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

(57) Abstract: The present invention relates to an organic electroluminescent compound and an organic electroluminescent device comprising the same. By using the organic electroluminescent compound according to the present invention, an organic electroluminescent device can have a low driving voltage, a long lifespan, and high power efficiency.



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Description

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

Technical Field

- [1] The present invention relates to organic electroluminescent compounds 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] The most important factor determining luminous efficiency in the organic EL device is light-emitting materials. Until now, fluorescent materials have been widely used as light-emitting material. However, in view of electroluminescent mechanisms, since phosphorescent materials theoretically enhance luminous efficiency by four (4) times compared to fluorescent materials, phosphorescent light-emitting materials are widely being researched. Iridium(III) complexes have been widely known as phosphorescent materials, including bis(2-(2'-benzothienyl)-pyridinato-N,C3')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.
- [4] At present, 4,4'-N,N'-dicarbazol-biphenyl (CBP) is the most widely known host material for phosphorescent materials. Recently, Pioneer (Japan) et al., developed a high performance organic EL device using bathocuproine (BCP) and aluminum(III)bis(2-methyl-8-quinolate)(4-phenylphenolate) (BALq) etc., as host materials, which were known as hole blocking materials.
- [5] Although these materials provide good light-emitting characteristics, they have the following disadvantages: (1) Due to their low glass transition temperature and poor thermal stability, their degradation may occur during a high-temperature deposition process in a vacuum. (2) The power efficiency of the organic EL device is given by $[(\pi/\text{voltage}) \times \text{current efficiency}]$, and the power efficiency is inversely proportional to the voltage. Although the organic EL device comprising phosphorescent host materials provides higher current efficiency (cd/A) than one comprising fluorescent materials, a significantly high driving voltage is necessary. Thus, there is no merit in terms of

power efficiency (lm/W). (3) Furthermore, the operational lifespan of the organic EL device is short, and luminous efficiency is still required in order to be improved.

[6] Korean Patent Application Laying-Open No. 2005-0100694 discloses compounds for an organic EL device, in which a benzocarbazole backbone is substituted with an aryl group; and Korean Patent Application Laying-Open No. 2010-0015581 discloses compounds for an organic EL device, in which a dibenzocarbazole backbone is substituted with a nitrogen-containing heteroaryl group. However, the above references fail to specifically disclose organic electroluminescent compounds, in which a cycloalkyl group, an aryl group, or a heteroaryl group is bonded to one of the carbon atoms of a benzocarbazole backbone and a nitrogen-containing heteroaryl group is bonded to a nitrogen atom of the benzocarbazole backbone.

[7] Korean Patent Application Laying-Open No. 2010-0108924 discloses compounds in which an aryl group is bonded to a carbon atom of a benzocarbazole and a nitrogen-containing heteroaryl group is bonded to a nitrogen atom of the benzocarbazole. However, the above reference fails to specifically disclose organic electroluminescent compounds, in which a substituent such as a cycloalkyl group, an aryl group, a hexahydrocarbazole group, or a heteroaryl group is bonded to the 2 position of a benzocarbazole. Furthermore, the device using the compound of the above reference needs to be improved in terms of driving voltage, lifespan, and power efficiency.

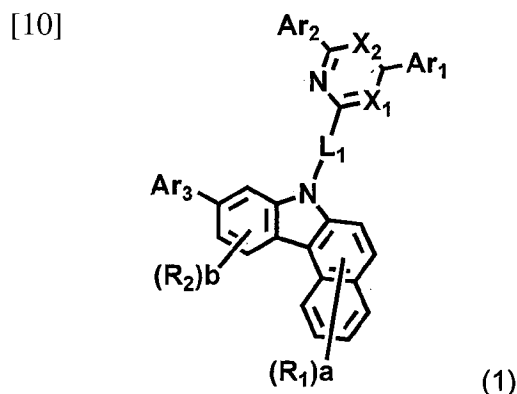
Disclosure of Invention

Technical Problem

[8] The objective of the present invention is to provide an organic electroluminescent compound, which can provide an organic electroluminescent device having a low driving voltage, a long lifespan, and high power efficiency.

Solution to Problem

[9] The present inventors found that the above objective can be achieved by a compound represented by the following formula 1:



[11] wherein

[12] L_1 represents a single bond, a substituted or unsubstituted (3- to 30-membered) het-

eroarylene, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (C6-C30)cycloalkylene;

- [13] X_1 and X_2 , each independently, represent -CH- or -N-;
- [14] Ar_1 and Ar_2 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl;
- [15] Ar_3 represents a substituted or unsubstituted (C6-C30)cycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted hexahydrocarbazole, or a substituted or unsubstituted (3- to 30-membered)heteroaryl;
- [16] R_1 and R_2 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (5- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl, $-NR_3R_4$, $-SiR_5R_6R_7$, $-SR_8$, $-OR_9$, a cyano, a nitro or a hydroxyl;
- [17] R_3 to R_9 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, a substituted or unsubstituted (5- to 7-membered)heterocycloalkyl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (3- to 30-membered), 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;
- [18] a represents an integer of 1 to 6; b represents an integer of 1 to 3; where a or b represents an integer of 2 or more, each of R_1 or R_2 may be the same or different; and
- [19] the heteroarylene, the heterocycloalkyl and the heteroaryl, each independently, contain at least one hetero atom selected from B, N, O, S, P(=O), Si, and P.

Advantageous Effects of Invention

- [20] The organic electroluminescent compound, according to the present invention, can provide an organic electroluminescent device having a low driving voltage, a long lifespan, and high power efficiency.

Mode for the Invention

- [21] Hereinafter, the present invention 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.
- [22] The present invention provides the organic electroluminescent compound of formula

1 above, an organic electroluminescent material comprising the same, and an organic electroluminescent device comprising the material.

[23] The compound of formula 1 of the present invention is described in detail.

[24] Herein, “alkyl” includes methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl, tert-butyl, etc. “Alkenyl” includes vinyl, 1-propenyl, 2-propenyl, 1-butenyl, 2-butenyl, 3-butenyl, 2-methylbut-2-enyl, etc. “Alkynyl” includes ethynyl, 1-propynyl, 2-propynyl, 1-butyne, 2-butyne, 3-butyne, 1-methylpent-2-ynyl, etc. “Cycloalkyl” includes cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, etc. “(5- to 7-membered) heterocycloalkyl” indicates a cycloalkyl having 5 to 7 ring backbone atoms including at least one hetero atom selected from B, N, O, S, P(=O), Si, and P, preferably O, S, and N, and includes tetrahydrofuran, pyrrolidine, thiolan, tetrahydropyran, etc. Furthermore, “aryl(ene)” indicates a monocyclic or fused ring derived from an aromatic hydrocarbon, and includes phenyl, biphenyl, terphenyl, naphthyl, binaphthyl, phenyl-naphthyl, naphthylphenyl, fluorenyl, phenylfluorenyl, benzofluorenyl, dibenzofluorenyl, phenanthrenyl, phenylphenanthrenyl, anthracenyl, indenyl, triphenylenyl, pyrenyl, tetracenyl, perylenyl, chrysenyl, naphthacenyl, fluoranthenyl, etc. “(3- to 30-membered) heteroaryl(ene)” indicates an aryl group having 3 to 30 ring backbone atoms including at least one, preferably 1 to 4, hetero atom selected from the group consisting of B, N, O, S, P(=O), Si, and P; may be a monocyclic ring, or a fused ring condensed with at least one benzene ring; may be partially saturated; may be one formed by linking at least one heteroaryl or aryl group to a heteroaryl group via a single bond(s); and includes a monocyclic ring-type heteroaryl such as furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, etc., and a fused ring-type heteroaryl such as benzofuranyl, benzothiophenyl, isobenzofuranyl, dibenzofuranyl, dibenzothiophenyl, benzoimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenoxazinyl, phenanthridinyl, benzo[dioxolyl, dihydroacridinyl, etc. Furthermore, “halogen” includes F, Cl, Br, and I.

[25] Herein, “substituted” in the expression “substituted or unsubstituted” means that a hydrogen atom in a certain functional group is replaced with another atom or group, i.e., a substituent. The substituents for the substituted groups of L₁, Ar₁ to Ar₃, and R₁ to R₉ of formula 1, each independently, are at least one selected from the group consisting of deuterium; a halogen; a (C1-C30)alkyl unsubstituted or substituted with a halogen; a (C1-C30)alkoxy; a (C6-C30)aryl; a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl; a (C3-C30)cycloalkyl; a (5- to 7-membered)heterocycloalkyl; 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; a (C2-C30)alkenyl; a (C2-C30)alkynyl; a cyano; a di(C1-C30)alkylamino; a di(C6-C30)arylramino; a (C1-C30)alkyl(C6-C30)arylramino; a di(C6-C30)arylboronyl; a di(C1-C30)alkylboronyl; a (C1-C30)alkyl(C6-C30)arylboronyl; a (C6-C30)aryl(C1-C30)alkyl; a (C1-C30)alkyl(C6-C30)aryl; a carboxyl; a nitro; and a hydroxyl; and preferably, at least one selected from the group consisting of deuterium; a halogen; a (C1-C6)alkyl; a (C1-C6)alkoxy; a (C6-C15)aryl; a (5- to 15-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl; a tri(C6-C10)arylsilyl; a (C1-C6)alkyldi(C6-C10)arylsilyl; a di(C6-C10)arylramino; and a (C1-C6)alkyl(C6-C15)aryl.

- [26] In formula 1, L_1 represents a single bond, a substituted or unsubstituted (3- to 30-membered)heteroarylene, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (C6-C30)cycloalkylene; preferably, a single bond, or a substituted or unsubstituted (C6-C20)arylene; and more preferably, a single bond, or a (C6-C15)arylene unsubstituted or substituted with a (C1-C6)alkyl.
- [27] X_1 and X_2 , each independently, represent -CH- or -N-.
- [28] Ar_1 and Ar_2 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl; preferably, each independently, hydrogen, a substituted or unsubstituted (C1-C10)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl; and, more preferably, each independently, hydrogen; a (C1-C6)alkyl; a (C6-C19)aryl unsubstituted or substituted with deuterium, a halogen, a (C1-C6)alkyl, a (C1-C6)alkoxy, a (5- to 15-membered)heteroaryl, a tri(C6-C10)arylsilyl, a (C1-C6)alkyldi(C6-C10)arylsilyl, a di(C6-C10)arylramino, or a (C1-C6)alkyl(C6-C15)aryl; or a (5- to 20-membered)heteroaryl unsubstituted or substituted with a (C1-C6)alkyl or a (C6-C10)aryl.
- [29] Ar_3 represents a substituted or unsubstituted (C6-C30)cycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted a hexahydrocarbazole, or a substituted or unsubstituted (3- to 30-membered)heteroaryl; and preferably, a substituted or unsubstituted (C6-C20)aryl, a substituted or unsubstituted hexahydrocarbazole, or a substituted or unsubstituted (5- to 20-membered)heteroaryl. More preferably, Ar_3 represents a (C1-C6)alkyl; a (C6-C19)aryl unsubstituted or substituted with a (5- to 15-membered)heteroaryl or a di(C6-C10)arylramino; a hexahydrocarbazole unsubstituted or substituted with a (C1-C6)alkyl or a (C6-C10)aryl; or a (5- to 19-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl.
- [30] R_1 and R_2 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a

substituted or unsubstituted (3- to 30-membered)heteroaryl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (5- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl, -NR₃R₄, -SiR₅R₆R₇, -SR₈, -OR₉, a cyano, a nitro or a hydroxyl; and preferably, each independently, hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl. More preferably, R₁ and R₂, each independently, represent hydrogen; a (C1-C6)alkyl; a (C6-C19)aryl unsubstituted or substituted with a (C1-C6)alkyl; or a (5- to 19-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl.

[31] R₃ to R₉, each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, a substituted or unsubstituted (5- to 7-membered)heterocycloalkyl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked with an adjacent substituent(s) to form a substituted or unsubstituted, (3- to 30-membered), 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.

[32] According to one embodiment of the present invention, in formula 1 above, L₁ represents a single bond, or a substituted or unsubstituted (C6-C20)arylene; X₁ and X₂, each independently, represent -CH- or -N-; Ar₁ and Ar₂, each independently, represent hydrogen, a substituted or unsubstituted (C1-C10)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl; Ar₃ represents a substituted or unsubstituted (C6-C20)aryl, a substituted or unsubstituted hexahydrocarbazole, or a substituted or unsubstituted (5- to 20-membered)heteroaryl; and R₁ and R₂, each independently, represent hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl.

