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(54) Title: A PLURALITY OF HOST MATERIALS AND ORGANIC ELECTROLUMINESCENT DEVICE COMPRISING THE SAME

(57) Abstract: The present disclosure relates to a plurality of host materials comprising a first host compound and a second host compound, wherein the first host compound is represented by formula 1 and the second host compound is represented by formula 1, and the first host compound and the second host compound are different from each other, and an organic electroluminescent device comprising the same. By comprising the plurality of host materials including a specific combination of compounds, it is possible to produce an organic electroluminescent device having excellent thermal stability, low driving voltage, high luminous efficiency, and/or improved lifespan properties.

Description

Title of Invention: A PLURALITY OF HOST MATERIALS AND ORGANIC ELECTROLUMINESCENT DEVICE COMPRISING THE SAME

Technical Field

[1] The present disclosure relates to a plurality of host materials and an organic electroluminescent device comprising the same.

Background Art

[2] A small molecular green organic electroluminescent device (OLED) was first developed by Tang, et al., of Eastman Kodak in 1987 by using TPD/ALq3 bi-layer consisting of a light-emitting layer and a charge transport layer. Thereafter, the development of OLEDs was rapidly effected and OLEDs have been commercialized. At present, OLEDs primarily use phosphorescent materials having excellent luminous efficiency in panel implementation. An OLED having high luminous efficiency and/or long lifespan characteristics is required for long time use and high resolution of a display.

[3] In order to enhance luminous efficiency, driving voltage and/or lifespan, various materials or concepts for an organic layer of an organic electroluminescent device have been proposed. However, they were not satisfactory to use practically.

[4] Korean Patent Application Laid-Open No. 2015-0121337 discloses a compound in which azulene, carbazole, etc., are fused. However, said reference does not specifically disclose that the compound is used as a plurality of host compounds. Thus, development of a host material for improving performances of an OLED device is still required.

Disclosure of Invention

Technical Problem

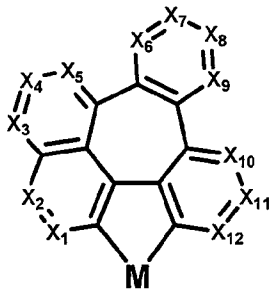
[5] The objective of the present disclosure is to provide an organic electroluminescent device having excellent thermal stability, low driving voltage, high luminous efficiency, and/or improved lifespan properties by comprising a plurality of host materials including a specific combination of compounds.

Solution to Problem

[6] It is advantageous that a light-emitting layer containing a phosphorescent dopant has excellent hole and electron current properties of a light-emitting material for low voltage, high efficiency, and long lifespan, and has excellent thermal stability of the material for improving lifespan. Further, for efficient energy transfer from a host to a

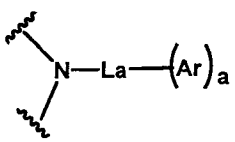
dopant of a light-emitting layer, a light-emitting material having a narrow energy band gap can minimize a charge trap to contribute to driving voltage and luminous efficiency. An azulene derivative included in the device of the present disclosure has a high internal conversion transition constant of $S_2 \rightarrow S_1$ of $7*10^{-8}$ s, whereas it has a low internal conversion transition constant of $S_1 \rightarrow S_0$ of $7*10^{-12}$ s, which increases the fluorescence quantum yield of $S_2 \rightarrow S_0$. Thus, the azulene derivative is one of the representative materials violating Kasha's rule. Phys. Chem. Chem. Phys. 2015, 17, 23573, J. Phys. Chem. A, Vol. 103, No. 15, 1999, 2529 reported that azulene can be advantageous in improving the phosphorescent light-emitting property, since the energy levels of S_2 and S_1 of azulene are 3.565 eV and 1.771 eV, respectively, and $T_1 \rightarrow S_0$ transition shows a very low level difference between T_1 and S_0 of 1.711 eV, as well as intersystem crossing transition to $S_2 \rightarrow T_n$ is improved according to the substitution material and the polarity of a solvent, resulting in increase of the transition to a triplet. Such azulene derivatives show a low $S_1 \rightarrow T_1$ energy gap, and have relatively high HOMO property compared to carbazole- or benzocarbazole-type compounds, and thus can have a narrow energy band gap. The present inventors found that the low driving voltage, high luminous efficiency, and/or long lifespan properties can be achieved by using azulene derivatives of the present disclosure by suitably mixing them as first and second hosts in a light-emitting layer. Specifically, the present inventors found that the above objective can be achieved by using a plurality of host materials comprising at least one first host compound and at least one second host compound, wherein the first host compound and the second host compound are represented by the following formula 1, and the first host compound and the second host compound are different from each other:

[7]



----- (1)

[8] wherein

[9] M represents 

, O or S;

[10] X_1 to X_{12}, each independently, represent N or CR_1;

[11] La represents a single bond, a substituted or unsubstituted (C1-C30)alkylene, a sub-

stituted or unsubstituted (C6-C30)arylene, a substituted or unsubstituted (3- to 30-membered)heteroarylene, or a substituted or unsubstituted (C3-C30)cycloalkylene;

[12] Ar and R_1, each independently, represent hydrogen, deuterium, a halogen, a cyano, 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 (C1-C30)alkoxy, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a substituted or unsubstituted mono- or di- (C1-C30)alkylamino, a substituted or unsubstituted mono- or di- (C6-C30)arylamino, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino; or adjacent Ar's may be linked to each other to form a ring, or adjacent R_1's may be linked to each other to form a ring, where if a plurality of R_1's are present, each of R_1 may be the same or different; and

[13] a represents an integer of 1 or 2, where if a is 2, each of Ar may be the same or different.

Advantageous Effects of Invention

[14] A plurality of host materials according to the present disclosure can provide an organic electroluminescent device having excellent thermal stability, low driving voltage, high luminous efficiency, and/or improved lifespan properties, and it is possible to produce a display device or a lighting device using the same.

Mode for the Invention

[15] Hereinafter, the present disclosure will be described in detail. However, the following description is intended to explain the invention, and is not meant in any way to restrict the scope of the invention.

[16] The term "organic electroluminescent material" in the present disclosure means a material that may be used in an organic electroluminescent device, and may comprise at least one compound. The organic electroluminescent material may be comprised in any layer constituting an organic electroluminescent device, as necessary. For example, the organic electroluminescent material may be a hole injection material, a hole transport material, a hole auxiliary material, a light-emitting auxiliary material, an electron blocking material, a light-emitting material (including a host material and a dopant material), an electron buffer material, a hole blocking material, an electron transport material, an electron injection material, etc.

[17] The term "a plurality of organic electroluminescent materials" in the present disclosure means an organic electroluminescent material comprising a combination of at least two compounds, which may be comprised in any layer constituting an organic

electroluminescent device. It may mean both a material before being comprised in an organic electroluminescent device (for example, before vapor deposition) and a material after being comprised in an organic electroluminescent device (for example, after vapor deposition). For example, a plurality of organic electroluminescent materials may be a combination of at least two compunds, which may be comprised in at least one layer of a hole injection layer, a hole transport layer, a hole auxiliary layer, a light-emitting auxiliary layer, an electron blocking layer, a light-emitting layer, an electron buffer layer, a hole blocking layer, an electron transport layer, and an electron injection layer. Such at least two compounds may be comprised in the same layer or different layers, and may be mixture-evaporated or co-evaporated, or may be individually evaporated.

[18] The term "a plurality of host materials" in the present disclosure means a host material comprising a combination of at least two compounds, which may be comprised in any light-emitting layer constituting an organic electroluminescent device. It may mean both a material before being comprised in an organic electroluminescent device (for example, before vapor deposition) and a material after being comprised in an organic electroluminescent device (for example, after vapor deposition). For example, a plurality of host materials of the present disclosure may be a combination of at least two host materials, and selectively may further comprise conventional materials comprised in an organic electroluminescent material. A plurality of host materials of the present disclosure may be comprised in any light-emitting layer constituting an organic electroluminescent device, and at least two compounds comprised in the plurality of host materials may be comprised together in one light-emitting layer or may respectively be comprised in different light-emitting layers. If at least two host materials are comprised in one layer, for example, the at least two compounds may be mixture-evaporated to form a layer, or may be individually evaporated at the same time to form a layer.

[19] Hereinafter, the compound represented by formula 1 will be described in more detail.

[20] Herein, the term "(C1-C30)alkyl(ene)" is meant to be a linear or branched alkyl(ene) having 1 to 30 carbon atoms constituting the chain, in which the number of carbon atoms is preferably 1 to 20, and more preferably 1 to 10. The above alkyl may include methyl, ethyl, *n*-propyl, *iso*-propyl, *n*-butyl, *iso*-butyl, *tert*-butyl, etc. The term "(C2-C30)alkenyl" is meant to be a linear or branched alkenyl having 2 to 30 carbon atoms constituting the chain, in which the number of carbon atoms is preferably 2 to 20, and more preferably 2 to 10. The above alkenyl may include vinyl, 1-propenyl, 2-propenyl, 1-butenyl, 2-butenyl, 3-butenyl, 2-methylbut-2-enyl, etc. The term "(C2-C30)alkynyl" is meant to be a linear or branched alkynyl having 2 to 30 carbon atoms constituting the chain, in which the number of carbon atoms is preferably 2 to

20, and more preferably 2 to 10. The above alkynyl may include ethynyl, 1-propynyl, 2-propynyl, 1-butynyl, 2-butynyl, 3-butynyl, 1-methylpent-2-ynyl, etc. The term "(C3-C30)cycloalkyl(ene)" is meant to be a mono- or polycyclic hydrocarbon having 3 to 30 ring backbone carbon atoms, in which the number of carbon atoms is preferably 3 to 20, and more preferably 3 to 7. The above cycloalkyl may include cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, etc. The term "(3- to 7-membered)heterocycloalkyl" is meant to be a cycloalkyl having 3 to 7, preferably 5 to 7, ring backbone atoms, and including at least one heteroatom selected from the group consisting of B, N, O, S, Si, and P, and preferably the group consisting of O, S, and N. The above heterocycloalkyl may include tetrahydrofuran, pyrrolidine, thiolan, tetrahydropyran, etc. The term "(C6-C30)aryl(ene)" is meant to be a monocyclic or fused ring radical derived from an aromatic hydrocarbon having 6 to 30 ring backbone carbon atoms, in which the number of the ring backbone carbon atoms is preferably 6 to 25, more preferably 6 to 18. The above aryl(ene) may be partially saturated, and may comprise a spiro structure. The above aryl may include phenyl, biphenyl, terphenyl, naphthyl, binaphthyl, phenylnaphthyl, naphthylphenyl, phenylterphenyl, fluorenyl, phenylfluorenyl, benzofluorenyl, dibenzofluorenyl, phenanthrenyl, phenylphenanthrenyl, anthracenyl, indenyl, triphenylenyl, pyrenyl, tetracenyl, perylenyl, chrysenyl, naphthacenyl, fluoranthenyl, spirobifluorenyl, etc. More specifically, the above aryl may include a phenyl group, a 1-naphthyl group, a 2-naphthyl group, a 1-anthryl group, a 2-anthryl group, a 9-anthryl group, a benzanthryl group, a 1-phenanthryl group, a 2-phenanthryl group, a 3-phenanthryl group, a 4-phenanthryl group, a 9-phenanthryl group, a naphthacenyl group, a pyrenyl group, a 1-chrysenyl group, a 2-chrysenyl group, a 3-chrysenyl group, a 4-chrysenyl group, a 5-chrysenyl group, a 6-chrysenyl group, a benzo[c]phenanthryl group, a benzo[g]chrysenyl group, a 1-triphenylenyl group, a 2-triphenylenyl group, a 3-triphenylenyl group, a 4-triphenylenyl group, a 1-fluorenyl group, a 2-fluorenyl group, a 3-fluorenyl group, a 4-fluorenyl group, a 9-fluorenyl group, a benzofluorenyl group, a dibenzofluorenyl group, a 2-biphenylyl group, a 3-biphenylyl group, a 4-biphenylyl group, an o-terphenyl group, an m-terphenyl-4-yl group, an m-terphenyl-3-yl group, an m-terphenyl-2-yl group, a p-terphenyl-4-yl group, a p-terphenyl-3-yl group, a p-terphenyl-2-yl group, an m-quaterphenyl group, a 3-fluoranthenyl group, a 4-fluoranthenyl group, an 8-fluoranthenyl group, a 9-fluoranthenyl group, a benzofluoranthenyl group, an o-tolyl group, an m-tolyl group, a p-tolyl group, a 2,3-xylyl group, a 3,4-xylyl group, a 2,5-xylyl group, a mesityl group, an o-cumenyl group, an m-cumenyl group, a p-cumenyl group, a p-t-butylphenyl group, a p-(2-phenylpropyl)phenyl group, a 4'-methylbiphenylyl group, a 4"-t-butyl-p-terphenyl-4-yl group, a 9,9-dimethyl-1-fluorenyl group, a 9,9-dimethyl-2-fluorenyl group, a 9,9-dimethyl-3-fluorenyl group, a

9,9-dimethyl-4-fluorenyl group, a 9,9-diphenyl-1-fluorenyl group, a 9,9-diphenyl-2-fluorenyl group, a 9,9-diphenyl-3-fluorenyl group, a 9,9-diphenyl-4-fluorenyl group, etc.

[21] The term "(3- to 30-membered)heteroaryl(ene)" is meant to be an aryl having 3 to 30 ring backbone atoms, and including at least one, preferably 1 to 4 heteroatoms selected from the group consisting of B, N, O, S, Si, and P. The above heteroaryl(ene) 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 may comprise a spiro structure. The above heteroaryl may include 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, and pyridazinyl, and a fused ring-type heteroaryl such as benzofuranyl, benzothiophenyl, isobenzofuranyl, dibenzofuranyl, dibenzothiophenyl, benzimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, benzoindolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, benzoquinazolinyl, quinoxalinyl, benzoquinoxalinyl, naphthyridinyl, carbazolyl, benzocarbazolyl, dibenzocarbazolyl, phenoxazinyl, phenothiazinyl, phenanthridinyl, benzodioxolyl, and dihydroacridinyl. More specifically, the above heteroaryl may include a 1-pyrrolyl group, a 2-pyrrolyl group, a 3-pyrrolyl group, a pyrazinyl group, a 2-pyridinyl group, a 2-pyrimidinyl group, a 4-pyrimidinyl group, a 5-pyrimidinyl group, a 6-pyrimidinyl group, a 1,2,3-triazin-4-yl group, a 1,2,4-triazin-3-yl group, a 1,3,5-triazin-2-yl group, a 1-imidazolyl group, a 2-imidazolyl group, a 1-pyrazolyl group, a 1-indolidinyl group, a 2-indolidinyl group, a 3-indolidinyl group, a 5-indolidinyl group, a 6-indolidinyl group, a 7-indolidinyl group, an 8-indolidinyl group, a 2-imidazopyridinyl group, a 3-imidazopyridinyl group, a 5-imidazopyridinyl group, a 6-imidazopyridinyl group, a 7-imidazopyridinyl group, an 8-imidazopyridinyl group, a 3-pyridinyl group, a 4-pyridinyl group, a 1-indolyl group, a 2-indolyl group, a 3-indolyl group, a 4-indolyl group, a 5-indolyl group, a 6-indolyl group, a 7-indolyl group, a 1-isoindolyl group, a 2-isoindolyl group, a 3-isoindolyl group, a 4-isoindolyl group, a 5-isoindolyl group, a 6-isoindolyl group, a 7-isoindolyl group, a 2-furyl group, a 3-furyl group, a 2-benzofuranyl group, a 3-benzofuranyl group, a 4-benzofuranyl group, a 5-benzofuranyl group, a 6-benzofuranyl group, a 7-benzofuranyl group, a 1-isobenzofuranyl group, a 3-isobenzofuranyl group, a 4-isobenzofuranyl group, a 5-isobenzofuranyl group, a 6-isobenzofuranyl group, a 7-isobenzofuranyl group, a 2-quinolyl group, a 3-quinolyl group, a 4-quinolyl group, a 5-quinolyl group, a 6-quinolyl group, a 7-quinolyl group, an 8-quinolyl group, a 1-isoquinolyl group, a 3-isoquinolyl group, a 4-isoquinolyl

group, a 5-isoquinolyl group, a 6-isoquinolyl group, a 7-isoquinolyl group, an 8-isoquinolyl group, a 2-quinoxalinyl group, a 5-quinoxalinyl group, a 6-quinoxalinyl group, a 1-carbazolyl group, a 2-carbazolyl group, a 3-carbazolyl group, a 4-carbazolyl group, a 9-carbazolyl group, an azacarbazolyl-1-yl group, an azacarbazolyl-2-yl group, an azacarbazolyl-3-yl group, an azacarbazolyl-4-yl group, an azacarbazolyl-5-yl group, an azacarbazolyl-6-yl group, an azacarbazolyl-7-yl group, an azacarbazolyl-8-yl group, an azacarbazolyl-9-yl group, a 1-phenanthridinyl group, a 2-phenanthridinyl group, a 3-phenanthridinyl group, a 4-phenanthridinyl group, a 6-phenanthridinyl group, a 7-phenanthridinyl group, an 8-phenanthridinyl group, a 9-phenanthridinyl group, a 10-phenanthridinyl group, a 1-acridinyl group, a 2-acridinyl group, a 3-acridinyl group, a 4-acridinyl group, a 9-acridinyl group, a 2-oxazolyl group, a 4-oxazolyl group, a 5-oxazolyl group, a 2-oxadiazolyl group, a 5-oxadiazolyl group, a 3-furazanyl group, a 2-thienyl group, a 3-thienyl group, a 2-methylpyrrol-1-yl group, a 2-methylpyrrol-3-yl group, a 2-methylpyrrol-4-yl group, a 2-methylpyrrol-5-yl group, a 3-methylpyrrol-1-yl group, a 3-methylpyrrol-2-yl group, a 3-methylpyrrol-4-yl group, a 3-methylpyrrol-5-yl group, a 2-t-butylpyrrol-4-yl group, a 3-(2-phenylpropyl)pyrrol-1-yl group, a 2-methyl-1-indolyl group, a 4-methyl-1-indolyl group, a 2-methyl-3-indolyl group, a 4-methyl-3-indolyl group, a 2-t-butyl-1-indolyl group, a 4-t-butyl-1-indolyl group, a 2-t-butyl-3-indolyl group, a 4-t-butyl-3-indolyl group, a 1-dibenzofuranyl group, a 2-dibenzofuranyl group, a 3-dibenzofuranyl group, a 4-dibenzofuranyl group, a 1-dibenzothiophenyl group, a 2-dibenzothiophenyl group, a 3-dibenzothiophenyl group, a 4-dibenzothiophenyl group, a 1-silafluorenyl group, a 2-silafluorenyl group, a 3-silafluorenyl group, a 4-silafluorenyl group, a 1-germafluorenyl group, a 2-germafluorenyl group, a 3-germafluorenyl group, and a 4-germafluorenyl group. Furthermore, "halogen" includes F, Cl, Br, and I.

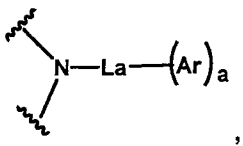
[22] Herein, "substituted" in the expression "substituted or unsubstituted" means that a hydrogen atom in a certain functional group is replaced with another atom or another functional group, i.e., a substituent. The substituents of the substituted (C1-C30)alkyl(ene), the substituted (C6-C30)aryl(ene), the substituted (3- to 30-membered)heteroaryl(ene), the substituted (C3-C30)cycloalkyl(ene), the substituted (C1-C30)alkoxy, the substituted tri(C1-C30)alkylsilyl, the substituted di(C1-C30)alkyl(C6-C30)arylsilyl, the substituted (C1-C30)alkyldi(C6-C30)arylsilyl, the substituted tri(C6-C30)arylsilyl, the substituted mono- or di- (C1-C30)alkylamino, the substituted mono- or di- (C6-C30)arylamino, and the substituted (C1-C30)alkyl(C6-C30)arylamino in the formulas of the present disclosure, each independently, are at least one selected from the group consisting of deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a (C1-C30)alkyl, a halo(C1-C30)alkyl, a (C2-C30)alkenyl, a (C2-C30)alkynyl, a (C1-C30)alkoxy, a (C1-C30)alkylthio, a

(C3-C30)cycloalkyl, a (C3-C30)cycloalkenyl, a (3- to 7-membered)heterocycloalkyl, a (C6-C30)aryloxy, a (C6-C30)arylthio, a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl, a (C6-C30)aryl unsubstituted or substituted with a (3- to 30-membered)heteroaryl, a tri(C1-C30)alkylsilyl, a tri(C6-C30)arylsilyl, a di(C1-C30)alkyl(C6-C30)arylsilyl, a (C1-C30)alkyldi(C6-C30)arylsilyl, an amino, a mono- or di- (C1-C30)alkylamino, a mono- or di- (C6-C30)arylamino unsubstituted or substituted with a (C1-C30)alkyl, a (C1-C30)alkyl(C6-C30)arylamino, a (C1-C30)alkylcarbonyl, a (C1-C30)alkoxycarbonyl, a (C6-C30)arylcarbonyl, a di(C6-C30)arylboronyl, a di(C1-C30)alkylboronyl, a (C1-C30)alkyl(C6-C30)arylboronyl, a (C6-C30)aryl(C1-C30)alkyl, and a (C1-C30)alkyl(C6-C30)aryl; preferably, at least one selected from the group consisting of a (C1-C20)alkyl, an unsubstituted (C6-C25)aryl, and a (5- to 25-membered)heteroaryl unsubstituted or substituted with a (C6-C25)aryl; more preferably, at least one selected from the group consisting of a (C1-C10)alkyl, an unsubstituted (C6-C18)aryl, and a (5- to 18-membered)heteroaryl substituted with a (C6-C18)aryl; and for example, at least one selected from the group consisting of a methyl, a phenyl, a diphenyltriazinyl, and a phenylquinoxalinyl.

[23] In the formulas of the present disclosure, if adjacent substituents are linked to each other to form a ring, the ring may be a substituted or unsubstituted, mono- or polycyclic, (3- to 30-membered) alicyclic or aromatic ring, or the combination thereof, in which the formed ring may contain at least one heteroatom selected from nitrogen, oxygen, and sulfur. For example, the fused ring may be a substituted or unsubstituted dibenzothiophene ring, a substituted or unsubstituted dibenzofuran ring, a substituted or unsubstituted naphthalene ring, a substituted or unsubstituted phenanthrene ring, a substituted or unsubstituted fluorene ring, a substituted or unsubstituted benzothiophene ring, a substituted or unsubstituted benzofuran ring, a substituted or unsubstituted indole ring, a substituted or unsubstituted indene ring, a substituted or unsubstituted benzene ring, or a substituted or unsubstituted carbazole ring.

[24] In the formulas of the present disclosure, the heteroaryl or heteroarylene may, each independently, contain at least one heteroatom selected from B, N, O, S, Si, and P. In addition, the heteroatom may be combined with at least one selected from the group consisting of hydrogen, deuterium, a halogen, a cyano, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (5- to 30-membered)heteroaryl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl,

a substituted or unsubstituted mono- or di- (C1-C30)alkylamino, a substituted or unsubstituted mono- or di- (C6-C30)arylamino, and a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino.

[25] In formula 1, M represents  O or S.

,

[26] In formula 1, X_1 to X_{12}, each independently, represent N or CR_1. According to one embodiment of the present disclosure, all of X_1 to X_{12} may represent CR_1. According to another embodiment of the present disclosure, any one of X_1 to X_{12} may represent N. According to further embodiment of the present disclosure, two of X_1 to X_{12} may represent N.

[27] In formula 1, La represents a single bond, a substituted or unsubstituted (C1-C30)alkylene, a substituted or unsubstituted (C6-C30)arylene, a substituted or unsubstituted (3- to 30-membered)heteroarylene, or a substituted or unsubstituted (C3-C30)cycloalkylene; preferably, a single bond, a substituted or unsubstituted (C6-C25)arylene, or a substituted or unsubstituted (5- to 25-membered)heteroarylene; more preferably, a single bond, an unsubstituted (C6-C18)arylene, or an unsubstituted (5- to 18-membered)heteroarylene. The heteroarylene may comprise at least one of N, O, and S, and preferably at least one of N and S. According to one embodiment of the present disclosure, La may represent a single bond, phenylene, naphthylene, biphenylene, pyridylene, pyrimidinylene, triazinylene, isoquinolinylene, quinazolinylene, naphthyridinylene, quinoxalinylene, benzoquinoxalinylene, indoloquinoxalinylene, benzothienopyrimidinylene, or benzoquinazolinylene.

[28] In formula 1, Ar and R_1, each independently, represent hydrogen, deuterium, a halogen, a cyano, 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 (C1-C30)alkoxy, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a substituted or unsubstituted mono- or di- (C1-C30)alkylamino, a substituted or unsubstituted mono- or di- (C6-C30)arylamino, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino; or adjacent Ar's may be linked to each other to form a ring, or adjacent R_1's may be linked to each other to form a ring, in which if a plurality of R_1's are present, each of R_1 may be the same or different.

[29] The above Ar may represent, preferably, a substituted or unsubstituted (C6-C25)aryl, a substituted or unsubstituted (5- to 25-membered)heteroaryl, or a substituted or unsub-

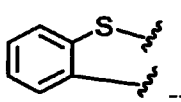
stituted di(C6-C25)arylamino, and more preferably, an unsubstituted (C6-C18)aryl, a (5- to 25-membered)heteroaryl unsubstituted or substituted with a (C1-C10)alkyl and/or a (C6-C12)aryl, or a di(C6-C25)arylamino unsubstituted or substituted with a (C1-C6)alkyl. According to one embodiment of the present disclosure, Ar may represent a substituted or unsubstituted phenyl, a substituted or unsubstituted naphthyl, a substituted or unsubstituted biphenyl, a substituted or unsubstituted terphenyl, a substituted or unsubstituted fluorenyl, a substituted or unsubstituted fluoranthenyl, a substituted or unsubstituted triazinyl, a substituted or unsubstituted pyridyl, a substituted or unsubstituted pyrimidinyl, a substituted or unsubstituted benzothienopyrimidinyl, a substituted or unsubstituted acenaphthopyrimidinyl, a substituted or unsubstituted quinazolinyl, a substituted or unsubstituted benzoquinazolinyl, a substituted or unsubstituted quinoxalinyl, a substituted or unsubstituted benzoquinoxalinyl, a substituted or unsubstituted dibenzoquinoxalinyl, a substituted or unsubstituted quinolyl, a substituted or unsubstituted benzoquinolyl, a substituted or unsubstituted isoquinolyl, a substituted or unsubstituted benzoisoquinolyl, a substituted or unsubstituted benzothienoquinolyl, a substituted or unsubstituted benzofuroquinolyl, a substituted or unsubstituted triazolyl, a substituted or unsubstituted pyrazolyl, a substituted or unsubstituted carbazolyl, a substituted or unsubstituted dibenzothiophenyl, a substituted or unsubstituted benzothiophenyl, a substituted or unsubstituted dibenzofuranyl, a substituted or unsubstituted benzofuranyl, a substituted or unsubstituted naphthyridinyl, a substituted or unsubstituted benzothiazolinyl, a substituted or unsubstituted phenanthroimidazolyl, a substituted or unsubstituted diphenylamino, a substituted or unsubstituted phenylbiphenylamino, a substituted or unsubstituted fluorenylphenylamino, a substituted or unsubstituted dibenzothiophenylphenylamino, or a substituted or unsubstituted dibenzofuranylphenylamino. According to another embodiment of the present disclosure, Ar may represent a phenyl unsubstituted or substituted with at least one of deuterium and naphthyl, an unsubstituted naphthyl, an unsubstituted biphenyl, a fluorenyl substituted with at least one methyl, an unsubstituted fluoranthenyl, a triazinyl unsubstituted or substituted with at least one of phenyl and naphthyl, a pyridyl unsubstituted or substituted with at least one phenyl, a pyrimidinyl unsubstituted or substituted with at least one phenyl, a quinazolinyl unsubstituted or substituted with at least one phenyl, an isoquinolyl substituted with at least one phenyl, a carbazolyl unsubstituted or substituted with at least one phenyl, an unsubstituted dibenzothiophenyl, an unsubstituted dibenzofuranyl, a naphthyridinyl substituted with at least one phenyl, an unsubstituted diphenylamino, an unsubstituted phenylbiphenylamino, a dimethylfluorenylphenylamino, a benzothienopyrimidinyl substituted with at least one phenyl, an unsubstituted benzothienoquinolyl, an unsubstituted benzofuroquinolyl, a benzoquinazolinyl substituted with at least one phenyl, a benzothiazolinyl substituted with at

least one phenyl, a benzoquinoxalinyl substituted with at least one phenyl, an unsubstituted dibenzoquinoxalinyl, a phenanthroimidazolyl substituted with at least one phenyl, an unsubstituted dibenzothiophenylphenylamino, an unsubstituted dibenzofuranylphenylamino, a nitrogen-containing 17-membered heteroaryl substituted with at least one methyl, a 25-membered heteroaryl containing nitrogen and oxygen, or an acenaphthopyrimidinyl substituted with at least one phenyl.

[30] The above R_1 may represent, preferably, a substituted or unsubstituted (C6-C25)aryl, or a substituted or unsubstituted (3- to 25-membered)heteroaryl; or adjacent R_1's may be linked to each other to form a substituted or unsubstituted, mono- or polycyclic, (3- to 25-membered) alicyclic or aromatic ring, or the combination thereof, whose carbon atom(s) may be replaced with at least one heteroatom selected from nitrogen, oxygen, and sulfur; more preferably, a substituted or unsubstituted (C6-C18)aryl, or a substituted or unsubstituted (5- to 18-membered)heteroaryl; or adjacent R_1's may be linked to each other to form a substituted or unsubstituted, mono- or polycyclic, (3- to 18-membered) aromatic ring, whose carbon atom(s) may be replaced with at least one heteroatom selected from nitrogen, oxygen, and sulfur; and even more preferably, a (C6-C12)aryl unsubstituted or substituted with a (5- to 18-membered)heteroaryl, or a (5- to 13-membered)heteroaryl unsubstituted or substituted with a (C6-C18)aryl; or adjacent R_1's may be linked to each other to form a substituted or unsubstituted, mono- or polycyclic, (3- to 10-membered) aromatic ring, whose carbon atom(s) may be replaced with at least one heteroatom selected from nitrogen, oxygen, and sulfur. According to one embodiment of the present disclosure, R_1 may represent a phenyl unsubstituted or substituted with diphenyltriazinyl, a diphenyltriazinyl, a quinazolinyl substituted with a phenyl(s), or an unsubstituted pyridyl; or adjacent R_1's may be linked to each other to form an unsubstituted benzene ring, an indene ring substituted with at least one of methyl and phenyl, an unsubstituted pyridine ring, an unsubstituted benzothiophene ring, an unsubstituted benzofuran ring, or an indole ring substituted with a phenyl(s) or a phenylquinoxalinyl(s).

[31] According to one embodiment of the present disclosure, two adjacent X_1 to X_{12} in formula 1 are CR_1, two adjacent R_1's may be linked to each other to form any one ring of the following formulas 2 to 6, and one or more of the rings may be formed in one compound represented by formula 1. For example, the ring may be a dibenzothiophene ring, a dibenzofuran ring, a naphthalene ring, a phenanthrene ring, or a substituted or unsubstituted carbazole ring.

[32]



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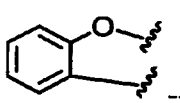

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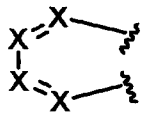

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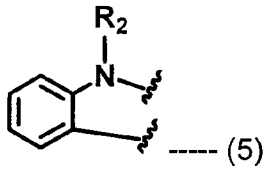
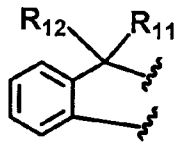
[33]  ----- (5)  ----- (6)

[34] In formulas 2 to 6, ~ represents a connecting site between C and R_1 in CR_1.

[35] In formula 4, X represents N or CH. According to one embodiment of the present disclosure, all of X may represent CH. According to another embodiment of the present disclosure, any one of X may represent N.

[36] In formula 5, R_2 represents hydrogen, deuterium, a halogen, a cyano, 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 (C1-C30)alkoxy, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a substituted or unsubstituted mono- or di- (C1-C30)alkylamino, a substituted or unsubstituted mono- or di- (C6-C30)arylamino, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino; preferably, a substituted or unsubstituted (C6-C25)aryl, or a substituted or unsubstituted (5- to 25-membered)heteroaryl; more preferably, an unsubstituted (C6-C18)aryl, or a (5- to 18-membered)heteroaryl unsubstituted or substituted with a (C6-C18)aryl. According to one embodiment of the present disclosure, R_2 may represent an unsubstituted phenyl, or a quinoxalinyl substituted with a phenyl(s).

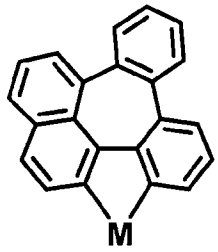
[37] In formula 6, R_{11} and R_{12}, each independently, represent hydrogen, deuterium, a halogen, a cyano, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked to each other to form a ring. Preferably, R_{11} and R_{12}, each independently, represent hydrogen, a substituted or unsubstituted (C1-C6)alkyl, or a substituted or unsubstituted (C6-C12)aryl; or may be linked to each other to form a substituted or unsubstituted, mono- or polycyclic, (5- to 10-membered) alicyclic or aromatic ring, or the combination thereof. More preferably, R_{11} and R_{12}, each independently, represent hydrogen, an unsubstituted (C1-C6)alkyl, or an unsubstituted (C6-C12)aryl; or may be linked to each other to form a spiro ring.

[38] In formula 1, a represents an integer of 1 or 2, where if a is 2, each of Ar may be the same or different.

[39] The compound represented by formula 1 may be represented by any one of the

following formulas 7 to 10:

[40]



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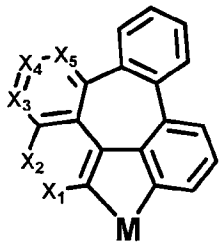
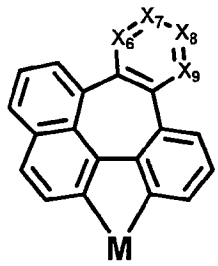


----- (8)

[41]



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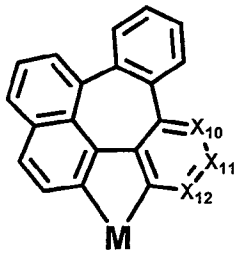


----- (10)

[42] wherein, X_1 to X_{12} and M are as defined in formula 1.

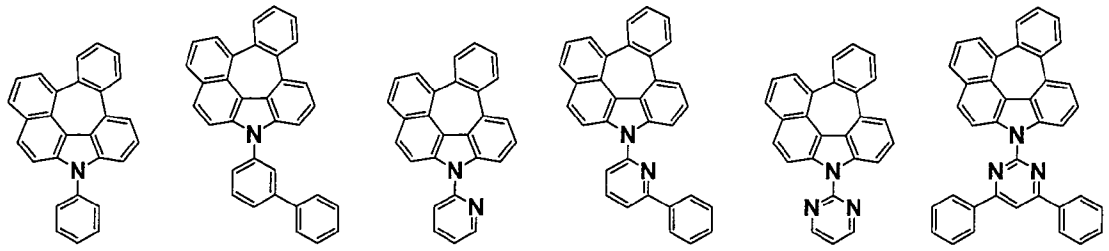
[43] According to one embodiment of the present disclosure, at least one of X_1 to X_5, at least one of X_6 to X_9, and at least one of X_{10} to X_{12} represent N or CR_1, in which R_1, each independently, represents a substituted or unsubstituted (C6-C25)aryl, or a substituted or unsubstituted (3- to 25-membered)heteroaryl; or may be linked to an adjacent substituent to form a substituted or unsubstituted, mono- or polycyclic, (3- to 25-membered) alicyclic or aromatic ring, or the combination thereof, whose carbon atom(s) may be replaced with at least one heteroatom selected from nitrogen, oxygen, and sulfur.

[44] According to one embodiment of the present disclosure, Ar in formula 1 of the first host compound represents a substituted or unsubstituted (3- to 30-membered)heteroaryl, and Ar in formula 1 of the second host compound represents a substituted or unsubstituted (3- to 30-membered)heteroaryl.

[45] According to another embodiment of the present disclosure, Ar in formula 1 of the first host compound represents a substituted or unsubstituted (3- to 30-membered)heteroaryl, and Ar in formula 1 of the second host compound represents 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, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino.

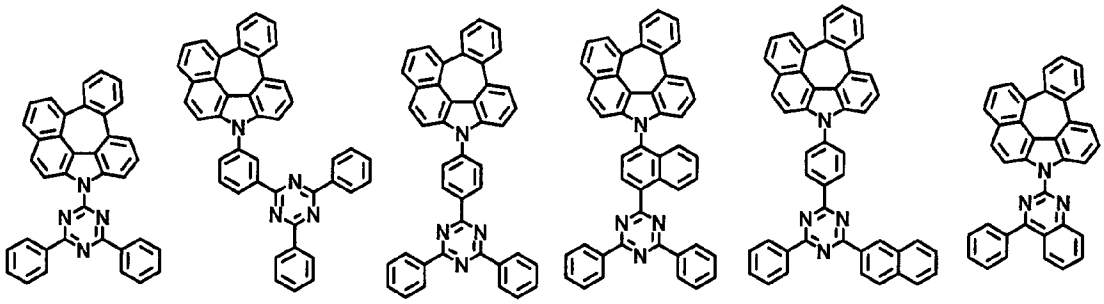
[46] The compound represented by formula 1 includes the following compounds, but is not limited thereto.

