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(54) **NOVEL COMPOUND AND ORGANIC ELECTROLUMINESCENCE DEVICE COMPRISING SAME**

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(57) **ABSTRACT**

The present invention relates to a novel compound and an organic electroluminescence device including the same, and the compound according to the present invention may be used in an organic material layer, preferably a light-emitting layer of an organic electroluminescence device, thereby enhancing the light-emitting efficiency, driving voltage, lifespan, and the like of the organic electroluminescence device.

NOVEL COMPOUND AND ORGANIC ELECTROLUMINESCENCE DEVICE COMPRISING SAME

TECHNICAL FIELD

[0001] The present invention relates to a novel compound and an organic electroluminescence device including the same.

BACKGROUND ART

[0002] When voltage is applied between two electrodes of the organic electroluminescence device, holes are injected into the organic material layer at the anode and electrons are injected into the organic material layer at the cathode, the injected holes and electrons meet each other to form an exciton, and when the formed exciton falls down to a bottom state, light is emitted. Materials used as the organic material layer may be classified into a light-emitting material, a hole injection material, a hole transporting material, an electron transporting material, an electron injection material, and the like according to the function.

[0003] The light-emitting materials may be divided into blue, green, and red light-emitting materials according to the light-emitting color, and into yellow and orange light-emitting materials required for implementing a much better natural color. Further, a host/dopant system may be used as a light-emitting material in order to enhance color purity and light-emitting efficiency through an energy transfer.

[0004] Dopant materials may be divided into a fluorescent dopant using an organic material and a phosphorescent dopant in which a metal complex compound including heavy atoms such as Ir and Pt is used. Since the development of the phosphorescent dopant may theoretically enhance light-emitting efficiency by up to 4 times compared to the development of the fluorescent dopant, studies on not only phosphorescent dopants, but also phosphorescent hosts have been conducted.

[0005] As the hole transporting material, the hole injection material, the electron transporting layer, and the like, NPB, BCP, Alq_3 and the like have been widely known until now, and as the light-emitting material, anthracene derivatives have been used. In particular, metal complex compounds including Ir and having a great advantage in terms of enhancing the efficiency, such as Firpic, $Ir(ppy)_3$ and $(acac)Ir(btp)_2$, are used as blue, green and red phosphorescent dopant materials, and CBP is used as a phosphorescent host material. In addition, the official gazette of Korean Patent Application Laid-Open No. 2012-0020816 discloses an organic electroluminescence device which uses an indolo benzofluoranthene derivative as the host material.

[0006] However, since light-emitting materials in the related art have good light-emitting characteristics, but have low glass transition temperature, and thus poor thermal stability, these materials fall short of a level that sufficiently satisfies the lifespan of the organic electroluminescence device.

DISCLOSURE

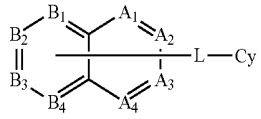
Technical Problem

[0007] In order to solve the aforementioned problems, an object of the present invention is to provide a novel compound which may enhance the efficiency, lifespan, stability, and the like of an organic electroluminescence device, and an organic electroluminescence device including the compound.

Technical Solution

[0008] In order to achieve the aforementioned object, the present invention provides a compound represented by the following Formula 1.

[Formula 1]



[0009] In Formula 1,

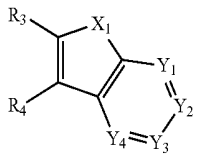
[0010] A_1 to A_4 are each independently CR_1 or N, and here, at least one thereof is N, and B_1 to B_4 are each independently CR_2 or N,

[0011] R_1 and R_2 are each independently selected from the group consisting of hydrogen, deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 60 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphosphine oxide group and a C_6 to C_{60} arylamine group, or may form a fused ring with an adjacent group.

[0012] L is a single bond, or a C_6 to C_{30} arylene group or a heteroarylene group having 5 to 30 nuclear atoms,

[0013] Cy is a compound represented by the following Formula 2, and

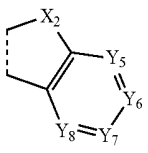
[Formula 2]



[0014] In Formula 2,

[0015] Y_1 to Y_4 are each independently CR_5 or N, and at least one of Y_1 and Y_2, Y_2 and Y_3 or Y_3 and Y_4 forms a fused ring represented by the following Formula 3;

[Formula 3]



[0016] In Formula 3,

[0017] the dotted line means a site where a fusion (condensation) with the compound of Formula 2 occurs, and Y_5 to Y_8 are each independently CR_6 or N,

[0018] X_1 and X_2 are each independently selected from the group consisting of O, S, Se, $N(Ar_1)$, $C(Ar_2)(Ar_3)$ and $Si(Ar_4)(Ar_5)$, and here, at least one of X_1 and X_2 is $N(Ar_1)$, and

[0019] R_3 to R_6 are each independently selected from the group consisting of hydrogen, deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 60 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphosphine oxide group and a C_6 to C_{60} arylamine group, or may form a fused ring with an adjacent group,

[0020] Ar_1 to Ar_5 are each independently selected from the group consisting of hydrogen, deuterium, halogen, a cyano group, a nitro group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 60 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphosphine oxide group and a C_6 to C_{60} arylamine group,

[0021] the alkyl group, the alkenyl group, the alkynyl group, the cycloalkyl group, the heterocycloalkyl group, the aryl group, the heteroaryl group, the alkyloxy group, the aryloxy group, the alkylsilyl group, the arylsilyl group, the alkylboron group, the arylboron group, the arylphosphine group, the arylphosphine oxide group and the arylamine group of R_1 to R_6 and Ar_1 to Ar_5 may be each independently substituted with one or more selected from the group consisting of deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group (preferably a C_1 to C_{10} alkyl group), a C_2 to C_{40} alkenyl group (preferably a C_2 to C_{10} alkenyl group), a C_2 to C_{40} alkynyl group (preferably a C_2 to C_{10} alkynyl group), a C_3 to C_{40} cycloalkyl group (preferably a C_3 to C_{18} cycloalkyl group), a heterocycloalkyl group having 3 to 40 nuclear atoms (preferably a heterocycloalkyl group having 3 to 18 nuclear atoms), a C_6 to C_{40} aryl group (preferably a C_6 to C_{18} aryl group), a heteroaryl group having 5 to 40 nuclear atoms (preferably a heteroaryl group having 5 to 18 nuclear atoms), C_1 to C_{40} alkyloxy group (preferably a C_1 to C_{10} alkyloxy group), a C_6 to C_{60} aryloxy group (preferably a C_6 to C_{18} aryloxy group), a C_1 to C_{40} alkylsilyl group (preferably a C_1 to C_{10} alkylsilyl group), a C_6 to C_{60} arylsilyl group (preferably a C_6 to C_{18} arylsilyl group), a C_1 to C_{40} alkyl boron group (preferably a C_1 to C_{10} alkyl boron group), a C_6 to C_{60} aryl boron group (preferably a C_6 to C_{18} aryl boron group), a C_6 to C_{60} arylphosphone group (preferably C_6 to C_{18} arylphosphine group), a C_6 to C_{60} arylphosphine oxide group (preferably a C_6 to C_{18} arylphosphine oxide group) and a C_6 to C_{60} arylamine group (preferably a C_6 to C_{20} arylamine group), and in this case, a plurality of substituents may be the same as or different from each other, and

[0022] L is linked to any one of A_1 to A_4 and B_1 to B_4 of Formula 1, and simultaneously to any one of X_1, X_2, R_3, R_4 and Y_1 to Y_8 of Formula 2.

[0023] The alkyl used in the present invention means a monovalent functional group obtained by removing a hydrogen atom from a linear or branched, saturated hydrocarbon having 1 to 40 carbon atoms, and non-limiting examples thereof include methyl, ethyl, propyl, isobutyl, sec-butyl, pentyl, iso-amyl, hexyl, and the like.

[0024] The alkenyl used in the present invention means a monovalent functional group obtained by removing a hydrogen atom from a linear or branched, unsaturated hydrocarbon having 2 to 40 carbon atoms, which has one or more carbon-carbon double bonds. Non-limiting examples thereof include vinyl, allyl, isopropenyl, 2-butenyl, and the like.

[0025] The alkynyl used in the present invention means a monovalent functional group obtained by removing a hydrogen atom from a linear or branched, unsaturated hydrocarbon having 2 to 40 carbon atoms, which has one or more carbon-carbon triple bonds. Non-limiting examples thereof include ethynyl, 2-propynyl, and the like.

[0026] The cycloalkyl used in the present invention means a monovalent functional group obtained by removing a hydrogen atom from a monocyclic or polycyclic non-aromatic hydrocarbon (saturated cyclic hydrocarbon) having 3 to 40 carbon atoms. Non-limiting examples thereof include cyclopropyl, cyclopentyl, cyclohexyl, norbornyl, adamantine, and the like.

[0027] The heterocycloalkyl used in the present invention means a monovalent functional group obtained by removing a hydrogen atom from a non-aromatic hydrocarbon (saturated cyclic hydrocarbon) having 3 to 40 nuclear atoms, and one or more carbons in the ring, preferably 1 to 3 carbons, are substituted with a heteroatom such as N, O, or S. Non-limiting examples thereof include morpholine, piperazine, and the like.

[0028] The aryl used in the present invention means a monovalent functional group obtained by removing a hydrogen atom from an aromatic hydrocarbon having 6 to 60 carbon atoms of a single ring or a combination of two or more rings. In this case, the two or more rings may be simply pendant to each other or pendant to each other in a fused form. Non-limiting examples thereof include phenyl, biphenyl, triphenyl, terphenyl, naphthyl, fluorenyl, phenanthryl, anthracenyl, indenyl, and the like.

[0029] The heteroaryl used in the present invention is a monovalent functional group obtained by removing a hydrogen atom from a monoheterocyclic or polyheterocyclic aromatic hydrocarbon having 5 to 60 nuclear atoms, and one or more carbons in the ring, preferably 1 to 3 carbons are substituted with a heteroatom such as nitrogen (N), oxygen (0), sulfur (S), or selenium (Se). In this case, the two or more rings may be simply pendant to each other or pendant to each other in a fused form in the heteroaryl, and furthermore, the heteroaryl may also include a fused form with an aryl group. Non-limiting examples of the heteroaryl include: a six-membered monocyclic ring such as pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, and triazinyl; a polycyclic ring such as phenoxathienyl, indolizinyl, indolyl, purinyl, quinolyl, benzothiazole, and carbazolyl; and 2-furanyl, N-imidazolyl, 2-isoxazolyl, 2-pyridinyl, 2-pyrimidinyl, and the like.

[0030] The alkyloxy used in the present invention means a monovalent functional group represented by RO—, and R is an alkyl having 1 to 40 carbon atoms, and may include a linear, branched, or cyclic structure. Non-limiting examples of the alkyloxy include methoxy, ethoxy, n-propoxy, 1-propoxy, t-butoxy, n-butoxy, pentoxy, and the like.

[0031] The aryloxy used in the present invention means a monovalent functional group represented by R'O—, and R' is

an aryl having 6 to 60 carbon atoms. Non-limiting examples of the aryloxy include phenyloxy, naphthyloxy, diphenyloxy, and the like.

[0032] The alkylsilyl used in the present invention means a silyl substituted with an alkyl having 1 to 40 carbon atoms, the arylsilyl means a silyl substituted with an aryl having 6 to 60 carbon atoms, and the arylamine means an amine substituted with an aryl having 6 to 60 carbon atoms.

[0033] The fused ring used in the present invention means a fused aliphatic ring, a fused aromatic ring, a fused heteroaliphatic ring, a fused heteroaromatic ring, or a combined form thereof.

[0034] Further, the present invention provides an organic electroluminescence device including: an anode; a cathode; and an organic material layer having one or more layers interposed between the anode and the cathode, in which at least one of the organic material layers having one or more layers includes the compound represented by Formula 1.

[0035] Here, the organic material layer including the compound represented by Formula 1 is selected from the group consisting of a hole injection layer, a hole transporting layer, and a light-emitting layer, and is preferably a light-emitting layer. In this case, the compound represented by Formula 1 may be used as a phosphorescent host material of the light-emitting layer.

Advantageous Effects

[0036] The compound represented by Formula 1 according to the present invention has excellent thermal stability and phosphorescent characteristics, and thus may be applied to an organic material layer, preferably a light-emitting layer of an organic electroluminescence device. Therefore, when the light-emitting layer of the organic electroluminescence device includes the compound represented by Formula 1 as a phosphorescent host material, the efficiency (light-emitting efficiency and power efficiency), lifespan, brightness, and driving voltage of the device may be enhanced as compared to the case in which a host material in the related art is included, and furthermore, performance and lifespan of a full-color organic electroluminescence panel may be greatly enhanced.

BEST MODE

[0037] Hereinafter, the present invention will be described in detail.

[0038] 1. Novel Compound

[0039] A novel compound according to the present invention has a basic structure in which an indole group fusion compound is bonded to a naphthalene derivative including nitrogen (N), and is represented by Formula 1.

[0040] The compound represented by Formula 1 according to the present invention has excellent phosphorescent characteristics and excellent electron and/or hole transporting capabilities, and thus may be used as a material for any one of a hole injection layer, a hole transporting layer, a light-emitting layer, an electron transporting layer, and an electron injection layer, which are the organic material layers of an organic electroluminescence device. The compound may be used preferably as a material for any one of a hole injection layer, a hole transporting layer, and a light-emitting layer, and more preferably as a material (particularly, a phosphorescent host material) for a light-emitting layer.

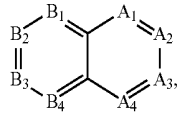
[0041] Specifically, the compound represented by Formula 1 according to the present invention is a compound into which various substituents are introduced and in which a naphthalene derivative including nitrogen (N) and an indole group fusion compound are combined, and since the mobility balance between holes and electrons may be controlled by bipolar characteristics which the compound has, the recombination efficiency of holes and electrons may be enhanced, thereby exhibiting excellent phosphorescent characteristics. Furthermore, the compound represented by Formula 1 according to the present invention may have a wide energy band gap (sky blue to red) because the energy level is controlled by various substituents introduced into a basic structure composed of a naphthalene derivative and an indole group fusion compound. Therefore, when the compound of Formula 1 according to the present invention is used in an organic electroluminescence device, phosphorescent characteristics of the device are improved, and simultaneously, hole injection capabilities and/or transporting capabilities, light-emitting efficiency, driving voltage, lifespan characteristics, and the like may be improved.

[0042] Further, the molecular weight of the compound represented by Formula 1 according to the present invention is significantly increased due to various substituents introduced into the basic structure, so that the glass transition temperature is enhanced, and accordingly, the compound represented by Formula 1 according to the present invention may have higher thermal stability than that of a material (for example, CBP [4,4-dicarbazolybiphenyl]) for the organic electroluminescence device in the related art.

[0043] Therefore, the compound according to the present invention may greatly contribute to the improvement of performance and the enhancement of lifespan, of the organic electroluminescence device, and furthermore, the enhancement of lifespan of the organic electroluminescence device may maximize the performance of a full color organic light-emitting panel.

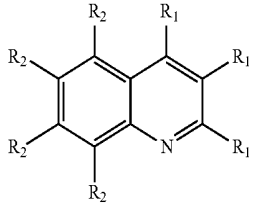
[0044] In the compound represented by Formula 1 of the present invention, A_1 to A_4 of the naphthalene derivative including nitrogen (N) are each independently CR_1 or N, and in this case, it is preferred that at least one thereof is nitrogen (N), and it is more preferred that two thereof are nitrogen (N). In addition, B_1 to B_4 are each independently CR_2 or N, and it is preferred that all of B_1 to B_4 are CR_2, or one of B_1 to B_4 is nitrogen (N).

[0045] Here, it is preferred that



which is a naphthalene derivative including nitrogen (N), is selected from the group consisting of structures represented by the following S-1 to S-30.

S-1



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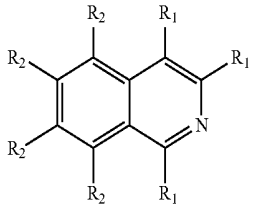
S-2



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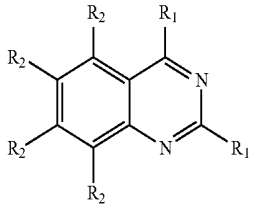

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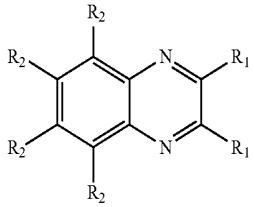

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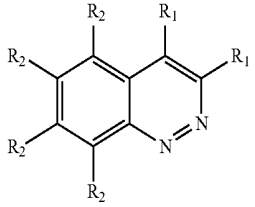

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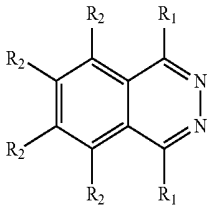

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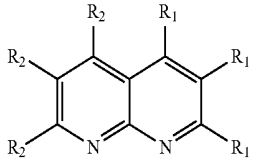

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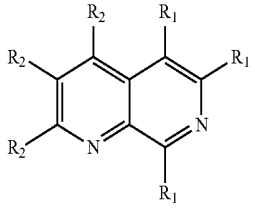

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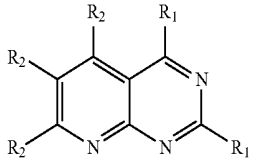

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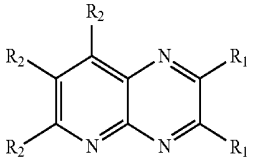
S-10



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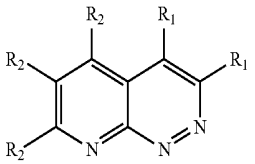

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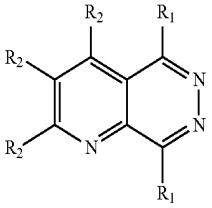

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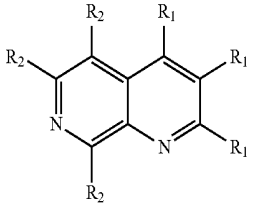

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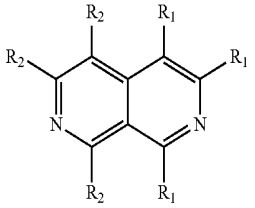

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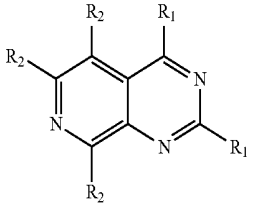
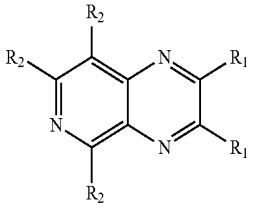
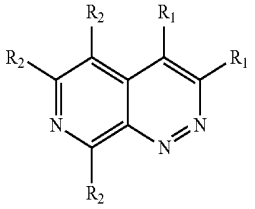


S-16



S-17



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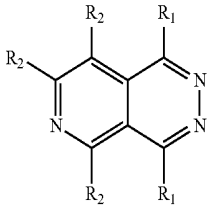

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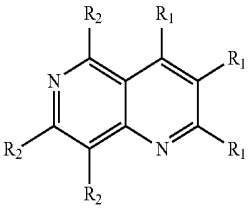

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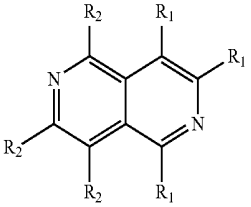

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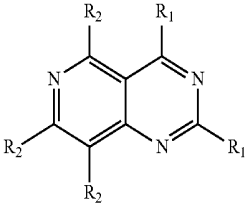

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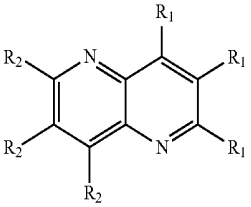

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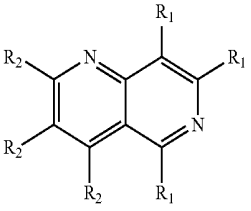

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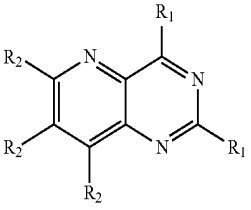

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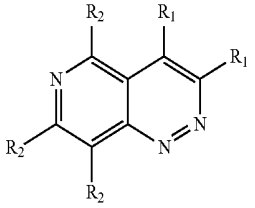

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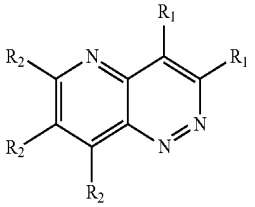

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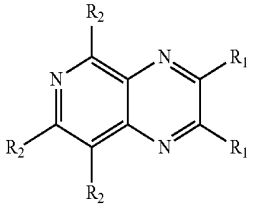

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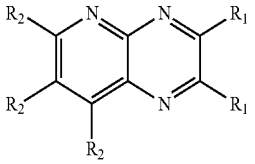
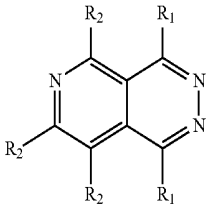
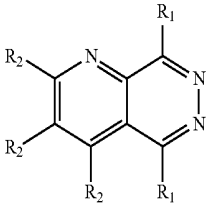


S-29



S-30

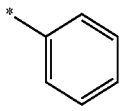


[0046] In the structures represented by S-1 to S-30, R_1 and R_2 are the same as those defined above, a plurality of R_1's may be the same as or different from each other, and a plurality of R_2's may also be the same as or different from each other.

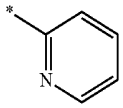
[0047] In this case, in consideration of efficiency and lifespan characteristics of the organic electroluminescence device, it is preferred that R_1 and R_2 are selected from the group consisting of hydrogen, a C_6 to C_{60} (preferably C_6 to C_{25}) aryl group, a heteroaryl group having 5 to 40 nuclear atoms (preferably 5 to 32 nuclear atoms), and a C_6 to C_{60} (preferably C_6 to C_{20}) arylamine group.

[0048] More preferably, R_1 and R_2 may be each independently selected from the group consisting of hydrogen, or structures represented by the following A1 to A70.

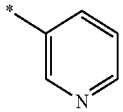
A1



A2



A3



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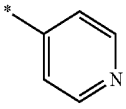

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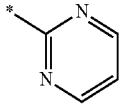

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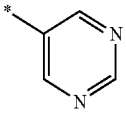

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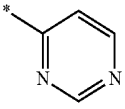

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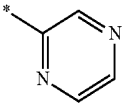

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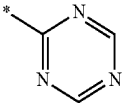

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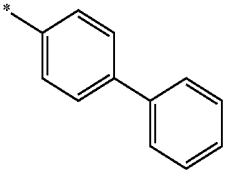

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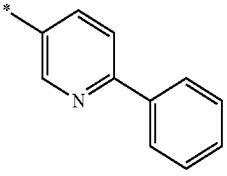

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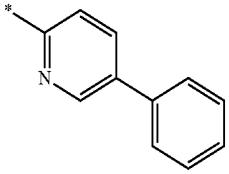

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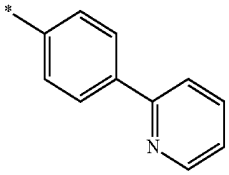

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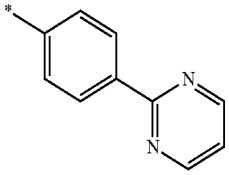

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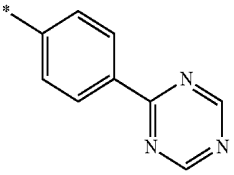

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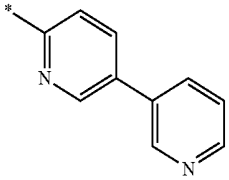

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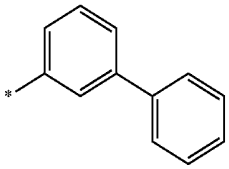

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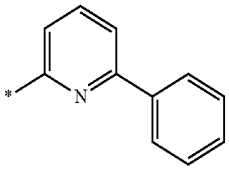

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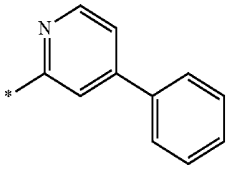

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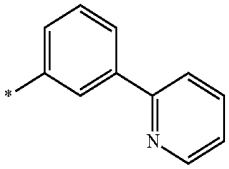

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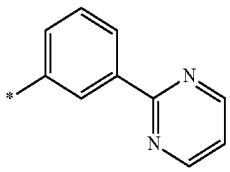

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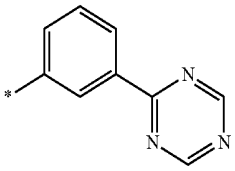

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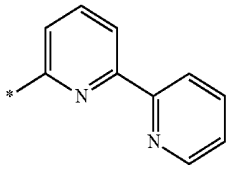

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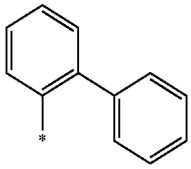

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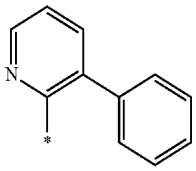

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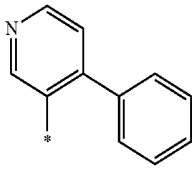

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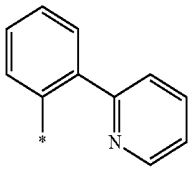

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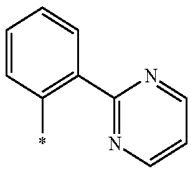

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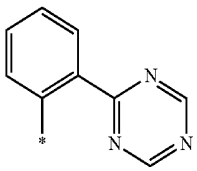

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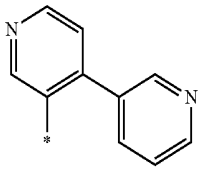

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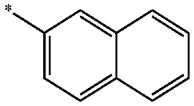

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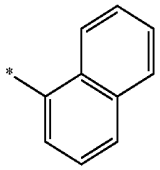

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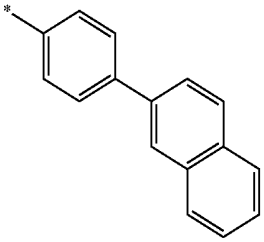

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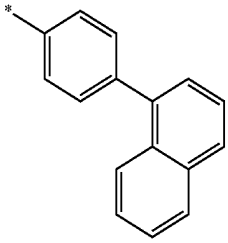

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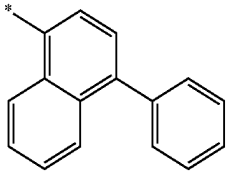

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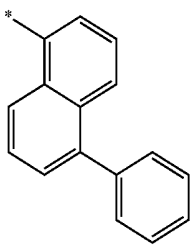

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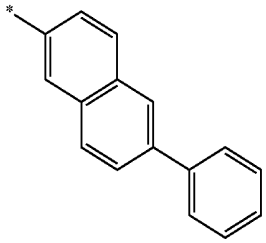

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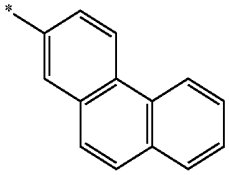

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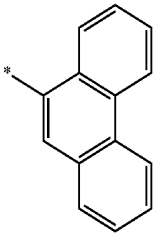

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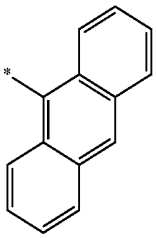

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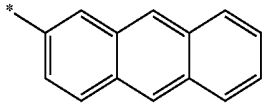

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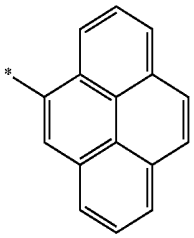

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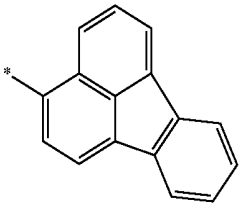

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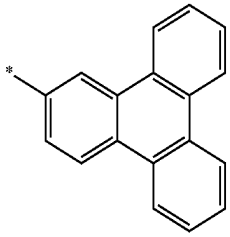
A44



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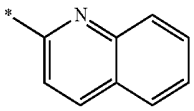

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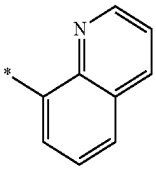

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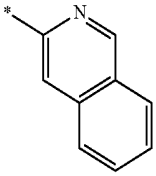

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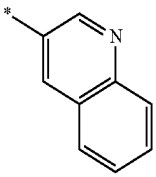

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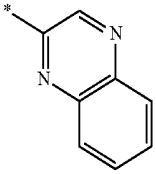

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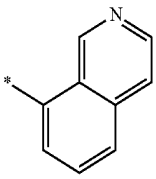

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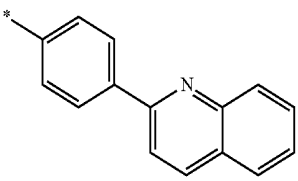

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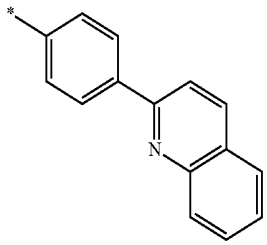

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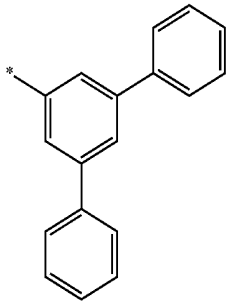

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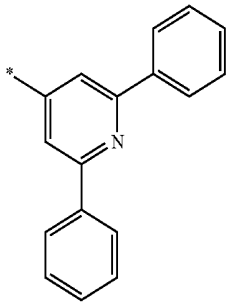

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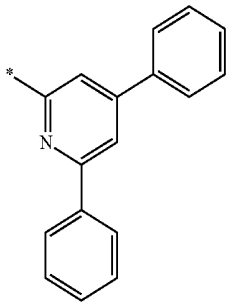

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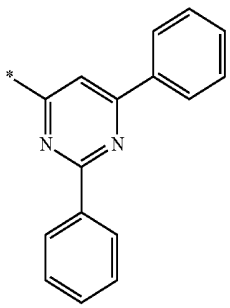

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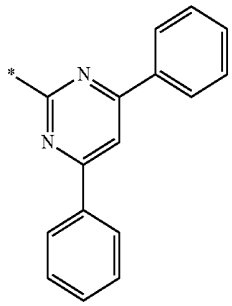

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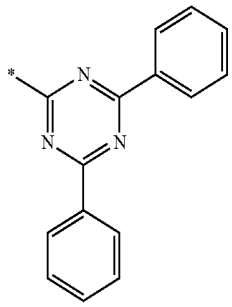

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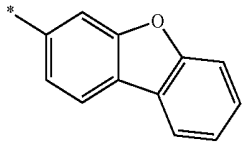

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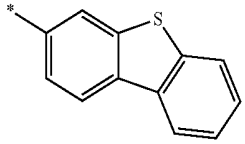

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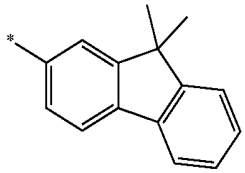

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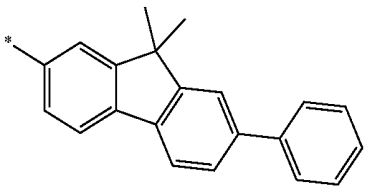

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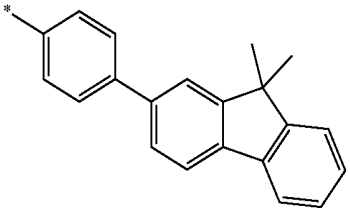

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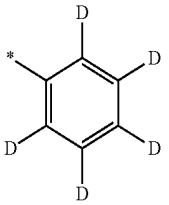

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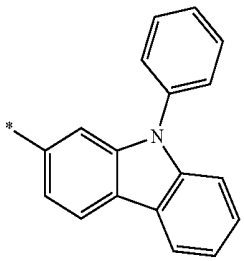

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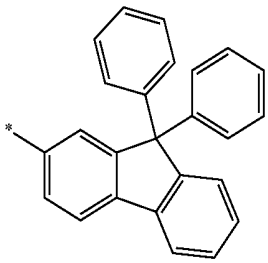

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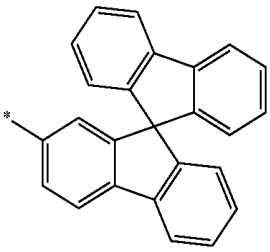

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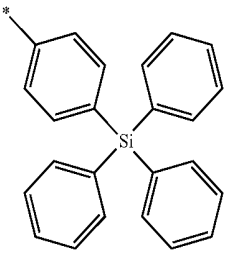

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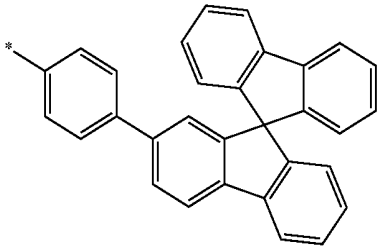

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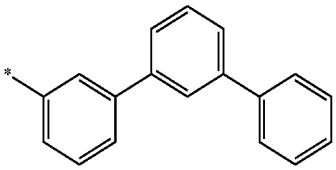
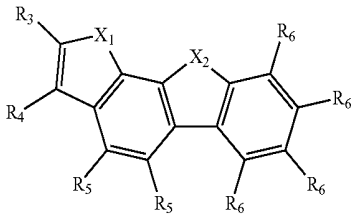
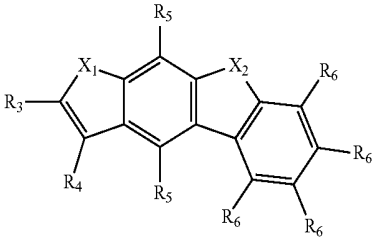


[0049] Meanwhile, in the compound represented by Formula 1 according to the present invention, it is preferred that the compound represented by Formula 2 which corresponds to Cy is selected from the group consisting of compounds represented by the following Formulae 2a to 2f.

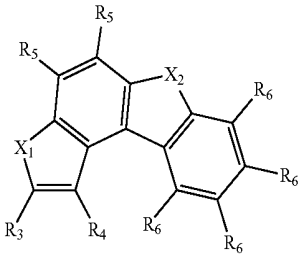
[Formula 2a]



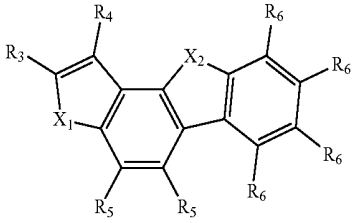
[Formula 2b]



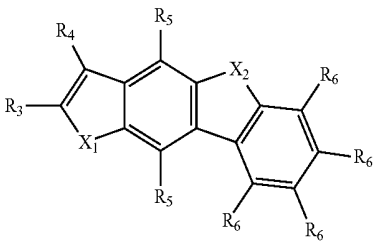
[Formula 2c]



[Formula 2d]



[Formula 2e]



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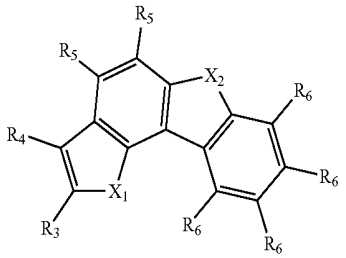
[Formula 2f]



[0050] In Formulae 2a to 2f, X_1, X_2 and R_3 to R_6 are the same as those defined above. In this case, a plurality of R_5's may be the same as or different from each other, and a plurality of R_6's may also be the same as or different from each other.

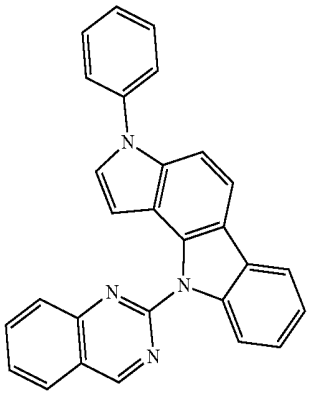
[0051] Meanwhile, in consideration of efficiency and lifespan characteristics of the organic electroluminescence device, in the compound represented by Formula 1 according to the present invention, it is preferred that L which links the naphthalene derivative including nitrogen (N) to one compound of the compounds represented by Formulae 2a to 2f is a single bond or phenylene.

[0052] In addition, in the compounds represented by Formulae 2a to 2f, it is preferred that both X_1 and X_2 are $N(Ar_1)$. In this case, Ar_1 of $N(Ar_1)$ to be combined as X_1 and Ar_1 of $N(Ar_1)$ to be combined as X_2 may be the same as or different from each other. It is preferred that Ar_1 is selected from the group consisting of hydrogen, a C_6 to C_{60} aryl group (preferably a C_6 to C_{18} aryl group) and a heteroaryl group having 5 to 40 nuclear atoms (preferably a heteroaryl group having 5 to 18 nuclear atoms).

[0053] In the compound represented by Formula 1 according to the present invention, the linking position of L and the compound represented by Formula 2 is not particularly limited, but it is preferred that L is linked to any one of X_1 and Y_5 to Y_8 of Formula 2.

[0054] The compound represented by Formula 1 according to the present invention may be specifically exemplified as the following compounds (C1 to C458), but is not limited thereto.

C1



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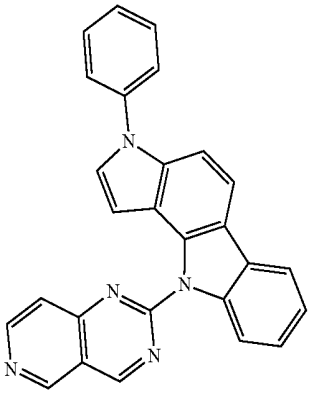
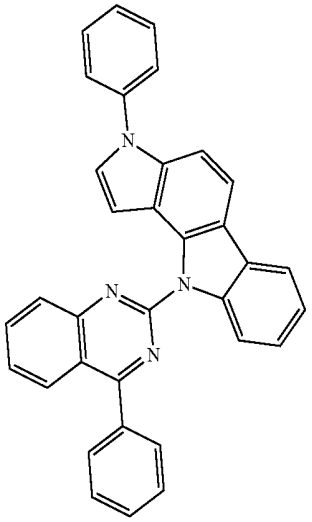
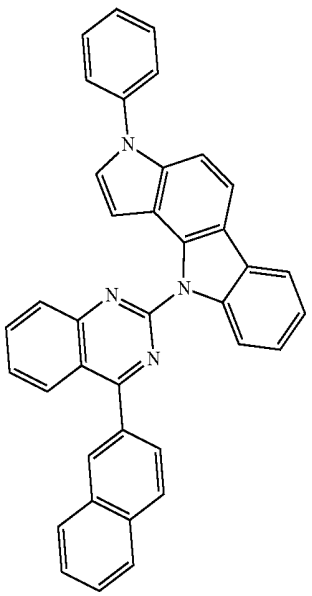
C2



C3



C4



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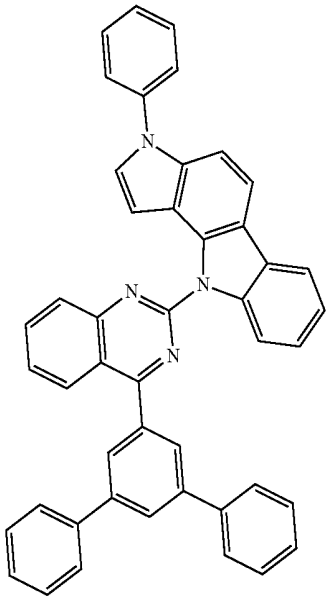
C5



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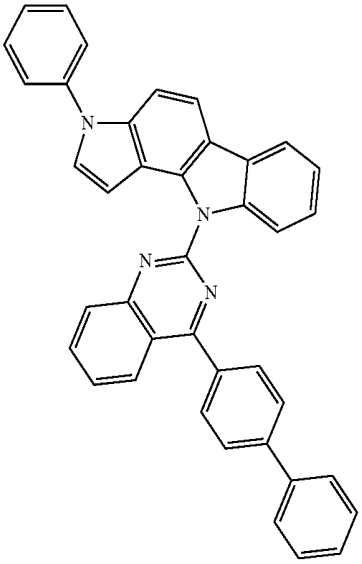
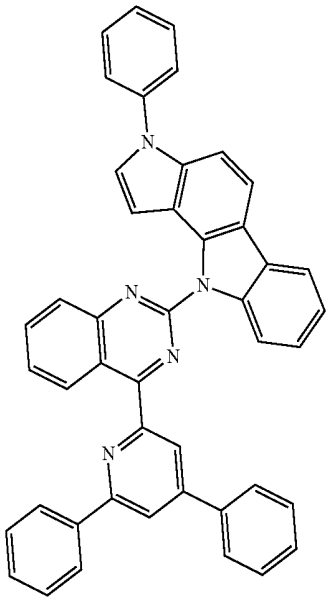
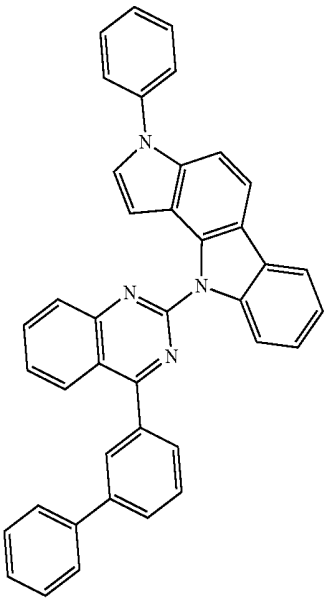
C7



C6



C8



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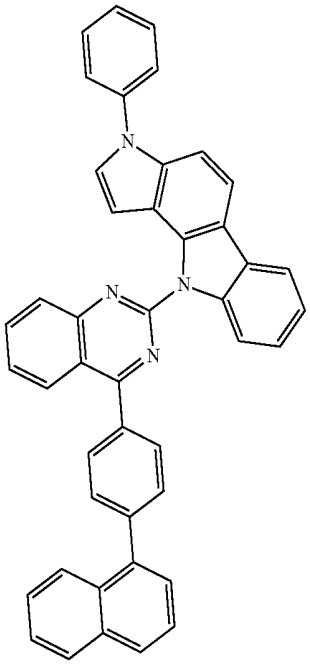
C9



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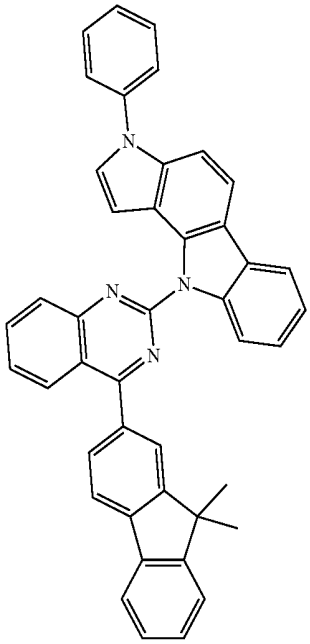
C11



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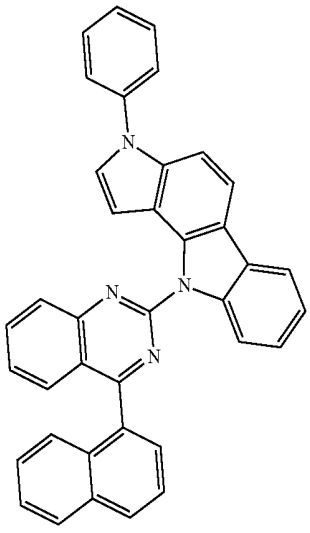

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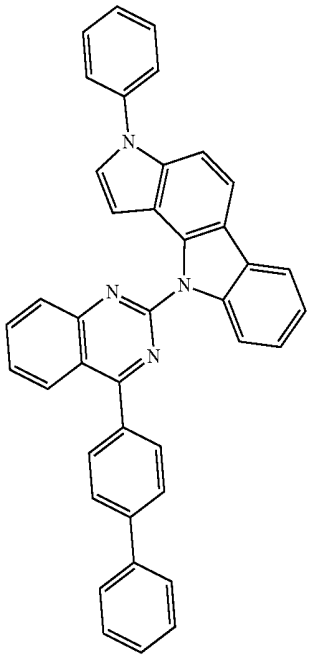

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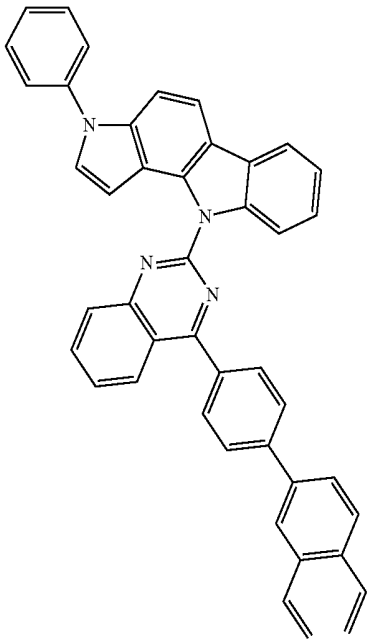
C13



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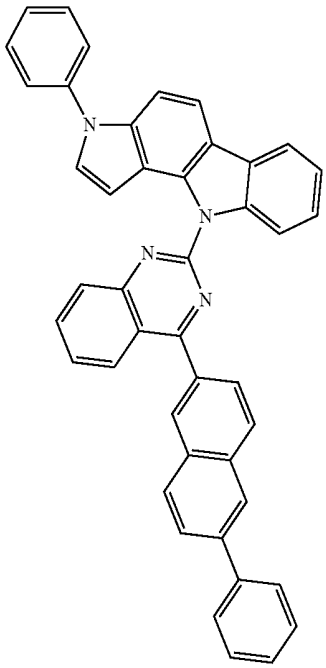

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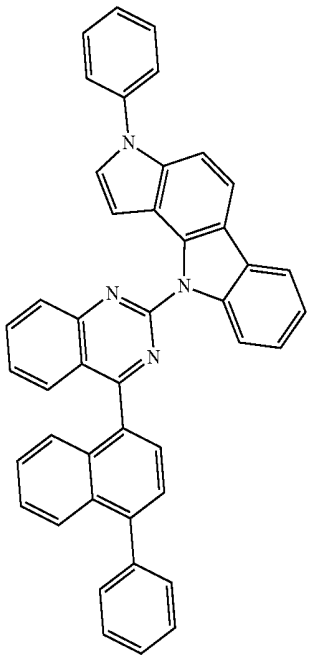
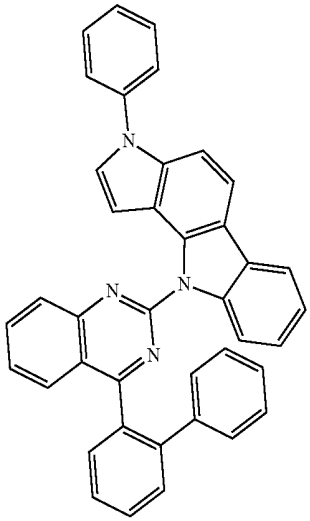


C16



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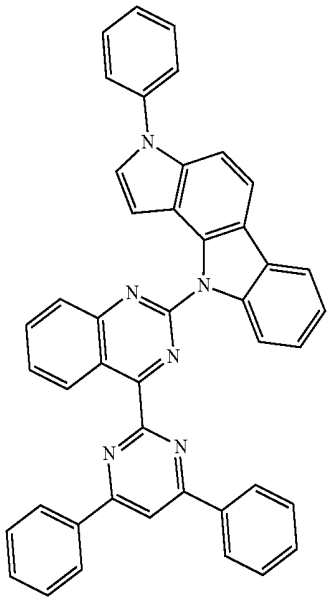

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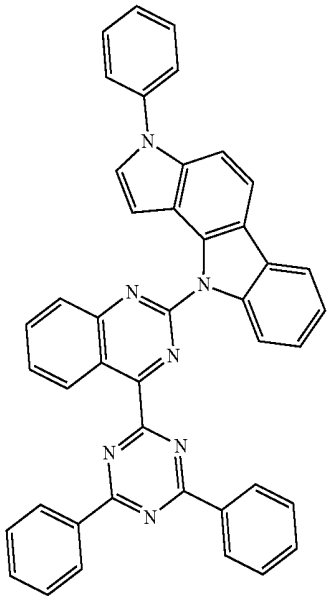

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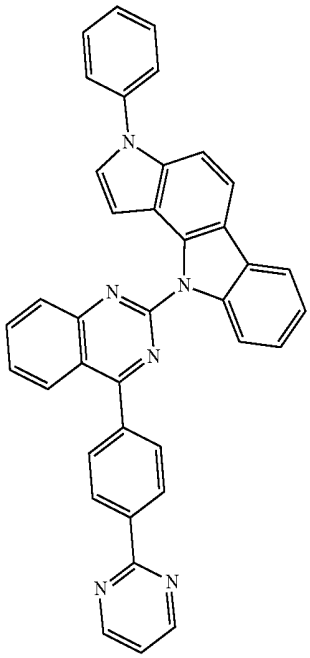

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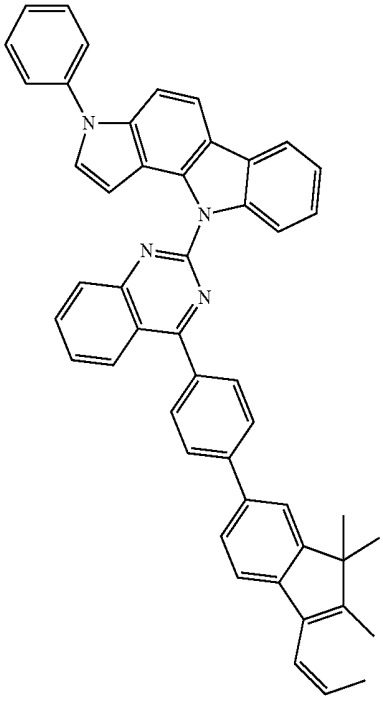

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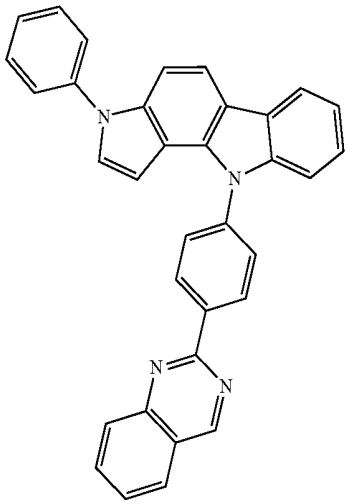

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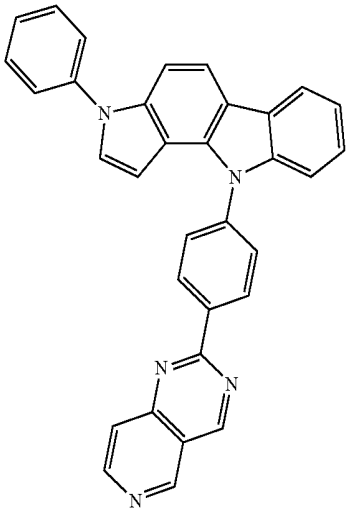
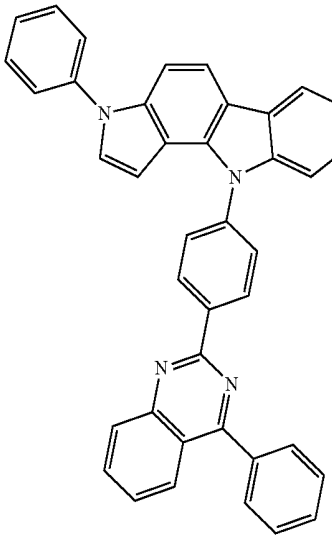


C23



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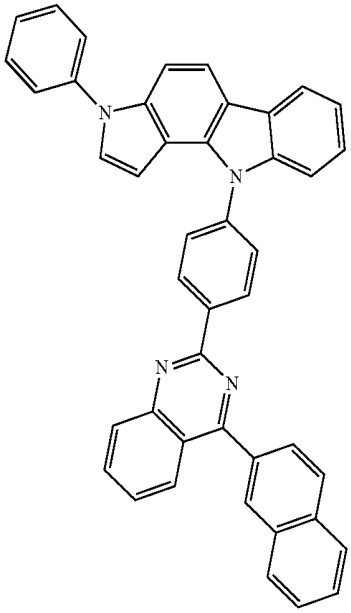

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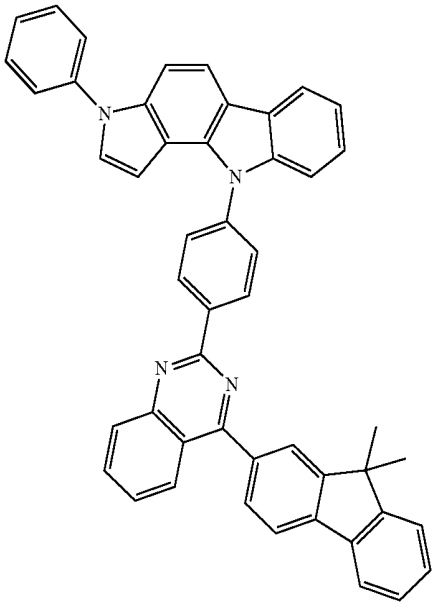

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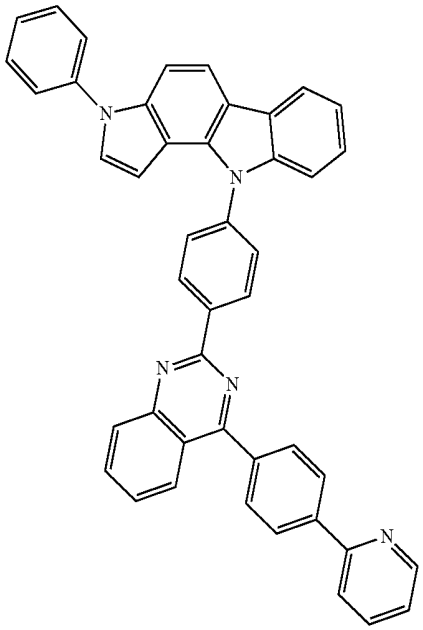

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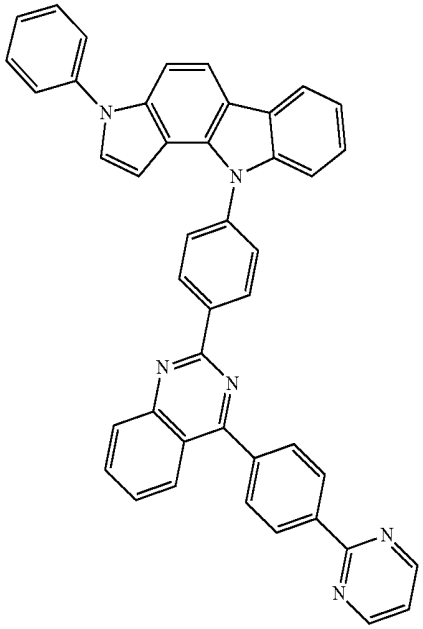