[33] According to another embodiment of the present invention, in formula 1 above, L₁ represents a single bond, or a (C6-C15)arylene unsubstituted or substituted with a (C1-C6)alkyl; X₁ and X₂, each independently, represent -CH- or -N-; Ar₁ and Ar₂, each independently, represent hydrogen; a (C1-C6)alkyl; a (C6-C19)aryl unsubstituted or substituted with deuterium, a halogen, a (C1-C6)alkyl, a (C1-C6)alkoxy, a (5- to 15-membered)heteroaryl, a tri(C6-C10)arylsilyl, a (C1-C6)alkyldi(C6-C10)arylsilyl, a di(C6-C10)arylamino or a (C1-C6)alkyl(C6-C15)aryl; or a (5- to 20-membered)heteroaryl unsubstituted or substituted with a (C1-C6)alkyl or a (C6-C10)aryl; Ar₃ represents a (C6-C19)aryl unsubstituted or substituted with a (C1-C6)alkyl, a (5- to 15-membered)heteroaryl or a di(C6-C10)arylamino; a hexahy-

drocarbazole unsubstituted or substituted with a (C1-C6)alkyl or a (C6-C10)aryl; or a (5- to 19-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl; and R_1 and R_2 , each independently, represent hydrogen, a (C1-C6)alkyl, a (C6-C19)aryl unsubstituted or substituted with a (C1-C6)alkyl, or a (5- to 19-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl.

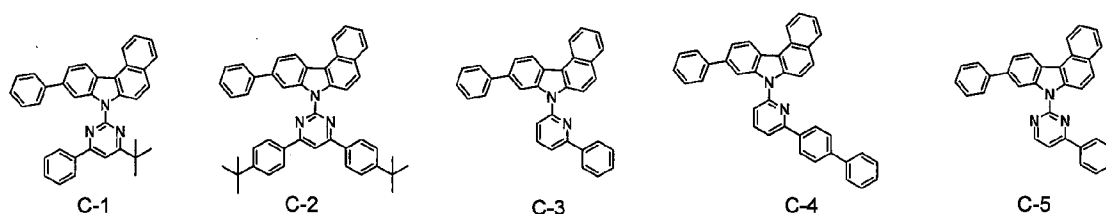
- [34] Specifically, L_1 represents a single bond, a (3- to 30-membered)heteroarylene or a (C6-C30)arylene; X_1 and X_2 , each independently, represent -CH- or -N-; Ar_1 and Ar_2 , each independently, represent hydrogen, a (C1-C30)alkyl, a (C6-C30)aryl or a (3- to 30-membered)heteroaryl; Ar_3 represents a (C6-C30)cycloalkyl, a (C6-C30)aryl or a (3- to 30-membered)heteroaryl; R_1 and R_2 , each independently, represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl, a (C6-C30)aryl, a (3- to 30-membered)heteroaryl, $-NR_3R_4$ or $-SiR_5R_6R_7$; R_3 to R_7 , each independently, represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl, a (C6-C30)aryl or a (3- to 30-membered)heteroaryl; the arylene and the heteroarylene of L_1 and the alkyl, the cycloalkyl, the aryl and the heteroaryl of Ar_1 , Ar_2 , and R_1 to R_9 may be further substituted with at least one selected from the group consisting of deuterium, a halogen, a (C1-C30)alkyl unsubstituted or substituted with a halogen, a (C6-C30)aryl, a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl, 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, a di(C1-C30)alkylamino, a di(C6-C30)arylamino, a (C1-C30)alkyl(C6-C30)arylamino, and a (C1-C30)alkyl(C6-C30)aryl.

- [35] More specifically, L_1 represents a single bond, phenylene, biphenylene, terphenylene, indenylene, fluorenylene, triphenylenylene, pyrenylene, perylenylene, chrysenylene, naphthacenylenylene, fluoranthenylenylene, thiophenylenylene, pyrrolylene, pyrazolylenylene, thiazolylenylene, oxazolylenylene, oxadiazolylenylene, triazinylene, tetrazinylenylene, triazolylenylene, furazanylenylene, pyridylene, benzofuranylenylene, benzothiophenylenylene, indolylenylene, benzoimidazolylenylene, benzothiazolylenylene, benzoisothiazolylenylene, benzoisoxazolylenylene, benzoxazolylenylene, benzothiadiazolylenylene, dibenzofuranylenylene or dibenzothiophenylenylene; Ar_1 and Ar_2 , each independently, represent hydrogen, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, biphenyl, fluorenyl, fluoranthenyl, terphenyl, pyrenyl, chrysenyl, naphthacenyl, perylenyl, pyridyl, pyrrolyl, furanyl, thiophenyl, imidazolyl, benzoimidazolyl, quinolyl, triazinyl, benzofuranyl, dibenzofuranyl, benzothiophenyl, dibenzothiophenyl, pyrazolyl, indolyl, carbazolyl, thiazolyl, oxazolyl, benzothiazolyl, benzoxazolyl, phenanthrolinyl, or quinoxalinyll; R_1 and R_2 , each independently, represent hydrogen, deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl,

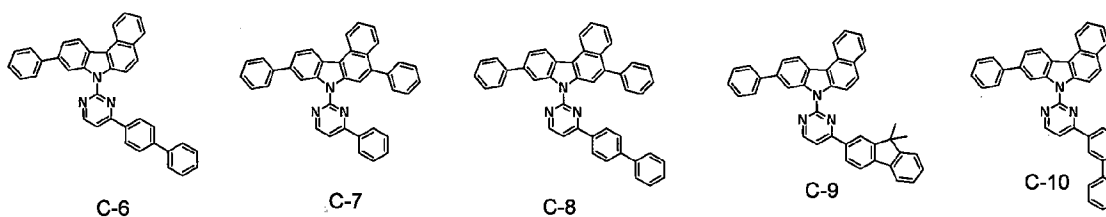
2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, naphthyl, anthryl, biphenyl, fluorenyl, fluoranthenyl, triphenylenyl, pyrenyl, chrysenyl, naphthacenyl, perylenyl, pyridyl, pyrrolyl, furanyl, thiophenyl, imidazolyl, benzoimidazolyl, indenyl, pyrazinyl, pyrimidinyl, pyridazinyl, quinolyl, triazinyl, benzofuranyl, dibenzofuranyl, benzothioiophenyl, dibenzothiophenyl, pyrazolyl, indolyl, carbazolyl, thiazolyl, oxazolyl, benzothiazolyl, benzoxazolyl, phenanthrolinyl, dimethylamino, diethylamino, methylphenylamino, diphenylamino, trimethylsilyl, triethylsilyl, tripropylsilyl, tri(t-butyl)silyl, t-butyl dimethylsilyl, dimethylphenylsilyl or triphenylsilyl; the groups of L₁, Ar₁, Ar₂, R₁ and R₂ may be further substituted with at least one selected from the group consisting of deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, naphthyl, biphenyl, 9,9-dimethylfluorenyl, 9,9-diphenylfluorenyl, fluoranthenyl, triphenylenyl, pyrenyl, chrysenyl, naphthacenyl, perylenyl, pyridyl, pyrrolyl, furanyl, thiophenyl, imidazolyl, benzoimidazolyl, pyrazinyl, pyrimidinyl, pyridazinyl, quinolyl, triazinyl, benzofuranyl, dibenzofuranyl, dibenzothiophenyl, benzothiophenyl, pyrazolyl, indolyl, carbazolyl, thiazolyl, oxazolyl, benzothiazolyl, benzoxazolyl, phenanthrolinyl, dimethylamino, diethylamino, methylphenylamino, diphenylamino, trimethylsilyl, triethylsilyl, tripropylsilyl, tri(t-butyl)silyl, t-butyl dimethylsilyl, dimethylphenylsilyl, methyl diphenylsilyl, triphenylsilyl, N-carbazolyl, and N-phenylcarbazolyl.

[36] Even more specifically, organic electroluminescent compounds of formula 1 of the present invention include the following, but are not limited thereto:

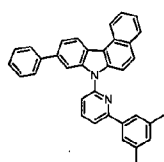
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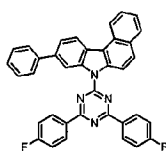
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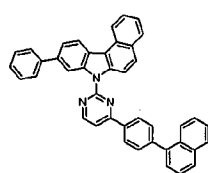
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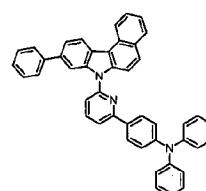
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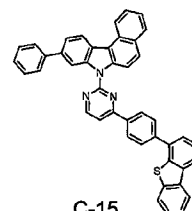
C-12



C-13

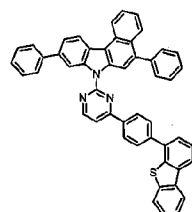


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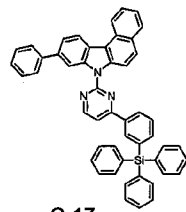


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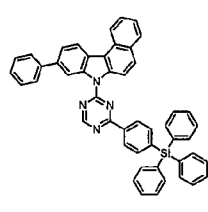
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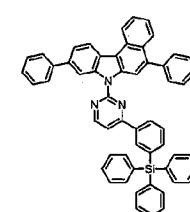
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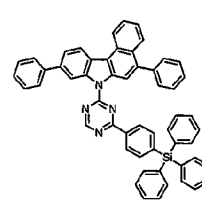
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C-18

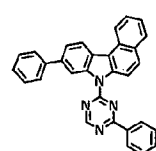


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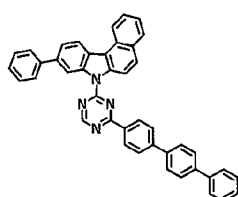


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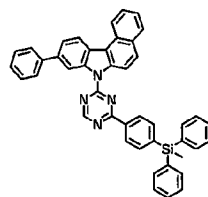
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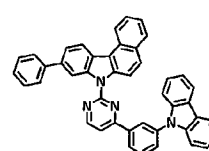
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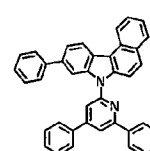
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C-23

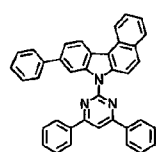


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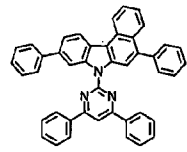


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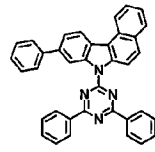
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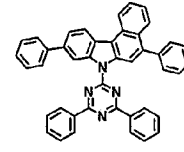
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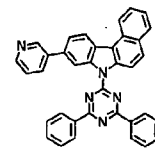
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C-28

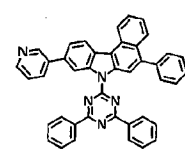


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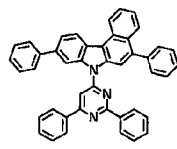


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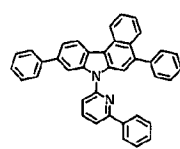
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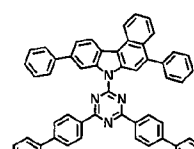
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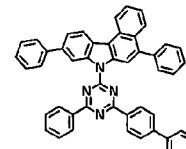
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C-33

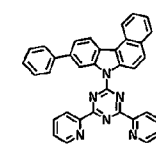


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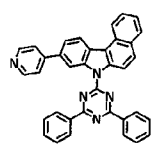


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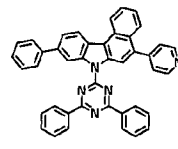
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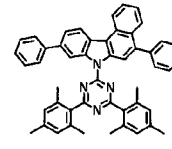
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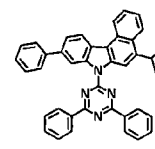
C-37



C-38

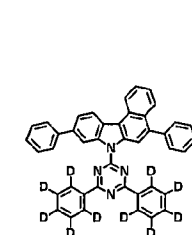


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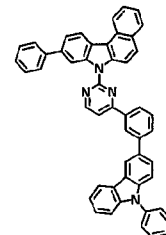


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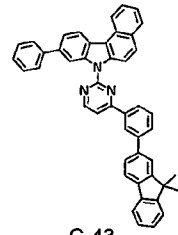
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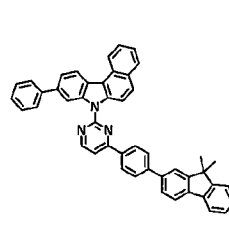
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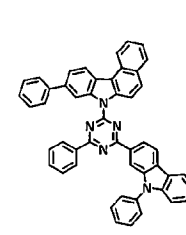
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C-43

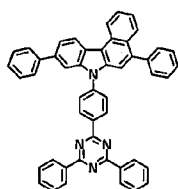


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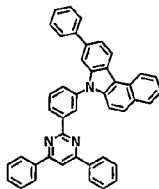


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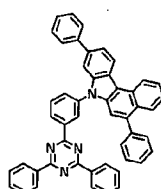
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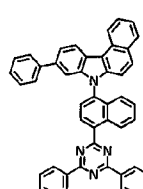
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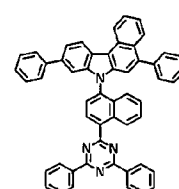
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C-48

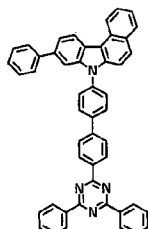


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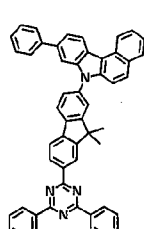


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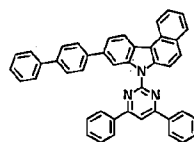
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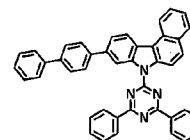
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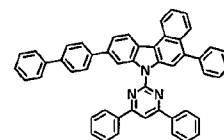
C-52