[47]



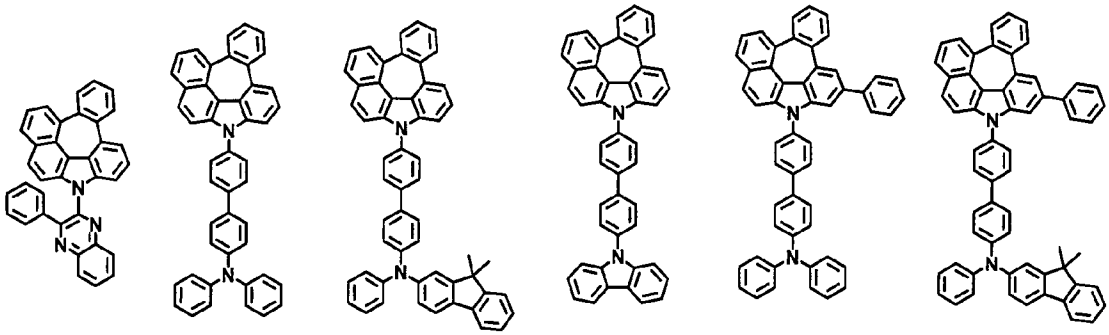
C-1 C-2 C-3 C-4 C-5 C-6

[48]



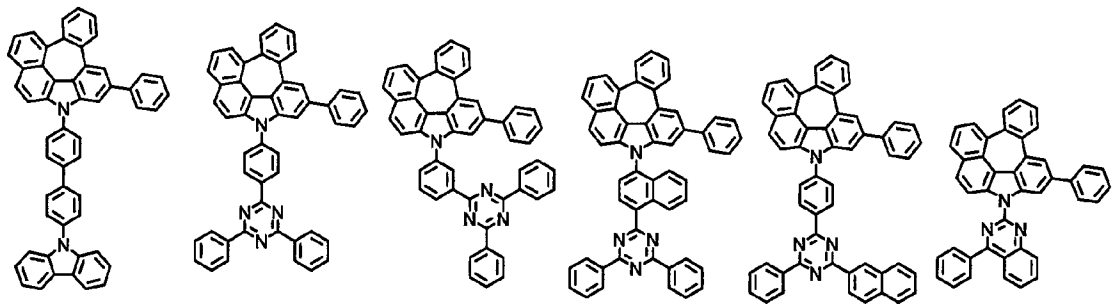
C-7 C-8 C-9 C-10 C-11 C-12

[49]



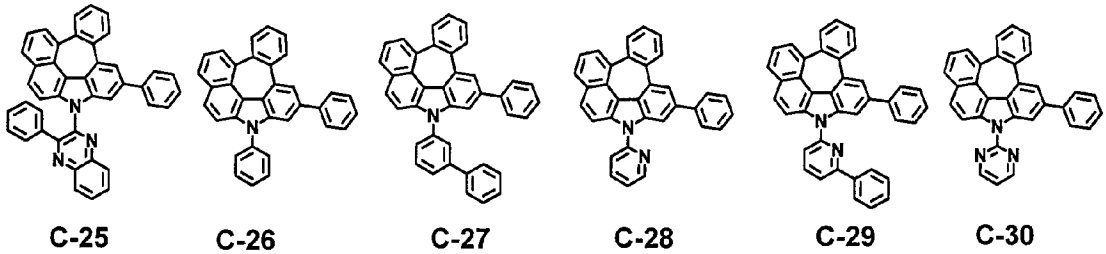
C-13 C-14 C-15 C-16 C-17 C-18

[50]



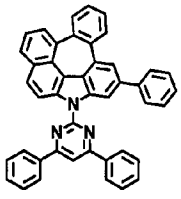
C-19 C-20 C-21 C-22 C-23 C-24

[51]



C-25 C-26 C-27 C-28 C-29 C-30

[52]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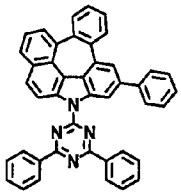
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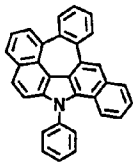
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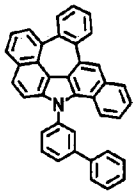
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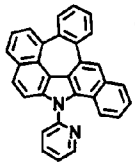
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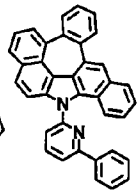
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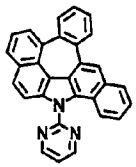
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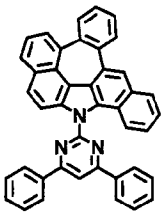
[53]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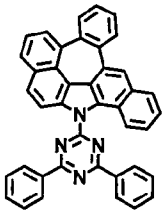
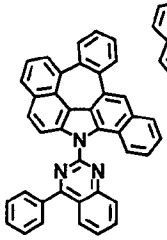

C-39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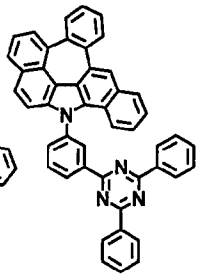
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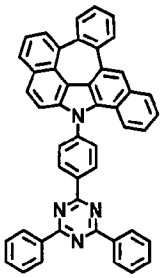
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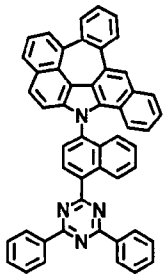
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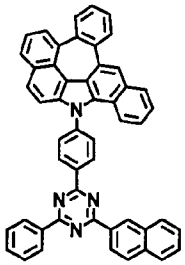
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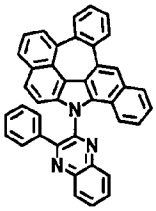
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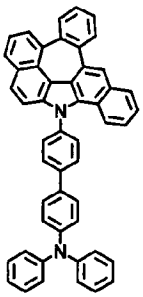
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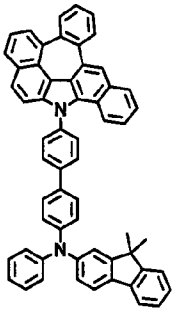
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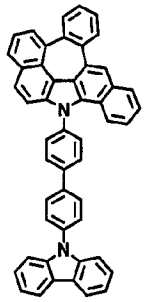
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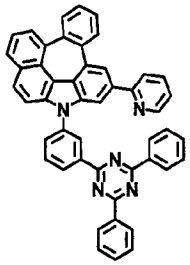
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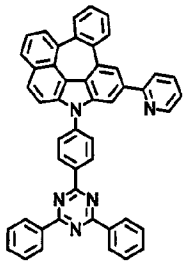
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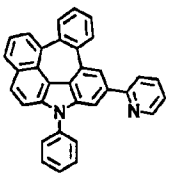
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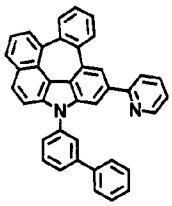
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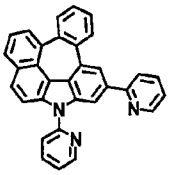
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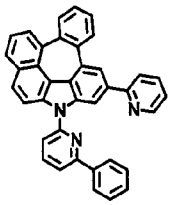
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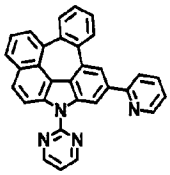
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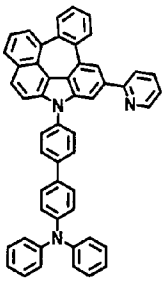
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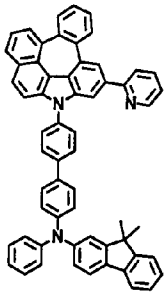
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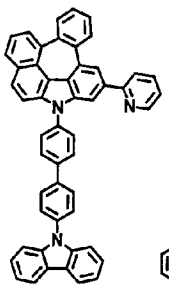
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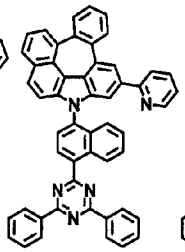
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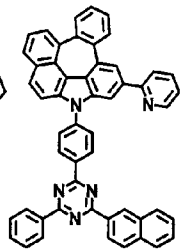
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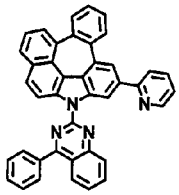
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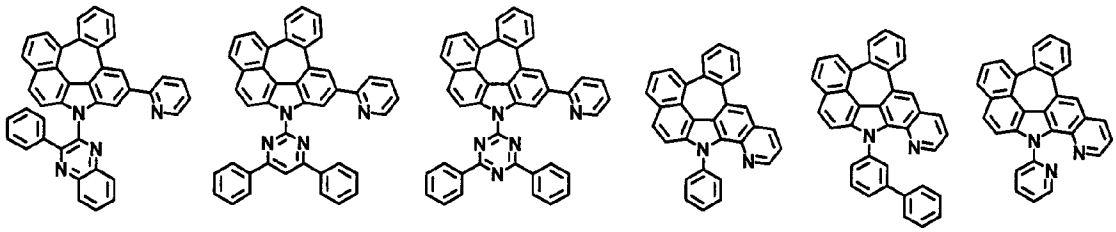

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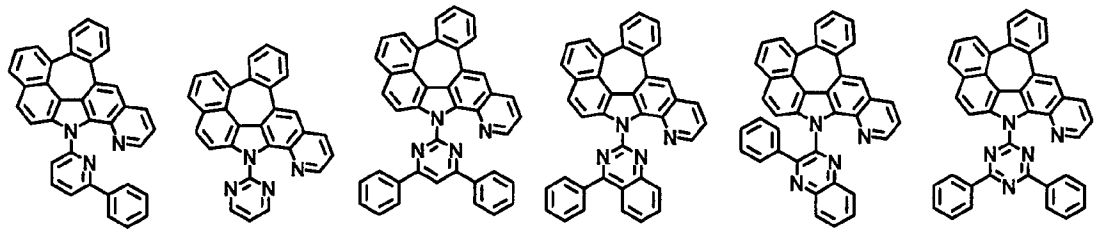

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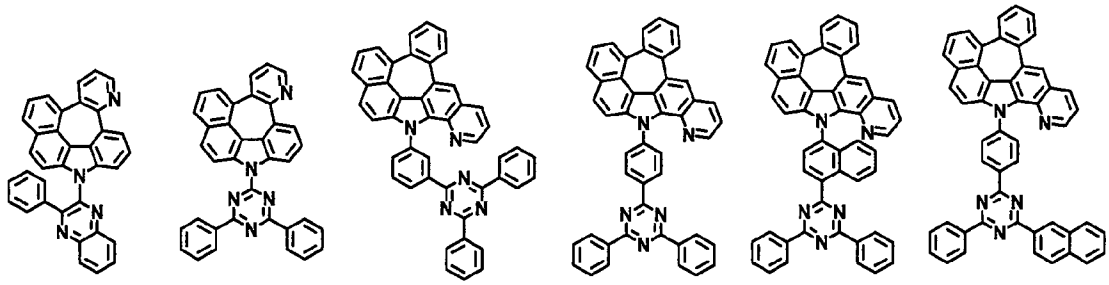

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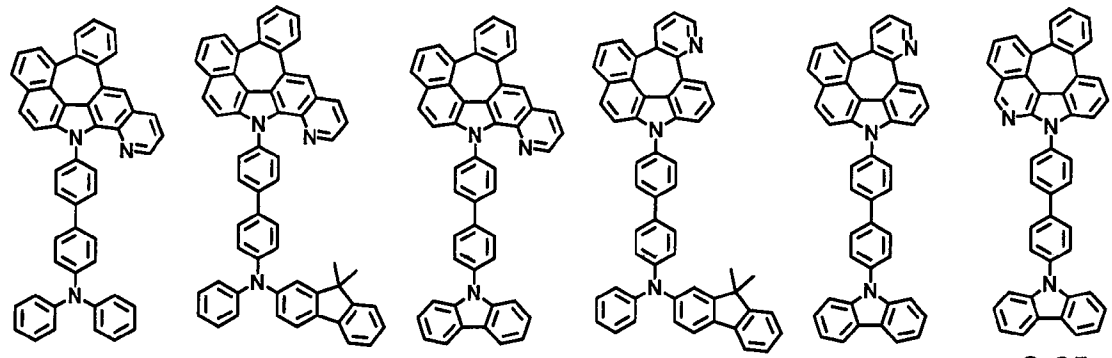

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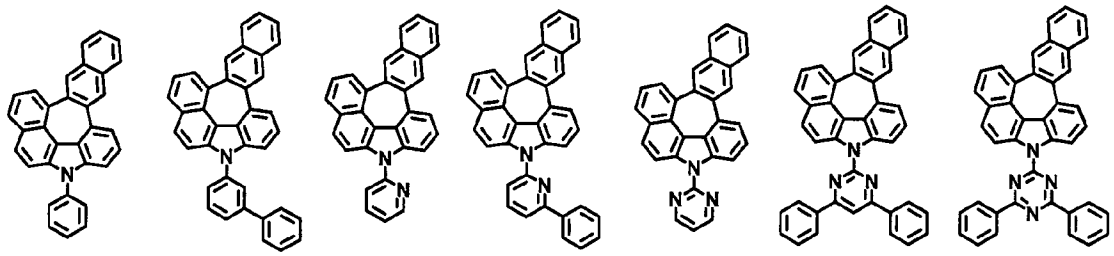

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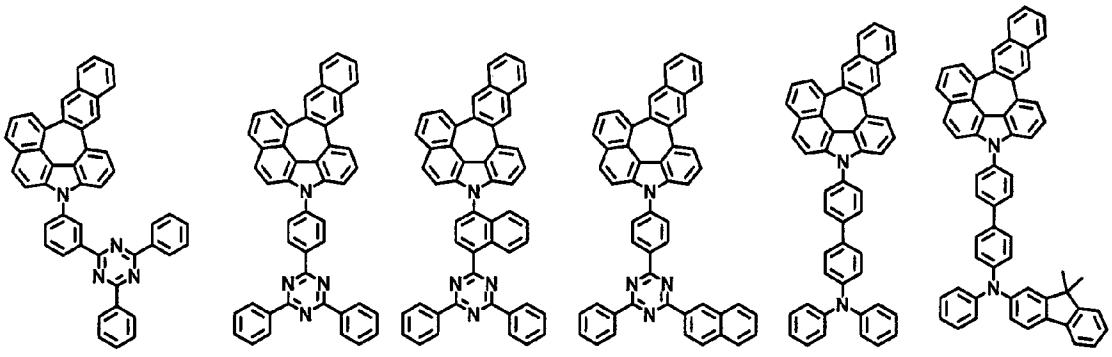

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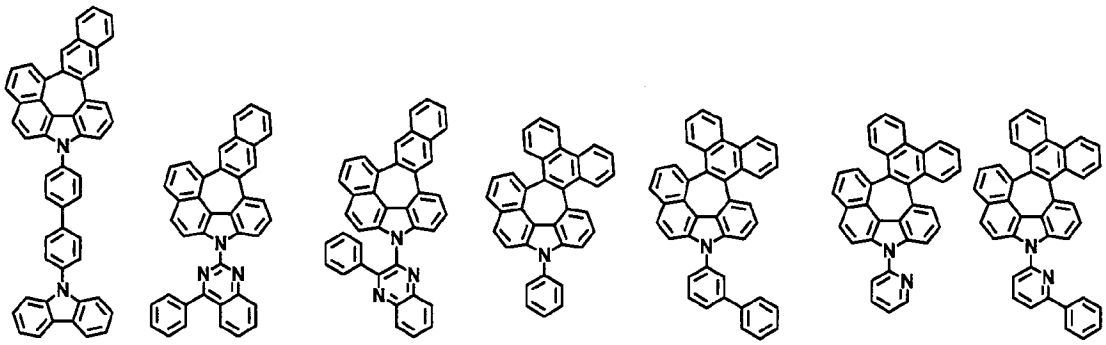

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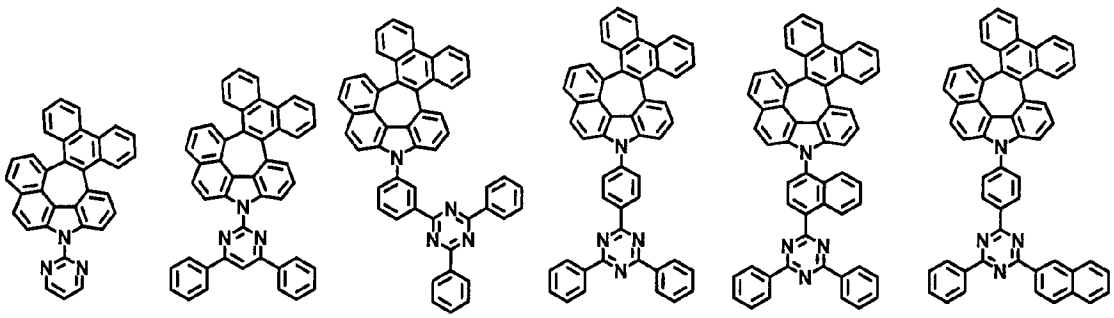

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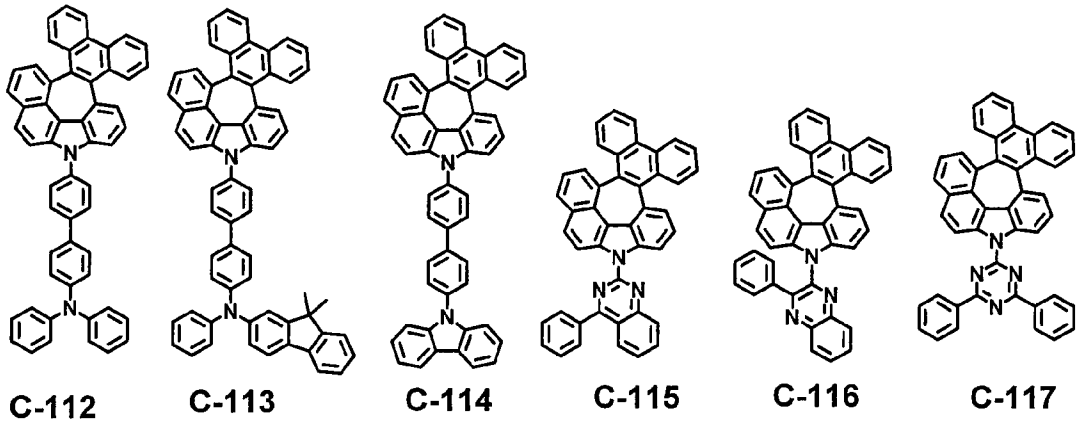

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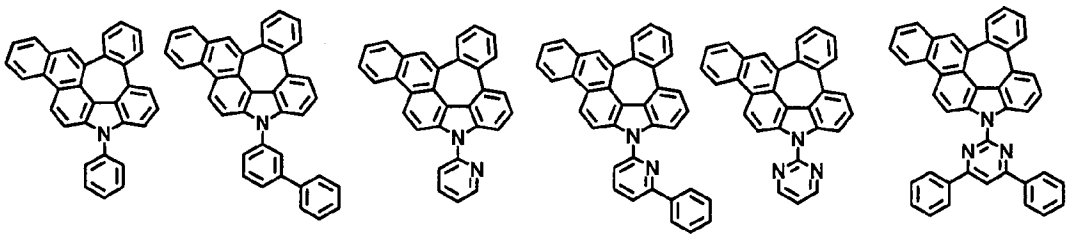

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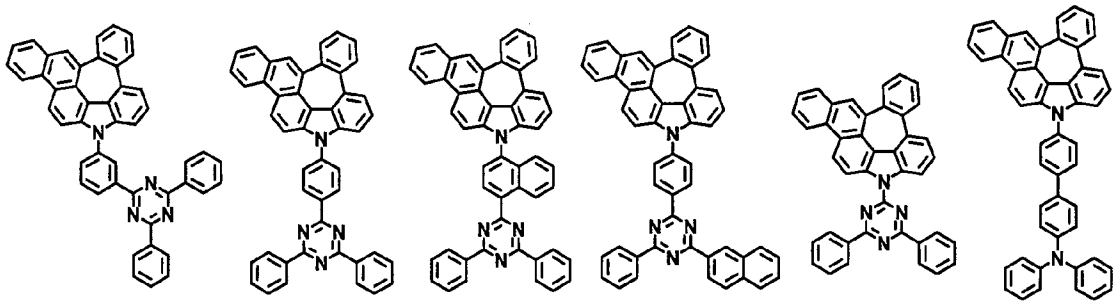

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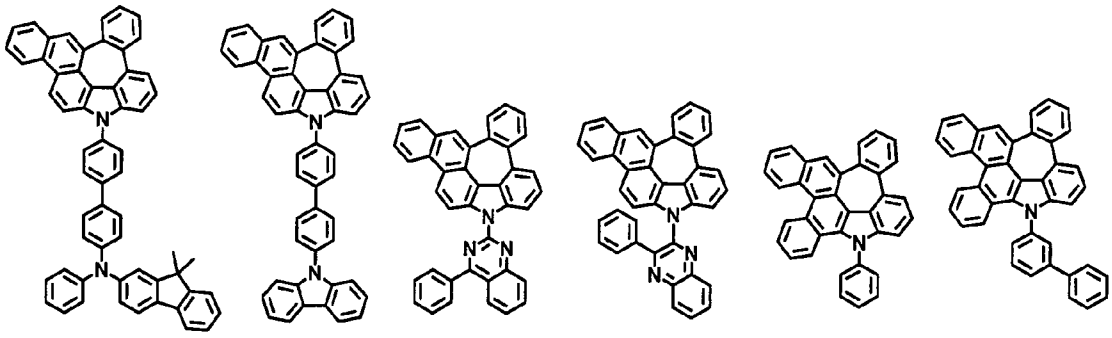

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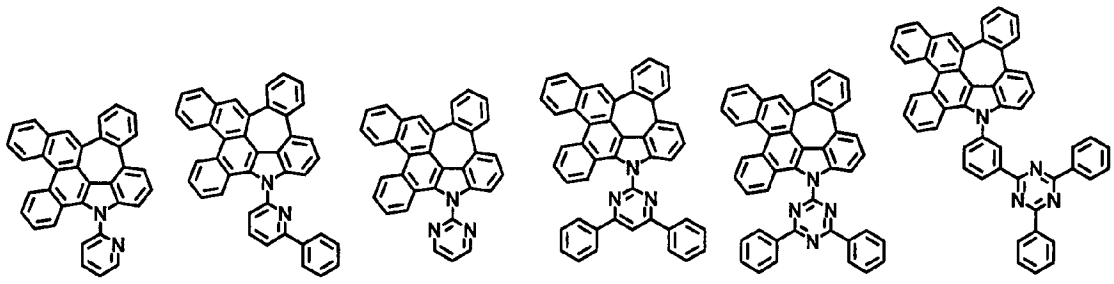

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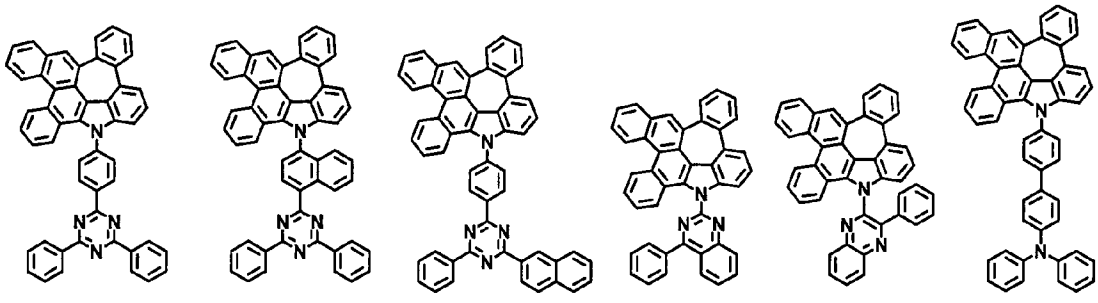

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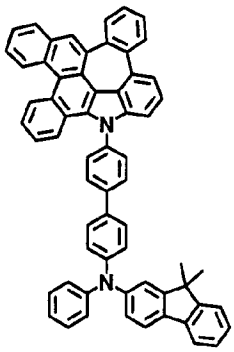

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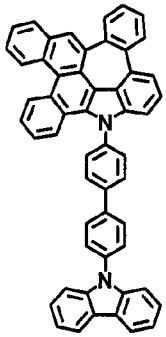

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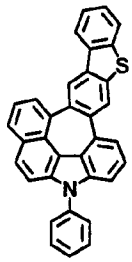

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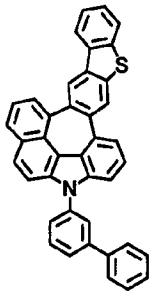

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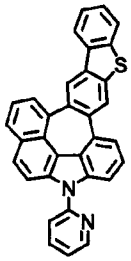

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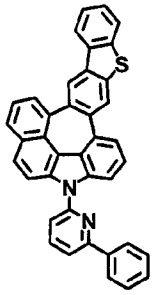

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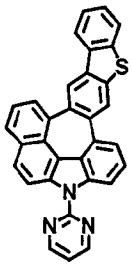

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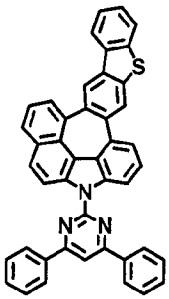

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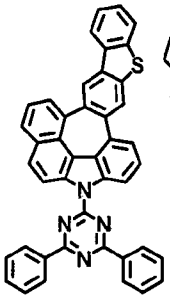

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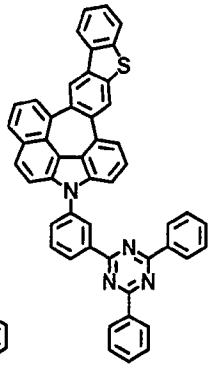

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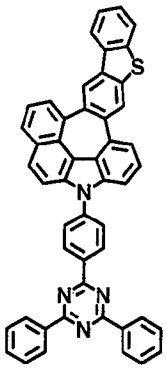

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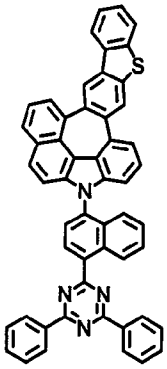

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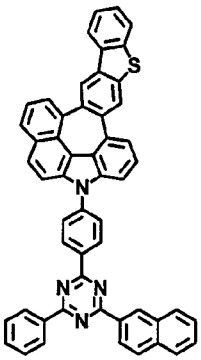

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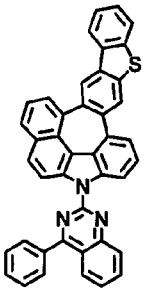

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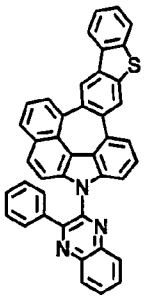

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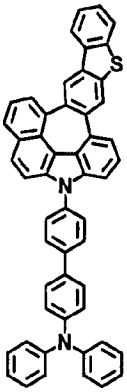
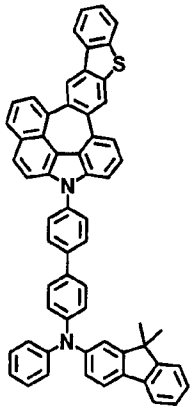
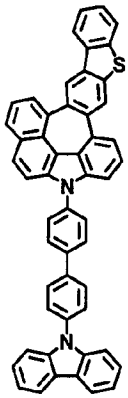


C-163



C-164



C-165

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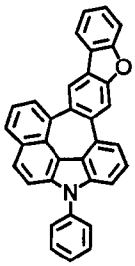

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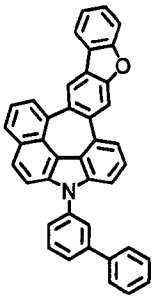

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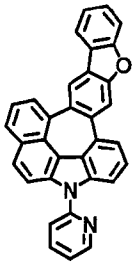

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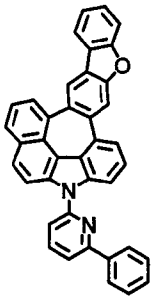

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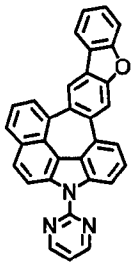

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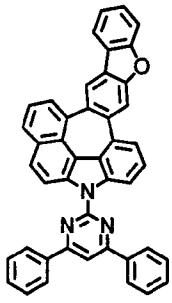

C-171

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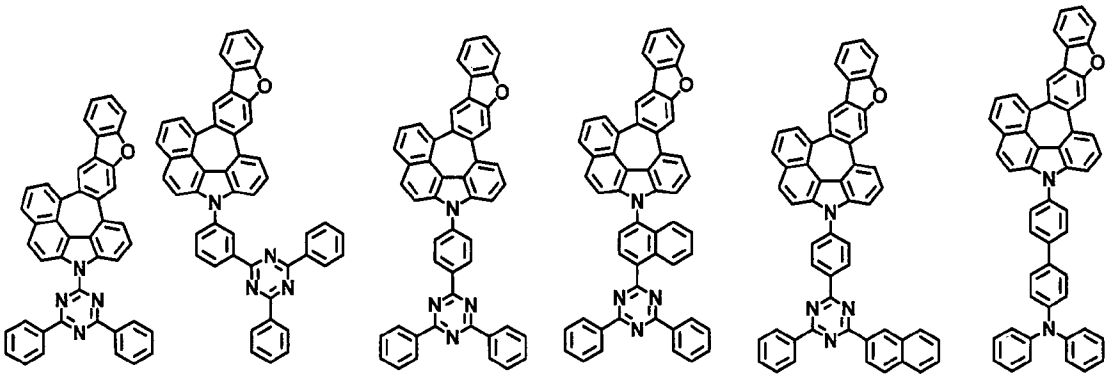

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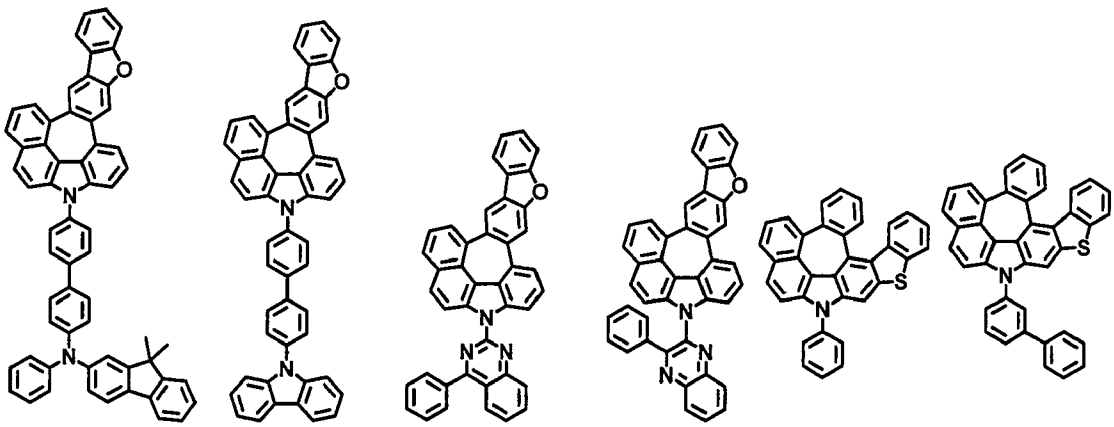

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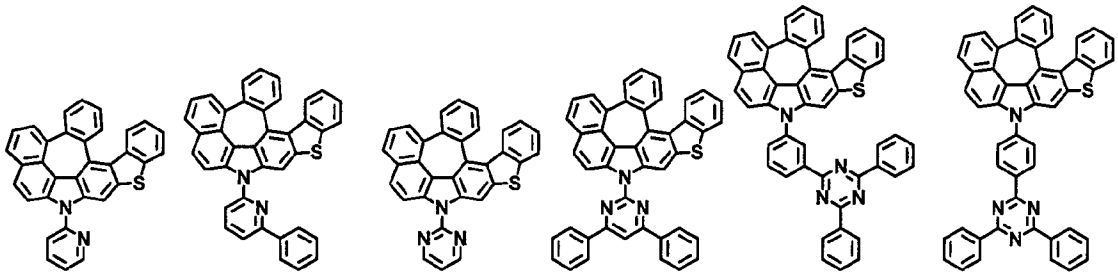

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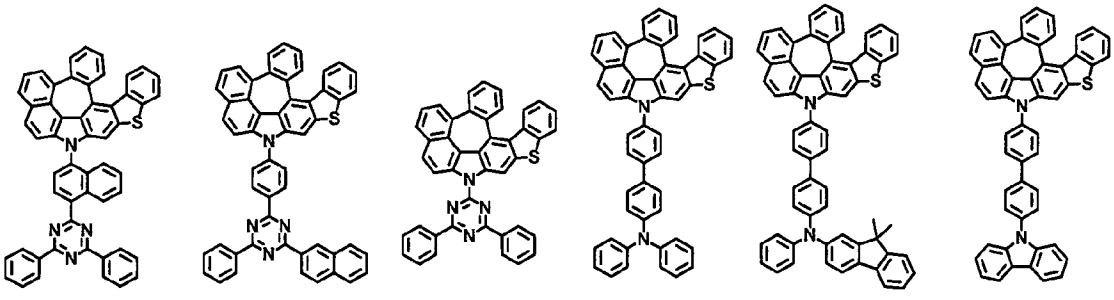

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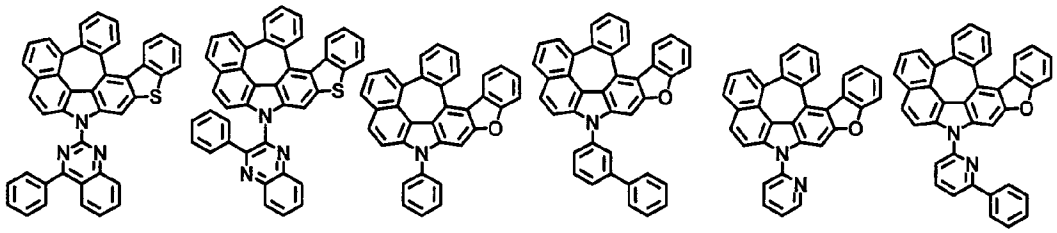

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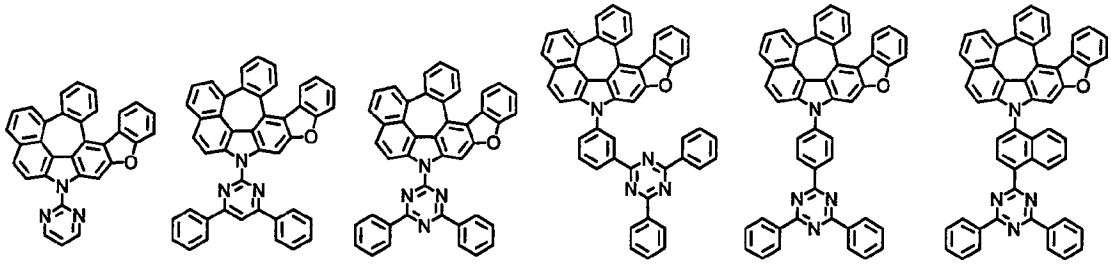

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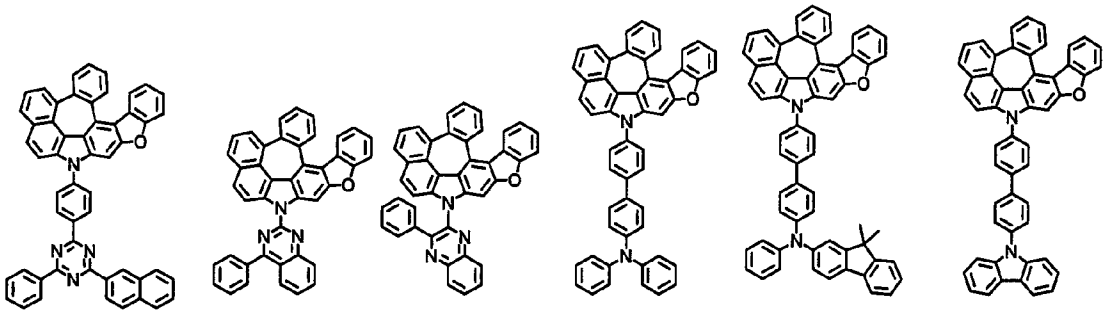

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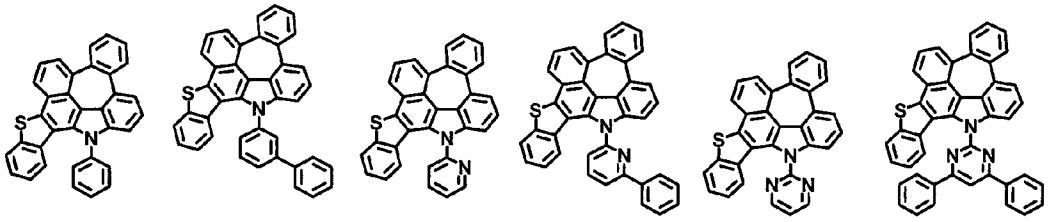

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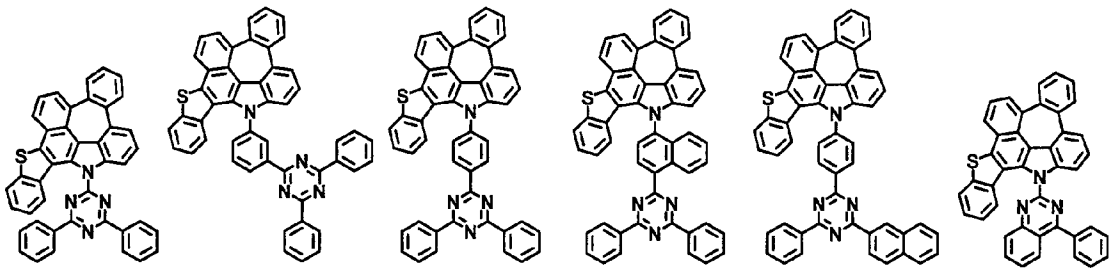

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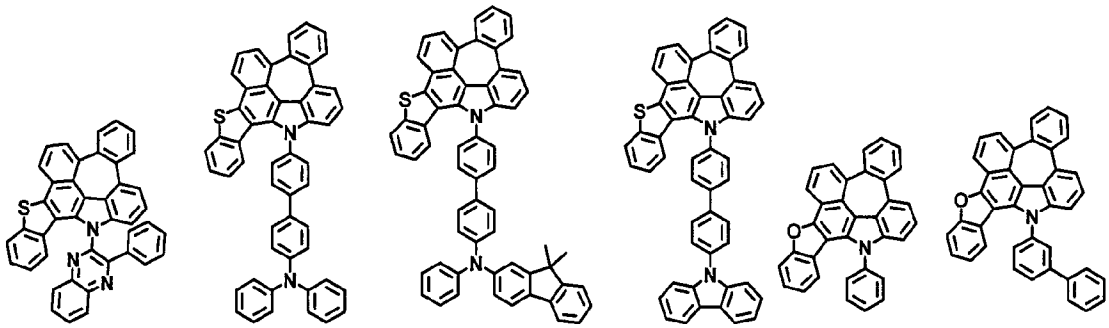

