃ (4.4g, 42mmol), and 2-ethoxyethanol (50mL) into a reaction vessel, the mixture was reacted at room temperature overnight. The mixture was filtered, and the obtained solid was subjected to column chromatography to obtain compound D-20 (2.2g, 24%).

[183]

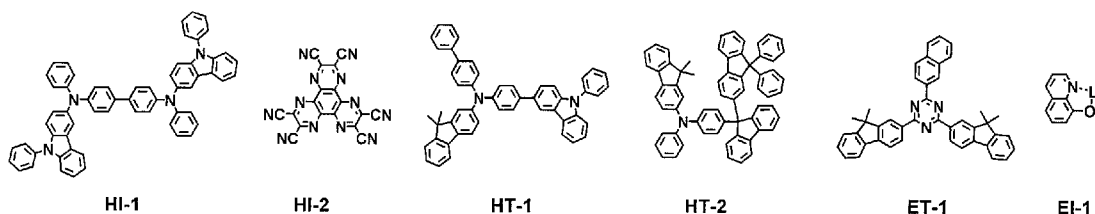
	Molecular Weight	MP (°C)	UV (nm)	PL (nm)
D-20	1104.49	365	246	619

[184] [Device Examples 1-1 to 1-5] OLED comprising the dopant of the present disclosure

[185] An organic electroluminescent device (OLED) was produced using the light-emitting compound of the present disclosure as follows. A transparent electrode indium tin oxide (ITO) thin film (10 Ω/sq) on a glass substrate for an OLED (Geomatec) was subjected to an ultrasonic washing with acetone, ethanol, and distilled water sequentially, and was then stored in isopropanol. The ITO substrate was then mounted on a substrate holder of a vacuum vapor depositing apparatus. **HI-1** was introduced into a cell of the vacuum vapor depositing apparatus, and then the pressure in the chamber of the apparatus was controlled to 10⁻⁶ torr. Thereafter, an electric current was applied to the cell to evaporate the above introduced material, thereby forming a first hole

injection layer having a thickness of 80 nm on the ITO substrate. **HI-2** was then introduced into another cell of said vacuum vapor depositing apparatus, and evaporated by applying electric current to the cell, thereby forming a second hole injection layer having a thickness of 5 nm on the first hole injection layer. **HT-1** was introduced into one cell of the vacuum vapor depositing apparatus, and evaporated by applying electric current to the cell, thereby forming a first hole transport layer having a thickness of 10 nm on the second hole injection layer. **HT-2** was introduced into another cell of the vacuum vapor depositing apparatus, and evaporated by applying electric current to the cell, thereby forming a second hole transport layer having a thickness of 60 nm on the first hole transport layer. Thereafter, compound **H2-16** was introduced into one cell of the vacuum vapor depositing apparatus as a host, and a dopant material shown in Table 1 below was introduced into another cell as a dopant. The two materials were evaporated at different rates, so that the dopant was deposited in a doping amount of 3 wt% based on the total amount of the host and dopant to form a light-emitting layer having a thickness of 40 nm on the second hole transport layer. **ET-1** and **EI-1** were introduced into two cells of the vacuum vapor depositing apparatus, respectively, and evaporated at a 1:1 rate to form an electron transport layer having a thickness of 30 nm on the light-emitting layer. After depositing **EI-1** as an electron injection layer having a thickness of 2 nm, an Al cathode having a thickness of 80 nm was then deposited by another vacuum vapor deposition apparatus on the electron injection layer to produce OLED.

[186]



[187]

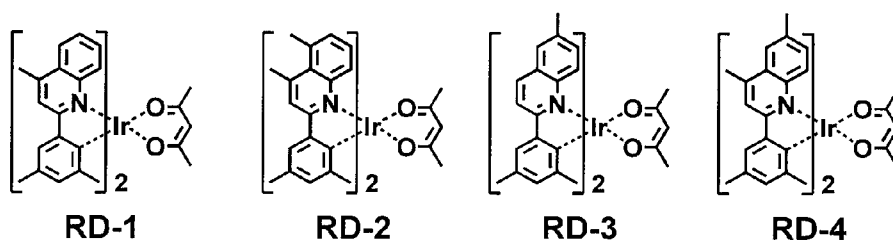
[188]

[189]

[190]

[Comparative Examples 1-1 to 1-4] OLED using a conventional organic electroluminescent compound

OLED was produced in the same manner as in Device Examples 1-1 to 1-5, except that a dopant shown in Table 1 below was used as a dopant for a light-emitting layer.



[191]

Organic electroluminescent devices produced in Device Examples 1-1 to 1-5 and Comparative Examples 1-1 to 1-4 were characterized as shown in Table 1 below.