C-53

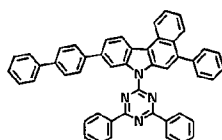


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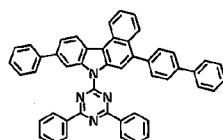


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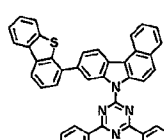
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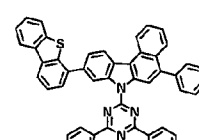
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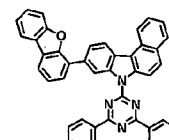
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C-58

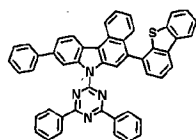


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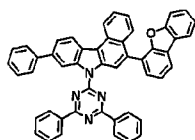


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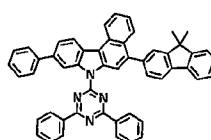
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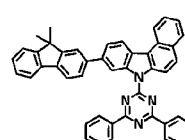
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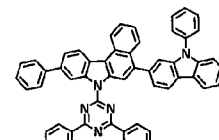
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C-63

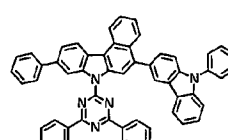


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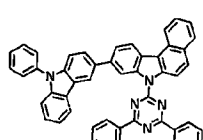


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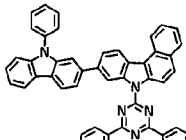
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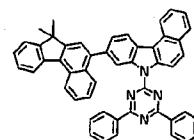
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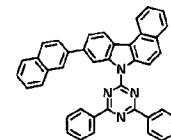
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C-68

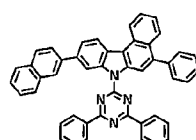


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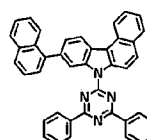


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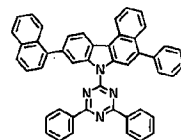
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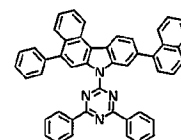
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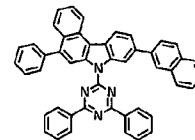
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C-73

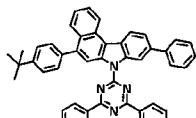


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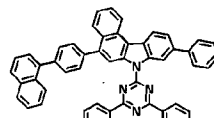


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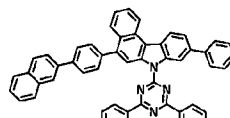
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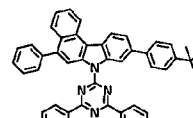
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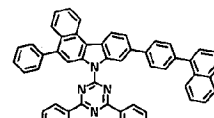
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C-78

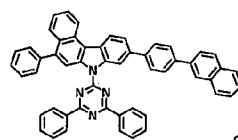


C-79

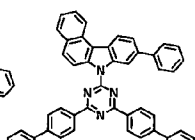


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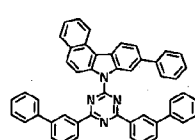
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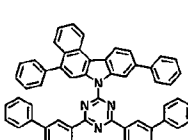
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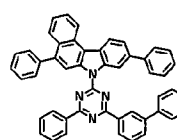
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C-83

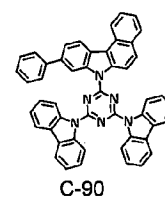
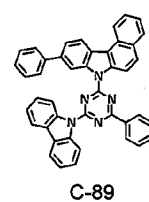
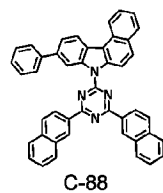
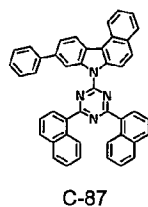
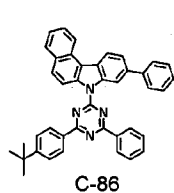


C-84

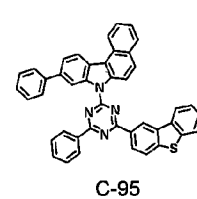
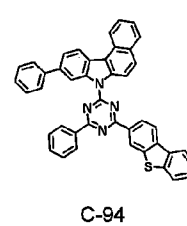
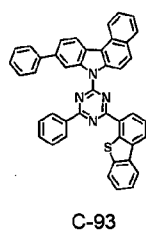
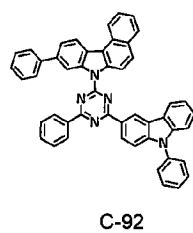
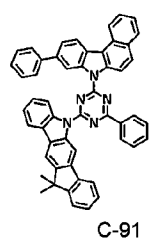


C-85

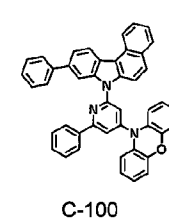
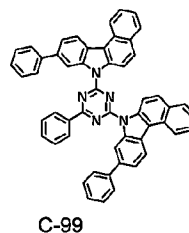
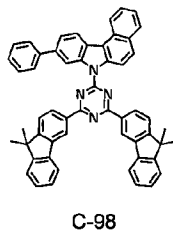
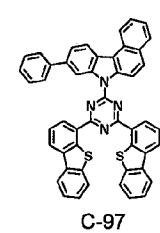
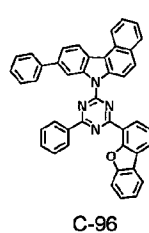
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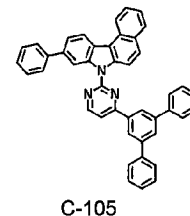
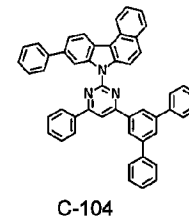
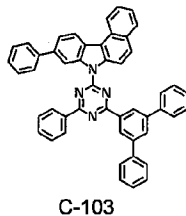
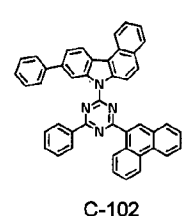
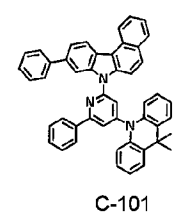
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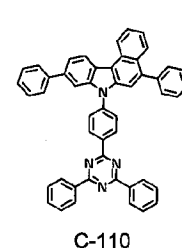
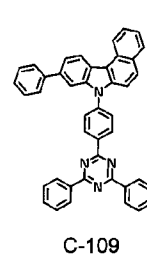
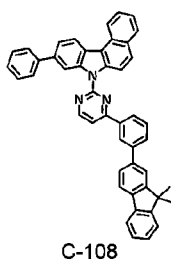
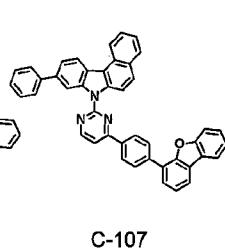
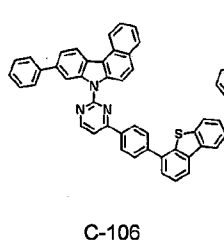
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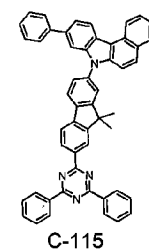
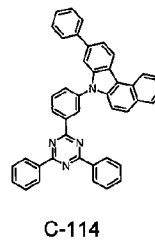
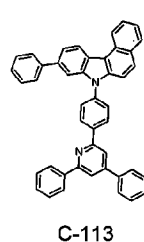
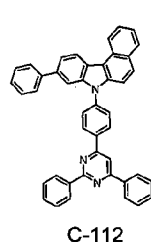
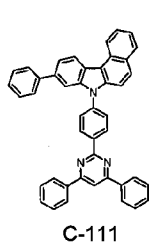
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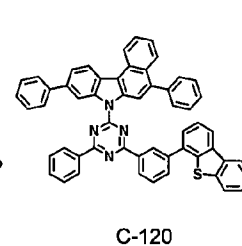
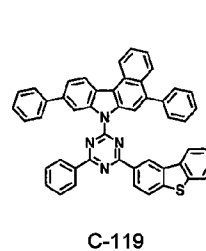
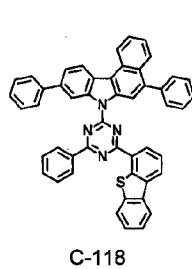
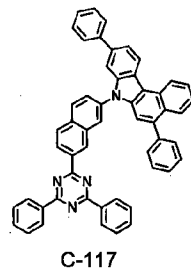
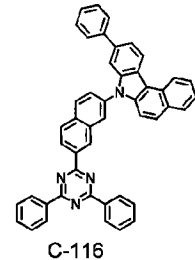
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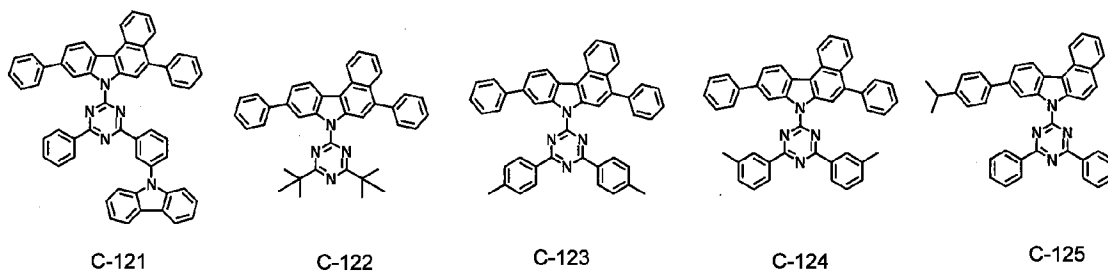
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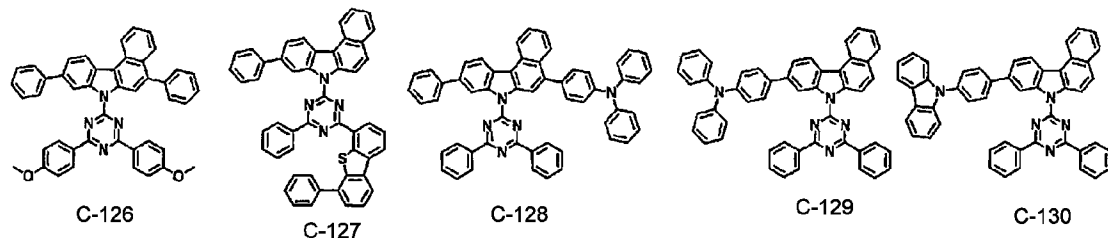
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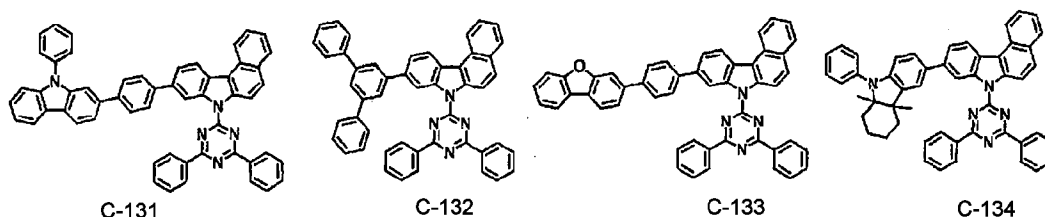
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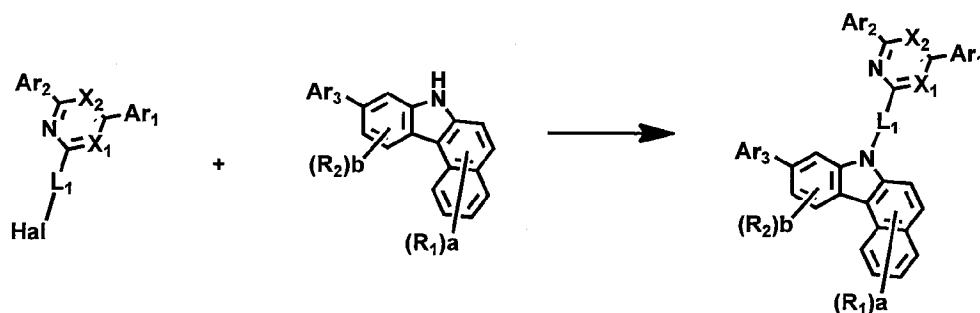
[63]



[64] The organic electroluminescent compounds of the present invention can be prepared by a synthetic method known to one skilled in the art. For example, they can be prepared according to the following reaction scheme 1.

[65] [Reaction Scheme 1]

[66]



[67] In reaction scheme 1, L₁, X₁, X₂, Ar₁ to Ar₃, R₁, R₂, a, and b are as defined in formula 1 above, and Hal represents a halogen.

[68] The present invention provides an organic electroluminescent material comprising the organic electroluminescent compound of formula 1, and an organic electroluminescent device comprising the material.

[69] The material may consist of the organic electroluminescent compound of formula 1. Otherwise, the material may further comprise a conventional compound(s) which has been comprised of an organic electroluminescent material, in addition to the compound of formula 1.

[70] The organic electroluminescent device 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 organic electroluminescent compound of formula 1.

[71] 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, and an electron blocking layer.