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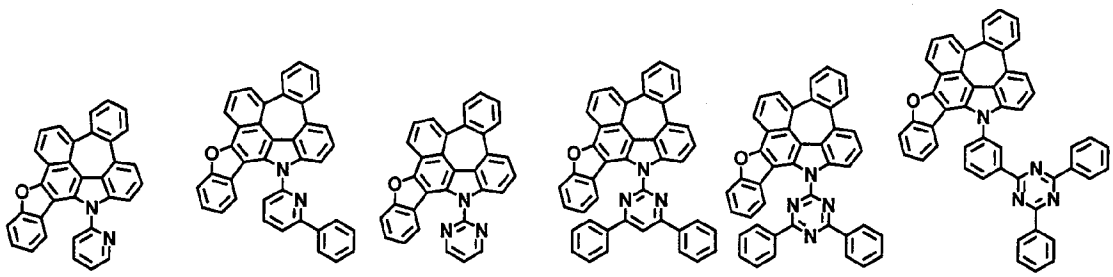

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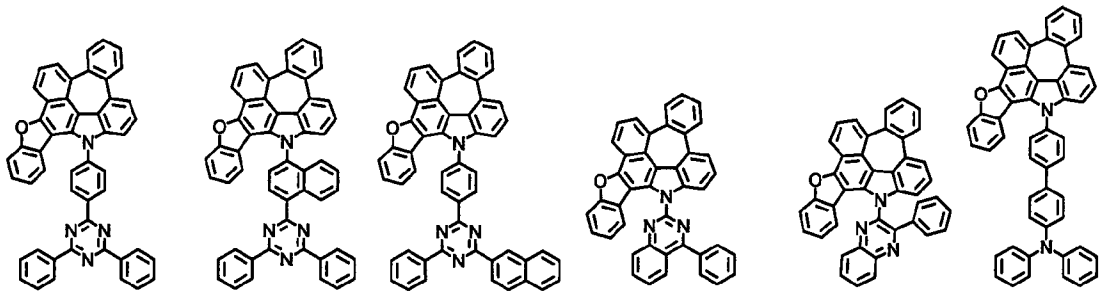

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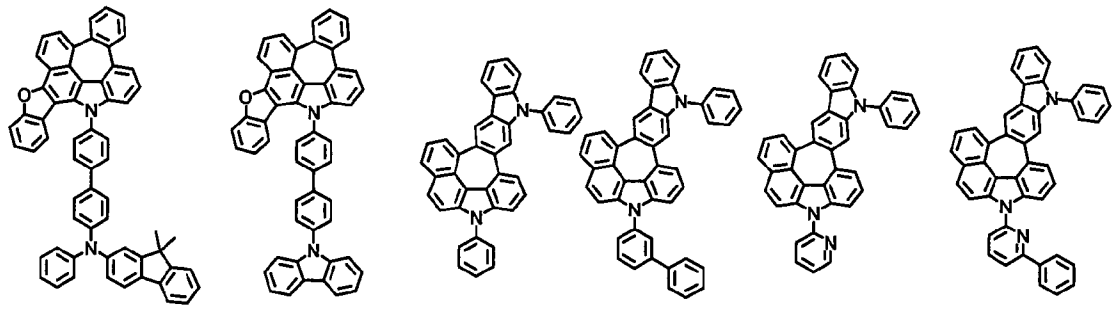

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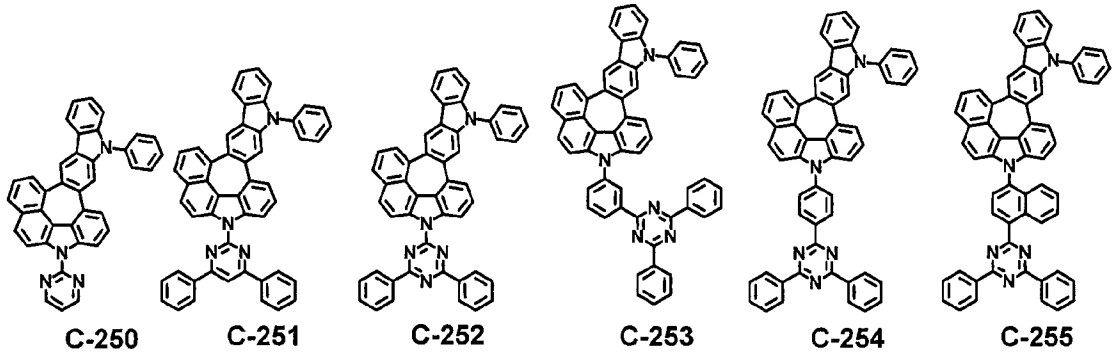

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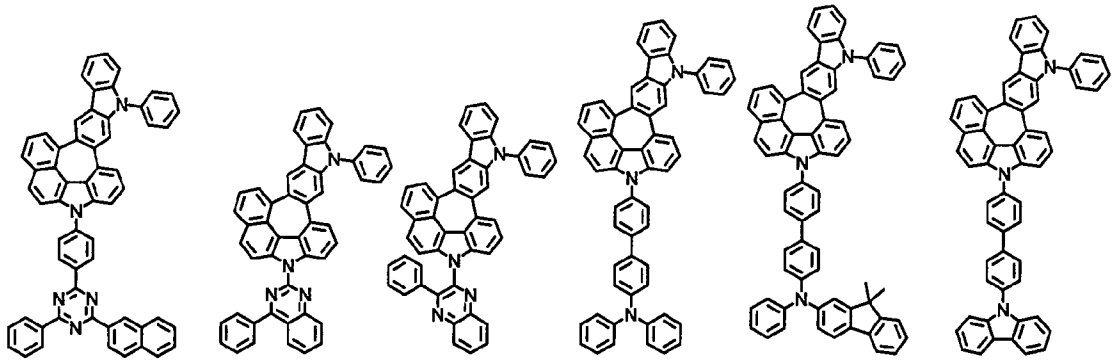

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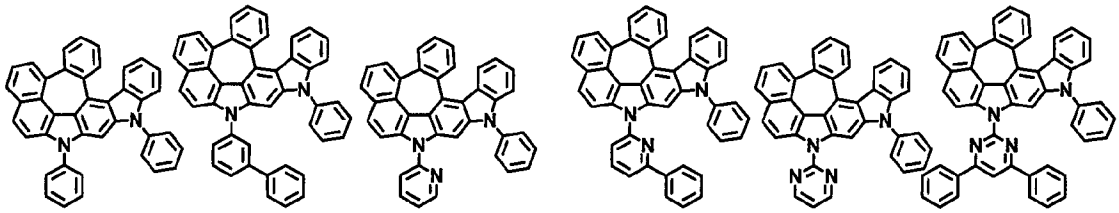

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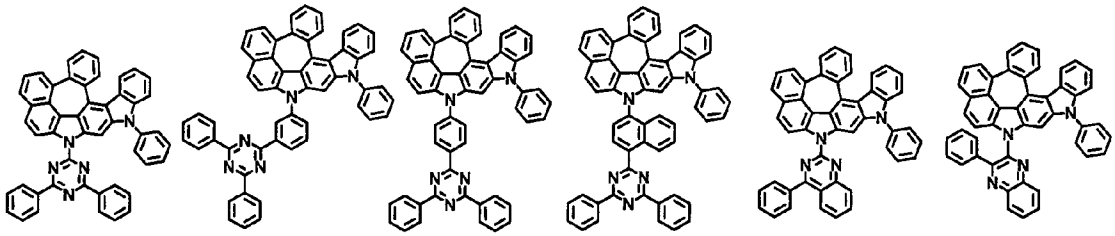

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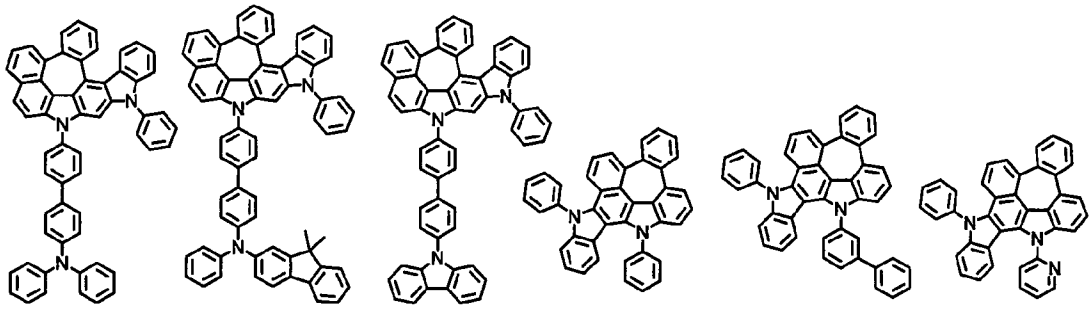

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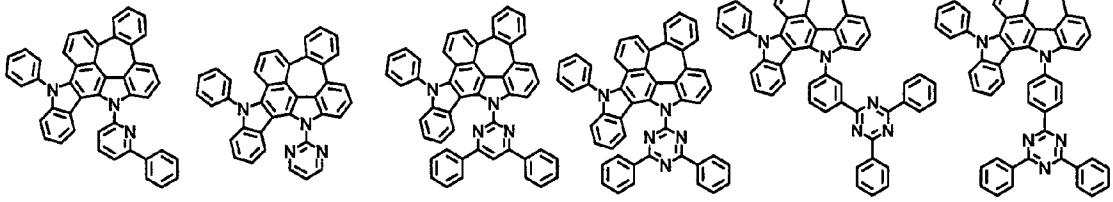

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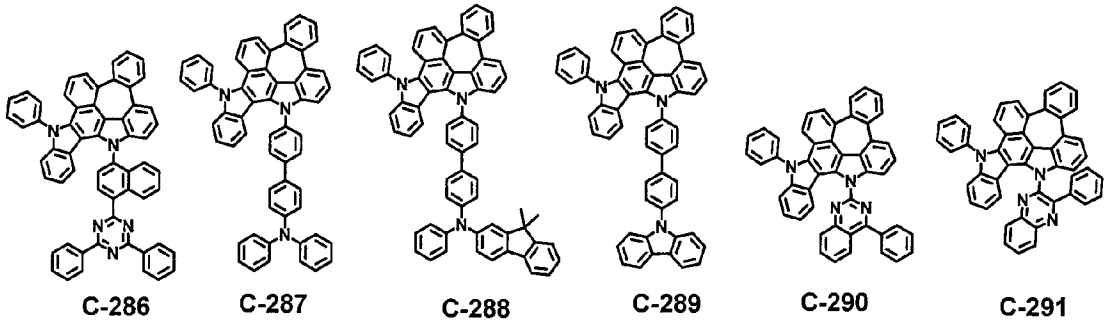

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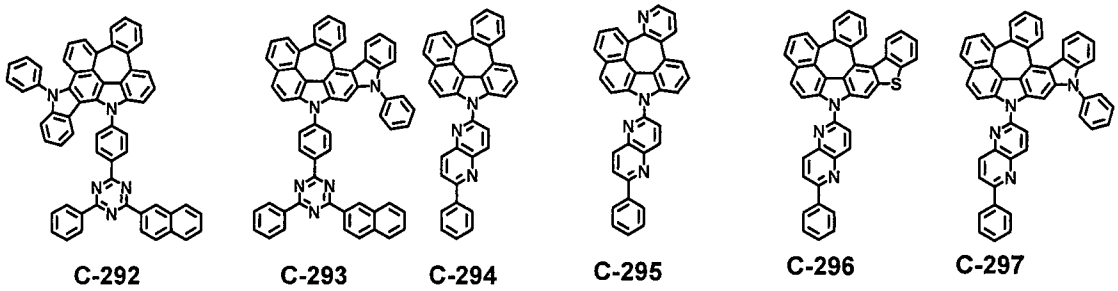

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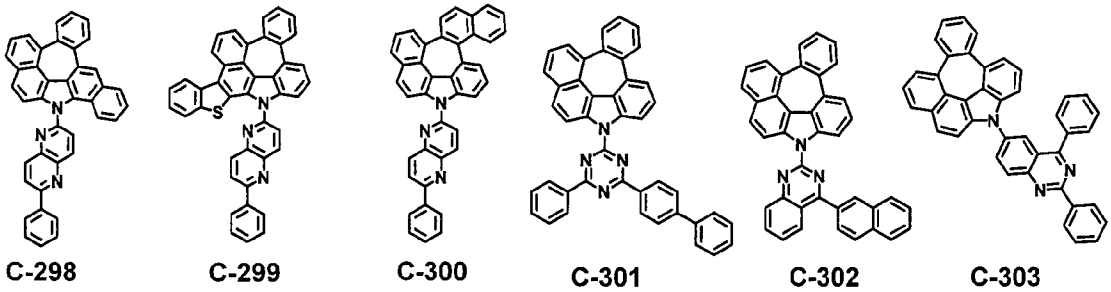

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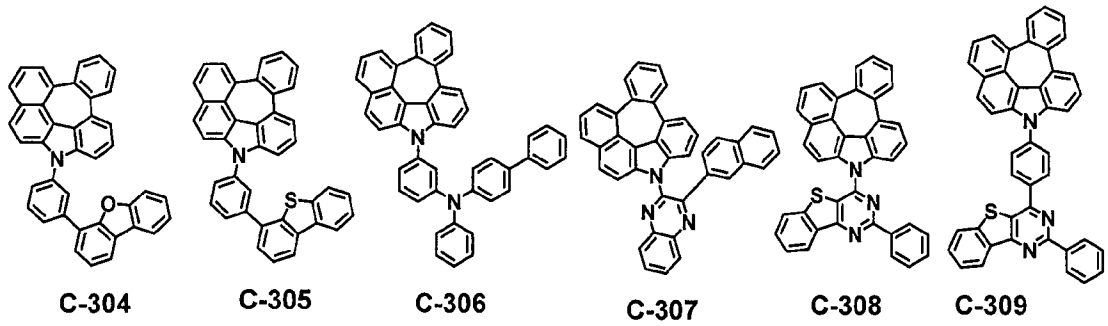

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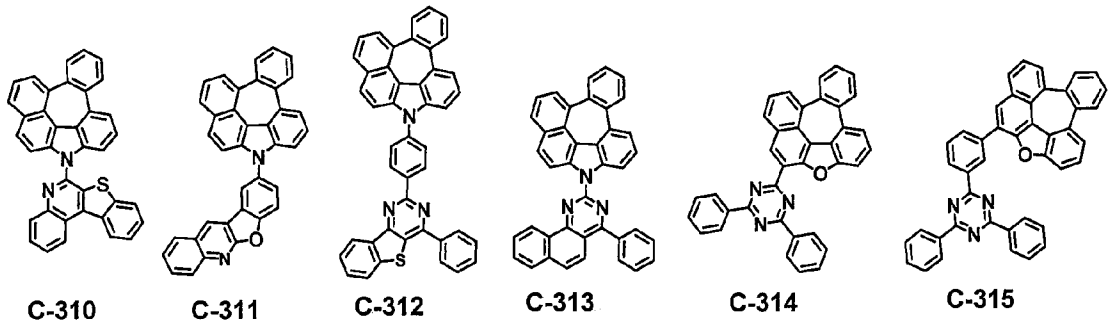

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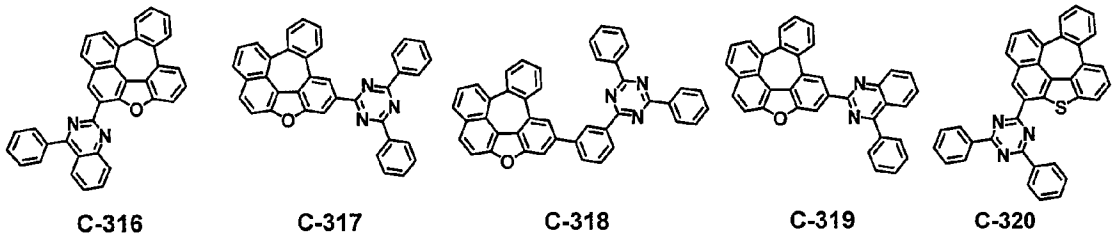

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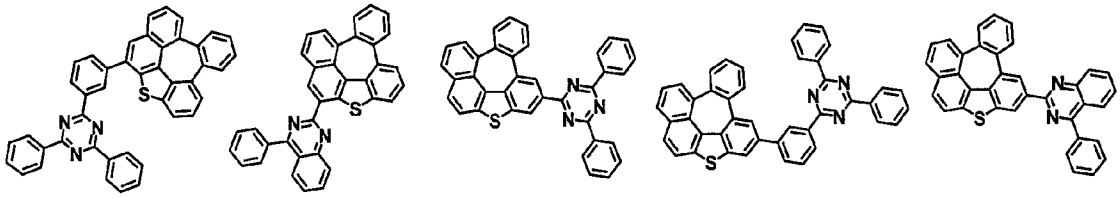

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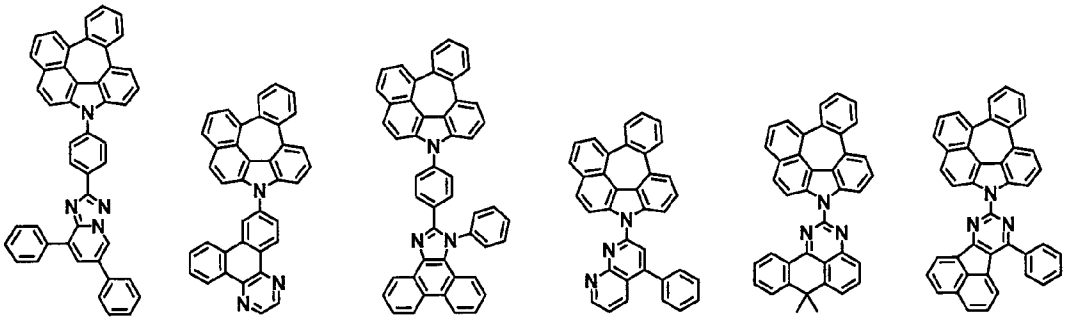

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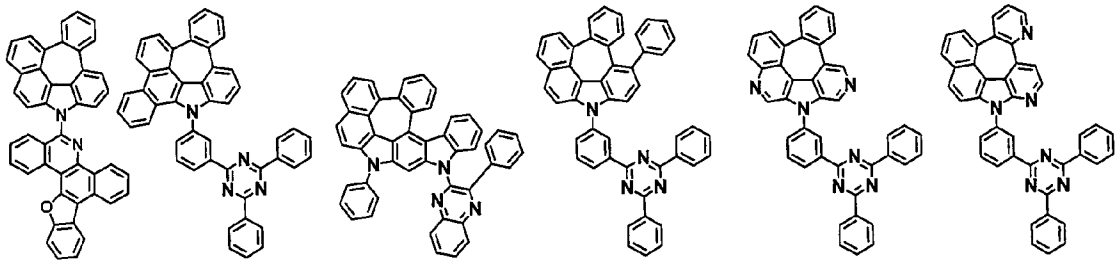

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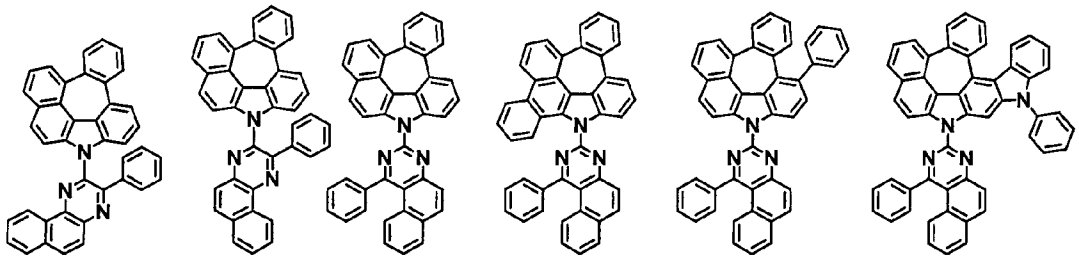

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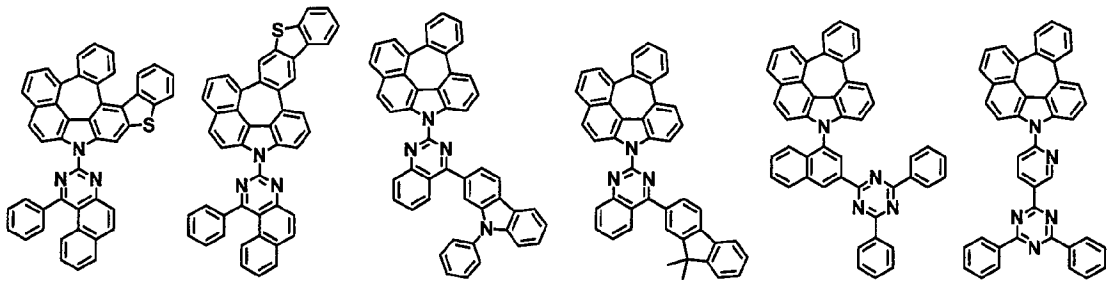

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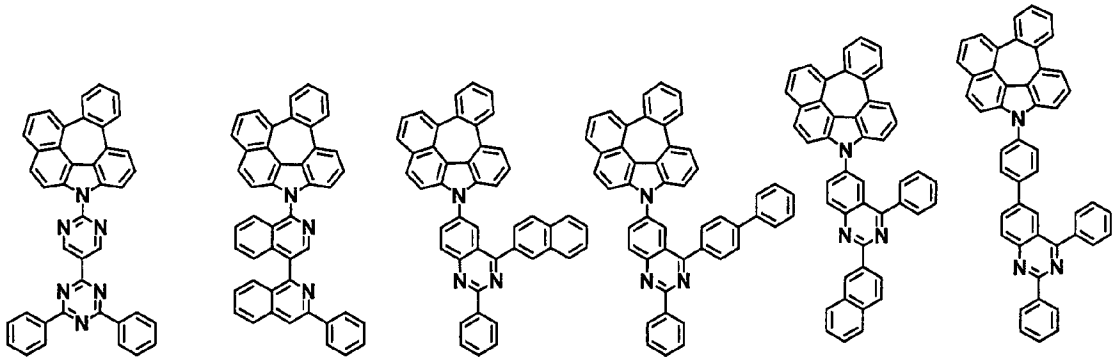

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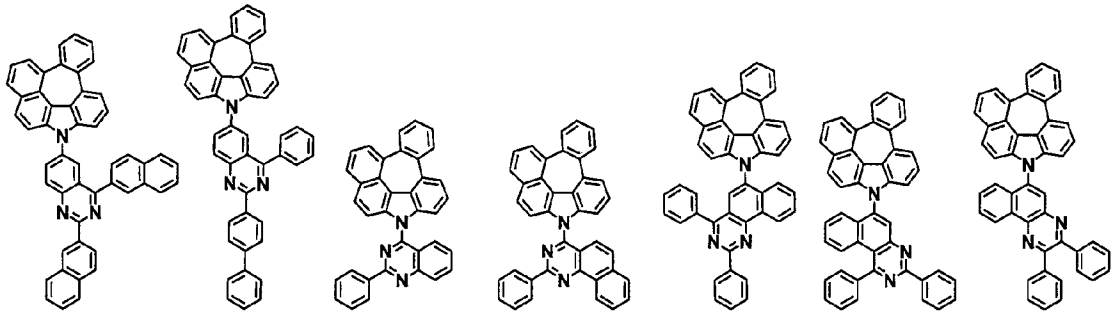

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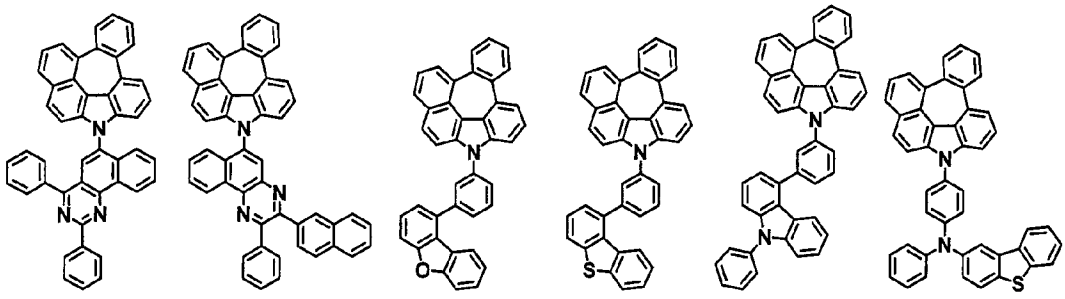

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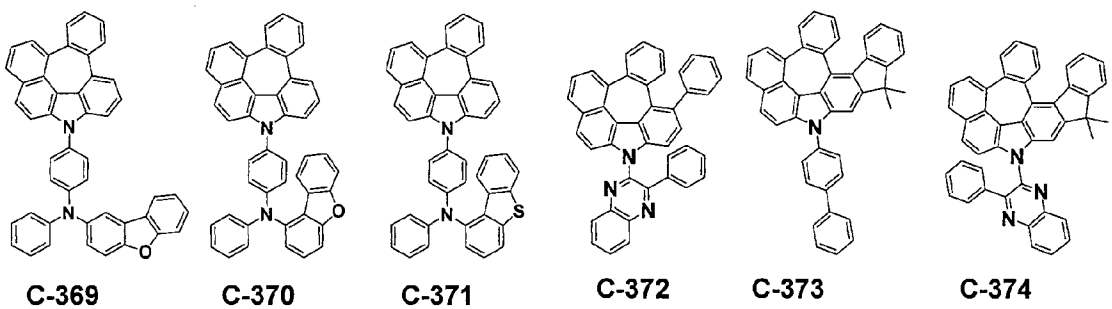

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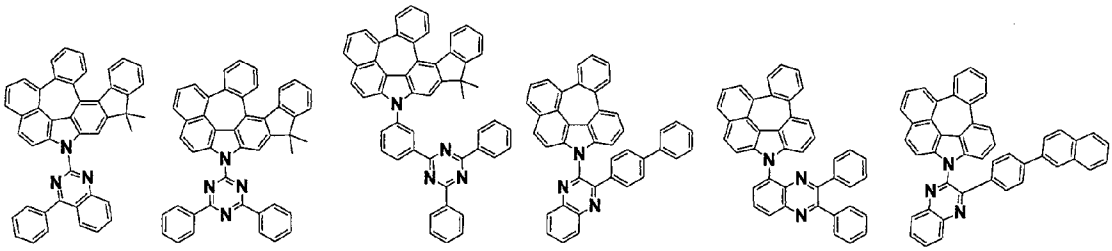

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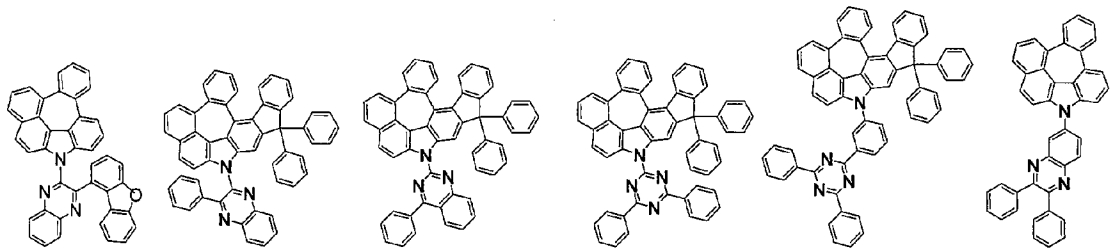

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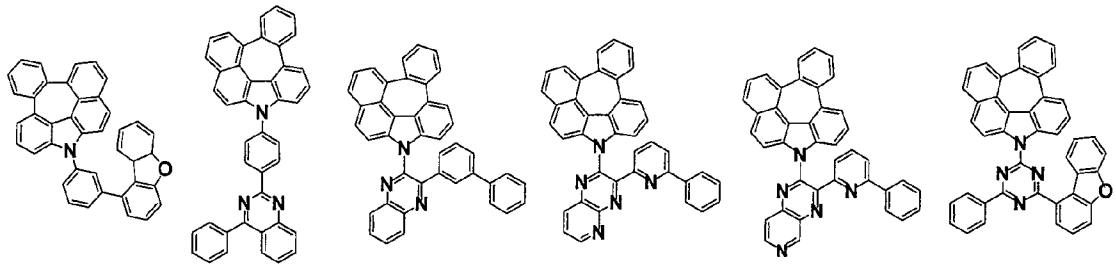

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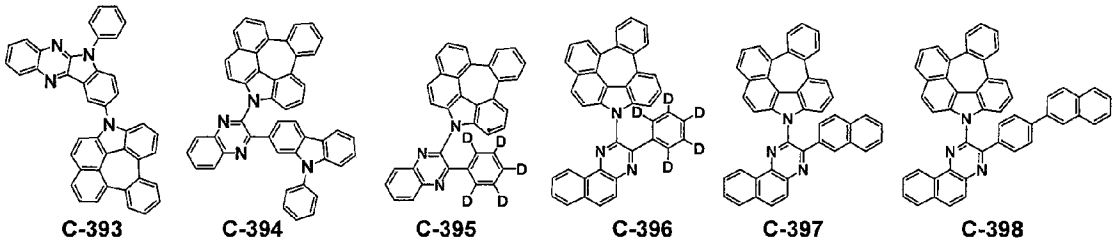

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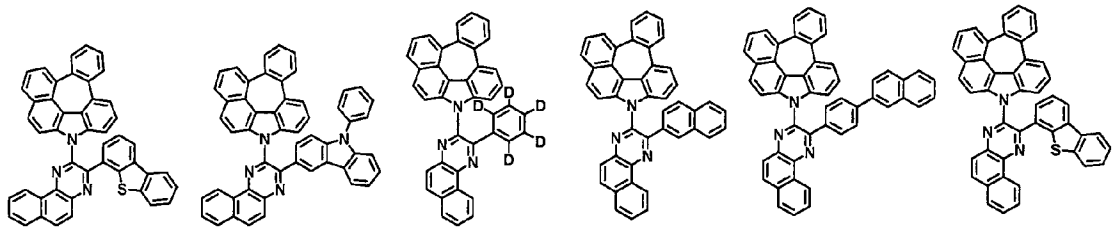

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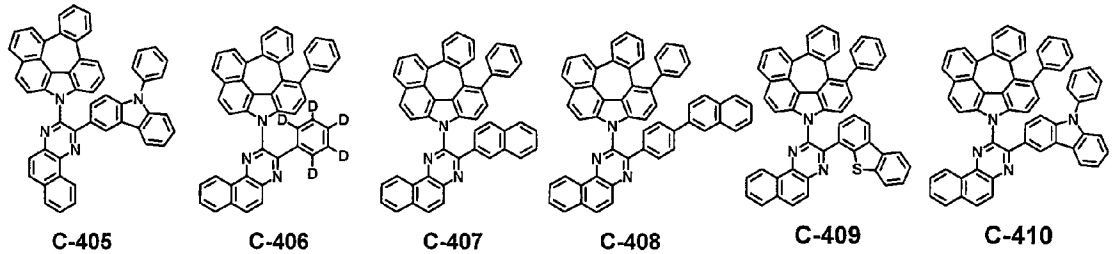

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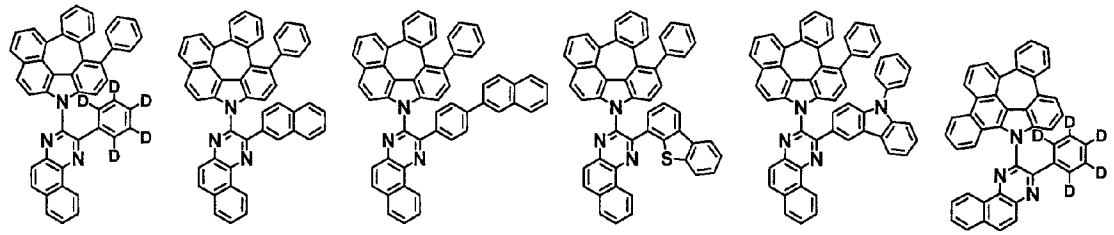
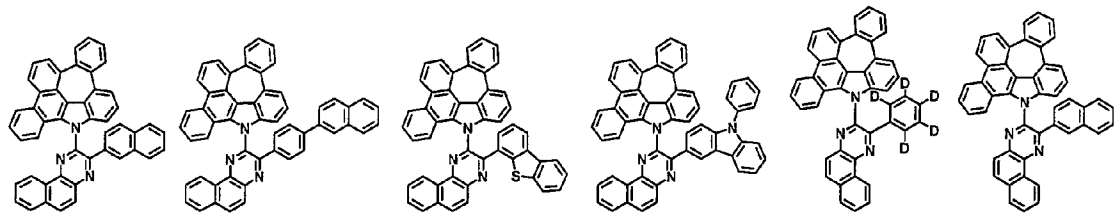


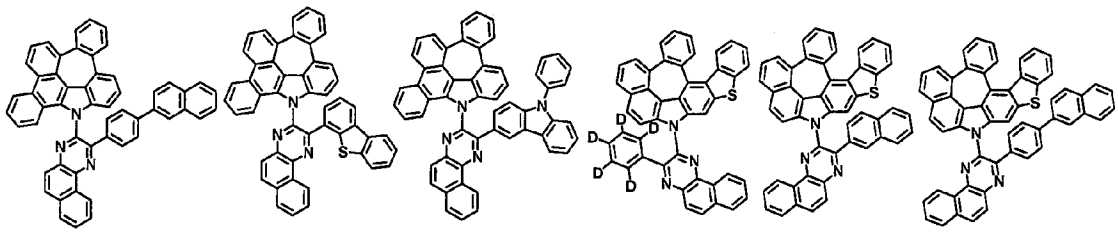
C-411 C-412 C-413 C-414 C-415 C-416

[116]



C-417 C-418 C-419 C-420 C-421 C-422

[117]



C-423 C-424 C-425 C-426 C-427 C-428

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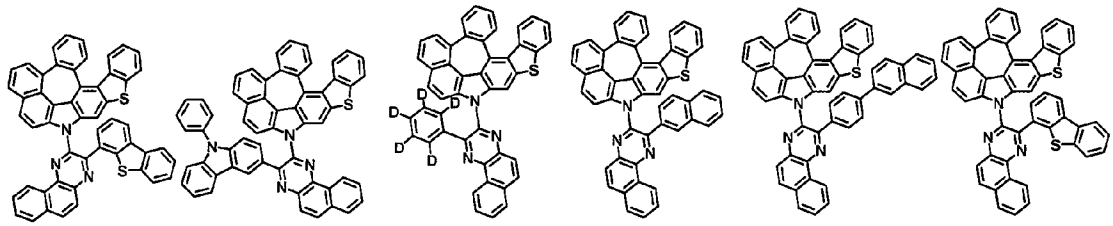
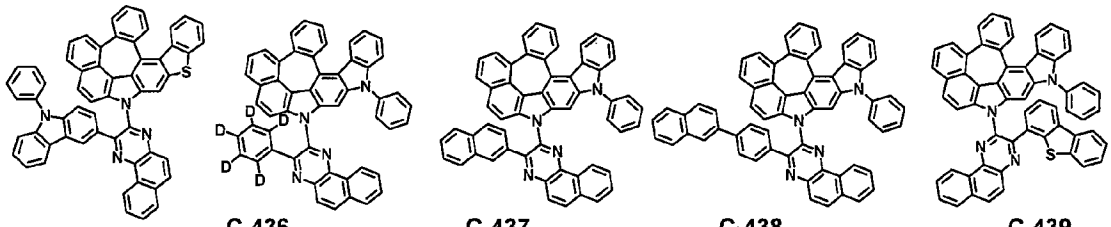


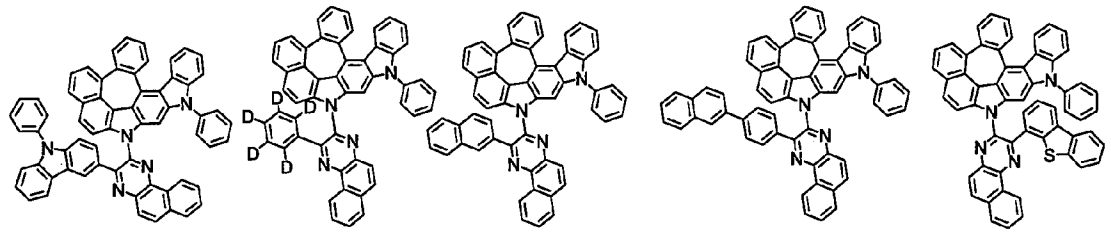
C-429 C-430 C-431 C-432 C-433 C-434

[119]



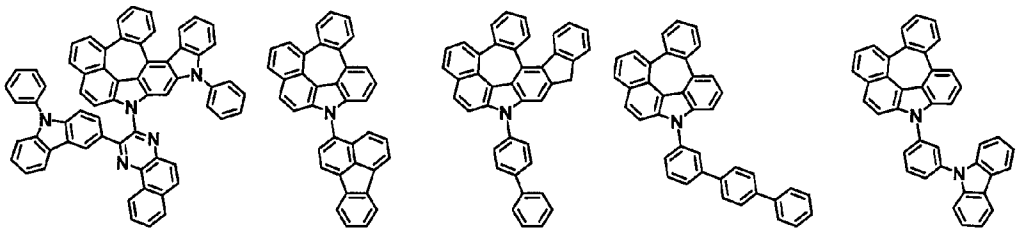
C-435 C-436 C-437 C-438 C-439

[120]



C-440 C-441 C-442 C-443 C-444

[121]



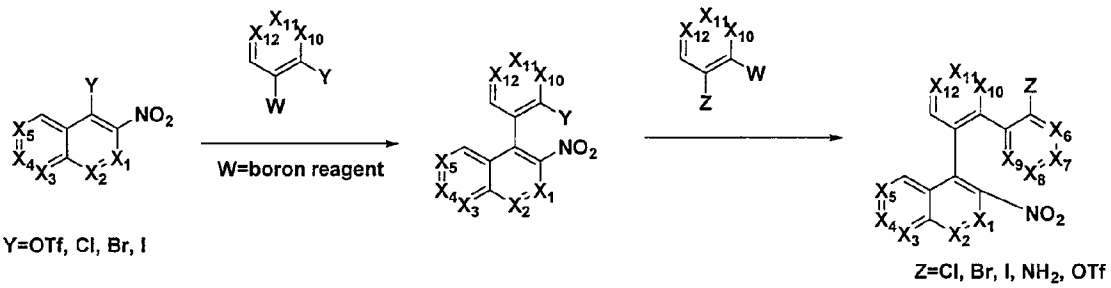
C-445 C-446 C-447 C-448 C-449

[122] Two or more of compounds C-1 to C-449 may be combined and used in an organic electroluminescent device.