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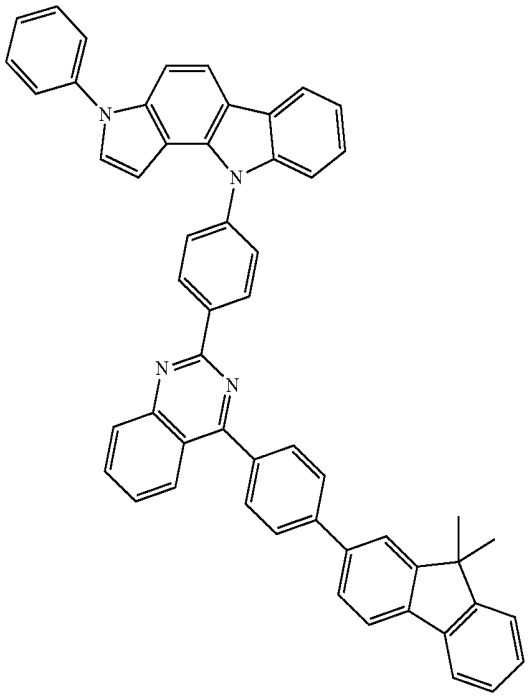

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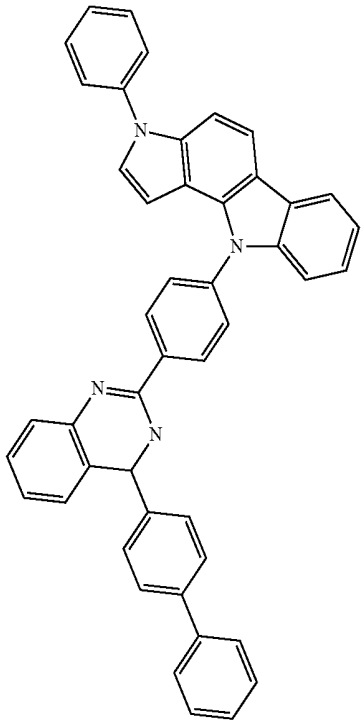

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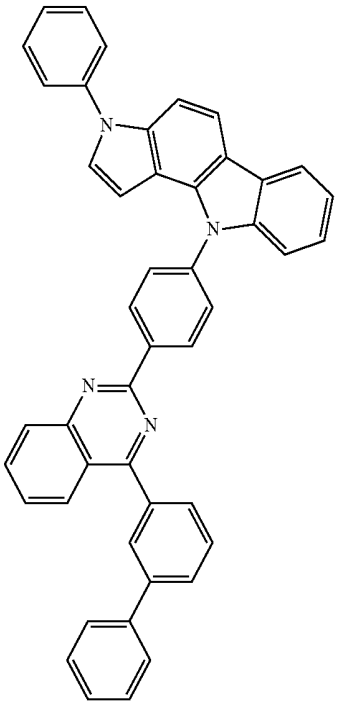

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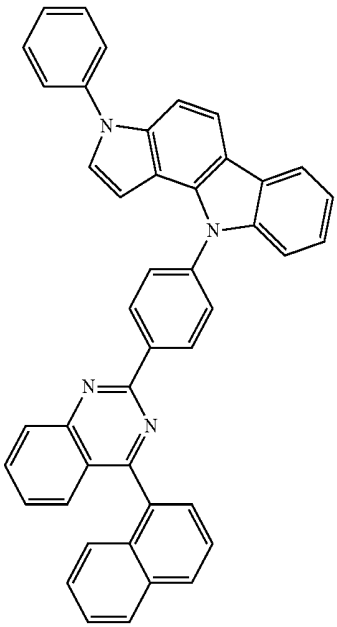

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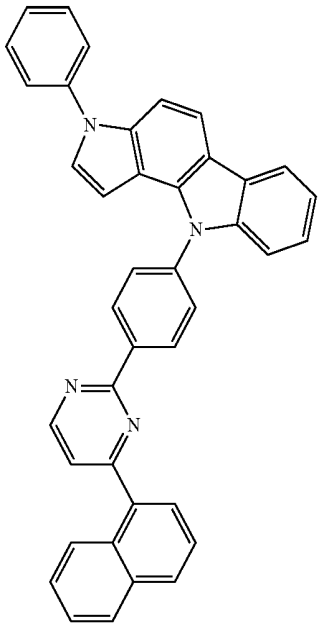

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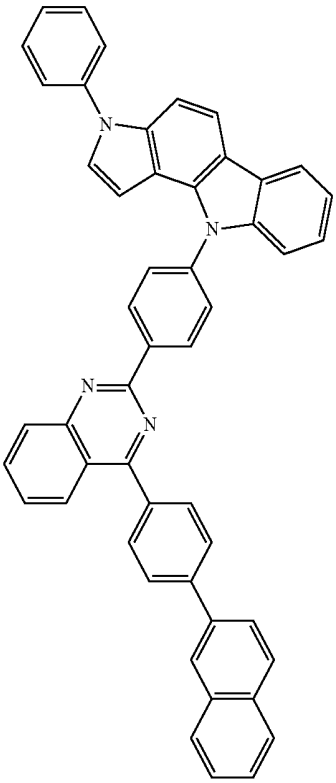

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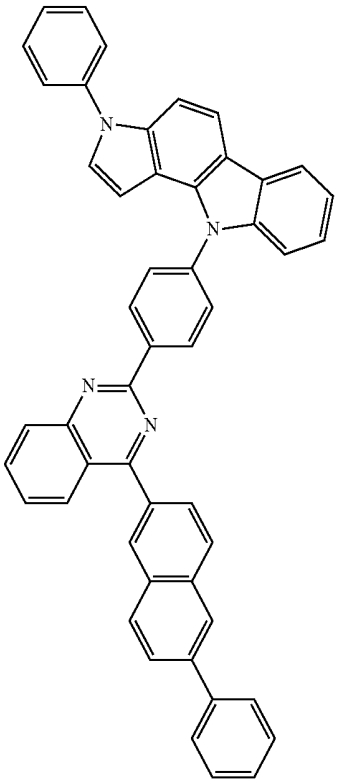

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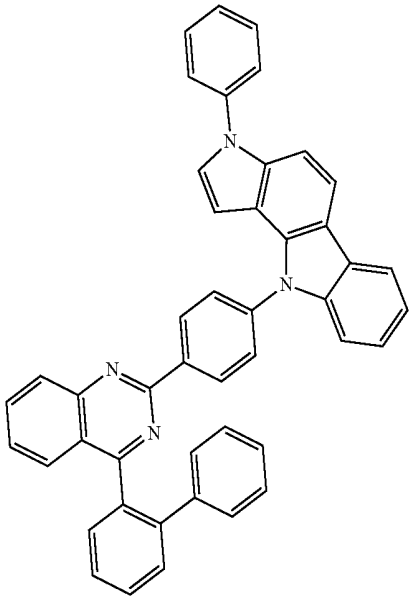

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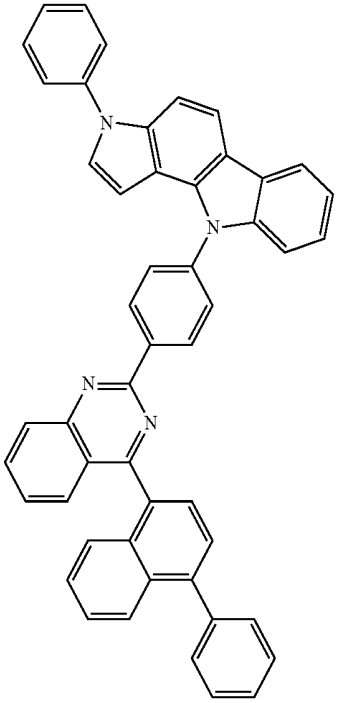

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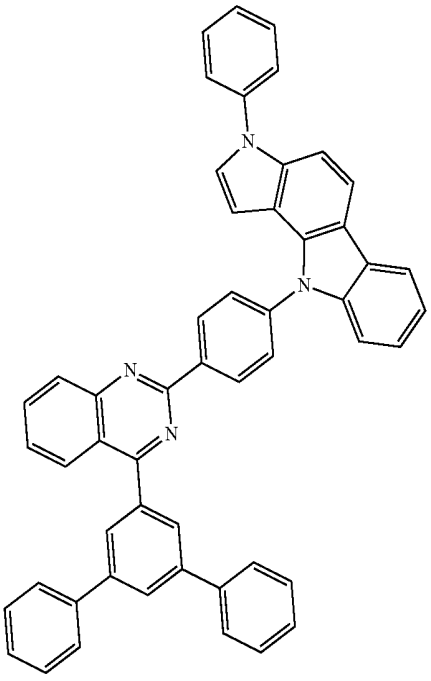

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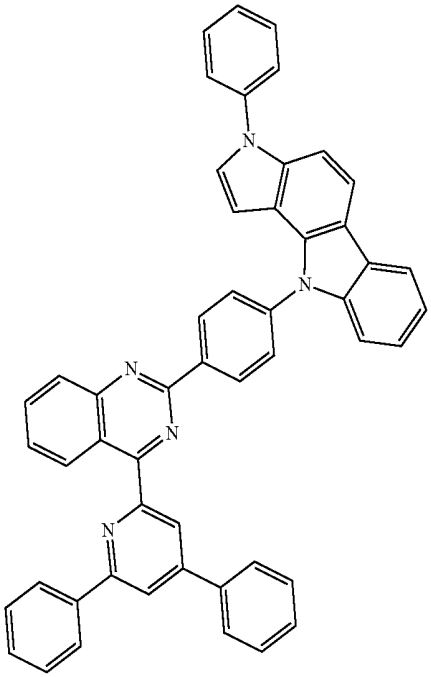

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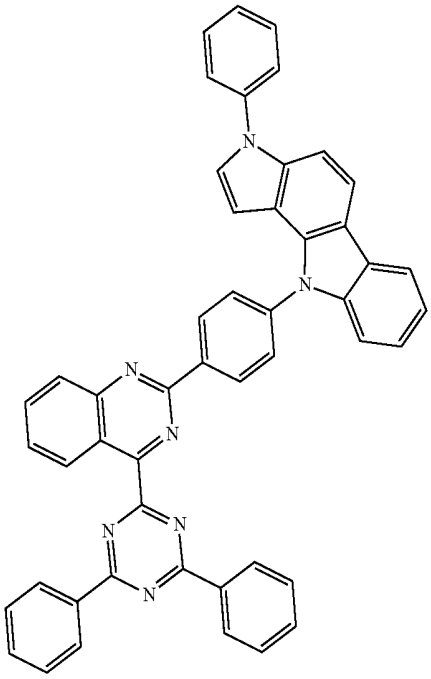

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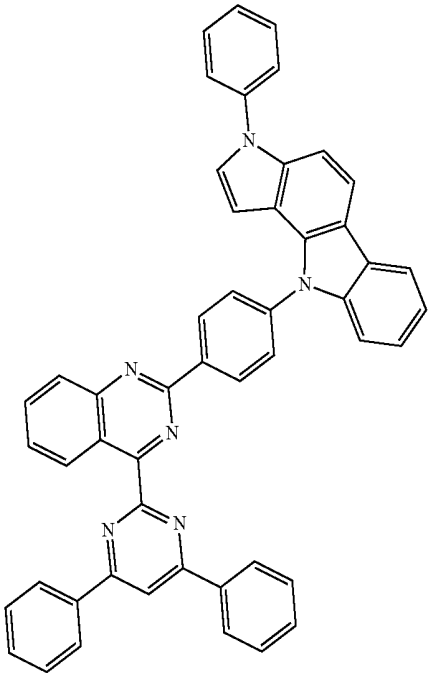

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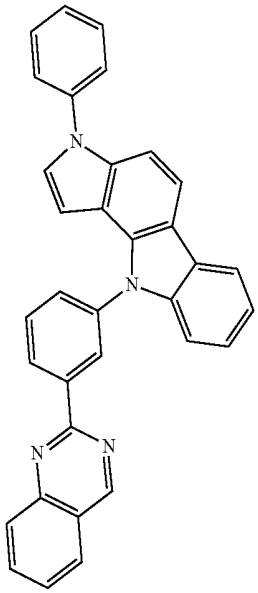

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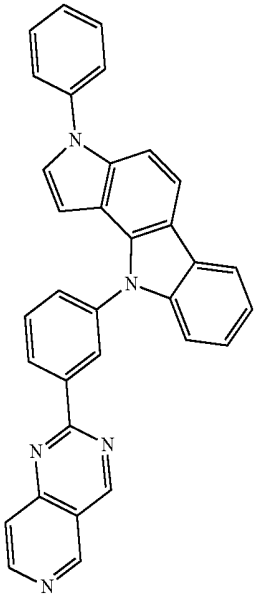

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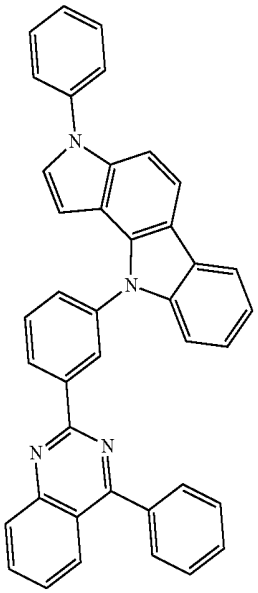

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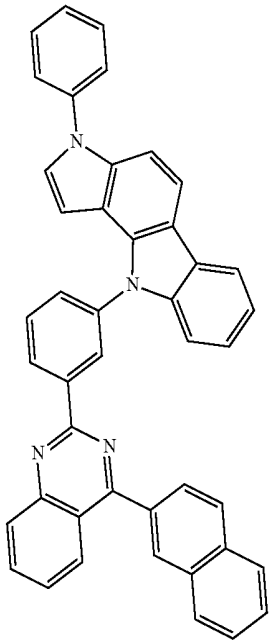

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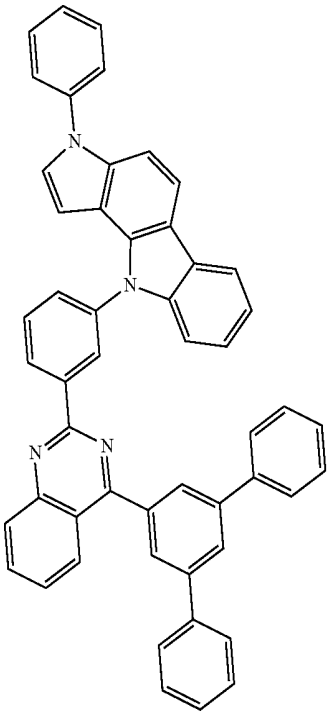

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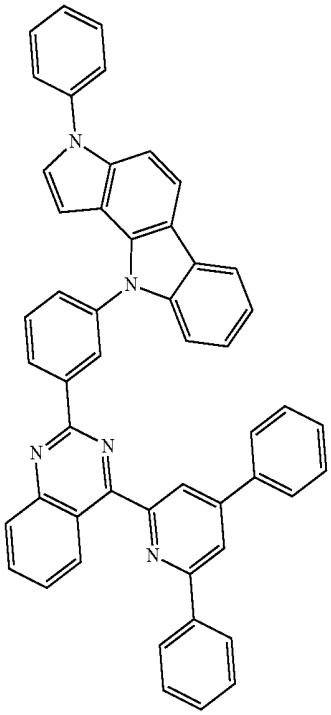

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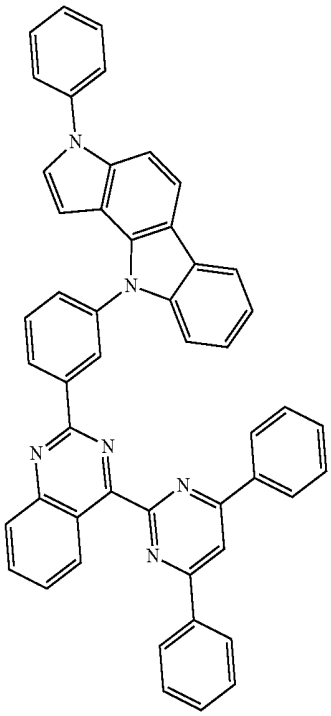

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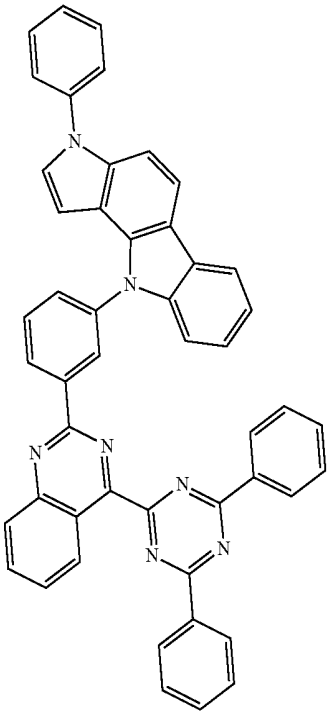

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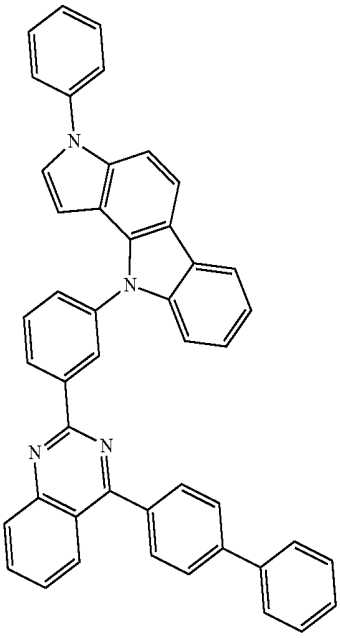

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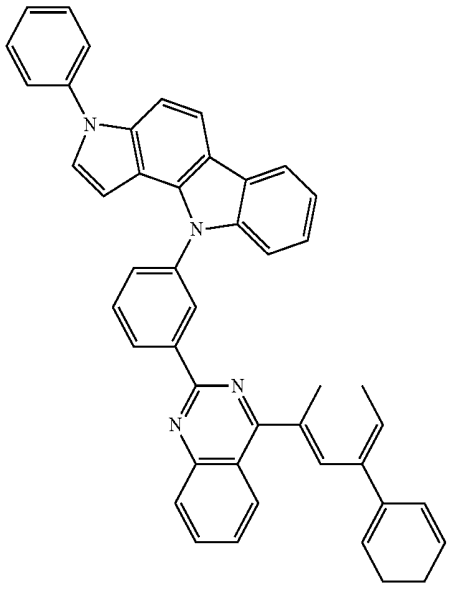

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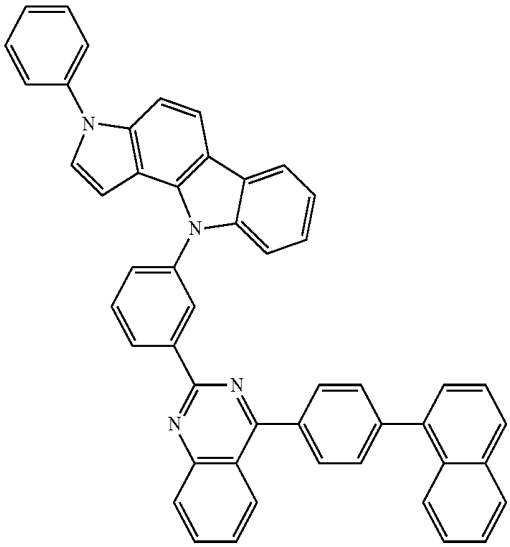

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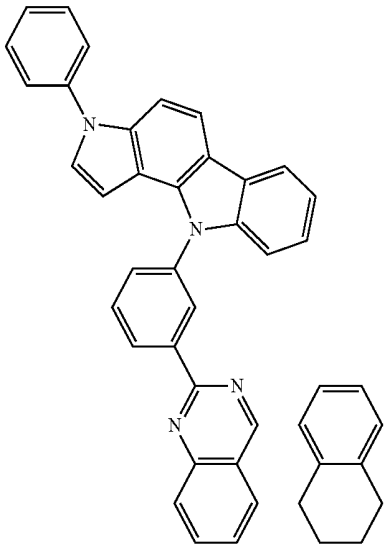

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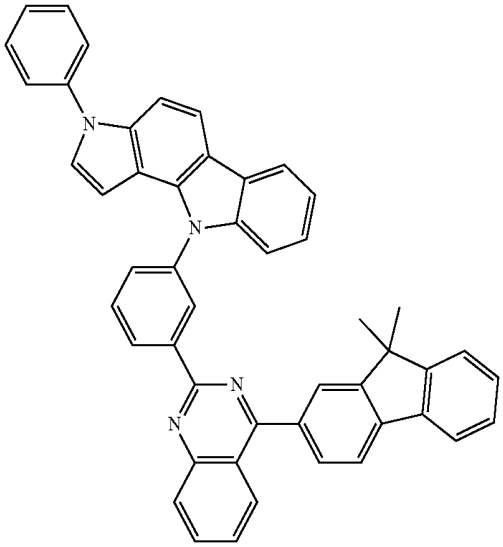

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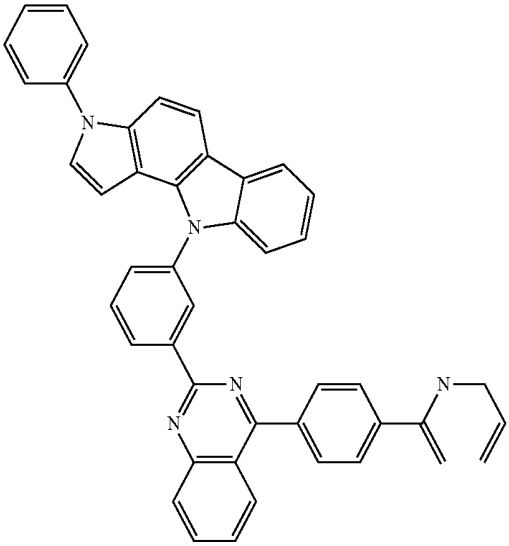

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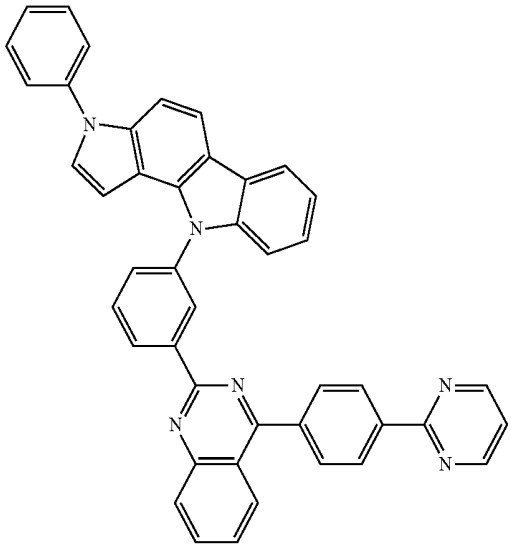

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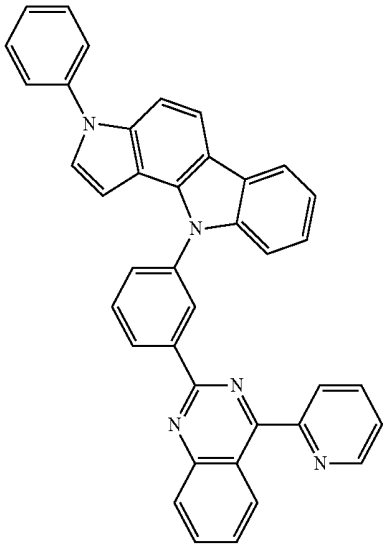

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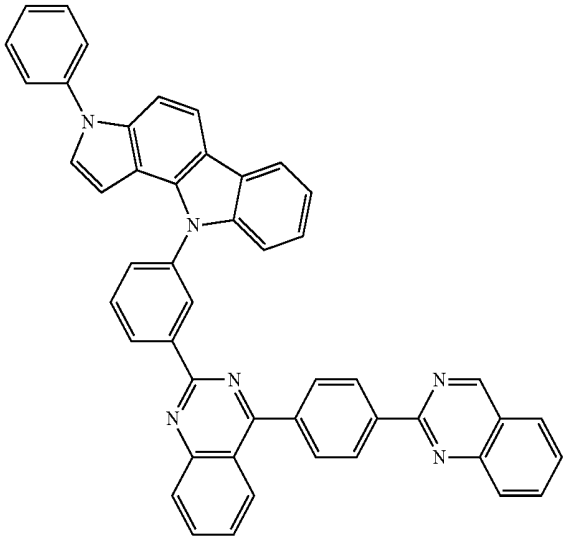

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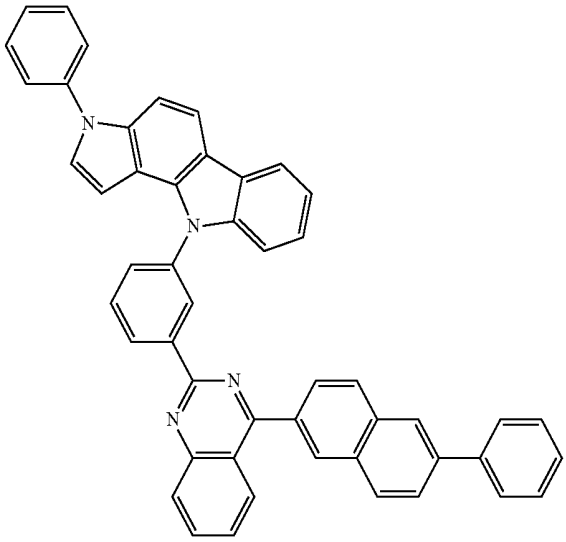

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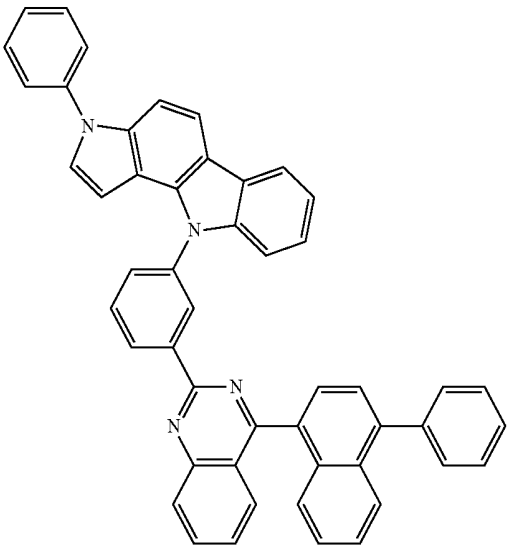

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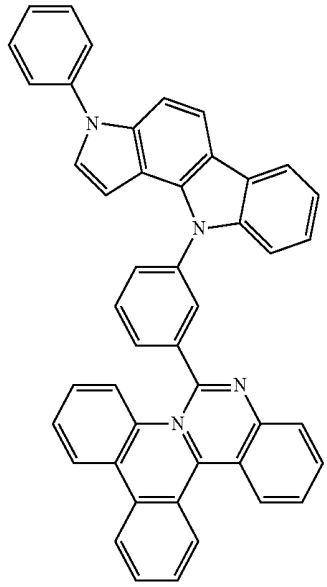

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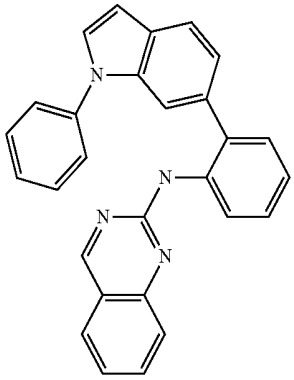

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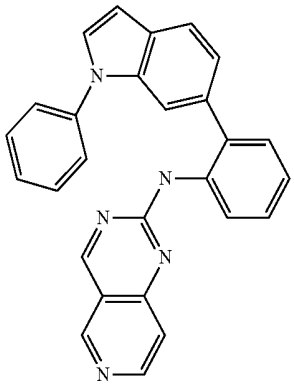

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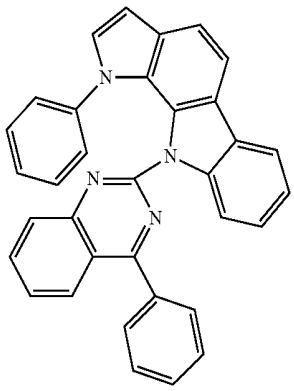

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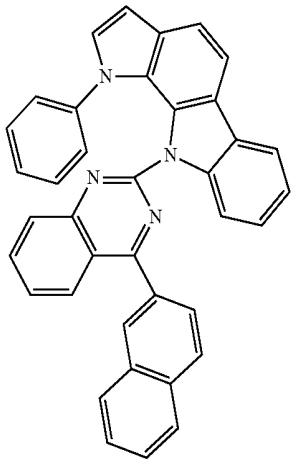

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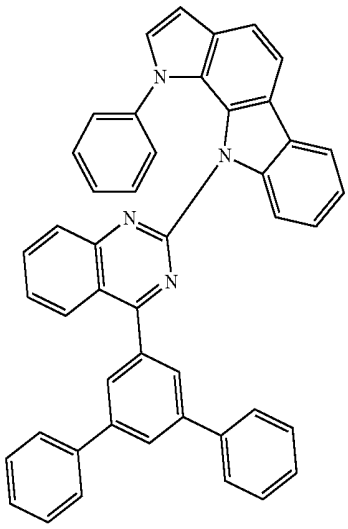

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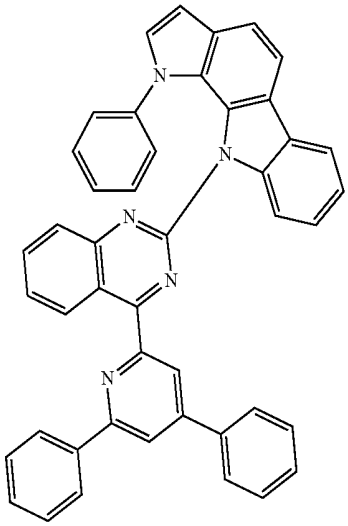

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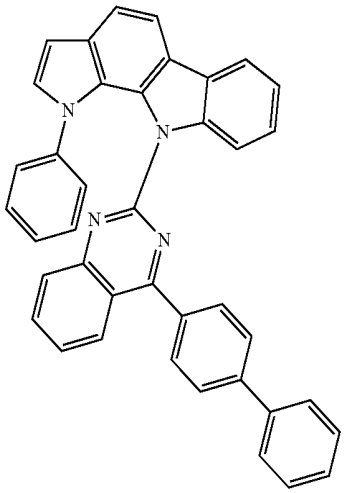

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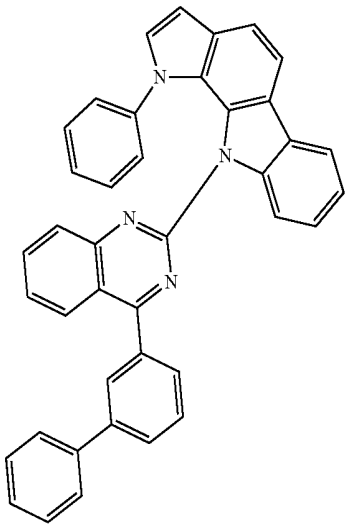

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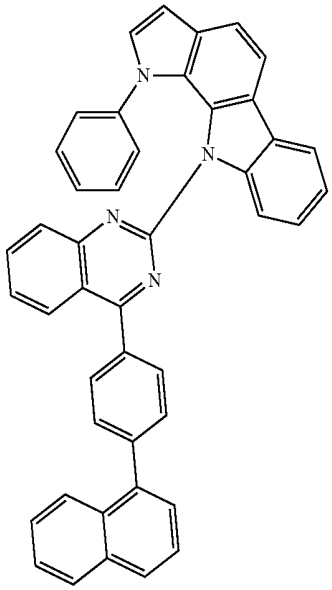

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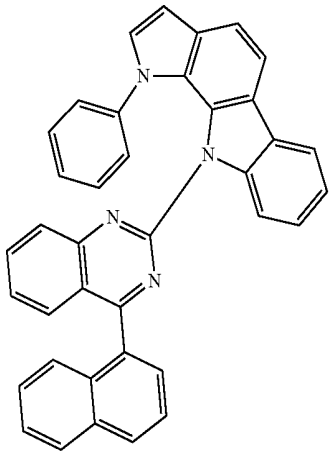

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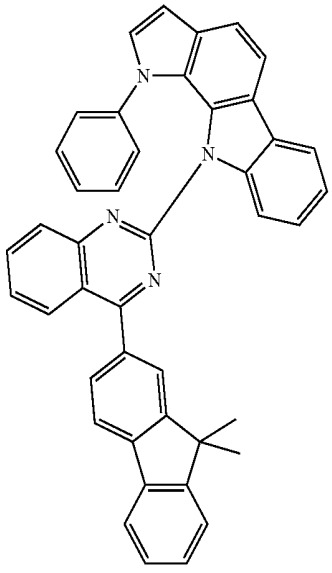

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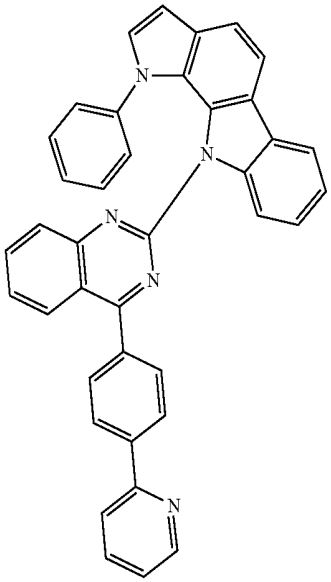

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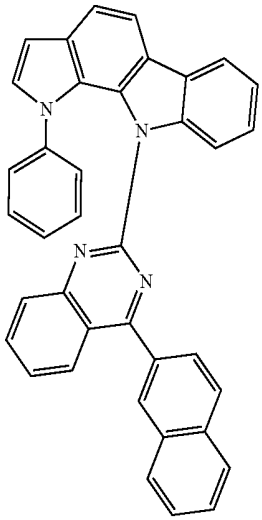

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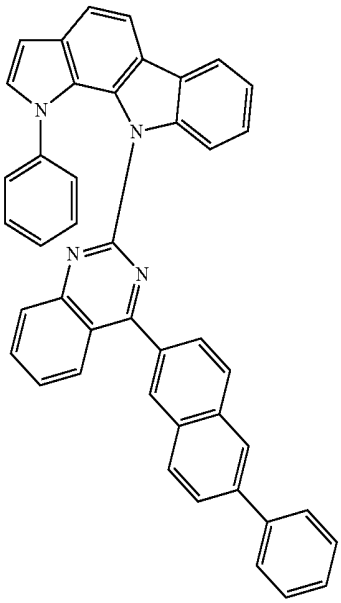

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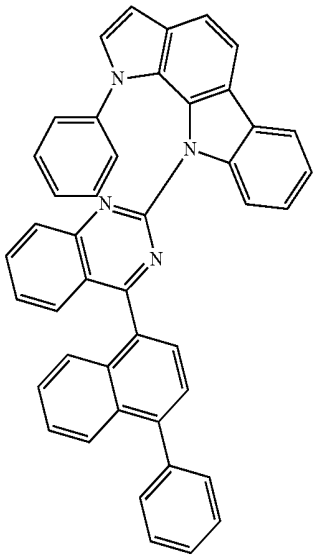

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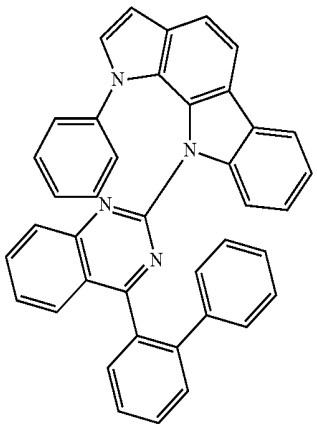

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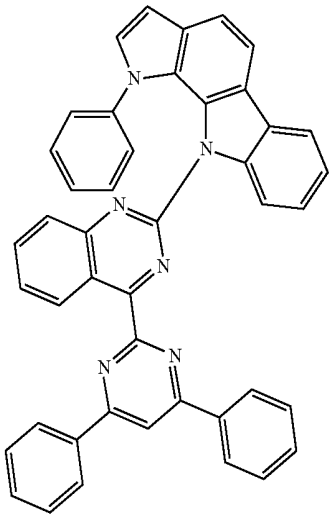

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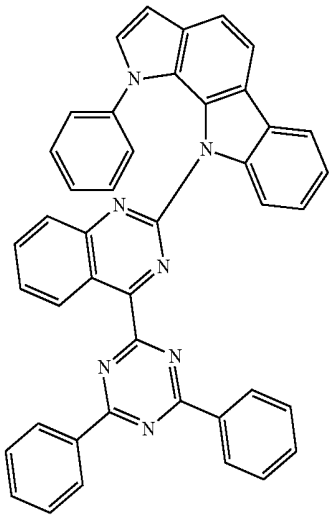

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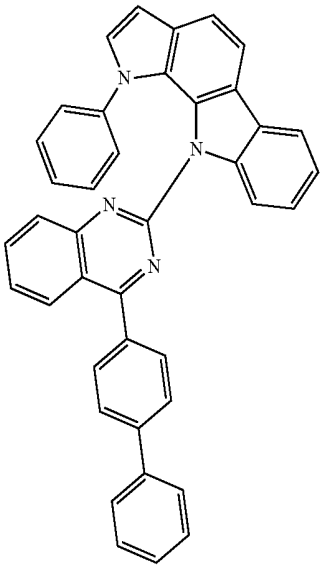

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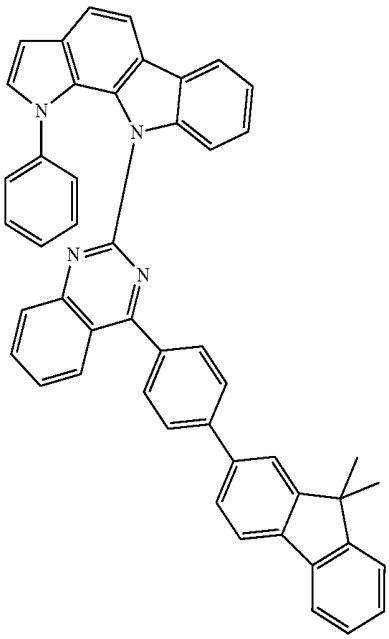

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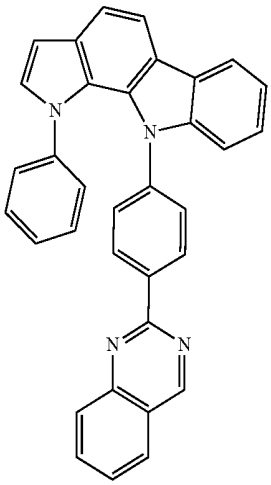

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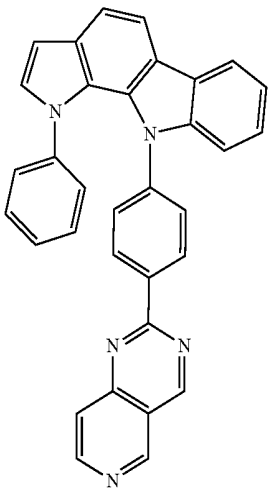

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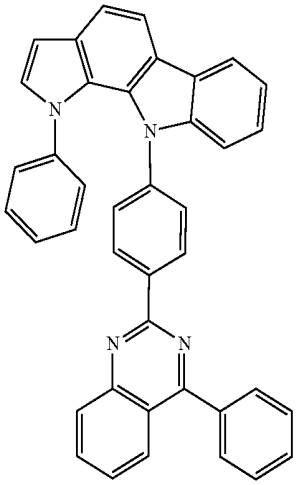

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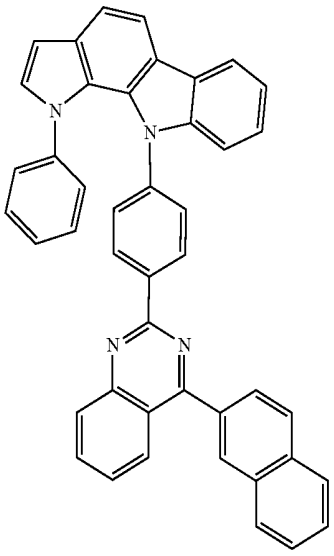

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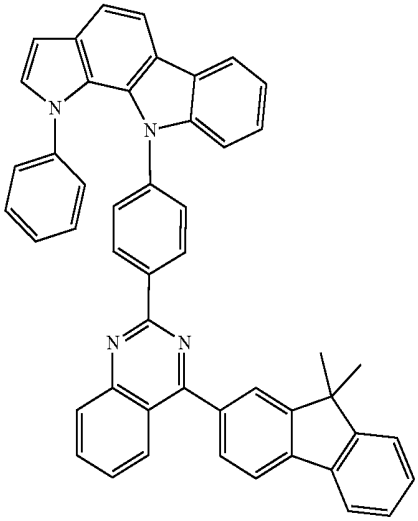

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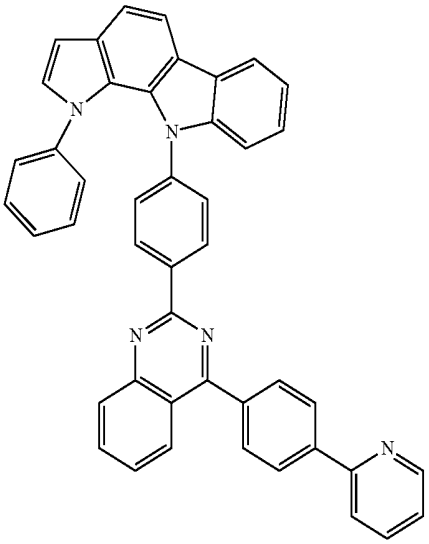

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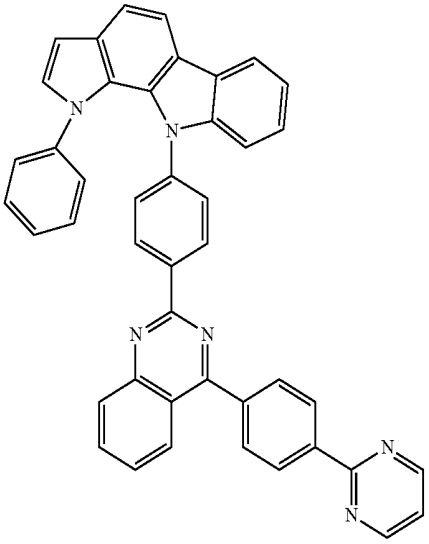

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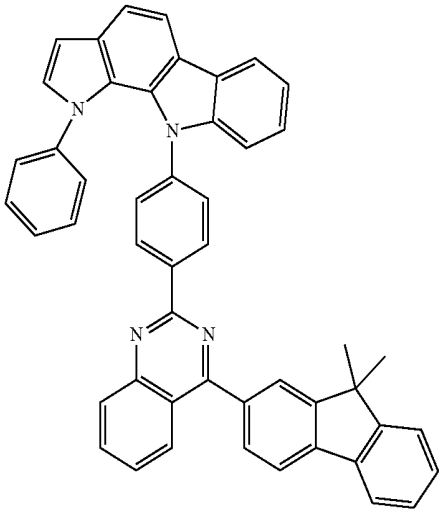

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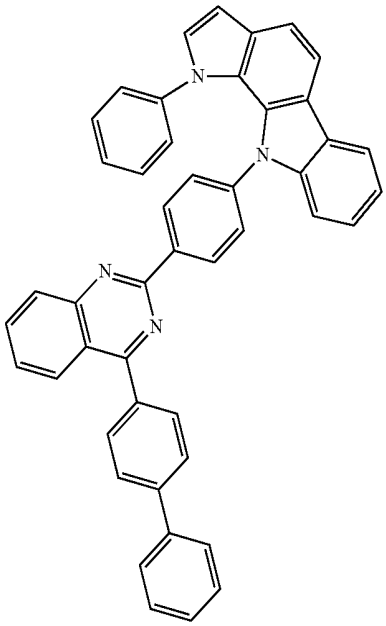

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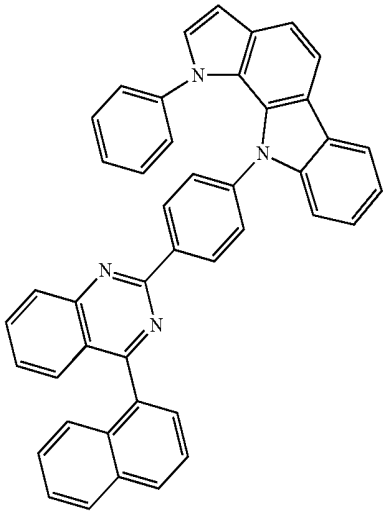

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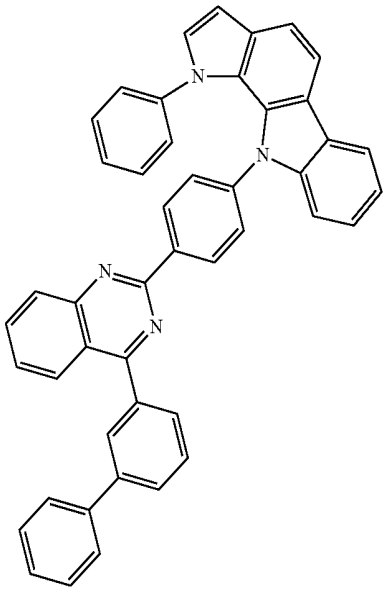

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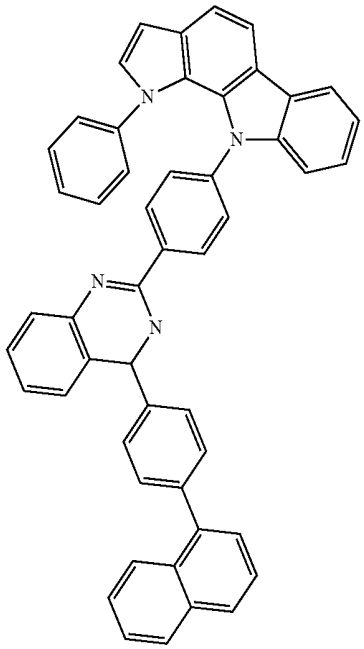

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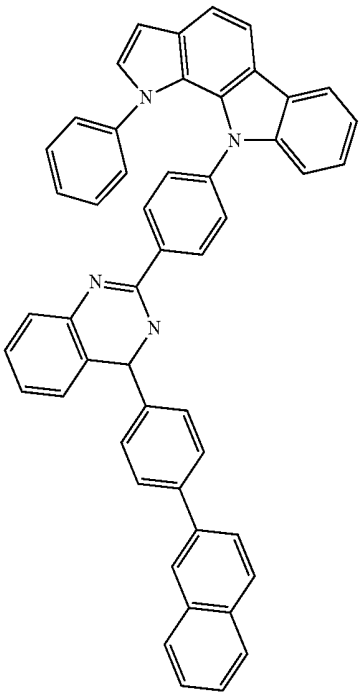

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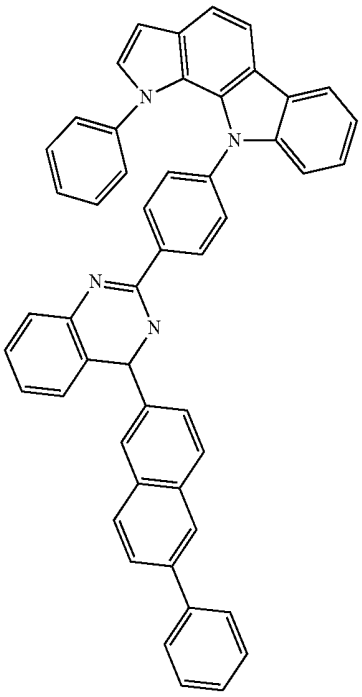

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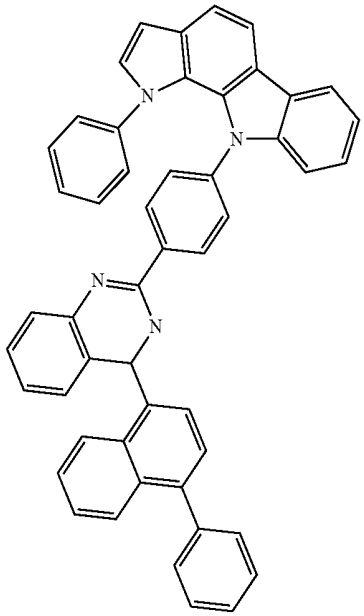

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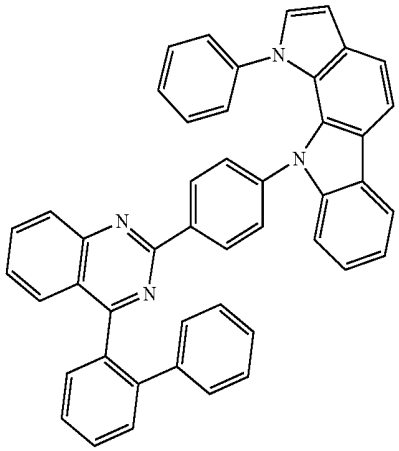

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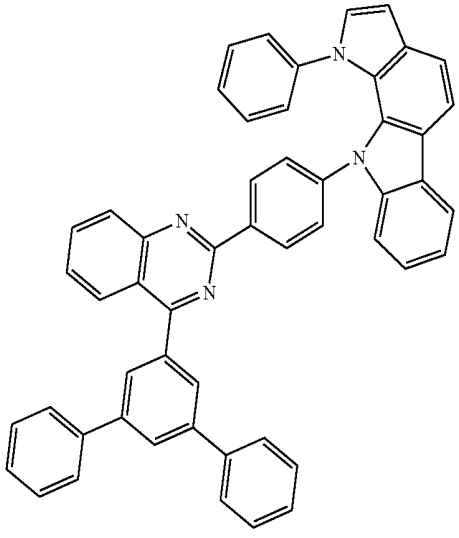

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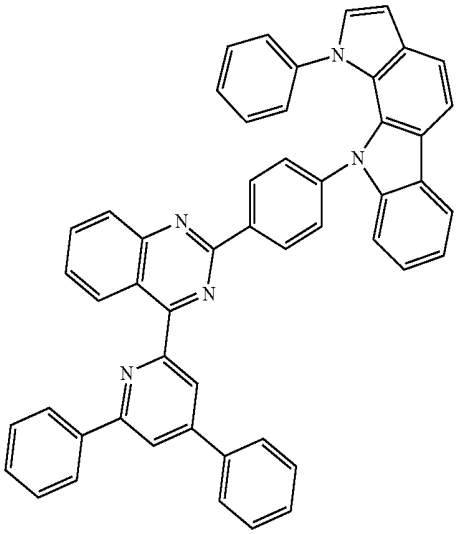

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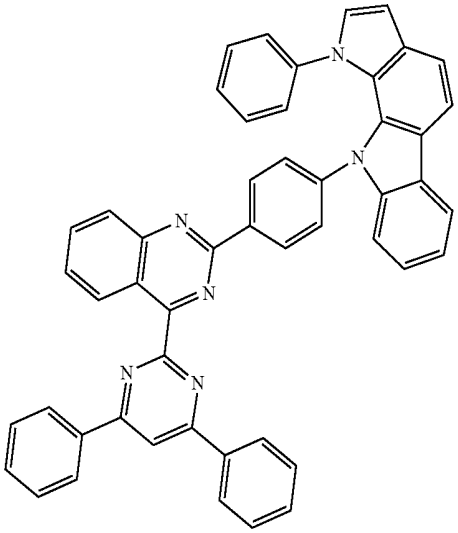

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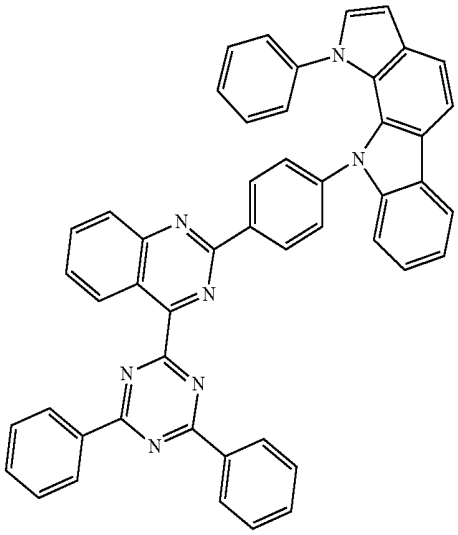

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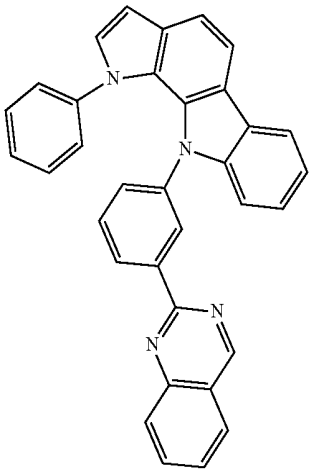

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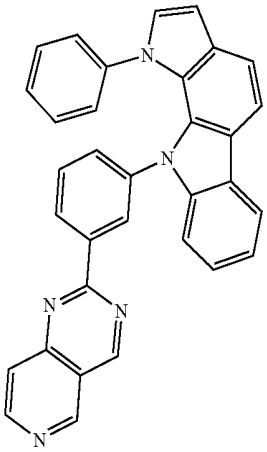

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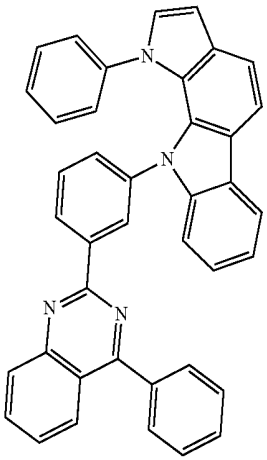

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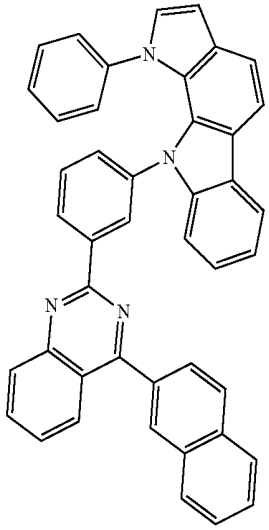

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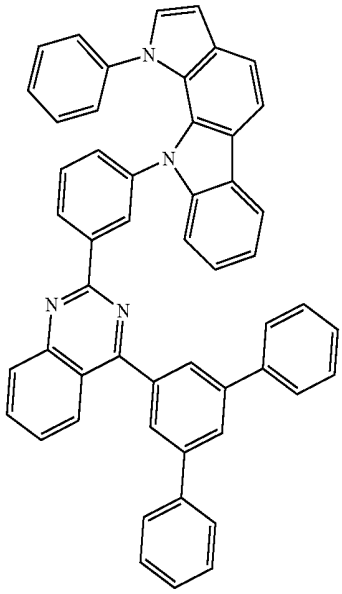