[72] Furthermore, the organic layer may comprise a light-emitting layer in which the organic electroluminescent compound of formula 1 may be comprised as a host material, and if needed, another compound(s) other than the compound of formula 1 may be further comprised.

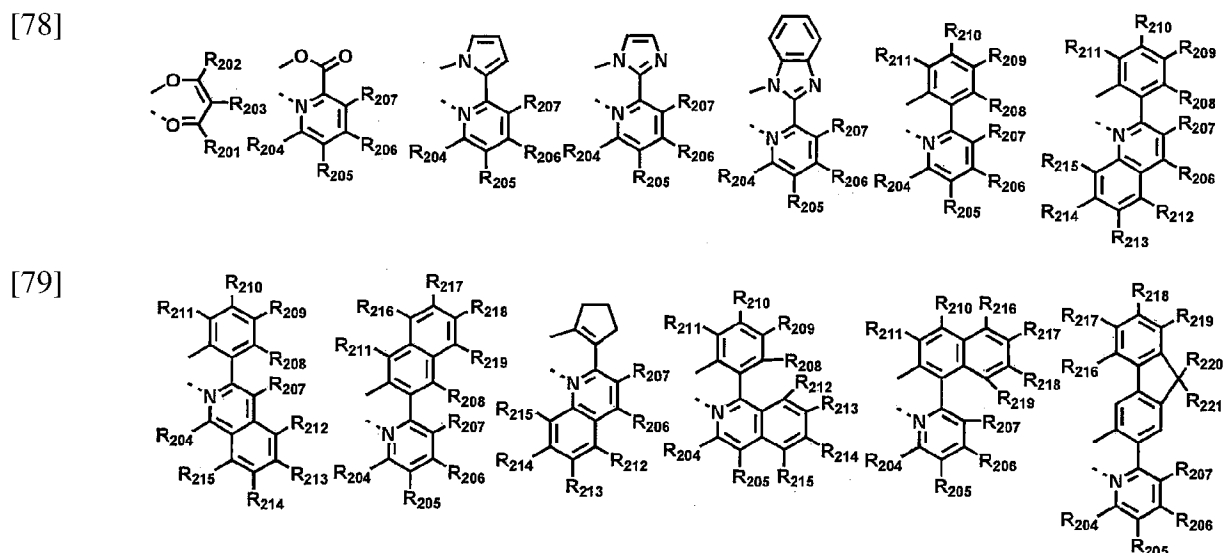
[73] In addition, a phosphorescent dopant, which is used for an organic electroluminescent device together with the host material according to the present invention, may be selected from the compounds represented by the following formula 2:

[74]
$$M^1 L^{101} L^{102} L^{103} \quad (2)$$

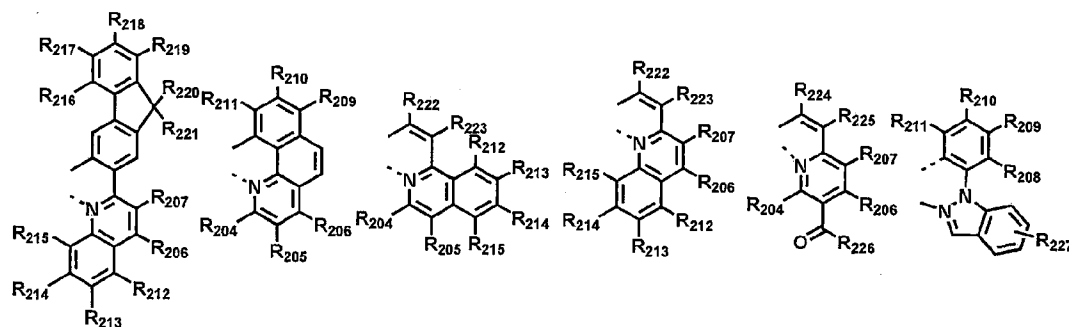
[75] wherein

[76] M^1 is selected from the group consisting of Ir, Pt, Pd and Os;

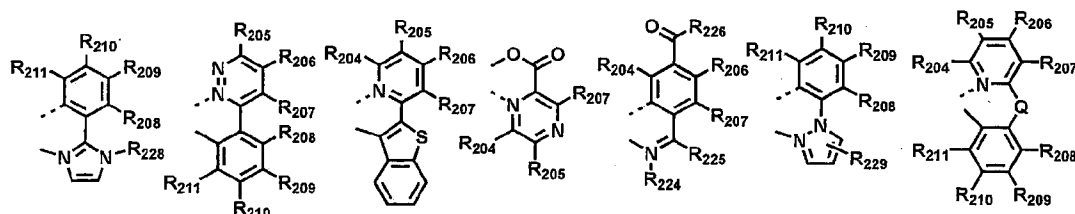
[77] L^{101} , L^{102} and L^{103} are each independently selected from the following structures:



[80]



[81]



[82] R₂₀₁ to R₂₀₃, each independently, represent hydrogen, deuterium, a (C1-C30)alkyl unsubstituted or substituted with a halogen, a (C6-C30)aryl unsubstituted or substituted with a (C1-C30)alkyl, or a halogen;

[83] R₂₀₄ to R₂₁₉, each independently, represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted mono- or di-(C1-C30)alkylamino, a substituted or unsubstituted mono- or di-(C6-C30)arylamino, SF₅, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a cyano or a halogen;

[84] R₂₂₀ to R₂₂₃, each independently, represent hydrogen, deuterium, a (C1-C30)alkyl unsubstituted or substituted with a halogen, or a (C6-C30)aryl unsubstituted or substituted with a (C1-C30)alkyl;

[85] R₂₂₄ and R₂₂₅, each independently, represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a halogen, or R₂₂₄ and R₂₂₅ may be linked with an adjacent substituent(s) to form a (C5-C30), mono- or polycyclic, alicyclic or aromatic ring;

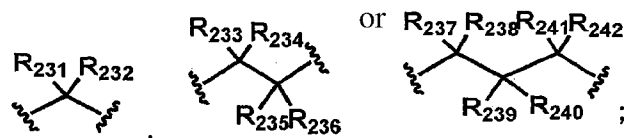
[86] R₂₂₆ represents a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (5- or 30-membered) heteroaryl or a halogen;

[87] R₂₂₇ to R₂₂₉, each independently, represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl or a halogen;

[88]

[89]

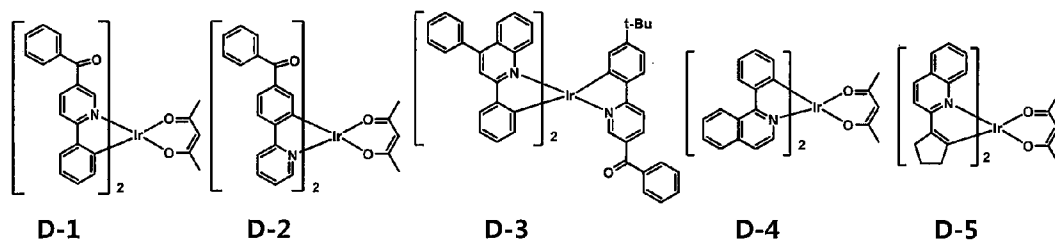
[90] Q represents



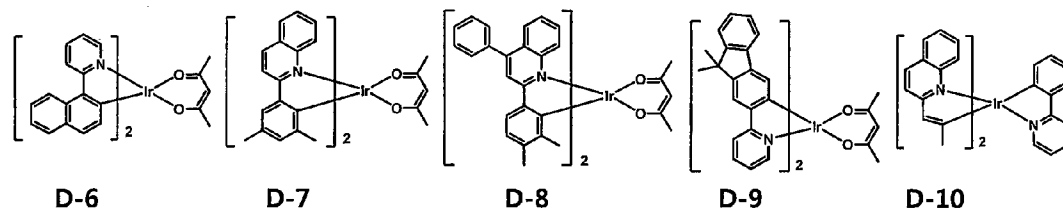
[91] R_{231} to R_{242} each independently represent hydrogen, deuterium, a (C1-C30)alkyl unsubstituted or substituted with a halogen, a (C1-C30)alkoxy, a halogen, a substituted or unsubstituted (C6-C30)aryl, a cyano, or a substituted or unsubstituted (C5-C30)cycloalkyl, or may be linked with an adjacent substituent(s) via alkylene or alkenylene to form a spiro ring or a fused ring, or may be linked with R_{207} or R_{208} via alkylene or alkenylene to form a saturated or unsaturated fused ring.

[92] Specifically, the following compounds are preferred as the dopants of formula 2, but the dopants of formula 2 are not limited thereto:

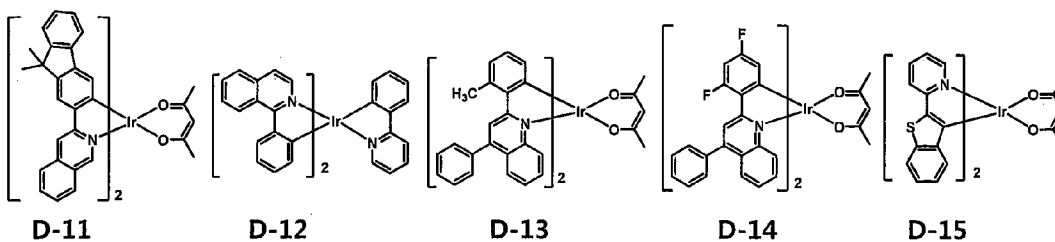
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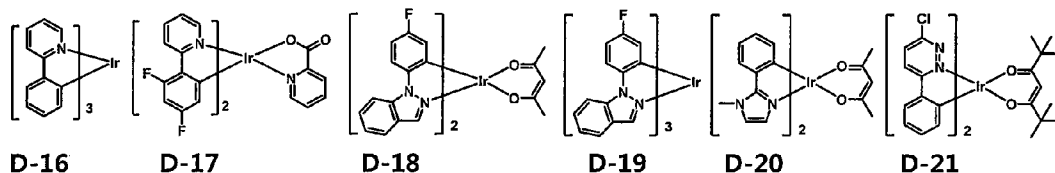
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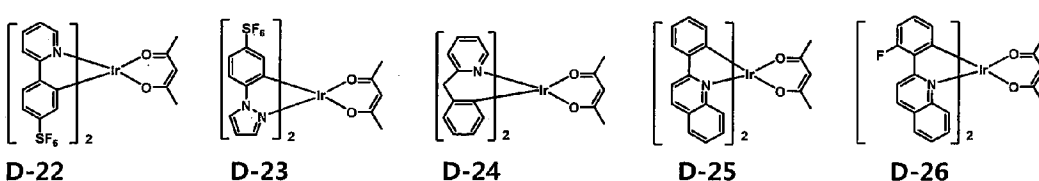
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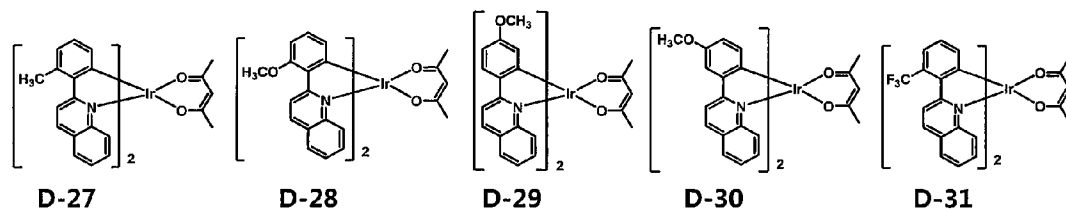
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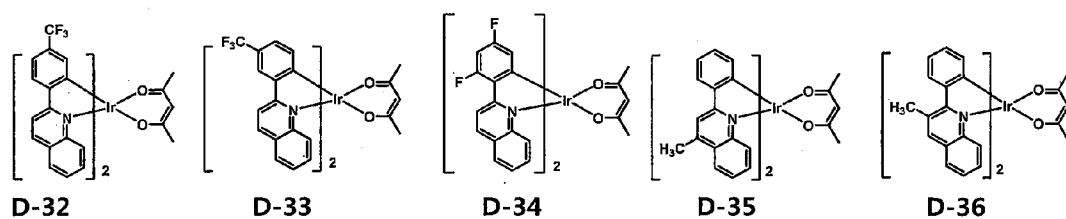
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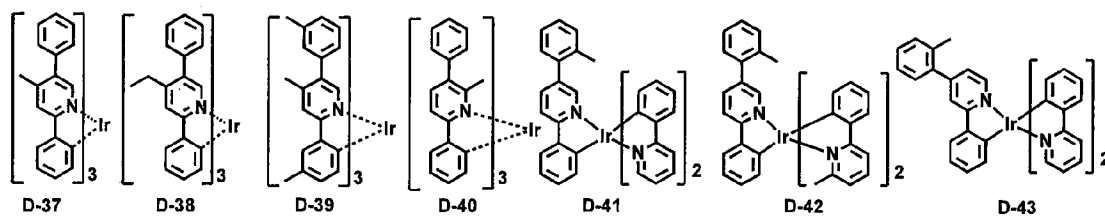
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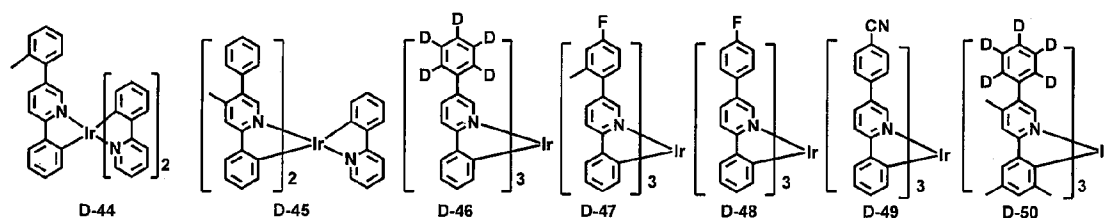
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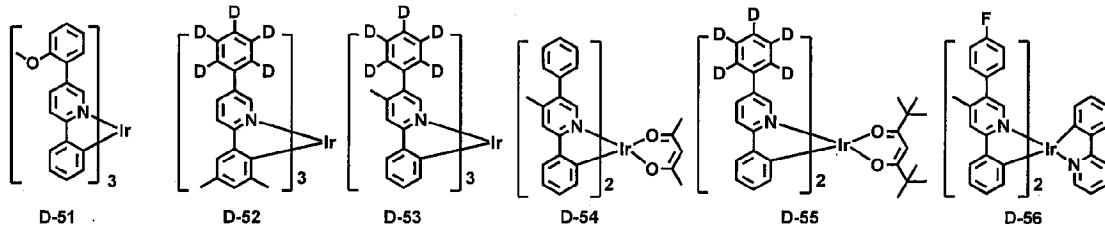
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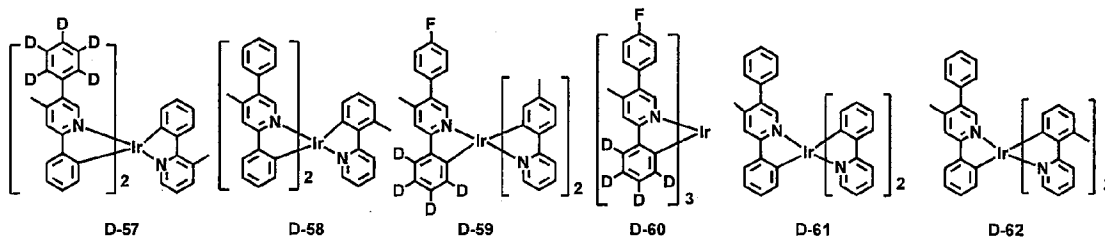
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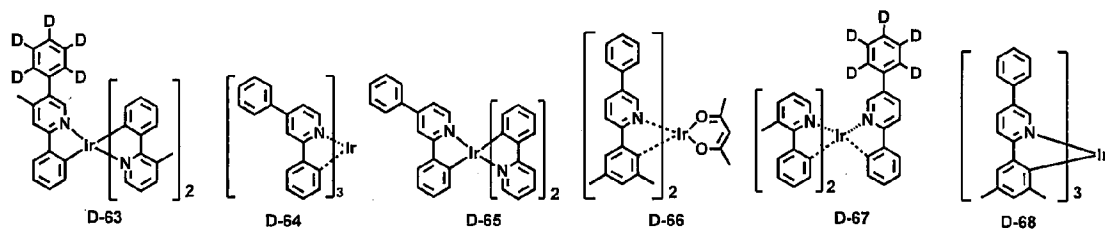
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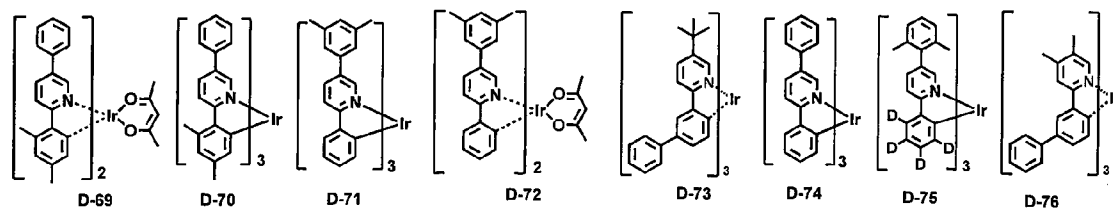
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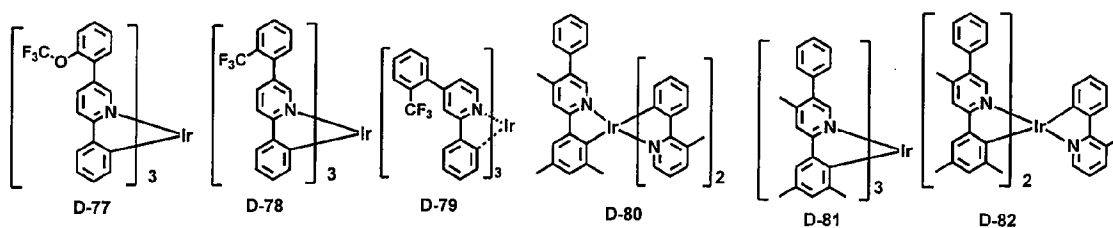
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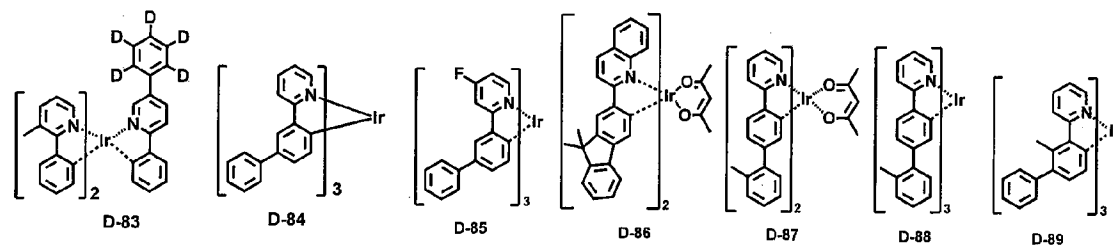
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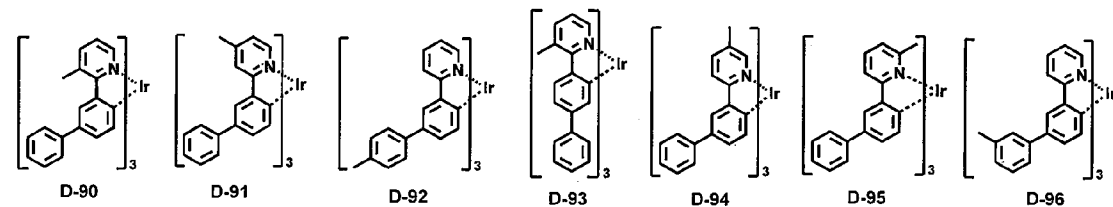
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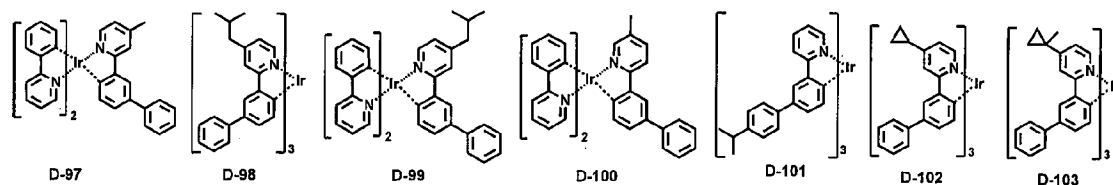
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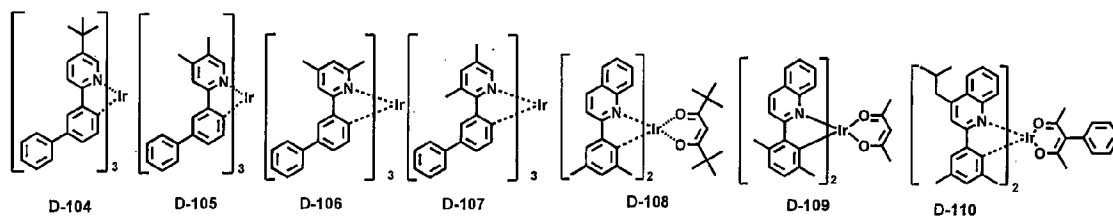
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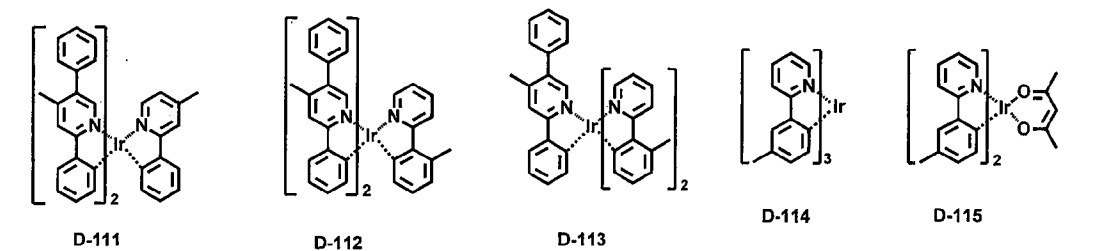
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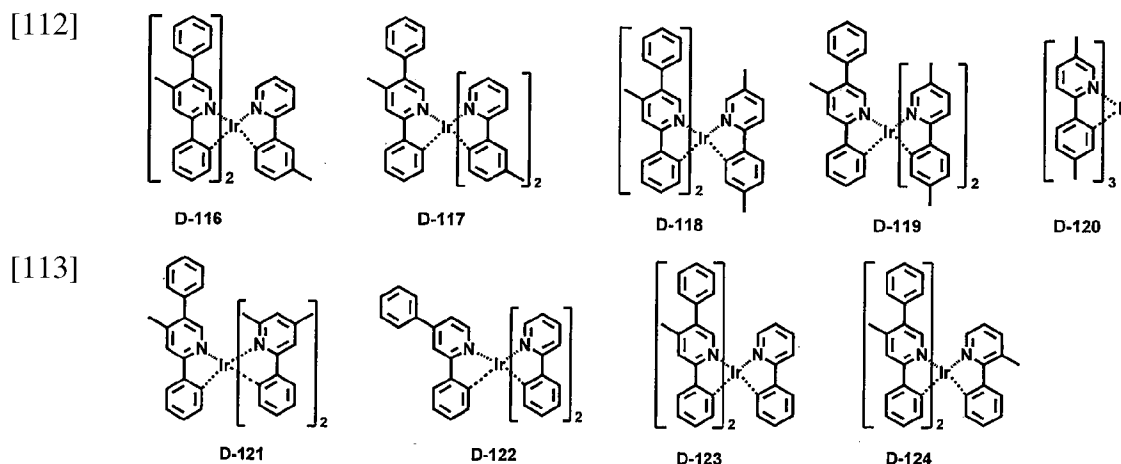


[110]



[111]



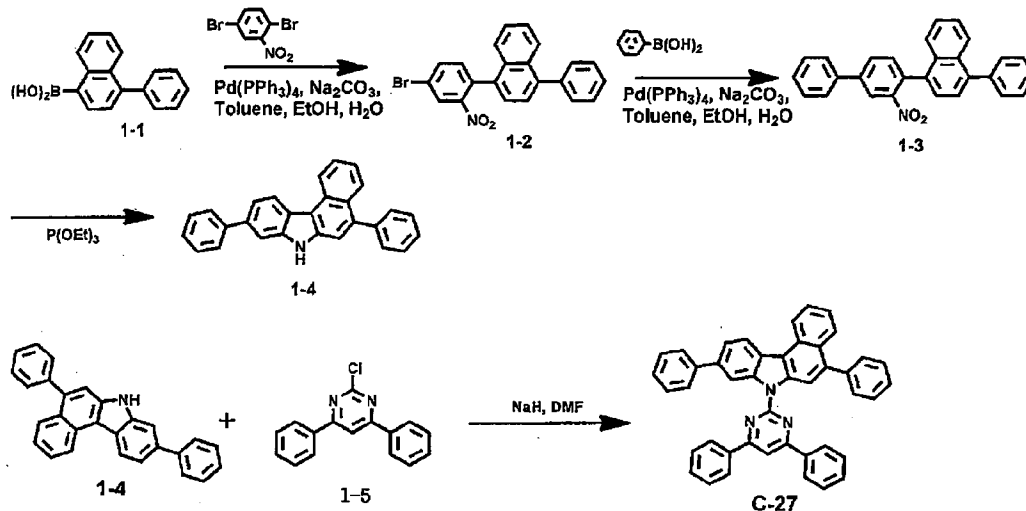


- [114] Furthermore, the present invention provides a composition for preparing an organic electroluminescent device. The composition may comprise the compound of the present invention as a host material.
- [115] The organic electroluminescent device of the present invention comprises a first electrode, a second electrode, and at least one organic layer disposed between the first and second electrodes. The organic layer comprises a light-emitting layer in which the composition of the present invention may be comprised.
- [116] The organic electroluminescent device of the present invention comprises the organic electroluminescent compound of formula 1 of the present invention, and may further comprise at least one compound selected from the group consisting of arylamine-based compounds and styrylarylamine-based compounds.
- [117] In the organic electroluminescent device of the present invention, 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 said metal. The organic layer may comprise a light-emitting layer and a charge generating layer.
- [118] In addition, the organic electroluminescent device of the present invention 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, besides the compound of the present invention.
- [119] In the organic electroluminescent device of the present invention, 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.