[192]

[Table 1]

	Dopant	Voltage (V)	Color Coordinates (x, y)		Color Gamut of NTSC Standards (%)	Lifespan (T97)
Device Example 1-1	D-1	3.9	668	331	100	188
Device Example 1-2	D-2	3.9	667	331	99	194
Device Example 1-3	D-7	4.0	665	333	99	165
Device Example 1-4	D-10	3.9	667	332	99	220
Device Example 1-5	D-20	4.0	670	329	100	118
Comparative Example 1-1	RD-1	4.0	635	364	92	60
Comparative Example 1-2	RD-2	4.0	612	318	89	97
Comparative Example 1-3	RD-3	4.2	648	351	95	4
Comparative Example 1-4	RD-4	4.0	624	375	90	73

[193] The data (voltage and color coordinates) of Device Examples 1-1 to 1-5 and Comparative Examples 1-1 to 1-4 shown in Table 1 were measured at a luminance of 1000 cd/m², except lifespan. Said lifespan is the time taken to be 97% of the luminance when the early luminance at 5000 cd/m² and a constant current is taken as 100% of the luminance.

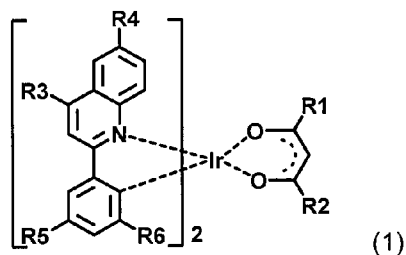
[194] The color gamut is calculated based on a color space which was made by US National Television System Committee (NTSC) in view of the color coordinate system defined by the CIE of the International Commission on Illumination. An area (t_0) of triangle made by three points of red (0.67, 0.33), green (0.21, 0.71), and blue (0.14, 0.08) defined by the NTSC was determined, and then, an area (t_1) of triangle made by blue and green points defined by the NTSC and a red point described in Table 1 above was determined. Thereafter, color gamut (%) was calculated as follows: Color gamut (%) = [t_1 (the area of color coordinate made by the present disclosure) / t_0 (an area of color coordinate based on NTSC standards)] * 100. Where the numerical value of the color gamut is larger and larger, the device can display a larger and larger number of colors. Therefore, the color gamut is better when it has a larger numerical value.

[195] By using the organic electroluminescent compound of the present disclosure, an organic electroluminescent device showing better color purity and lifespan is provided, compared with conventional organic electroluminescent compound.

Claims

[Claim 1]

A compound represented by the following formula 1:



wherein

 R_1 and R_2 , each independently, represent a (C1-C5)alkyl, R_3 represents a (C3-C5)alkyl unsubstituted or substituted with deuterium, R_4 represents phenyl unsubstituted or substituted with a (C1-C5)alkyl unsubstituted or substituted with deuterium, and R_5 and R_6 , each independently, represent methyl unsubstituted or substituted with deuterium.

[Claim 2]

The compound according to claim 1, wherein R_4 is phenyl unsubstituted or substituted with a (C1-C4)alkyl.

[Claim 3]

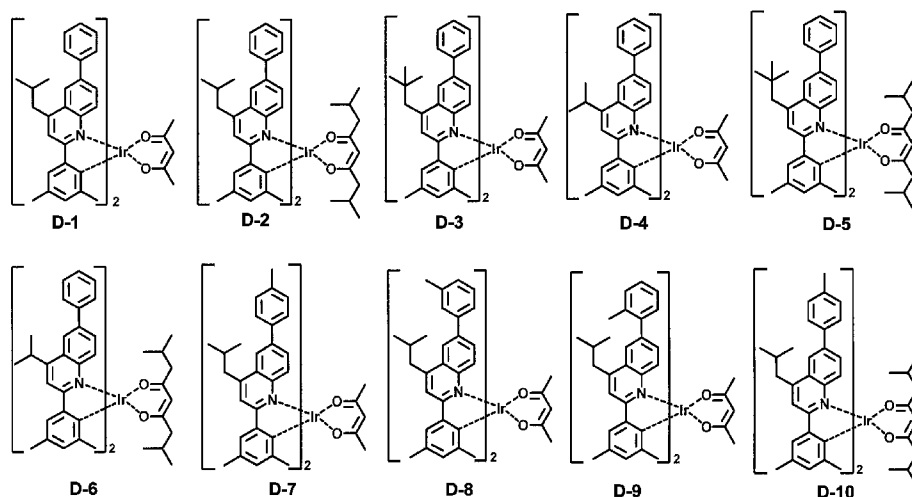
The compound according to claim 1, wherein R_3 is a branched (C3-C5)alkyl unsubstituted or substituted with deuterium, and R_4 is phenyl unsubstituted or substituted with methyl unsubstituted or substituted with deuterium.