[123] The compound of formula 1 according to the present disclosure may be produced by a synthetic method known to one skilled in the art, and for example, as shown in the following reaction schemes 1 to 7, but is not limited thereto:

[124] [Reaction Scheme 1]

[125]



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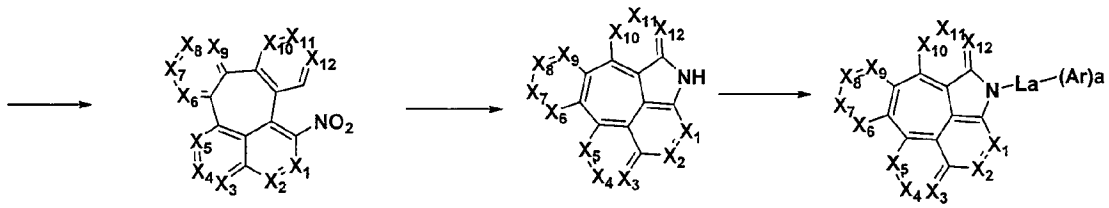
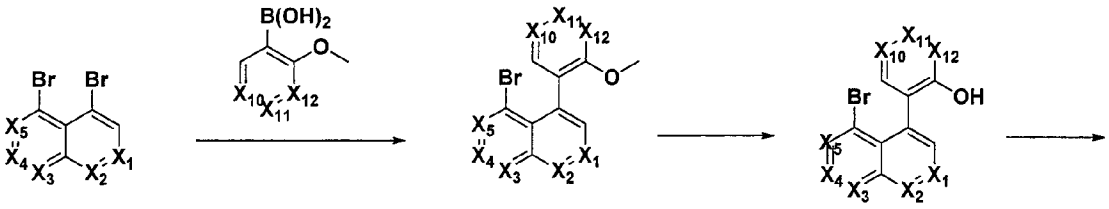
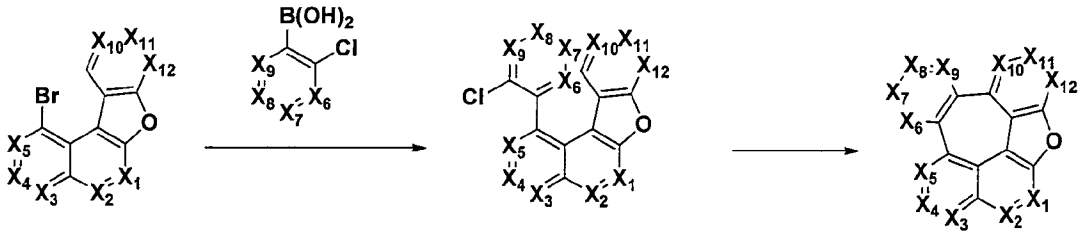


[127] [Reaction Scheme 2]

[128]

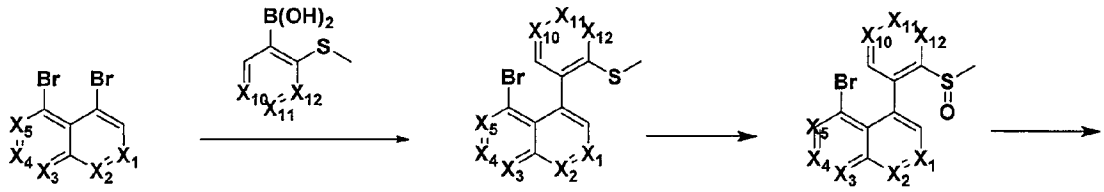


[129]



[130] [Reaction Scheme 3]

[131]



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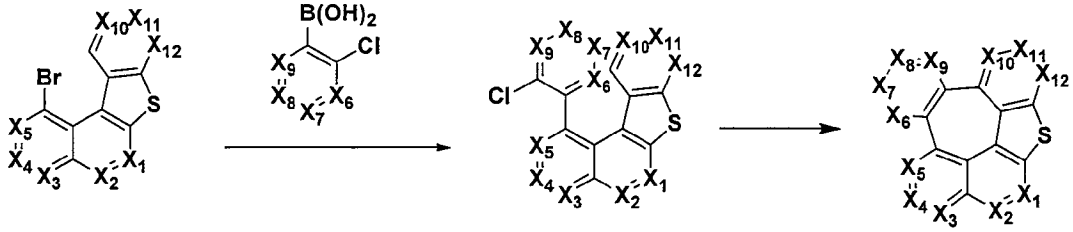
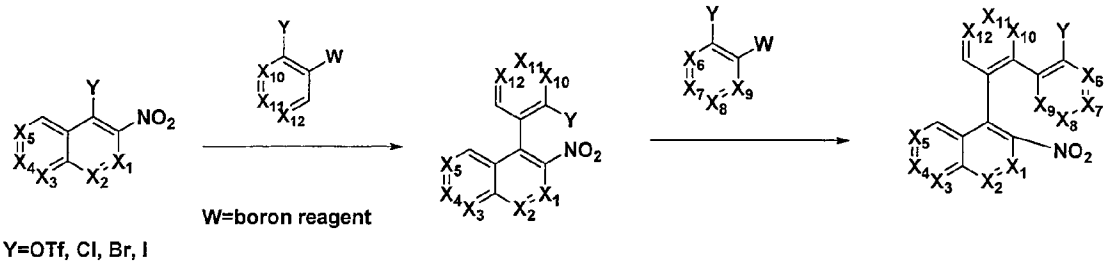


[133] [Reaction Scheme 4]

[134]



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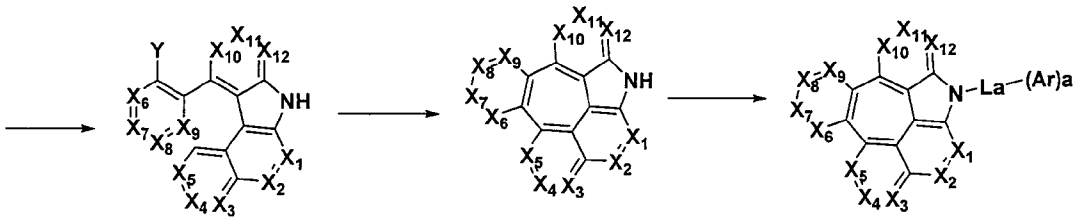
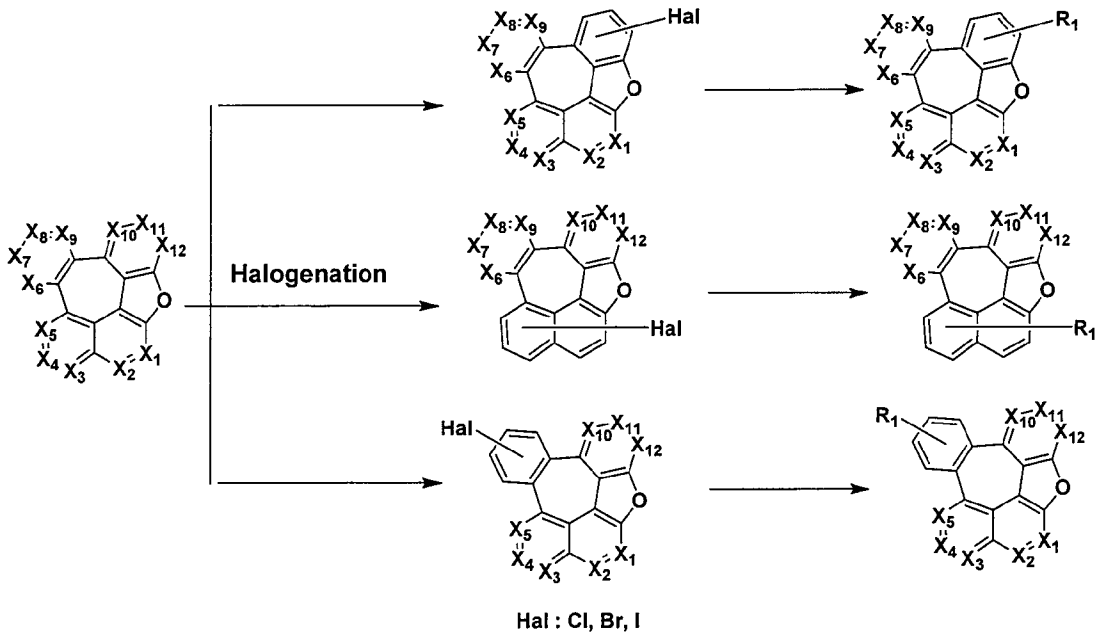


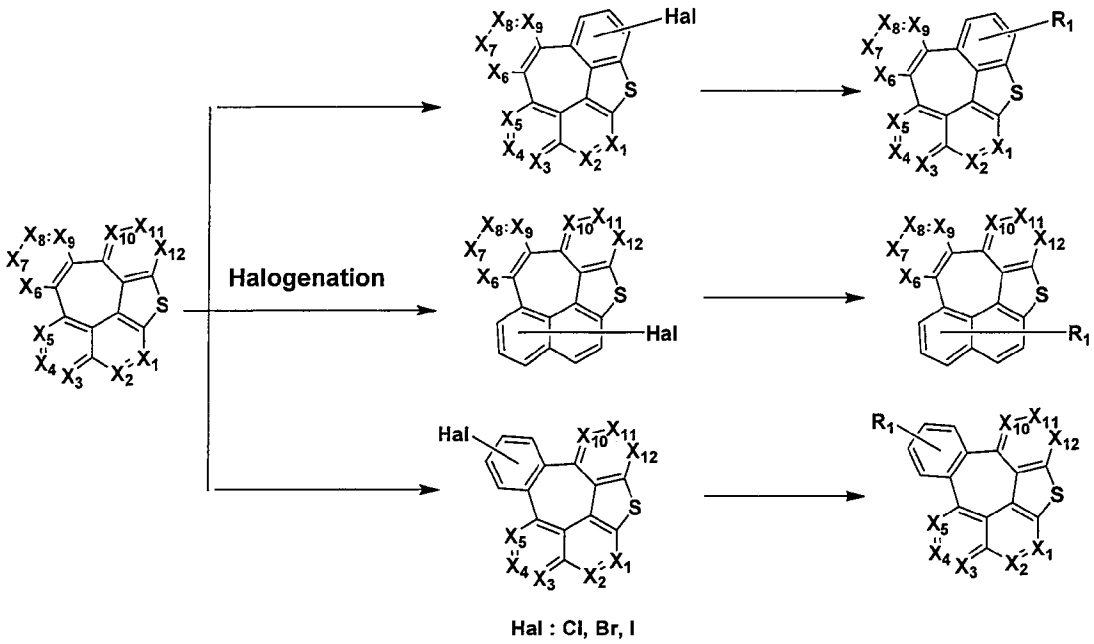
[136] [Reaction Scheme 5]

[137]



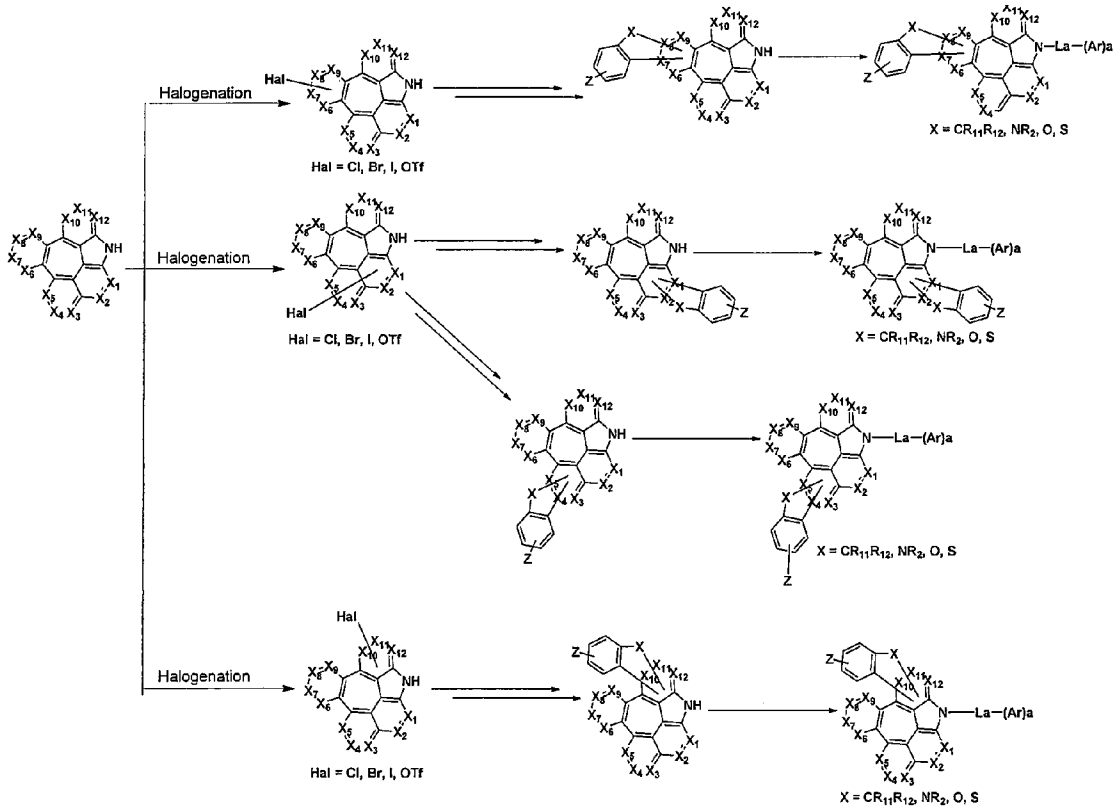
[138] [Reaction Scheme 6]

[139]



[140] [Reaction Scheme 7]

[141]



[142] In reaction schemes 1 to 7, X_1 to X_{12}, R_1, La, Ar, and a are as defined in formula 1; R_2, R_{11}, and R_{12} are as defined in formulas 5 and 6; Z is identical to the definition of R_1; and OTf represents a trifluoromethanesulfonate.

[143] The organic electroluminescent device of the present disclosure may comprise a first electrode, a second electrode, and at least one organic layer between the first and

second electrodes.

[144] 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, a hole auxiliary layer, a light-emitting auxiliary layer, an electron transport layer, an electron buffer layer, an electron injection layer, an interlayer, a hole blocking layer, and an electron blocking layer. The second electrode may be a transflective electrode or a reflective electrode, and may be a top emission type, a bottom emission type, or both-sides emission type according to the kinds of the material. In addition, the hole injection layer may be further doped with a p-dopant, and the electron injection layer may be further doped with an n-dopant.

[145] The organic electroluminescent device according to the present disclosure may comprise an anode, a cathode, and at least one organic layer between the anode and cathode, in which the organic layer may comprise a plurality of organic electroluminescent materials including different compounds represented by formula 1 as the first organic electroluminescent material and the second organic electroluminescent material. The organic electroluminescent device according to the present disclosure may comprise an anode, a cathode, and at least one light-emitting layer between the anode and cathode, in which the light-emitting layer may comprise two or more different compounds represented by formula 1.

[146] The light-emitting layer includes a host and a dopant, in which the host includes a plurality of host materials, and the compound represented by formula 1 may be included as the first and second host compounds of the plurality of host materials. The weight ratio of the first host compound and the second host compound is about 1:99 to about 99:1, preferably about 10:90 to about 90:10, more preferably about 30:70 to about 70:30, even more preferably about 40:60 to about 60:40, and further more preferably about 50:50.

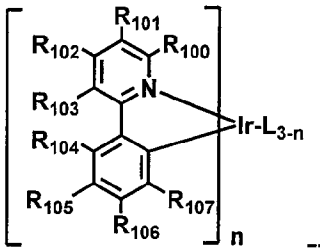
[147] Herein, the light-emitting layer is a layer from which light is emitted, and may be a single layer or a multi-layer of which two or more layers are stacked. All of the first host material and the second host material may be included in one layer, or the first host material and the second host material may be included in respective different light-emitting layers. According to one embodiment of the present disclosure, the doping concentration of the dopant compound with respect to the host compound in the light-emitting layer may be less than 20 wt%.

[148] The organic electroluminescent device of the present disclosure may further comprise at least one layer selected from a hole injection layer, a hole transport layer, a hole auxiliary layer, a light-emitting auxiliary layer, an electron transport layer, an electron injection layer, an interlayer, an electron buffer layer, a hole blocking layer,

and an electron blocking layer. According to one embodiment of the present disclosure, the organic electroluminescent device of the present disclosure may further comprise an amine-based compound besides the plurality of host materials of the present disclosure as at least one of a hole injection material, a hole transport material, a hole auxiliary material, a light-emitting material, a light-emitting auxiliary material, and an electron blocking material. Further, according to one embodiment of the present disclosure, the organic electroluminescent device of the present disclosure may further comprise an azine-based compound besides the plurality of host materials of the present disclosure as at least one of an electron transport material, an electron injection material, an electron buffer material, and a hole blocking material.

[149] The dopant comprised in the organic electroluminescent device of the present disclosure may be at least one phosphorescent or fluorescent dopont, and is preferably at least one phosphorescent dopant. The phosphorescent dopant material applied to the organic electroluminescent device of the present disclosure is not particularly limited, but may be preferably selected from the metallated complex compounds of iridium (Ir), osmium (Os), copper (Cu), and platinum (Pt), more preferably selected from ortho-metallated complex compounds of iridium (Ir), osmium (Os), copper (Cu), and platinum (Pt), and even more preferably ortho-metallated iridium complex compounds.

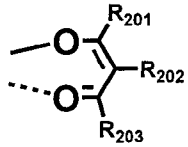
[150] The dopant comprised in the organic electroluminescent device of the present disclosure may comprise a compound represented by the following formula 101, but is not limited thereto.

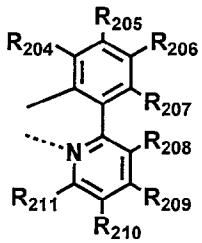
[151] 

--- (101)

[152] In formula 101, L is selected from the following structures 1 and 2:

[153] [Structure 1] [Structure 2]





[154] R_{100} to R_{103}, each independently, represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl unsubstituted or substituted with a halogen(s), a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a cyano, a

substituted or unsubstituted (3- to 30-membered)heteroaryl, or a substituted or unsubstituted (C1-C30)alkoxy; or may be linked to an adjacent substituent to form a ring, e.g., a substituted or unsubstituted, quinoline, benzofuropyridine, benzothienopyridine, benzothienoquinoline, or indenoquinoline ring, together with pyridine;

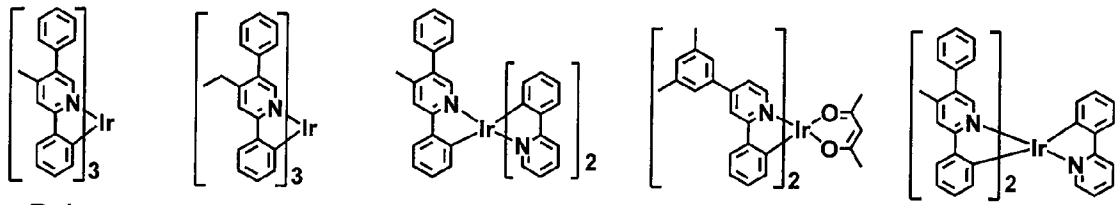
[155] R_{104} to R_{107}, each independently, represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl unsubstituted or substituted with a halogen(s), a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, a cyano, or a substituted or unsubstituted (C1-C30)alkoxy; or may be linked to an adjacent substituent to form a ring, e.g., a substituted or unsubstituted, naphthyl, fluorene, dibenzothiophene, dibenzofuran, indenopyridine, benzofuropyridine or benzothienopyridine ring, together with benzene;

[156] R_{201} to R_{211}, each independently, represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl unsubstituted or substituted with a halogen(s), a substituted or unsubstituted (C3-C30)cycloalkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent to form a ring; and

[157] n represents an integer of 1 to 3.

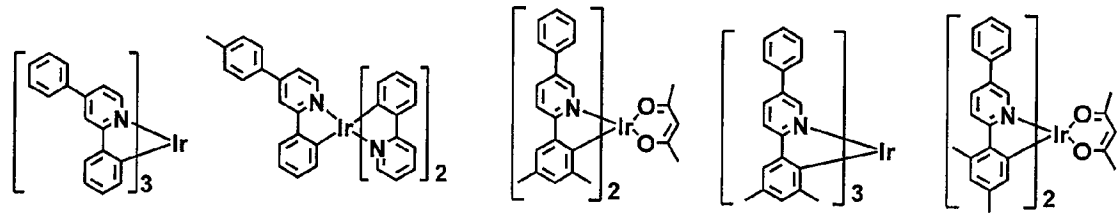
[158] The specific examples of the dopant compound are as follows, but are not limited thereto.

[159]



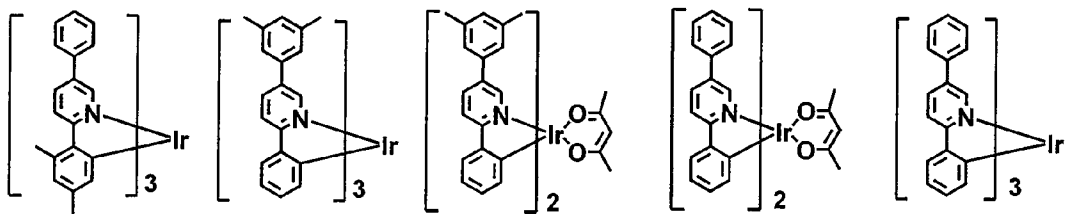
D-1 D-2 D-3 D-4 D-5

[160]



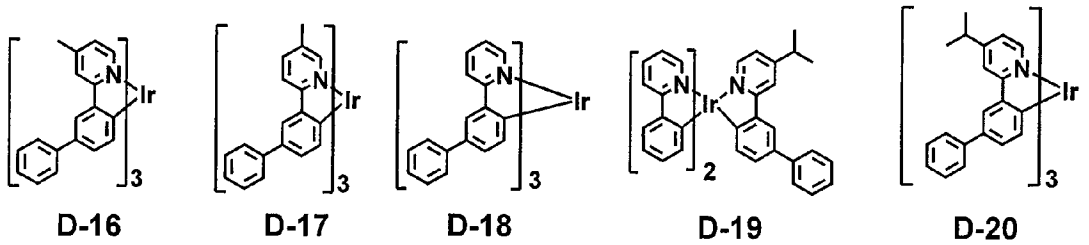
D-6 D-7 D-8 D-9 D-10

[161]



D-11 D-12 D-13 D-14 D-15

[162]



D-16 D-17 D-18 D-19 D-20

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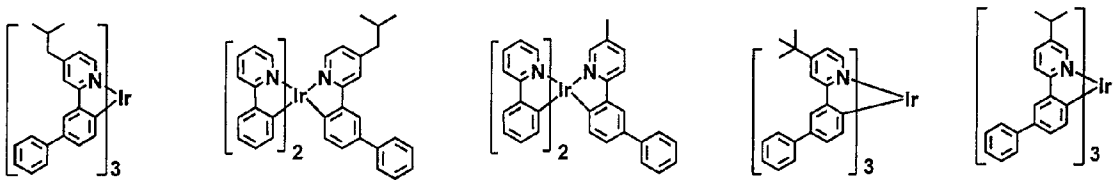
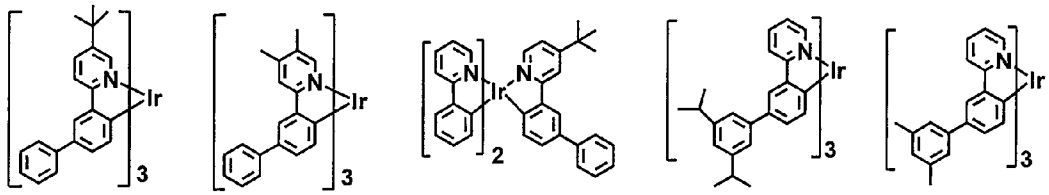


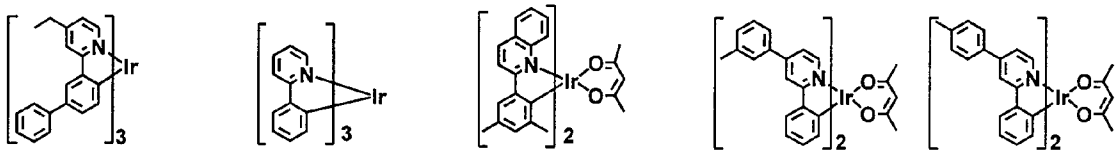
D-21 D-22 D-23 D-24 D-25

[164]



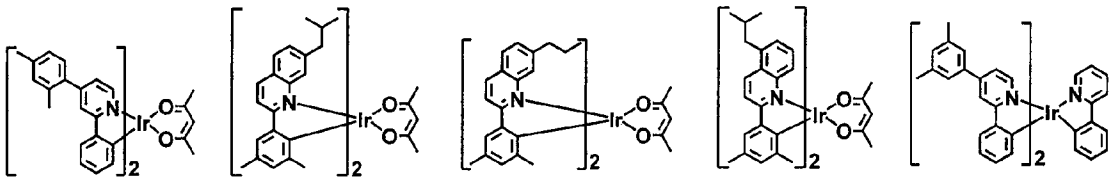
D-26 D-27 D-28 D-29 D-30

[165]



D-31 D-32 D-33 D-34 D-35

[166]



D-36 D-37 D-38 D-39 D-40

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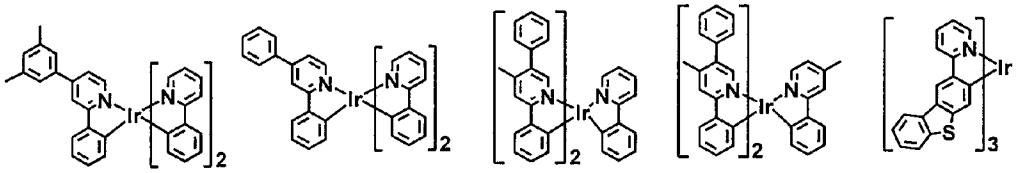

D-41 D-42 D-43 D-44 D-45

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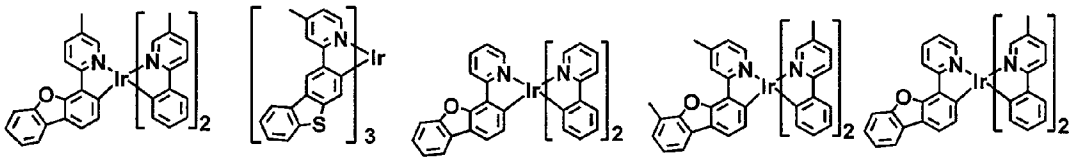
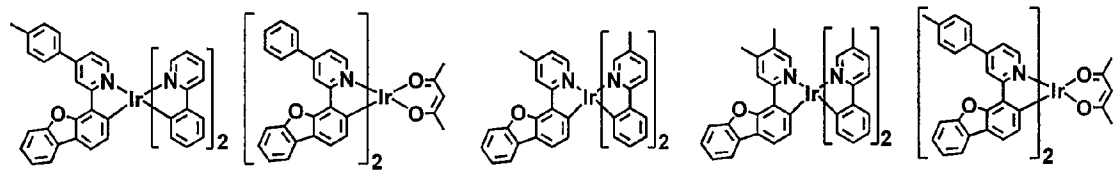


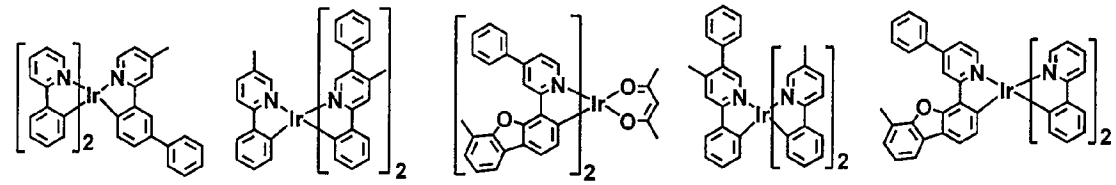
D-46 D-47 D-48 D-49 D-50

[169]



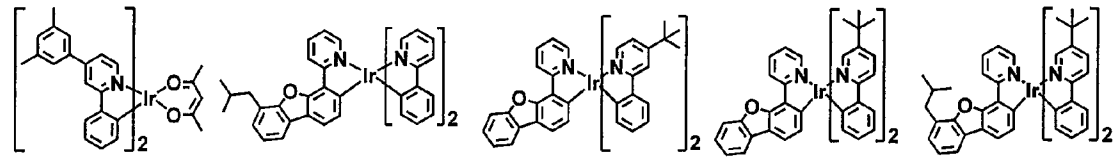
D-51 D-52 D-53 D-54 D-55

[170]



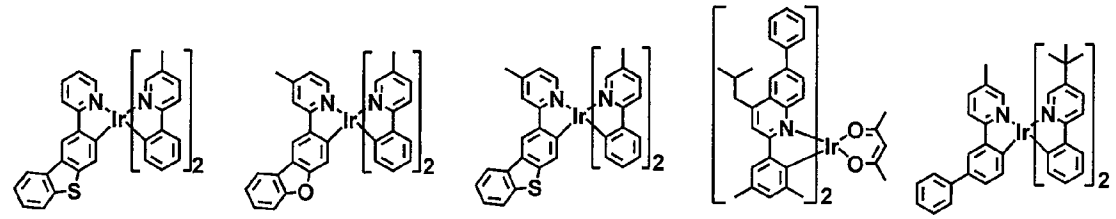
D-56 D-57 D-58 D-59 D-60

[171]



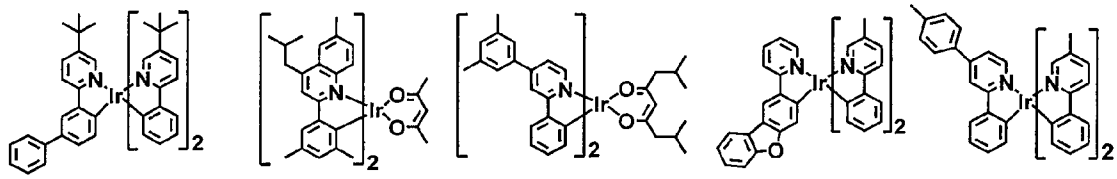
D-61 D-62 D-63 D-64 D-65

[172]



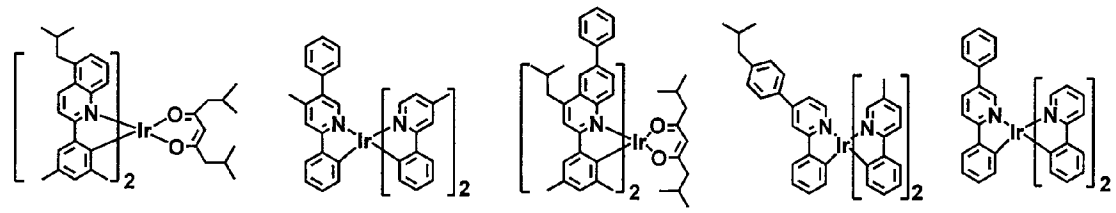
D-66 D-67 D-68 D-69 D-70

[173]



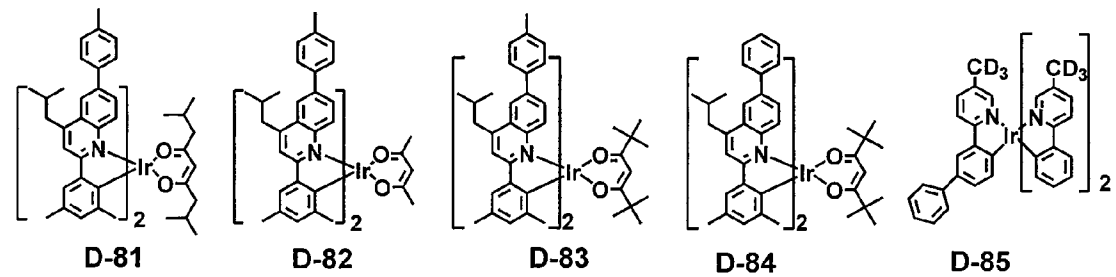
D-71 D-72 D-73 D-74 D-75

[174]



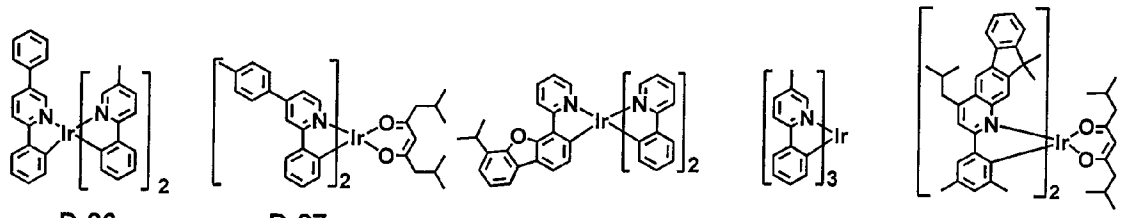
D-76 D-77 D-78 D-79 D-80

[175]



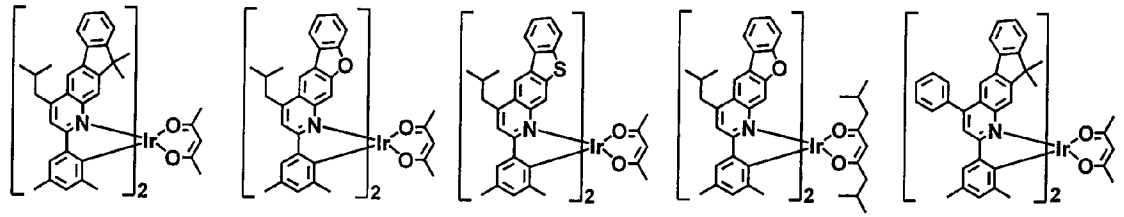
D-81 D-82 D-83 D-84 D-85

[176]



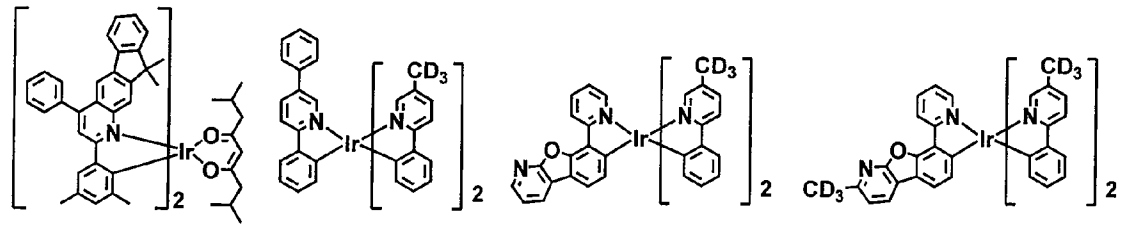
D-86 D-87 D-88 D-89 D-90

[177]



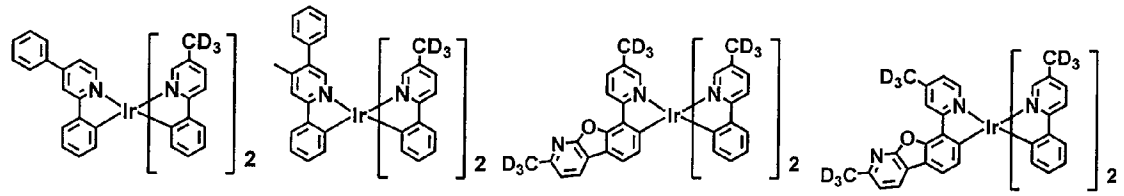
D-91 D-92 D-93 D-94 D-95

[178]



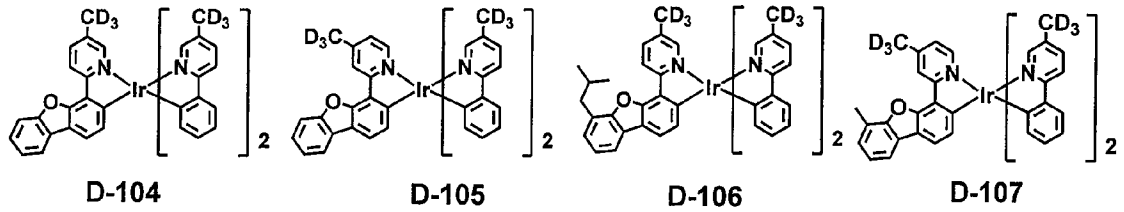
D-96 D-97 D-98 D-99

[179]



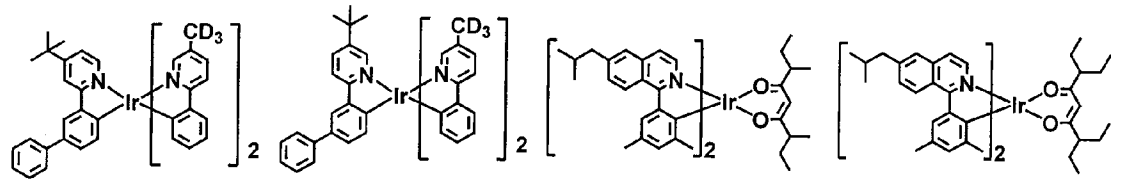
D-100 D-101 D-102 D-103

[180]



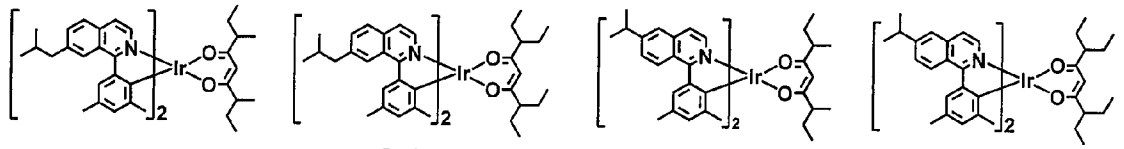
D-104 D-105 D-106 D-107

[181]

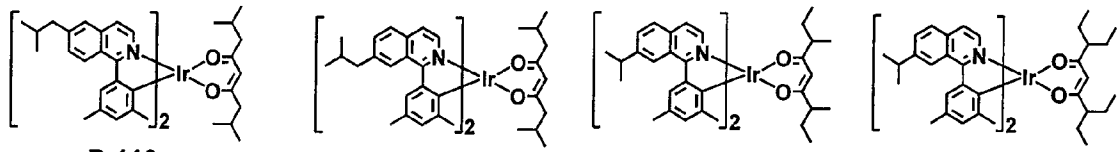


D-108 D-109 D-110 D-111

[182]



D-112 D-113 D-114 D-115

[183] 

D-116 D-117 D-118 D-119

[184] In the organic electroluminescent device of the present disclosure, a hole injection layer, a hole transport layer, an electron blocking layer, or a combination thereof can be used between the anode and the light-emitting layer. The hole injection layer may be multilayers in order to lower the hole injection barrier (or hole injection voltage) from the anode to the hole transport layer or the electron blocking layer, wherein each of the multilayers may use two compounds simultaneously. The hole transport layer or the electron blocking layer may also be multilayers.