- [120] In the organic electroluminescent device of the present invention, 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 electroluminescent layers and emitting white light.
- [121] In order to form each layer of the organic electroluminescent device of the present invention, dry film-forming methods such as vacuum evaporation, sputtering, plasma and ion plating methods, or wet film-forming methods such as spin coating, dip coating, and flow coating methods can be used.
- [122] 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.
- [123] Hereinafter, the organic electroluminescent compound, the preparation method of the compound, and the luminescent characteristics of the device will be explained in detail with reference to the following examples.
- [124] **Example 1: Preparation of compound C-27**

[125]

[126] Preparation of compound 1-2

[127] Compound 1-1 (18.5 g, 66 mmol), 2,5-dibromonitrobenzene (18 g, 72.6 mmol), Na_2CO_3 (16.8 g, 158.4 mmol), and $\text{Pd(PPh}_3)_4$ (3.8 g, 3.3 mmol) were added to a mixture of toluene (320 mL), ethanol (80 mL), and purified water (80 mL). The mixture was stirred at 90-100 °C for 3 hours. After completing the reaction, the mixture was stood to remove an aqueous layer. The organic layer was concentrated, was subjected to trituration with methylene chloride (MC), and was filtered to obtain compound 1-2 (19 g, 71.2%).

[128] Preparation of compound 1-3

[129] Compound 1-2 (10 g, 24.7 mmol), phenylboronic acid (3.6 g, 29.7 mmol), Na_2CO_3 (7.8 g, 74.1 mmol) and $\text{Pd(PPh}_3)_4$ (1.4 g, 1.2 mmol) were added to a mixture of toluene (150 mL), ethanol (37 mL), and purified water (37 mL). The mixture was stirred at 90-100 °C for 3 hours. After completing the reaction, the mixture was cooled to room temperature, and then was stood to remove an aqueous layer. The organic layer was concentrated, was subjected to trituration with MC, and was filtered to obtain compound 1-3 (9 g, 90.9%).

[130] Preparation of compound 1-4

[131] Compound 1-3 (9 g, 22.4 mmol) was dissolved in P(OEt)_3 (100 mL). The mixture was stirred at 160 °C for a day, and then was distilled under vacuum to remove P(OEt)_3 . Thereafter, the mixture was extracted with MC and distilled water, was subjected to trituration with MC, and then was filtered to obtain compound 1-4 (4.9 g, 60%).

[132] Preparation of compound C-27

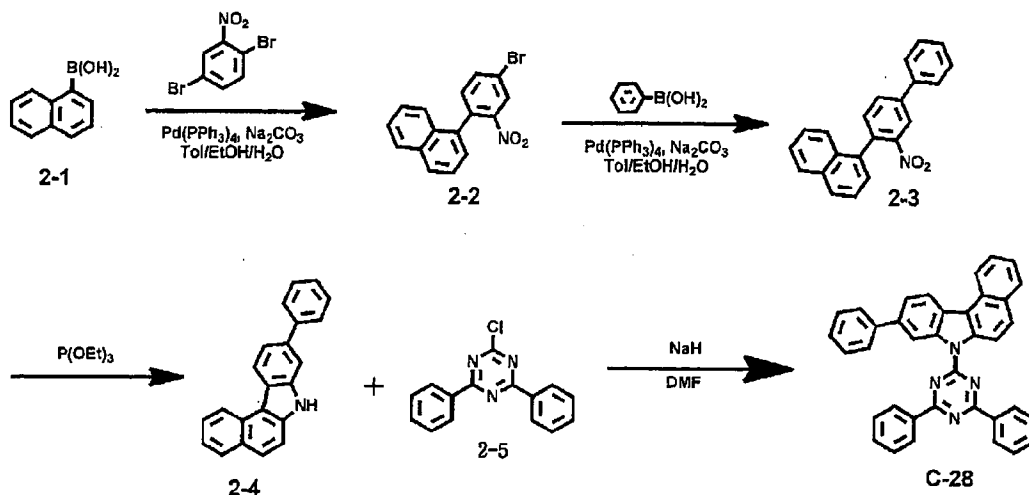
[133] After suspending compound 1-4 (4.0 g, 10.83 mmol) and compound 1-5 (3.1 g, 11.91 mmol) in dimethylformamide (DMF) (80 mL), 60% NaH (702 mg, 16.1 mmol) was added to the mixture at room temperature. Thereafter, the mixture was stirred for 12 hours, and then purified water (1L) was added thereto. After a filtration under reduced

pressure, the obtained solids was subjected to trituration with methanol/ethylacetate (EA), was dissolved in MC, was filtered through silica, and then was subjected to trituration with MC/n-hexane to obtain compound **C-27** (4.5 g, 69%).

[134] MW : 600.71, UV : 382 nm, PL : 493 nm, melting point : 324 °C

[135] **Example 2: Preparation of compound C-28**

[136]



[137] **Preparation of compound 2-2**

[138] Compound **2-2** (14.2 g, 41%) was prepared in the same manner as in the preparation of compound **1-2** of Example 1 by using compound **2-1** (22 g, 128.16 mmol) and 2,5-dibromonitrobenzene (30 g, 106.80 mmol).

[139] **Preparation of compound 2-3**

[140] Compound **2-3** (12 g, 92%) was prepared in the same manner as in the preparation of compound **1-2** of Example 1 by using compound **2-2** (14.2 g, 43.27 mmol) and phenylboronic acid (5.3 g, 43.27 mmol).

[141] **Preparation of compound 2-4**

[142] After dissolving compound **2-3** (12 g, 36.88 mmol) in triethylphosphate (120 mL), compound **2-4** (6.4 g, 62%) was prepared in the same manner as in the preparation of compound **1-3** of Example 1.

[143] **Preparation of compound C-28**

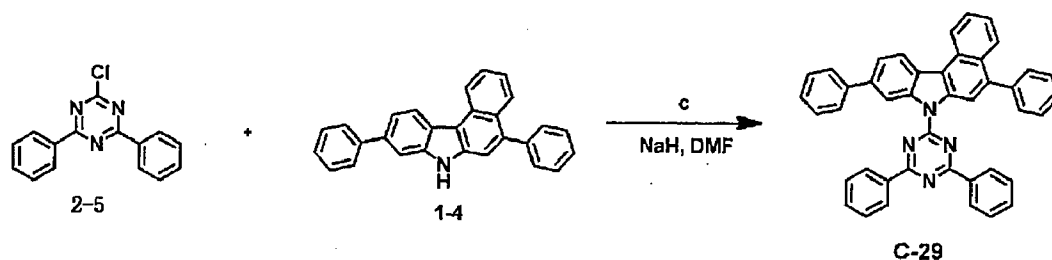
[144] Compound **C-28** (6.4 g, 58%) was prepared in the same manner as in the preparation of compound **C-27** of Example 1 by using compound **2-4** (6.4 g, 21.81 mmol) and compound **2-5** (5.8 g, 23.99 mmol).

[145] MW : 524.61, UV : 334 nm, PL : 495 nm, melting point: 273 °C

[146]

[147] **Example 3: Preparation of compound C-29**

[148]

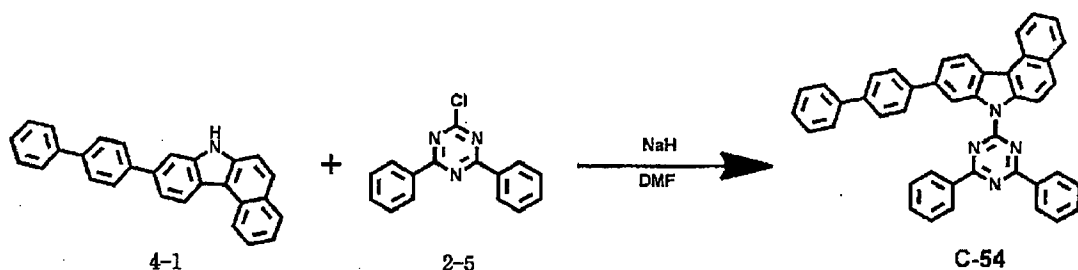


[149] Compound C-29 (6.5 g, 81%) was prepared in the same manner as in the preparation of compound C-27 of Example 1 by using compound 2-5 (3.6 g, 13.4 mmol) and compound 1-4 (4.8 g, 13.4 mmol).

[150] MW : 600.71, UV : 334 nm, PL : 385 nm, melting point: 349 °C

[151] **Example 4: Preparation of compound C-54**

[152]

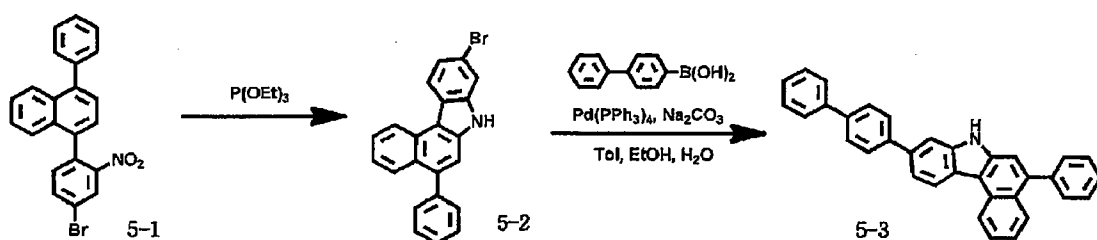


[153] Compound C-54 (6.0 g, 60%) was prepared in the same manner as in the preparation of compound C-27 of Example 1 by using compound 4-1 (6.4 g, 17.30 mmol) and compound 2-5 (5.1 g, 19.10 mmol).

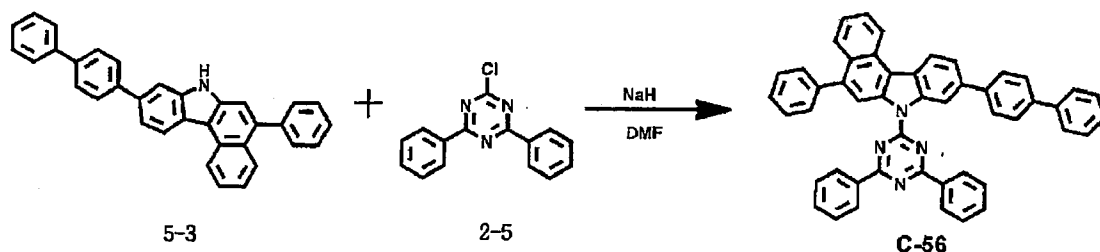
[154] MW : 676.81, UV : 344 nm, PL : 495 nm, melting point: 336 °C

[155] **Example 5: Preparation of compound C-56**

[156]



[157]



[158] **Preparation of compound 5-2**

[159] After dissolving compound 5-1 (35 g, 86.60 mmol) in triethylphosphate (350 mL), compound 5-2 (7.0 g, 22%) was prepared in the same manner as in the preparation of

compound 1-4 of Example 1.

[160] Preparation of compound 5-3

[161] Compound 5-3 (7.6 g, 92%) was prepared in the same manner as in the preparation of compound 1-2 of Example 1 by using compound 5-2 (7.0 g, 18.80 mmol) and [1,1'-biphenyl]-4-yl boronic acid (4.1 g, 20.70 mmol).

[162] Preparation of compound C-56

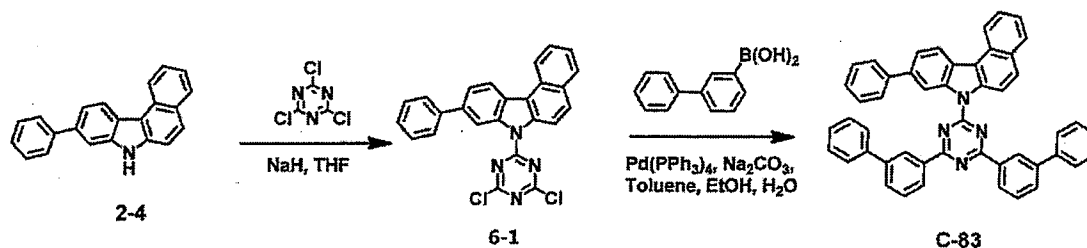
[163] Compound C-56 (4 g, 70%) was prepared in the same manner as in the preparation of compound C-27 of Example 1 by using compound 5-3 (3.8 g, 8.53 mmol) and compound 2-5 (2.5 g, 9.38 mmol).

[164] MW : 599.72, UV : 324 nm, PL : 485 nm, melting point: 264 °C

[165]

[166] Example 6: Preparation of compound C-83

[167]



[168] Preparation of compound 6-1

[169] After dissolving compound 2-4 (3.7 g, 13 mmol) and cyanuric acid (12 g, 63 mmol) in tetrahydrofuran (THF) (300 mL), compound 6-1 (4.3 g, 77%) was prepared in the same manner as in the preparation of compound C-27 of Example 1.