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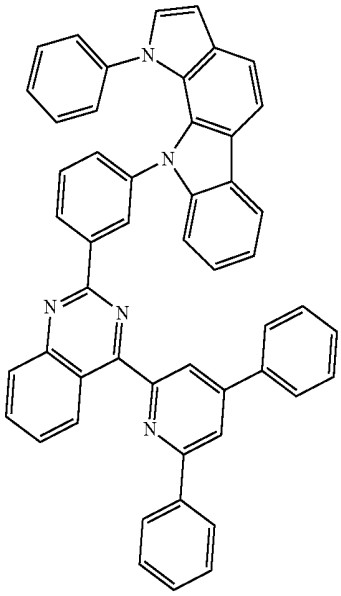

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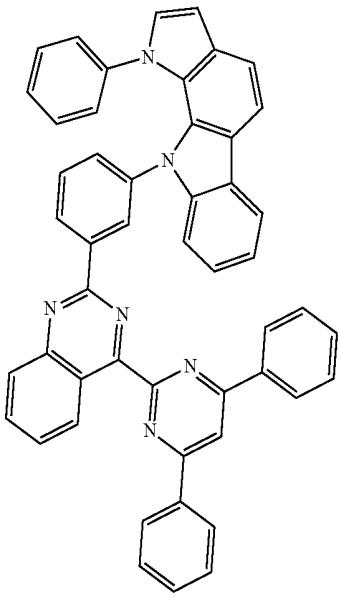

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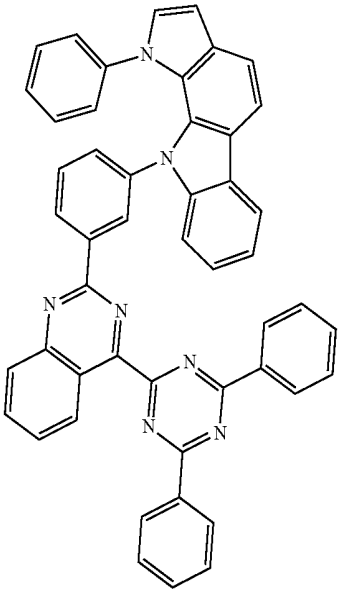

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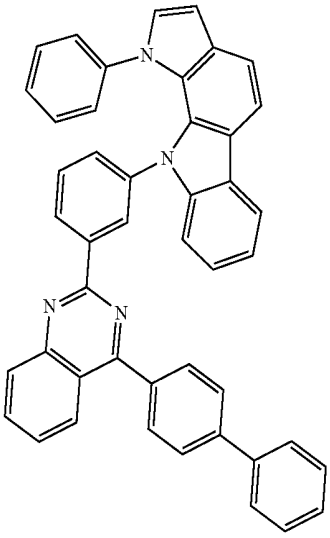

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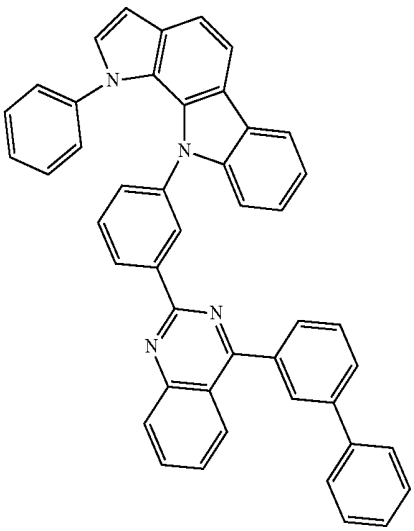

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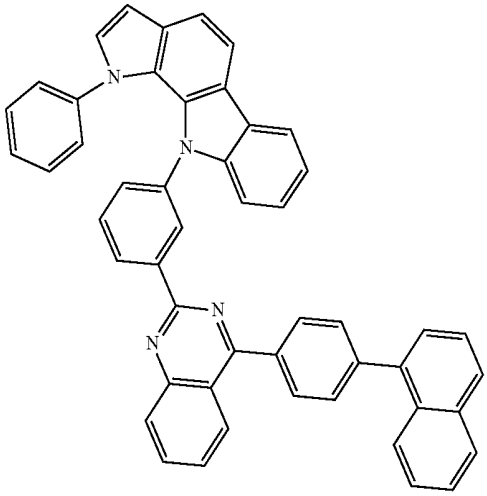

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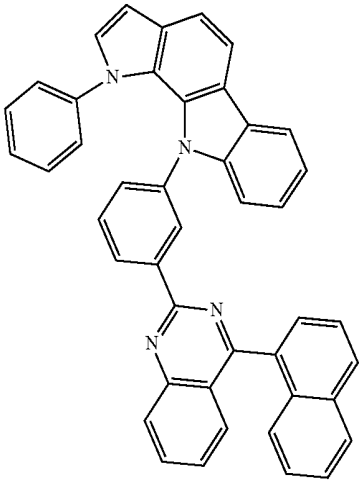

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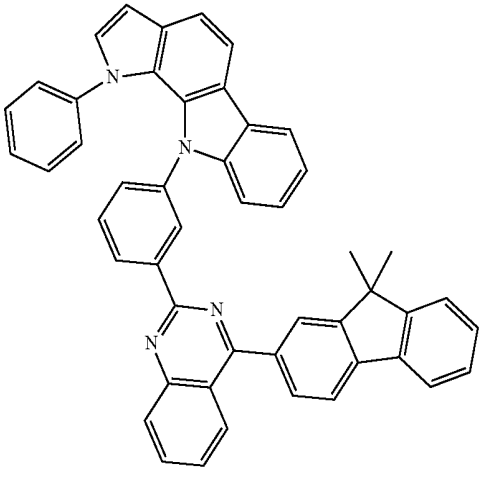

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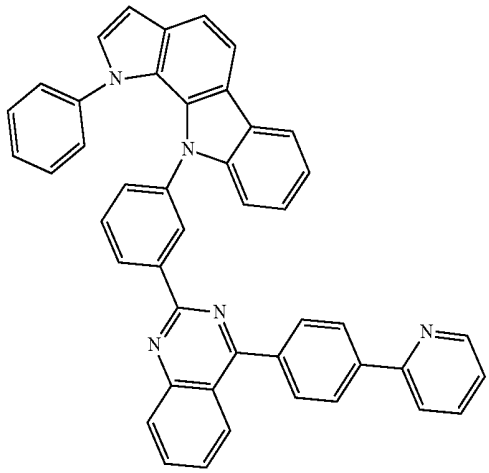

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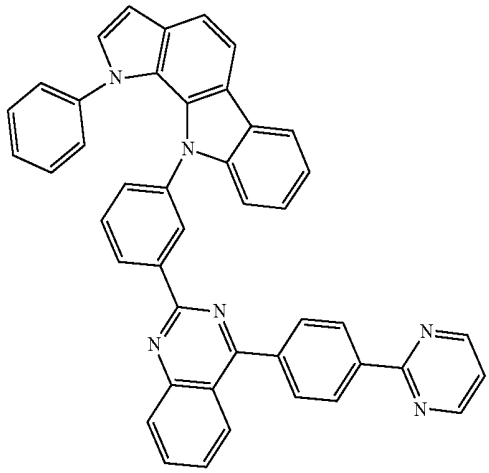

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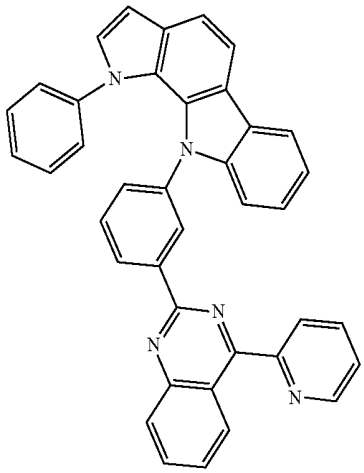

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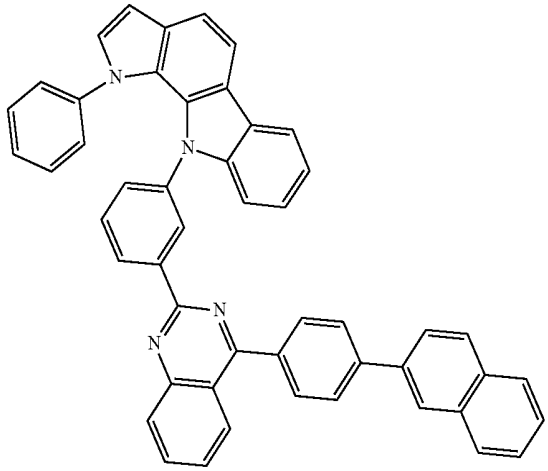

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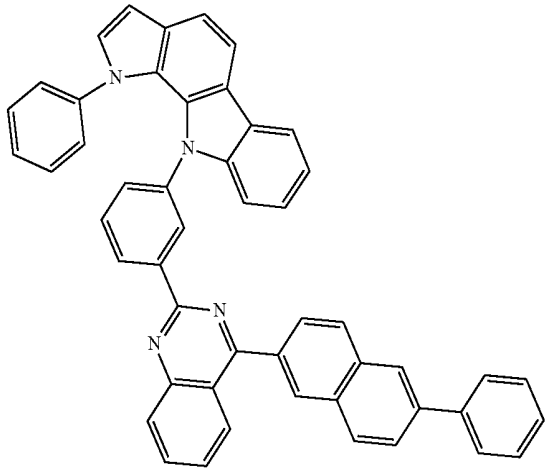

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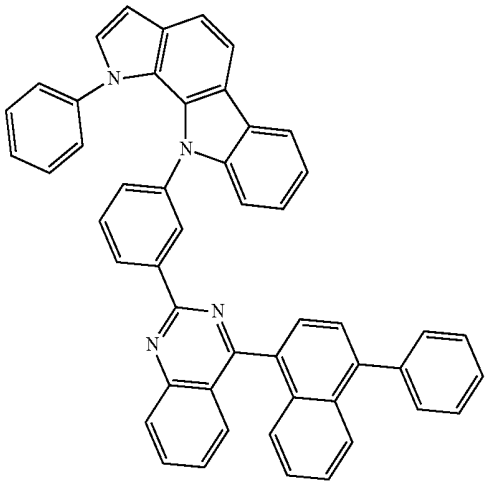

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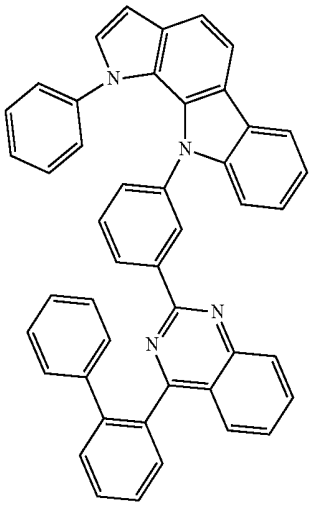

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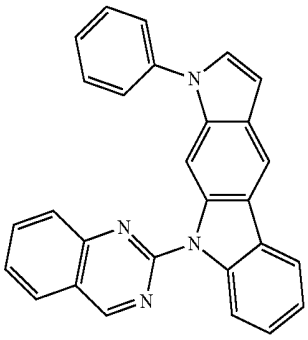

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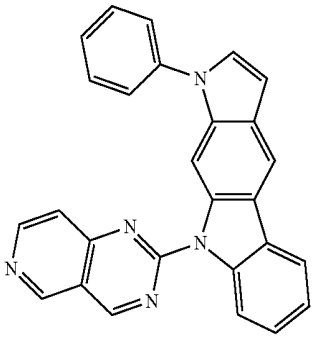

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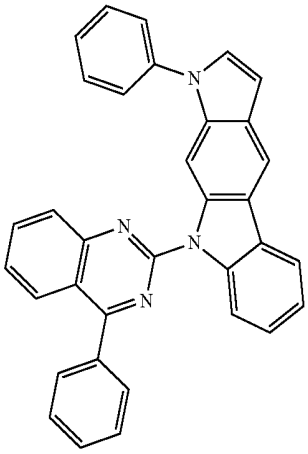

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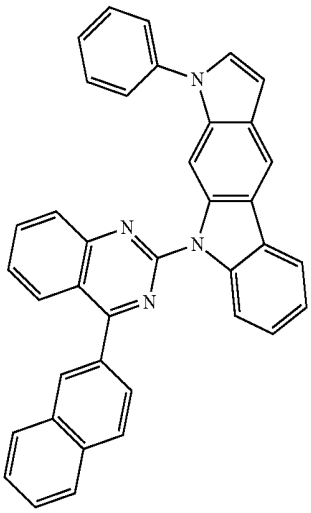

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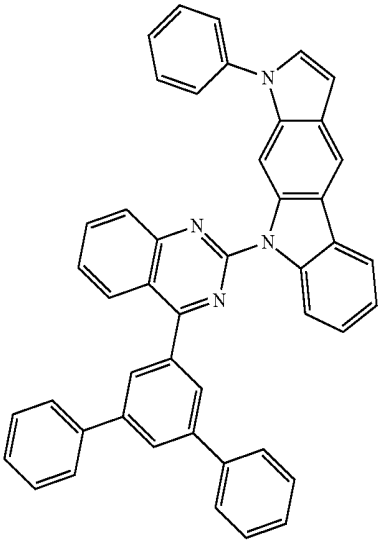

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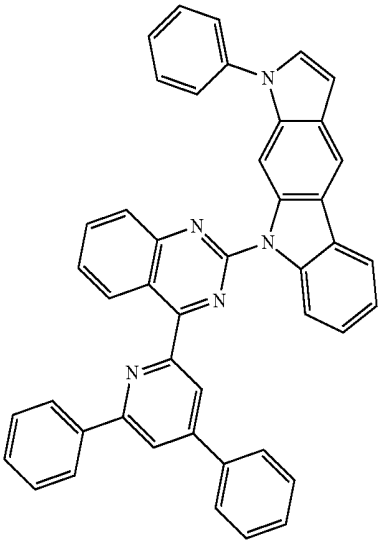

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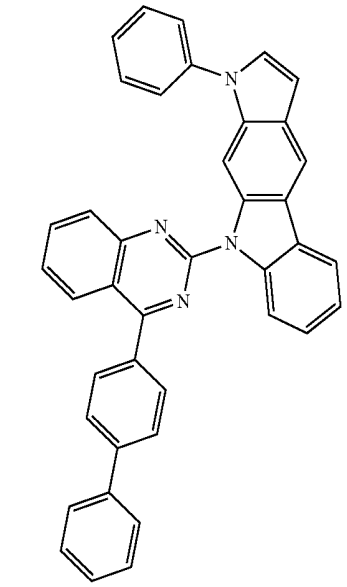

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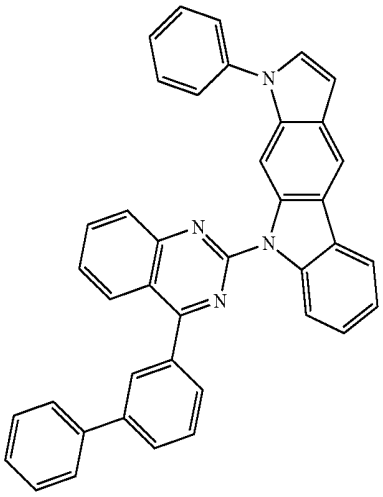

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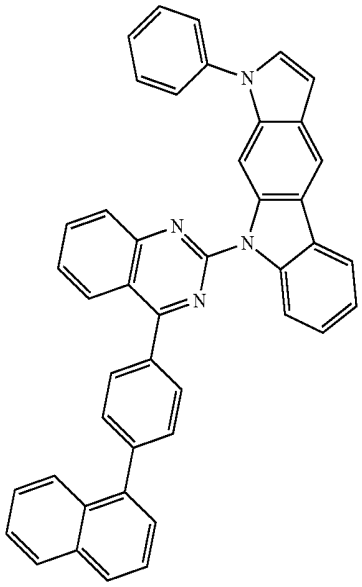

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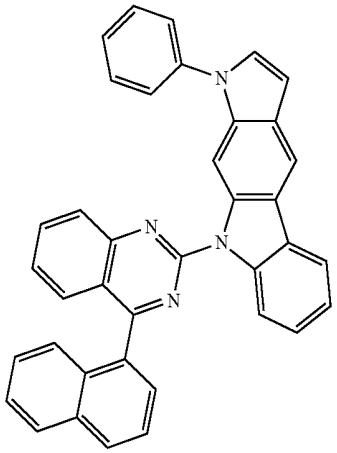

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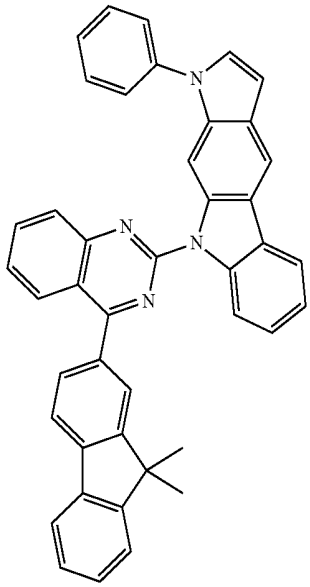

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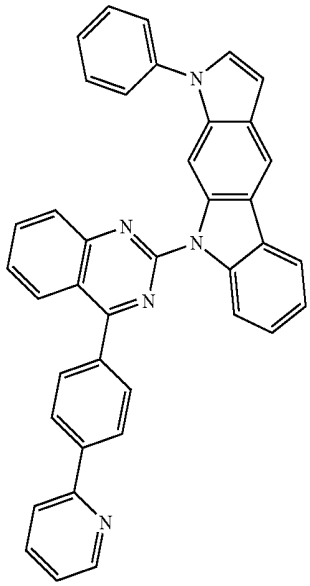

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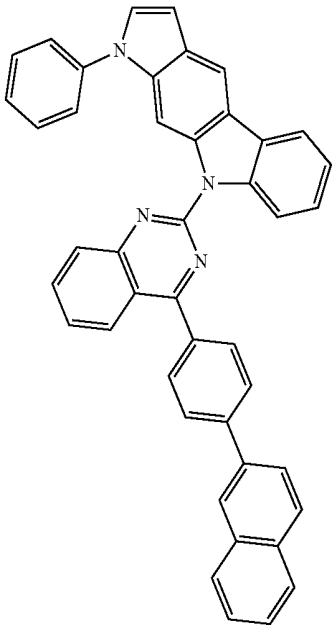

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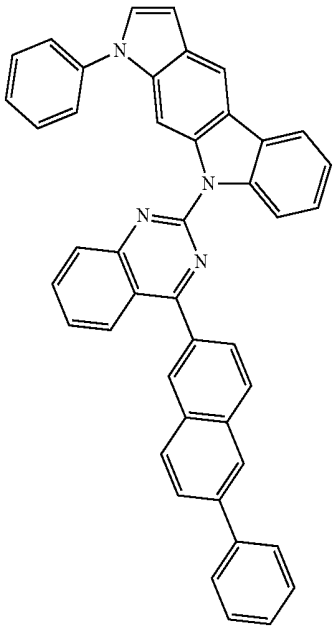

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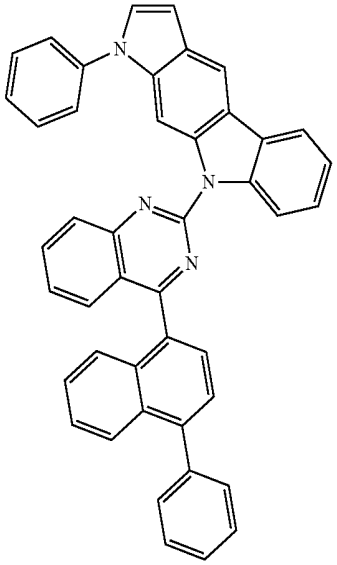

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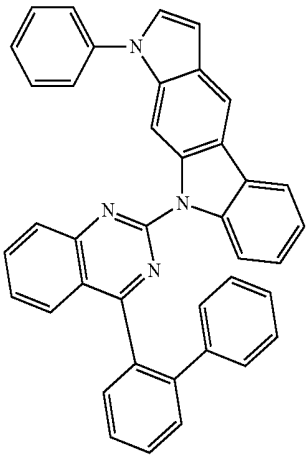

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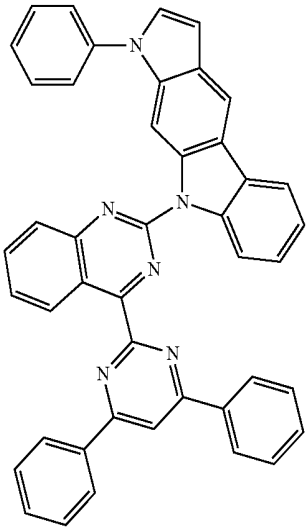

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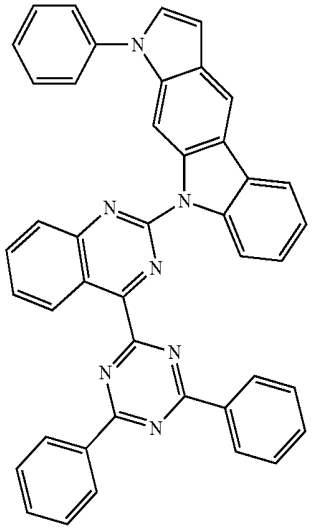

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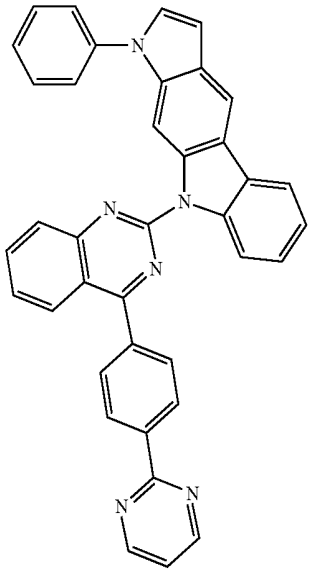

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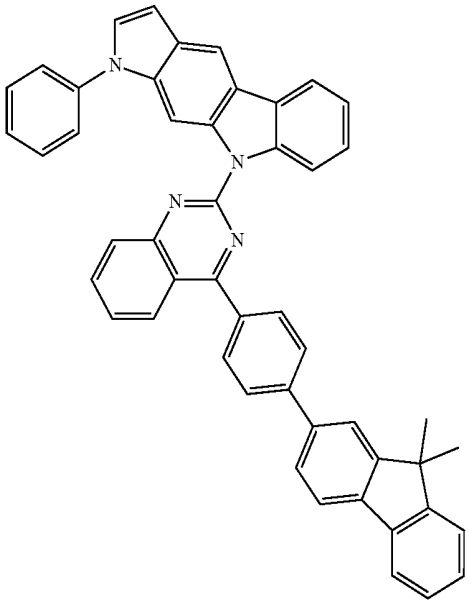

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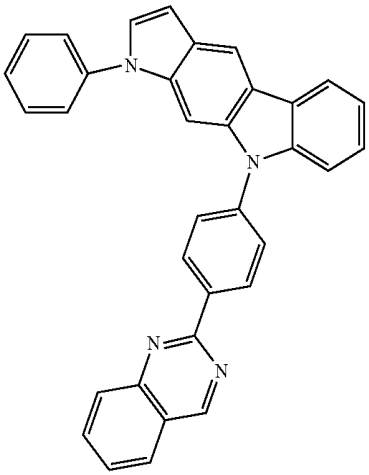

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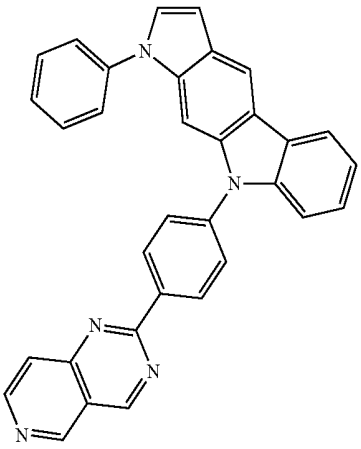

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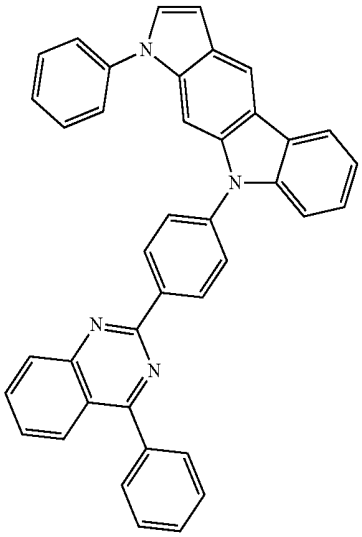

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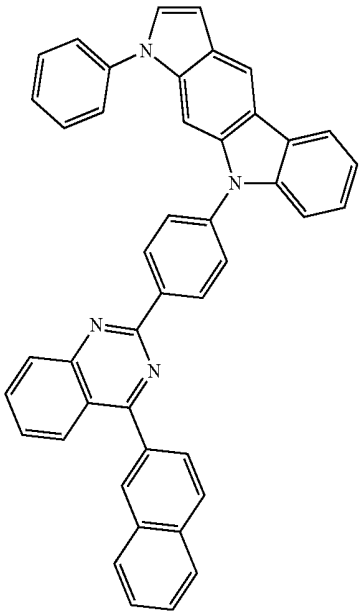

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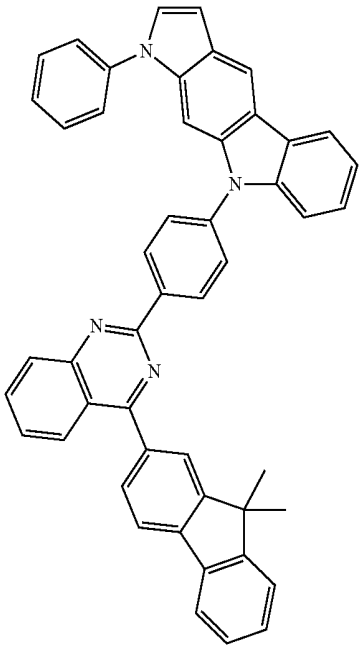

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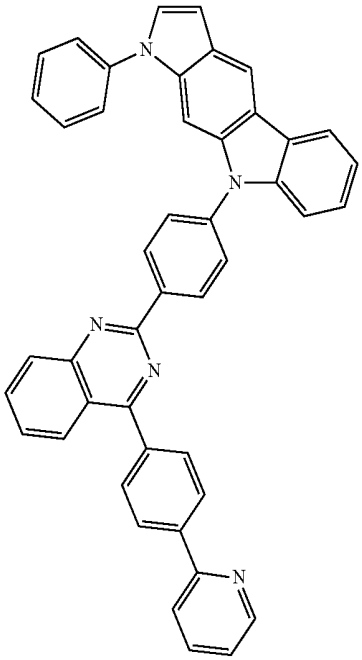

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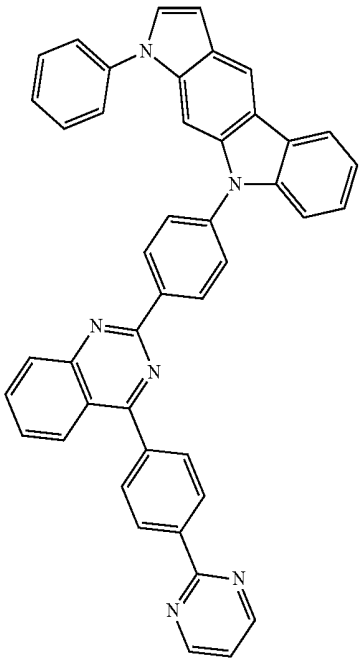

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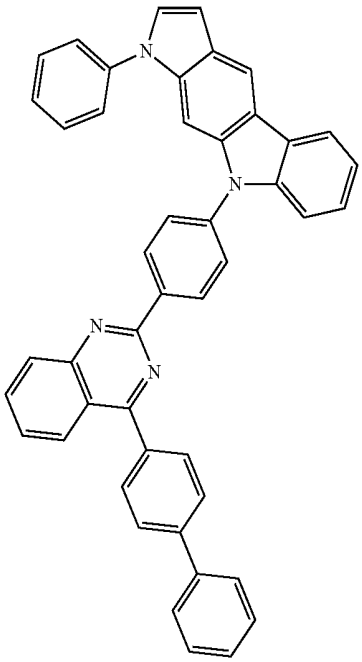

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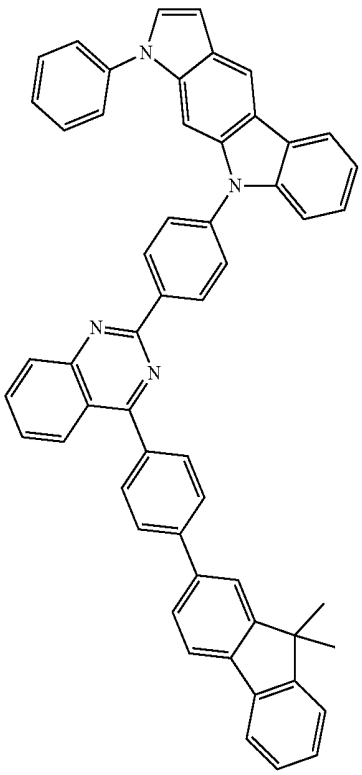

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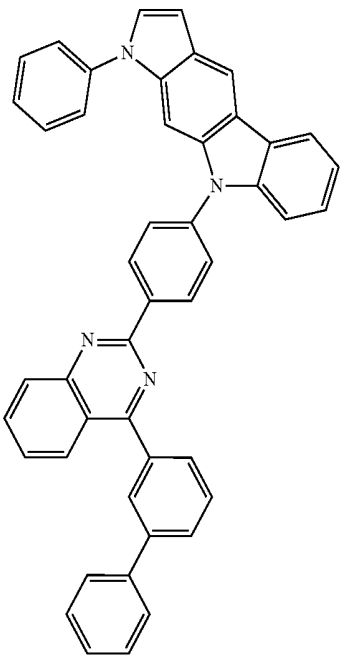

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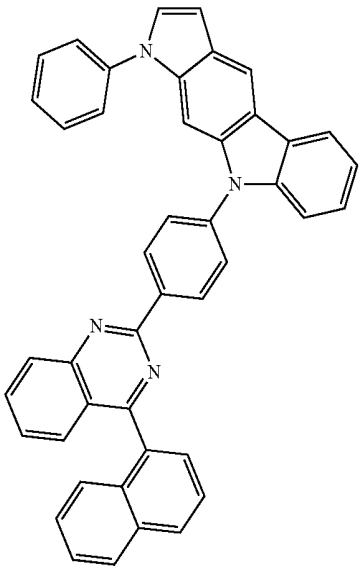

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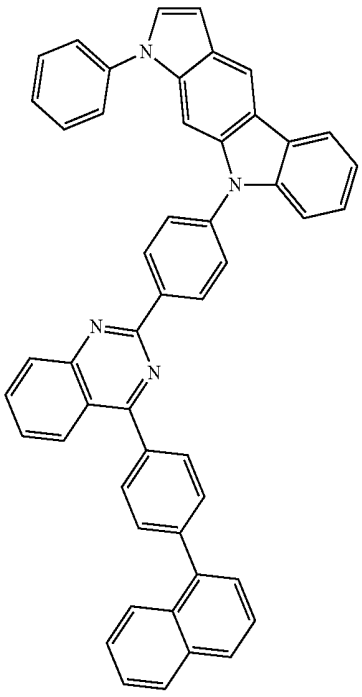

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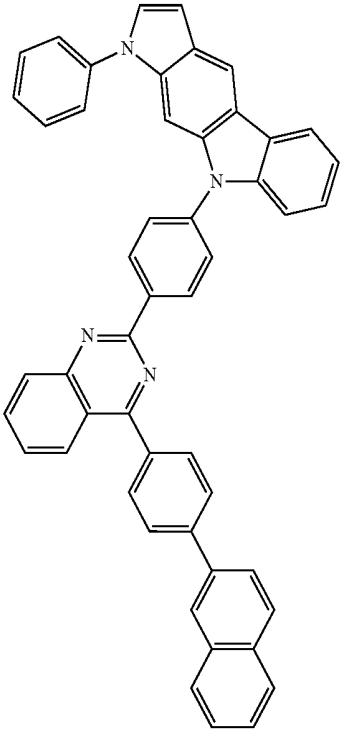

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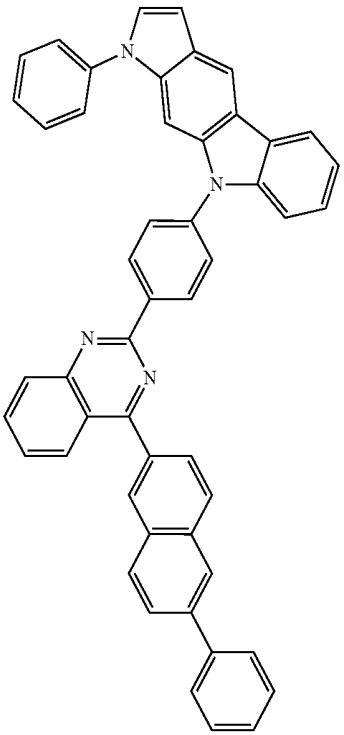

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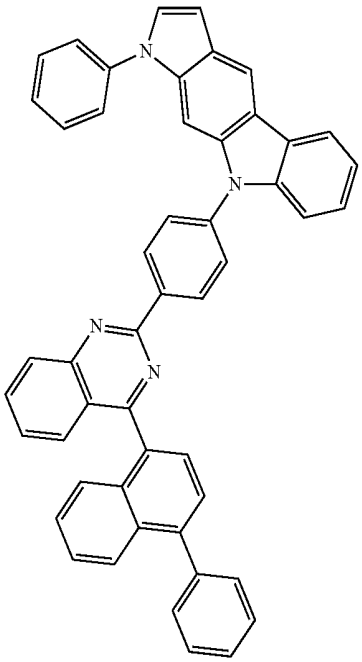

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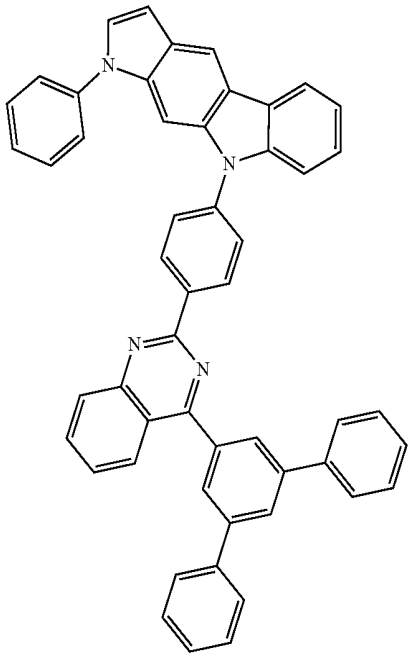

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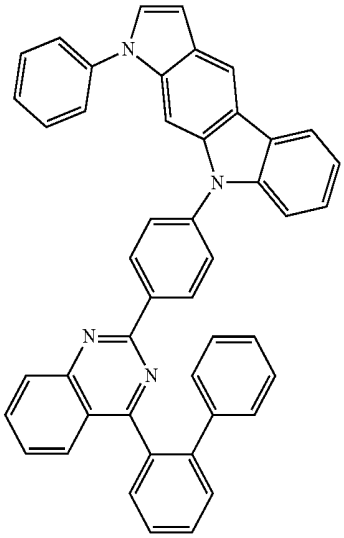

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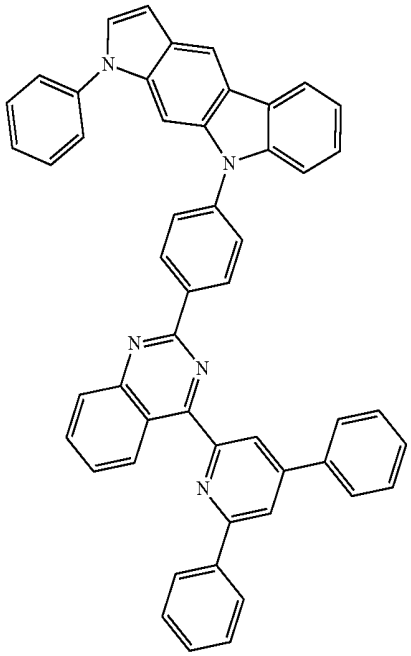

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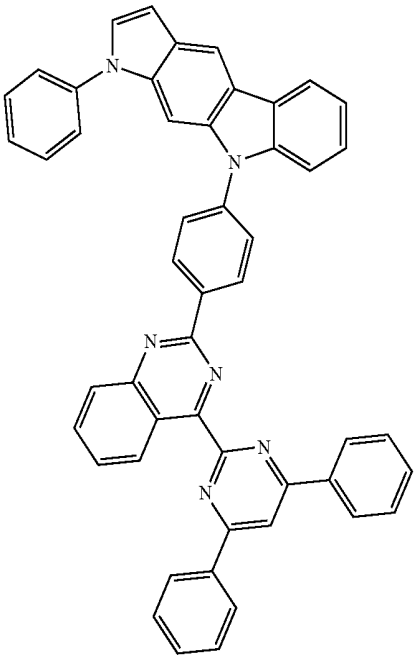

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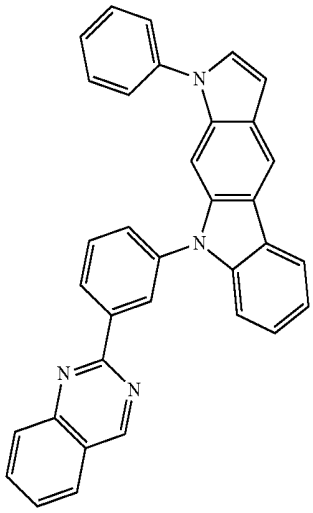

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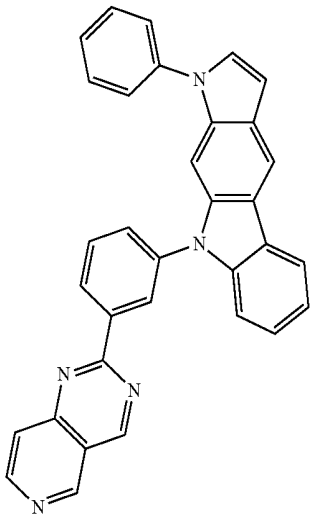

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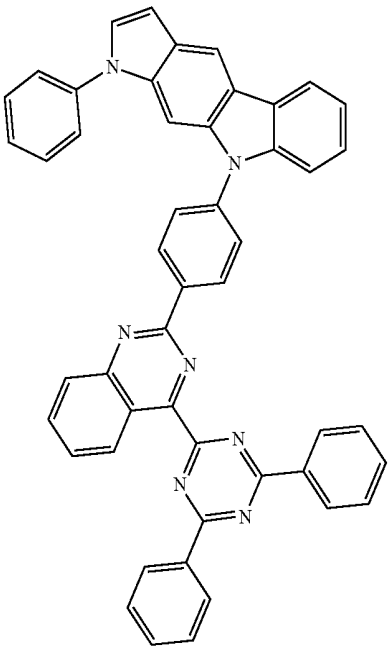

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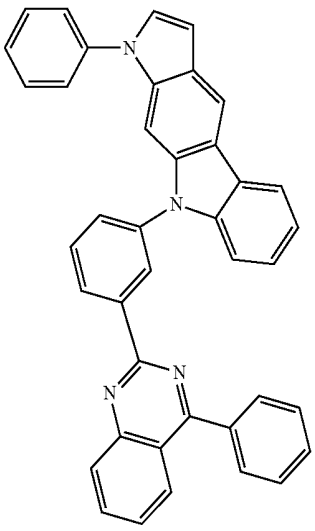

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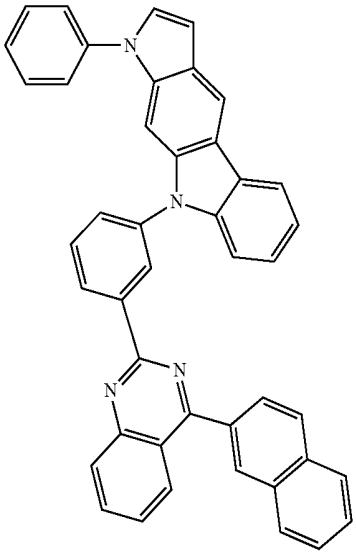

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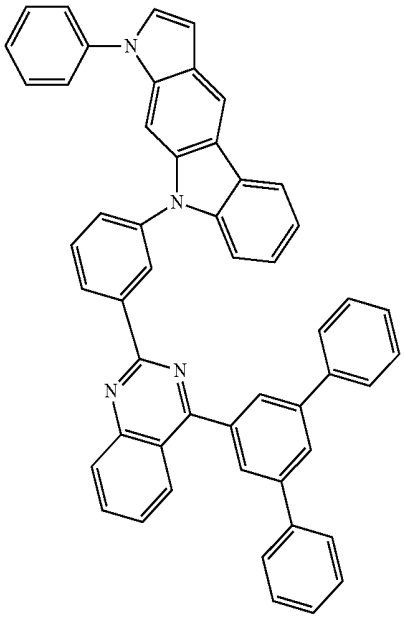

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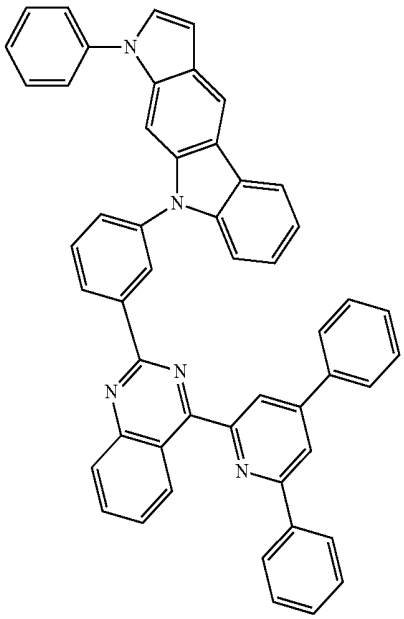

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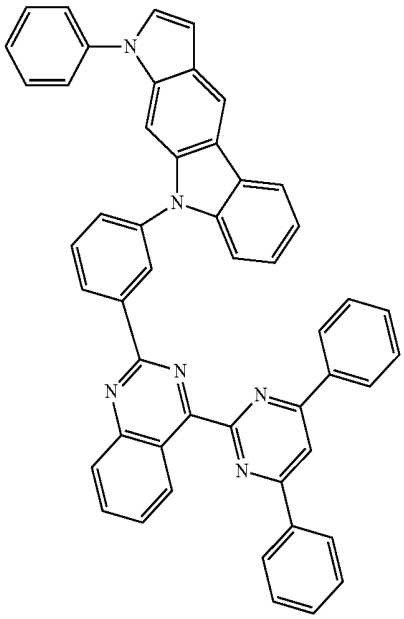

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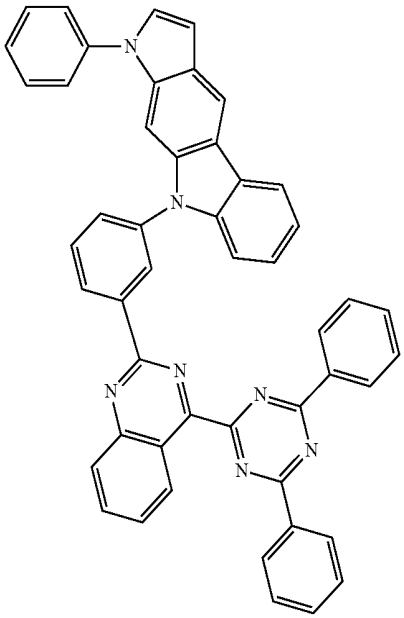

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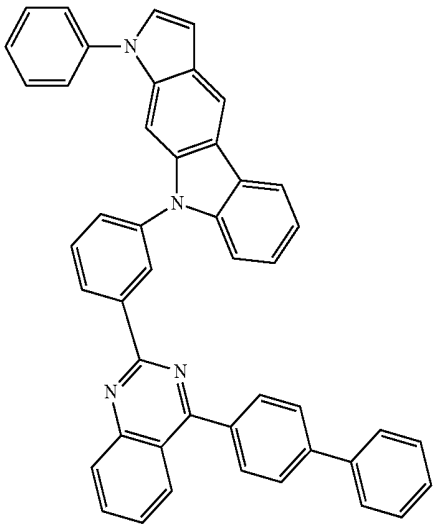

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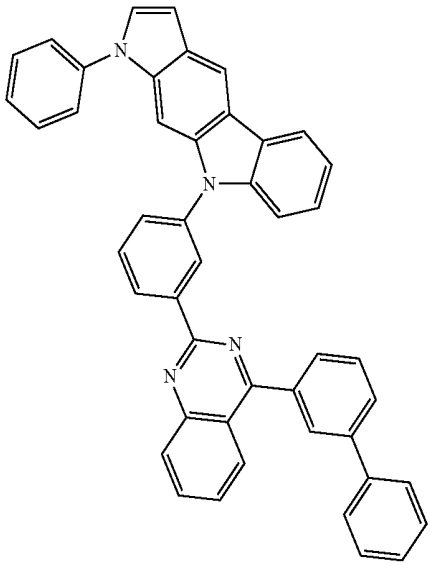

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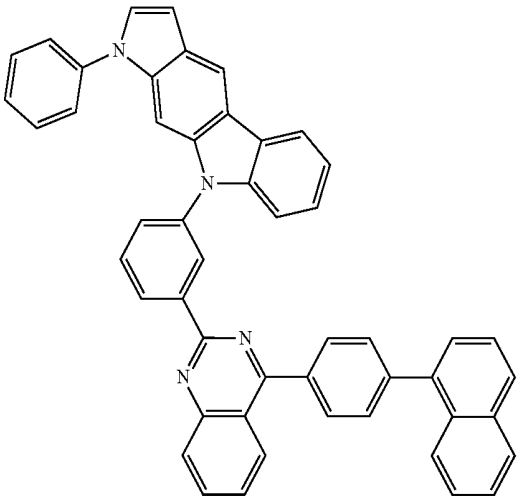

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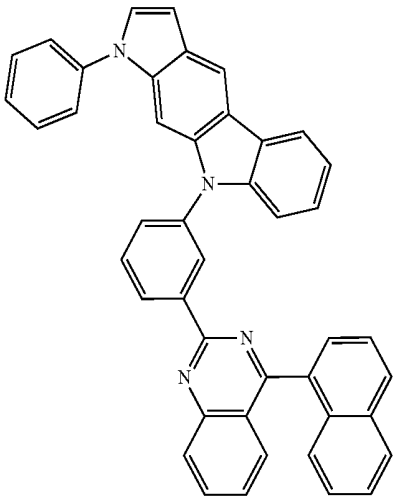

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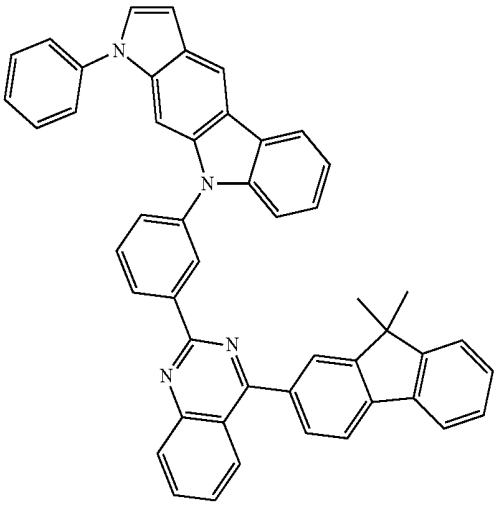

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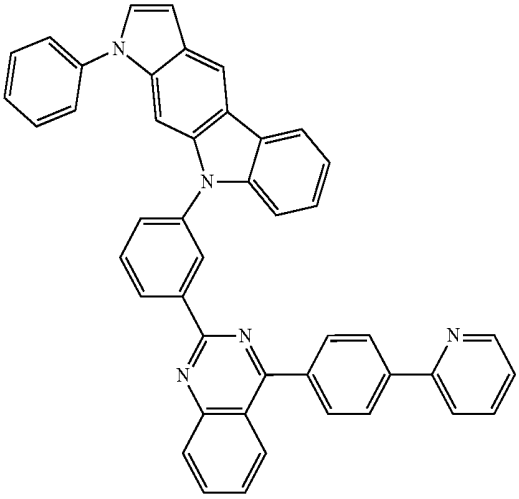

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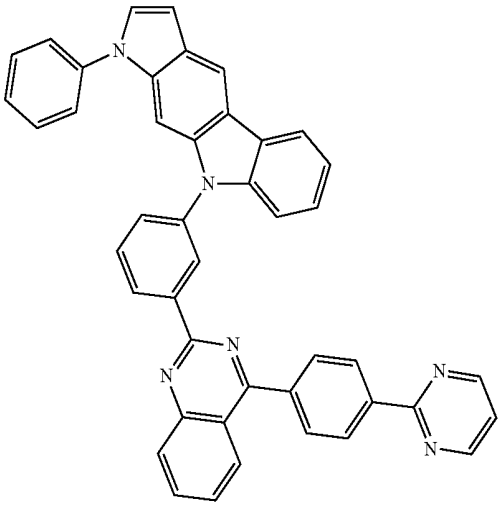

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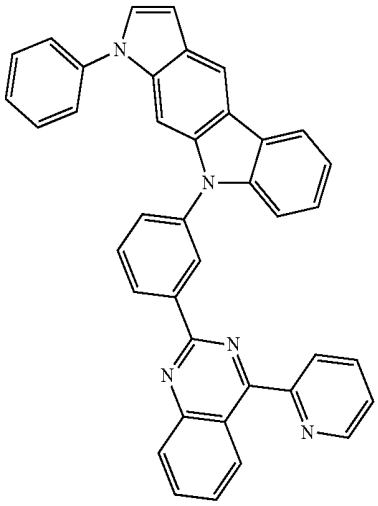

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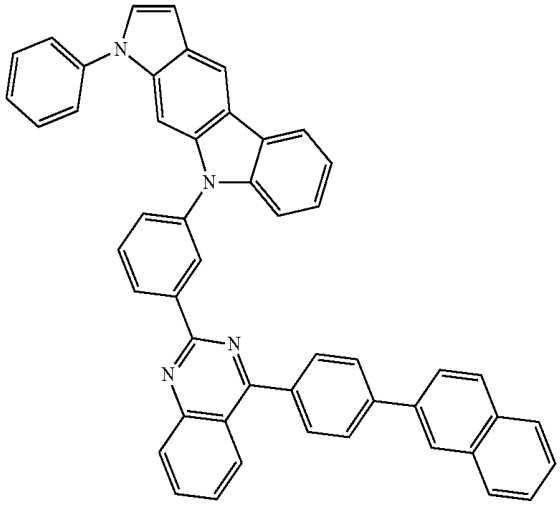

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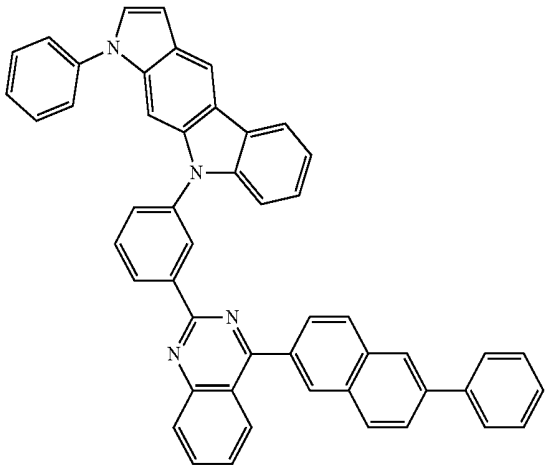

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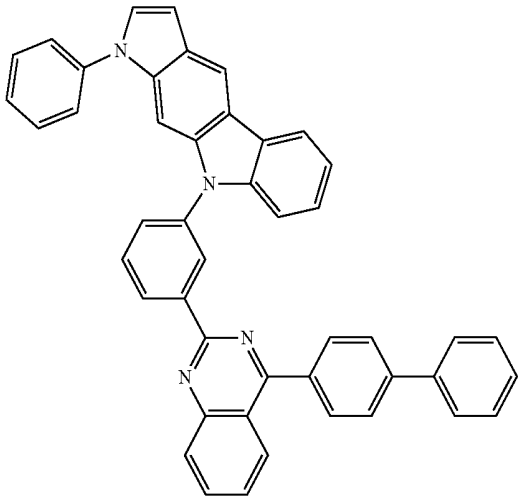

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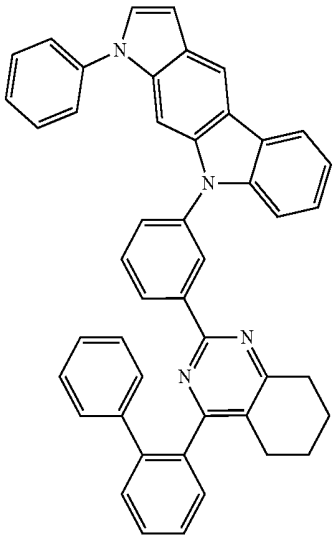

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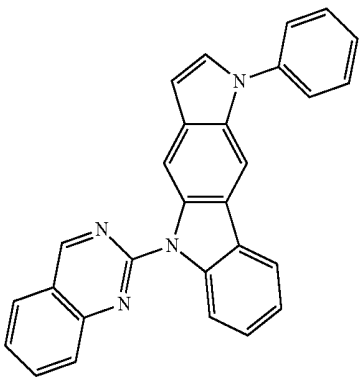

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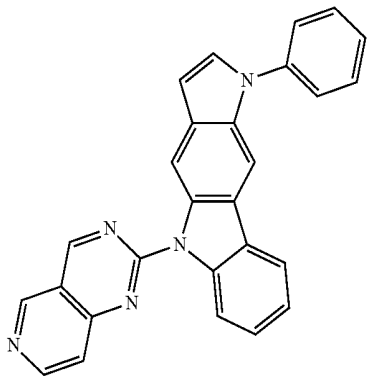

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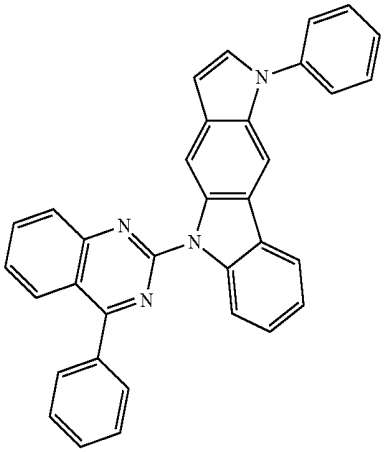

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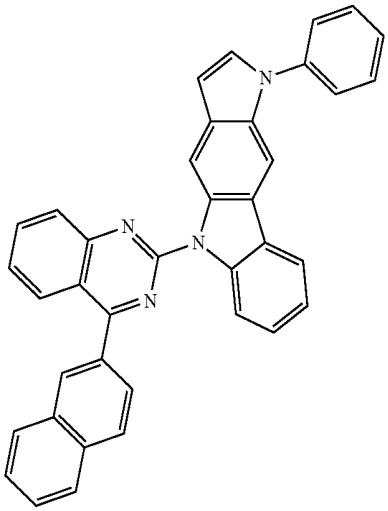