[185] An electron buffer layer, a hole blocking layer, an electron transport layer, an electron injection layer, or a combination thereof can be used between the light-emitting layer and the cathode. The electron buffer layer may be multilayers in order to control the injection of the electron and improve the interfacial properties between the light-emitting layer and the electron injection layer, wherein each of the multilayers may use two compounds simultaneously. The hole blocking layer or the electron transport layer may also be multilayers, wherein each of the multilayers may use a plurality of compounds.

[186] In addition, the organic electroluminescent compound or the plurality of host materials according to the present disclosure may also be applied to an organic electro-luminescent device comprising a QD (quantum dot).

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

[188] 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.

[189] The first and the second host compounds of the present disclosure may be film-formed by the above-listed methods, commonly by a co-evaporation process or a mixture-evaporation process. The co-evaporation is a mixed deposition method in which two or more materials are placed in a respective individual crucible source and a current is applied to both cells at the same time to evaporate the materials. The

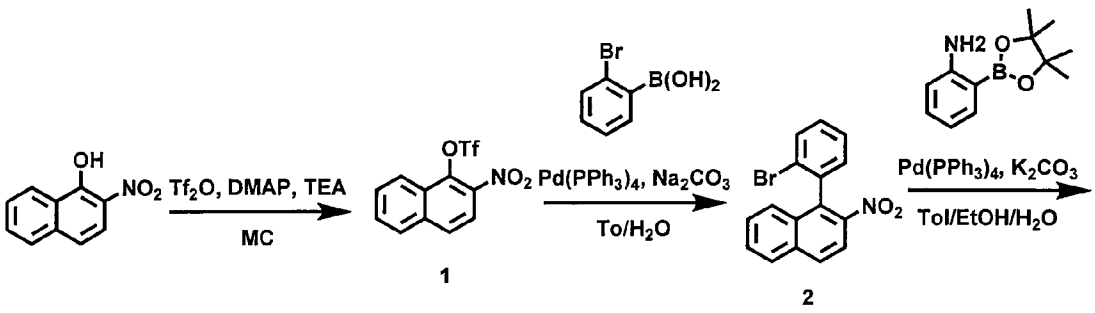
mixture-evaporation is a mixed deposition method in which two or more materials are mixed in one crucible source before evaporating them, and a current is applied to the cell to evaporate the materials. Further, if the first and the second host compounds are present in the same layer or different layers in an organic electroluminescent device, the two host compounds may individually form films. For example, the second host compound may be deposited after depositing the first host compound.

[190] The present disclosure may provide a display device by using the plurality of host materials including two or more different compounds represented by formula 1. Also, by using the organic electroluminescent device of the present disclosure, it is possible to manufacture a display system or a lighting system. Specifically, by using the organic electroluminescent device of the present disclosure, a display system, for example, for smart phones, tablets, notebooks, PCs, TVs, or cars; or a lighting system, for example an outdoor or indoor lighting system, can be produced.

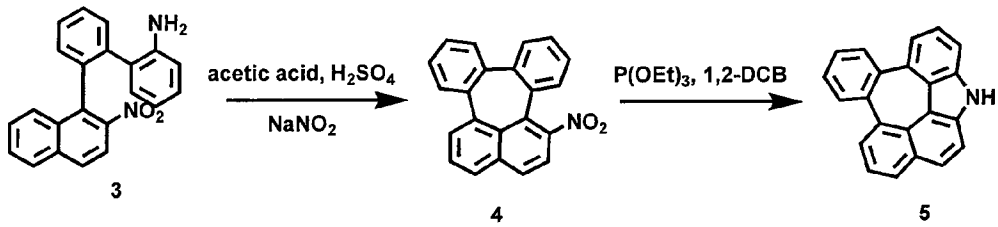
[191] Hereinafter, the preparation method of the compound of the present disclosure and the properties thereof, and the properties of an organic electroluminescent device comprising the plurality of host materials of the present disclosure will be explained in detail with reference to the representative compounds of the present disclosure. However, the present disclosure is not limited by the following examples.

[192] **Example 1: Preparation of compound C-8**

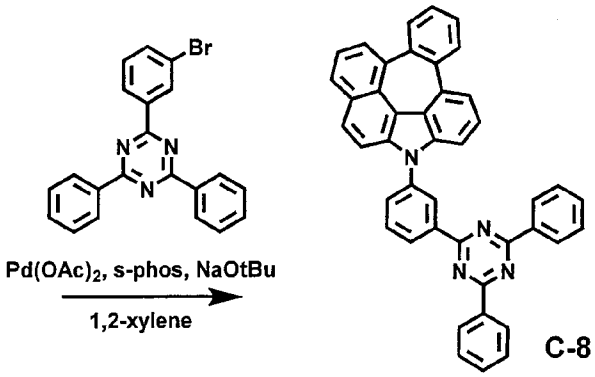
[193]



[194]



[195]



[196] Synthesis of compound **1**

[197] 70 g of 2-nitro-1-naphthol (370 mmol) and 4.5 g of 4-(dimethylamino)pyridine (DMAP) (37 mmol) were dissolved in 1800 mL of methylene chloride (MC) in a flask. 62 mL of triethylamine (TEA) (444 mmol) were added dropwise at 0°C and stirred for 20 minutes. 125.3 g of trifluoromethane sulfonic anhydride (444 mmol) was slowly added dropwise to the reactant at the same temperature and stirred for 1 hour. After the reaction was completed, the organic layer was extracted with MC, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 96.2 g of compound **1** (yield: 81%).

[198] Synthesis of compound **2**

[199] 96.2 g of compound **1** (299 mmol), 72.1 g of 2-bromophenylboronic acid (359 mmol), 17.3 g of tetrakis(triphenylphosphine)palladium(0) (15 mmol), and 79.3 g of sodium carbonate (749 mmol) were dissolved in 1400 mL of toluene, 350 mL of ethanol, and 350 mL of water in a flask and refluxed for 1 hour. After the reaction was completed, the organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 98 g of compound **2** (yield: 99%).

[200] Synthesis of compound **3**

[201] 98 g of compound **2** (299 mmol), 78.5 g of 2-aminophenylboronic acid pinacol ester (358 mmol), 17.2 g of tetrakis(triphenylphosphine)palladium(0) (15 mmol), and 103g of potassium carbonate (747 mmol) were dissolved in 1300 mL of toluene, 350 mL of ethanol and 350 mL of water in a flask and refluxed for 20 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 54 g of compound **3** (yield: 53%).

[202] Synthesis of compound **4**

[203] 25 g of compound **3** (73 mmol) was dissolved in 250 mL of acetic acid and 25 mL of sulfuric acid in a flask, 6.5 g of sodium nitrite (95 mmol) was slowly added dropwise at 0°C and stirred for 40 minutes. After the reaction was completed, the reaction

product was added dropwise to water and filtered to remove moisture. The residue was dried and separated by column chromatography to obtain 2 g of compound **4** (yield: 8.4%).

[204] Synthesis of compound **5**

[205] 4.7g of compound **4** (15 mmol) was dissolved in 48 mL of triethylphosphite and 48 mL of 1,2-dichlorobenzene in a flask and refluxed for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 2.7 g of compound **5** (yield: 63%).

[206] Synthesis of compound **C-8**

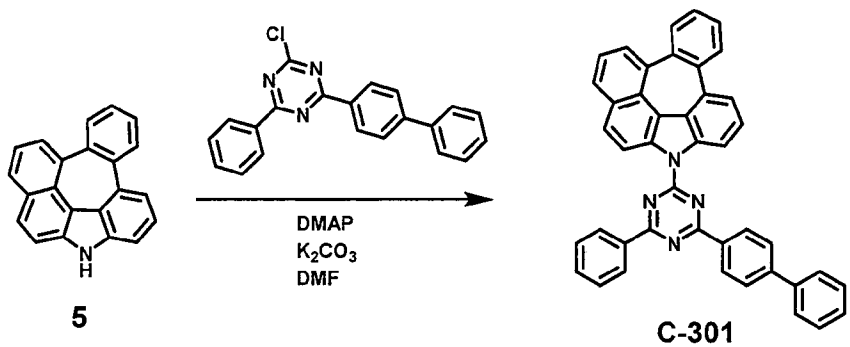
[207] 2.1 g of compound **5** (7 mmol), 3.1 g of 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (8 mmol), 0.81 g of palladium (II) acetate (0.36 mmol), 0.3 g of 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (S-Phos) (0.7 mmol), and 1.7 g of sodium *tert*-butoxide (18 mmol) were dissolved in 72 mL of 1,2-xylene in a flask and refluxed for 4 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 2.5 g of compound **C-8** (yield: 58%).

[208]

Compound	MW	UV	PL	M.P.	Tg
C-8	598.71	308 nm	495 nm	285°C	132.37°C

[209] **Example 2: Preparation of compound C-301**

[210]



[211] 5.0 g of compound **5** (17 mmol), 7.08 g of 2-([1,1'-biphenyl]-4-yl)-4-chloro-6-phenyl-1,3,5-triazine (21 mmol), 105 mg of DMAP (0.858 mmol), and 7.1 g of potassium carbonate (51 mmol) were dissolved in 85 mL of dimethylformamide (DMF) in a flask and refluxed for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The

residue was dried and separated by column chromatography to obtain 4.8 g of compound **C-301** (yield: 47%).

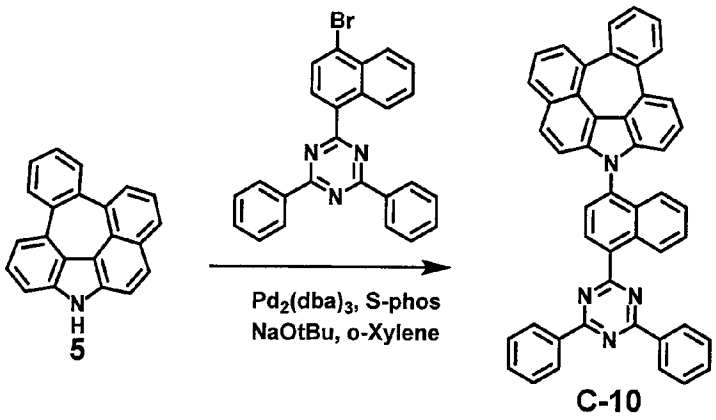
[212] ^{1}H NMR (600MHz, CDCl3) 9.09-9.07 (d, *J= 12 Hz*, 1H), 8.93-8.91 (d, *J = 12 Hz*, 1H), 8.74-8.73 (d, *J= 6 Hz*, 2H), 8.71-8.69 (d, *J= 12 Hz*, 2H), 7.80-7.75 (m, 6H), 7.73-7.69 (m, 3H), 7.64-7.57 (m, 3H), 7.52-7.38 (m, 8H)

[213]

Compound	MW	Tg	M.P.
C-301	598.71	124.4°C	236°C

[214] **Example 3: Preparation of compound C-10**

[215]



[216] 5.0 g of compound **5** (17 mmol), 11.28 g of 2-(4-bromonaphthalene-1-yl)-4,6-diphenyl-1,3,5-triazine) (21 mmol), 625 mg of tris(dibenzylideneacetone)dipalladium(0) (0.686 mmol), 565 mg of S-Phos (1 mmol), and 4.9 g of sodium *tert*-butoxide (51 mmol) were dissolved in 100 mL of o-xylene in a flask and refluxed for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 3.6 g of compound **C-10** (yield: 32%).

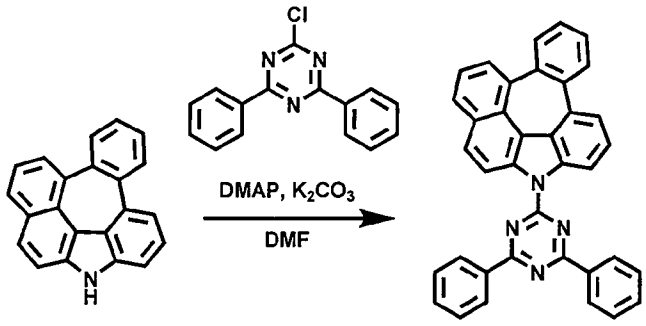
[217] ^{1}H NMR (600MHz, CDCl3) 9.25-9.24 (d, J=6Hz, 1H), 8.85-8.83 (sd, J=12Hz, 4H), 8.68-8.67 (d, J=6Hz, 1H), 7.94-7.92 (m, 1H), 7.82-7.79 (m, 3H), 7.74-7.61 (m, 10H), 7.49-7.42 (m, 5H), 7.31-7.29 (t, J=6Hz, 1H), 7.16-7.15 (d, J=6Hz,1H), 6.96-6.94 (d, J=12Hz, 1H)

[218]

Compound	MW	Tg	M.P.
C-10	648.7	159.5°C	176°C

[219] **Example 4: Preparation of compound C-7**

[220]



5 C-7

[221] 5 g of compound **5** (17.1 mmol), 5.5 g of 2-chloro-4,6-diphenyl-1,3,5-triazine (20.5 mmol), 0.1 g of DMAP (0.85 mmol), and 7.1 g of potassium carbonate (51.4 mmol) were dissolved in 85 mL of DMF in a flask and refluxed for 3 hours. After the reaction was completed, the reaction product was cooled, methanol and water were added thereto, and the mixture was filtered. The residue was dried and separated by column chromatography to obtain 4.4 g of compound **C-7** (yield: 49%).

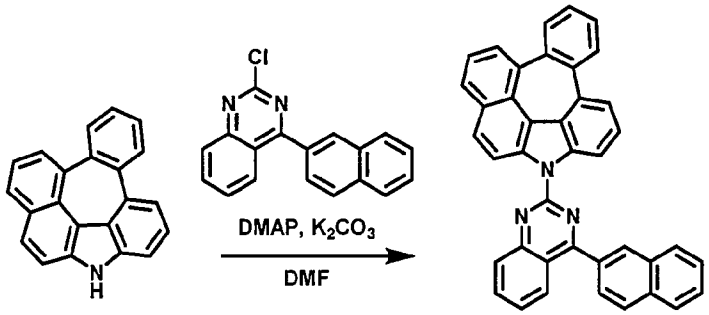
[222] ^{1}H NMR (600MHz, CDCl3) 9.13-9.11(d, J=12Hz, 1H), 8.97-8.95 (d, J=12Hz, 1H), 8.75-8.73 (d, J=12Hz, 4H), 7.83-7.75 (m, 5H), 7.64-7.59(m, 6H), 7.54-7.51 (m, 3H), 7.48-7.45 (t, J=12Hz, 3H), 7.40-7.39 (m, 2H)

[223]

Compound	MW	Tg	M.P.
C-7	522.6	105°C	209°C

[224] **Example 5: Preparation of compound C-302**

[225]



5 C-302

[226] 4.5 g of compound **5** (15.4 mmol), 5.4 g of 2-chloro-4-(naphthalen-2-yl)quinazoline (18.5 mmol), 0.09 g of DMAP (0.7 mmol), and 6.4 g of potassium carbonate (46.3 mmol) were dissolved in 77 mL of DMF in a flask and refluxed for 1.5 hours. After the reaction was completed, the reaction product was filtered, dried and separated by column chromatography to obtain 7.5 g of compound **C-302** (yield: 80%).

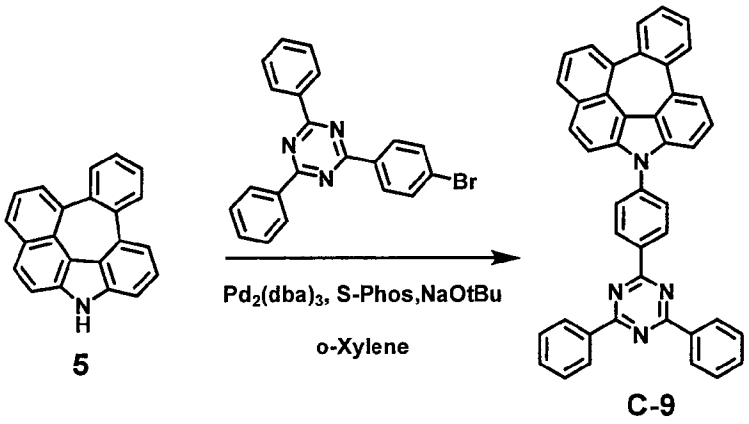
[227] ^{1}H NMR (600MHz, CDCl3) 9.03-9.02 (d, J=6Hz, 1H), 8.88-8.86 (d, J=12Hz, 1H), 8.39 (s, 1H), 8.22-8.21 (d, J=6Hz, 1H), 8.20-8.17 (d, J=18 Hz, 1H), 8.15-8.05 (m, 2H), 8.00-7.98 (t, J=6Hz, 2H), 7.91-7.89 (m, 1H), 7.76-7.72 (m, 5H), 7.63-7.61 (m, 2H), 7.54-7.52 (m, 2H), 7.43-7.36 (m, 4H)

[228]

Compound	MW	Tg	M.P.
C-302	545.65	120.6°C	257°C

[229] **Example 6: Preparation of compound C-9**

[230]



[231] 5.0 g of compound **5** (17.16 mmol), 6.6 g of 2-(4-bromophenyl)-4,6-diphenyl-1,3,5-triazine (17.16 mmol), 0.6 g of tris(dibenzylideneacetone)dipalladium(0) (0.686 mmol), 0.7 g of S-Phos (1.176 mmol), and 4.0 g of sodium *tert*-butoxide (42.9 mmol) were dissolved in 90 mL of o-xylene in a flask and refluxed for 4 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 6.2 g of compound **C-9** (yield: 62%).

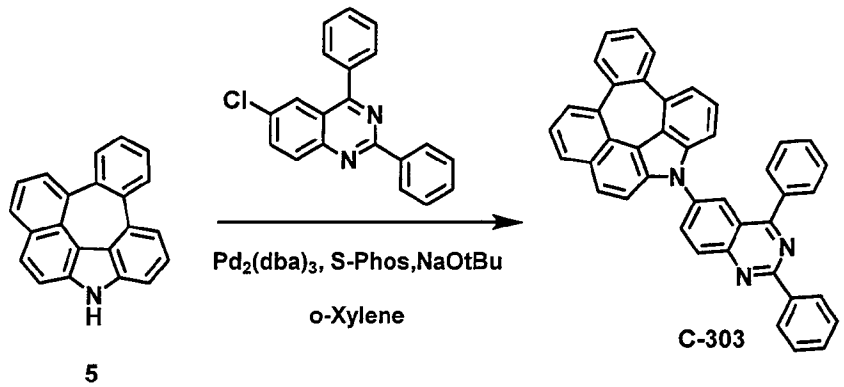
[232] ^{1}H NMR (600MHz, CDCl3,δ) 9.06-9.05 (d, J=6.0Hz, 2H), 8.85-8.83 (d, J=12Hz, 4H), 7.90-7.89 (m, 1H), 7.82-7.78 (m, 4H), 7.74-7.72 (m, 2H), 7.66-7.58 (m, 8H), 7.45-7.43 (m, 3H), 7.42-7.39 (m, 2H)

[233]

Compound	MW	Tg	M.P.
C-9	598.71	140.59°C	260°C

[234] **Example 7: Preparation of compound C-303**

[235]



[236] 4.3 g of compound **5** (14.83 mmol), 4.7 g of 6-chloro-2,4-diphenylquinazoline (14.83 mmol), 0.5 g of $Pd_2(dba)_3$ (0.593 mmol), 0.6 g of S-Phos (1.483 mmol), and 3.6 g of

sodium *tert*-butoxide (37.07 mmol) were dissolved in 80 mL of o-xylene in a flask and refluxed for 4 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 1.8 g of compound **C-303** (yield: 21%).

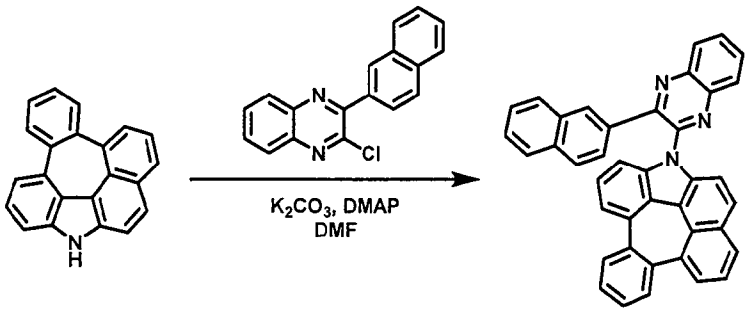
[237] ^{1}H NMR (600MHz, CDCl3,δ) 8.74-8.73 (d, J=6.0 Hz, 2H), 8.37-8.36 (d, J=6.0Hz, 1H), 8.28-8.27 (d, J=6.0Hz, 1H), 8.05-8.04 (d, J=6.0Hz, 1H), 7.89-7.88 (d, J=6.0Hz, 2H), 7.85-7.83 (m, 1H), 7.75-7.73 (d, J=12Hz, 2H), 7.69-7.67 (m, 2H), 7.57-7.50 (m, 7H), 7.42-7.37 (m, 4H), 7.34-7.31 (m, 1H), 7.22-7.21 (m, 1H)

[238]

Compound	MW	Tg	M.P.
C-303	571.67	140.16°C	189.3°C

[239] **Example 8: Preparation of compound C-307**

[240]



5 C-307

[241] 5.4 g of compound **5** (18.53 mmol), 4.5 g of 2-chloro-3-naphthylquinoxaline (15.44 mmol), 2.1 g of potassium carbonate (15.44 mmol), and 0.9 g of DMAP (7.72 mmol) were dissolved in 80 mL of DMF in a flask and refluxed for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water was added thereto. The organic layer was extracted with MC, and residual moisture was removed by using magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 2.3 g of compound **C-307** (yield: 47%).

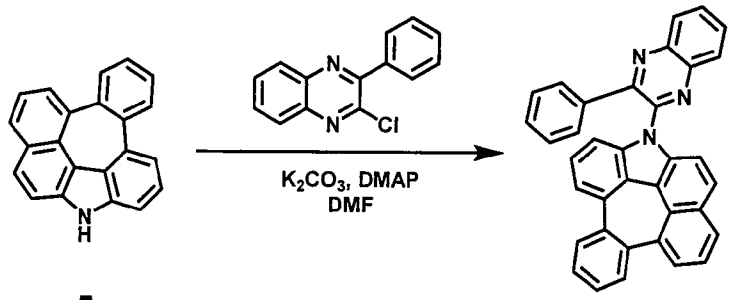
[242] ^{1}H NMR (600MHz, CDCl3,δ) 8.36-8.34 (d, J=6.0Hz, 1H), 8.23 (s, 1H), 8.17-8.16 (d, J=6.0HZ, 1H), 7.90-7.86 (m, 3H), 7.73-7.71 (d, J=12Hz, 1H), 7.68-7.63 (m, 4H), 7.50-7.48(m, 2H), 7.40-7.35 (m, 6H), 7.32-7.24 (m, 2H)

[243]

Compound	MW	Tg	M.P.
C-307	545.65	133°C	152°C

[244] **Example 9: Preparation of compound C-13**

[245]



5 C-13

[246] 4.0 g of compound **5** (13.73 mmol), 4.0 g of 2-chloro-3-phenylquinoxaline (16.47 mmol), 3.8 g of potassium carbonate (27.46 mmol), and 0.84 g of DMAP (6.87 mmol) were dissolved in 68 mL of DMF in a flask and refluxed for 18 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water was added thereto. The organic layer was extracted with MC, and residual moisture was removed by using magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 2.3 g of compound **C-13** (yield: 33.8%).

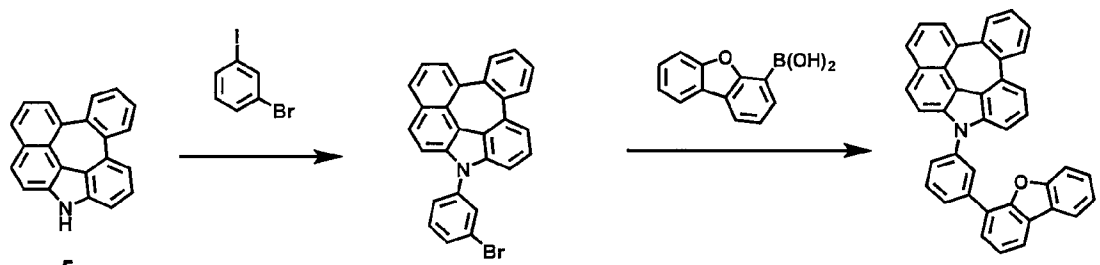
[247] ^{1}H NMR (600MHz, CDCl3,δ) 8.32-8.30 (m, 1H), 8.16-8.15 (m, 1H), 7.89-7.83 (m, 3H), 7.73 (d,J=7.38Hz, 1H), 7.69-7.68 (m, 2H), 7.60-7.54 (m, 2H), 7.50 (d, J=9.00Hz, 1H), 7.42-7.37 (m, 3H), 7.29-7.27 (m, 3H), 7.21-7.15 (m, 4H)

[248]

Compound	MW	Tg	M.P.
C-13	495.59	124.88°C	154-164°C

[249] **Example 10: Preparation of compound C-304**

[250]



5 10-1 C-304

[251] Synthesis of compound **10-1**

[252] 155 mL of toluene was added to 9 g of compound **5** (30.89 mmol), 10.6 g of 1-bromo-3-iodobenzene (61.78 mmol), 3 g of CuI (15.44 mmol), 1.8 g of EDA (30.89 mmol), and 16.4 g of K_3PO_4 (77.22 mmol) and stirred under reflux for one day. After the reaction was completed, the reaction product was cooled to room temperature, and the resulting solid was filtered under reduced pressure. The solid was dissolved in $CHCl_3$ and separated by column chromatography using MC/Hex to obtain 10 g of compound **10-1** (yield: 75%).

[253] Synthesis of compound **C-304**

[254] 50 mL of toluene, 13 mL of EtOH, and 13 mL of purified water were added to 5.7 g of compound **10-1** (12.77 mmol), 0.73 g of $Pd(PPh_3)_4$ (0.638 mmol), and 3.5 g of K_2CO_3 (25.54 mmol) and stirred under reflux for 2 hours. After the reaction was completed, the reaction product was cooled to room temperature, and the resulting solid was filtered under reduced pressure. The solid was dissolved in $CHCl_3$ and separated by column chromatography using MC/Hex to obtain 2.9 g of compound **C-304** (yield: 43%).

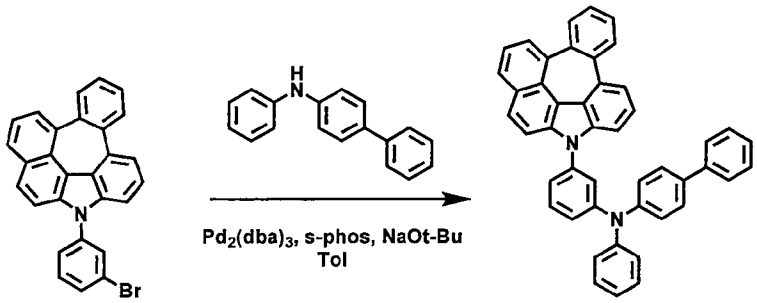
[255] ^{1}H NMR (600MHz, DMSO-d6,δ) 8.232-8.206 (m, 3H), 8.111-8.098 (d, 1H), 7.962-7.946 (m, 1H), 7.929-7.903 (m, 3H), 7.896-7.882 (d, 1H), 7.806-7.802 (d, 2H), 7.783-7.759 (t, 2H), 7.738-7.723 (d, 1H), 7.635-7.620 (m, 1H), 7.581-7.548 (m, 2H), 7.513-7.440 (m, 6H)

[256]

Compound	MW	Tg	M.P.
C-304	533.6	119°C	208°C

[257] **Example 11: Preparation of compound C-306**

[258]



10-1 C-306

[259] 5.0 g of compound **10-1** (11.2 mmol), 3.0 g of N-phenyl-[1,1'-biphenyl]-4-amine (12.3 mmol), 0.51 g of $Pd_2(dba)_3$ (0.56 mmol), 0.46 g of S-Phos (1.12 mmol), and 2.7 g of sodium *tert*-butoxide (28 mmol) were added to 60 mL of toluene in a flask and refluxed for 4 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 2.3 g of compound **C-306** (yield: 34%).

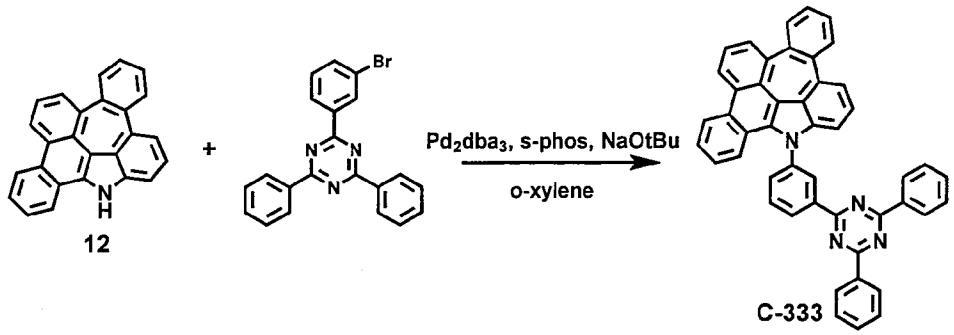
[260] ^{1}H NMR (600MHz, DMSO-d6,δ) 7.896-7.880 (m, 1H), 7.863-7.850 (d, 1H), 7.805-7.790 (d, 1H), 7.758-7.745 (d, 1H), 7.733-7.720 (d, 1H), 7.669-7.650 (m, 2H), 7.640-7.627 (d, 1H), 7.604-7.566 (m, 2H), 7.522-7.507 (d, 1H), 7.447-7.384 (m, 7H), 7.373-7.347 (t, 1H), 7.335-7.311 (t, 1H), 7.269-7.237 (m, 6H), 7.175-7.156 (d, 1H), 7.147-7.122 (t, 1H), 7.069-7.062 (t, 1H)

[261]

Compound	MW	Tg	M.P.
C-306	610.8	114°C	132°C

[262] **Example 12: Preparation of compound C-333**

[263]



[264] 2.6 g of compound **12** (7.6 mmol), 2.95 g of 2-(3-bromophenyl)-4,6-diphenyl-1,3,5-triazine (7.6 mmol), 0.27 g of tris(dibenzylideneacetone)dipalladium(0) (0.3 mmol), 0.3 g of 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (0.7 mmol), and 1.8 g of sodium *tert*-butoxide (19 mmol) were dissolved in 50 mL of 1,2-dimethyl benzene in a flask and refluxed for 12 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 1.9 g of compound **C-333** (yield: 38%).

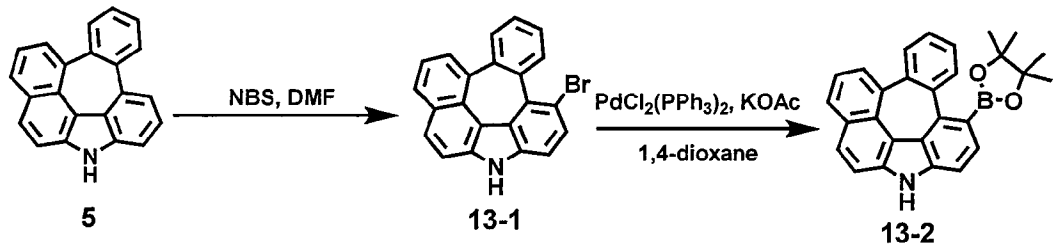
[265] ^{1}H NMR (600MHz, DMSO-d6,δ) 9.086-9.072 (d, 1H), 8.887-8.882 (t, 1H), 8.821-8.807 (d, 1H), 8.714-8.699 (d, 4H), 8.676-8.663 (d, 1H), 8.014-7.988 (t, 1H), 7.883-7.833 (m, 3H), 7.781-7.768 (d, 1H), 7.691-7.665 (t, 2H), 7.640-7.575 (m, 6H), 7.540-7.485 (m, 3H), 7.399-7.343 (m, 3H), 6.982-6.968 (d, 1H)

[266]

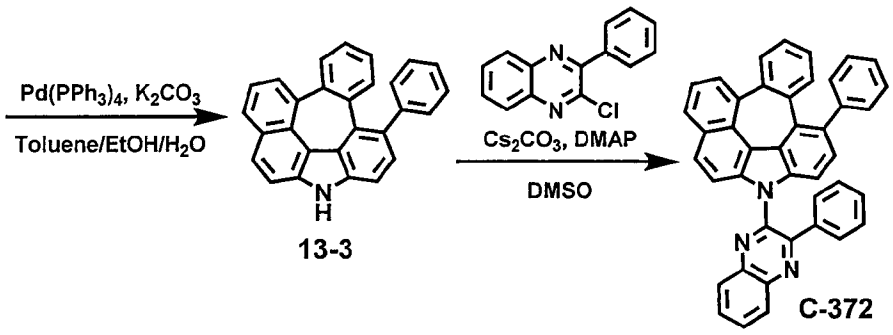
Compound	MW	M.P.	Tg
C-333	648.77	195°C	165°C

[267] **Example 13: Preparation of compound C-372**

[268]



[269]



[270] Synthesis of compound **13-1**

[271] 70 g of compound **5** (240 mmol), and 40.6 g of N-bromosuccinimide (255 mmol) were dissolved in 1200 mL of dimethylformamide in a flask, and stirred at 0℃ for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 68 g of compound **13-1** (yield: 76%).

[272] Synthesis of compound **13-2**

[273] 47.3 g of compound **13-1** (127 mmol), 42 g of bis(pinacolato)diboron (166 mmol), 4.5 g of bis(triphenylphosphine)palladium (II) dichloride (6.4 mmol), and 25 g of potassium acetate (255 mmol) were dissolved in 635 mL of 1,4-dioxane in a flask and refluxed for 4 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 31.5 g of compound **13-2** (yield: 59%).

[274] Synthesis of compound **13-3**

[275] 4.5 g of compound **13-2** (10.7 mmol), 1.9 g of 1-bromobenzene (11.85 mmol), 0.63 g of tetrakis(triphenylphosphine)palladium(0) (0.54 mmol), and 3.7 g of potassium carbonate (26.95 mmol) were dissolved in 54 mL of toluene, 13 mL of ethanol, and 13 mL of water in a flask and refluxed for 12 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 2.2 g of compound **13-3** (yield: 56%).

[276] Synthesis of compound **C-372**

[277] 2.2 g of compound **13-3** (5.9 mmol), 1.58 g of 2-chloro-3-phenylquinoxaline (6.57 mmol), 3.89 g of cesium carbonate (11.96 mmol), and 0.36 g of 4-dimethylaminopyridine (2.99 mmol) were dissolved in 30 mL of dimethyl sulfur monoxide in a flask and stirred at 100℃ for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water was added thereto. The organic layer was extracted with ethyl acetate, and residual moisture was

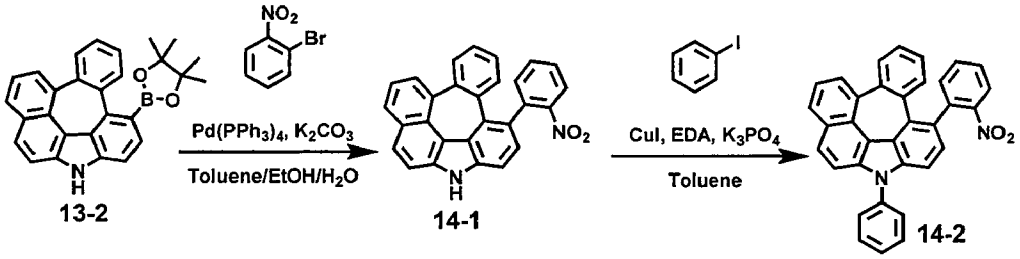
removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 2.9 g of compound **C-372** (yield: 85%).

[278]

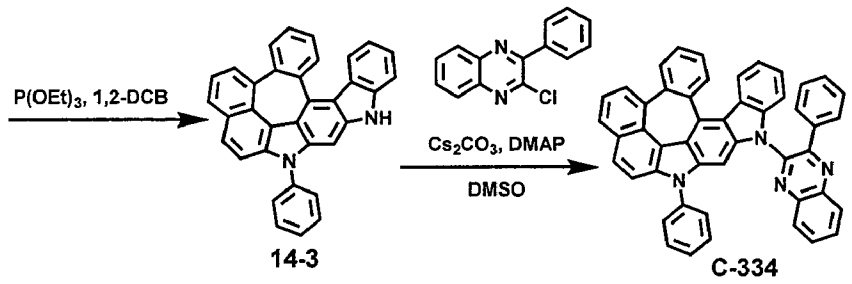
Compound	MW	M.P.	Tg
C-372	571.68	210°C	167°C

[279] **Example 14: Preparation of compound C-334**

[280]



[281]



[282] Synthesis of compound **14-1**

[283] 27 g of compound **13-2** (64.7 mmol), 14.4 g of 1-bromo-2-nitrobenzene (71.2 mmol), 3.7 g of tetrakis(triphenylphosphine)palladium(0) (3.2 mmol), and 22.4 g of potassium carbonate (162 mmol) were dissolved in 320 mL of toluene, 80 mL of ethanol, and 80 mL of water in a flask and refluxed for 12 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 26.7 g of compound **14-1** (yield: 100%).

[284] Synthesis of compound **14-2**

[285] 26.7 g of compound **14-1** (64.7 mmol), 18 mL of 1-iodobenzene (162 mmol), 18.5 g of copper iodide (CuI) (97 mmol), 13 mL of ethylenediamine (194 mmol), and 27.4 g of potassium phosphate (129 mmol) were dissolved in 325 mL of toluene in a flask and refluxed for 2 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 15.7 g of compound **14-2** (yield: 49%).

[286] Synthesis of compound **14-3**

[287] 13.1 g of compound **14-2** (26.8 mmol) was added to 180 mL of triethylphosphite and 180 mL of 1,2-dichlorobenzene in a flask and stirred at 200°C for 2 hours. After the

reaction was completed, the solvent was distilled off under reduced pressure, the reaction product was cooled to room temperature, and hexane was added thereto to obtain a solid. The resulting solid was filtered through a filter to remove the solvent and separated by column chromatography to obtain 0.71 g of compound **14-3** (yield: 5.8%).