[170] Preparation of compound C-83

[171] Compound C-83 (37 g, 62%) was prepared in the same manner of in the preparation of compound 1-2 of Example 1 by using compound 6-1 (4 g, 9 mmol) and 3-biphenyl boronic acid (7.2 g, 36 mmol).

[172] MW : 599.72, UV : 324 nm, PL : 485 nm, melting point: 264 °C

[173]

[174] [Device Example 1] Production of an OLED device using the organic electroluminescent compound of the present invention

[175] OLED device was produced using the compound of the present invention. A transparent electrode indium tin oxide (ITO) thin film (15 Ω/sq) on a glass substrate for an organic light-emitting diode (OLED) device (Samsung Corning, Republic of Korea) was subjected to an ultrasonic washing with trichloroethylene, acetone, ethanol, and distilled water, sequentially, and then was stored in isopropanol. The ITO substrate was then mounted on a substrate holder of a vacuum vapor depositing apparatus. N¹,N^{1'}-([1,1'-biphenyl]-4,4'-diyl)bis(N¹-(naphthalen-1-yl)-N⁴,N⁴-diphenylbenzene-1,4-diamine) was introduced into a cell of said vacuum vapor depositing apparatus, and then the

pressure in the chamber of said 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 hole injection layer having a thickness of 60 nm on the ITO substrate. N,N'-di(4-biphenyl)-N,N'-di(4-biphenyl)-4,4'-diaminobiphenyl was then introduced into another cell of said vacuum vapor depositing apparatus, and was evaporated by applying an electric current to the cell, thereby forming a hole transport layer having a thickness of 20 nm on the hole injection layer. Thereafter, compound **C-28** was introduced into one cell of the vacuum vapor depositing apparatus, as a host material, and compound **D-11** 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 4 wt% based on the total amount of the host and dopant to form a light-emitting layer having a thickness of 30 nm on the hole transport layer. 2-(4-(9,10-di(naphthalene-2-yl)anthracen-2-yl)phenyl)-1-phenyl-1H-benzo[d]imidazole was then introduced into one cell, and lithium quinolate was introduced into another cell. The two materials were evaporated at the same rate, so that they were respectively deposited in a doping amount of 50 wt% to form an electron transport layer having a thickness of 30 nm on the light-emitting layer. After depositing lithium quinolate as an electron injection layer having a thickness of 2 nm on the electron transport layer, an Al cathode having a thickness of 150 nm was then deposited by another vacuum vapor deposition apparatus on the electron injection layer. Thus, an OLED device was produced. All the material used for producing the OLED device were those purified by vacuum sublimation at 10^{-6} torr.

[177] The produced OLED device showed red emission having a luminance of 1,030 cd/m² and a current density of 8.7 mA/cm² at a driving voltage of 4.1 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 60 hours or more.

[178]

[179] **[Device Example 2] Production of an OLED device using the organic**
 [180] **electroluminescent compound of the present invention**

[181] OLED device was produced in the same manner as in Device Example 1, except for using compound **C-29** as a host material and compound **D-7** as a dopant to form a light-emitting layer.

[182] The produced OLED device showed red emission having a luminance of 980 cd/m² and a current density of 5.5 mA/cm² at a driving voltage of 3.8 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 90 hours or more.

[183]

[184] **[Device Example 3] Production of an OLED device using the organic**
 [185] **electroluminescent compound of the present invention**

[186] OLED device was produced in the same manner as in Device Example 1, except for

using compound **C-54** as a host material and compound **D-11** as a dopant to form a light-emitting layer.

[187] The produced OLED device showed red emission having a luminance of 1,020 cd/m² and a current density of 11.0 mA/cm² at a driving voltage of 3.7 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 60 hours or more.

[188]

[189] **[Device Example 4] Production of an OLED device using the organic**
[190] **electroluminescent compound of the present invention**

[191] OLED device was produced in the same manner as in Device Example 1, except for using compound **C-83** as a host material and compound **D-11** as a dopant to form a light-emitting layer.

[192] The produced OLED device showed red emission having a luminance of 950 cd/m² and a current density of 10.7 mA/cm² at a driving voltage of 3.8 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 75 hours or more.

[193]

[194] **[Device Example 5] Production of an OLED device using the organic**
[195] **electroluminescent compound of the present invention**

[196] OLED device was produced in the same manner as in Device Example 1, except for using compound **C-56** as a host material and compound **D-7** as a dopant to form a light-emitting layer.

[197] The produced OLED device showed red emission having a luminance of 980 cd/m² and a current density of 7.2 mA/cm² at a driving voltage of 3.5 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 90 hours or more.

[198]

[199] **[Device Example 6] Production of an OLED device using the organic**
[200] **electroluminescent compound of the present invention**

[201] OLED device was produced in the same manner as in Device Example 1, except for using compound **C-27** as a host material and compound **D-7** as a dopant to form a light-emitting layer.

[202] The produced OLED device showed red emission having a luminance of 1,050 cd/m² and a current density of 6.6 mA/cm² at a driving voltage of 3.7 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 90 hours or more.

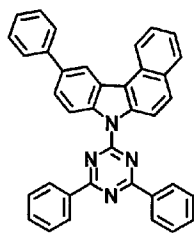
[203]

[204] **[Comparative Device Example 1] Production of an OLED device by using**
[205] **conventional organic electroluminescent compounds**

[206] An OLED device was produced in the same manner as in Device Example 1, except for using compound **A-1** shown below as a host material and compound **D-11** as a dopant to form a light-emitting layer.

[207] The produced OLED device showed red emission having a luminance of 1,000 cd/m² and a current density of 10.6 mA/cm² at a driving voltage of 4.7 V. The time taken to be reduced to 90% of the luminance at 5,000 nit was 20 hours or more.

[208]



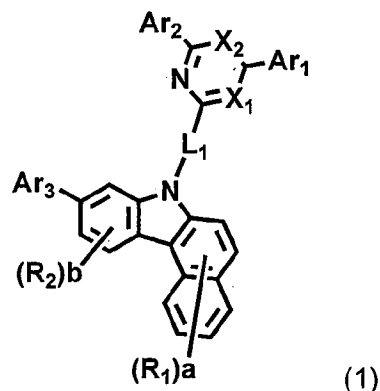
A-1

[209] The organic electroluminescent compound of the present invention can produce an organic electroluminescent device having an excellent lifespan and a lowered driving voltage so that power efficiency is improved. Furthermore, by using the compound of the present invention, it is possible to omit a hole blocking layer which has been necessary for an organic electroluminescent device using a conventional compound.

Claims

[Claim 1]

An organic electroluminescent compound represented by the following formula 1:



wherein

L_1 represents a single bond, a substituted or unsubstituted (3- to 30-membered) heteroarylene, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (C6-C30)cycloalkylene;

X_1 and X_2 , each independently, represent -CH- or -N-;

Ar_1 and Ar_2 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl;

Ar_3 represents a substituted or unsubstituted (C6-C30)cycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted hexahydrocarbazole, or a substituted or unsubstituted (3- to 30-membered)heteroaryl;

R_1 and R_2 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (5- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl, -NR₃R₄, -SiR₅R₆R₇, -SR₈, -OR₉, a cyano, a nitro or a hydroxyl;

R_3 to R_9 , each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, a substituted or unsubstituted (5- to

7-membered)heterocycloalkyl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (3- to 30-membered), 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;

a represents an integer of 1 to 6; b represents an integer of 1 to 3; where a or b represents an integer of 2 or more, each of R₁ or R₂ may be the same or different; and

the heteroarylene, the heterocycloalkyl and the heteroaryl, each independently, contain at least one hetero atom selected from B, N, O, S, P(=O), Si, and P.

[Claim 2]

The organic electroluminescent compound according to claim 1, wherein the substituents for the substituted groups of L₁, Ar₁ to Ar₃, and R₁ to R₉, each independently, are at least one selected from the group consisting of deuterium; a halogen; a (C1-C30)alkyl unsubstituted or substituted with a halogen; a (C1-C30)alkoxy; a (C6-C30)aryl; a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl; a (C3-C30)cycloalkyl; a (5- to 7-membered) heterocycloalkyl; 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; a (C2-C30)alkenyl; a (C2-C30)alkynyl; a cyano; a di(C1-C30)alkylamino; a di(C6-C30)arylamino; a (C1-C30)alkyl(C6-C30)arylamino; a di(C6-C30)arylboronyl; a di(C1-C30)alkylboronyl; a (C1-C30)alkyl(C6-C30)arylboronyl; a (C6-C30)aryl(C1-C30)alkyl; a (C1-C30)alkyl(C6-C30)aryl; a carboxyl; a nitro; and a hydroxyl.

[Claim 3]

The organic electroluminescent compound according to claim 1, wherein

L₁ represents a single bond, or a substituted or unsubstituted (C6-C20)arylene;

X₁ and X₂, each independently, represent -CH- or -N-;

Ar₁ and Ar₂, each independently, represent hydrogen, a substituted or unsubstituted (C1-C10)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl;

Ar₃ represents a substituted or unsubstituted (C6-C20)aryl, a substituted or unsubstituted hexahydrocarbazole, or a substituted or unsubstituted

(5- to 20-membered)heteroaryl; and

R₁ and R₂, each independently, represent hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl.

[Claim 4]

The organic electroluminescent compound according to claim 1, wherein

L₁ represents a single bond, or an (C6-C15)arylene unsubstituted or substituted with a (C1-C6)alkyl;

X₁ and X₂, each independently, represent -CH- or -N-;

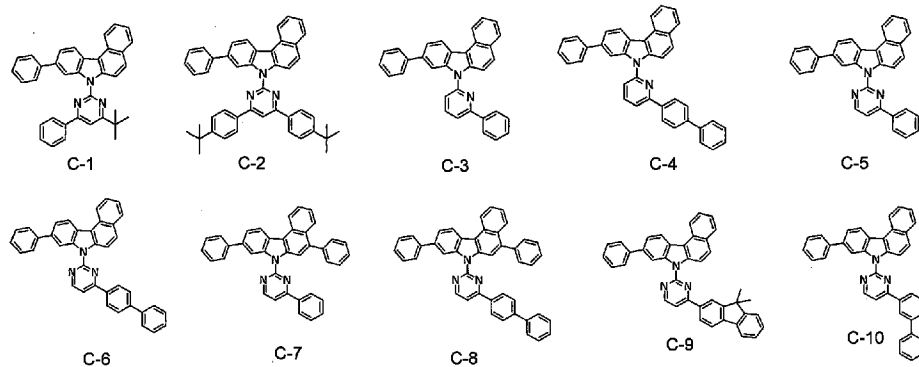
Ar₁ and Ar₂, each independently, represent hydrogen; a (C1-C6)alkyl; a (C6-C19)aryl unsubstituted or substituted with deuterium, a halogen, a (C1-C6)alkyl, a (C1-C6)alkoxy, a (5- to 15-membered)heteroaryl, a tri(C6-C10)arylsilyl, a (C1-C6)alkyldi(C6-C10)arylsilyl, a di(C6-C10)arylamino, or a (C1-C6)alkyl(C6-C15)aryl; or a (5- to 20-membered)heteroaryl unsubstituted or substituted with a (C1-C6)alkyl or a (C6-C10)aryl;