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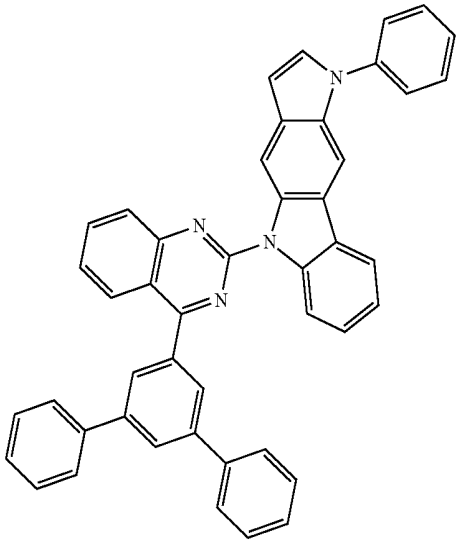

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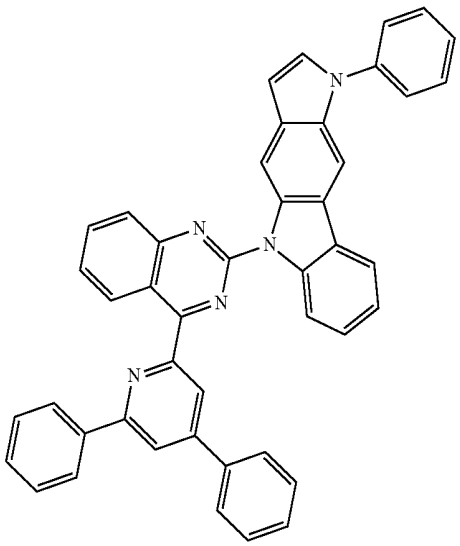

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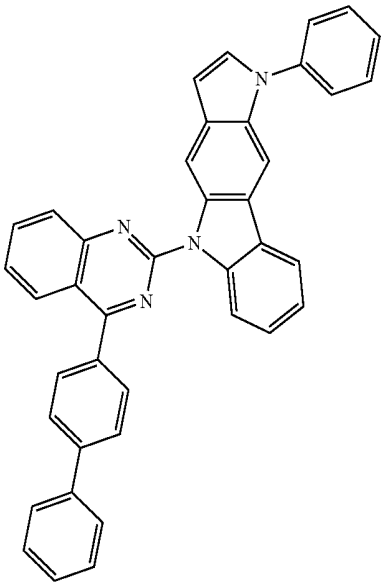

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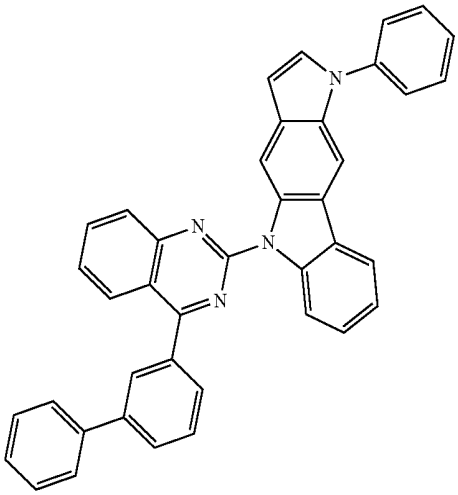

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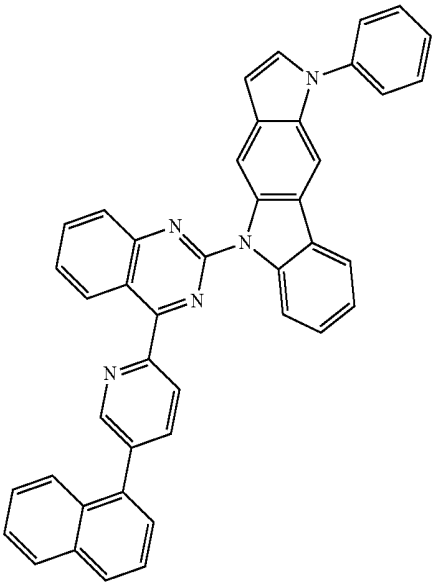

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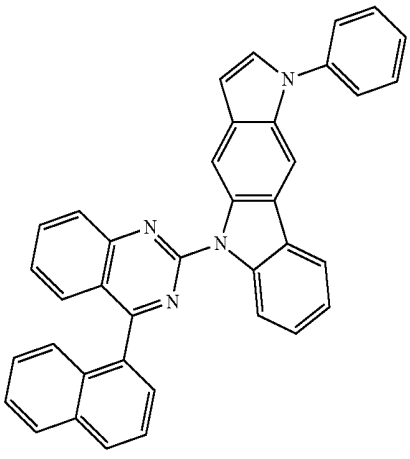

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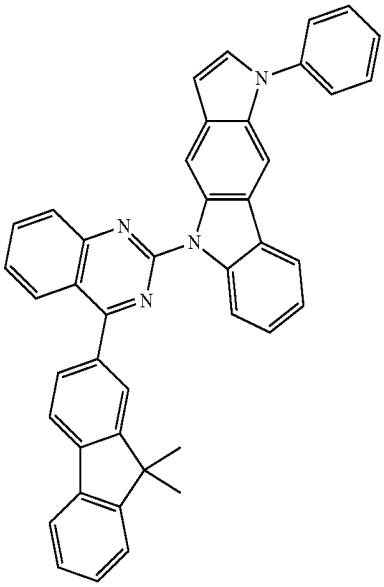

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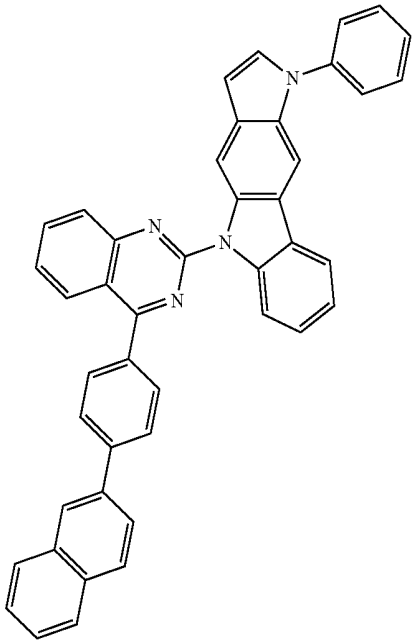

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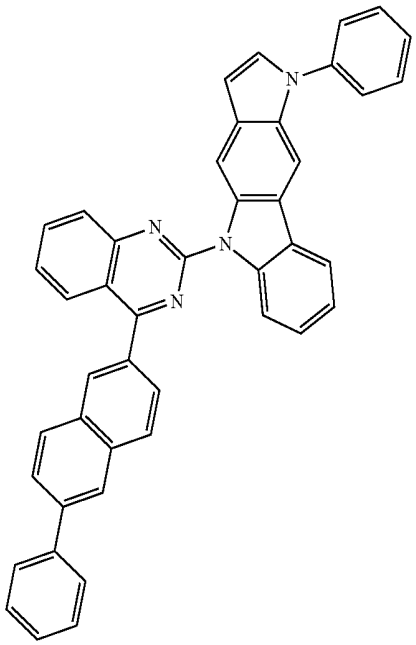

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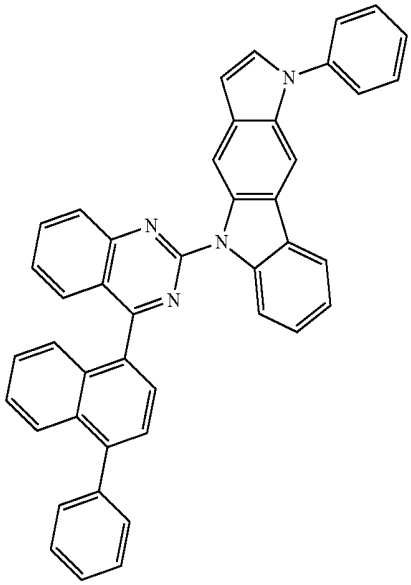

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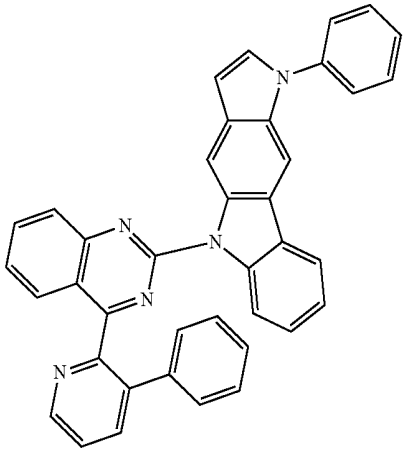

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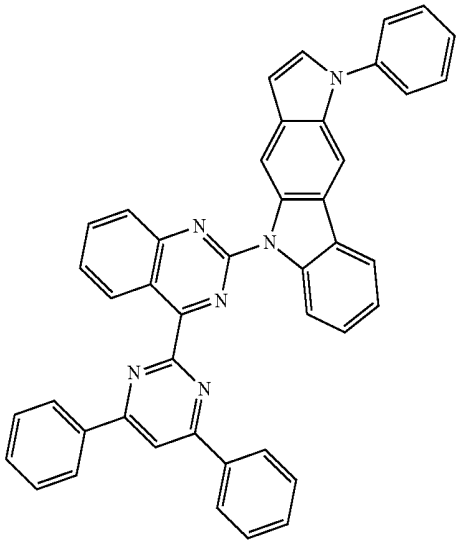

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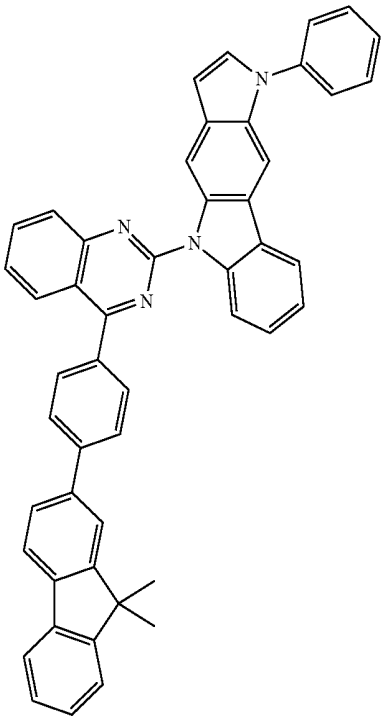
C200



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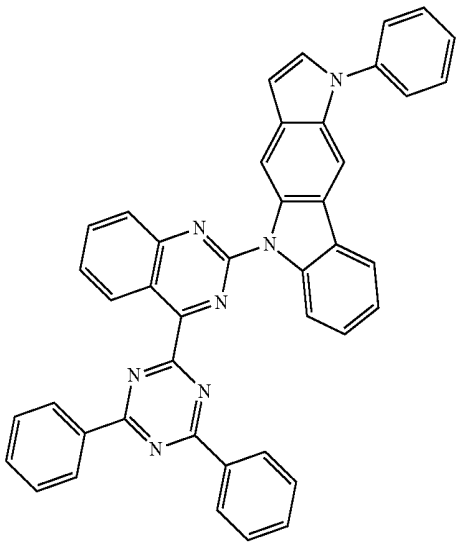

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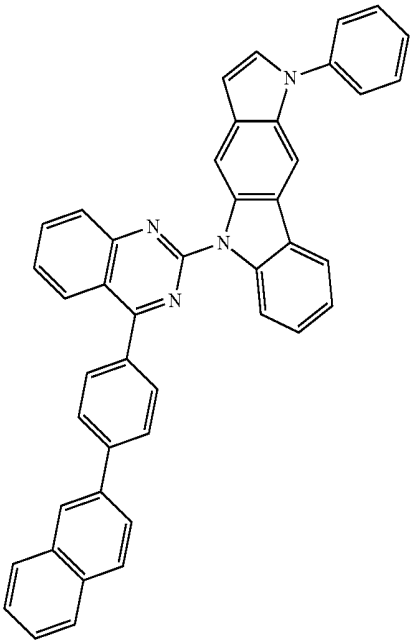

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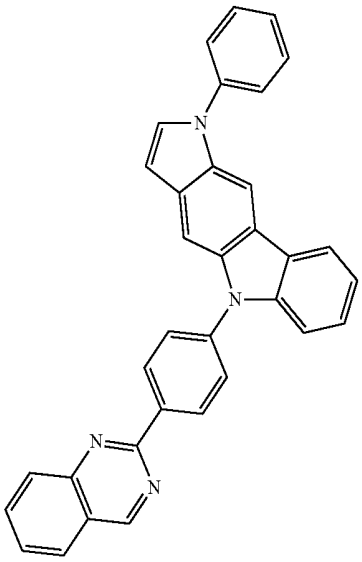

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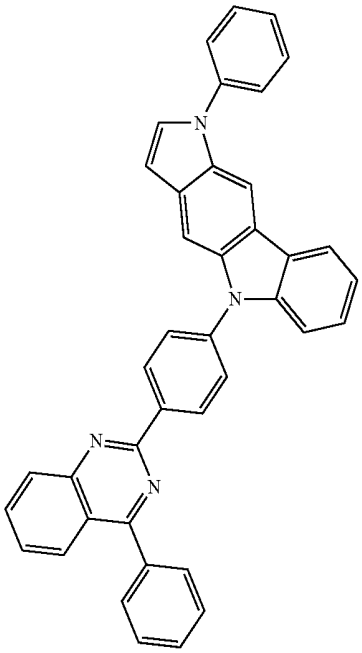

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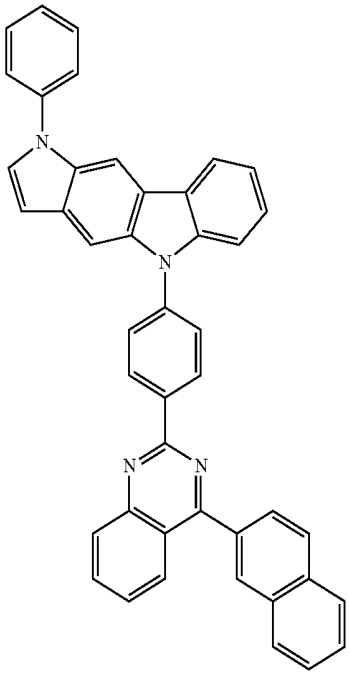

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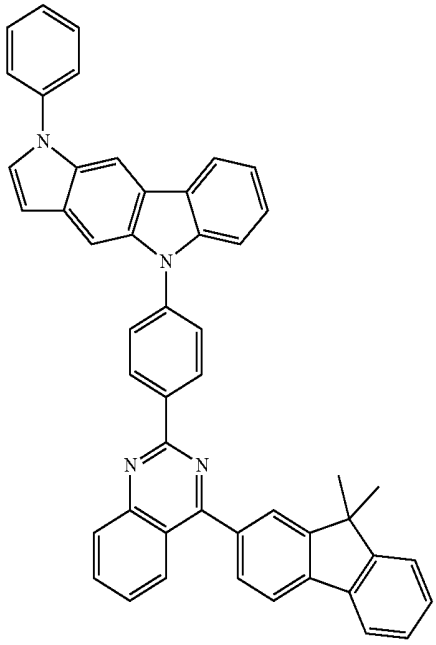

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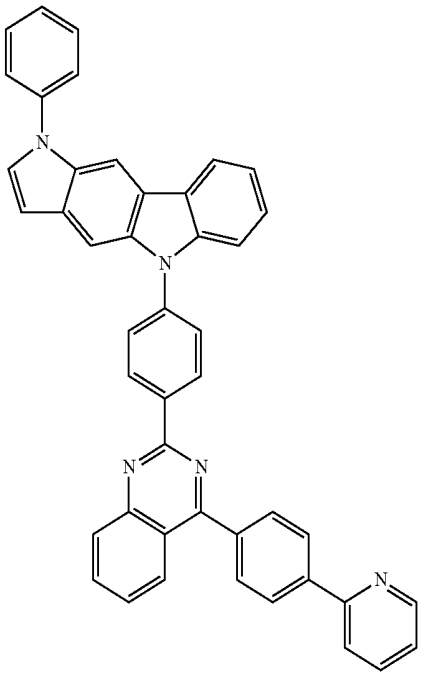

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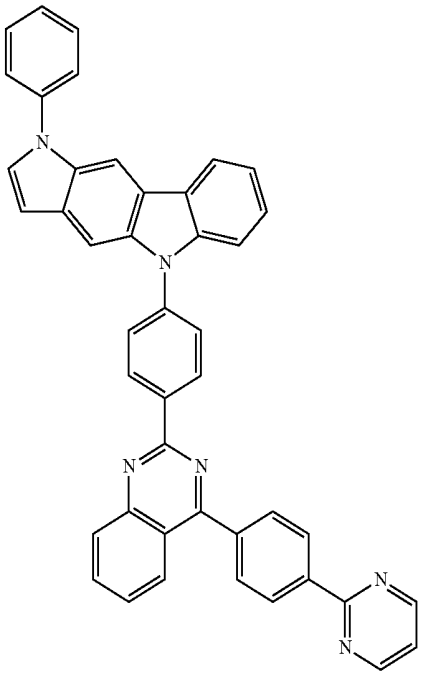

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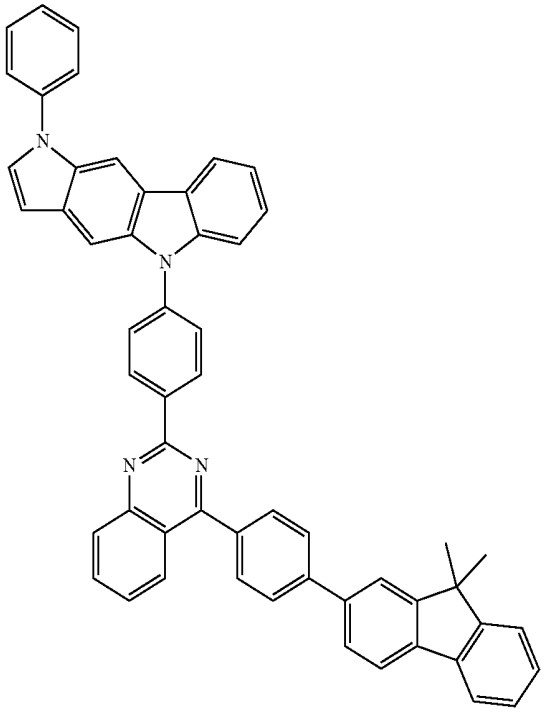

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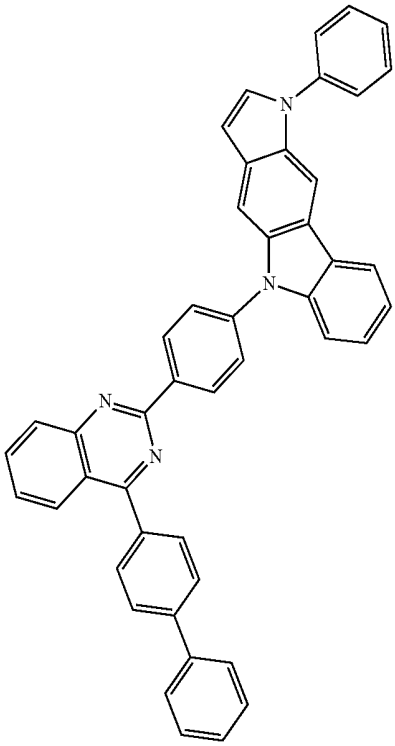

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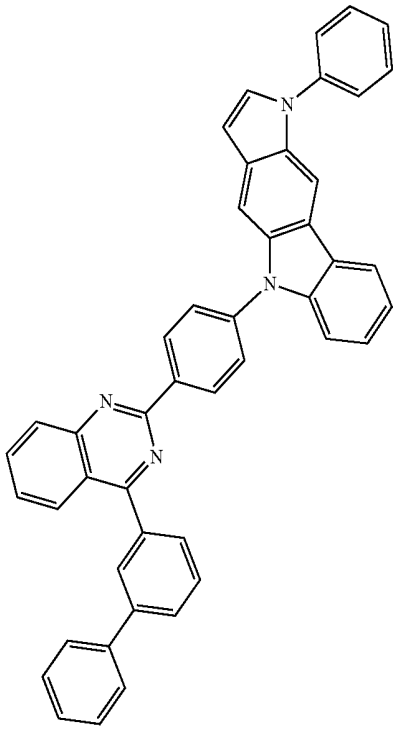

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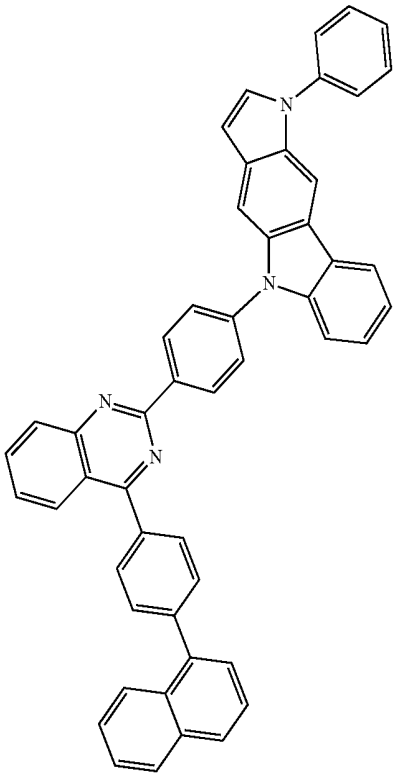

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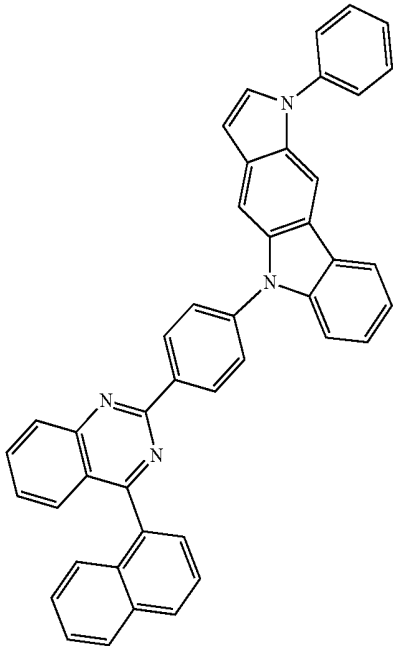

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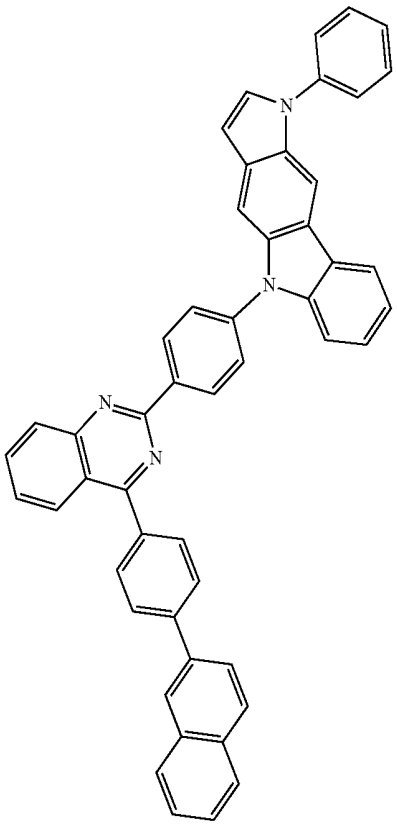

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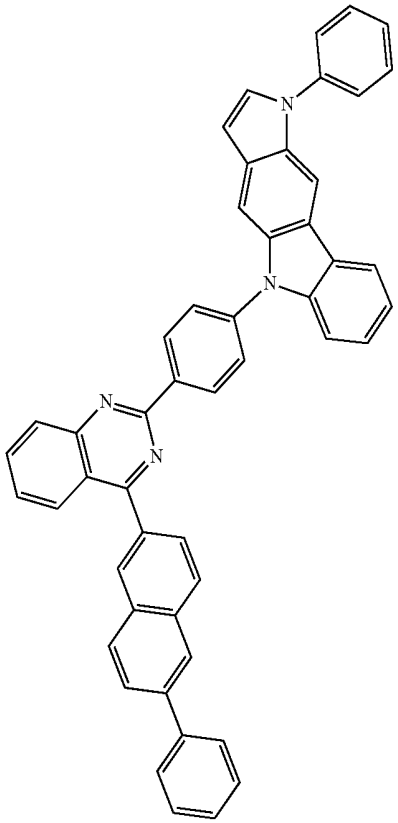

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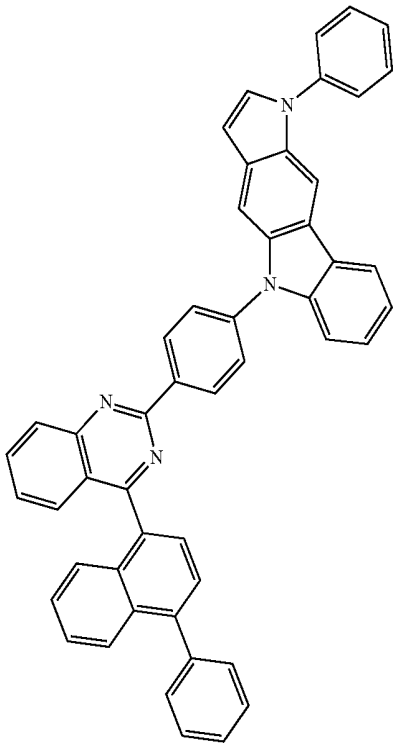

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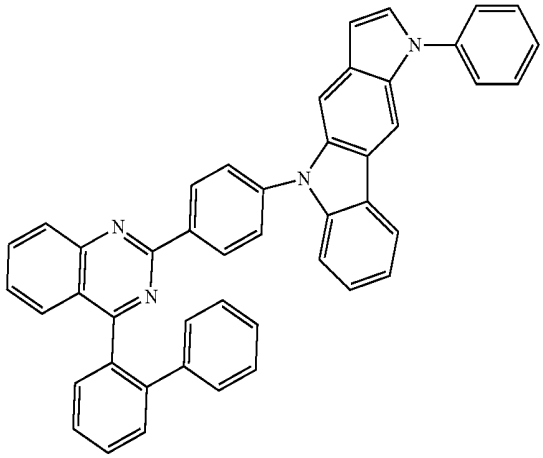

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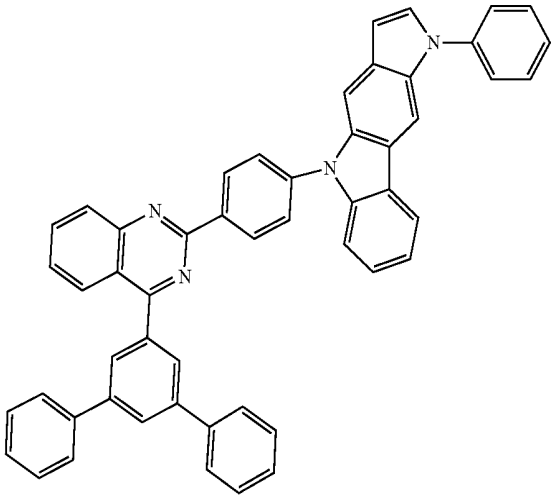

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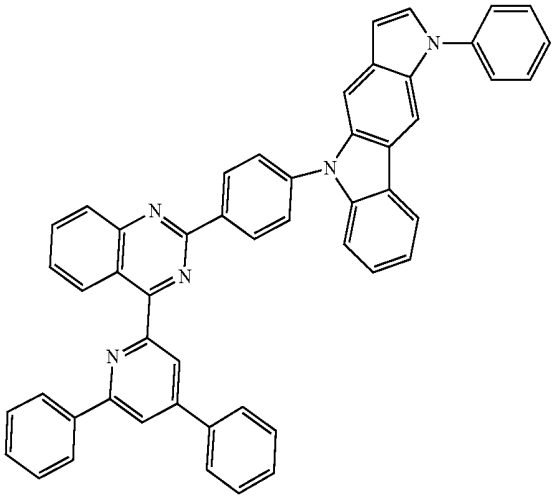

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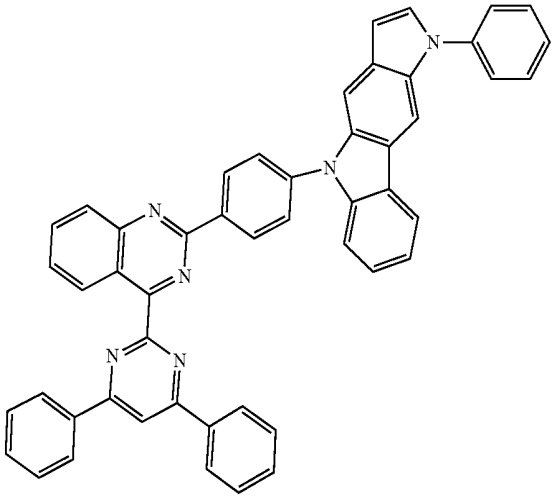

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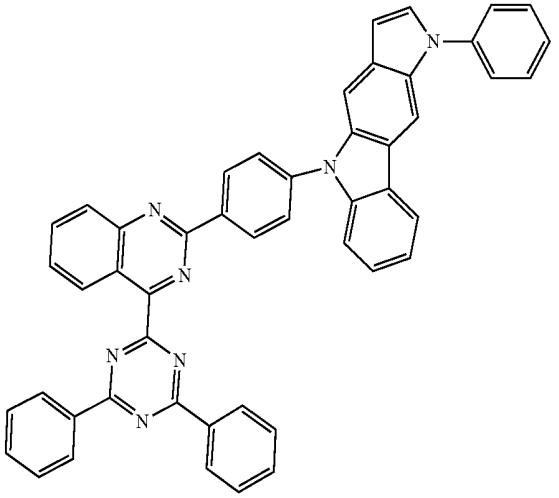

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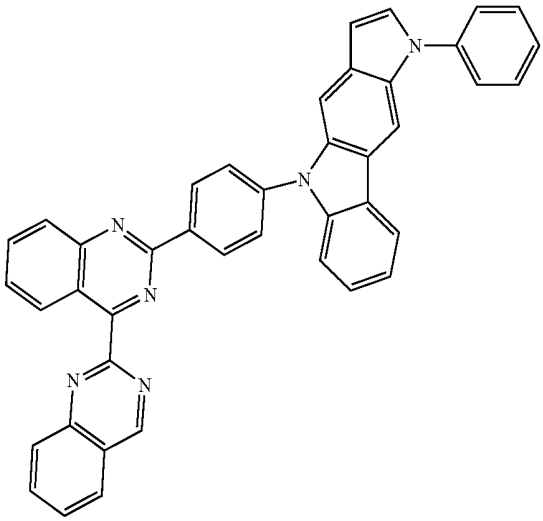

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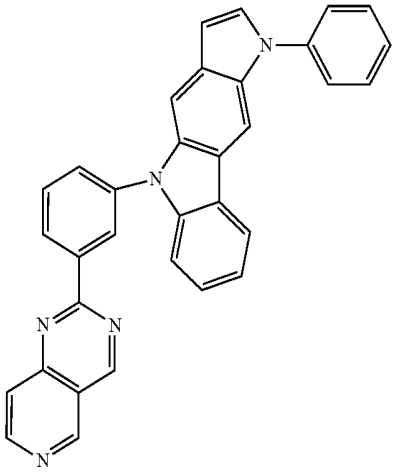

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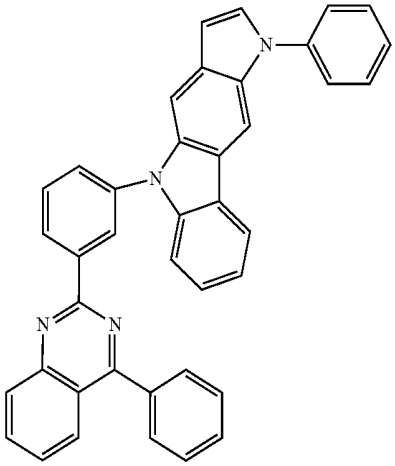

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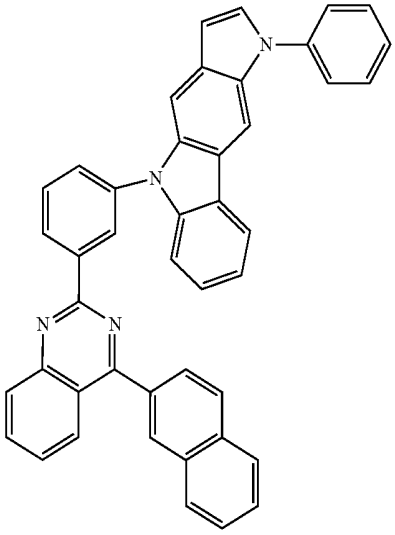

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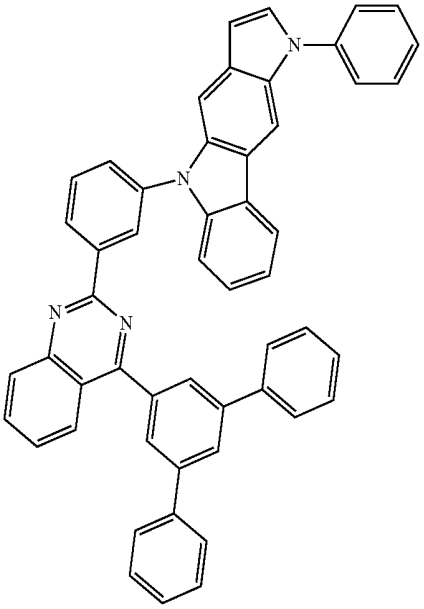

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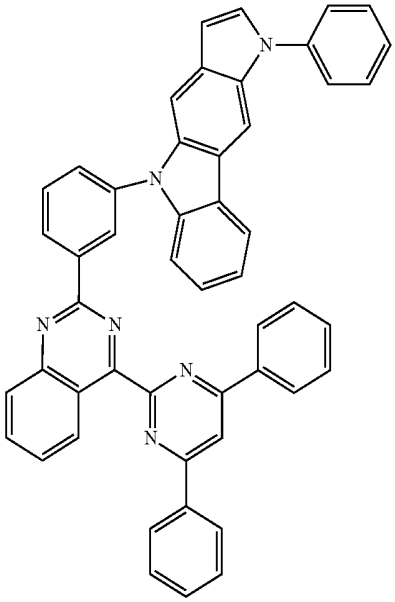

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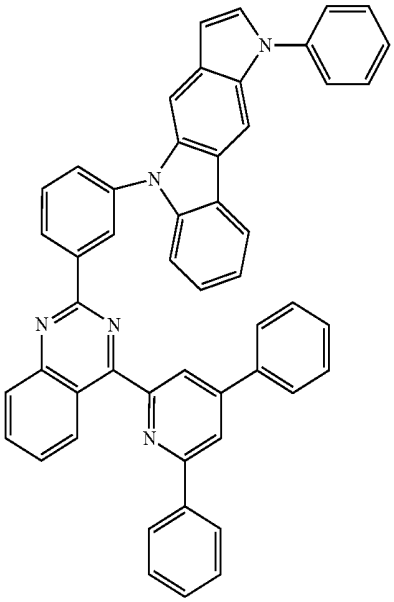

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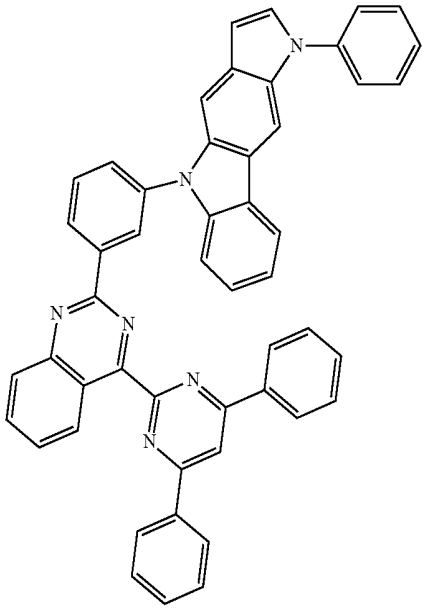

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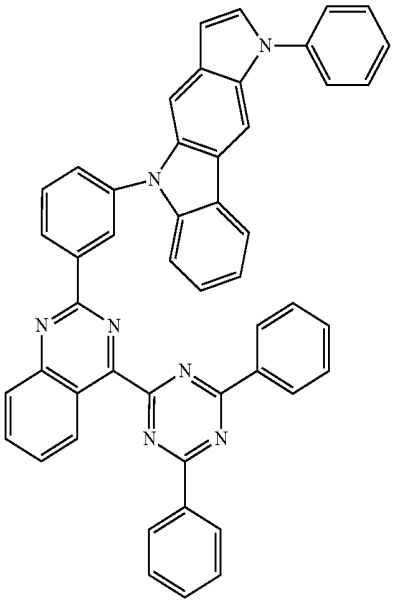

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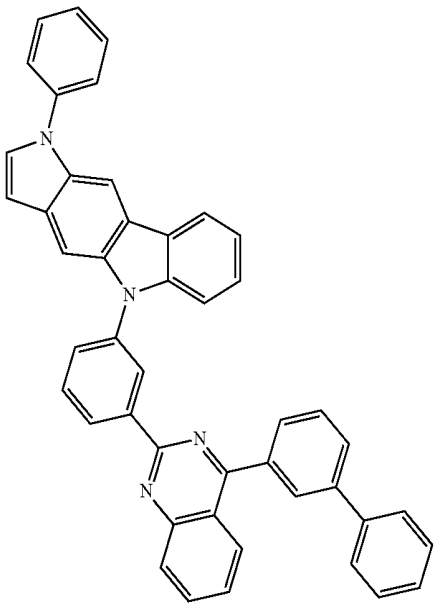

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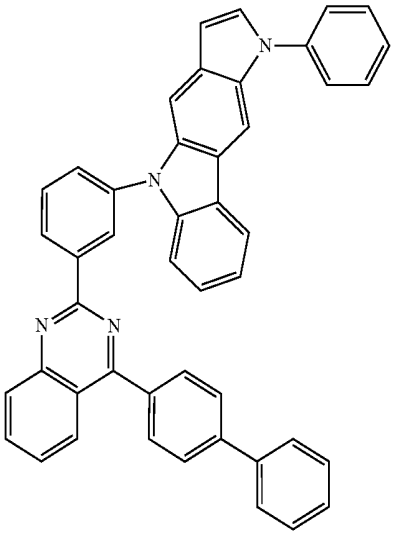

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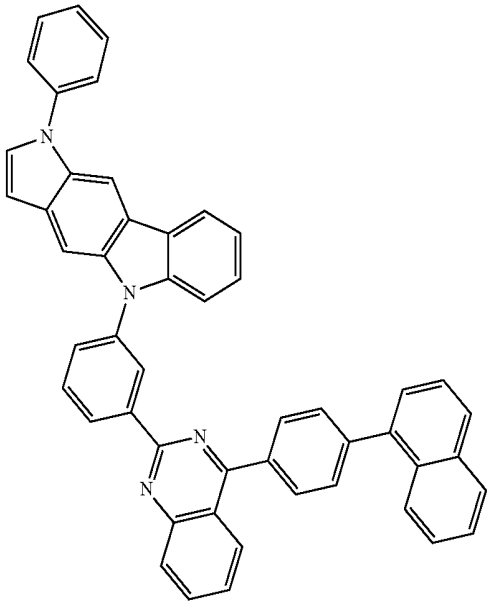

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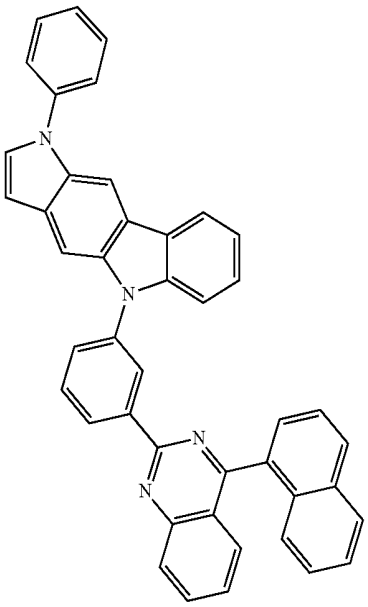

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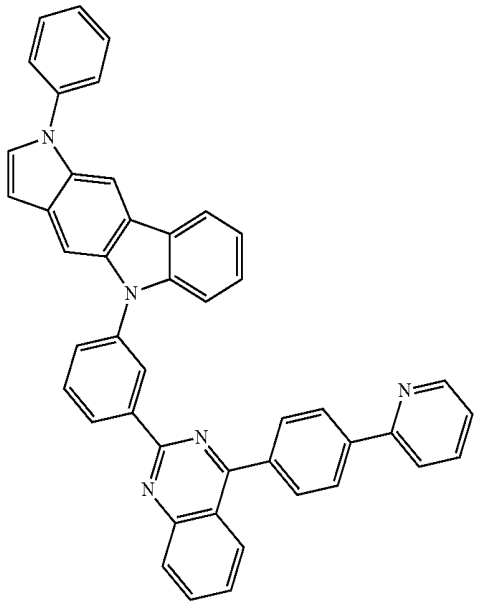

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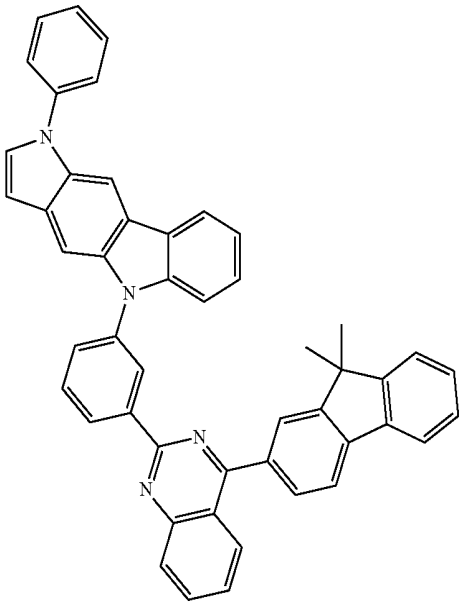

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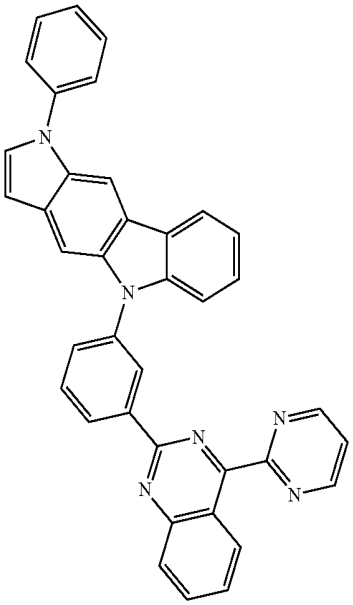

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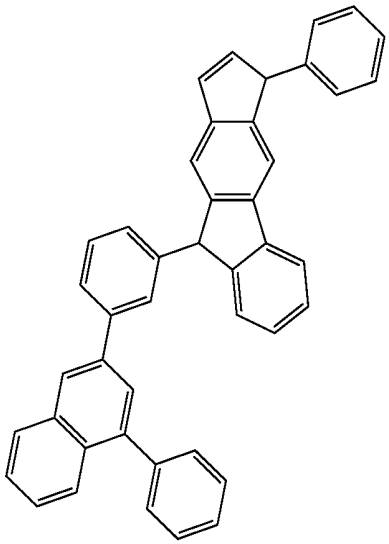

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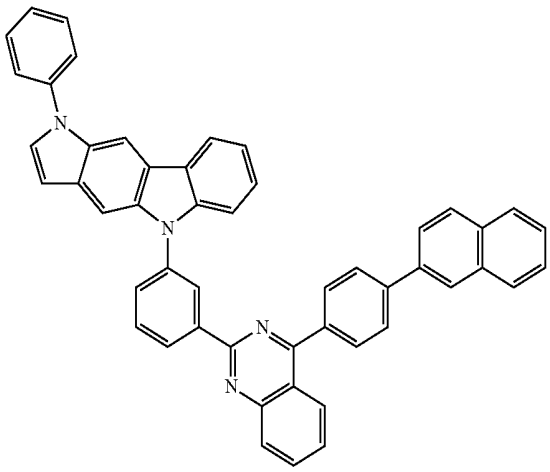

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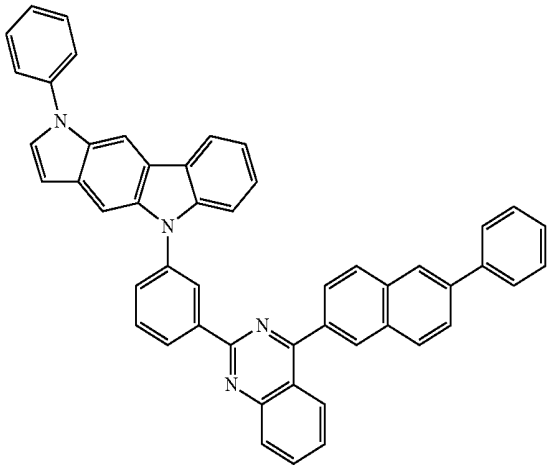

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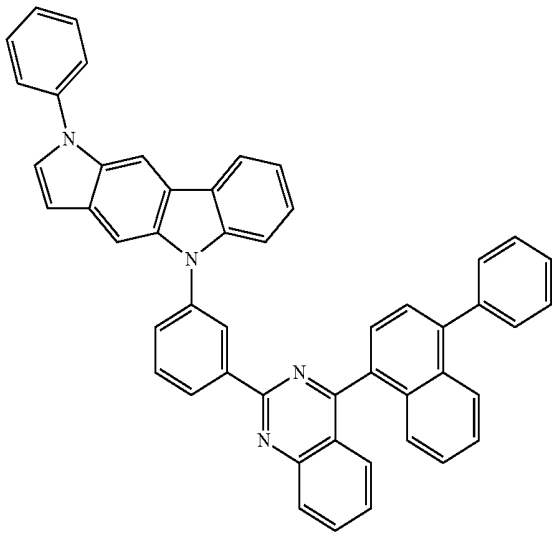

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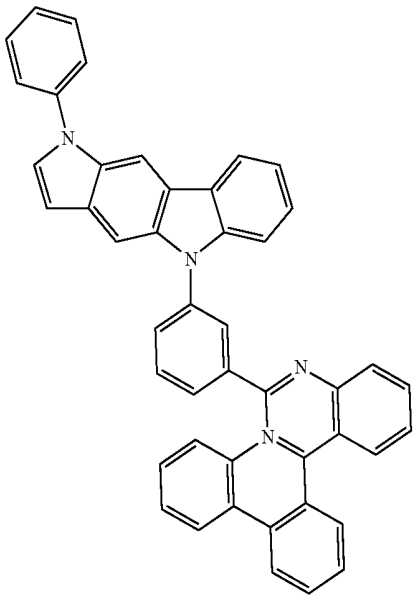

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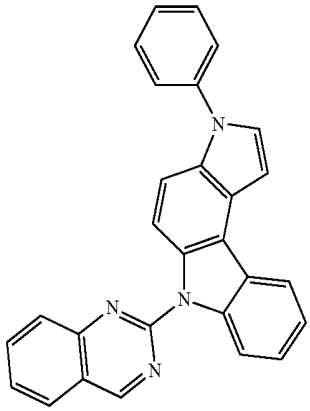

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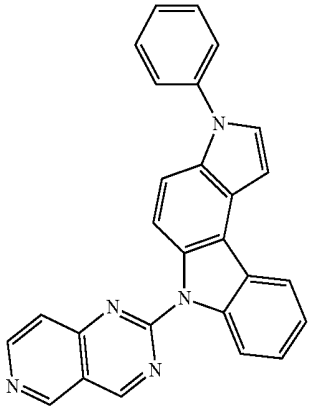

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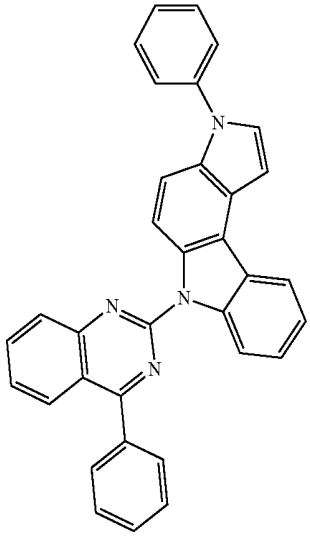

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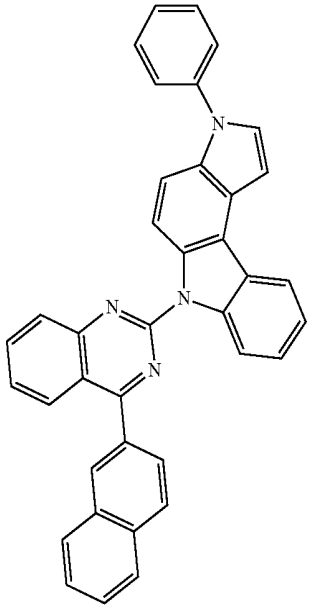

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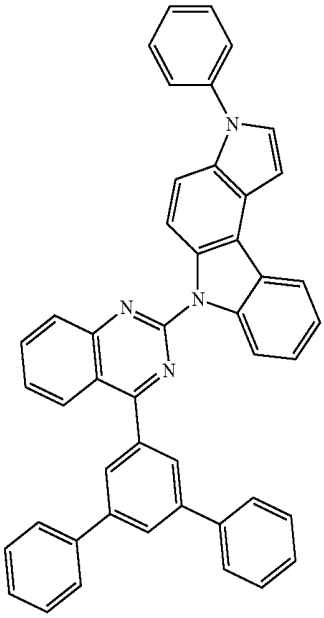

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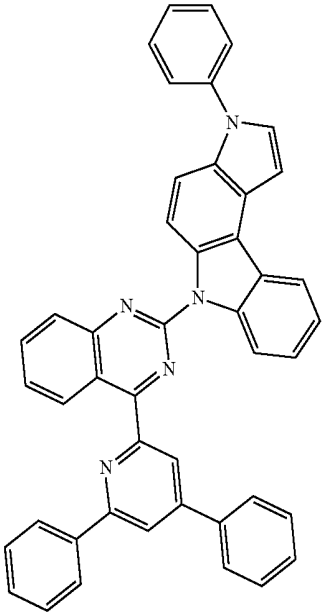

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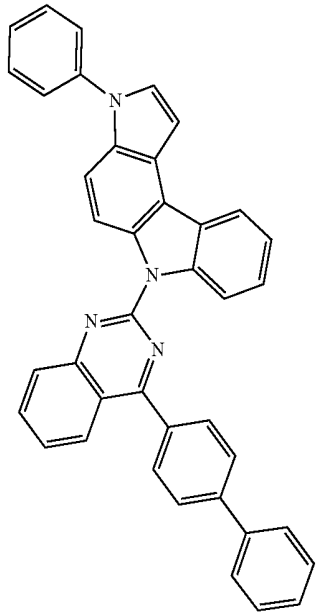

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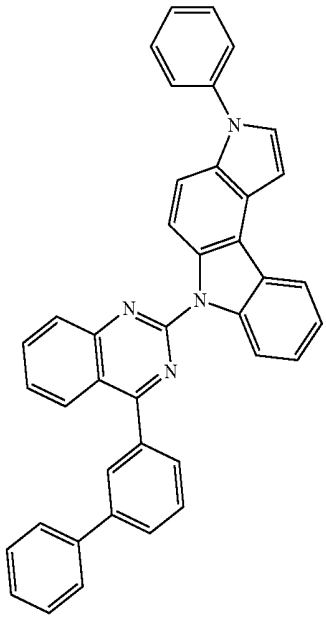

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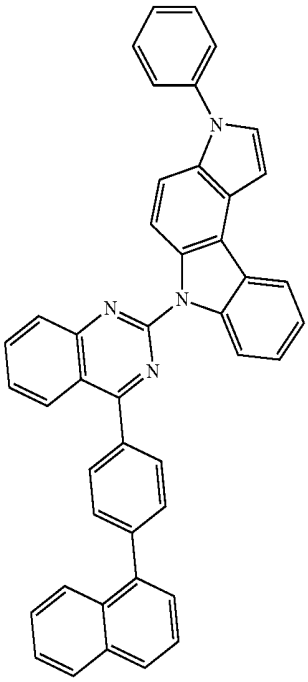

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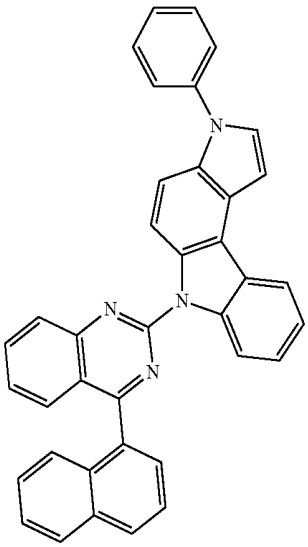

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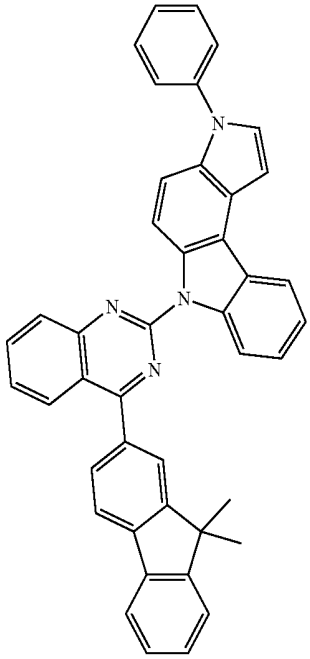

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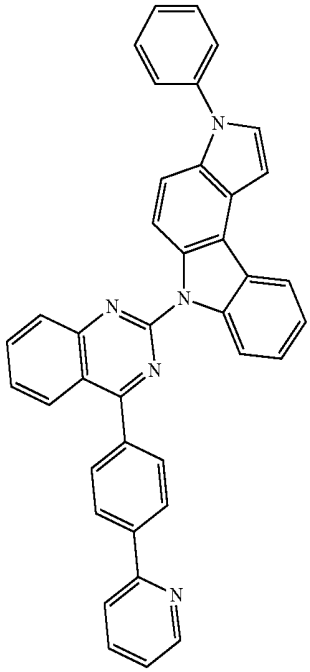

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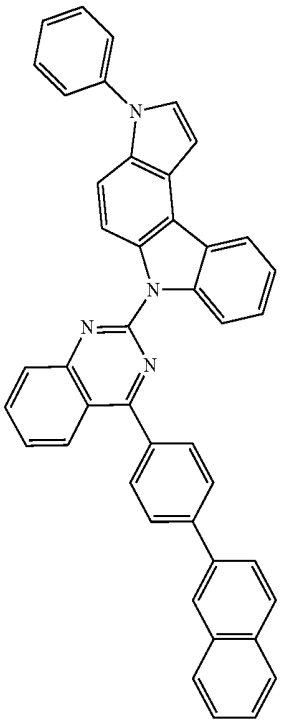