[288] Synthesis of compound **C-334**

[289] 0.71 g of compound **14-3** (1.56 mmol), 0.45 g of 2-chloro-3-phenylquinoxaline (1.87 mmol), 1.01 g of cesium carbonate (3.12 mmol), and 0.095 g of 4-dimethylaminopyridine (0.78 mmol) were dissolved in 30 mL of dimethyl sulfur monoxide in a flask and stirred at 100°C for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water and methanol were added thereto. The resulting solid was filtered through a filter to remove the solvent and separated by column chromatography to obtain 0.50 g of compound **C-334** (yield: 49%).

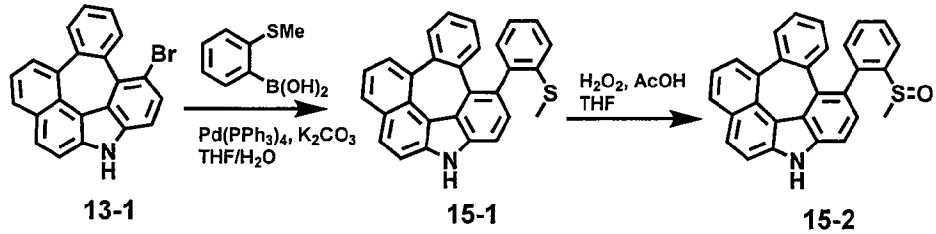
[290] ^{1}H NMR (600MHz, $CDCl_3$,δ) 8.333-8.248 (m, 3H), 8.192-8.099 (m, 1H), 7.911-7.820 (m, 3H), 7.767-7.754 (d, 1H), 7.613-7.526 (m, 5H), 7.488-7.410 (m, 4H), 7.395-7.347 (m, 3H), 7.329-7.296 (m, 2H), 7.230-7.205 (m, 2H), 7.179-7.153 (m, 1H), 7.130-7.075 (m, 1H), 7.056-7.030 (m, 1H), 6.874-6.688 (m, 1H)

[291]

Compound	MW	M.P.
C-334	660.78	290°C

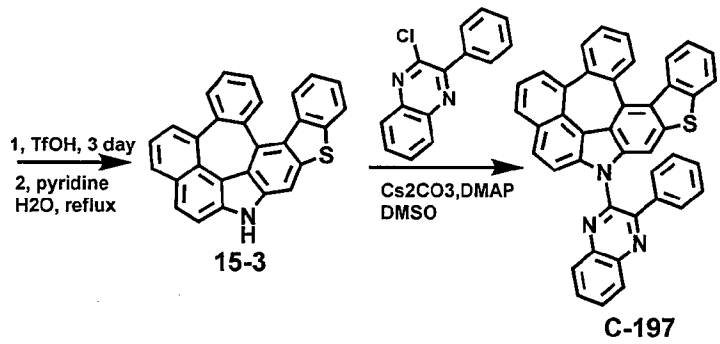
[292] **Example 15: Preparation of compound C-197**

[293]



13-1 15-1 15-2

[294]



15-3 C-197

[295] Synthesis of compound **15-1**

[296] 40 g of compound **13-1** (108 mmol), 25.4 g of (2-methylthiophenyl)boronic acid

(153.5 mmol), 6.26 g of tetrakis(triphenylphosphine)palladium(0) (5.40 mmol), and 26.3 g of potassium carbonate (272.0 mmol) were dissolved in 536 mL of tetrahydrofuran and 134 mL of distilled water in a flask and refluxed at 100℃ for 18 hours. After the reaction was completed, an organic layer was extracted with ethyl acetate, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 40 g of compound **15-1** (yield: 89%).

[297] Synthesis of compound **15-2**

[298] 40 g of compound **15-1** (96.8 mmol) was dissolved in 400 mL of tetrahydrofuran, 200 mL of acetic acid, and 12.6 mL of 34.5% hydrogen peroxide (145.2 mmol) in a flask and stirred at room temperature for 20 hours. After the reaction was completed, the mixture was concentrated, and an organic layer was extracted with methylene chloride and an aqueous solution of sodium hydrogencarbonate, and then residual moisture was removed by using magnesium sulfate. The residue was dried to obtain 42 g of compound **15-2** (yield: 100%).

[299] Synthesis of compound **15-3**

[300] 42 g of compound **15-2** (96.4 mmol) was dissolved in 190 mL of trifluoromethanesulfonic acid and stirred at room temperature for 3 days. After the reaction was completed, 50 mL of pyridine and 1M aqueous NaOH solution were added to the mixture at 0℃ to adjust the pH to 7 to 8, and the mixture was refluxed at 100℃ for 1 hour. The resulting solid was filtered through a filter to remove the solvent and separated by column chromatography to obtain 9.1 g of compound **15-3** (yield: 24%).

[301] Synthesis of compound **C-197**

[302] 4 g of compound **15-3** (10.1 mmol), 3 g of 2-chloro-3-phenylquinoxaline (12.1 mmol), 6.6 g of cesium carbonate (20.2 mmol), and 0.62 g of 4-dimethylaminopyridine (5.1 mmol) were dissolved in 50 mL of dimethyl sulfur monoxide in a flask and stirred at 100℃ for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water and methanol were added thereto. The resulting solid was filtered through a filter to remove the solvent and separated by column chromatography to obtain 4.8 g of compound **C-197** (yield: 79%).

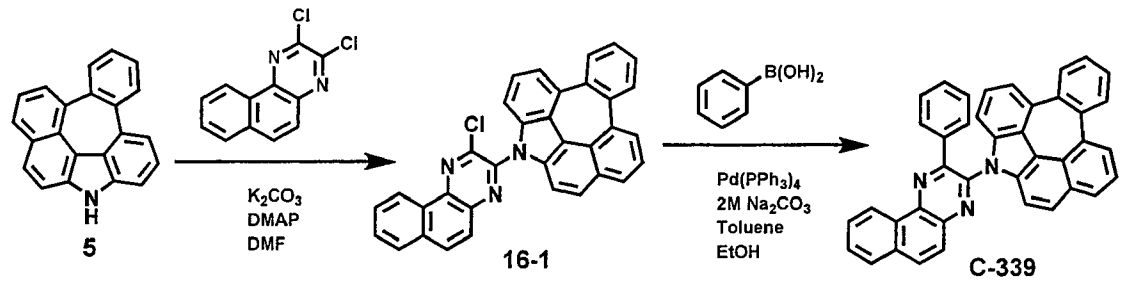
[303] ^{1}H NMR (600MHz, $CDCl_3$,δ) 8.337-8.310 (m, 1H), 8.247-8.202 (m, 1H), 8.196-8.151 (m, 1H), 7.957-7.945 (m, 1H), 7.928 (s, 1H), 7.912-7.837 (m, 3H), 7.794-7.728 (m, 3H), 7.685-7.672 (d, 1H), 7.531-7.498 (m, 1H), 7.469-7.414 (m, 2H), 7.348-7.300 (m, 2H), 7.262-7.173 (m, 4H), 7.102-7.087 (d, 1H), 7.036-6.955 (m, 1H)

[304]

Compound	MW	M.P.	Tg
C-197	601.73	317°C	194°C

[305] **Example 16: Preparation of compound C-339**

[306]



[307] Synthesis of compound **16-1**

[308] 15.6 g of compound **5** (53.5 mmol), 20 g of 2,3-dichlorobenzo[*f*]quinoxaline (80.3 mmol), 15 g of potassium carbonate (107.0 mmol), and 3.3 g of N,N-dimethyl-4-pyridineamine (26.7 mmol) were added to 270 mL of N,N-dimethylformamide and stirred at 150°C for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature and the solvent was removed by a rotary evaporator. The residue was separated by column chromatography to obtain 2.2 g of compound **16-1** (yield: 8%).

[309] Synthesis of compound **C-339**

[310] 2.2 g of compound **16-1** (4.4 mmol), 800 mg of phenylboronic acid (6.6 mmol), 250 mg of tetrakis(triphenylphosphine)palladium (0.2 mmol), and 1.2 g of sodium carbonate (10.9 mmol), 20 mL of toluene, and 5 mL of ethanol were added to a reaction vessel, and the mixture was stirred at 130°C for 3 hours. After the reaction was completed, the reaction product was cooled to room temperature and the solvent was removed by a rotary evaporator. The residue was separated by column chromatography to obtain 1.8 g of compound **C-339** (yield: 76%).

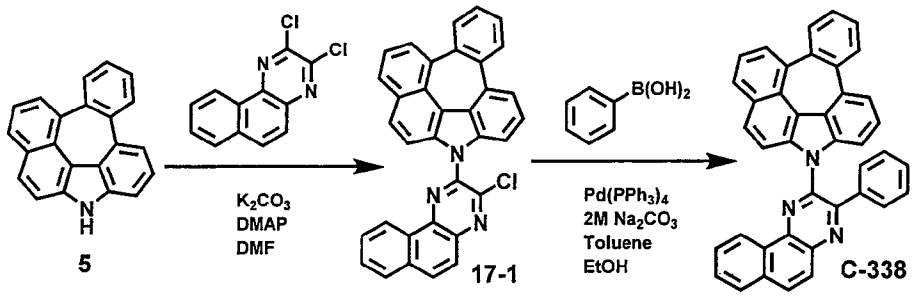
[311] ^{1}H NMR (600MHz, $CDCl_3$,δ) 9.403-9.390 (d, 1H), 8.119-8.105 (d, 1H), 8.012-7.997 (d, 1H), 7.994-7.979 (d, 1H), 7.867-7.851 (m, 1H), 7.847-7.822 (td, 1H), 7.815-7.788 (td, 1H), 7.734-7.722 (d, 1H), 7.686-7.656 (m, 4H), 7.600-7.585 (m, 1H), 7.509-7.494 (d, 1H), 7.404-7.389 (m, 2H), 7.385-7.359 (t, 1H), 7.295-7.264 (m, 2H), 7.250-7.219 (t, 1H), 7.208-7.182 (m, 3H)

[312]

Compound	MW	M.P.	Tg
C-339	545.65	247°C	148°C

[313] **Example 17: Preparation of compound C-338**

[314]



[315] Synthesis of compound **17-1**

[316] 15.6 g of compound **5** (53.5 mmol), 20 g of 2,3-dichlorobenzo[*f*]quinoxaline (80.3 mmol), 15 g of potassium carbonate (107.0 mmol), and 3.3 g of N,N-dimethyl-4-pyridineamine (26.7 mmol) were added to 270 mL of N,N-dimethylformamide and stirred at 150°C for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature and the solvent was removed by a rotary evaporator. The residue was separated by column chromatography to obtain 2.8 g of compound **17-1** (yield: 10%).

[317] Synthesis of compound **C-338**

[318] 2.7 g of compound **17-1** (5.4 mmol), 1 g of phenylboronic acid (8.0 mmol), 310 mg of tetrakis(triphenylphosphine)palladium (0.3 mmol), 1.4 g of sodium carbonate (13.4 mmol), 28 mL of toluene, and 7 mL of ethanol were added to a reaction vessel, and the mixture was stirred at 130°C for 3 hours. After the reaction was completed, the reaction product was cooled to room temperature and the solvent was removed by a rotary evaporator. The residue was separated by column chromatography to obtain 2.5 g of compound **C-338** (yield: 86%).

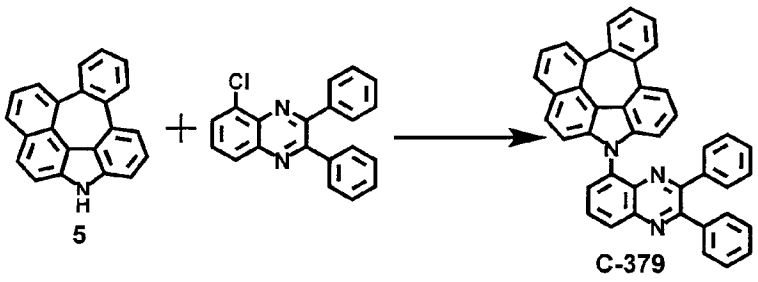
[319] ^{1}H NMR (600MHz, $CDCl_3$,δ) 9.119-9.106 (d,1H), 8.160-8.125 (dd, 2H), 8.001-7.988 (d, 1H), 7.878-7.862 (m, 1H), 7.782-7.755 (td, 1H), 7.748-7.726 (m, 2H), 7.709-7.685 (t, 2H), 7.623-7.594 (m, 3H), 7.518-7.503 (d, 1H), 7.418-7.371 (m, 4H), 7.305-7.271 (m, 2H), 7.200-7.182 (m, 3H)

[320]

Compound	MW	M.P.	Tg
C-338	545.65	299°C	149°C

[321] **Example 18: Preparation of compound C-379**

[322]



[323] 4.0 g of compound **5** (13.73 mmol), 5.2 g of 5-chloro-2,3-diphenylquinoxaline (16.47 mmol), 0.629 g of tris(dibenzylideneacetone)dipalladium(0) (0.686 mmol), 0.564 mg of 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (1.0 mmol), and 3.9 g of sodium *tert*-butoxide (41 mmol) were dissolved in 80 mL of 1,2-dimethylbenzene in a flask and refluxed for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water was added thereto. The organic layer was extracted with MC and dried over magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 2.8 g of compound **C-379** (yield: 35.67%).

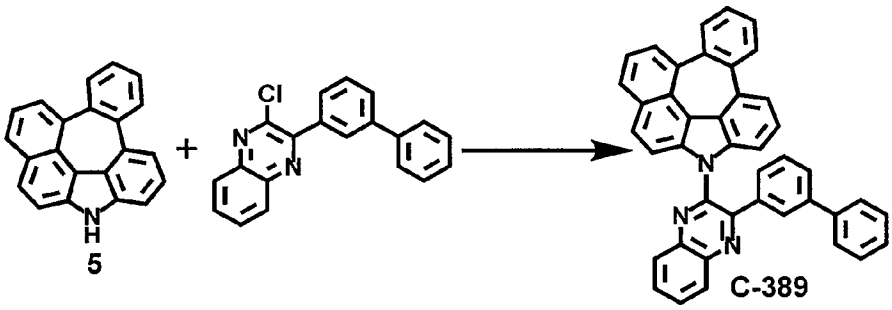
[324] ^{1}H NMR (600MHz, CDCl3, δ) 8.323-8.307 (d, J=7.2Hz, 1H), 7.947-7.935 (m, 2H), 7.883-7.867 (m, 1H), 7.762-7.749 (d, J=7.2Hz, 2H), 7.686-7.673 (d, J=7.8Hz, 1H), 7.633-7.603 (m, 2H), 7.568-7.556 (d, J=7.2Hz, 2H), 7.404-7.337 (m, 6H), 7.307-7.281 (t, J=7.8Hz, 1H), 7.195-7.281 (m, 3H), 7.144-7.110 (t, J=7.2HZ, 1H), 7.087-7.074 (d, J=7.8HZ, 1H), 7.010-6.990 (m, 2H)

[325]

Compound	MW	Tg	M.P.
C-379	571.67	135.60°C	142°C

[326] **Example 19: Preparation of compound C-389**

[327]



[328] 6.0 g of compound **5** (21 mmol), 7.8 g of 2-([1,1'-biphenyl]-3-yl)-3-chloroquinoxaline (25 mmol), 8.5 g of potassium carbonate (62 mmol), and 0.126 g of 4-dimethylaminopyridine (1 mmol) were dissolved in 100 mL of dimethyl formamide in a flask and refluxed for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature, and distilled water was added thereto. The organic layer was extracted with MC and dried over magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 8.8 g of compound **C-389** (yield: 74%).

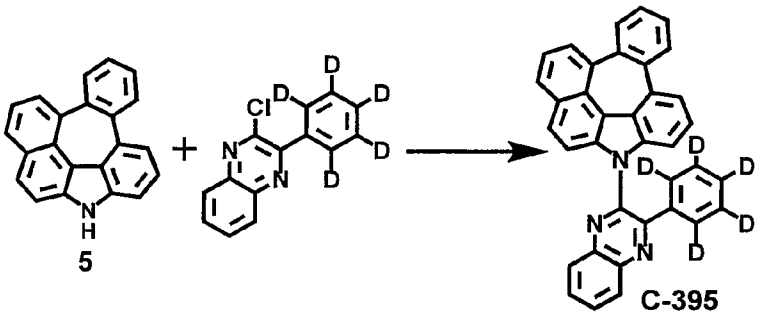
[329] ^{1}H NMR (600MHz, CDCl3, δ) 8.338-8.325 (d, J=7.8HZ, 1H), 8.228-8.212 (d, J=8.7HZ, 1H), 7.907-7.877 (m, 3H), 7.783-7.758 (m, 2H), 7.686-7.683 (d, J=7.8Hz, 2H), 7.630-7.590 (m, 1H), 7.523-7.508 (d, J=9Hz, 2H), 7.447-7.390 (m, 3H), 7.341-7.332 (m, 2H), 7.284-7.236 (m, 3H), 7.205 (s, 1H), 7.088-7.066 (m, 1H), 7.016-7.002 (d, J=7.8Hz, 2H), 6.903-6.877 (m, 2H)

[330]

Compound	MW	Tg	M.P.
C-389	571.67	120.06°C	202°C

[331] **Example 20: Preparation of compound C-395**

[332]



[333] 7.9 g of compound **5** (27 mmol), 7.9 g of 2-chloro-3-(phenyl-D5)quinoxaline (33 mmol), 11.24 g of potassium carbonate (81 mmol), and 0.166 g of 4-dimethylaminopyridine (1 mmol) were dissolved in 135 mL of dimethyl formamide in a flask and refluxed for 4 hours. After the reaction was completed, the reaction product was cooled to room temperature and distilled water was added thereto. The organic layer was extracted with MC and dried over magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 3.2 g of compound **C-395** (yield: 23.7%).

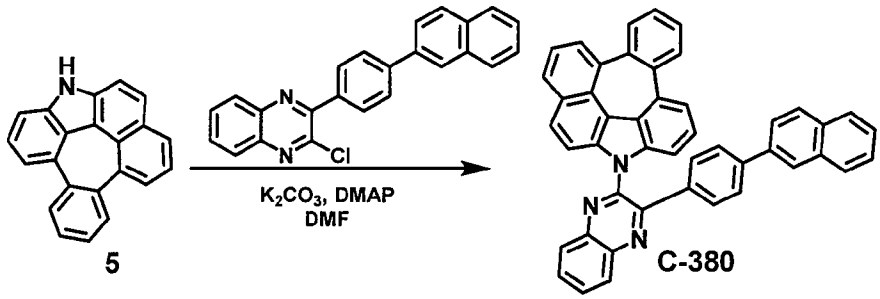
[334] ^{1}H NMR (600MHz, CDCl3, δ) 8.318-8.305 (d, J=7.8Hz, 1H), 8.164-8.151 (d, J= 7.8Hz, 1H), 7.892-7.834 (m, 3H), 7.740-7.728 (d, J=7.2Hz, 1H), 7.691-7.679 (d, J=7.2Hz, 2H), 7.603-7.587 (m, 1H), 7.508-7.493 (d, J=9Hz, 1H), 7.413-7.370 (m, 3H), 7.291-7.250 (m, 2H), 7.212-7.197 (d, J=9Hz, 1H)

[335]

Compound	MW	Tg	M.P.
C-395	500.62	127°C	158°C

[336] **Example 21: Preparation of compound C-380**

[337]



[338] 10 g of compound **5** (28.82 mmol), 7.0 g of 2-chloro-3-(4-(naphthalen-2-yl)phenyl)quinoxaline (24.02 mmol), 1.5 g of 4-(dimethylamino)pyridine (12.01 mmol), and 3.3 g of potassium carbonate (24.02 mmol) were dissolved in 130 mL of dimethyl formamide in a flask and refluxed for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 8.8 g of compound **C-380** (yield: 59%).

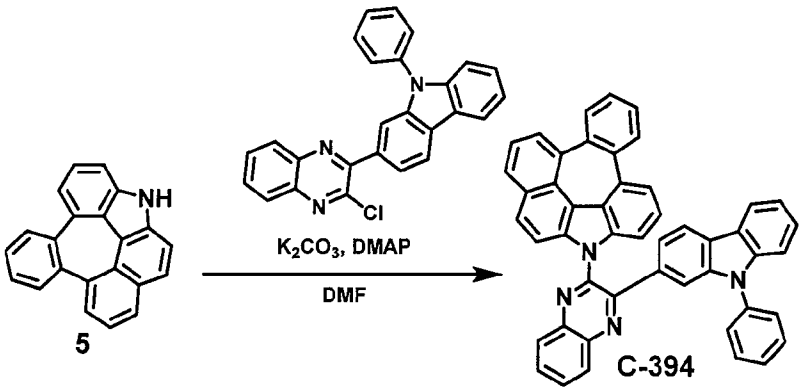
[339] ^{1}H NMR (600MHz, CDCl3, δ) 8.33-8.32 (d, J=6.0 Hz, 1H), 8.16-8.15 (d, J= 6.0 Hz, 1H), 7.88-7.84 (m, 4H), 7.80-7.77 (m, 3H), 7.74-7.73(d, J= 6.0 Hz, 1H), 7.69-7.66 (m, 4H), 7.57-7.56 (m, 2H), 7.53-7.50 (m, 3H), 7.43-7.37 (m, 5H), 7.32-7.23 (m, 3H)

[340]

Compound	MW	Tg	M.P.
C-380	621.74	145.6°C	262.7°C

[341] **Example 22: Preparation of compound C-394**

[342]



[343] 6 g of compound **5** (20.59 mmol), 9.1 g of 2-(3-chloroquinoxalin-2-yl)-9-phenyl-9H-carbazole (22.65 mmol), 1.2 g of 4-(dimethylamino)pyridine (10.29 mmol), and 2.8 g of potassium carbonate (20.59 mmol) were dissolved in 100 mL of dimethyl formamide in a flask and refluxed for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 9.6 g of compound **C-394** (yield: 70%).

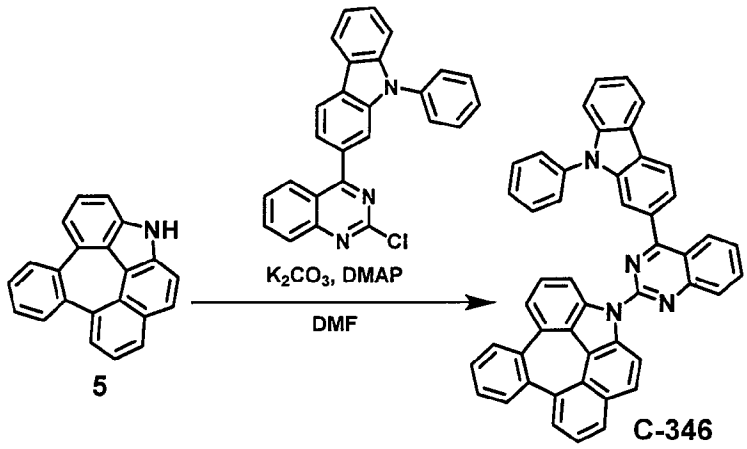
[344] ^{1}H NMR (600MHz, CDCl3, δ) 8.31-8.30 (d, J= 6.0 Hz, 1H), 8.13-8.11 (d, J= 12.0 Hz, 1H), 8.04-8.03 (d, J= 6.0Hz, 1H), 7.94-7.93 (d, J= 6.0 Hz, 1H), 7.86-7.81 (m, 3H), 7.74-7.73 (d, J=6.0 Hz, 1H), 7.65-7.63 (d, J= 12.0 Hz, 2H), 7.61-7.60 (m, 1H), 7.44-7.36 (m, 4H), 7.30-7.28 (m, 1H), 7.23-7.15 (m, 6H), 6.98-6.93 (m, 3H), 6.88-6.87 (m, 2H)

[345]

Compound	MW	Tg	M.P.
C-394	660.78	154.09°C	290.5°C

[346] **Example 23: Preparation of compound C-346**

[347]



[348] 6.0 g of compound **5** (20.59 mmol), 9.1 g of 2-(2-chloroquinazolin-4-yl)-9-phenyl-9H-carbazole (22.65 mmol), 1.2 g of 4-(dimethylamino)pyridine (10.29 mmol), and 2.8 g of potassium carbonate (20.59

mmol) were dissolved in 100 mL of dimethyl formamide in a flask and refluxed for 3 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 10 g of compound **C-346** (yield: 77%).

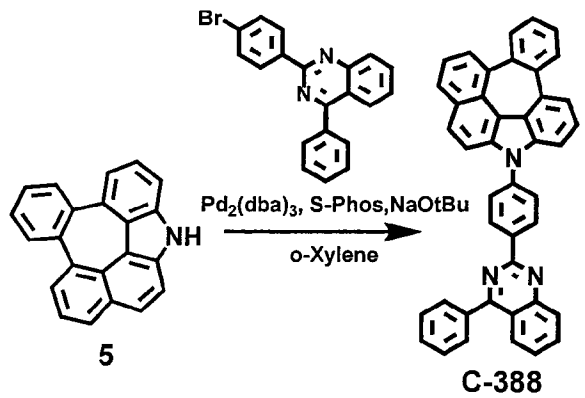
[349] ^{1}H NMR (600MHz, CDCl3, δ) 9.01-9.00 (d, J=6.0 Hz, 1H), 8.85-8.84 (d, J=6.0 Hz, 1H), 8.34-8.33 (d, J=6.0 Hz, 1H), 8.23-8.22 (d, J=6.0 Hz, 2H), 8.11-8.10 (d, J=6.0 Hz, 1H), 8.05 (s, 1H), 7.86-7.82 (m, 2H), 7.79-7.77 (m, 1H), 7.75-7.71 (m, 3H), 7.67-7.64 (m. 3H), 7.59-7.57 (m, 2H), 7.53-7.52 (m, 1H), 7.50-7.47 (m, 3H), 7.43-7.37 (m, 2H), 7.36-7.35 (m, 4H)

[350]

Compound	MW	Tg	M.P.
C-346	660.78	158°C	189.9°C

[351] **Example 24: Preparation of compound C-388**

[352]



[353] 12 g of compound **5** (41.1 mmol), 14.8 g of 2-(4-bromophenyl)-4-phenylquinazoline (41.1 mmol), 1.5 g of tris(dibenzylideneacetone)dipalladium(0) (1.6 mmol), 1.7 g of 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (4.1 mmol), and 9.8 g of sodium *tert*-butoxide (102.9 mmol) were dissolved in 274 mL of o-xylene in a flask and refluxed for 4 hours. After the reaction was completed, the reaction product was cooled and separated by column chromatography to obtain 1.1 g of compound **C-388** (yield: 4.7%).

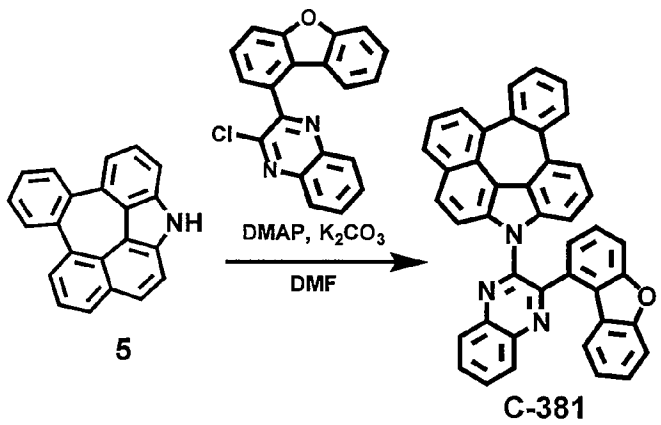
[354] ^{1}H NMR (600MHz, CDCl3, δ) 8.927-8.912 (d, J=7.8Hz, 2H), 8.199-8.160 (m, 2H), 7.925-7.910 (m, 3H), 7.865-7.855 (m, 1H),7.759-7.672 (m, 6H), 7.620-7.587 (m, 5H), 7.540-7.525 (d, J=9Hz, 1H), 7.401-7.375 (m, 3H), 7.339-7.328 (m, 2H)

[355]

Compound	MW	Tg	M.P.
C-388	571.6	133°C	241°C

[356] **Example 25: Preparation of compound C-381**

[357]



[358] 5.7 g of compound **5** (19.5 mmol), 7.7 g of 2-chloro-3-(dibenzo[b,d]furan-1-yl)quinoxaline (23.2 mmol), 0.1 g of 4-(dimethylamino)pyridine (0.9 mmol), and 8.1 g of potassium carbonate (58.5 mmol) were dissolved in 99 mL of dimethyl formamide in a flask and refluxed for 3 hours and 30 minutes. After the reaction was completed, the reaction product was cooled, and methanol and water were added thereto and filtered. The residue was dried and separated by column chromatography to obtain 6 g of compound **C-381** (yield: 52%).

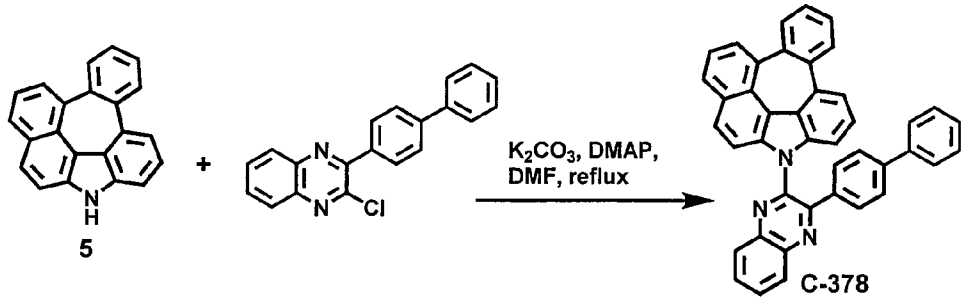
[359] ^{1}H NMR (600MHz, CDCl3, δ) 8.324-8.271 (m, 2H), 7.962-7.942 (m, 2H), 7.867-7.855 (d, J=7.2Hz, 1H), 7.821-7.805 (m, 1H), 7.705-7.693 (d, J=7.2Hz,1H), 7.655-7.595 (m, 3H), 7.567-7.537 (m, 2H), 7.394-7.272 (m, 8H), 7.124-7.155 (m, 1H), 6.984-6.958 (t, J=7.2Hz, 1H), 6.830-6.817 (d, J=7.8Hz, 1H)

[360]

Compound	MW	Tg	M.P.
C-381	585.6	154.79°C	233°C

[361] **Example 26: Preparation of compound C-378**

[362]



[363] 3.8 g of compound **5** (13 mmol), 5.0 g of 2-([1,1'-biphenyl]-4-yl)-3-chloroquinoxaline (16 mmol), 800 mg of DMAP (7 mmol), and 3.6 g of potassium carbonate (26 mmol) were dissolved in 55 mL of dimethyl formamide in a flask and refluxed for 18 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 1.4 g of compound **C-378** (yield: 19%).

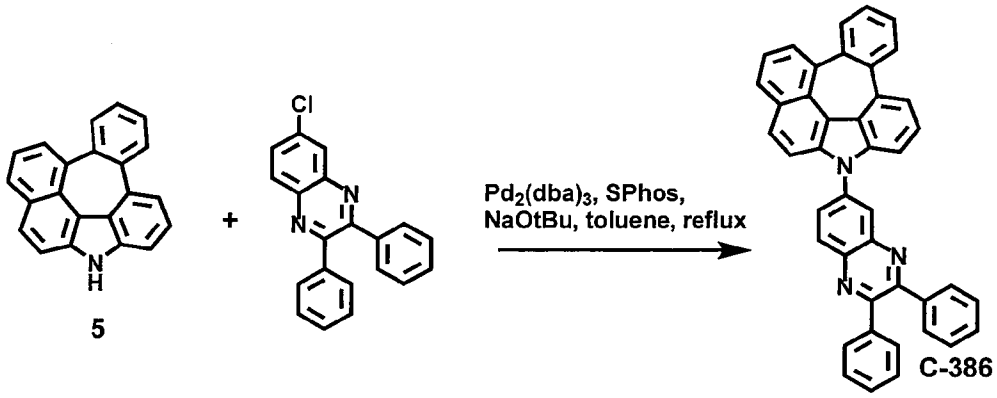
[364] ^{1}H NMR (600MHz, CDCl3, δ) 8.33-8.32(m, 1H), 8.17-8.16 (m, 1H), 7.90-7.84 (m, 3H), 7.74 (d, J=7.50 Hz, 1H), 7.69 (t, J= 6.72 Hz, 2H), 7.63 (d, J=8.4 Hz, 2H), 7.61-7.59 (m, 1H), 7.51 (d, J=9.00 Hz, 1H), 7.45-7.37 (m, 7H), 7.35-7.27 (m, 5H), 7.23 (d, J= 8.79 Hz, 1H)

[365]

Compound	MW	Tg	M.P.
C-378	571.68	137.6°C	189°C

[366] **Example 27: Preparation of compound C-386**

[367]



[368] 5.1 g of compound **5** (17 mmol), 5.0 g of 6-chloro-2,3-diphenylquinoxaline (16 mmol), 578 mg of tris(dibenzylideneacetone)dipalladium(0) (0.631 mmol), 648 mg of 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (2 mmol), and 3.8 g of sodium *tert* -butoxide (39 mmol) were dissolved in 100 mL of toluene in a flask and refluxed for 16 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 7.6 g of compound **C-386** (yield: 84%).

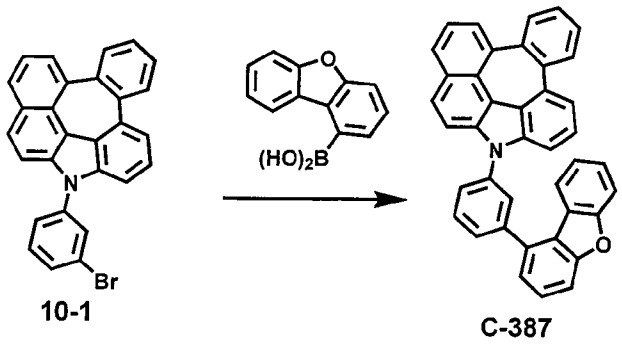
[369] ^{1}H NMR (600MHz, CDCl3, δ) 8.01 (s, 1H), 8.40 (d, J= 5.4 Hz, 1H), 7.99 (dd, J= 5.4 Hz; 2.22 Hz, 1H), 7.89-7.87 (m, 1H), 7.79-7.77 (m, 2H), 7.74-7.70 (m, 2H), 7.63-7.60 (m, 2H), 7.59-7.56 (m, 4H), 7.44 - 7.34 (m, 11H)

[370]

Compound	MW	Tg	M.P.
C-386	571.68	138.80°C	295°C

[371] **Example 28: Preparation of compound C-387**

[372]



[373] 6.6 g of compound **10-1** (14.78 mmol), 3.4 g of dibenzo[b,d]furan-1-yl-boronic acid (16.24 mmol), 0.85 g of tetrakis(triphenylphosphine)palladium(0) (0.739 mmol), and 4 g of potassium carbonate (29.57 mmol) were added to 60 mL of toluene, 15 mL of ethanol, and 15 mL of purified water and stirred under reflux for one day. After the reaction was completed, the reaction product was cooled to room temperature, and the resulting solid was filtered under reduced pressure. The solid was dissolved in $CHCl_3$ and separated by column chromatography using MC/Hex to obtain 3.5 g of compound **C-387** (yield: 45%).

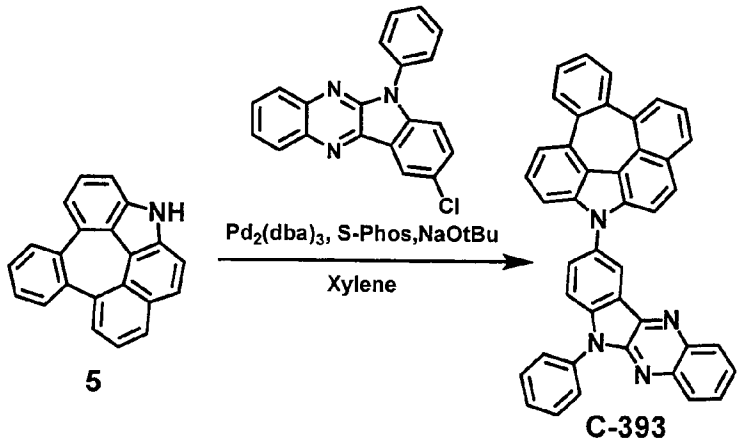
[374] ^{1}H NMR (600MHz, DMSO,δ) 7.953-7.927 (m,2H), 7.896-7.872 (t,2H), 7.848-7.810 (m,3H), 7.793-7.746 (m,4H), 7.656-7.601 (m,4H), 7.539-7.511 (t,1H), 7.485-7.443 (m,4H), 7.419-7.393 (t,1H), 7.369-7.356 (d,1H), 7.294-7.269 (t,1H)

[375]

Compound	MW	M.P.	Tg
C-387	533.6	224°C	117°C

[376] **Example 29: Preparation of compound C-393**

[377]



[378] 4.4 g of compound **5** (15.16 mmol), 5.0 g of 9-chloro-6-phenyl-6H-indolo[2,3,b]quinoxaline (15.16 mmol), 0.5 g of tris(dibenzylideneacetone)dipalladium(0) (0.606 mmol), 0.6 g of 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (1.516 mmol), and 12 g of sodium *tert*-butoxide (37.90 mmol) were dissolved in 100 mL of 1,2-dimethylbenzene in a

flask and refluxed for 4 hours. After the reaction was completed, the organic layer was extracted with ethyl acetate after distillation under reduced pressure, and residual moisture was removed by using magnesium sulfate. The residue was dried and separated by column chromatography to obtain 1.9 g of compound **C-393** (yield: 21%).