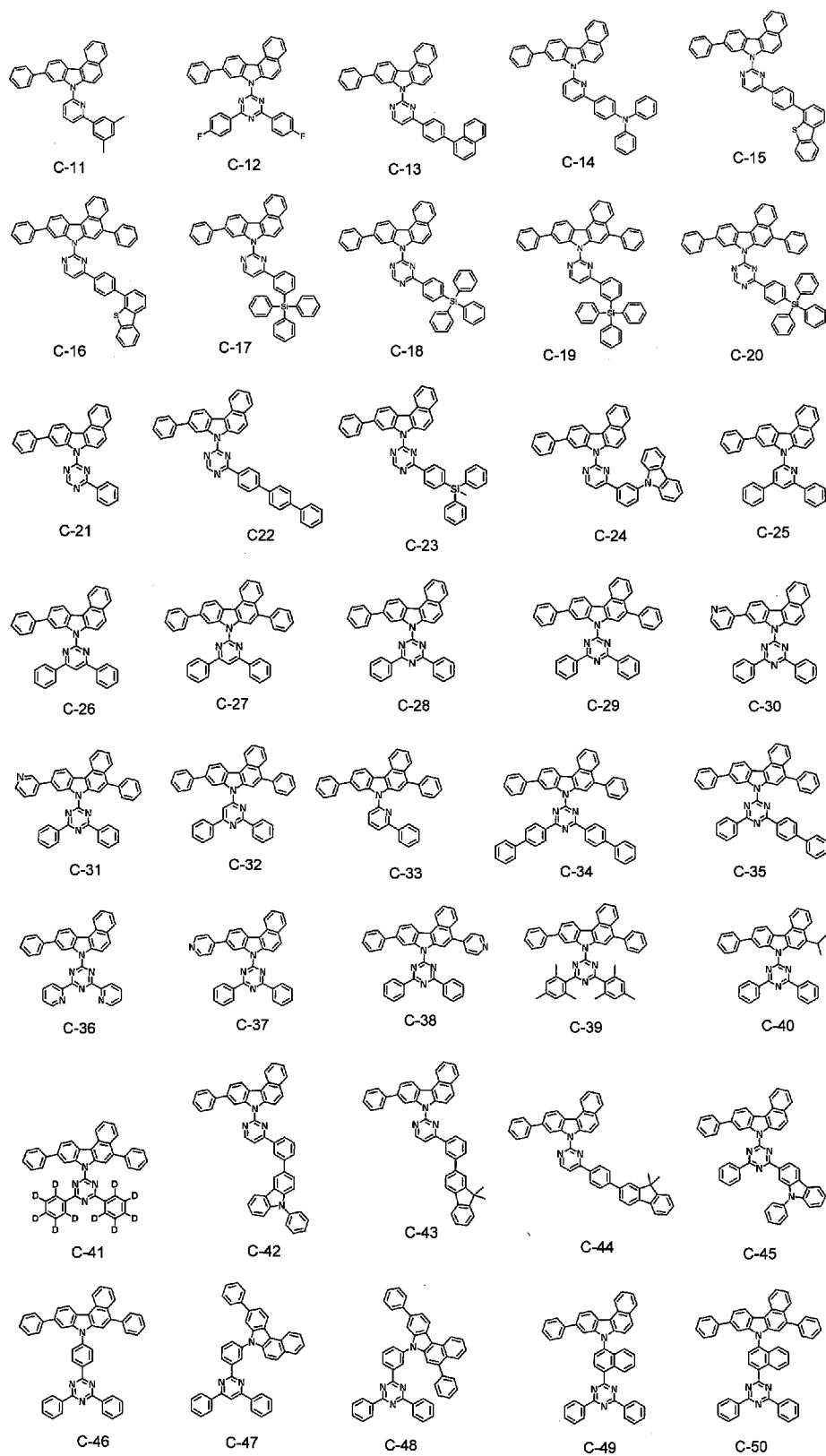
Ar₃ represents a (C6-C19)aryl unsubstituted or substituted with a (C1-C6)alkyl, a (5- to 15-membered)heteroaryl, or a di(C6-C10)arylamino; a hexahydrocarbazole unsubstituted or substituted with a (C1-C6)alkyl or a (C6-C10)aryl; or a (5- to 19-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl; and

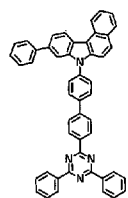
R₁ and R₂, each independently, represent hydrogen, a (C1-C6)alkyl, a (C6-C19)aryl unsubstituted or substituted with a (C1-C6)alkyl, or a (5- to 19-membered)heteroaryl unsubstituted or substituted with a (C6-C10)aryl.

[Claim 5]

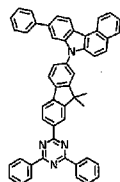
The organic electroluminescent compound according to claim 1, wherein the compound of formula 1 is selected from the group consisting of:



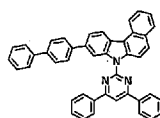




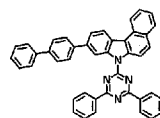
C-51



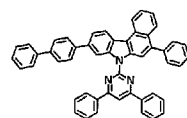
C-52



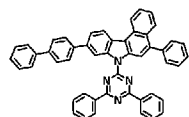
C-53



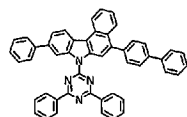
C-54



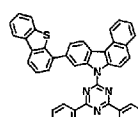
C-55



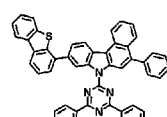
C-56



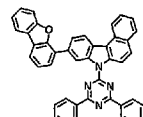
C-57



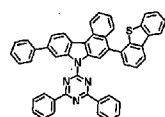
C-58



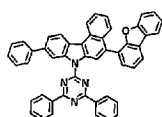
C-59



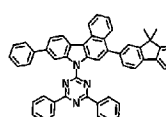
C-60



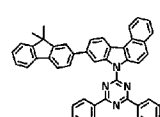
C-61



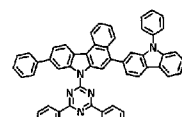
C-62



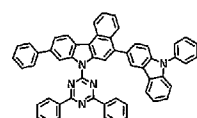
C-63



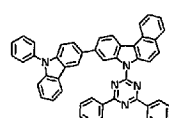
C-64



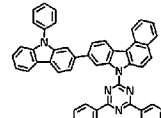
C-65



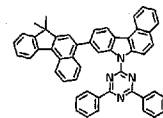
C-66



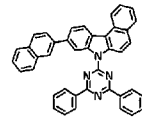
C-67



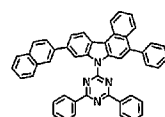
C-68



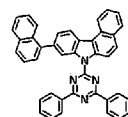
C-69



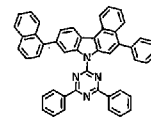
C-70



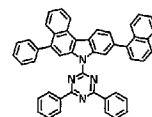
C-71



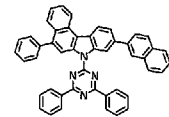
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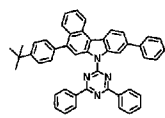
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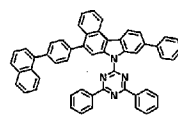
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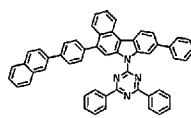
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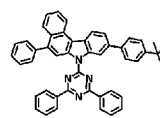
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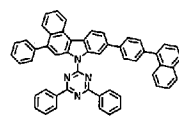
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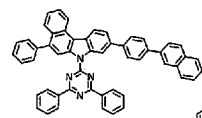
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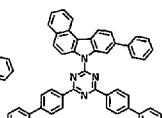
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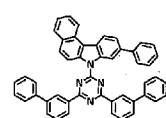
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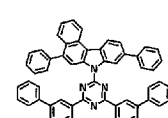
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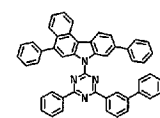
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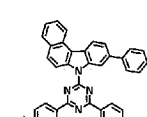
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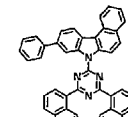
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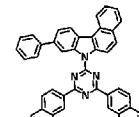
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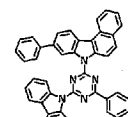
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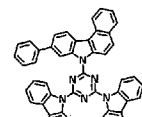
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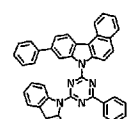
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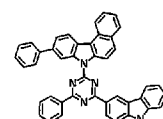
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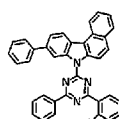
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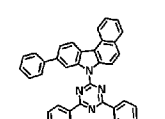
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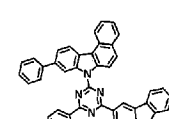
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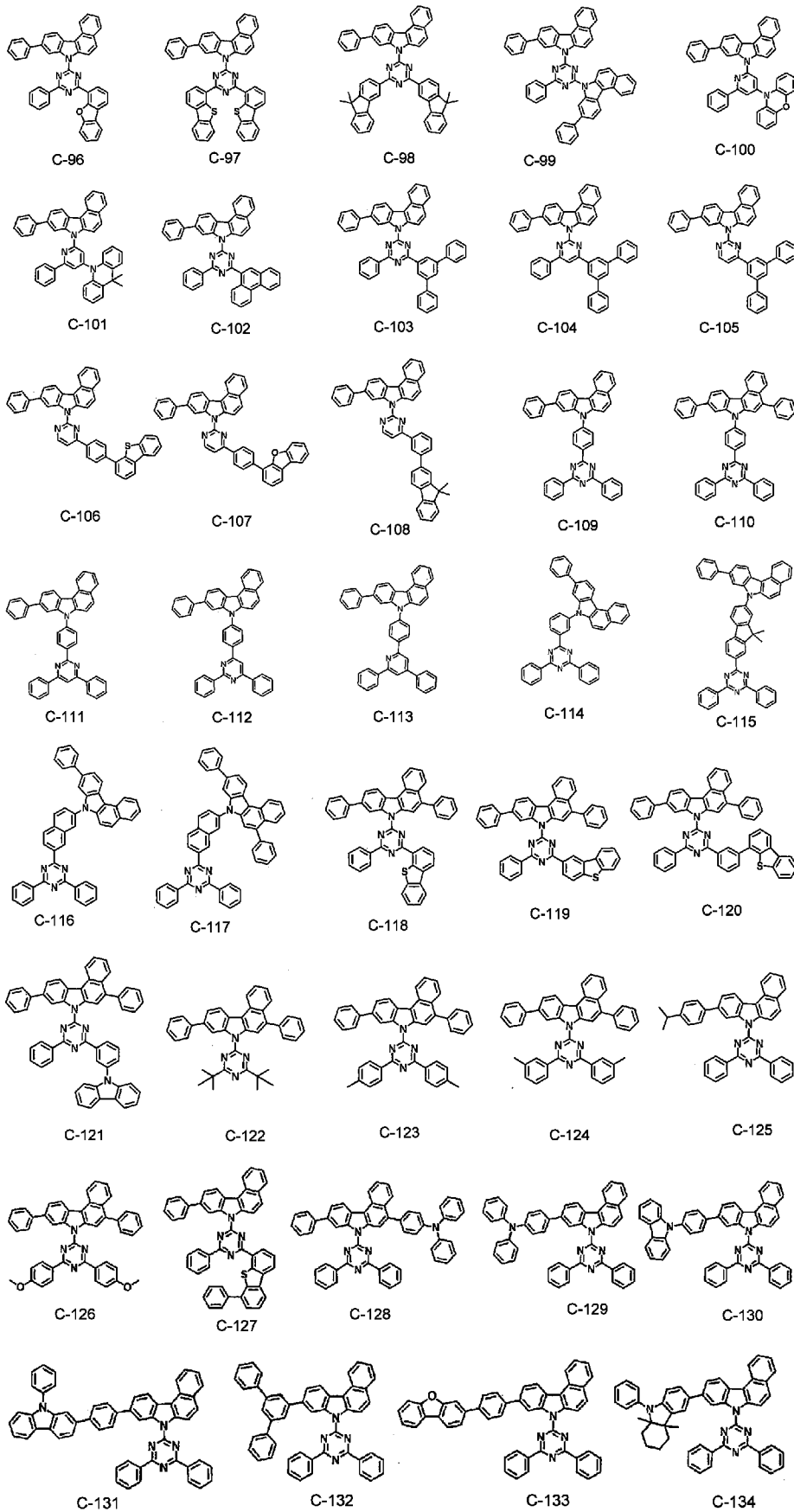
C-93



C-94



C-95



[Claim 6]

An organic electroluminescent device comprising the organic electrolu-

minescent compound according to claim 1.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2013/012123

A. CLASSIFICATION OF SUBJECT MATTER

C07D 401/04 (2006.01) C07D 401/14 (2006.01) C07D 403/04 (2006.01) C07D 403/14 (2006.01) C07D 407/14 (2006.01)
C07D 409/14 (2006.01) C07D 413/14 (2006.01) C07F 7/10 (2006.01) C09K 11/06 (2006.01) H01L 51/50 (2006.01)
H01L 51/54 (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)

Registry and Caplus: Substructure search based on formula (1).

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

* Special categories of cited documents:	
"A" 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
11 February 2014

Date of mailing of the international search report
11 February 2014

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INTERNATIONAL SEARCH REPORT		International application No.
C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT		PCT/KR2013/012123
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	KR 10-2012-0021203 A (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 08 March 2012 First structure on page 3, Abstract, pages 4-8, 14-16	1-6
A	WO 2011/019156 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 11 February 2011 Formula 1, paragraphs [1]-[3]), compounds 18, 19 etc.	1-6
P,X	WO 2013/105747 A1 (DUKSAN HIGH METAL CO. LTD) 18 July 2013 Formula at paragraph [8], at pages 8-9, formulae 4, 5, 7, 8, 14, 15, 17 and 18, examples such as 5-3, 5-4, 5-7 to 5-10 etc.	1-6
P,X	US 2013/0048956 A1 (BALAGANESAN et. al.) 28 February 2013 Abstract, claim 1, formula (I), compounds 1-27 to 1-30 etc.	1-6

INTERNATIONAL SEARCH REPORT Information on patent family members		International application No. PCT/KR2013/012123	
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.			
Patent Document/s Cited in Search Report		Patent Family Member/s	
Publication Number	Publication Date	Publication Number	Publication Date
KR 10-2012-0021203 A	08 Mar 2012	None	
WO 2011/019156 A1	11 Feb 2011	KR 20110015836 A	17 Feb 2011
		TW 201120186 A	16 Jun 2011
		US 2012235123 A1	20 Sep 2012
		WO 2011019156 A1	17 Feb 2011
WO 2013/105747 A1	18 Jul 2013	WO 2013105747 A1	18 Jul 2013
US 2013/0048956 A1	28 Feb 2013	JP 2013046067 A	04 Mar 2013
		KR 20130022391 A	06 Mar 2013
		TW 201309675 A	01 Mar 2013
		US 2013048956 A1	28 Feb 2013
End of Annex			
Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001. Form PCT/ISA/210 (Family Annex)(July 2009)			