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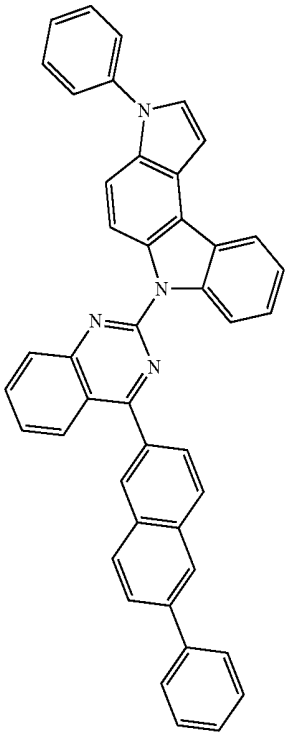

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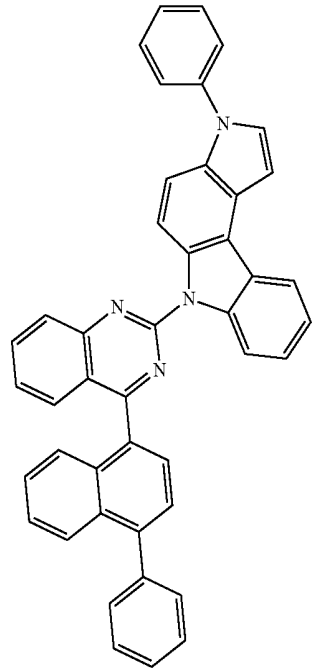

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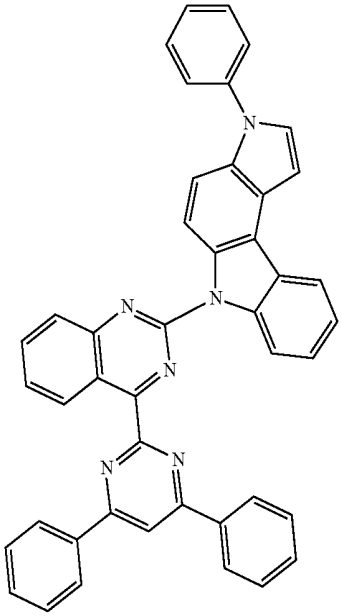

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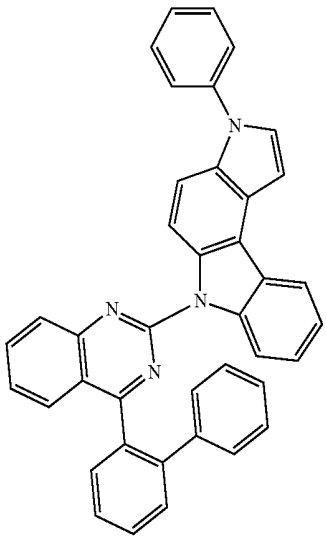

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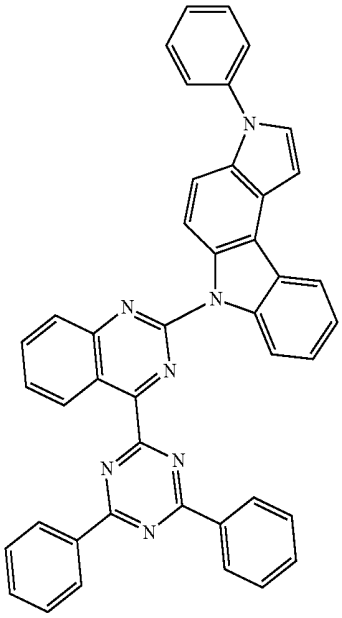

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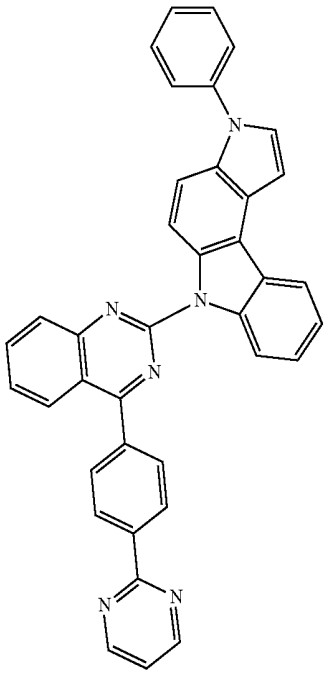

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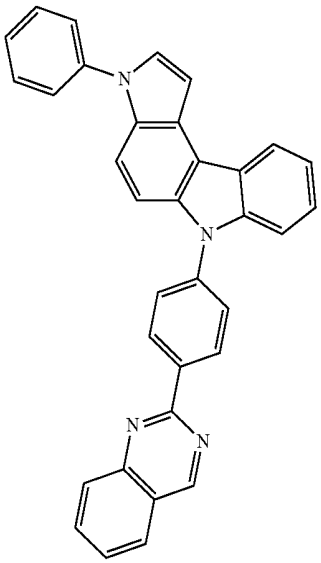

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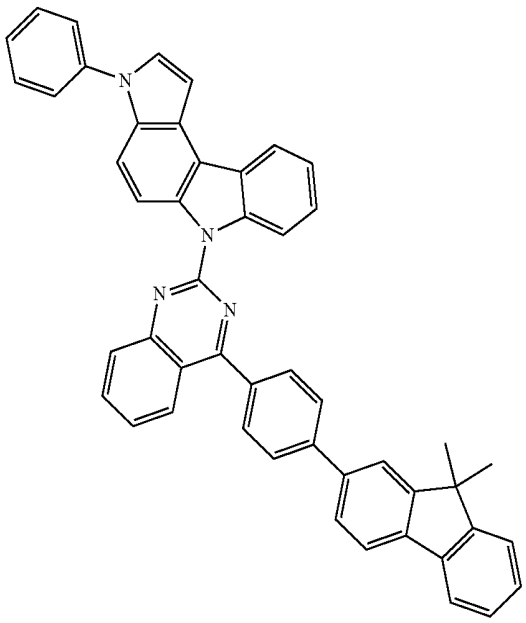

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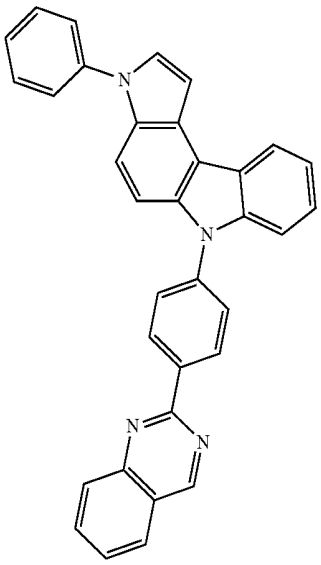

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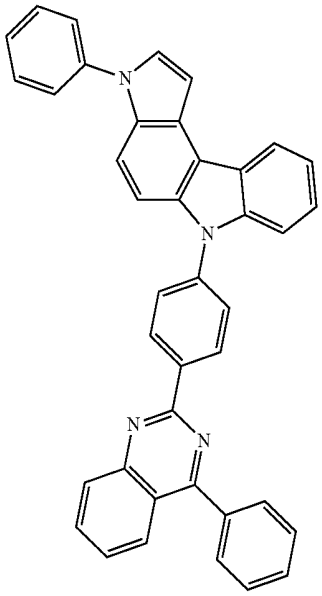

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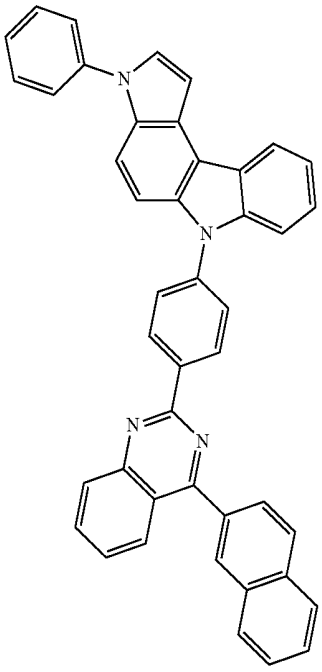

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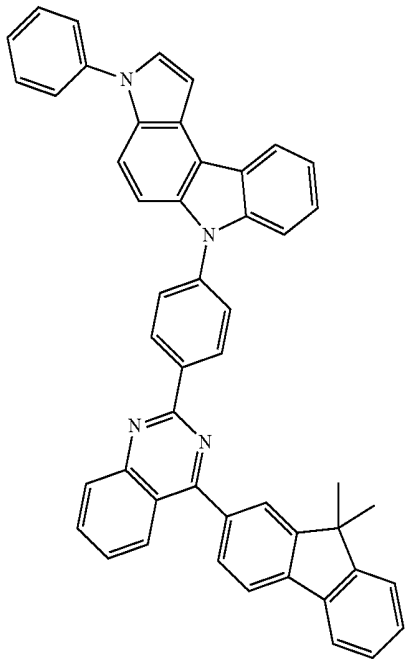

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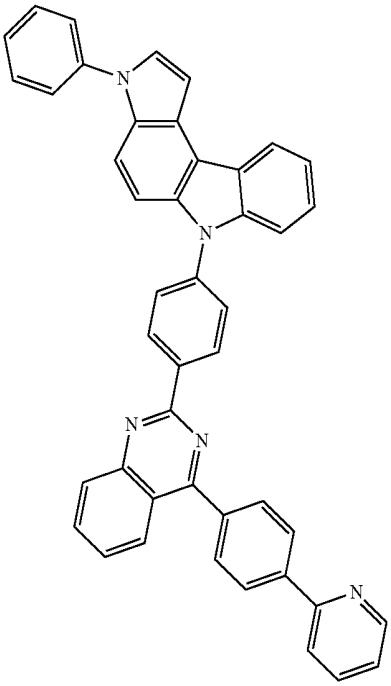

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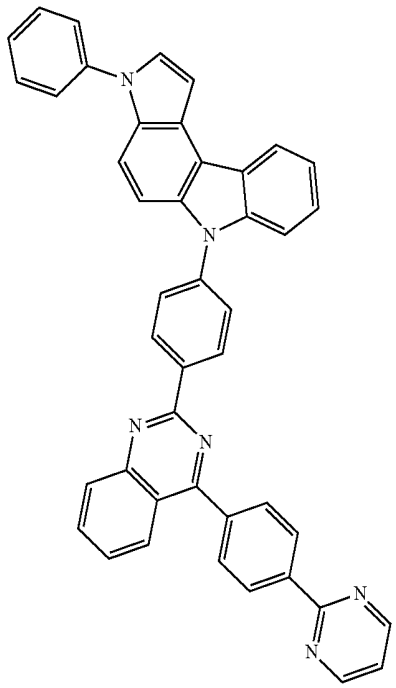

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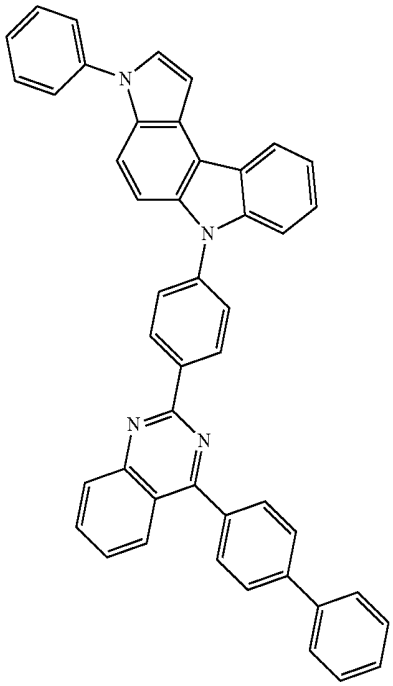

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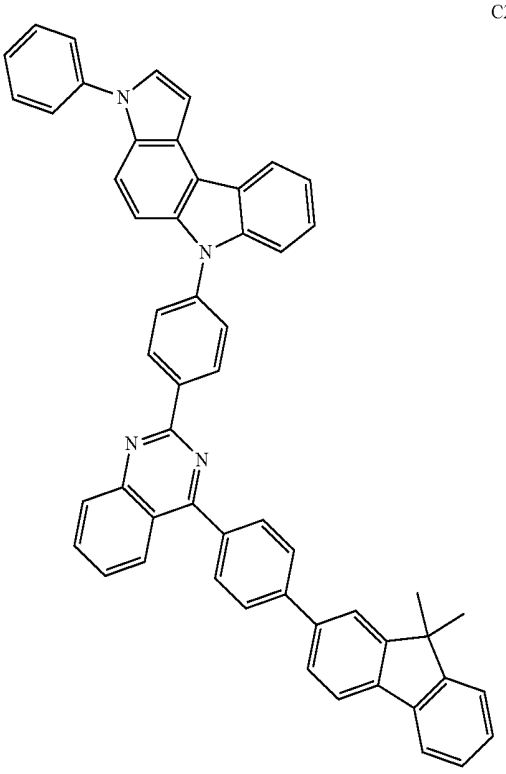

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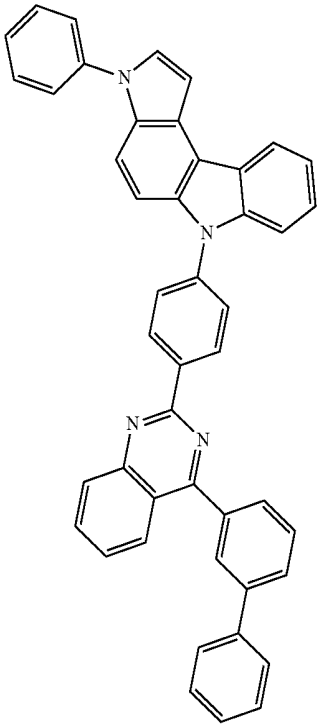

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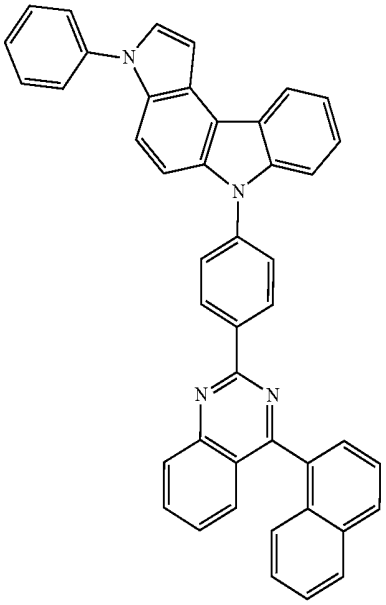

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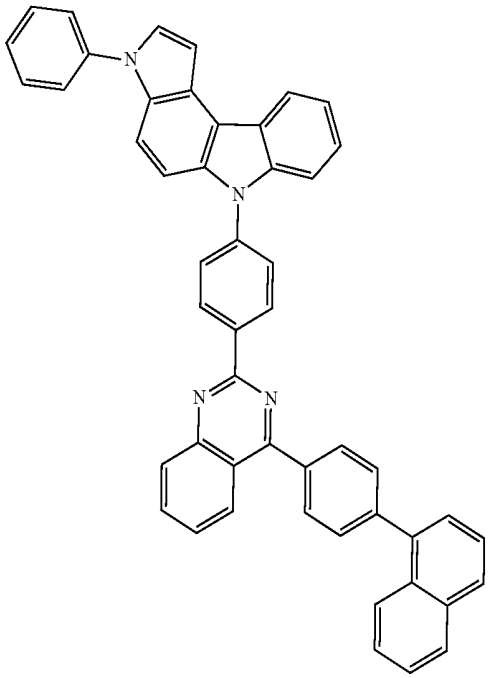

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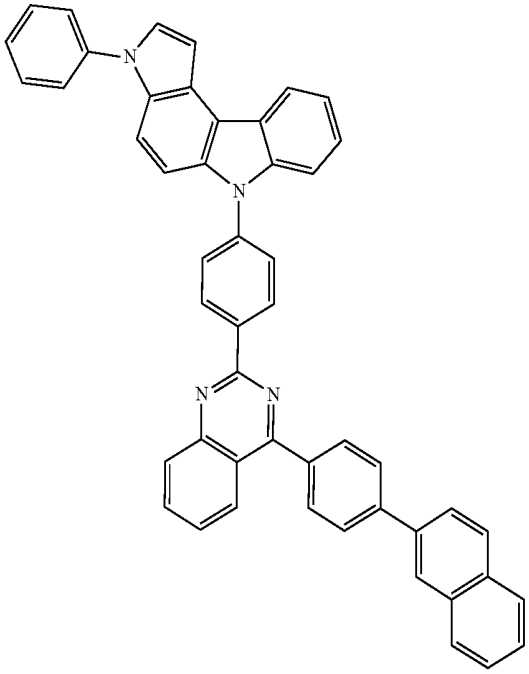

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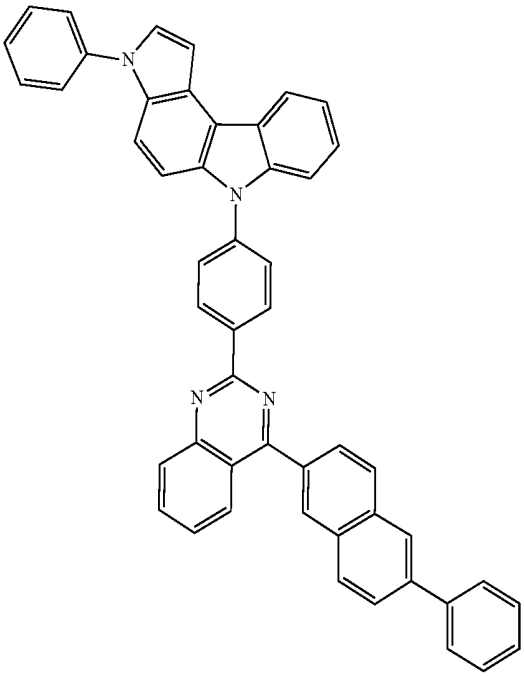

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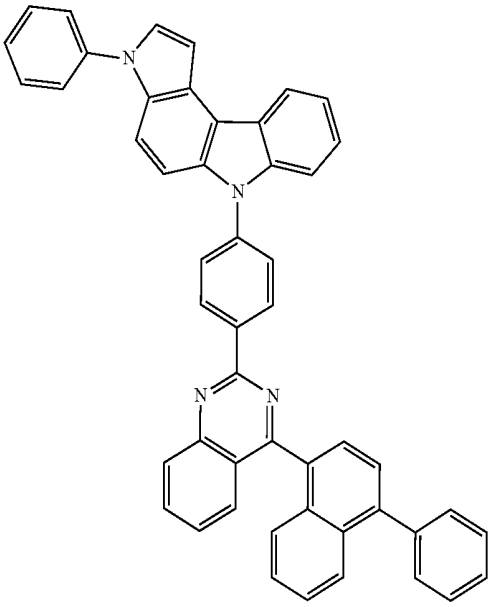

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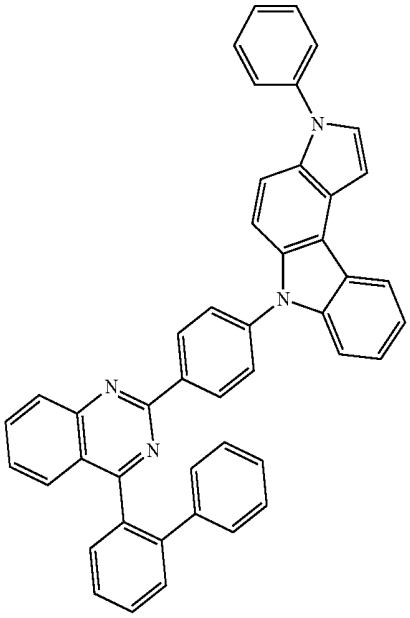

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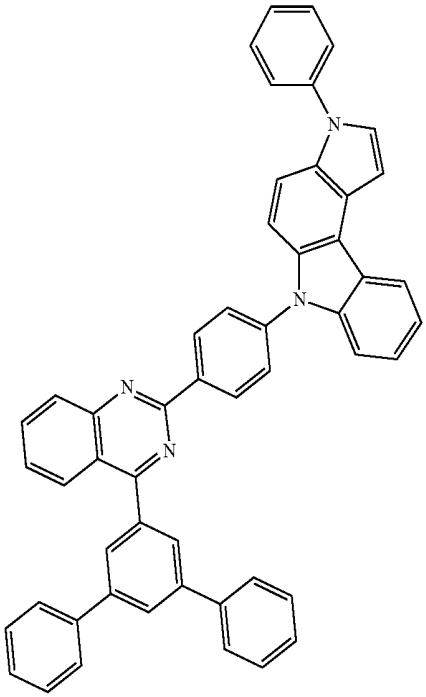

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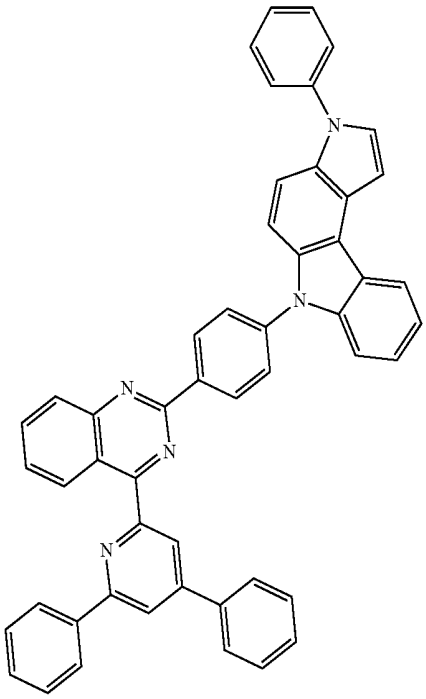

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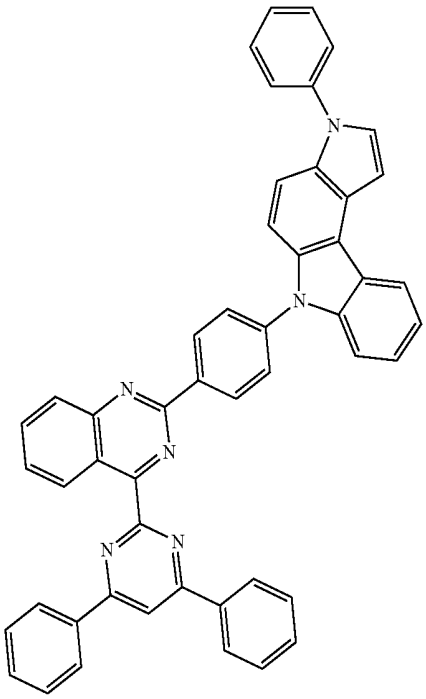

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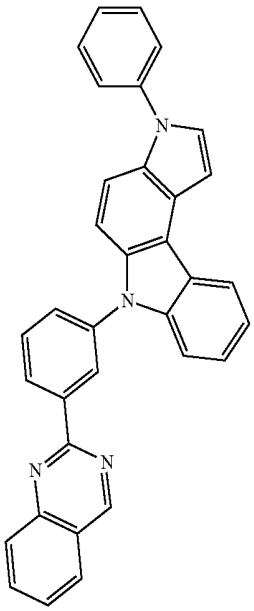

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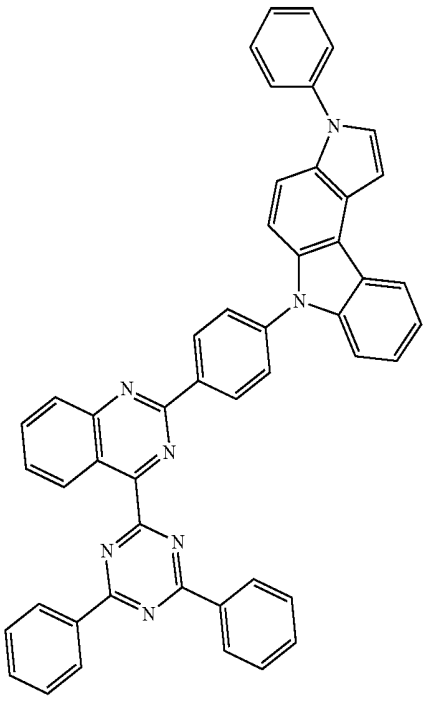

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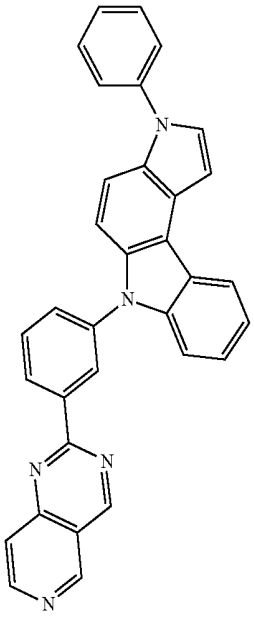

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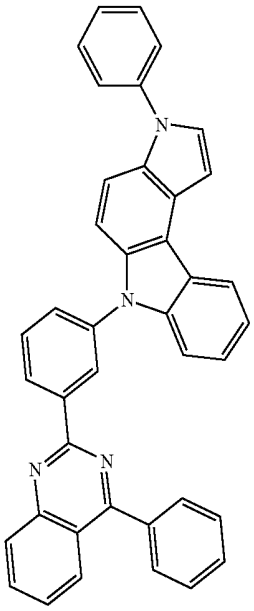

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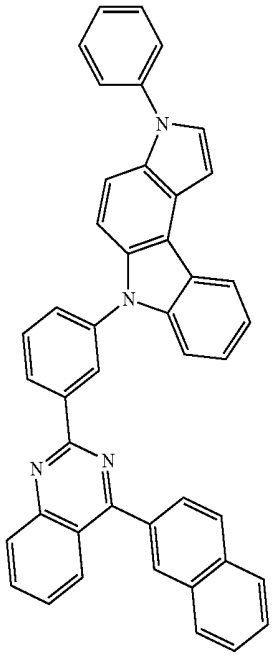

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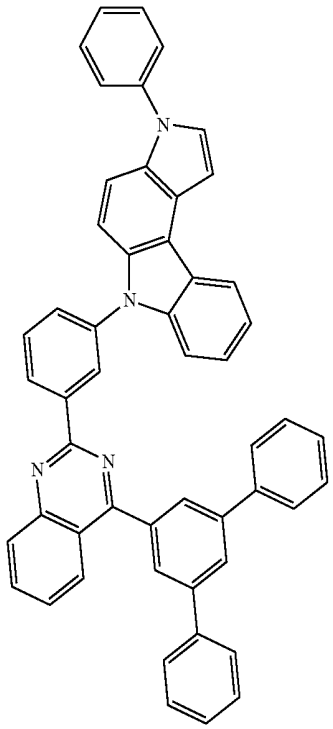

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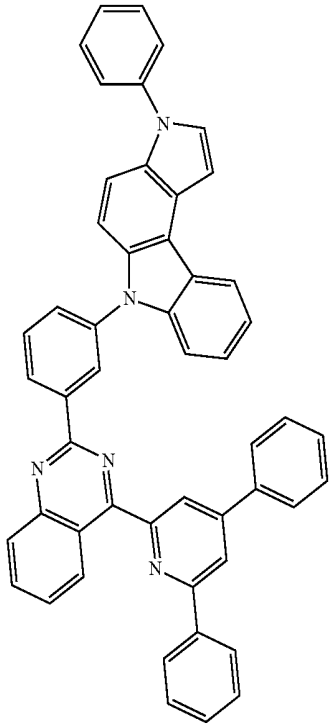

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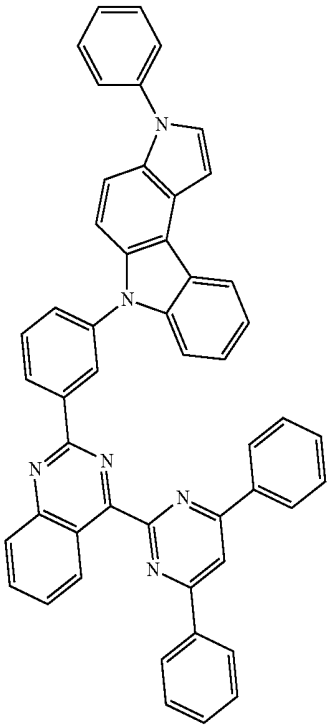

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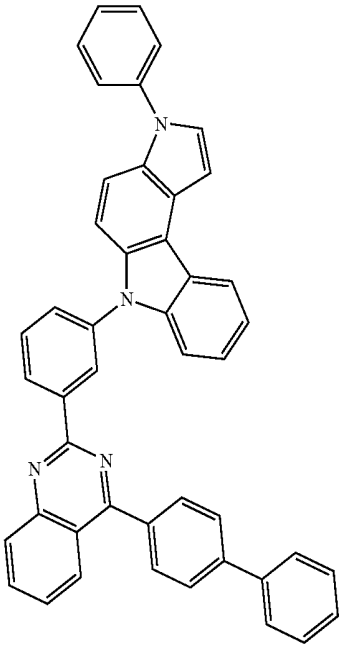

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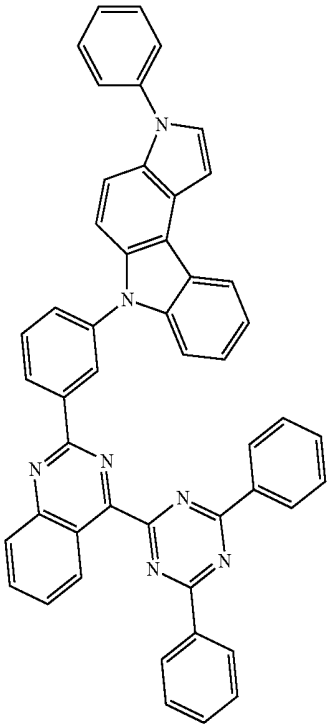

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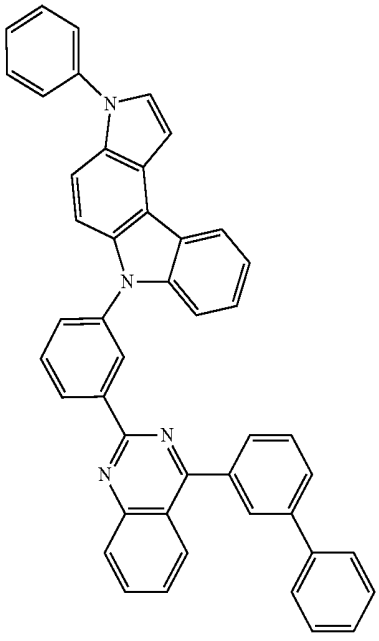

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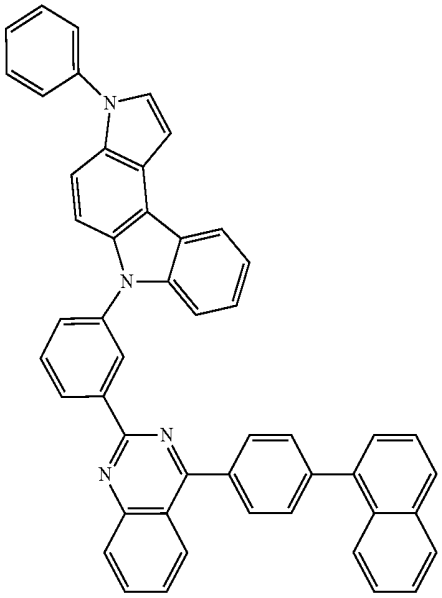

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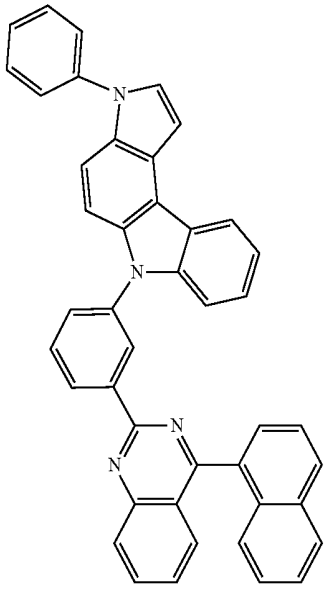

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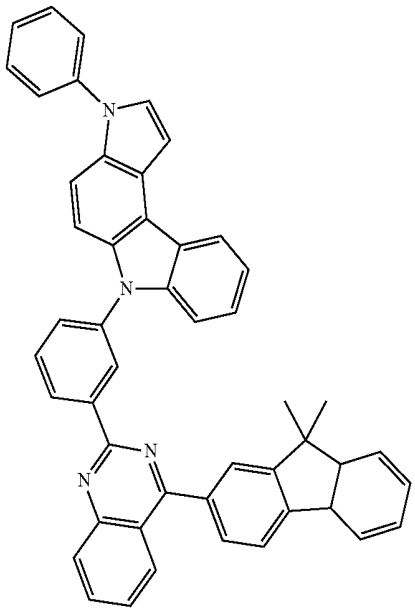

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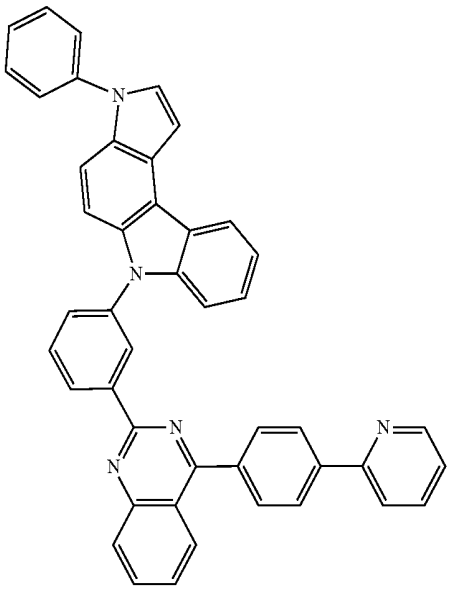

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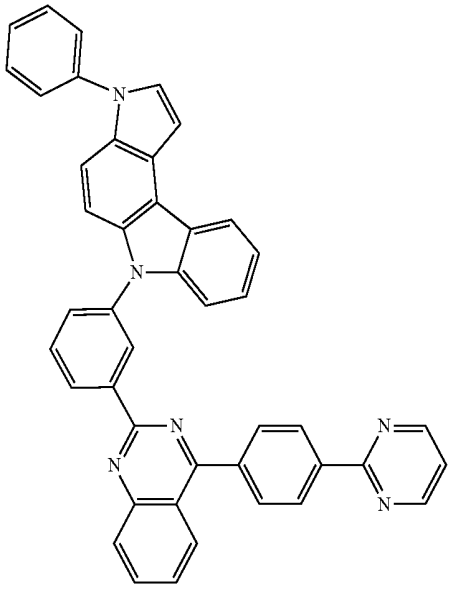

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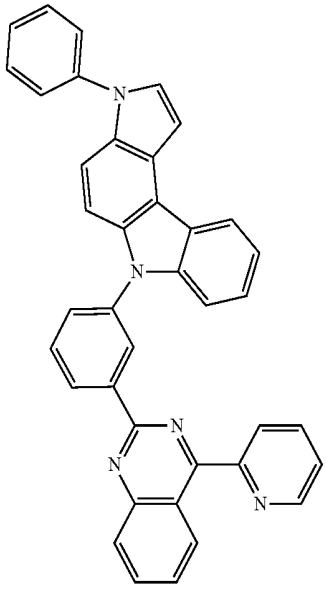

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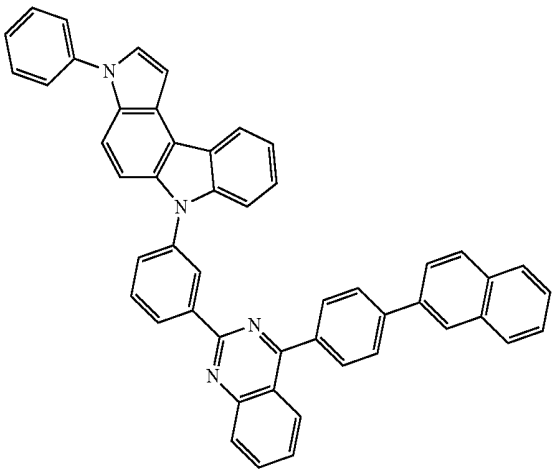

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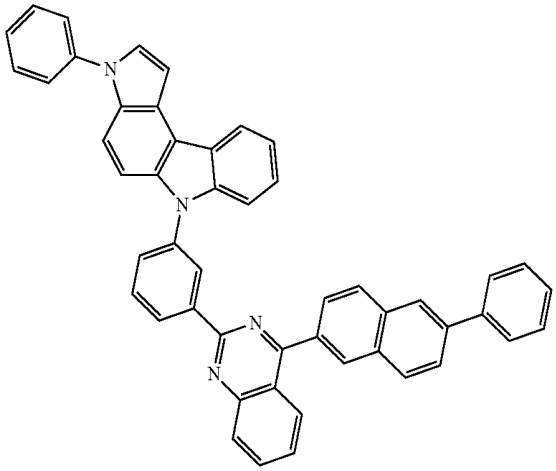

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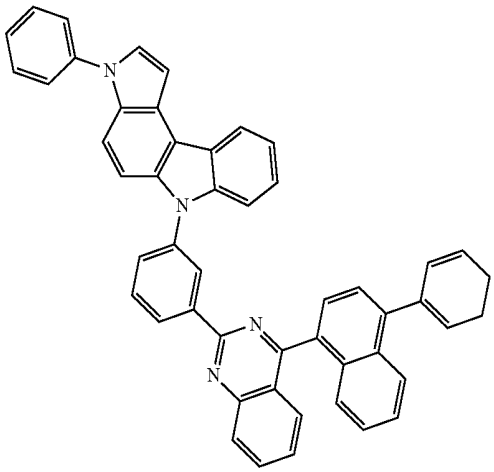

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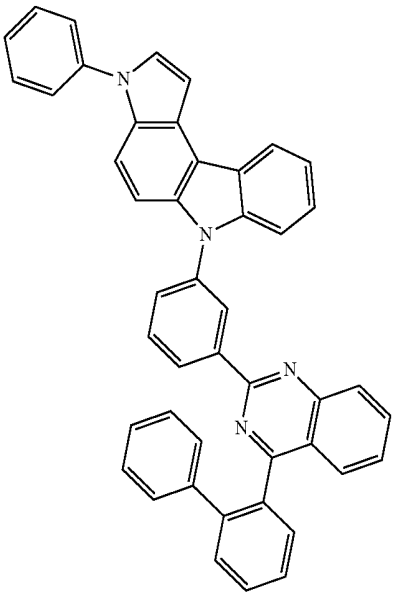

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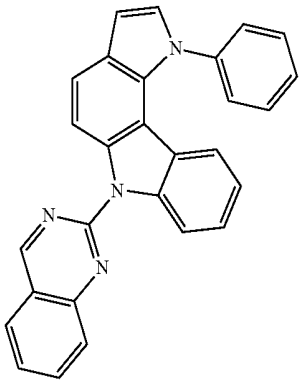

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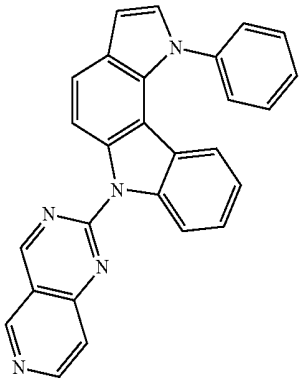

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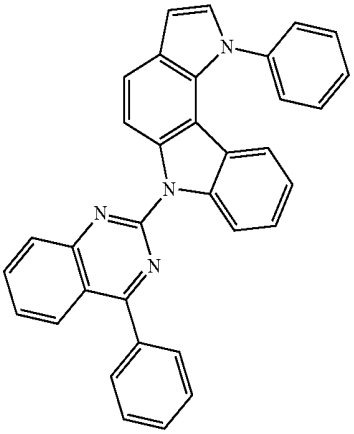

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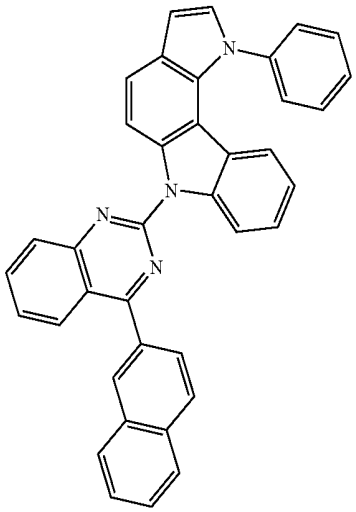

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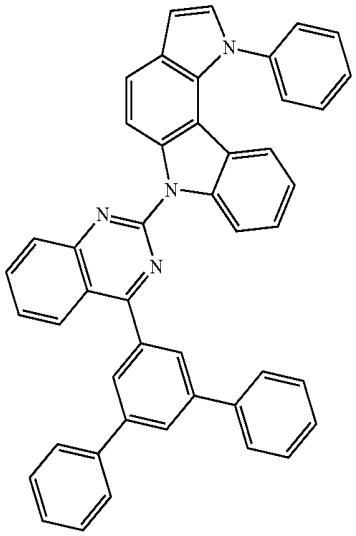

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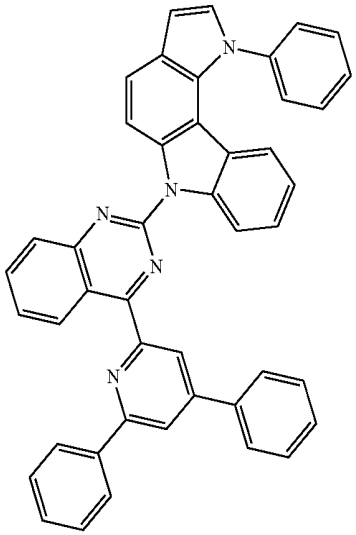

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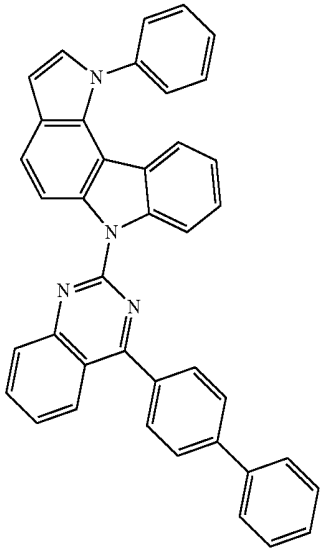

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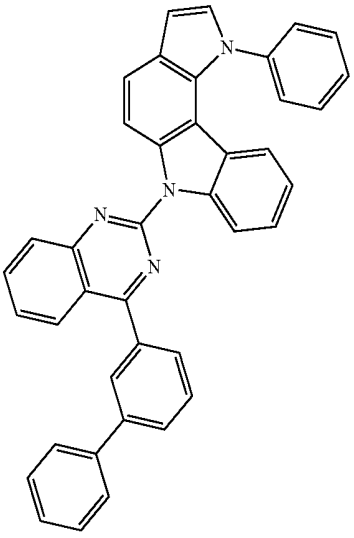

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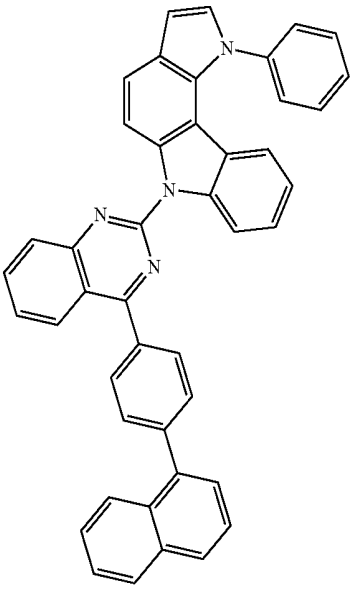

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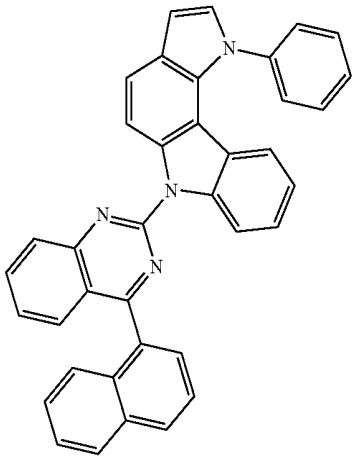

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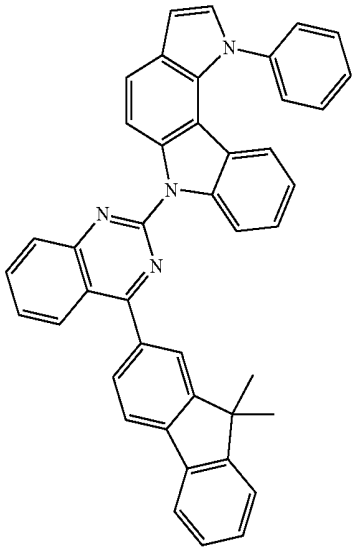

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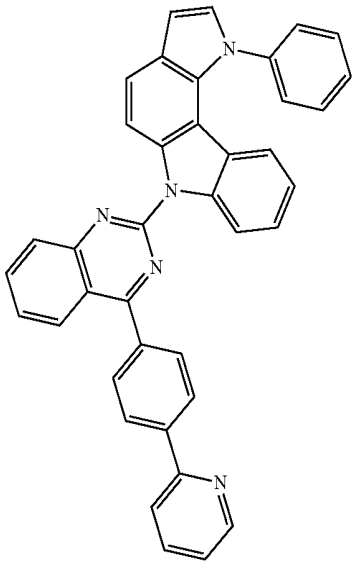

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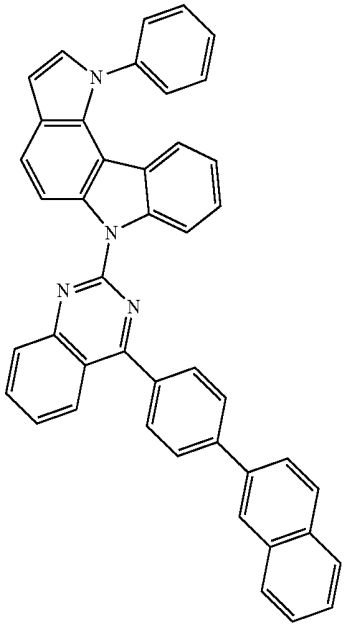

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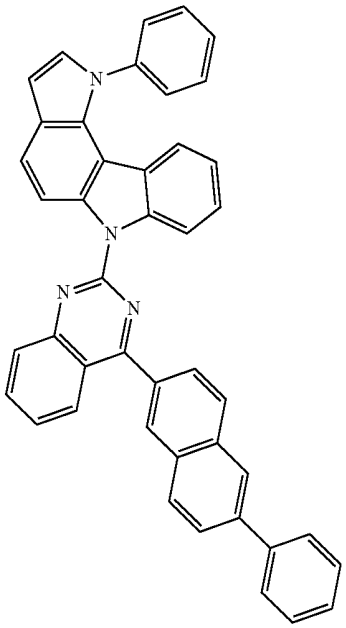

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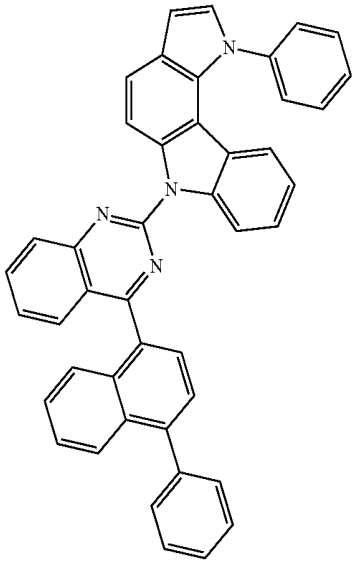
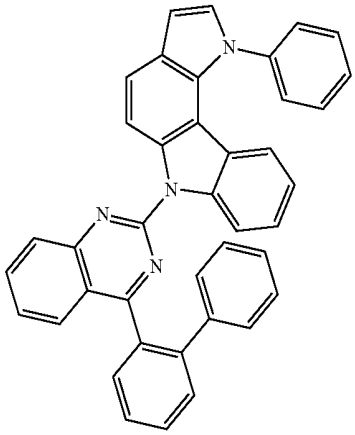
C315



C316



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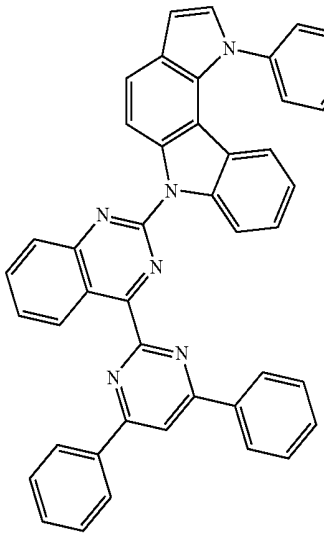

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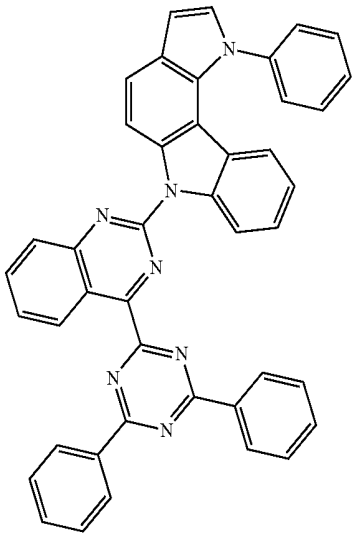

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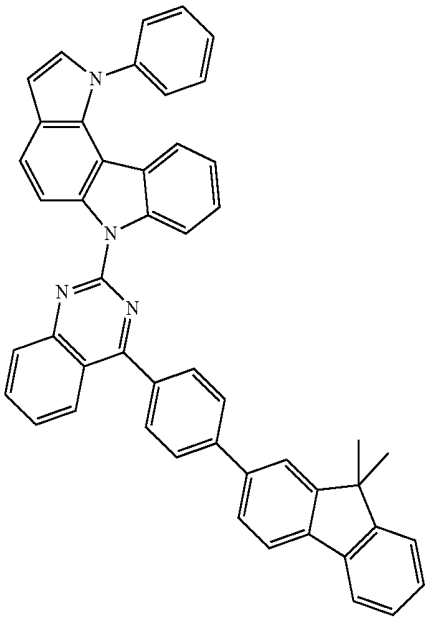

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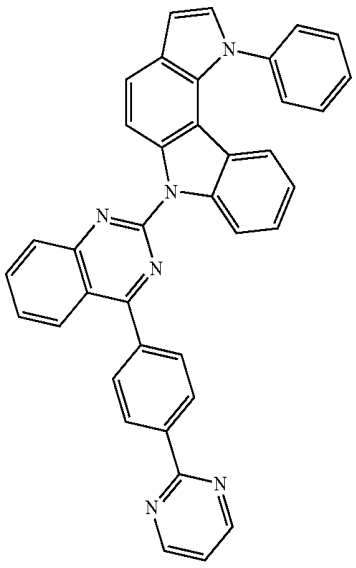

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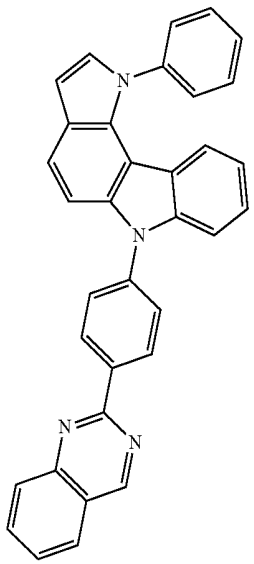

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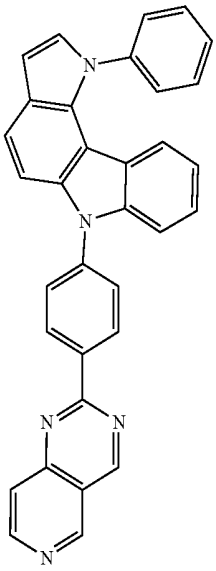

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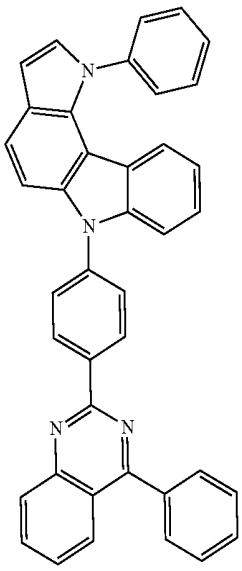

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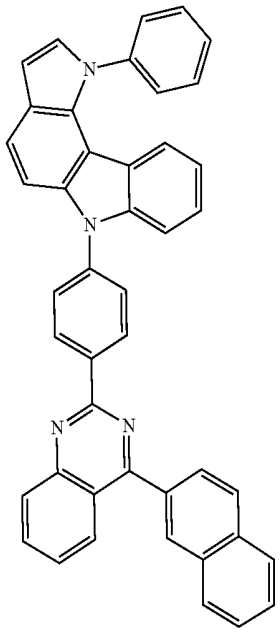

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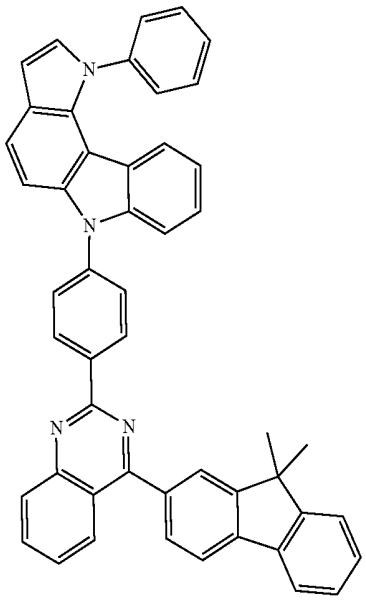

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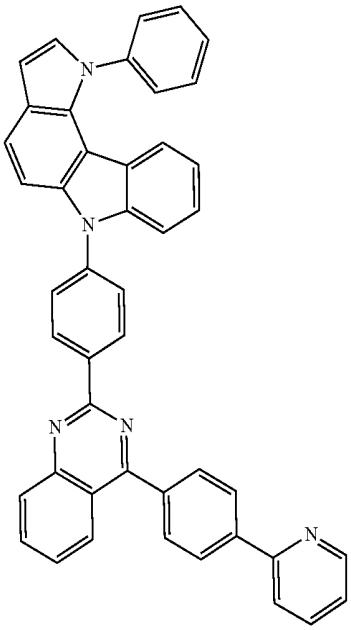

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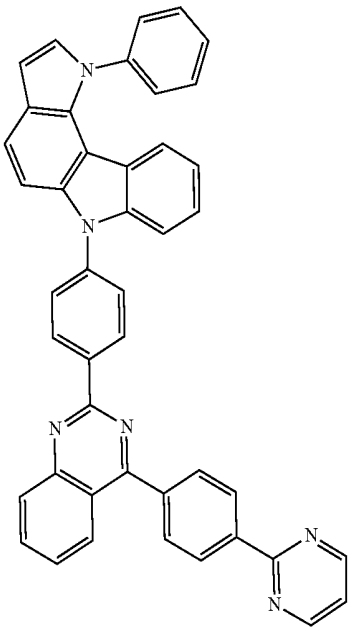