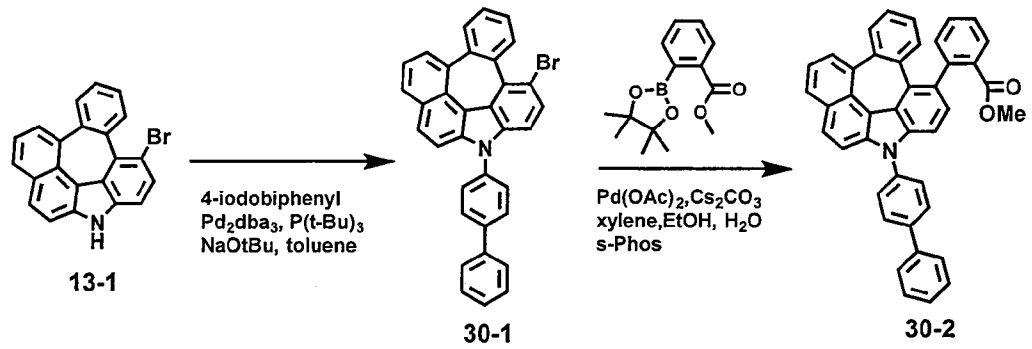
[379] ^{1}H NMR (600MHz, CDCl3,δ) 8.74 (s, 1H), 8.33-8.32 (d, J=6.0Hz, 1H), 8.15-8.14 (d, J=6.0Hz, 1H), 7.91-7.90 (m, 1H), 7.84-8.73 (m, 2H), 7.80-7.78 (m, 5H), 7.77-7.69 (m, 5H), 7.64-7.63 (m. 1H), 7.60-7.59 (m, 1H), 7.50-7.49 (d, J=6.0Hz, 1H), 7.43-7.41 (m, 3H), 7.36-7.34 (t, J=6.0 Hz, 1H), 7.28-7.27 (m, 1H)

[380]

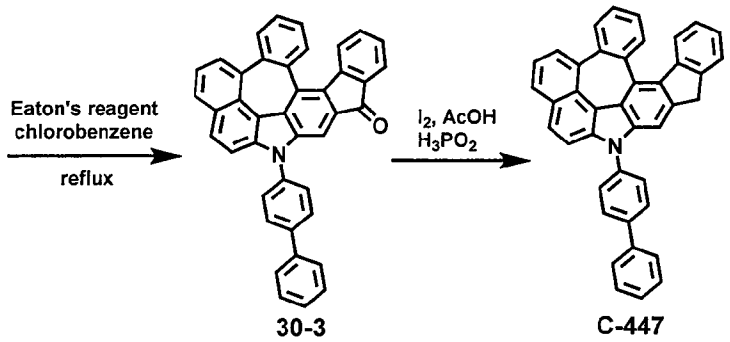
Compound	MW	Tg	M.P.
C-393	584.67	129.07°C	294°C

[381] **Example 30: Preparation of compound C-447**

[382]



[383]



[384] Synthesis of compound **30-1**

[385] 8.0 g of compound **13-1** (21.6 mmol), 12.1 g of 4-iodobiphenyl (43.2 mmol), 1.0 g of tris(dibenzylideneacetone)dipalladium(0) (1.08 mmol), 0.87 mL of tri-*tert* -butylphsophine (2.16 mmol, 50% toluene solution), and 5.2 g of sodium *tert*-butoxide (54.0 mmol) were dissolved in 216 mL of toluene in a flask and refluxed for 18 hours. After the reaction was completed, the reaction solution was cooled to room temperature, and the solvent was removed by a rotary evaporator. The residue was separated by column chromatography to obtain 7.5 g of compound **30-1** (yield: 66%).

[386] Synthesis of compound **30-2**

[387] 7.5 g of compound **30-1** (14.4 mmol), 4.5 g of methyl

2-(4,4,5,5-tetramethyl-1,3,2-dioxylboren-2-yl)benzoate (17.3 mmol), 323 mg of palladium acetate ($Pd(OAc)_2$) (1.44 mmol), 1.2 g of ligand (2-dicyclohexylphosphonium-2',6'-dimethoxybiphenyl) (2.88 mmol), 14 g of cesium carbonate (43.2 mmol), 80 mL of xylene, 40 mL of ethanol, and 40 mL of distilled water were added to a flask, and stirred under reflux for 18 hours. The mixture was cooled to room temperature and distilled water was added thereto. The organic layer was extracted with MC, and dried over magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 2.2 g of compound **30-2** (yield: 27%).

[388] Synthesis of compound **30-3**

[389] 2.2 g of compound **30-2** (3.8 mmol), 2 mL of Eaton's reagent, and 13 mL of benzene chloride were added to a flask and stirred under reflux for 18 hours. The mixture was cooled to room temperature and an aqueous solution of sodium hydrogencarbonate was added thereto. The organic layer was extracted with ethyl acetate (EA) and dried over magnesium sulfate. The residue was distilled under reduced pressure and separated by column chromatography to obtain 1.5 g of compound **30-3** (yield: 71%).

[390] Synthesis of compound **C-447**

[391] 244 mg of iodine (0.96 mmol), 0.48 mL of hypophosphorous acid (4.4 mmol, 50% aqueous solution), and 14 mL of acetic acid were added to a flask and stirred at 80°C for 30 minutes. 1.5 g of compound **30-3** (2.75 mmol) was slowly added dropwise thereto and stirred under reflux for 4 hours. The reaction solution was cooled to room temperature, and the precipitated solid was filtered and washed with a large amount of water and ethanol. The resulting solid was filtered through a filter to remove the solvent. The residue was separated by column chromatography to obtain 270 mg of compound **C-447** (yield: 18%).

[392] ^{1}H NMR (600MHz, $CDCl_3$,δ) 8.051-8.036 (dd, 1H), 7.967-7.953 (m, 1H), 7.920-7.909 (d, 1H), 7.857-7.843 (d, 2H), 7.797-7.784 (d, 1H), 7.720-7.698 (m, 2H), 7.669-7.643 (m, 3H), 7.562-7.500 (m, 5H), 7.463-7.416 (m, 5H), 7.217-7.190 (m, 2H), 4.153-4.188 (d, 1H), 3.949-3.913 (d, 1H)

[393] **Comparative Example 1: Producing an OLED device comprising a**

[394] **conventional compound as a host**

[395] OLED devices were produced by using a conventional compound not according to the present disclosure as a host. A transparent electrode indium tin oxide (ITO) thin film (10 Ω/sq) on a glass substrate for an OLED device (GEOMATEC CO., LTD., Japan) was subjected to an ultrasonic washing with acetone and isopropylalcohol, sequentially, and then was stored in isopropanol. The ITO substrate was then mounted on a substrate holder of a vacuum vapor deposition apparatus. Compound **HI-1** was introduced into a cell of the vacuum vapor deposition apparatus, and then the pressure in the chamber of the apparatus was controlled to 10^{-7} torr. Thereafter, an electric current

was applied to the cell to evaporate the above-introduced material, thereby forming a first hole injection layer having a thickness of 80 nm on the ITO substrate. Next, compound **HI-2** was introduced into another cell of the vacuum vapor deposition apparatus and was evaporated by applying an electric current to the cell, thereby forming a second hole injection layer having a thickness of 5 nm on the first hole injection layer. Compound **HT-1** was then introduced into a cell of the vacuum vapor deposition apparatus and was evaporated by applying an electric current to the cell, thereby forming a first hole transport layer having a thickness of 10 nm on the second hole injection layer. Compound **HT-3** was then introduced into another cell of the vacuum vapor deposition apparatus and was evaporated by applying an electric current to the cell, thereby forming a second hole transport layer having a thickness of 60 nm on the first hole transport layer. After forming the hole injection layers and the hole transport layers, a light-emitting layer was formed thereon as follows: **CBP** was introduced into one cell of the vacuum vapor depositing apparatus as a host, and compound **D-39** was introduced into another cell as a dopant. The two materials were evaporated at a different rate and the dopant was deposited in a doping amount of 3 wt% based on the total amount of the host and the dopant to form a light-emitting layer having a thickness of 40 nm on the second hole transport layer. Compounds **ETL-1:EIL-1** were deposited in a weight ratio of 50:50 to form an electron transport layer having a thickness of 35 nm on the light-emitting layer. After depositing compound **EIL-1** as an electron injection layer having a thickness of 2 nm on the electron transport layer, an Al cathode having a thickness of 80 nm was deposited on the electron injection layer by another vacuum vapor deposition apparatus. All the materials used for producing the OLED were purified by vacuum sublimation at 10^{-6} torr.

[396] **Device Examples 1 to 5: Producing an OLED device comprising the**

[397] **plurality of host materials according to the present disclosure**

[398] OLED devices were produced in the same manner as in Comparative Example 1, except that a light-emitting layer was formed as follows: The first host compound and the second compound shown in Table 1 were introduced into two cells of the vacuum vapor depositing apparatus as a host, and compound **D-39** was introduced into another cell as a dopant. The two host materials were evaporated at a rate of 1:1 and the dopant material was simulataneously evaporated at a different rate, and the dopant was deposited in a doping amount of 3 wt% based on the total amount of the host and the dopant to form a light-emitting layer having a thickness of 40 nm on the second hole transport layer.

[399] The driving voltage and the luminous efficiency at a luminance of 5,000 nit, and the time taken for luminance to decrease from 100% to 98% at a luminance of 5,000 nit

(lifespan; T98) of the OLED devices produced in Comparative Example 1 and Device Examples 1 to 5 are provided in Table 1 below.

[400] [Table 1]

	First Host	Second Host	Driving Voltage (V)	Luminous Efficiency (cd/A)	Lifespan (T98, hr)
Comparative Example 1		CBP	11.6	9.3	0.07
Device Example 1	C-387	C-8	4.1	25.8	358.6
Device Example 2	C-306	C-8	3.9	25.1	282.1
Device Example 3	C-449	C-8	4.4	25.5	428.3
Device Example 4	C-448	C-8	4.0	24.5	168.9
Device Example 5	C-7	C-8	3.8	23.4	265.3

[401] **Device Example 6: Producing an OLED device comprising the plurality of**

[402] **host materials according to the present disclosure**

[403] An OLED device was produced in the same manner as in Comparative Example 1, except that compound **HT-2** was used as a second hole transport material instead of compound **HT-3**, and a light-emitting layer was formed as follows: The first host compound (**C-339**) and the second compound (**C-338**) were introduced into two cells of the vacuum vapor depositing apparatus as a host, and compound **D-39** was introduced into another cell as a dopant. The two host materials were evaporated at a rate of 1:1 and the dopant material was simulataneously evaporated at a different rate, and the dopant was deposited in a doping amount of 3 wt% based on the total amount of the host and the dopant to form a light-emitting layer having a thickness of 40 nm on the second hole transport layer.

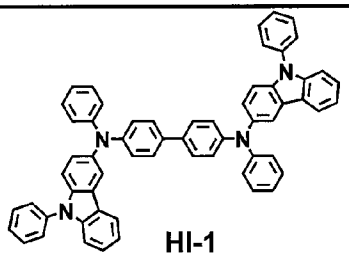
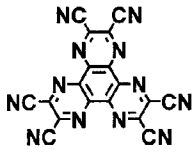
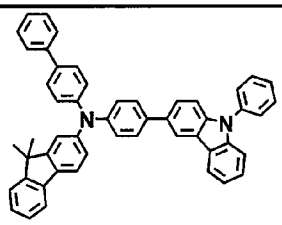
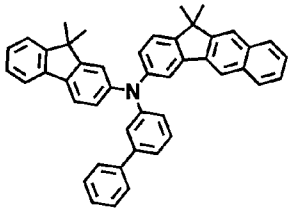
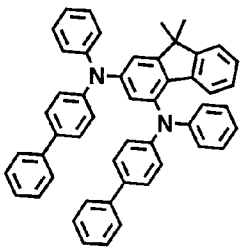
[404] The driving voltage and luminous efficiency based on a luminance of 1,000 nit of the OLED device produced in Device Example 6 was 2.8 V and 29.0 cd/A, respectively, and the time taken to be reduced from 100% to 98% of the luminance (lifespan; T98) based on a luminance of 5,000 nit was 169.8 hr.

[405] From Table 1 and Device Example 6 above, it can be seen that the OLED devices comprising the plurality of host materials of the present disclosure have low driving voltage, high luminous efficiency, and/or improved lifespan properties compared to the

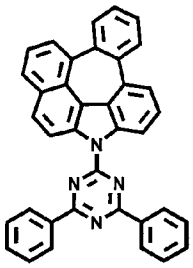
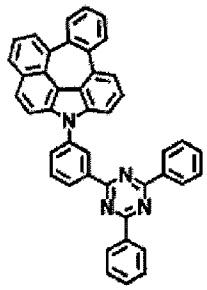
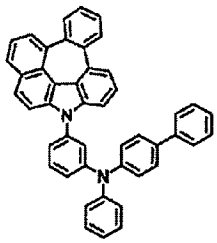
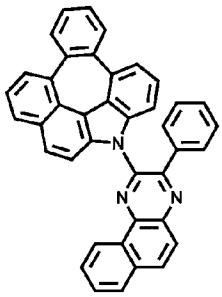
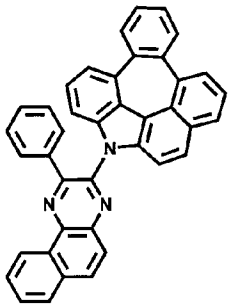
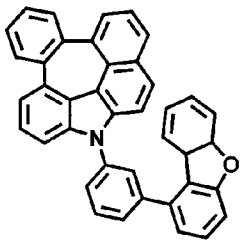
OLED device comprising a conventional organic electroluminescent compound.

[406] The compounds used in the Device Examples and the Comparative Example are shown in Table 2 below.

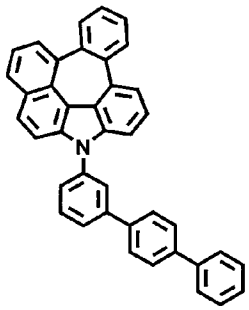
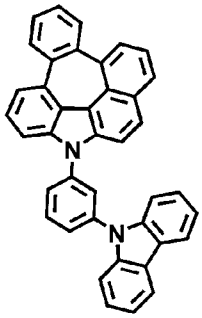
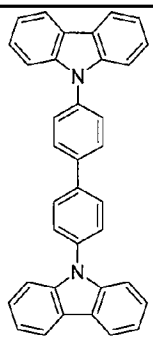
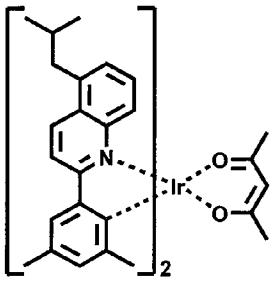
[407] [Table 2]

Hole Injection Layer/ Hole Transport Layer	 HI-1  HI-2  HT-1  HT-2  HT-3

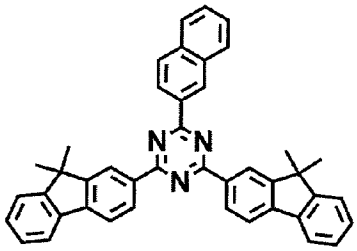
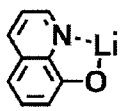
[408]

Light-Emitting Layer	 C-7  C-8  C-306  C-338  C-339  C-387

[409]

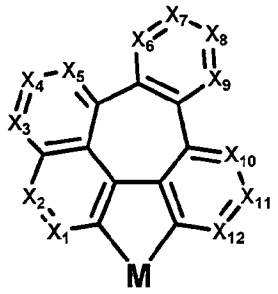
Light-Emitting Layer	 C-448  C-449  CBP  D-39

[410]

Electron Transport Layer/ Electron Injection Layer	 ETL-1  EIL-1

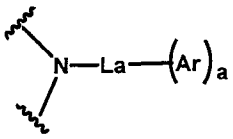
Claims

[Claim 1] A plurality of host materials comprising a first host compound and a second host compound, wherein the first host compound and the second host compound are represented by the following formula 1, and the first host compound and the second host compound are different from each other:



----- (1)

wherein

M represents  O or S;

,

X_1 to X_{12}, each independently, represent N or CR_1;

La represents a single bond, a substituted or unsubstituted (C1-C30)alkylene, a substituted or unsubstituted (C6-C30)arylene, a substituted or unsubstituted (3- to 30-membered)heteroarylene, or a substituted or unsubstituted (C3-C30)cycloalkylene;

Ar and R_1, each independently, represent hydrogen, deuterium, a halogen, a cyano, 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 (C1-C30)alkoxy, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsubstituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a substituted or unsubstituted mono- or di-(C1-C30)alkylamino, a substituted or unsubstituted mono- or di-(C6-C30)arylamino, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino; or adjacent Ar's may be linked to each other to form a ring, or adjacent R_1's may be linked to each other to form a ring, where if a plurality of R_1's are present, each of R_1 may be the same or different; and

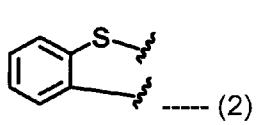
a represents an integer of 1 or 2, where if a is 2, each of Ar may be the same or different.

[Claim 2] The plurality of host materials according to claim 1, wherein the substituents of the substituted (C1-C30)alkyl(ene), the substituted (C6-C30)aryl(ene), the substituted (3- to 30-membered)heteroaryl(ene), the substituted (C3-C30)cycloalkyl(ene), the substituted (C1-C30)alkoxy, the substituted tri(C1-C30)alkylsilyl, the substituted di(C1-C30)alkyl(C6-C30)arylsilyl, the substituted (C1-C30)alkyldi(C6-C30)arylsilyl, the substituted tri(C6-C30)arylsilyl, the substituted mono- or di- (C1-C30)alkylamino, the substituted mono- or di- (C6-C30)arylamino, and the substituted (C1-C30)alkyl(C6-C30)arylamino in La, Ar, and R_1, each independently, are at least one selected from the group consisting of deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a (C1-C30)alkyl, a halo(C1-C30)alkyl, a (C2-C30)alkenyl, a (C2-C30)alkynyl, a (C1-C30)alkoxy, a (C1-C30)alkylthio, a (C3-C30)cycloalkyl, a (C3-C30)cycloalkenyl, a (3- to 7-membered)heterocycloalkyl, a (C6-C30)aryloxy, a (C6-C30)arylthio, a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl, a (C6-C30)aryl unsubstituted or substituted with a (3- to 30-membered)heteroaryl, a tri(C1-C30)alkylsilyl, a tri(C6-C30)arylsilyl, a di(C1-C30)alkyl(C6-C30)arylsilyl, a (C1-C30)alkyldi(C6-C30)arylsilyl, an amino, a mono- or di-(C1-C30)alkylamino, a mono- or di- (C6-C30)arylamino unsubstituted or substituted with a (C1-C30)alkyl, a (C1-C30)alkyl(C6-C30)arylamino, a (C1-C30)alkylcarbonyl, a (C1-C30)alkoxycarbonyl, a (C6-C30)arylcarbonyl, a di(C6-C30)arylboronyl, a di(C1-C30)alkylboronyl, a (C1-C30)alkyl(C6-C30)arylboronyl, a (C6-C30)aryl(C1-C30)alkyl, and a (C1-C30)alkyl(C6-C30)aryl.

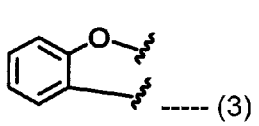
[Claim 3] The plurality of host materials according to claim 1, wherein Ar represents a substituted or unsubstituted phenyl, a substituted or unsubstituted naphthyl, a substituted or unsubstituted biphenyl, a substituted or unsubstituted terphenyl, a substituted or unsubstituted fluorenyl, a substituted or unsubstituted fluoranthenyl, a substituted or unsubstituted triazinyl, a substituted or unsubstituted pyridyl, a substituted or unsubstituted pyrimidinyl, a substituted or unsubstituted benzothienopyrimidinyl, a substituted or unsubstituted acenaphthopyrimidinyl,

a substituted or unsubstituted quinazolinyl, a substituted or unsubstituted benzoquinazolinyl, a substituted or unsubstituted quinoxalinyl, a substituted or unsubstituted benzoquinoxalinyl, a substituted or unsubstituted dibenzoquinoxalinyl, a substituted or unsubstituted quinolyl, a substituted or unsubstituted benzoquinolyl, a substituted or unsubstituted isoquinolyl, a substituted or unsubstituted benzoisoquinolyl, a substituted or unsubstituted benzothienoquinolyl, a substituted or unsubstituted benzofuroquinolyl, a substituted or unsubstituted triazolyl, a substituted or unsubstituted pyrazolyl, a substituted or unsubstituted carbazolyl, a substituted or unsubstituted dibenzothiophenyl, a substituted or unsubstituted benzothiophenyl, a substituted or unsubstituted dibenzofuranyl, a substituted or unsubstituted benzofuranyl, a substituted or unsubstituted naphthyridinyl, a substituted or unsubstituted benzothiazolinyl, a substituted or unsubstituted phenanthroimidazolyl, a substituted or unsubstituted diphenylamino, a substituted or unsubstituted phenylbiphenylamino, a substituted or unsubstituted fluorenylphenylamino, a substituted or unsubstituted dibenzothiophenylphenylamino, or a substituted or unsubstituted dibenzofuranylphenylamino.

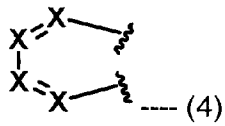
[Claim 4] The plurality of host materials according to claim 1, wherein two adjacent X_1 to X_{12} are CR_1, two adjacent R_1's are linked to each other to form any one ring of the following formulas 2 to 6, and one or more of the rings are formed in one compound represented by formula 1:



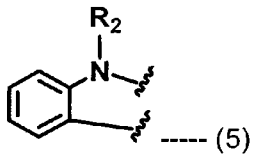
----- (2)



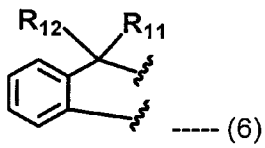
----- (3)



---- (4)



----- (5)



----- (6)

wherein

R_2 represents hydrogen, deuterium, a halogen, a cyano, 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 (C1-C30)alkoxy, a substituted or unsubstituted tri(C1-C30)alkylsilyl, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl, a substituted or unsub-

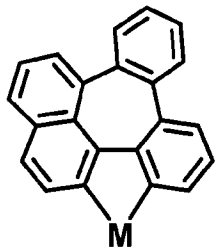
stituted (C1-C30)alkyldi(C6-C30)arylsilyl, a substituted or unsubstituted tri(C6-C30)arylsilyl, a substituted or unsubstituted mono- or di-(C1-C30)alkylamino, a substituted or unsubstituted mono- or di-(C6-C30)arylamino, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino;

X represents N or CH;

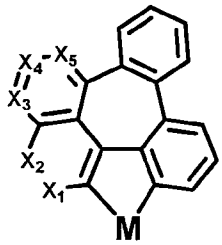
R_{11} and R_{12}, each independently, represent hydrogen, deuterium, a halogen, a cyano, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked to each other to form a ring; and

~ represents a connecting site between C and R_1 in CR_1.

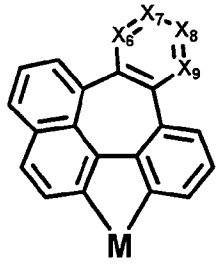
[Claim 5] The plurality of host materials according to claim 1, wherein formula 1 is represented by any one of the following formulas 7 to 10:



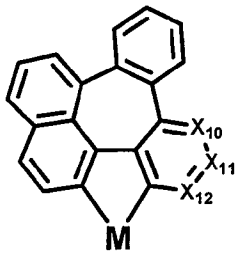
----- (7)



----- (8)



----- (9)

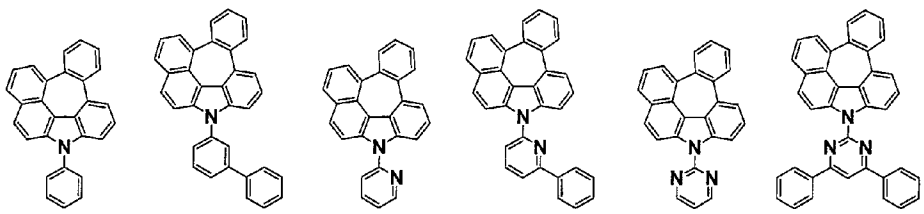


----- (10)

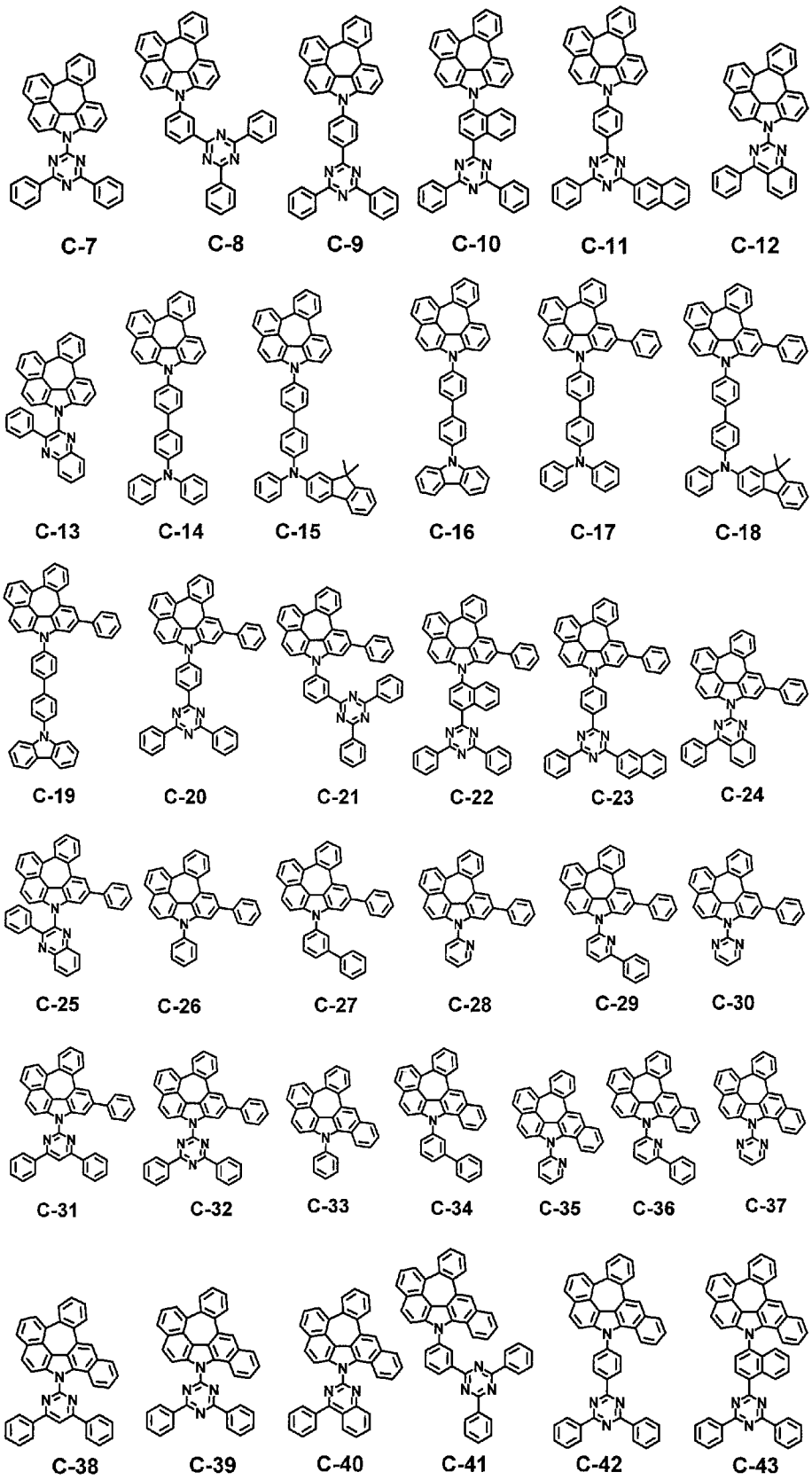
wherein

X_1 to X_{12} and M are as defined in claim 1.

[Claim 6] The plurality of host materials according to claim 1, wherein the compound represented by formula 1 is selected from the following compounds:



C-1 C-2 C-3 C-4 C-5 C-6


C-7
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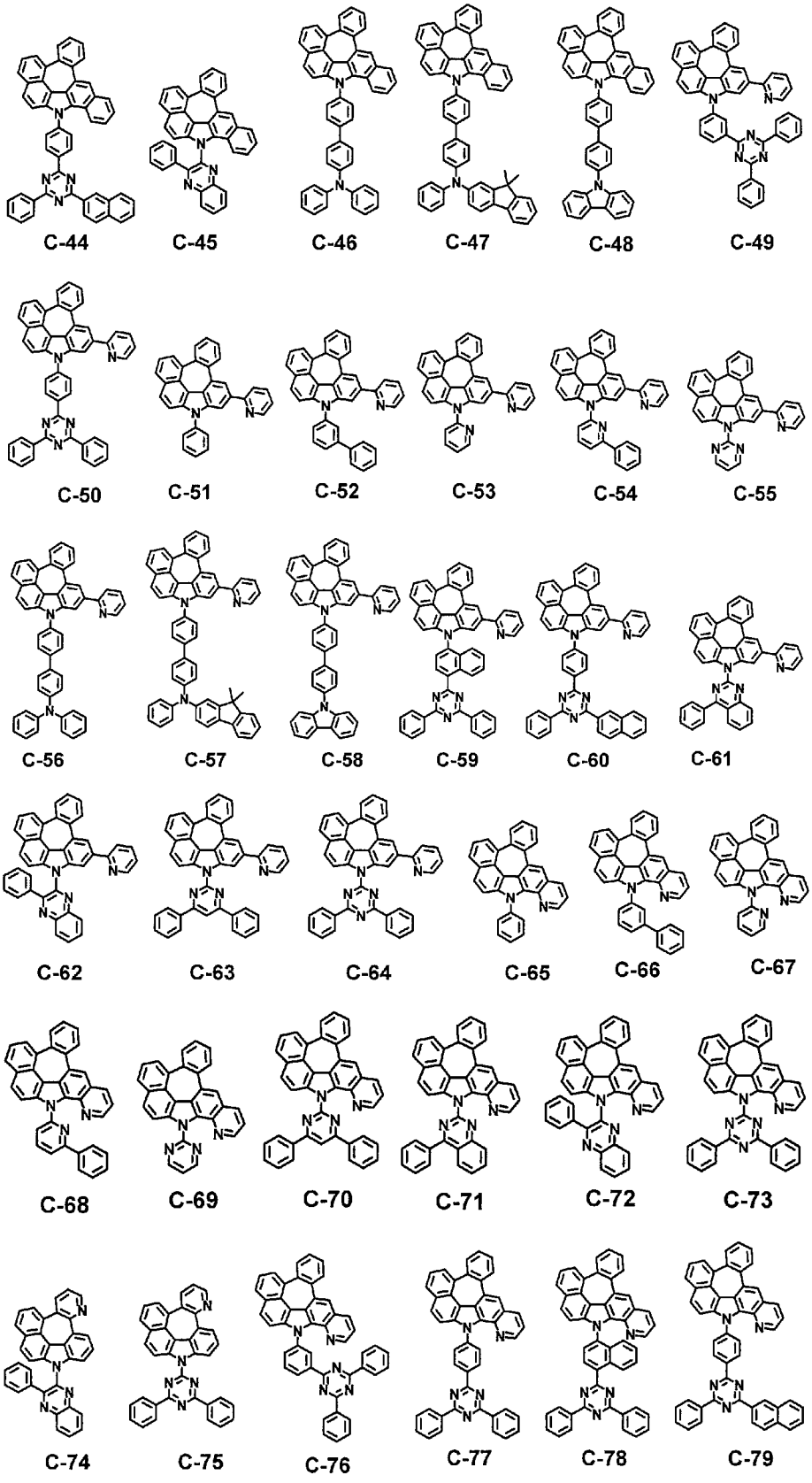
C-43


C-44
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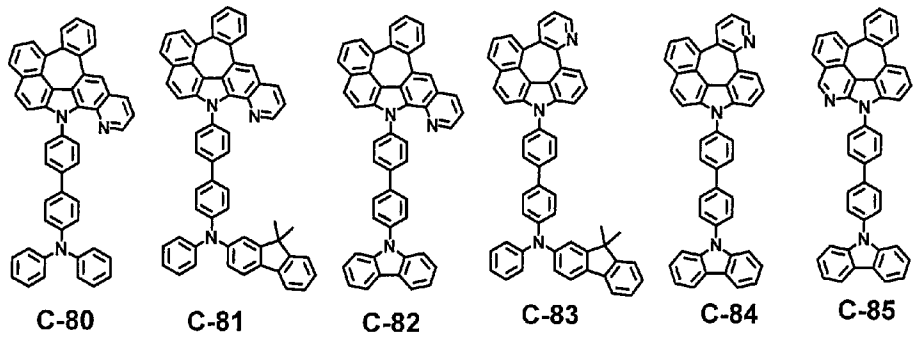
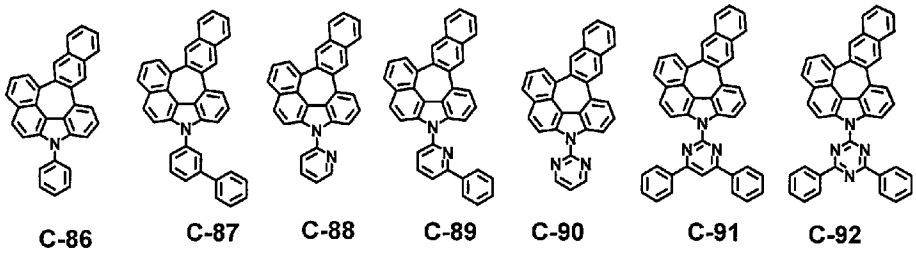
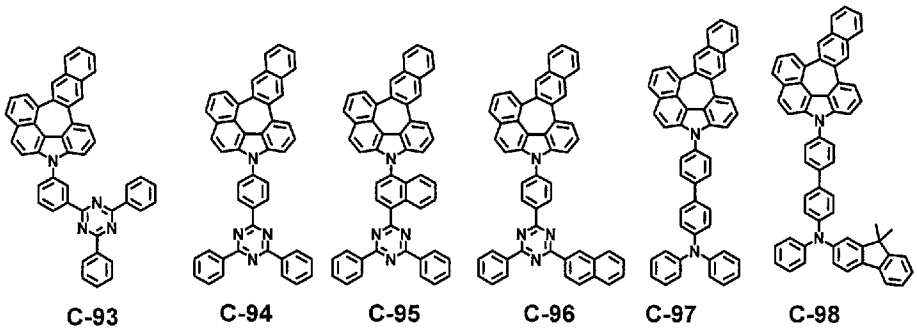
C-78
C-79



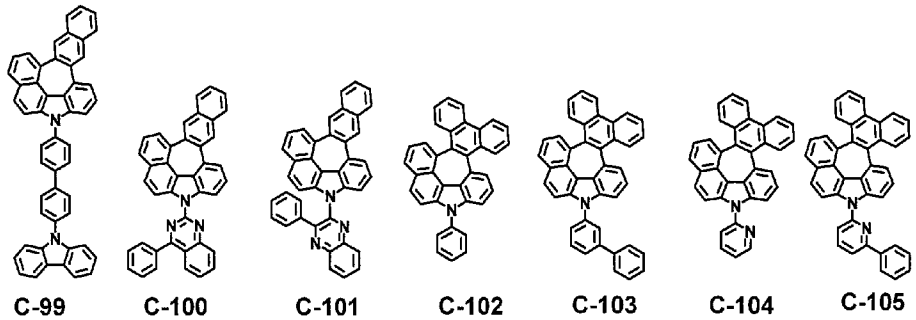
C-80 C-81 C-82 C-83 C-84 C-85



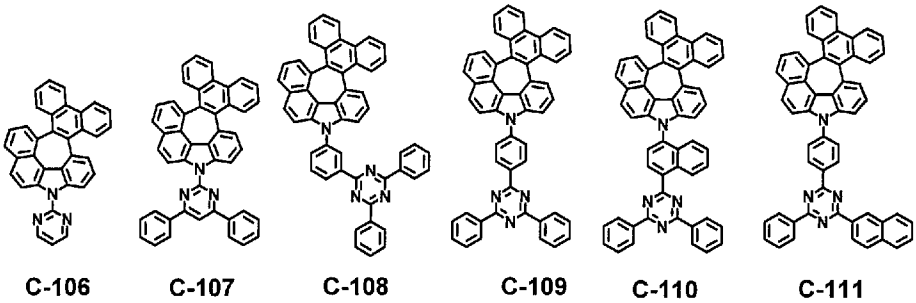
C-86 C-87 C-88 C-89 C-90 C-91 C-92



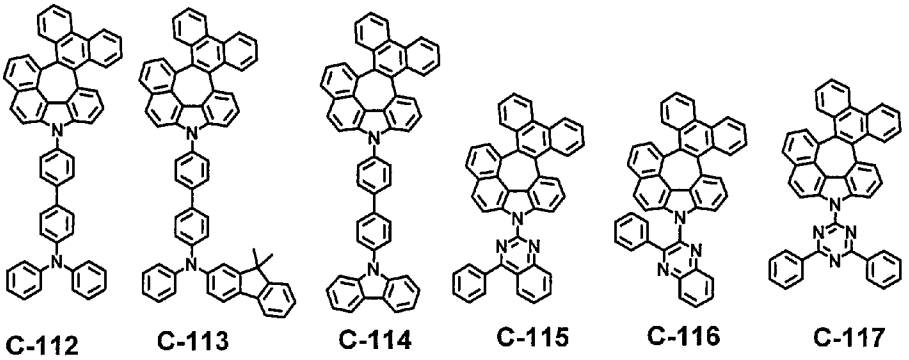
C-93 C-94 C-95 C-96 C-97 C-98



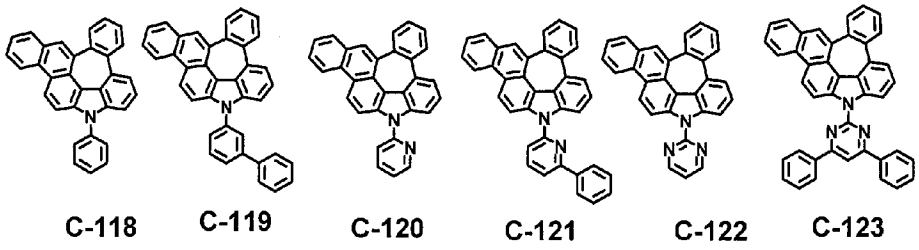
C-99 C-100 C-101 C-102 C-103 C-104 C-105



C-106 C-107 C-108 C-109 C-110 C-111



C-112 C-113 C-114 C-115 C-116 C-117



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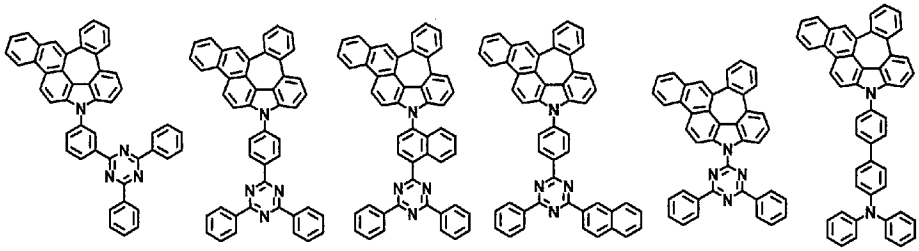