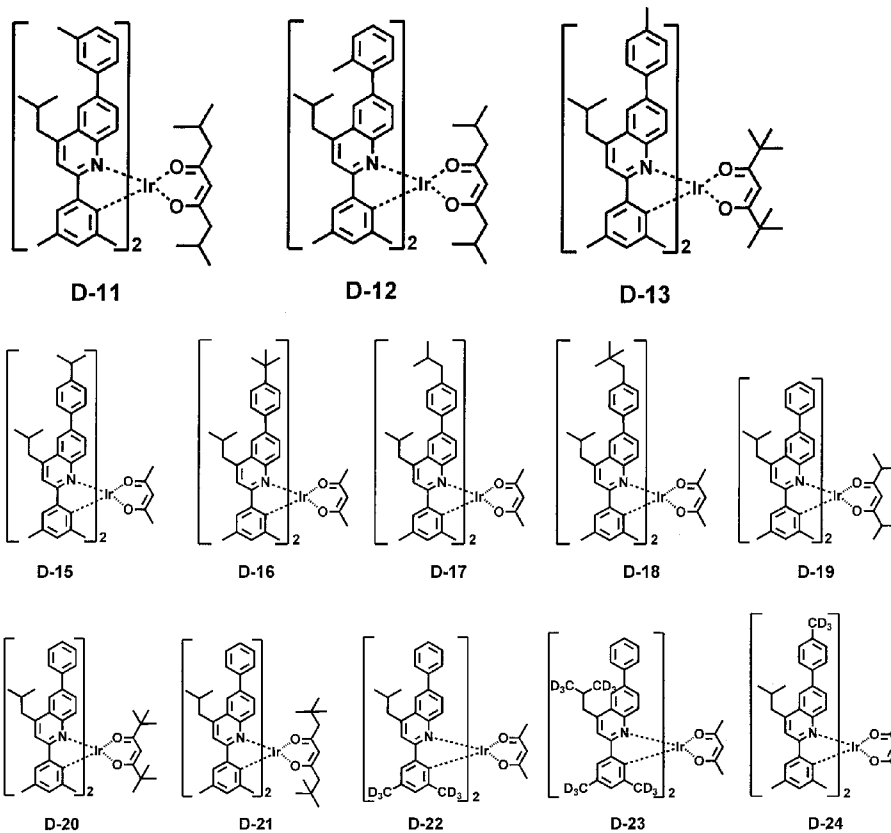
[Claim 4]

The compound according to claim 1, wherein R_1 and R_2 , each independently, are selected from methyl, ethyl, and a branched (C3-C5)alkyl.

[Claim 5]

The compound according to claim 1, wherein the compound of formula 1 is selected from the group consisting of:





[Claim 6]

An organic electroluminescent device comprising the compound according to claim 1.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2015/011888

A. CLASSIFICATION OF SUBJECT MATTER

**C09K 11/06 (2006.01) H01L 27/32 (2006.01) H01L 51/00 (2006.01) C07D 215/00 (2006.01) H05B 33/14 (2006.01)
C07F 15/00 (2006.01)**

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

STN Registry, Caplus: Substructure search of compounds of formula (1)

Patentscope, Espacenet: Applicant and/or inventor search with keywords: ROHM AND HAAS ELECTRONIC MATERIALS, Electroluminescent.

Applicant/ Inventors names were also searched in internal databases provided by IP Australia

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
	Documents are listed in the continuation of Box C	



Further documents are listed in the continuation of Box C



See patent family annex

* "A"	Special categories of cited documents: document defining the general state of the art which is not considered to be of particular relevance	"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"E"	earlier application or patent but published on or after the international filing date	"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"O"	document referring to an oral disclosure, use, exhibition or other means	"&"	document member of the same patent family
"P"	document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 16 February 2016	Date of mailing of the international search report 16 February 2016
Name and mailing address of the ISA/AU AUSTRALIAN PATENT OFFICE PO BOX 200, WODEN ACT 2606, AUSTRALIA Email address: pct@ipaustalia.gov.au	Authorised officer Pina Potenza AUSTRALIAN PATENT OFFICE (ISO 9001 Quality Certified Service) Telephone No. +61 399359614

INTERNATIONAL SEARCH REPORT C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT		International application No. PCT/KR2015/011888
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	EP 2053112 B1 (GRACEL DISPLAY INC.) 24 August 2011 (Abstract; Reaction Schemes 1-4, pages 11-12; Paragraph [0017], first 2 subsidiary ligands; Claim 8, first 2 ligands; Generic disclosure of Chemical Formula I, paragraph [0008], page 3, lines 33-34 and Claim 1; Paragraphs [0007] and [0025]; Paragraph [0015], first compound; Claim 5, first compound; Table 1, Compound No. 1, page 23)	1-6
X	EP 2034001 A2 (GRACEL DISPLAY INC.) 11 March 2009 (Abstract; Paragraph [0018], first and seventh compounds; Paragraph [0019], page 110, seventh compound; Claim 12, page 153, fourth compound)	1-6
X	EP 2080795 A1 (GRACEL DISPLAY INC.) 22 July 2009 (Abstract; Paragraph [0026], first and seventh compounds; Paragraph [0028], Compound D-112, page 59)	1-6

INTERNATIONAL SEARCH REPORT		International application No.	
Information on patent family members		PCT/KR2015/011888	
This Annex lists known patent family members relating to the patent documents cited in the above-mentioned international search report. The Australian Patent Office is in no way liable for these particulars which are merely given for the purpose of information.			
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End of Annex			
Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001.			