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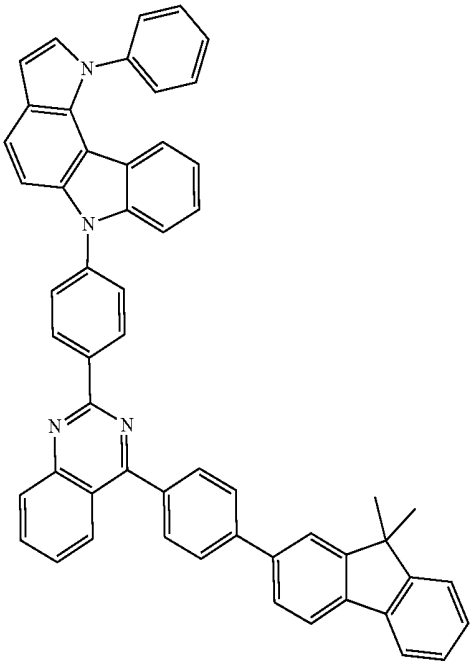

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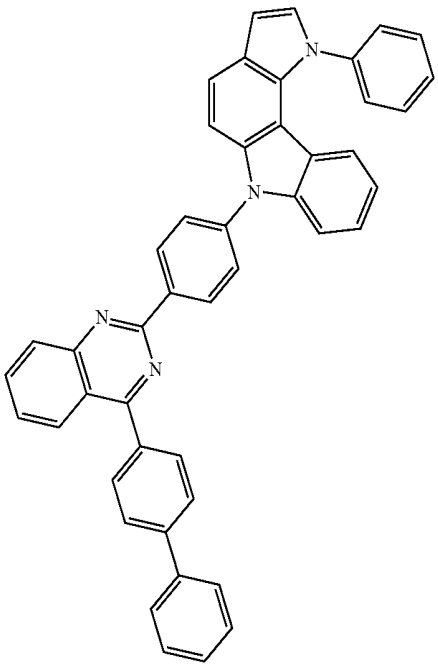

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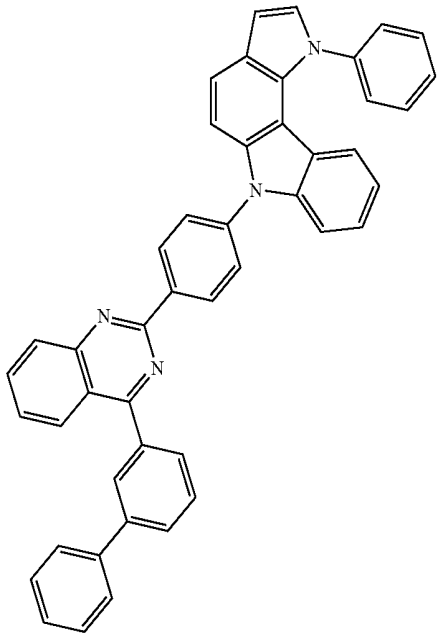

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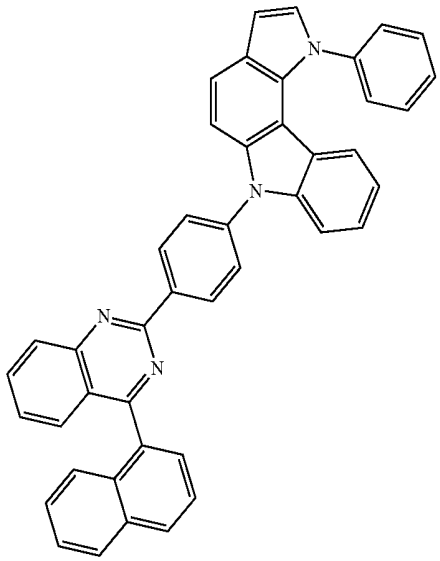

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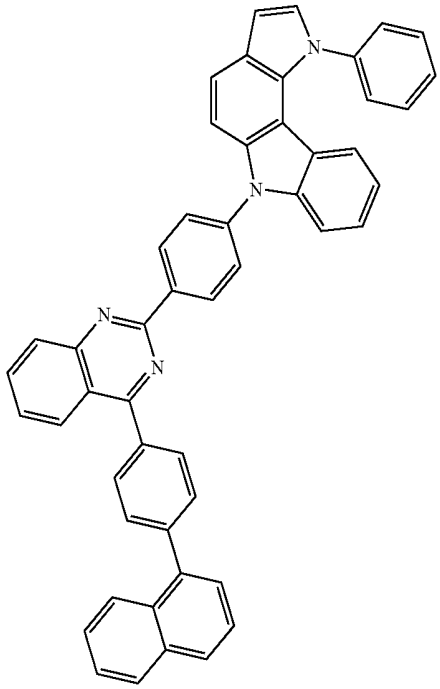

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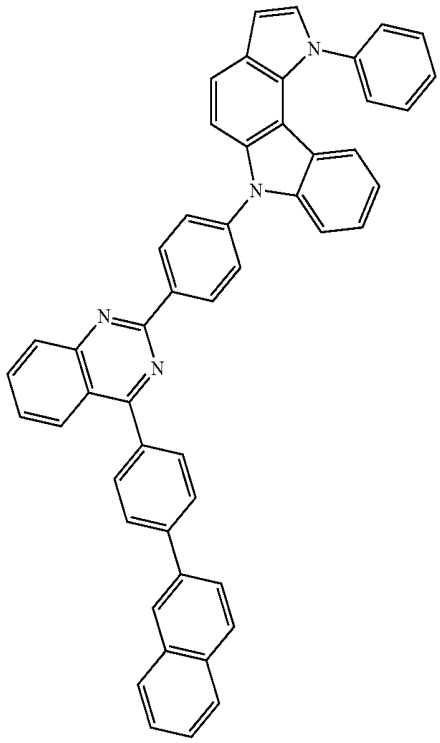

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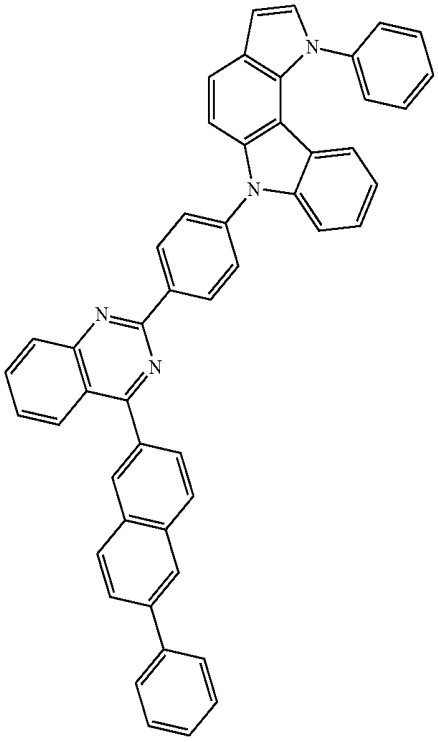

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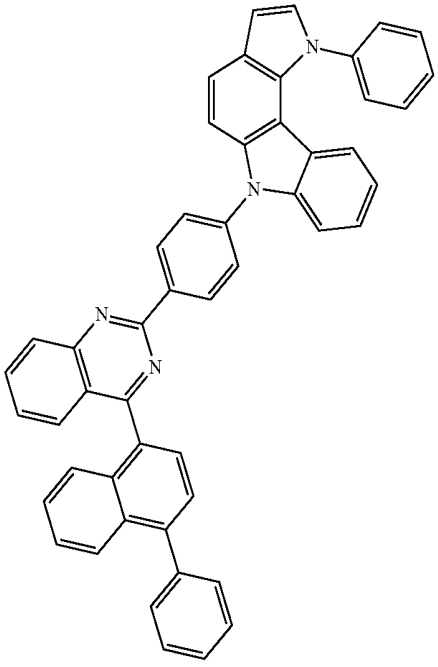

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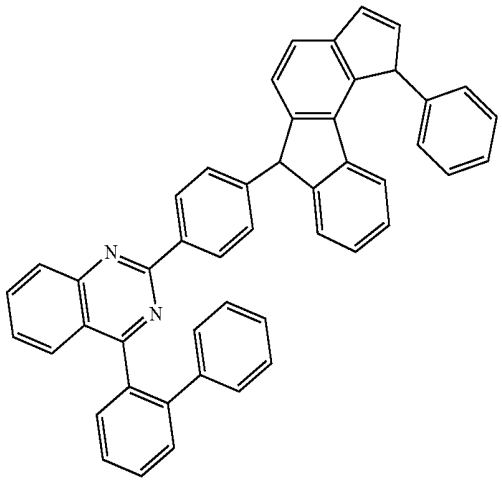

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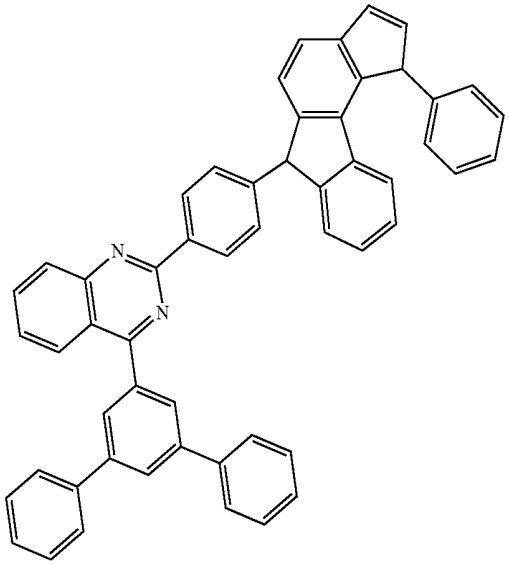

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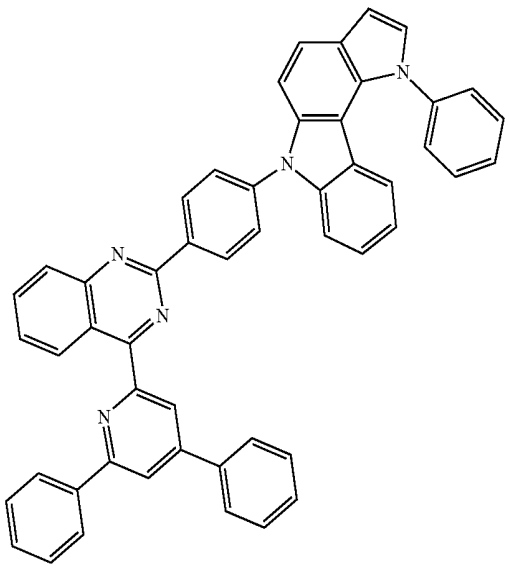

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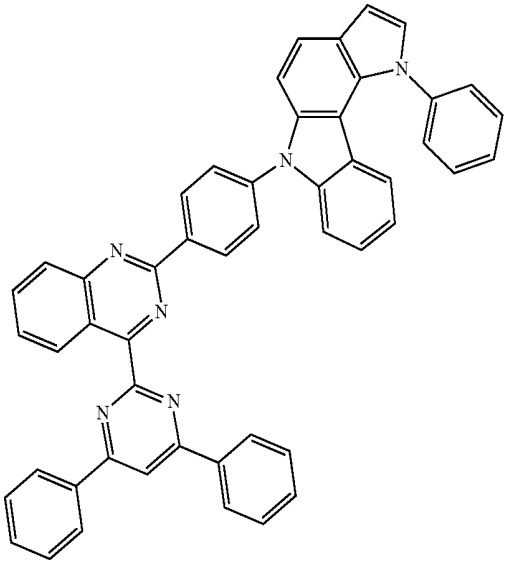

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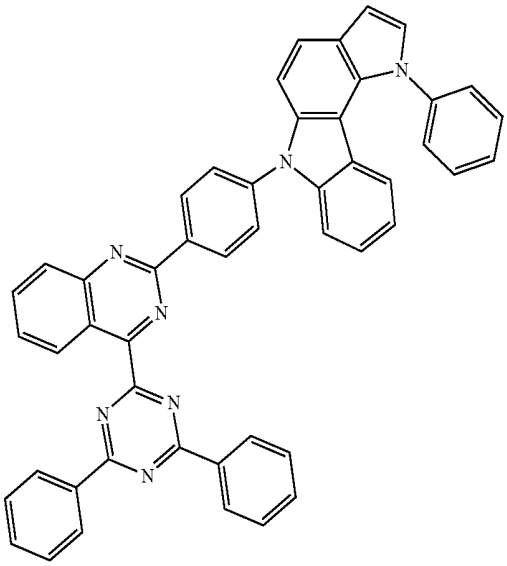

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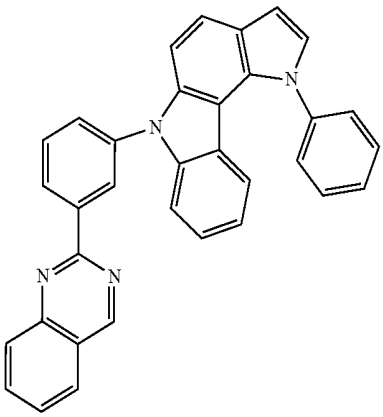

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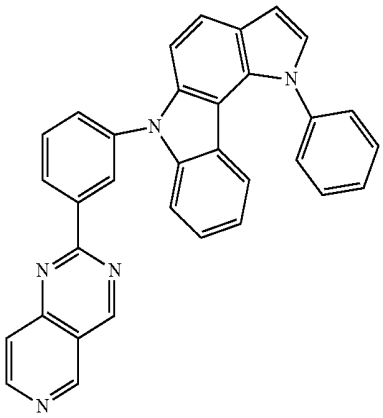

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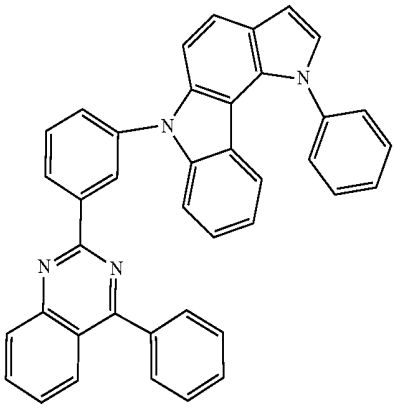

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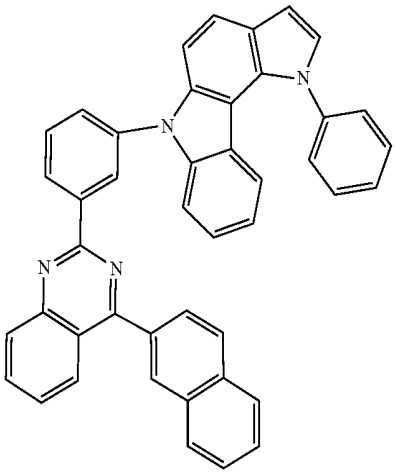

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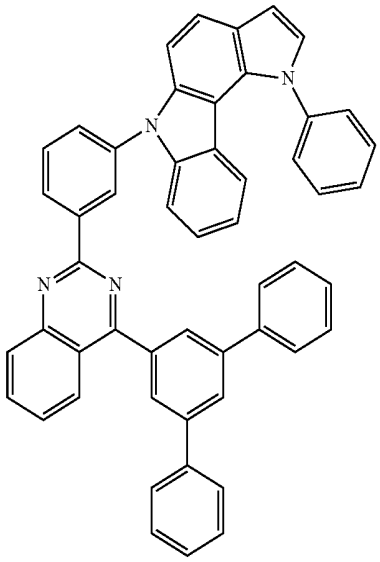

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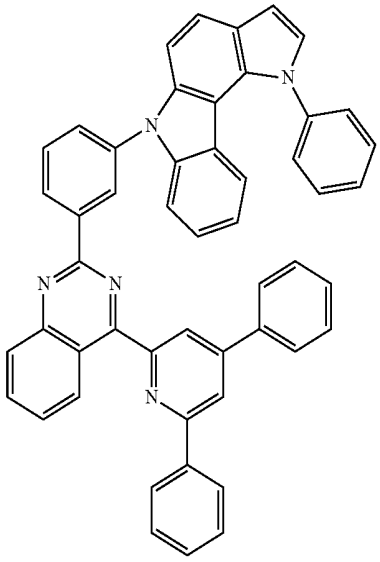

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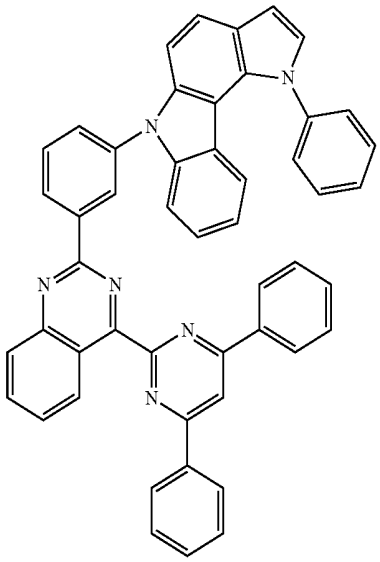

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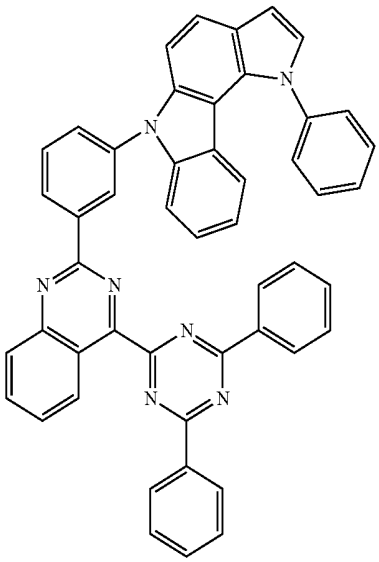

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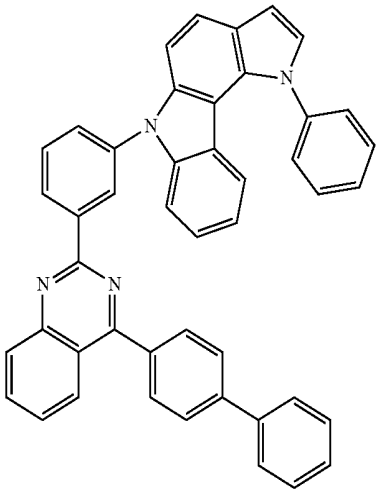

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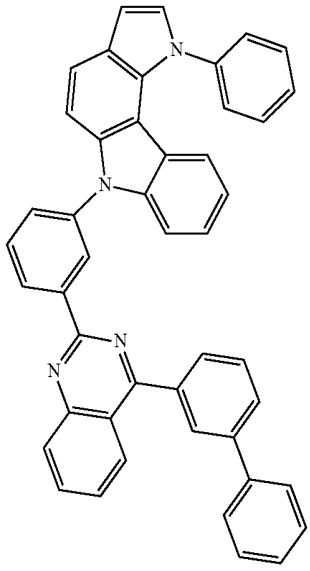

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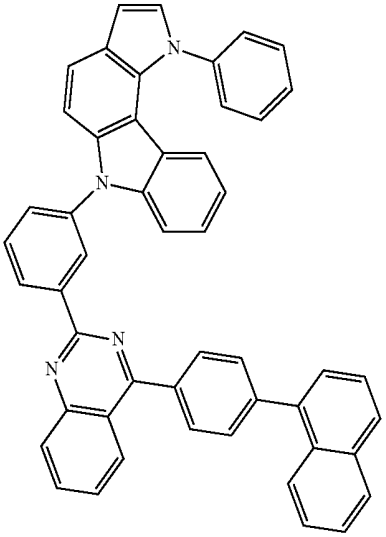

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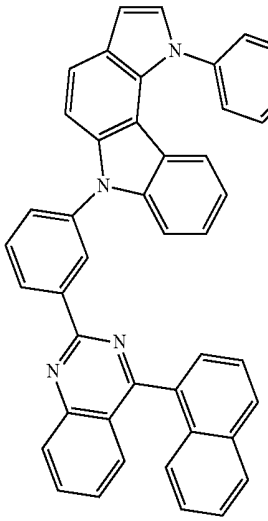

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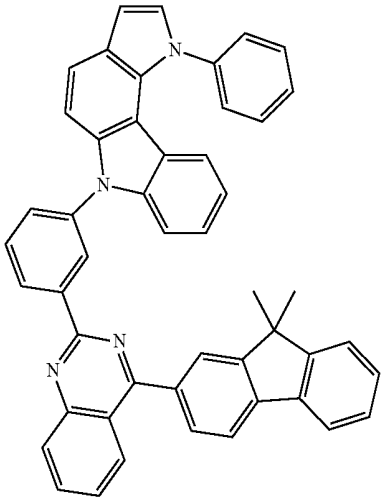

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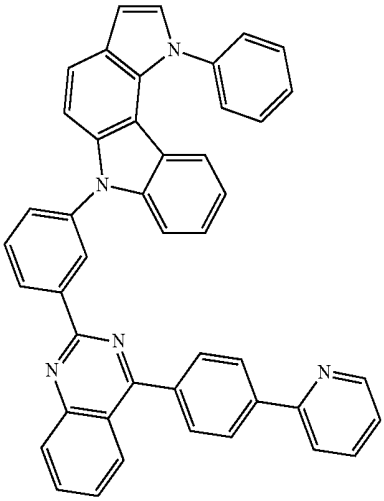

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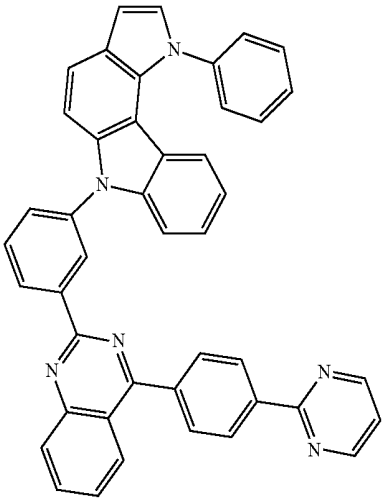

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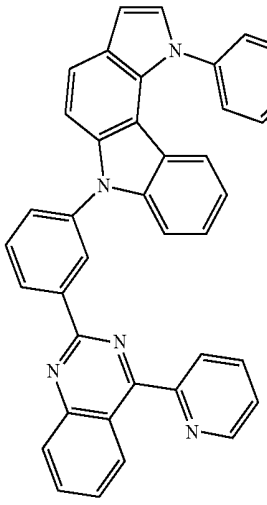

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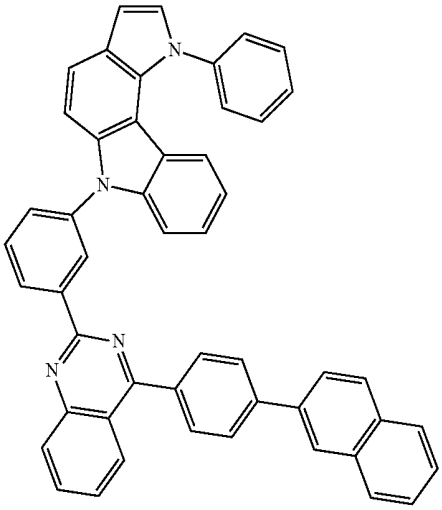

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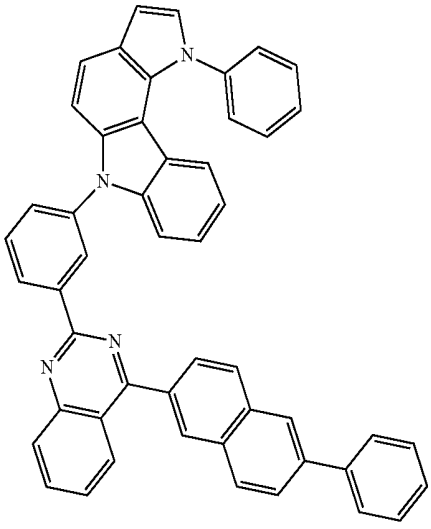

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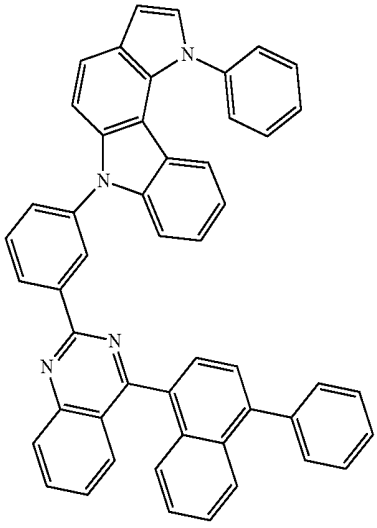

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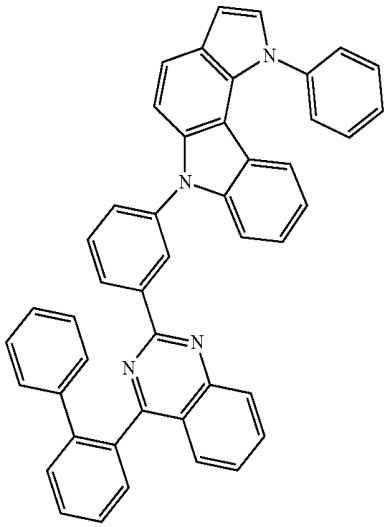

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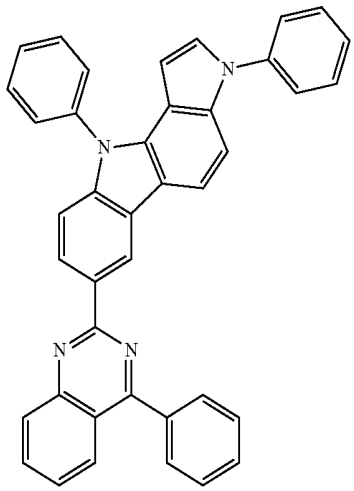

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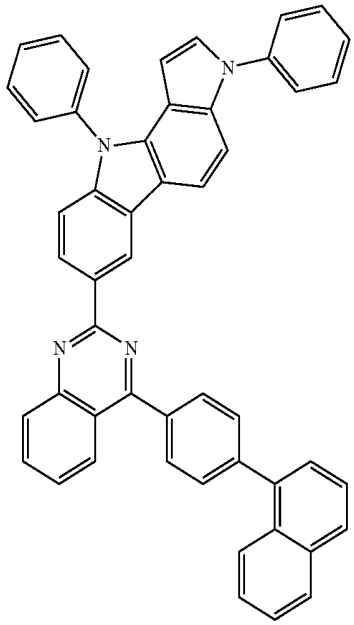

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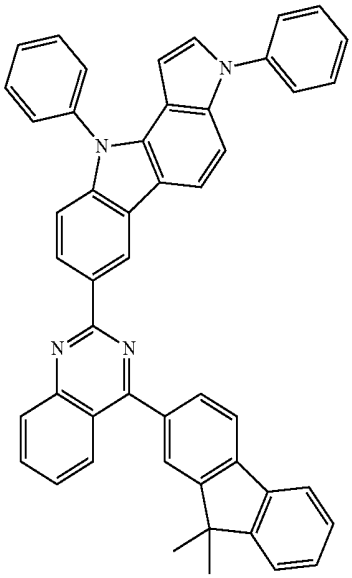

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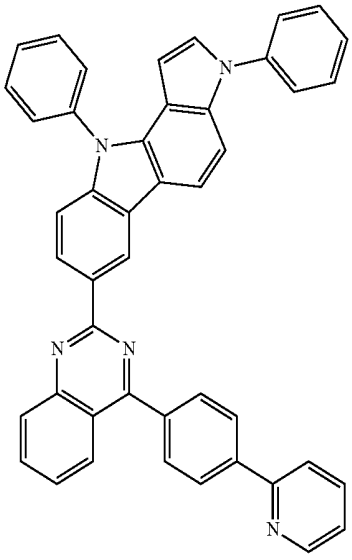

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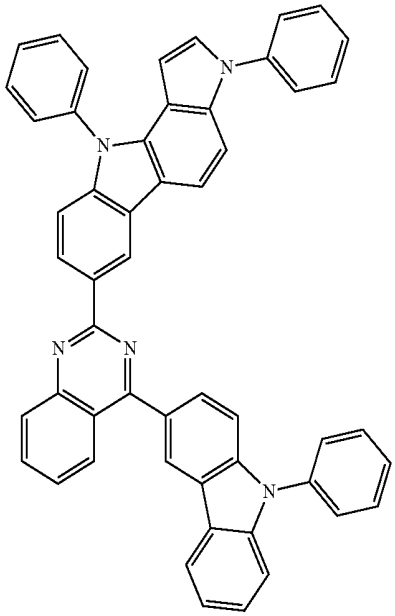

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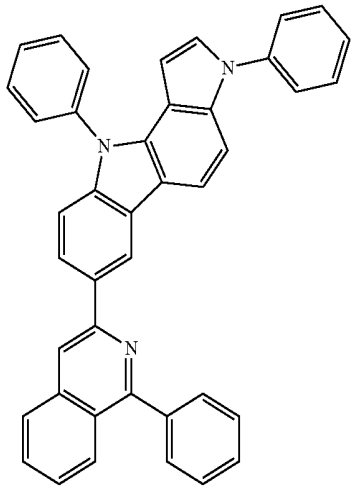

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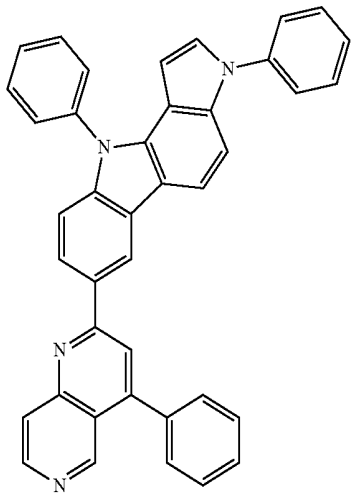

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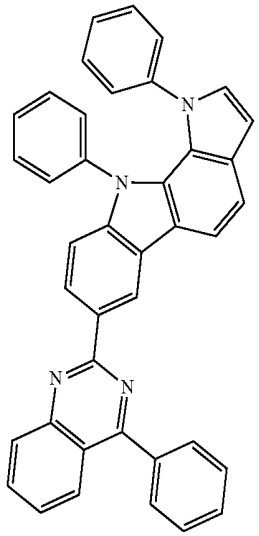

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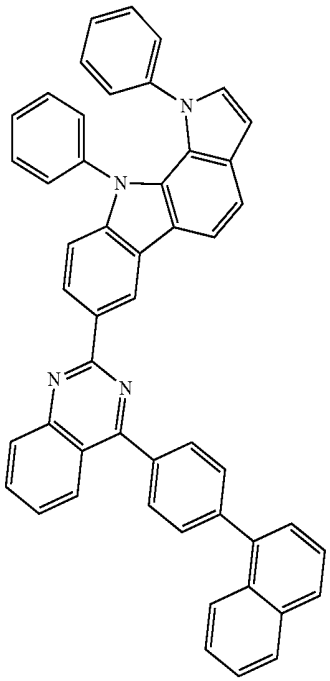

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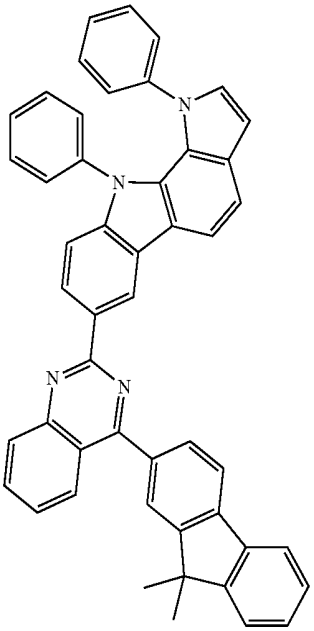

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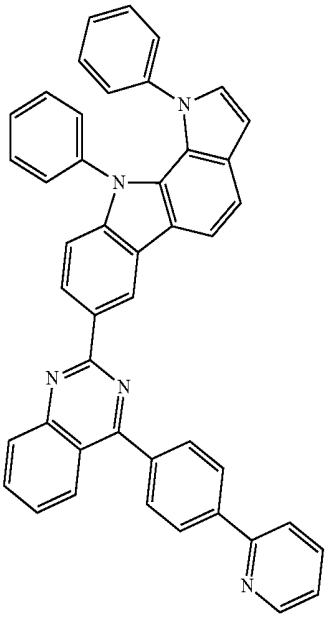

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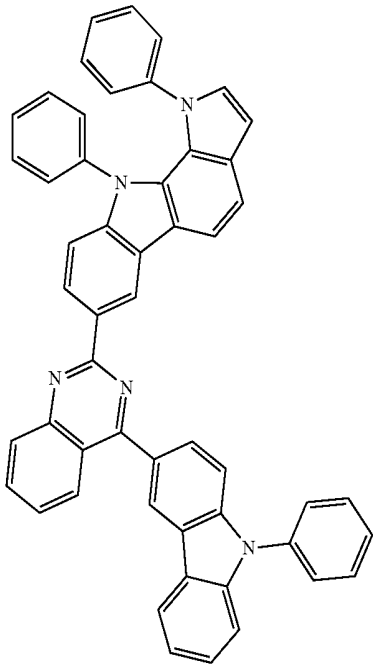

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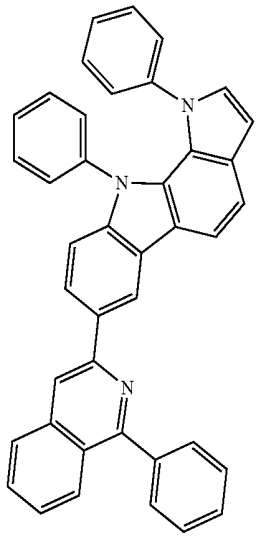

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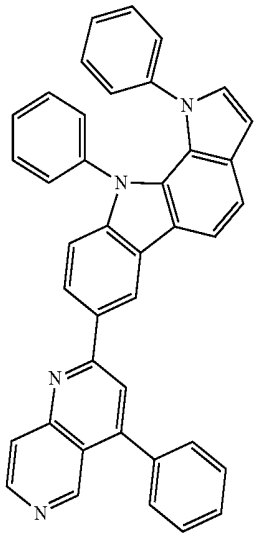
C374



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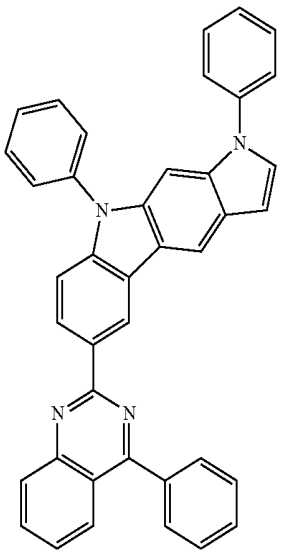

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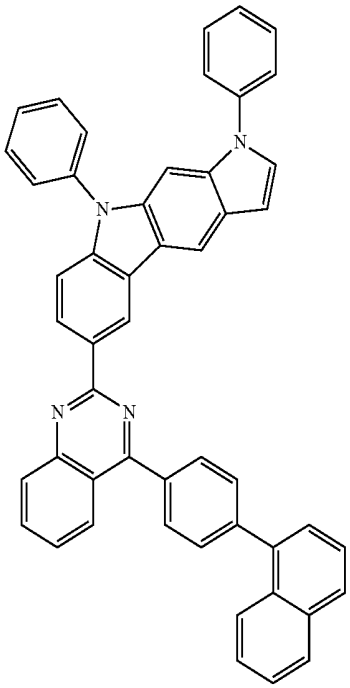

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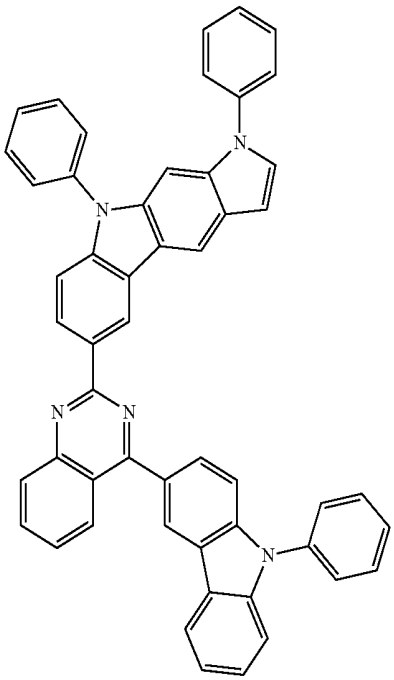

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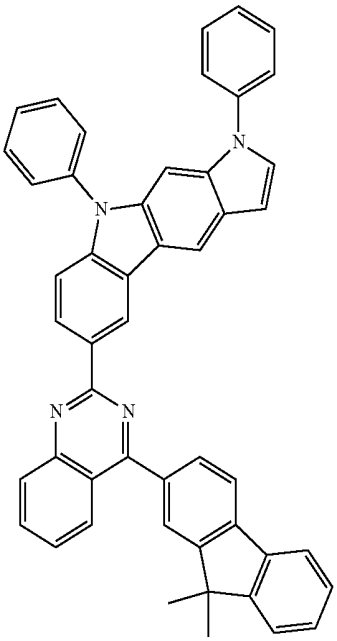

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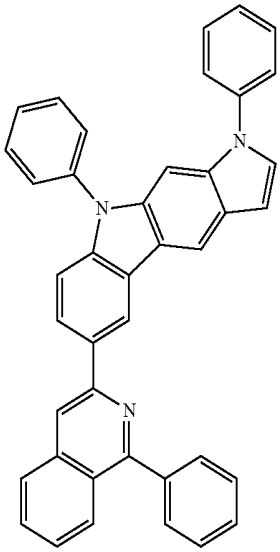

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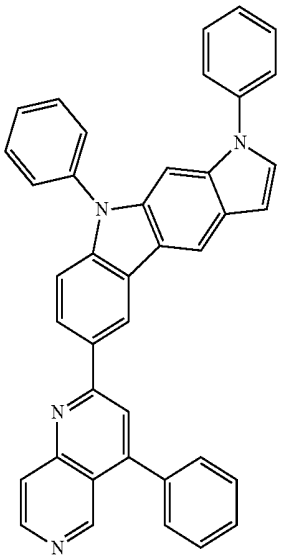

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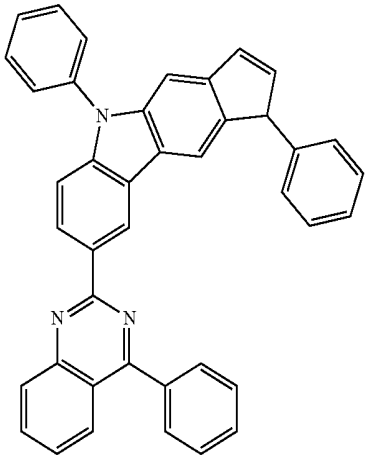

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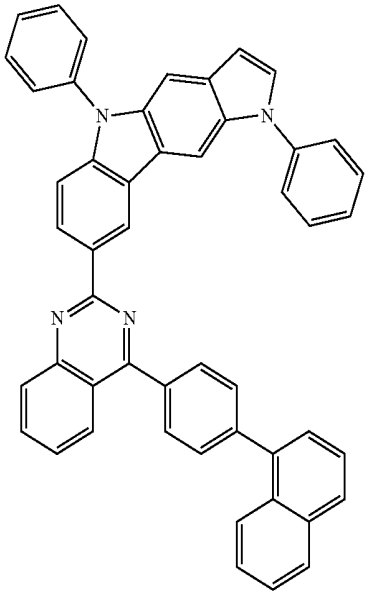

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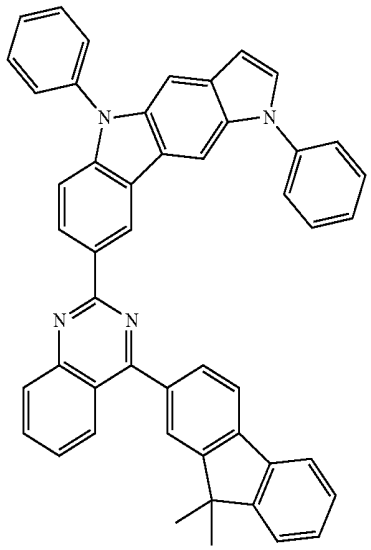

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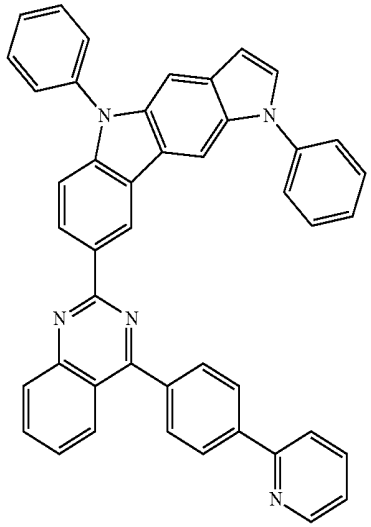

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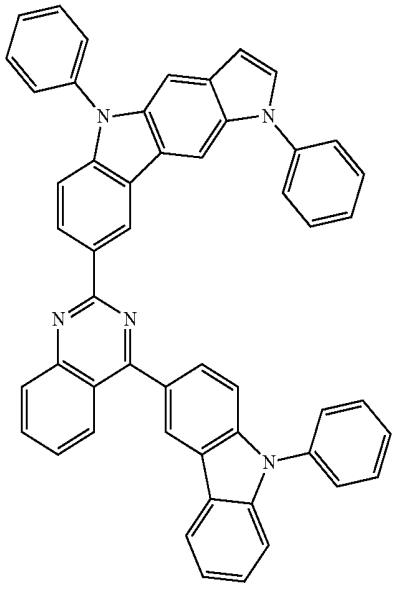

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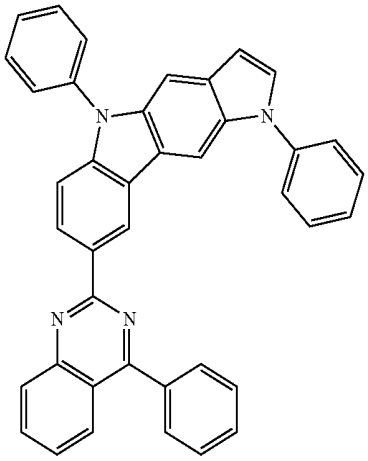

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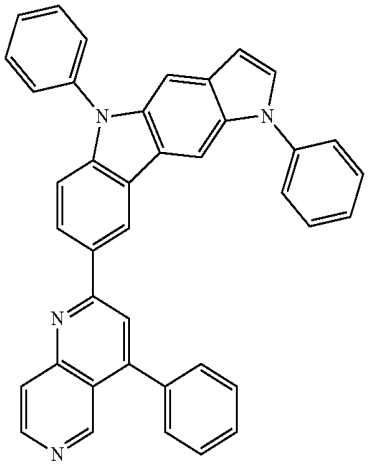

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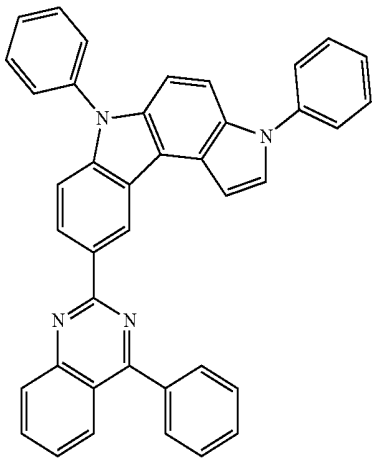

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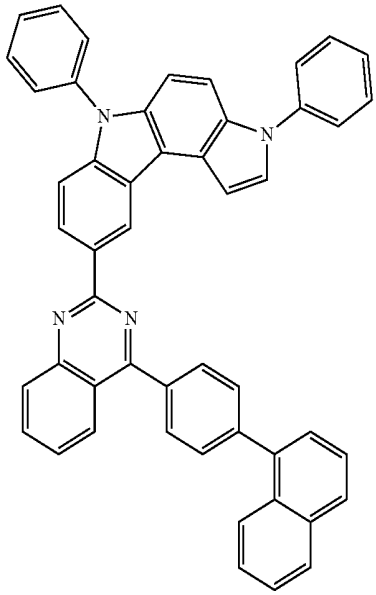

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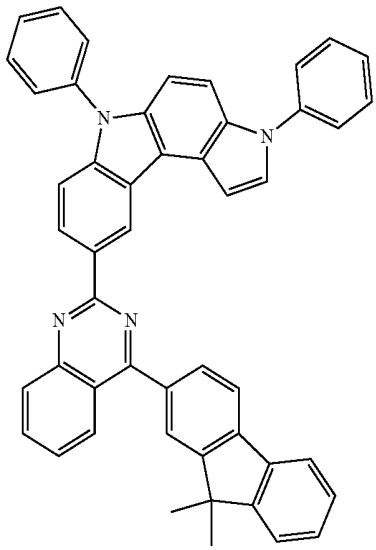

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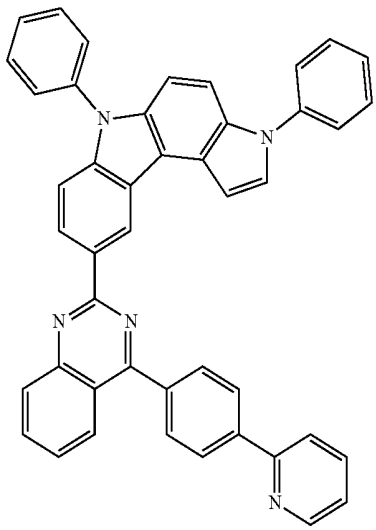

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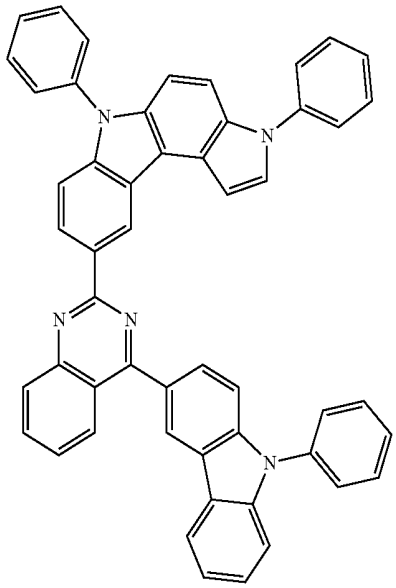

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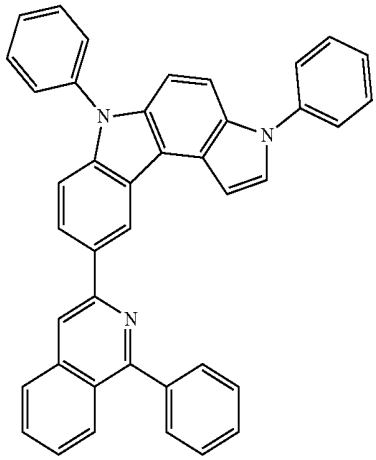

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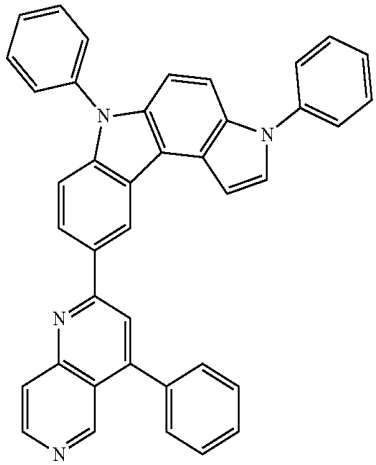

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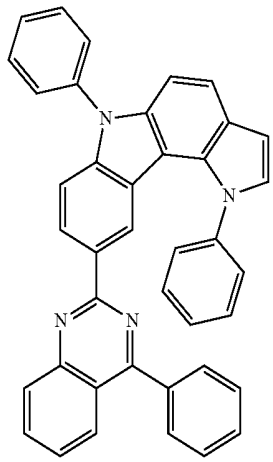

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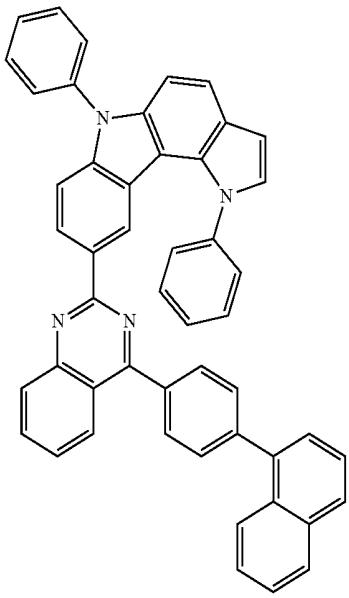

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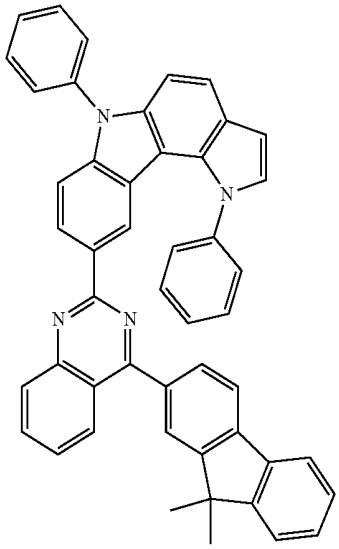

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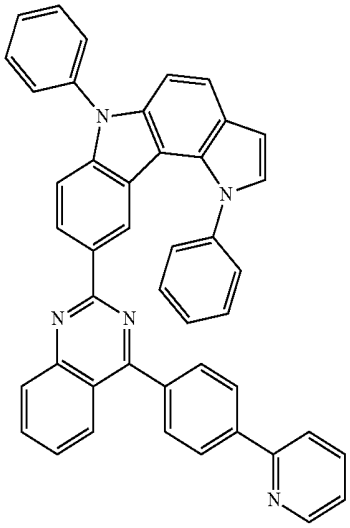

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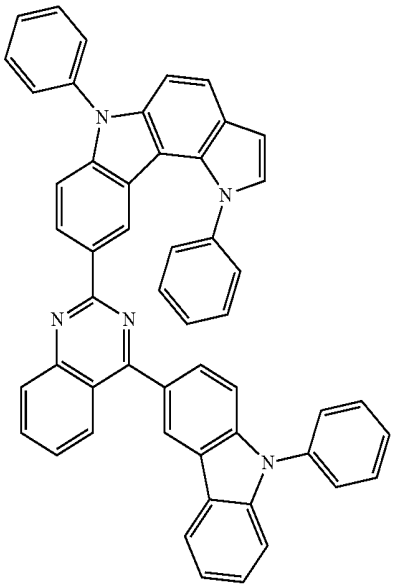

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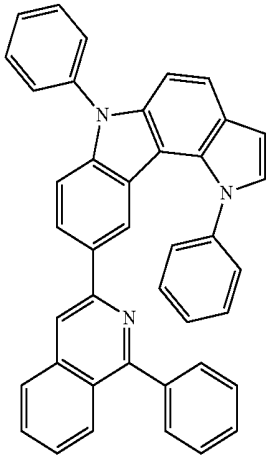

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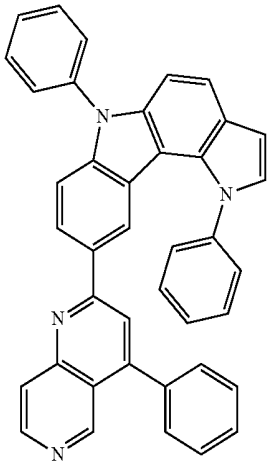

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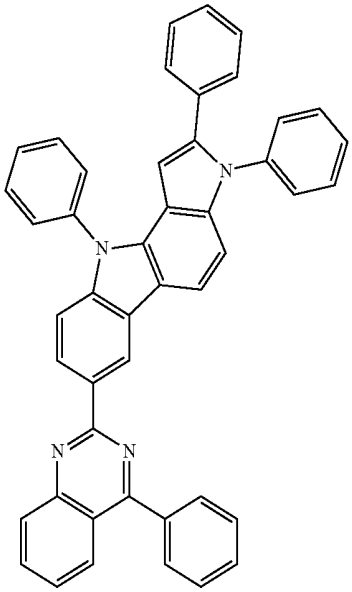

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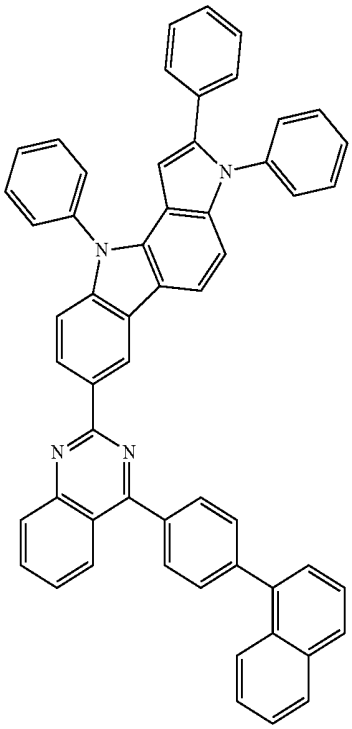

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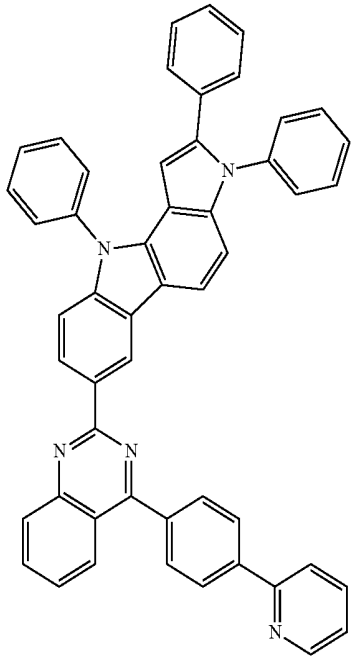

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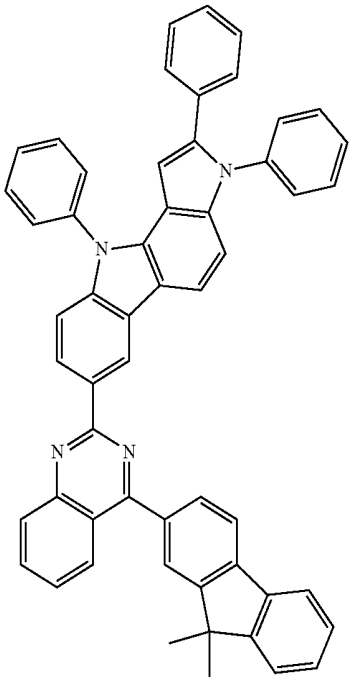

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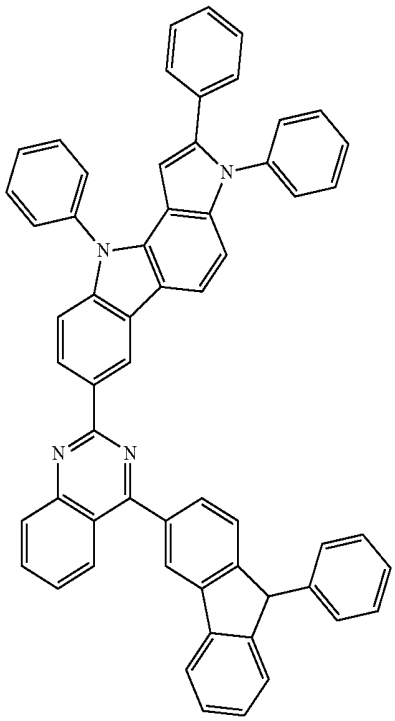