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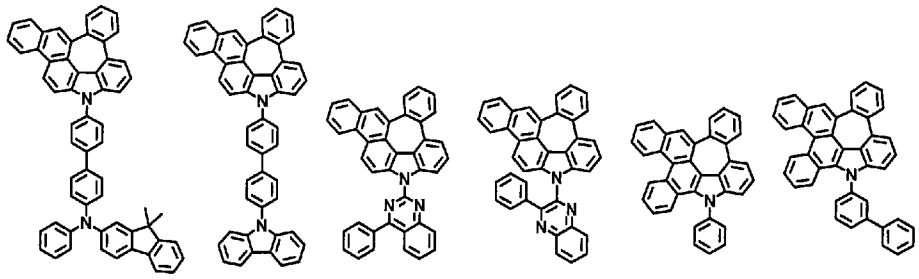

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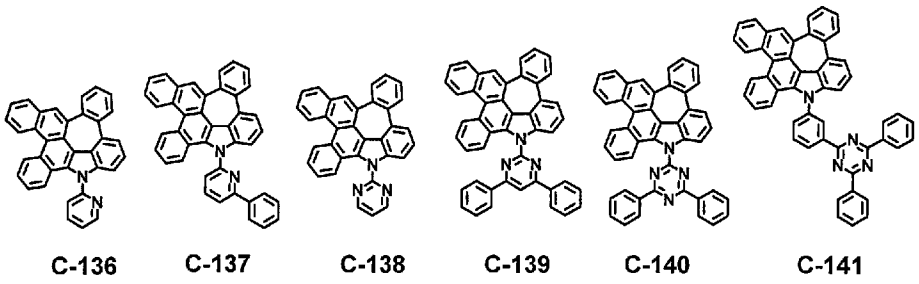

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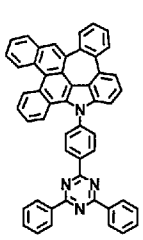

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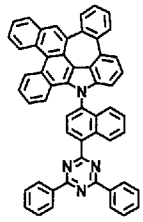

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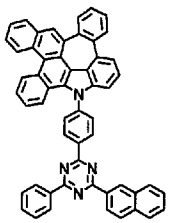

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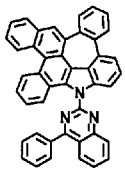

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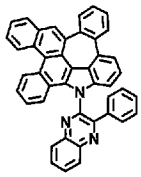

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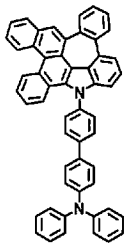

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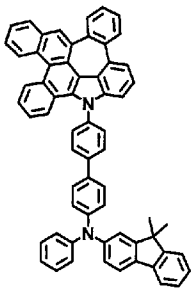

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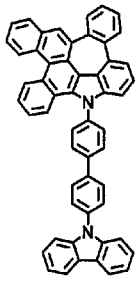

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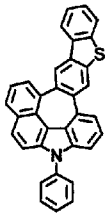

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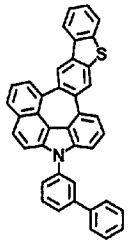

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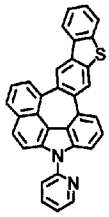

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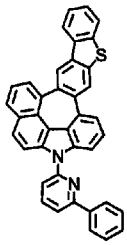

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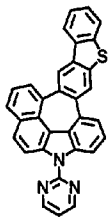

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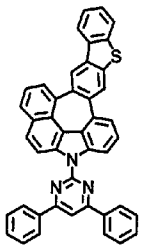

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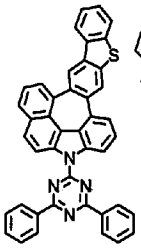

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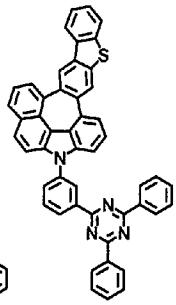

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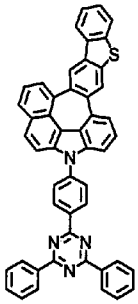

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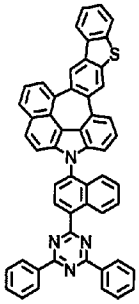

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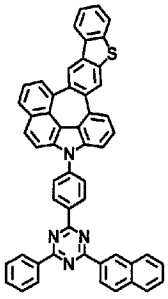

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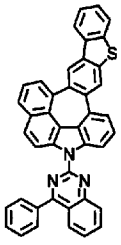

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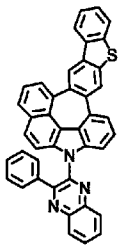

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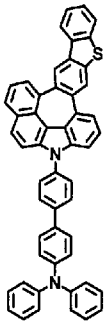

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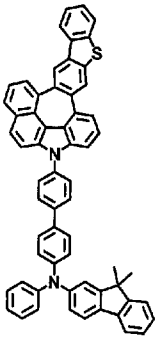

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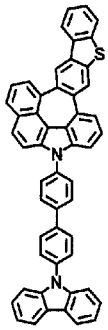

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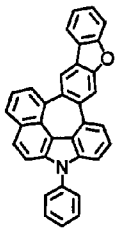

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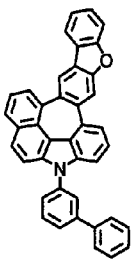

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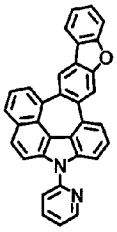

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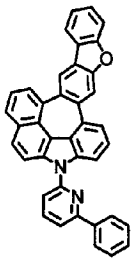

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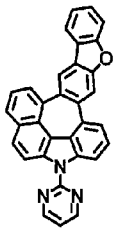

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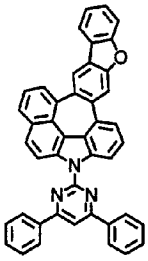

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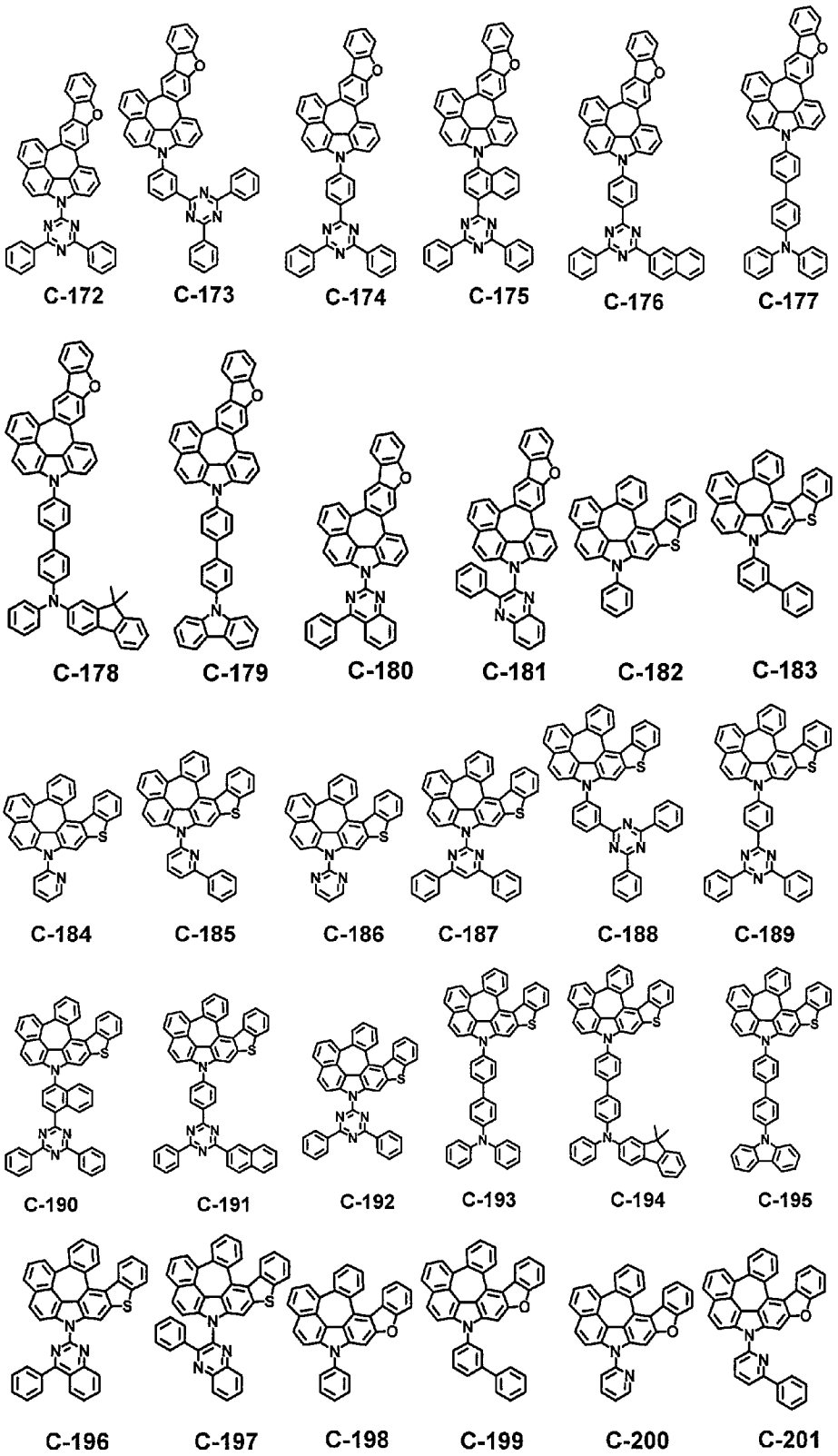
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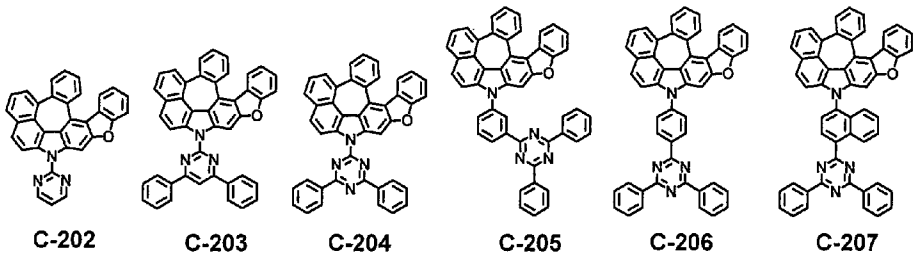

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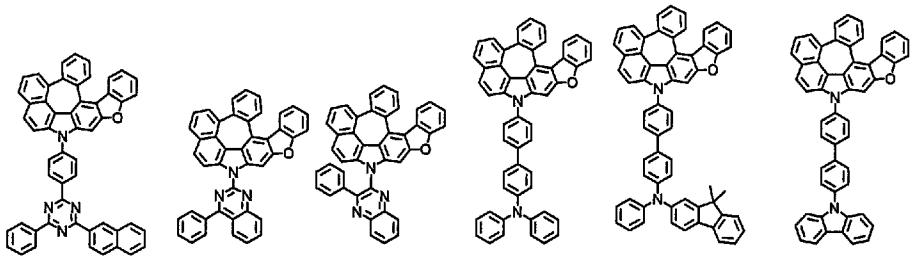

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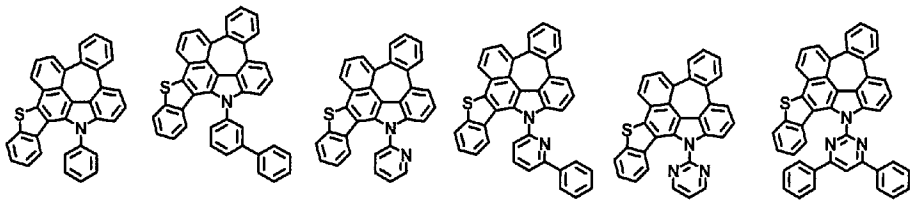

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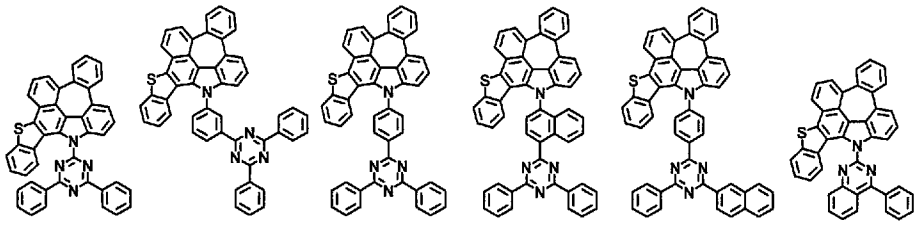

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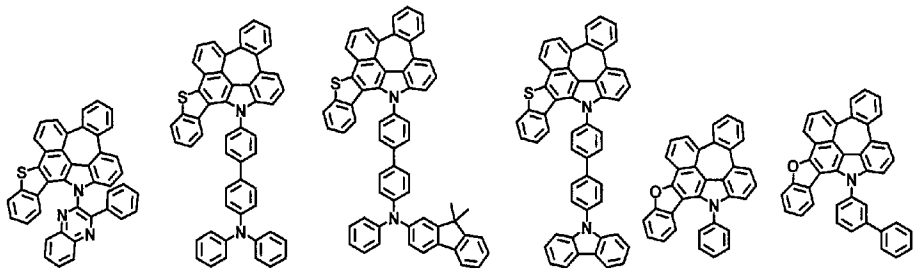

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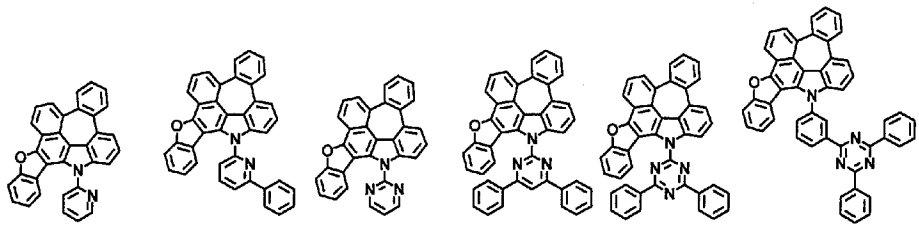

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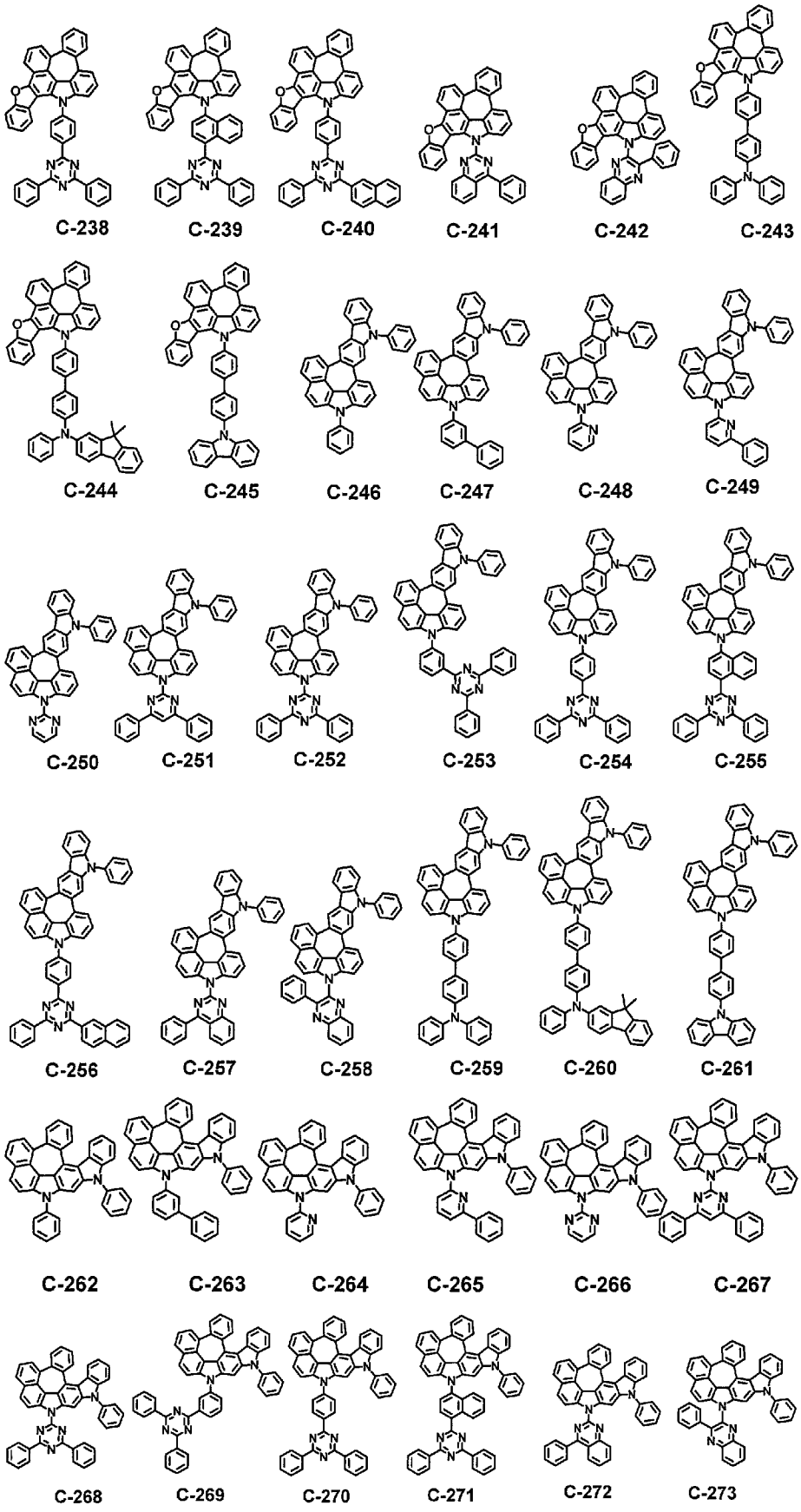
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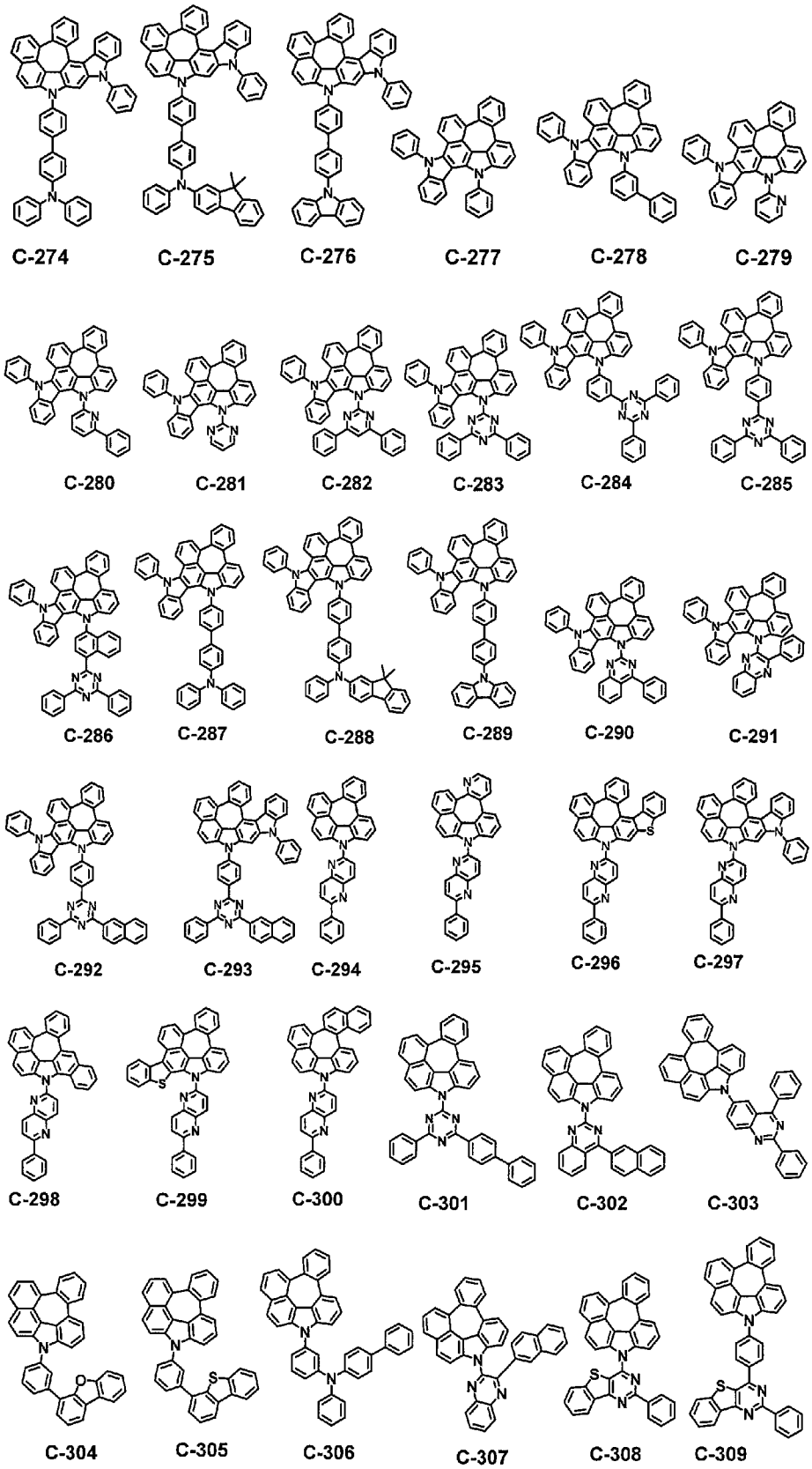
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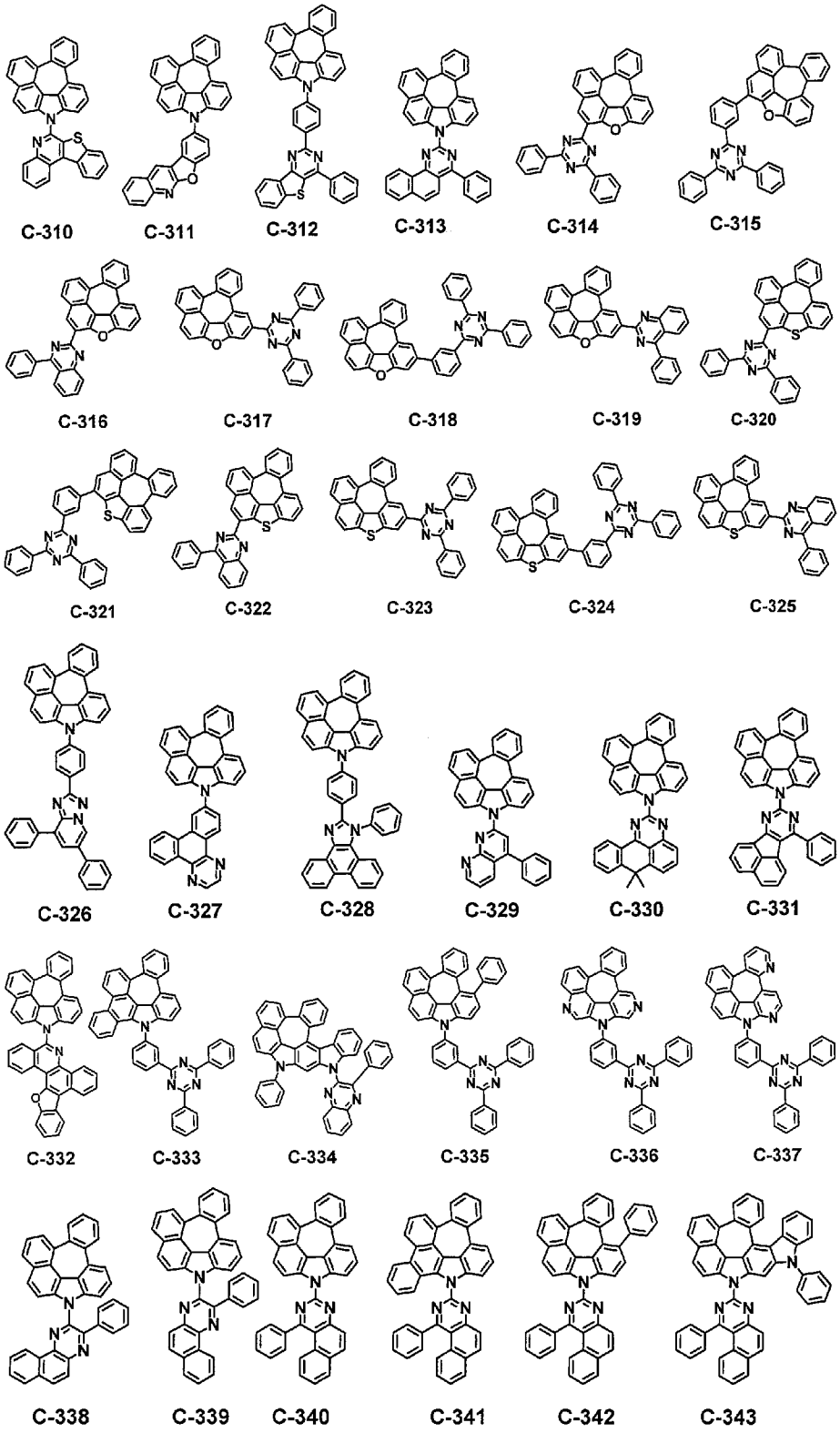
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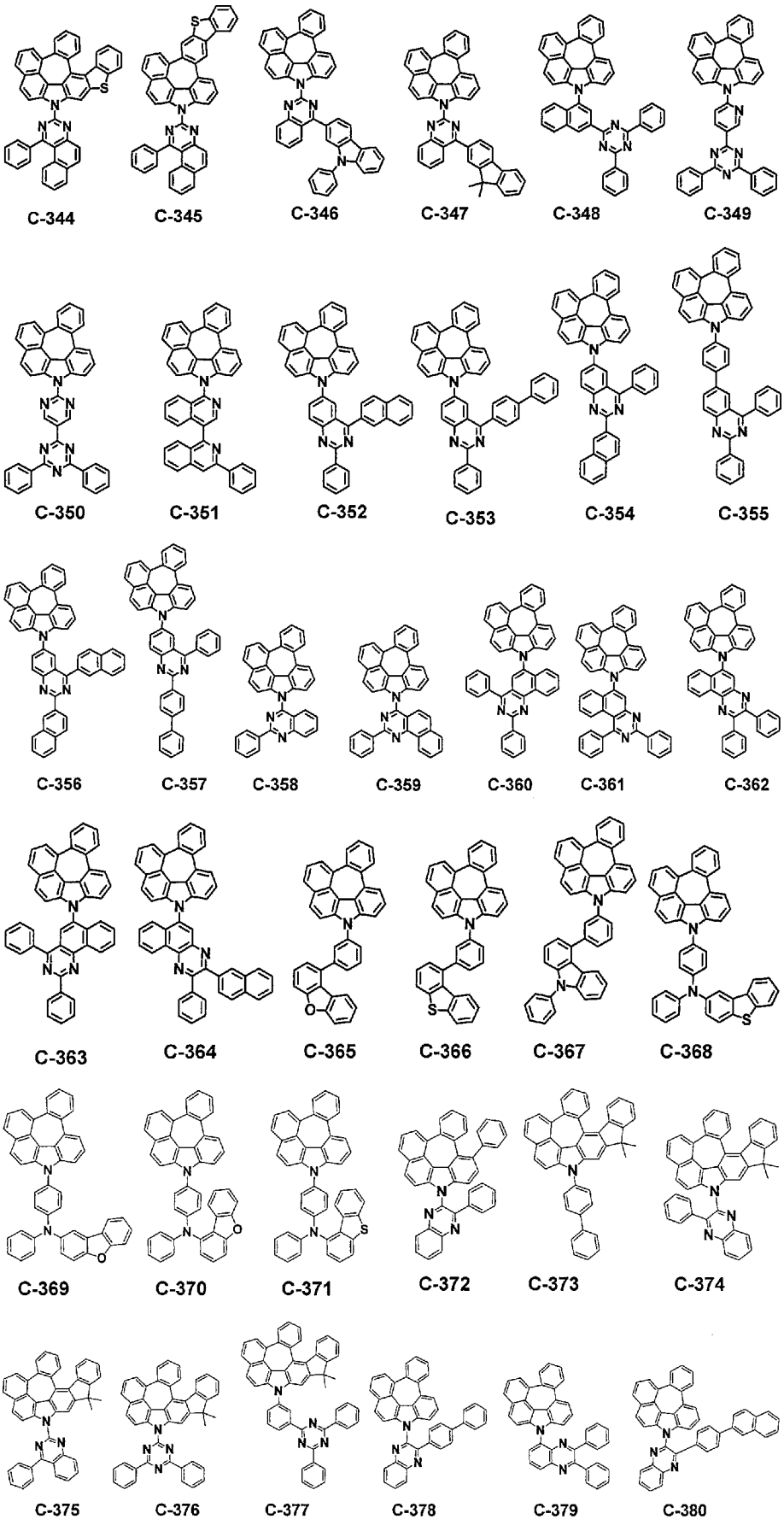
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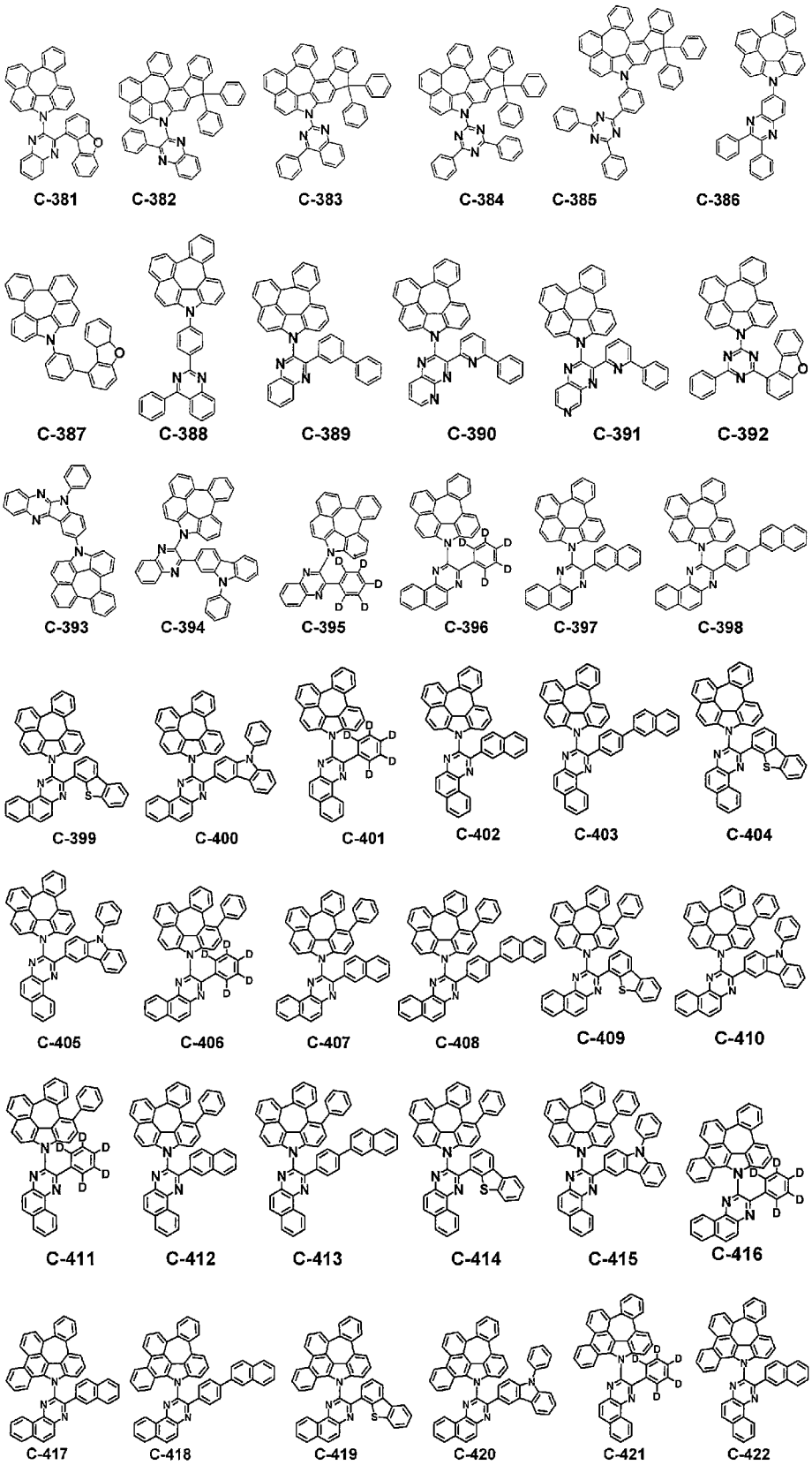
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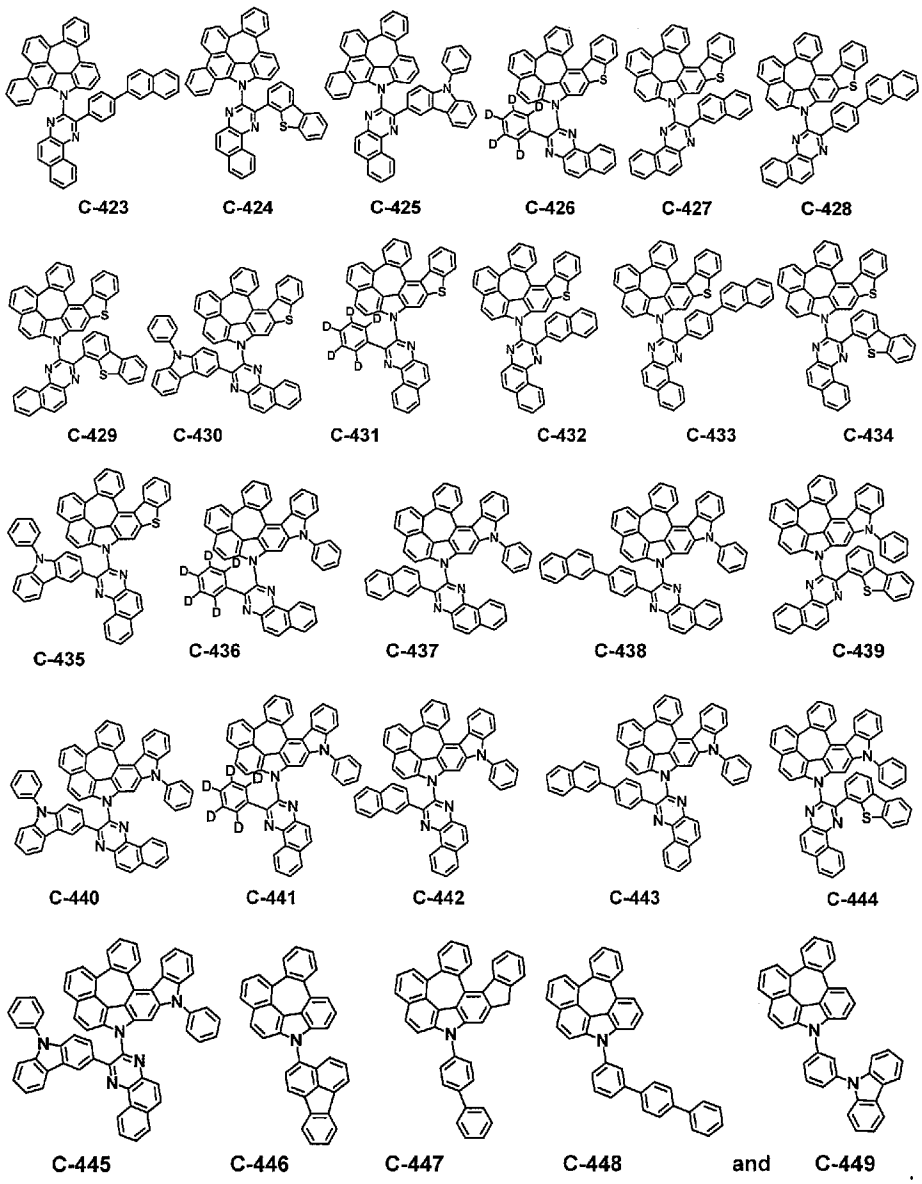

[Claim 7] The plurality of host materials according to claim 1, wherein Ar in formula 1 of the first host compound represents a substituted or unsubstituted (3- to 30-membered)heteroaryl, and Ar in formula 1 of the second host compound represents a substituted or unsubstituted (3- to 30- membered)heteroaryl.

[Claim 8] The plurality of host materials according to claim 1, wherein Ar in formula 1 of the first host compound represents a substituted or unsubstituted (3- to 30-membered)heteroaryl, and Ar in formula 1 of the second host compound represents 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, or a substituted or unsubstituted (C1-C30)alkyl(C6-C30)arylamino.

[Claim 9] An organic electroluminescent device comprising an anode, a cathode, and at least one light-emitting layer between the anode and the cathode, wherein at least one of the light-emitting layers comprises the plurality of host materials according to claim 1.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2019/008086

A. CLASSIFICATION OF SUBJECT MATTER

H01L 51/00(2006.01)i, H01L 51/50(2006.01)i, H01L 51/52(2006.01)i

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)
H01L 51/00; C07D 209/82; C07D 209/86; C07D 239/26; C07D 487/04; C09K 11/02; C09K 11/06; H01L 51/50; H01L 51/52

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched
Korean utility models and applications for utility models
Japanese utility models and applications for utility models

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
eKOMPASS(KIPO internal) , STN(Registry, Caplus) & Keywords: host compound, organic luminescent device

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	KR 10-2015-0121337 A (DUK SAN NEOLUX CO., LTD.) 29 October 2015 See claims 1, 3-5; paragraphs [0046]-[0050], [0226]-[0230].	1-3,7-9
A		4-6
A	US 2018-0175306 A1 (UNIVERSAL DISPLAY CORPORATION) 21 June 2018 See the whole document.	1-9
A	US 2017-0077409 A1 (UNIVERSAL DISPLAY CORPORATION) 16 March 2017 See the whole document.	1-9
A	US 2017-0213978 A1 (NICHEM FINE TECHNOLOGY CO., LTD.) 27 July 2017 See the whole document.	1-9
PX	KR 10-2018-0099547 A (ROHM & HAAS ELECT MATERIALS KOREA LTD.) 05 September 2018 See claims 1-5; compounds C-234, C-235.	1-9

☐ 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
"D" document cited by the applicant in the international application
"E" earlier application or patent but published on or after the international filing date
"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)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"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
"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
"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
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
23 September 2019 (23.09.2019)	**23 September 2019 (23.09.2019)**

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INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No.
PCT/KR2019/008086

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