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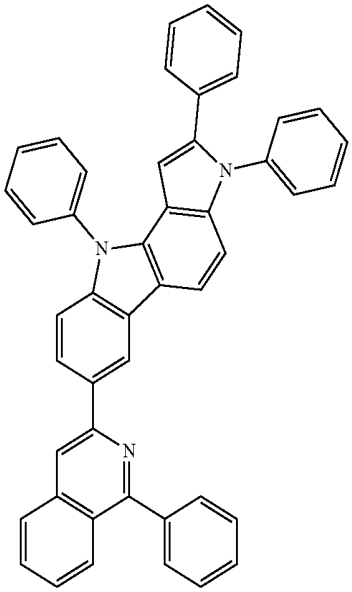

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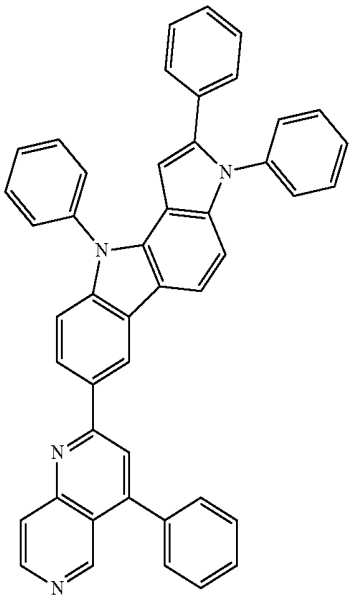

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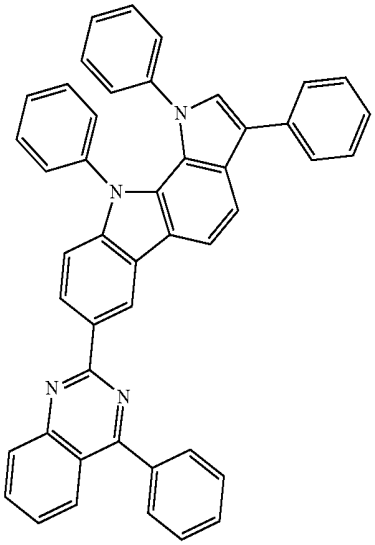

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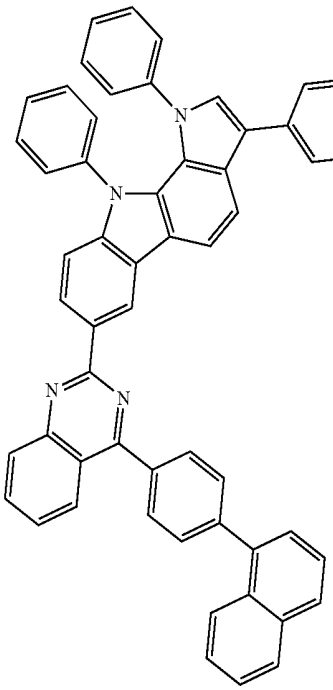

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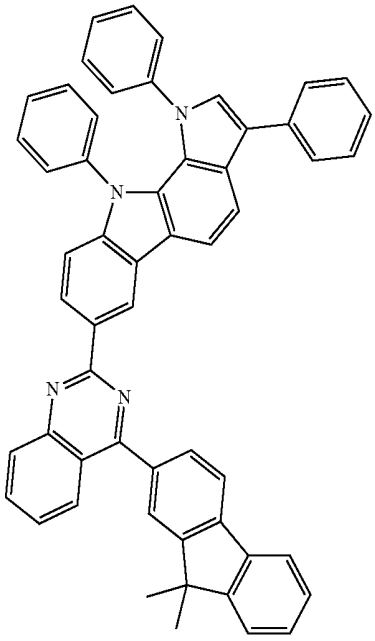

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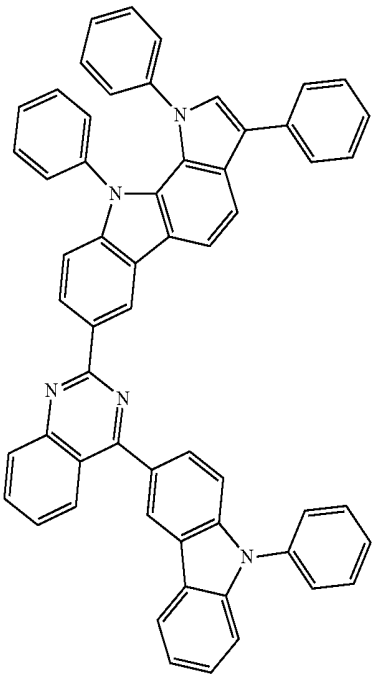

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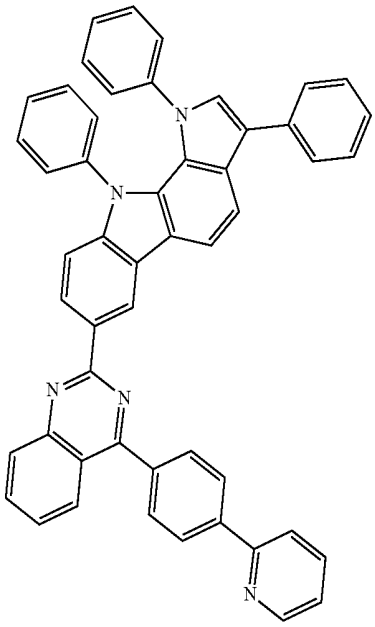

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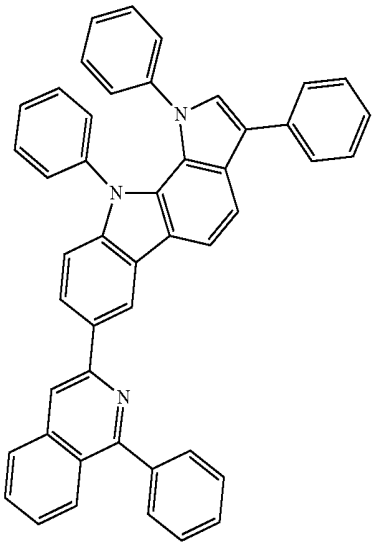

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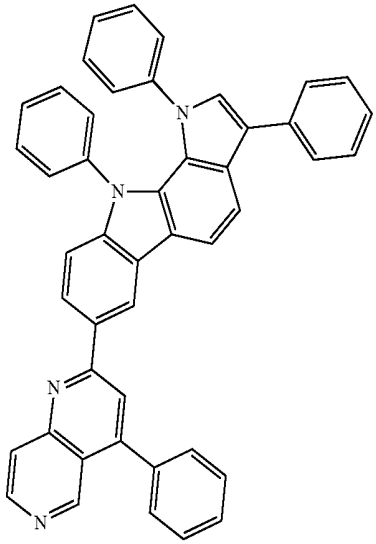

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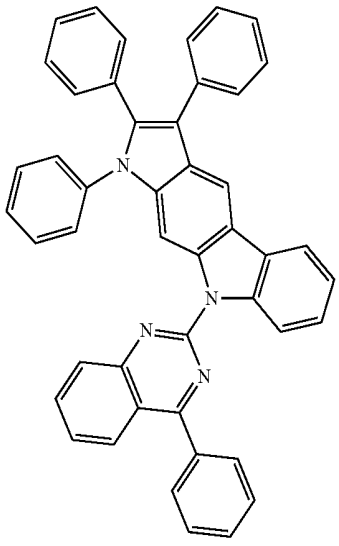

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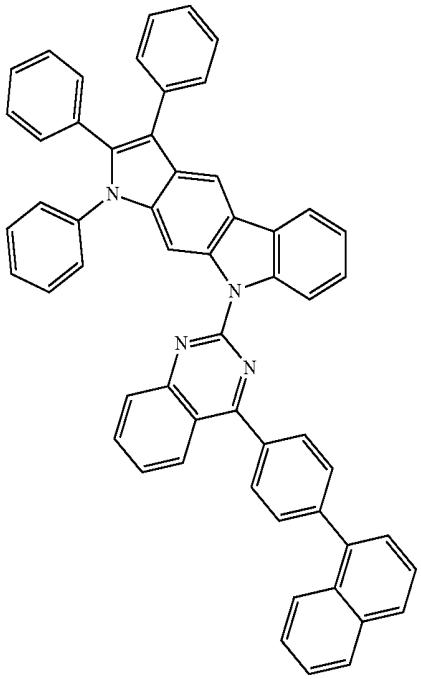

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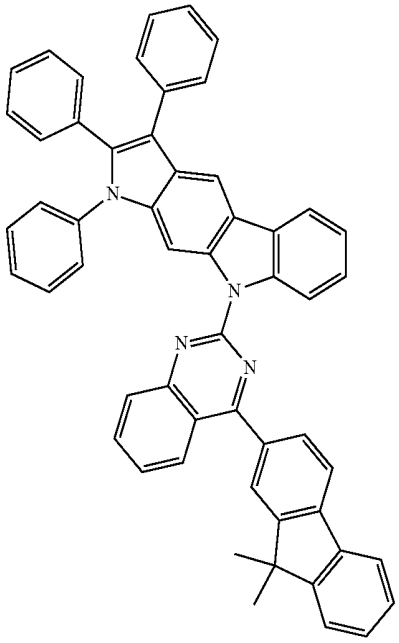

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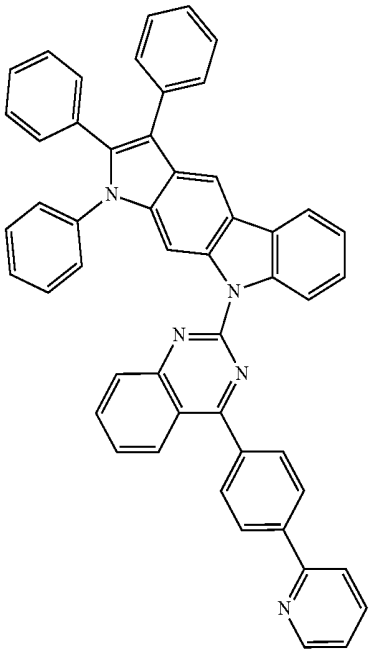

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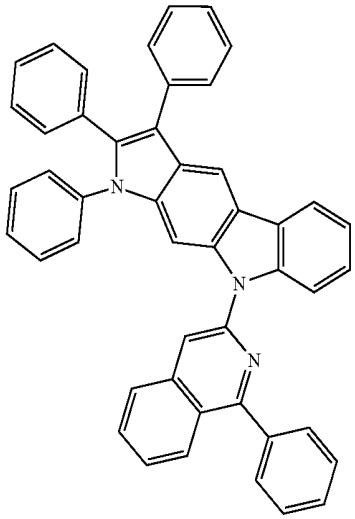

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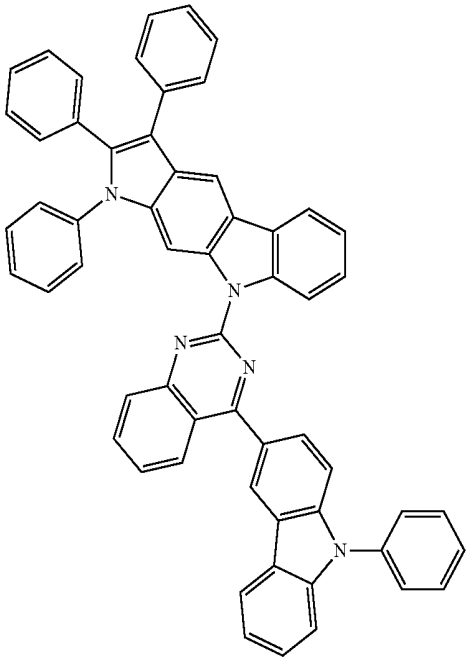

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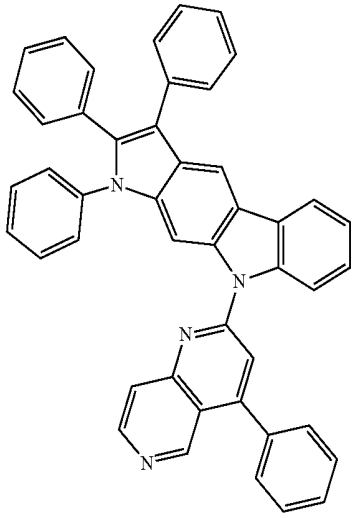

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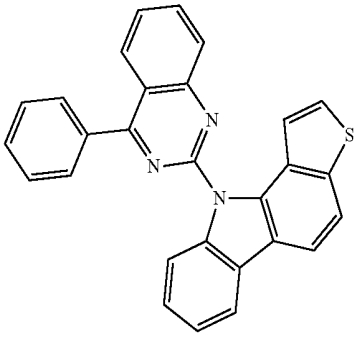

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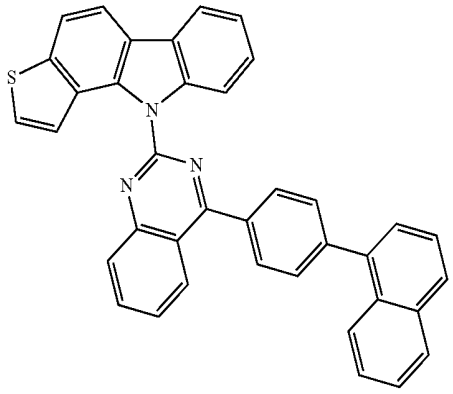

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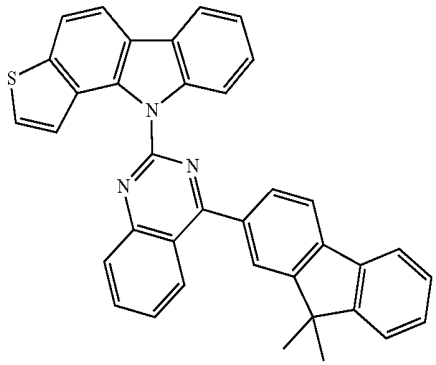

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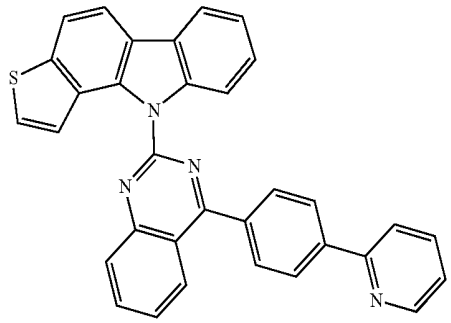

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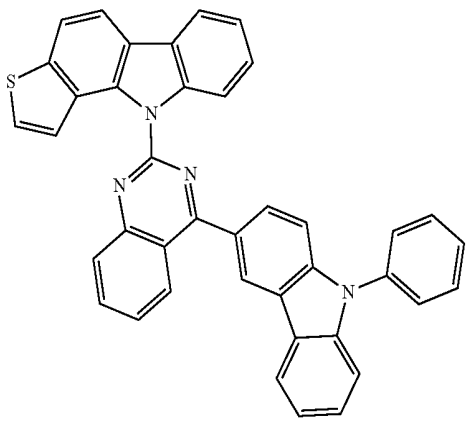

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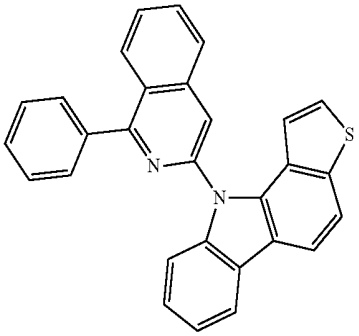

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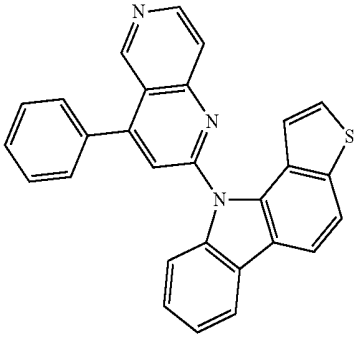

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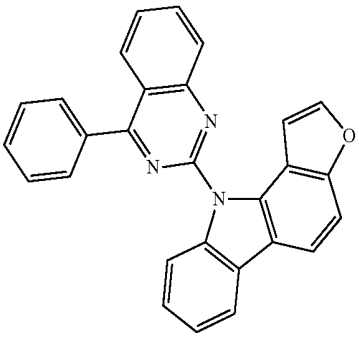

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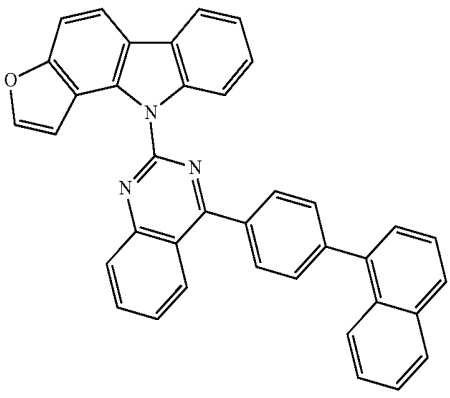

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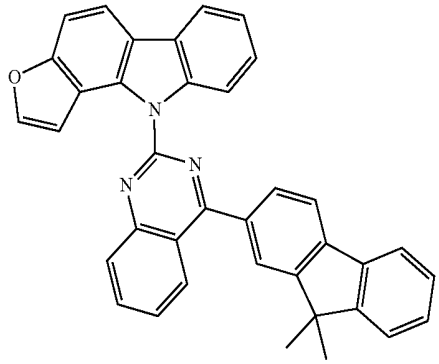

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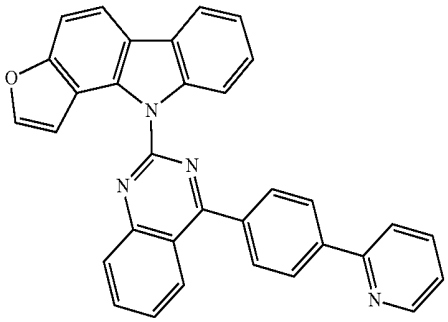

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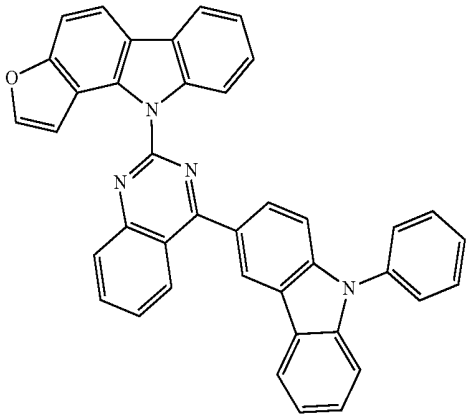

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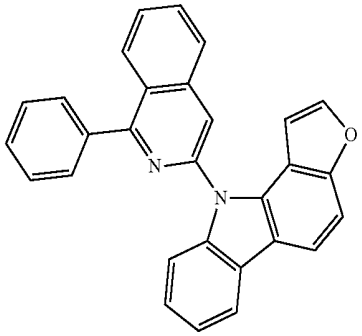

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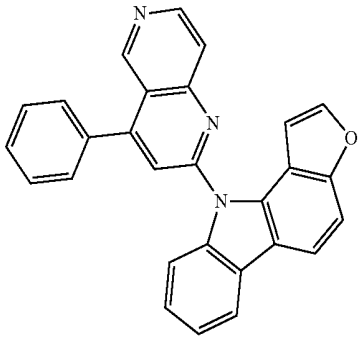

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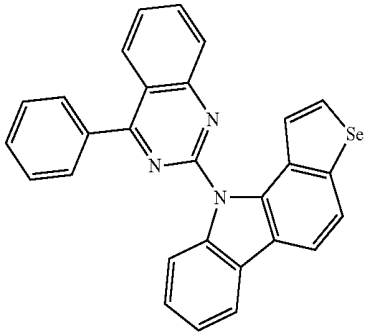

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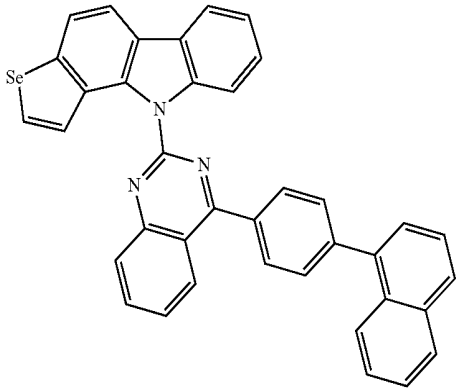

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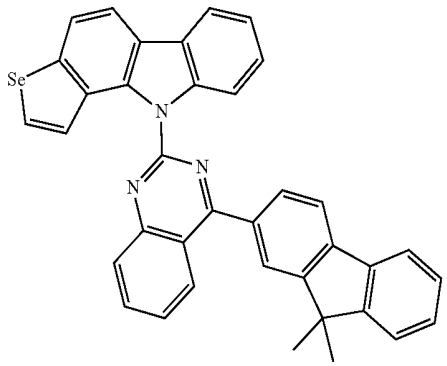

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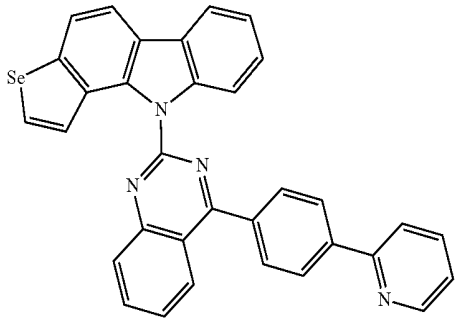

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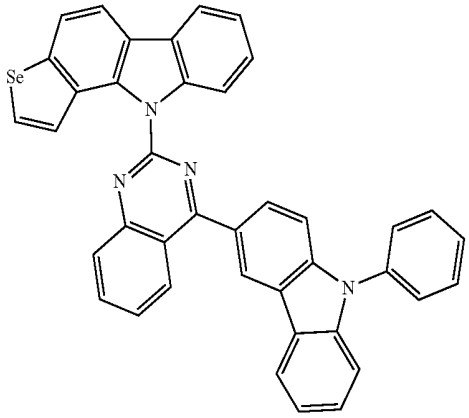

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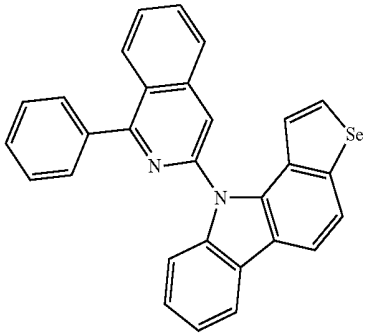

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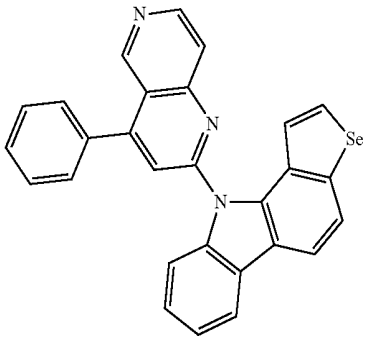

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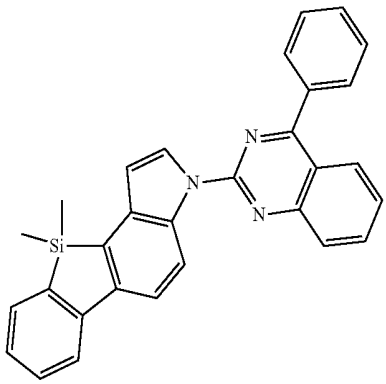

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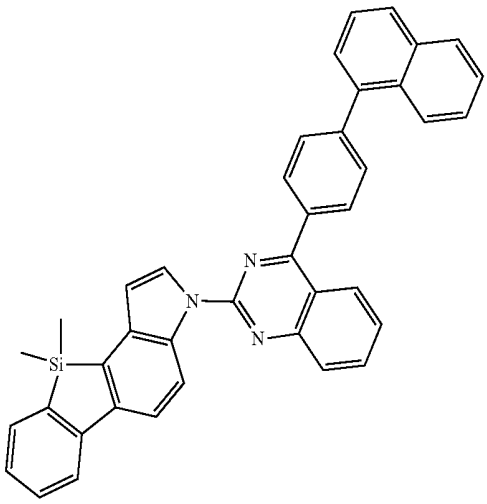

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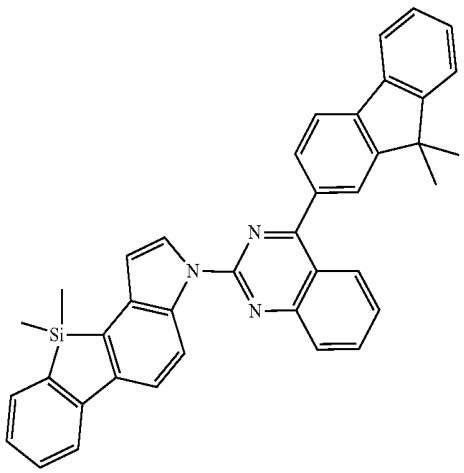

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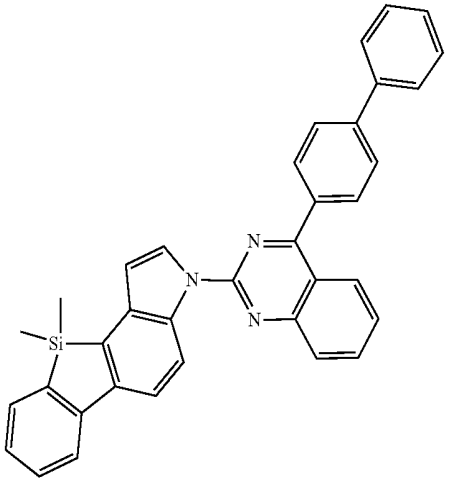

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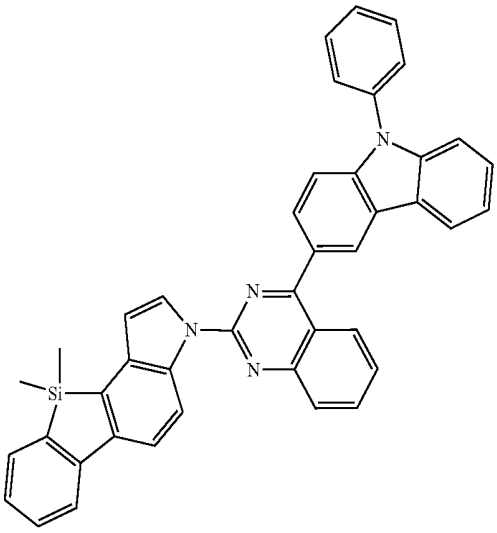

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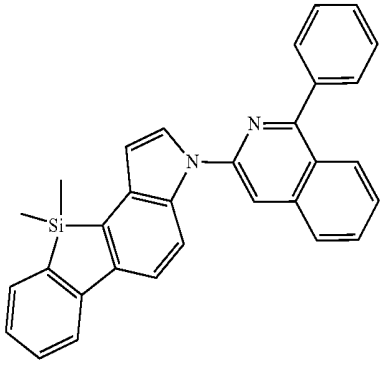

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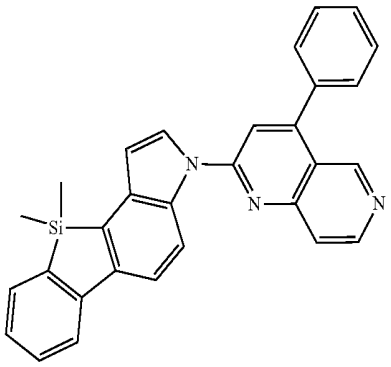

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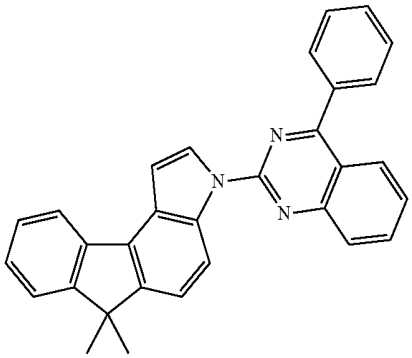

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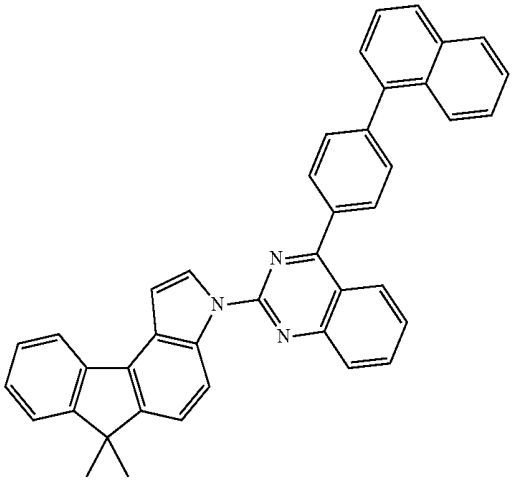

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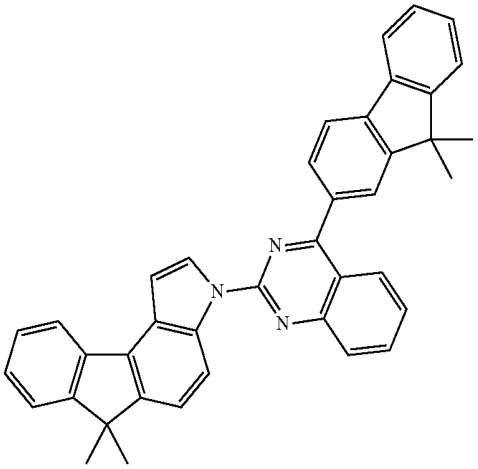

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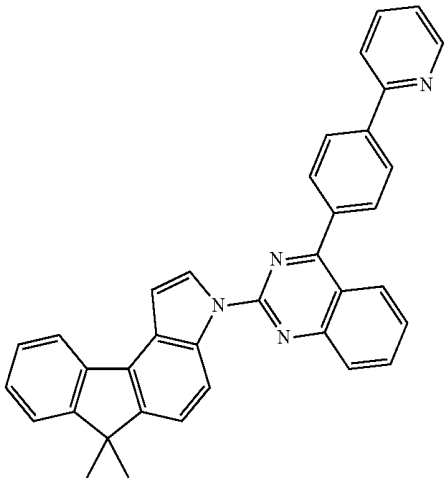

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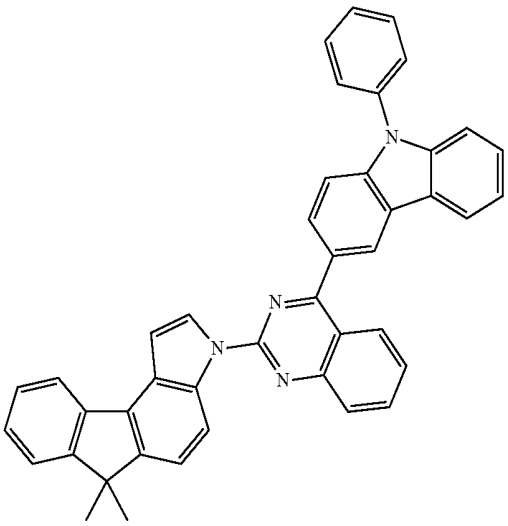

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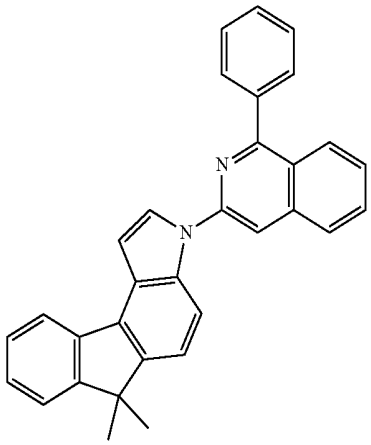

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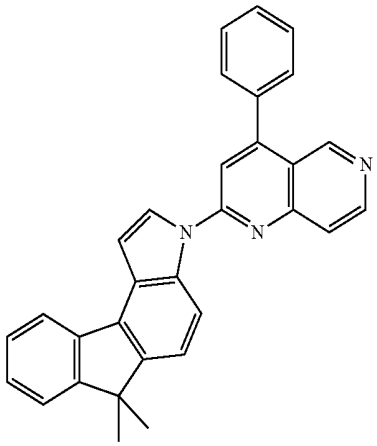


[0055] The compound represented by Formula 1 according to the present invention as described above may be synthesized in various manners with reference to the synthesis procedure of the following Examples.

[0056] 2. Organic Electroluminescence Device

[0057] The present invention provides an organic electroluminescence device including the compound represented by Formula 1.

[0058] Specifically, the organic electroluminescent device according to the present invention includes (i) an anode, (ii) a cathode, and (iii) an organic material layer having one or more layers interposed between the anode and the cathode, in which at least one of the organic material layer having one or more layers includes the compound represented by Formula 1.

[0059] The organic material layer including the compound represented by Formula 1 may be one or more of a hole injection layer, a hole transporting layer, a light-emitting layer, an electron transporting layer, and an electron injection layer. The organic material layer including the compound of Formula 1 may be preferably a hole injection layer, a hole transporting layer, or a light-emitting layer, and more preferably a light-emitting layer.

[0060] The light-emitting layer of the organic electroluminescence device according to the present invention may contain a host material (preferably a phosphorescent host material), and in this case, as the host material, the compound represented by Formula 1 may be used. When the light-emitting layer includes the compound represented by For-

mula 1 as described above, hole transporting capabilities are increased, so that the binding force of holes and electrons is increased in the light-emitting layer, thereby providing an organic electroluminescence device having excellent efficiency (light-emitting efficiency and power efficiency), lifespan, brightness, driving voltage, and the like.

[0061] The structure of the organic electroluminescence device according to the present invention is not particularly limited, but as a non-limiting example thereof, the organic electroluminescence device may have a structure in which a substrate, an anode, a hole injection layer, a hole transporting layer, a light-emitting layer, an electron transporting layer, and a cathode are sequentially laminated. Here, an electron injection layer may also be additionally laminated on the electron transporting layer. Furthermore, the organic electroluminescence device according to the present invention may have a structure in which an anode, an organic material layer including one or more layers, and a cathode are sequentially laminated and may also have a structure in which an insulating layer or an adhesive layer may be inserted into the interface between the electrode and the organic material layer.

[0062] Meanwhile, a material which may be used as the anode included in the organic electroluminescence device according to the present invention is not particularly limited, but as non-limiting examples thereof, it is possible to use: a metal, such as vanadium, chromium, copper, zinc, and gold, or alloys thereof; a metal oxide, such as zinc oxide, indium oxide, indium tin oxide (ITO), and indium zinc oxide (IZO); a combination of metal and oxide, such as ZnO:Al or SnO_2:Sb; an electrically conductive polymer, such as polythiophene, poly(3-methylthiophene), poly[3,4-(ethylene-1,2-dioxy)thiophene] (PEDT), polypyrrole, or polyaniline; and carbon black, and the like.

[0063] Furthermore, a material which may be used as the cathode included in the organic electroluminescence device according to the present invention is not particularly limited, but as non-limiting examples thereof, it is possible to use: a metal, such as magnesium, calcium, sodium, potassium, titanium, indium, yttrium, lithium, gadolinium, aluminum, silver, tin, and lead, or alloys thereof; and a multi-layer structured material, such as LiF/Al or LiO_2/Al, and the like.

[0064] The organic material layer included in the organic electroluminescence device according to the present invention may be formed by using materials and methods known in the art, except that the compound represented by Formula 1 is used in any one of a hole injection layer, a hole transporting layer, a light-emitting layer, an electron transporting layer, and an electron injection layer, preferably any one of a hole injection layer, a hole transporting layer, and a light-emitting layer, and more preferably a light-emitting layer.

[0065] A material which may be used as a substrate included in the organic electroluminescence device according to the present invention is not particularly limited, but as non-limiting examples thereof, a silicon wafer, quartz, a glass plate, a metal plate, a plastic film, a sheet, and the like may be used.

[0066] The organic electroluminescence device of the present invention as described above may be manufactured by a method publicly known in the art, and in this case, the light-emitting layer included in the organic material layer may be manufactured by a vacuum deposition method or a solution application method. Here, examples of the solution application method include spin coating, dip coating, doctor blading, inkjet printing, or a thermal transfer method, but are not limited thereto.

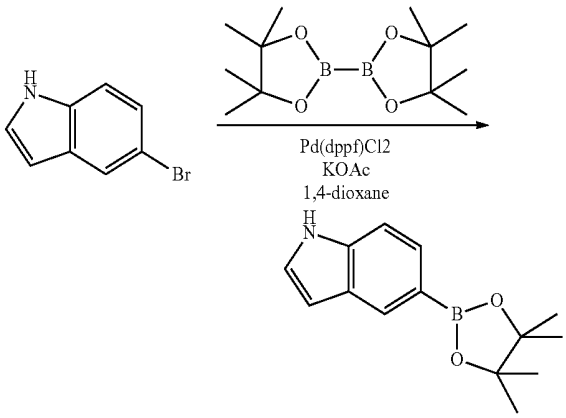
[0067] Hereinafter, the present invention will be described in detail as follows through Examples. However, the following Examples are only for exemplifying the present invention, and the present invention is not limited by the following Examples.

Preparation Example 1

Synthesis of IC-1

<Step 1> Synthesis of 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0068]

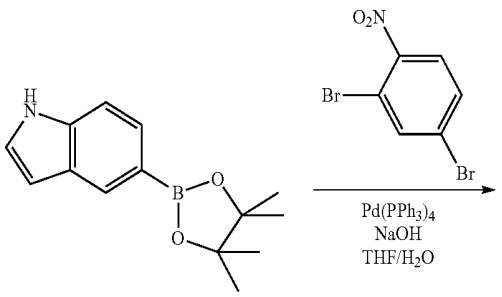


[0069] 5-bromo-1H-indole (25 g, 0.128 mol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (48.58 g, 0.191 mol), $Pd(dppf)Cl_2$ (5.2 g, 5 mol %), KOAc (37.55 g, 0.383 mol), and 1,4-dioxane (500 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 130° C. for 12 hours.

[0070] After the reaction was terminated, 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole (22.32 g, yield 72%) was obtained by performing extraction with ethyl acetate, removing moisture over $MgSO_4$, and refinement was performed by column chromatography (Hexane:EA=10:1 (v/v)).

<Step 2> Synthesis of 5-(5-bromo-2-nitrophenyl)-1H-indole

[0071]



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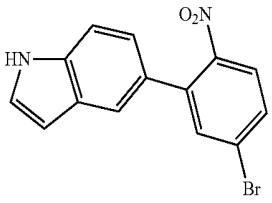
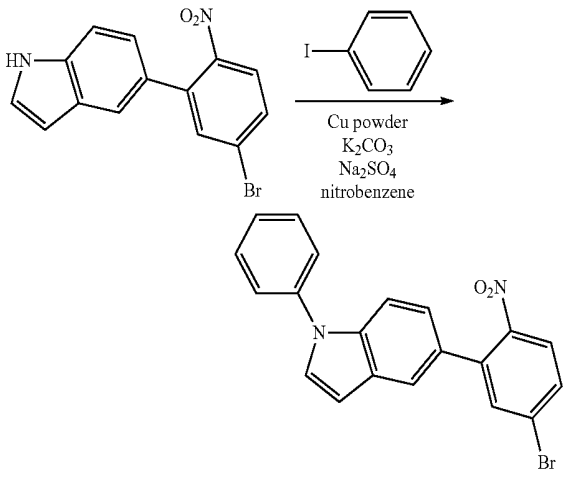


[0072] 2,4-dibromo-1-nitrobenzene (21.18 g, 75.41 mmol), the product (22 g, 90.49 mmol) in <Step 1>, NaOH (9.05 g, 226.24 mmol), and THF/H_2O (400 ml/200 ml) were mixed under nitrogen flow, $Pd(PPh_3)_4$ (4.36 g, 5 mol %) was added thereto at 40° C., and the resulting mixture was stirred at 80° C. for 12 hours.

[0073] After the reaction was terminated, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 5-(5-bromo-2-nitrophenyl)-1H-indole (9.6 g, yield 40%) was obtained by removing the solvent from the obtained organic layer, and refinement was performed by column chromatography (Hexane:EA=3:1 (v/v)).

<Step 3> Synthesis of 5-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole

[0074]

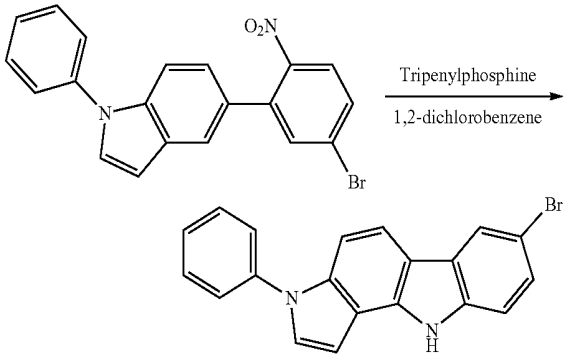


[0075] The product (14.64 g, 46.17 mmol) in <Step 2>, iodobenzene (14.13 g, 69.26 mmol), Cu powder (0.29 g, 4.62 mmol), K_2CO_3 (6.38 g, 46.17 mmol), Na_2SO_4 (6.56 g, 46.17 mmol), and nitrobenzene (200 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 190° C. for 12 hours.

[0076] After the reaction was terminated, nitrobenzene was removed, the organic layer was separated by methylene chloride, and water was removed by using $MgSO_4$. 545-bromo-2-nitrophenyl)-1-phenyl-1H-indole (12.89 g, yield 71%) was obtained by removing the solvent from the organic layer which water had been removed, and refinement was performed by column chromatography (Hexane:MC=3:1 (v/v)).

<Step 4> Synthesis of 7-bromo-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole

[0077]

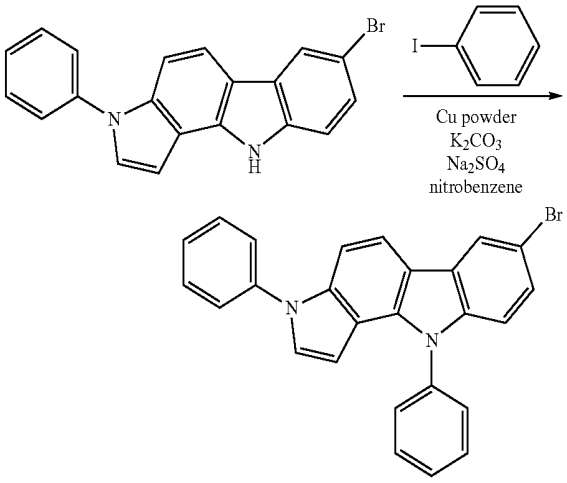


[0078] The product (6.25 g, 15.91 mmol) in <Step 3>, triphenylphosphine (10.43 g, 39.77 mmol), and 1,2-dichlorobenzene (50 ml) were mixed under nitrogen flow, and the resulting mixture was stirred for 12 hours.

[0079] After the reaction was terminated, 1,2-dichlorobenzene was removed, and extraction was performed with dichloromethane. 7-bromo-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole (3.04 g, yield 53%) was obtained by removing water from the obtained organic layer over $MgSO_4$, and refinement was performed by column chromatography (Hexane:MC=3:1 (v/v)).

<Step 5> Synthesis of 7-bromo-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole

[0080]



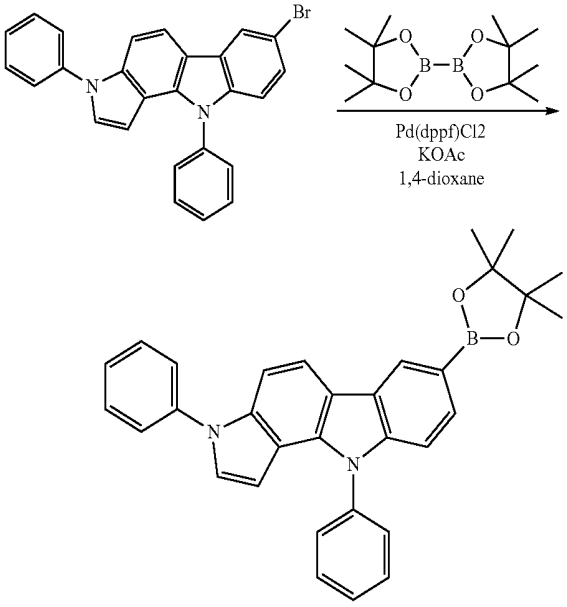
[0081] The product (5 g, 13.84 mmol) in <Step 4>, iodobenzene (4.24 g, 20.76 mmol), Cu powder (0.09 g, 1.38 mmol), K_2CO_3 (1.91 g, 13.84 mmol), Na_2SO_4 (1.97 g, 13.84 mmol), and nitrobenzene (70 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 190° C. for 12 hours.

[0082] After the reaction was terminated, nitrobenzene was removed, the organic layer was separated by methylene chloride, and water was removed by using $MgSO_4$. 7-bromo-3,

10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole (3.63 g, yield 60%) was obtained by removing the solvent from the organic layer which water had been removed, and refinement was performed by column chromatography (Hexane: MC=3:1 (v/v)).

<Step 6> Synthesis of IC-1

[0083]



[0084] The product (10 g, 22.93 mmol) in <Step 5>, 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (7 g, 27.52 mmol), $Pd(dppf)Cl_2$ (0.8 g, 5 mol %), KOAc (6.75 g, 68.79 mmol), and 1,4-dioxane (250 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 130° C. for 12 hours.

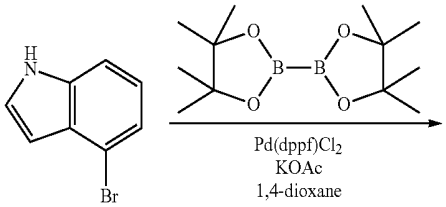
[0085] After the reaction was terminated, IC-1 (7.77 g, yield 70%) was obtained by performing extraction with ethyl acetate, removing moisture over $MgSO_4$, and refinement was performed by column chromatography (Hexane:EA=10:1 (v/v)).

Preparation Example 2

Synthesis of IC-2

<Step 1> Synthesis of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0086]



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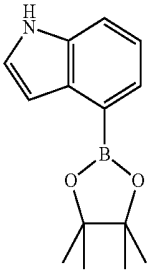
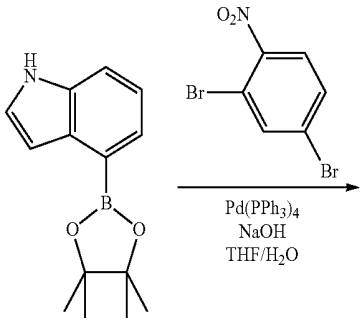
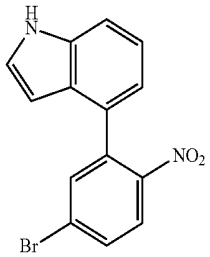


<Step 2> Synthesis of 4-(5-bromo-2-nitrophenyl)-1H-indole

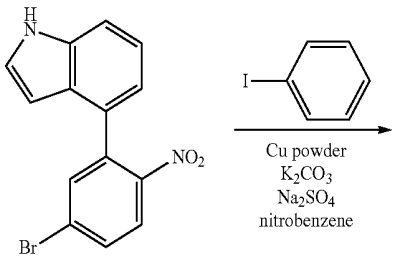
[0087]





<Step 3> Synthesis of 4-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole

[0088]



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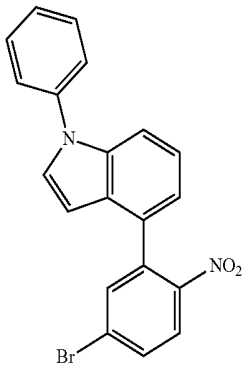
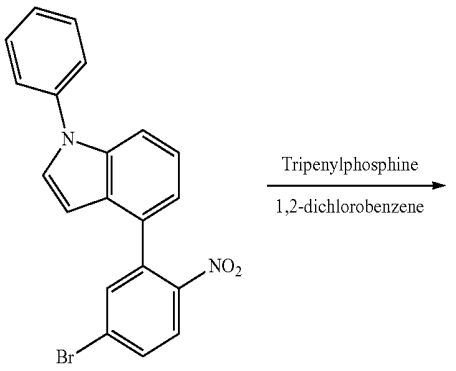
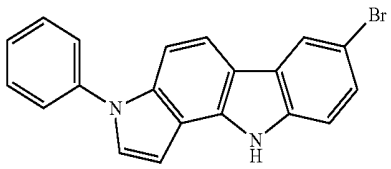


<Step 4> Synthesis of 7-bromo-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole

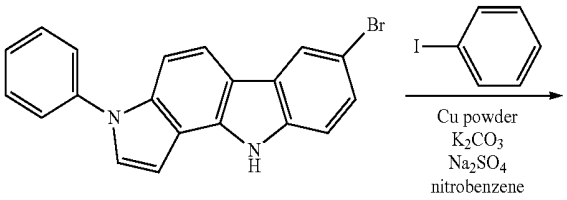
[0089]





<Step 5> Synthesis of 3,6-diphenyl-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,6-dihydropyrrolo[2,3-c]carbazole

[0090]



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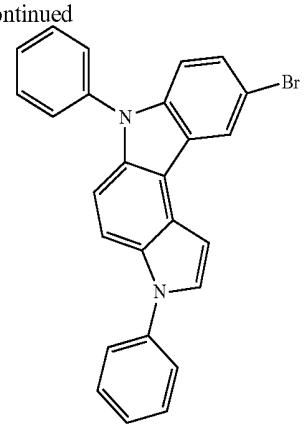
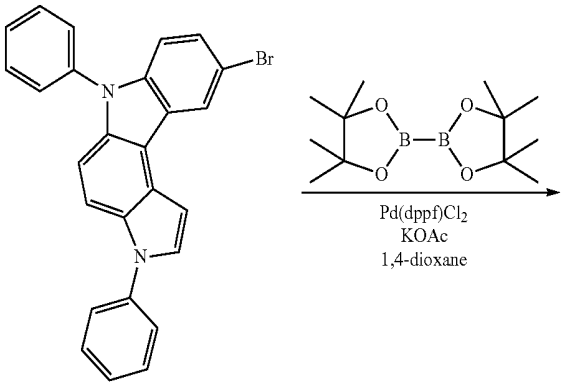
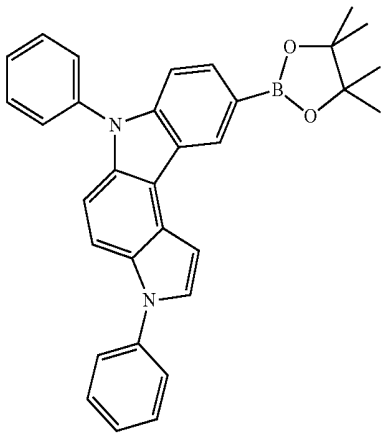


<Step 6> Synthesis of IC-2

[0091]





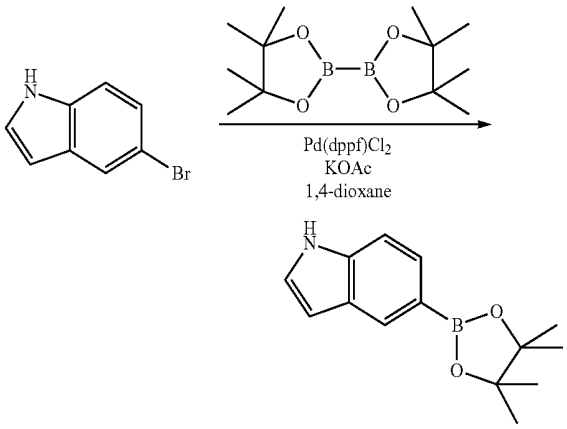
[0092] IC-2 was obtained by performing the same procedure as in Preparation Example 1, except that 4-bromo-1H-indole was used instead of 5-bromo-1H-indole.

Preparation Example 3

Synthesis of IC-3

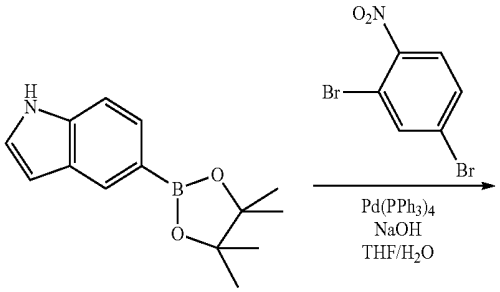
<Step 1> Synthesis of 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0093]



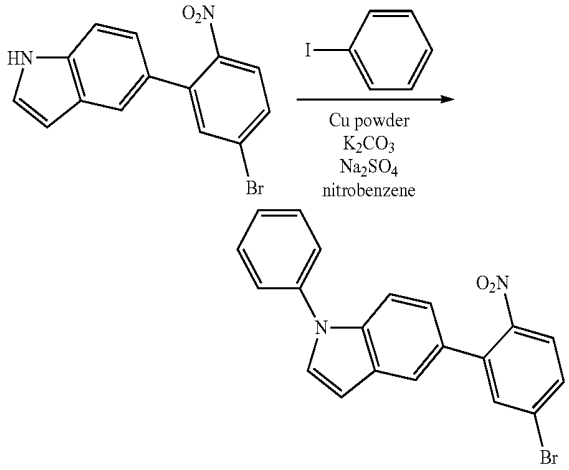
<Step 2> Synthesis of 5-(5-bromo-2-nitrophenyl)-1H-indole

[0094]



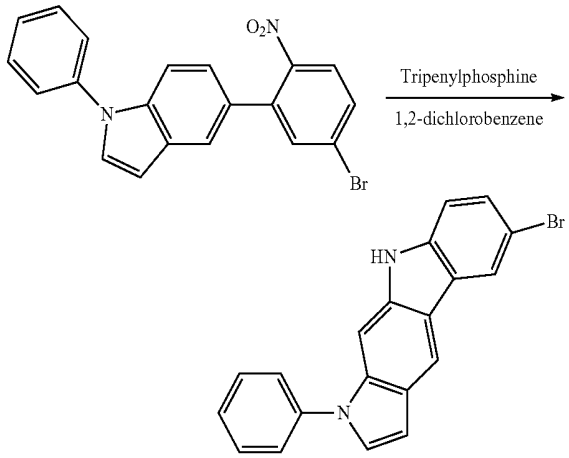
<Step 3> Synthesis of 5-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole

[0095]



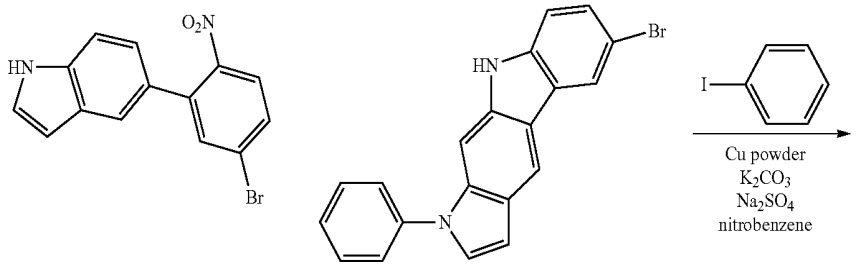
<Step 4> Synthesis of 6-bromo-1-phenyl-1,9-dihydropyrrolo[2,3-b]carbazole

[0096]



<Step 5> Synthesis of 6-bromo-1,9-diphenyl-1,9-dihydropyrrolo[2,3-b]carbazole

[0097]



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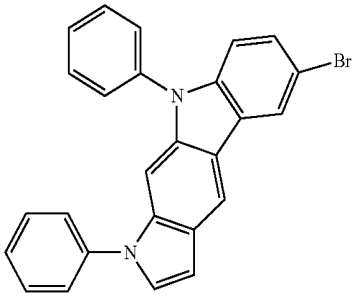
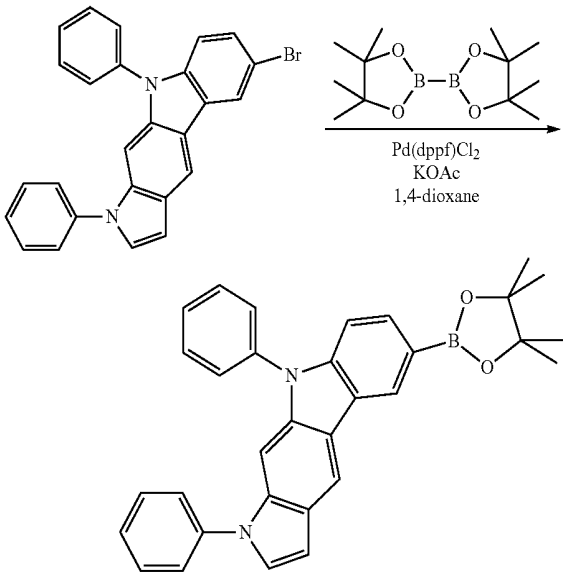


<Step 6> Synthesis of IC-3

[0098]



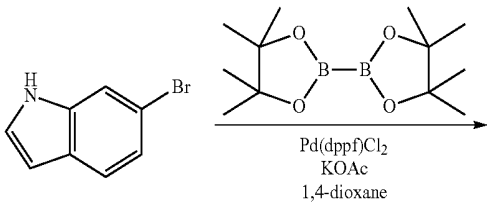
[0099] IC-3 was obtained by performing the same procedure as in Preparation Example 1, except that 7-bromo-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole which is an isomer produced together with the product in <Step 4> of Preparation Example 1 was used.

Preparation Example 4

Synthesis of IC-4

<Step 1> Synthesis of 6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0100]



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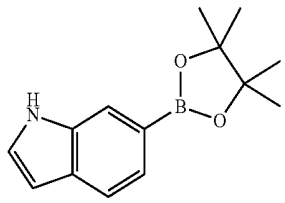
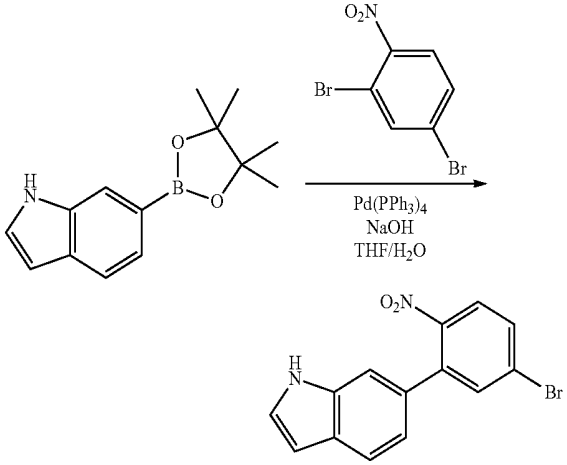


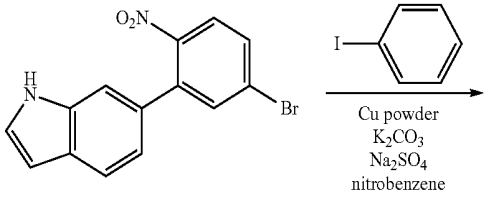
<Step 2> Synthesis of 6-(5-bromo-2-nitrophenyl)-1H-indole

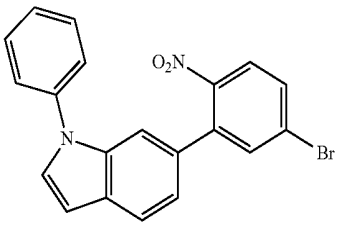
[0101]



<Step 3> Synthesis of 6-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole

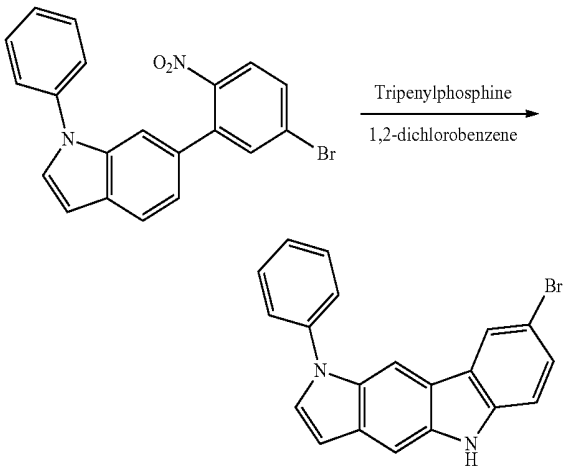
[0102]





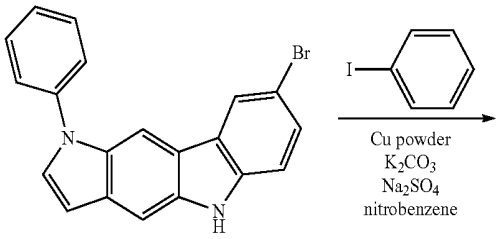
<Step 4> Synthesis of 8-bromo-1-phenyl-1,5-dihydropyrrolo[3,2-b]carbazole

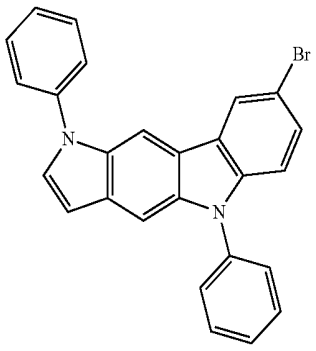
[0103]



<Step 5> Synthesis of 8-bromo-1,5-diphenyl-1,5-dihydropyrrolo[3,2-b]carbazole

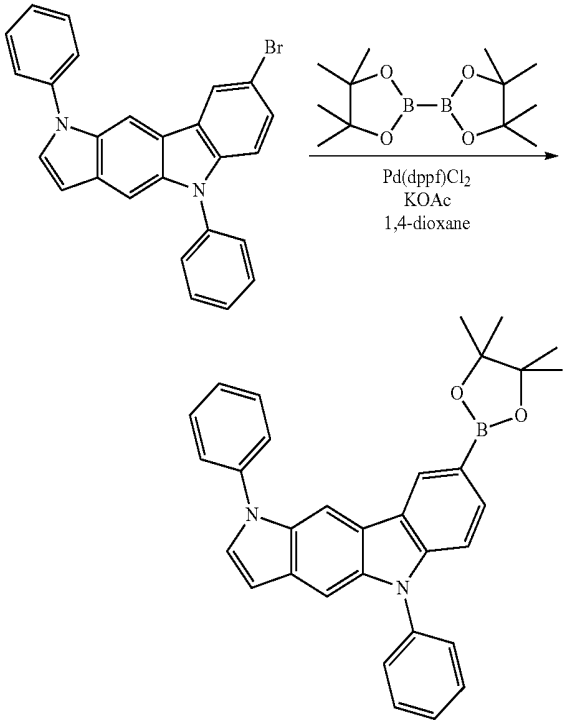
[0104]





<Step 6> Synthesis of IC-4

[0105]



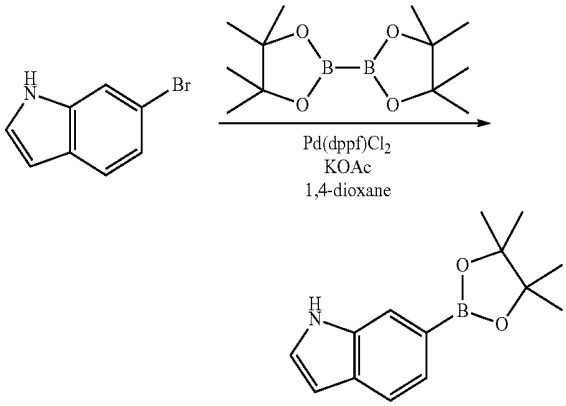
[0106] IC-4 was obtained by performing the same procedure as in Preparation Example 1, except that 6-bromo-1H-indole was used instead of 5-bromo-1H-indole, and 8-bromo-1-phenyl-1,5-dihydropyrrolo[3,2-b]carbazole of the two isomers produced in <Step 4> was used.

Preparation Example 5

Synthesis of IC-5

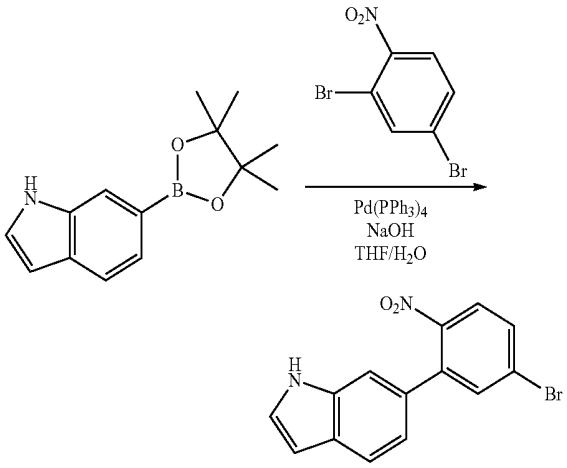
<Step 1> Synthesis of 6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0107]



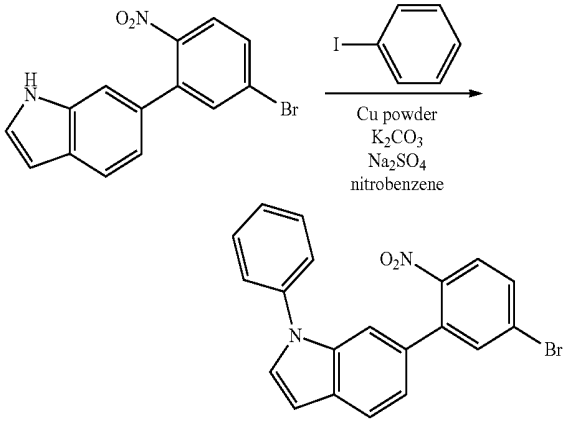
<Step 2> Synthesis of 6-(5-bromo-2-nitrophenyl)-1H-indole

[0108]



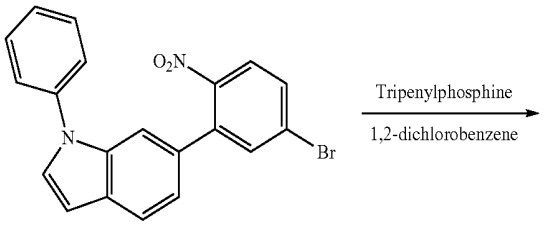
<Step 3> Synthesis of 6-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole

[0109]



<Step 4> Synthesis of 7-bromo-1-phenyl-1,10-dihydropyrrolo[2,3-a]carbazole

[0110]



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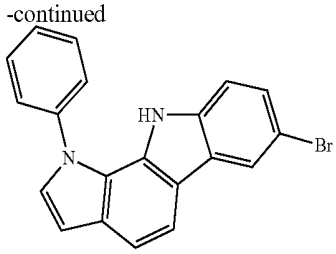
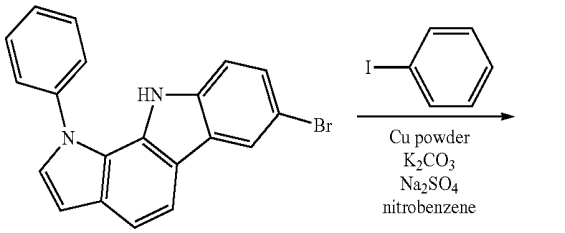


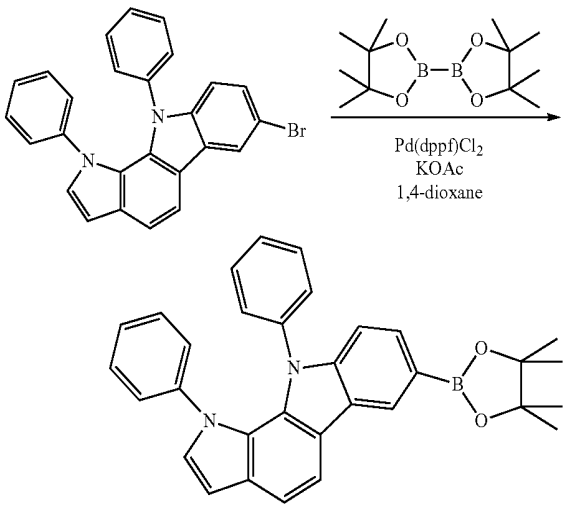
<Step 5> Synthesis of 7-bromo-1,10-diphenyl-1,10-dihydropyrrolo[2,3-a]carbazole

[0111]



<Step 6> Synthesis of IC-5

[0112]



[0113] IC-5 was obtained by performing the same procedure as in Preparation Example 1, except that 6-bromo-1H-indole was used instead of 5-bromo-1H-indole, and 7-bromo-

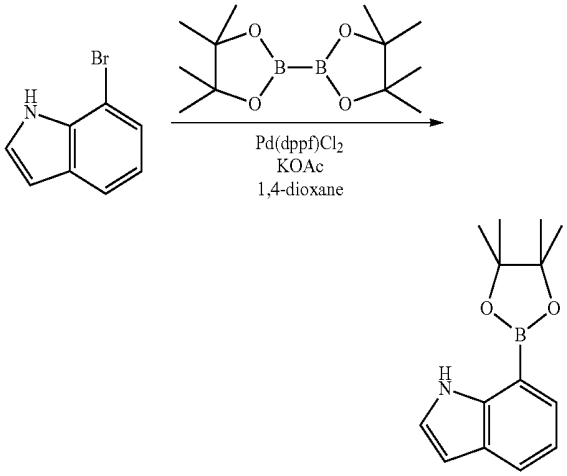
1-phenyl-1,10-dihydropyrrolo[2,3-a]carbazole of the two isomers produced in <Step 4> was used.

Preparation Example 6

Synthesis of IC-6

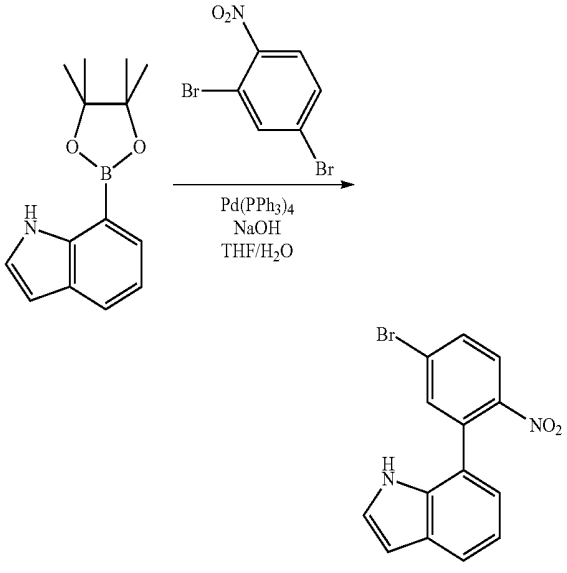
<Step 1> Synthesis of 7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0114]



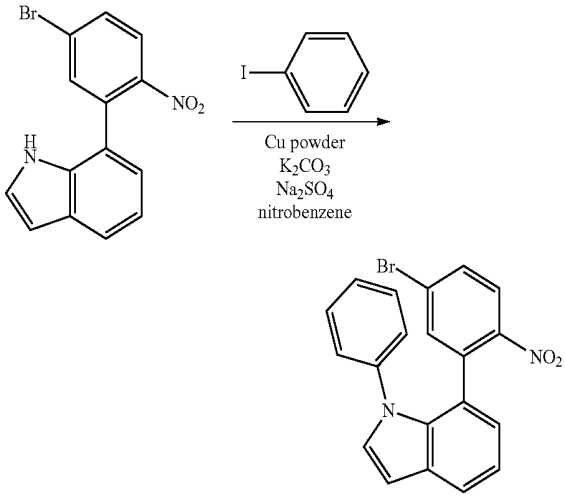
<Step 2> Synthesis of 7-(5-bromo-2-nitrophenyl)-1H-indole

[0115]



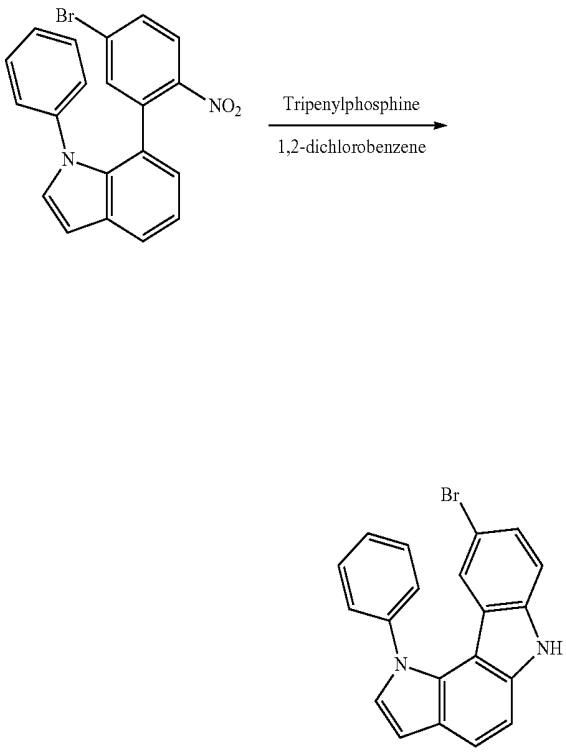
<Step 3> Synthesis of 7-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole

[0116]



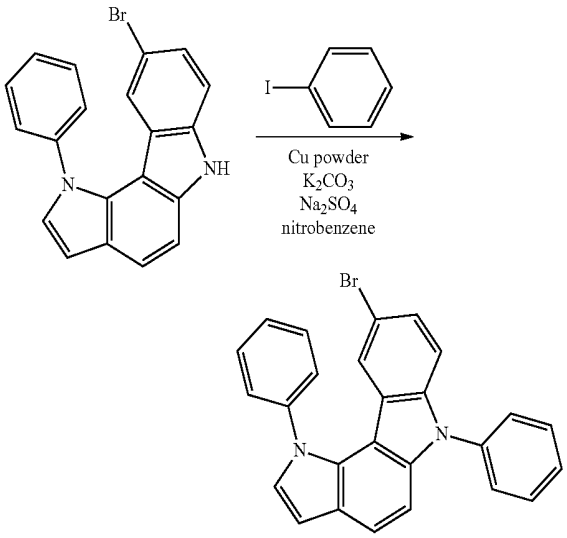
<Step 4> Synthesis of 9-bromo-1-phenyl-1,6-dihydropyrrolo[3,2-c]carbazole

[0117]



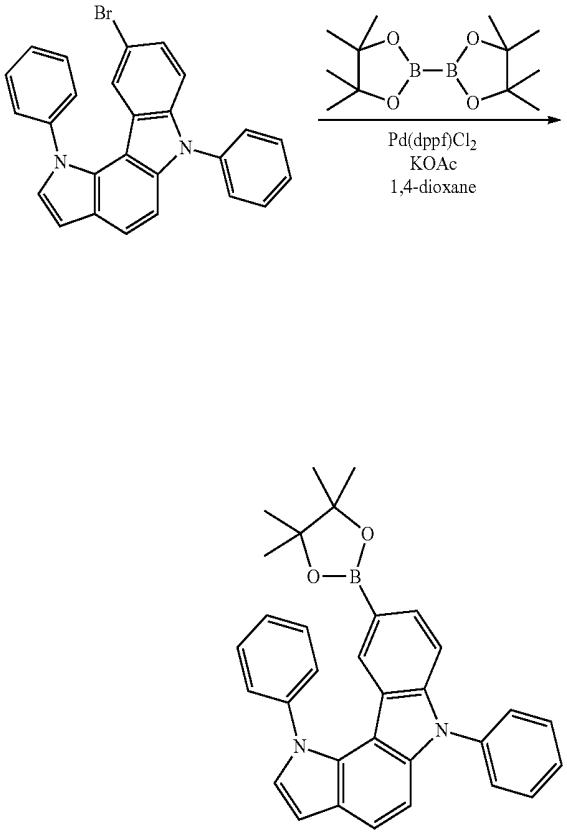
<Step 5> Synthesis of 9-bromo-1,6-diphenyl-1,6-dihydropyrrolo[3,2-c]carbazole

[0118]



<Step 6> Synthesis of IC-6

[0119]



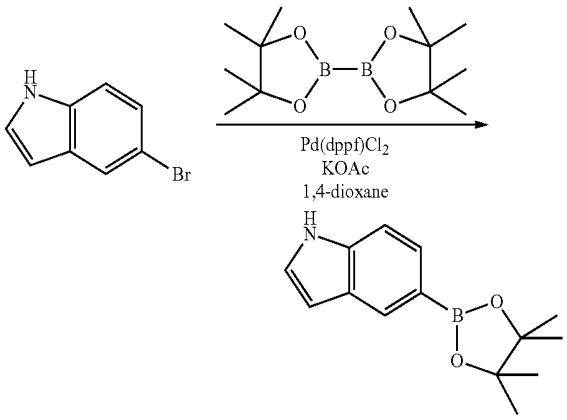
[0120] IC-6 was obtained by performing the same procedure as in Preparation Example 1, except that 7-bromo-1H-indole was used instead of 5-bromo-1H-indole.

Preparation Example 7

Synthesis of IC-7

<Step 1> Synthesis of 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

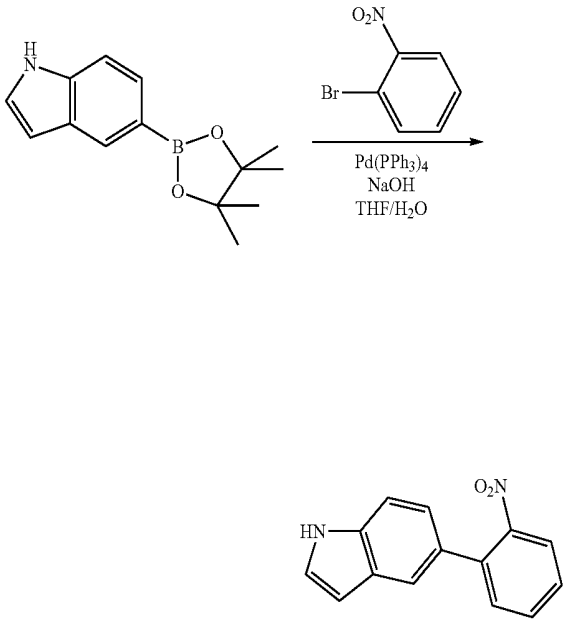
[0121]



[0122] 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole was obtained by performing the same procedure as in <Step 1> of Preparation Example 1.

<Step 2> Synthesis of 5-(2-nitrophenyl)-1H-indole

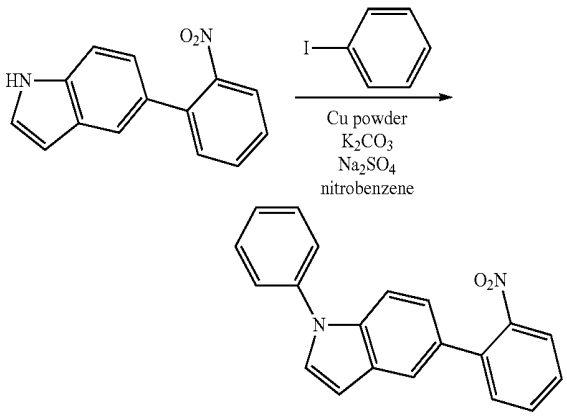
[0123]



[0124] 5-(2-nitrophenyl)-1H-indole was obtained by performing the same procedure as in <Step 2> of Preparation Example 1, except that 1-bromo-2-nitrobenzene was used instead of 2,4-dibromo-1-nitrobenzene.

<Step 3> Synthesis of 5-(2-nitrophenyl)-1-phenyl-1H-indole

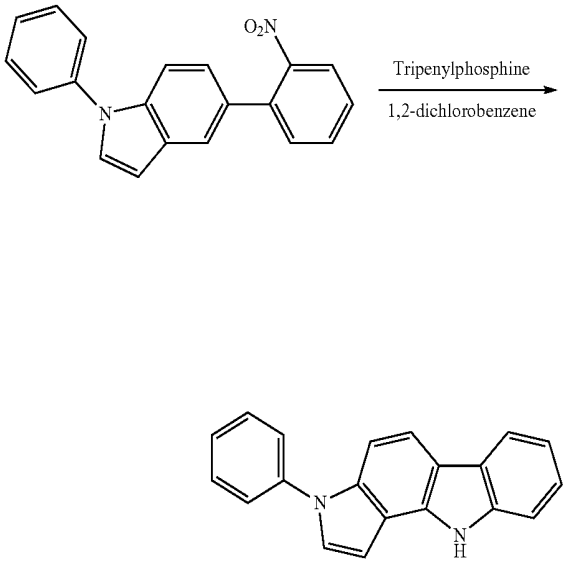
[0125]



[0126] 5-(2-nitrophenyl)-1-phenyl-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 1, except that 5-(2-nitrophenyl)-1H-indole was used instead of 5-(5-bromo-2-nitrophenyl)-1H-indole.

<Step 4> Synthesis of IC-7

[0127]



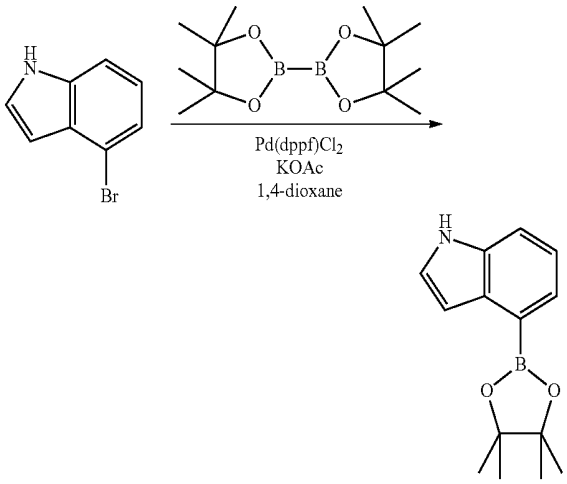
[0128] IC-7 was obtained by performing the same procedure as in <Step 4> of Preparation Example 1, except that the product in <Step 3> was used instead of 5-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole.

Preparation Example 8

Synthesis of IC-8

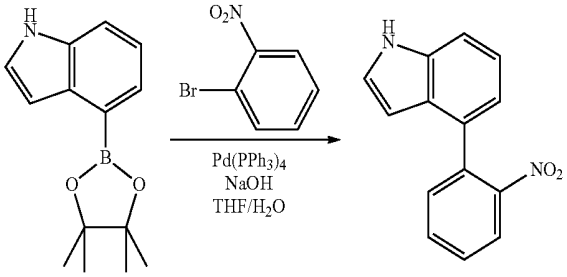
<Step 1> Synthesis of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0129]



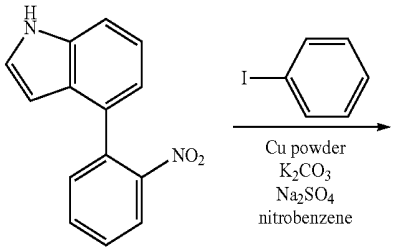
<Step 2> Synthesis of 4-(2-nitrophenyl)-1H-indole

[0130]



<Step 3> Synthesis of 4-(2-nitrophenyl)-1-phenyl-1H-indole

[0131]



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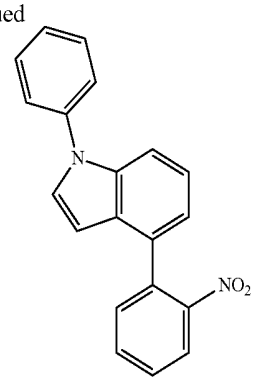
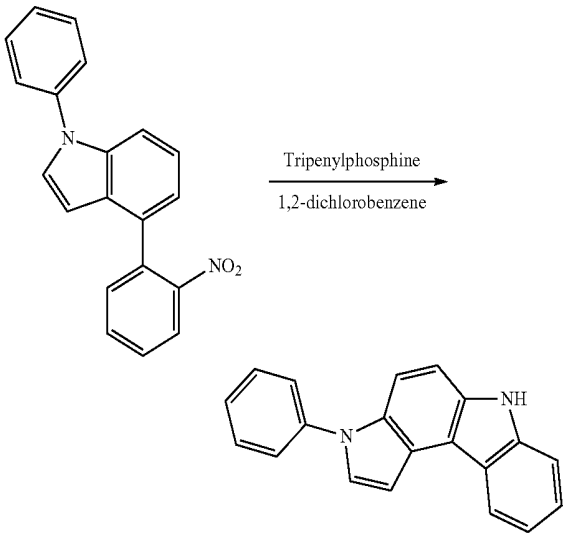


<Step 4> Synthesis of IC-8

[0132]



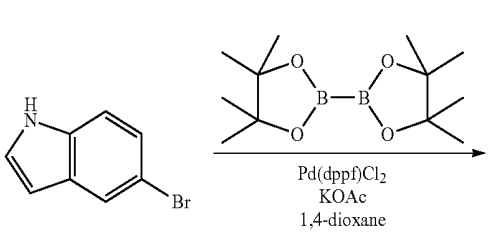
[0133] IC-8 was obtained by performing the same procedure as in Preparation Example 7, except that 4-bromo-1H-indole was used instead of 5-bromo-1H-indole.

Preparation Example 9

Synthesis of IC-9

<Step 1> Synthesis of 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0134]



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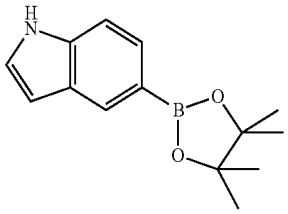
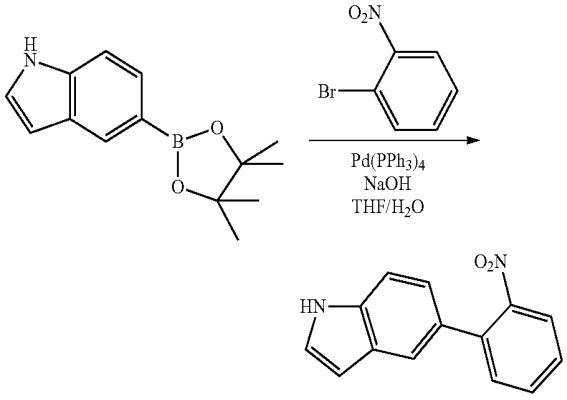


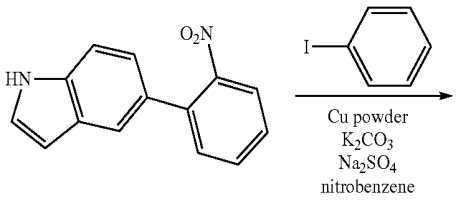
<Step 2> Synthesis of 5-(2-nitrophenyl)-1H-indole

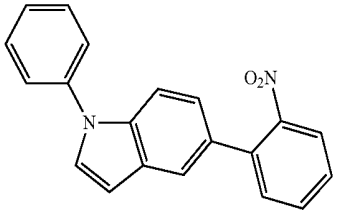
[0135]



<Step 3> Synthesis of 5-(2-nitrophenyl)-1-phenyl-1H-indole

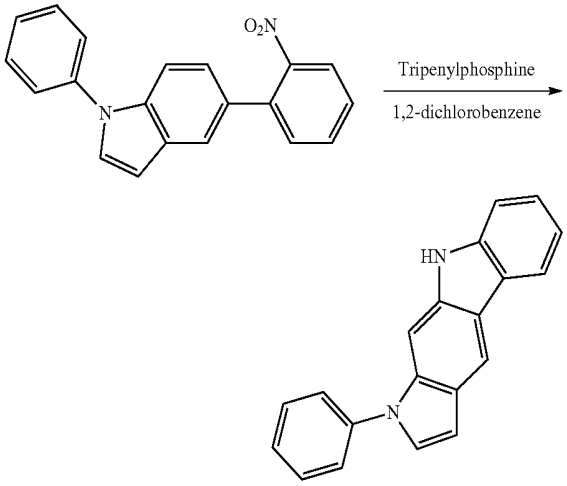
[0136]





<Step 4> Synthesis of IC-9

[0137]



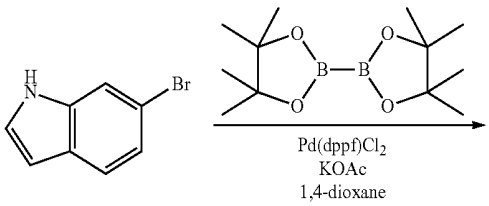
[0138] IC-9 which is the structural isomer of IC-7 was obtained by performing the same procedure as in Preparation Example 7.

Preparation Example 10

Synthesis of IC-10

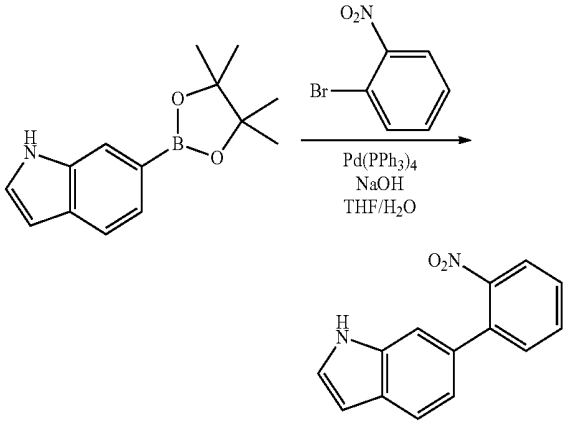
<Step 1> Synthesis of 6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0139]



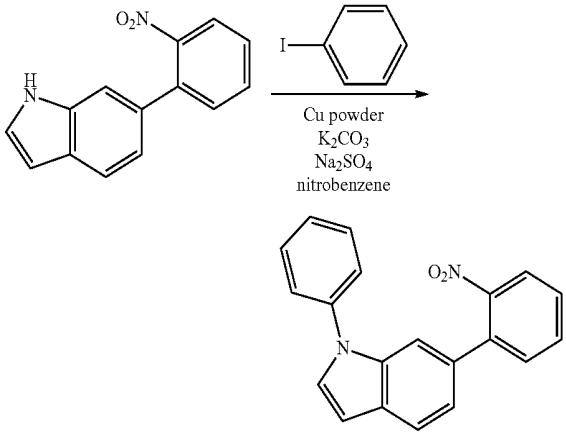
<Step 2> Synthesis of 6-(2-nitrophenyl)-1H-indole

[0140]



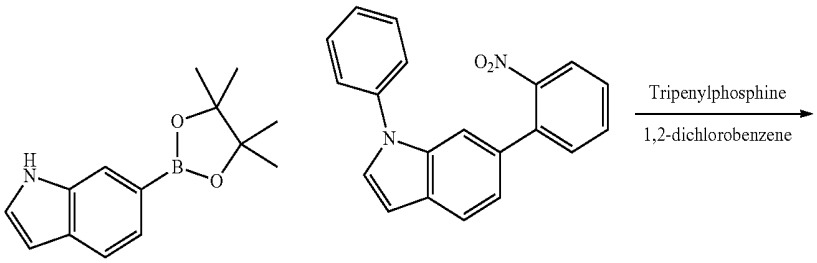
<Step 3> Synthesis of 6-(2-nitrophenyl)-1-phenyl-1H-indole

[0141]



<Step 4> Synthesis of IC-10

[0142]



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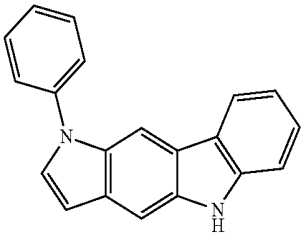


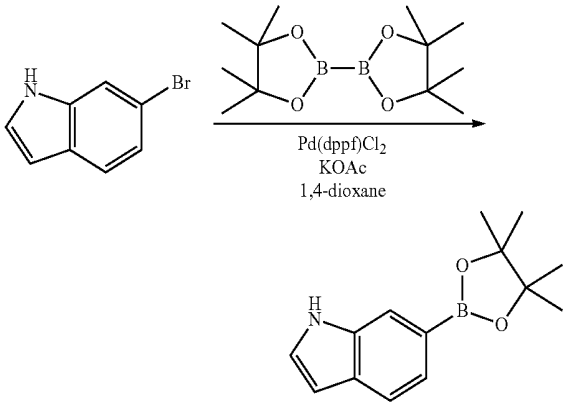
[0143] IC-10 was obtained by performing the same procedure as in Preparation Example 7, except that 6-bromo-1H-indole was used instead of 5-bromo-1H-indole.

Preparation Example 11

Synthesis of IC-11

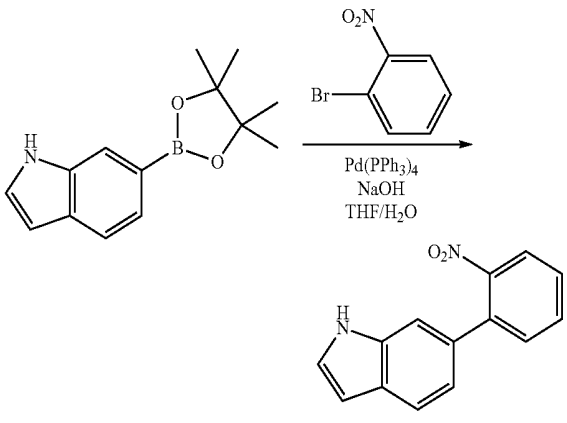
<Step 1> Synthesis of 6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0144]



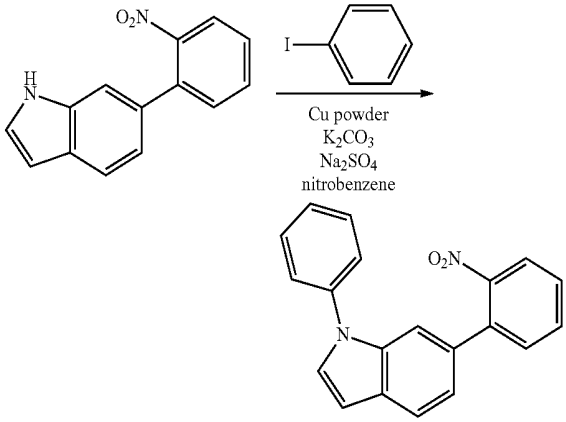
<Step 2> Synthesis of 6-(2-nitrophenyl)-1H-indole

[0145]



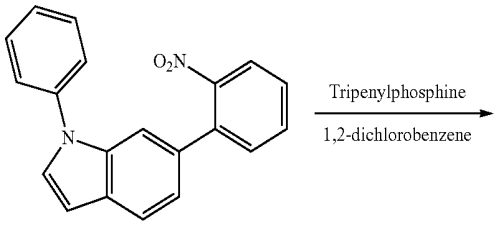
<Step 3> Synthesis of 6-(2-nitrophenyl)-1-phenyl-1H-indole

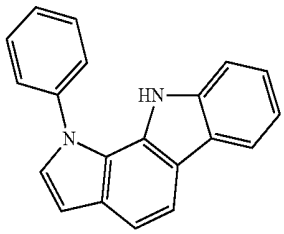
[0146]



<Step 4> Synthesis of IC-11

[0147]





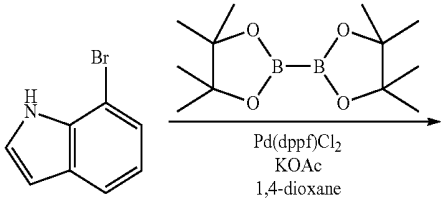
[0148] IC-11 which is the structural isomer of IC-10 was obtained by performing the same procedure as in Preparation Example 7, except that 6-bromo-1H-indole was used instead of 5-bromo-1H-indole.

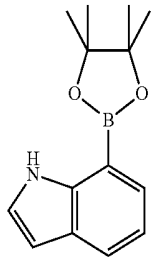
Preparation Example 12

Synthesis of IC-12

<Step 1> Synthesis of 7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

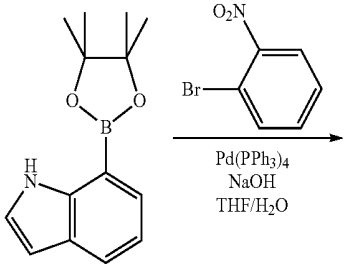
[0149]

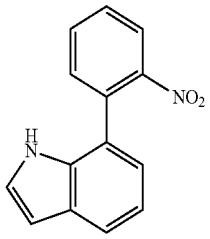




<Step 2> Synthesis of 7-(2-nitrophenyl)-1H-indole

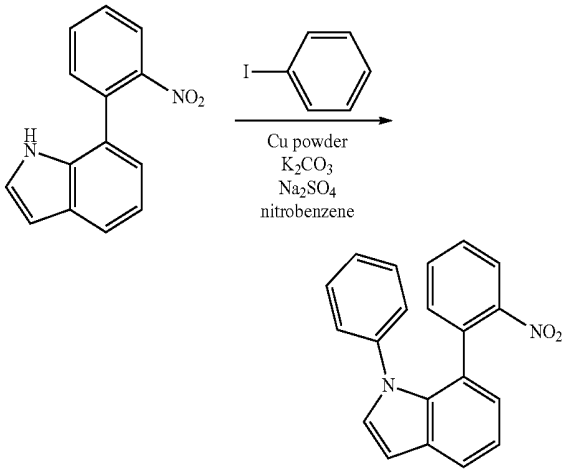
[0150]





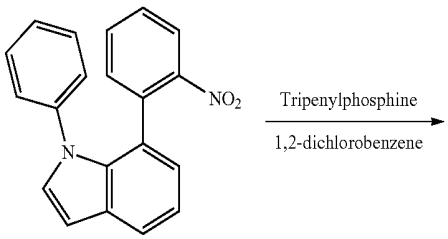
<Step 3> Synthesis of 7-(2-nitrophenyl)-1-phenyl-1H-indole

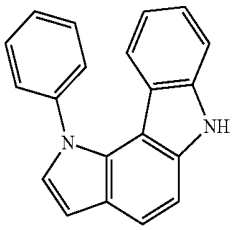
[0151]



<Step 4> Synthesis of IC-12

[0152]





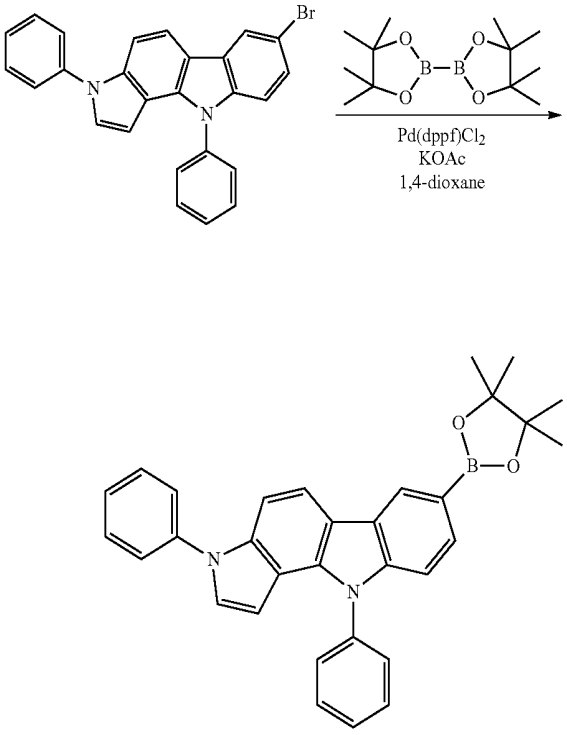
[0153] IC-12 was obtained by performing the same procedure as in Preparation Example 7, except that 7-bromo-1H-indole was used instead of 5-bromo-1H-indole.

Preparation Example 13

Synthesis of IC-13

<Step 1> Synthesis of 3,10-diphenyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole

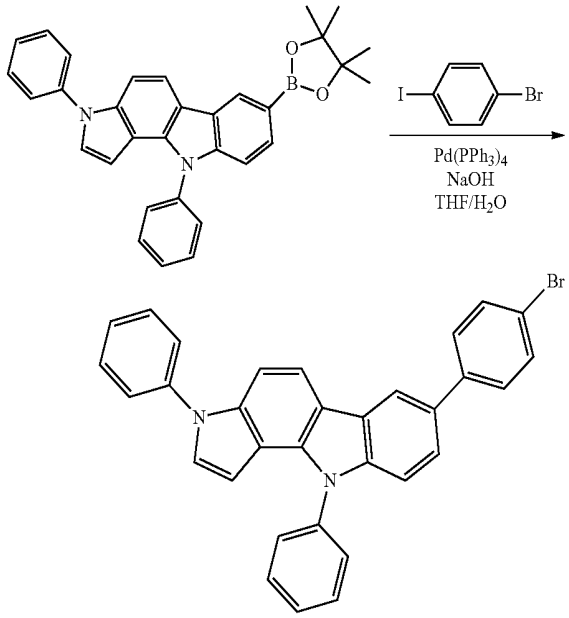
[0154]



[0155] 3,10-diphenyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole was obtained by performing the same procedure as in <Step 1> of Preparation Example 1, except that IC-1 was used instead of 5-bromo-1H-indole.

<Step 2> Synthesis of 7-(4-bromophenyl)-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole

[0156]

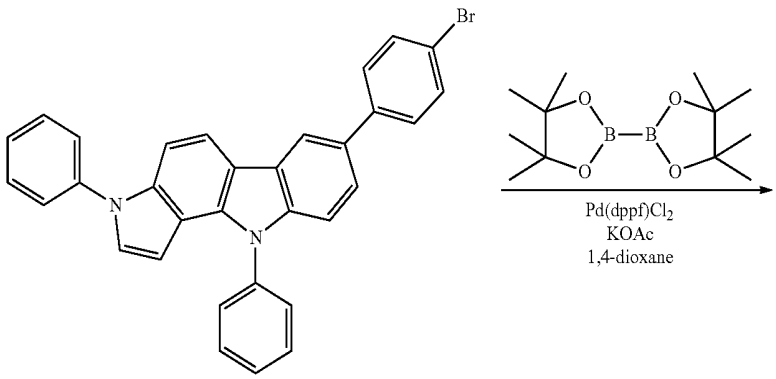


[0157] 1-bromo-4-iodobenzene (6.98 g, 24.78 mmol), the product (10 g, 20.65 mmol) in <Step 1>, NaOH (2.48 g, 61.95 mmol), and THF/H_2O (200 ml/30 ml) were mixed under nitrogen flow, $Pd(PPh_3)_4$ (0.72 g, 0.6195 mmol) was added thereto at 40° C., and the resulting mixture was stirred at 80° C. for 12 hours.

[0158] After the reaction was terminated, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 7-(4-bromophenyl)-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole (4.1 g, yield 40%) was obtained by removing the solvent from the obtained organic layer, and refinement was performed by recrystallization.

<Step 3> Synthesis of IC-13

[0159]



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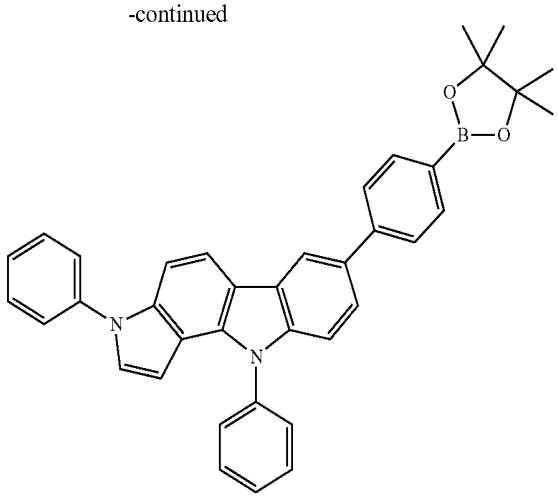


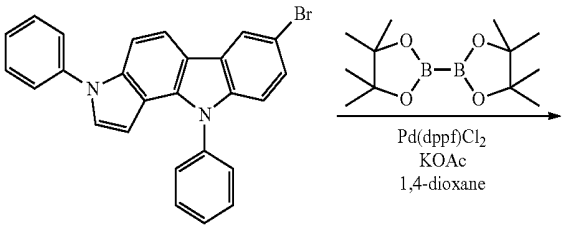
[0160] IC-13 was obtained by performing the same procedure as in <Step 1> of Preparation Example 1, except that 7-(4-bromophenyl)-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole was used instead of 5-bromo-1H-indole.

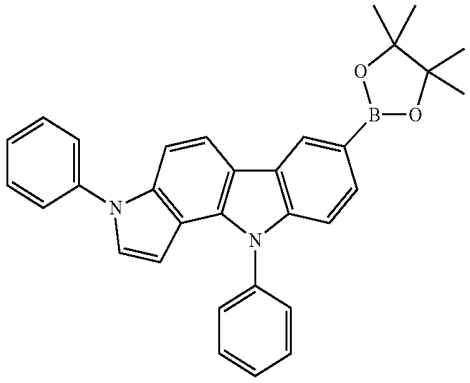
Preparation Example 14

Synthesis of IC-14

<Step 1> Synthesis of 3,10-diphenyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole

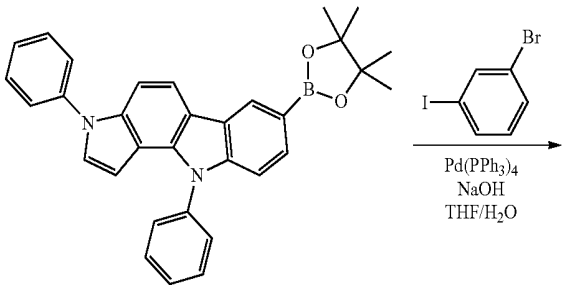
[0161]

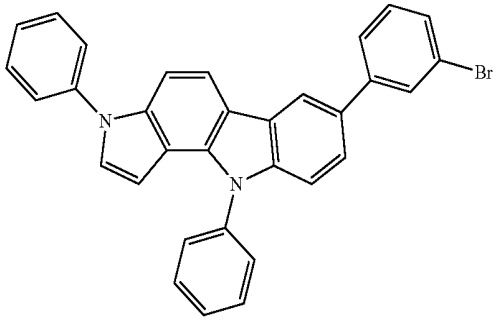




<Step 2> Synthesis of 7-(3-bromophenyl)-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole

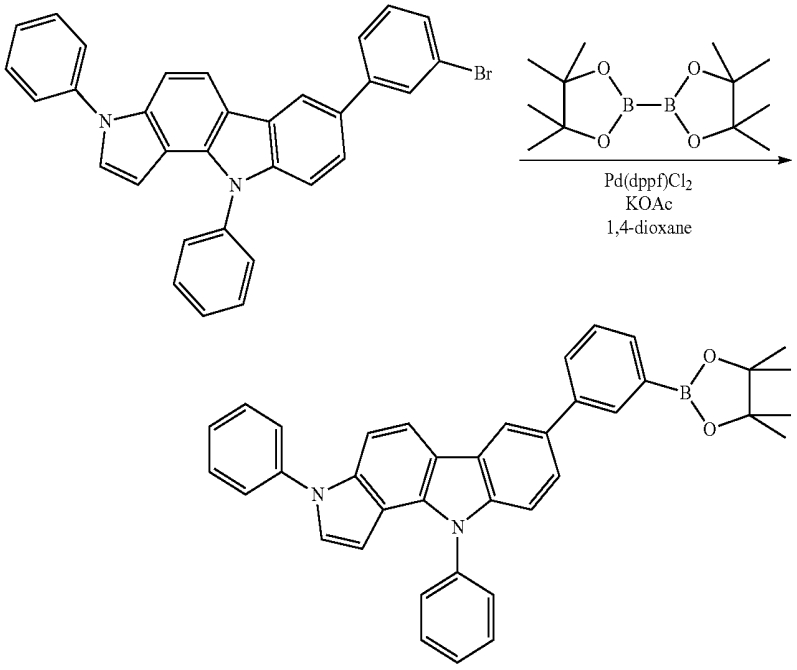
[0162]





<Step 3> Synthesis of IC-14

[0163]



[0164] IC-14 was obtained by performing the same procedure as in Preparation Example 13, except that 1-bromo-3-iodobenzene was used instead of 1-bromo-4-iodobenzene.

Preparation Example 15

Synthesis of IC-15

<Step 1> Synthesis of 3,10-diphenyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole

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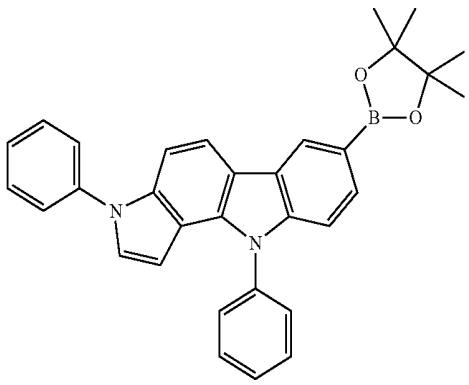
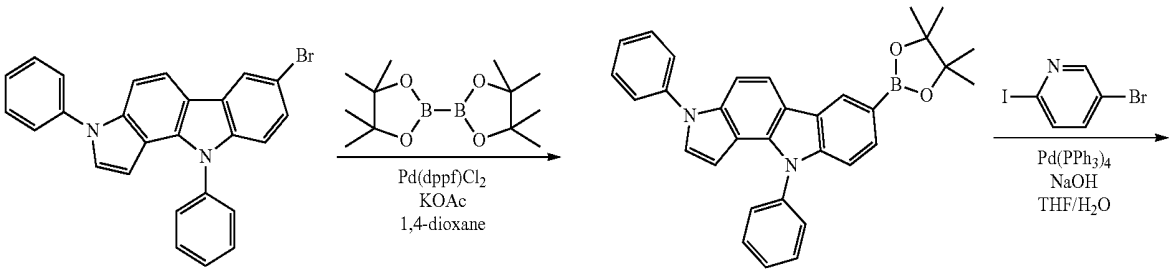


[0165]

<Step 2> Synthesis of 7-(5-bromopyridin-2-yl)-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole

[0166]



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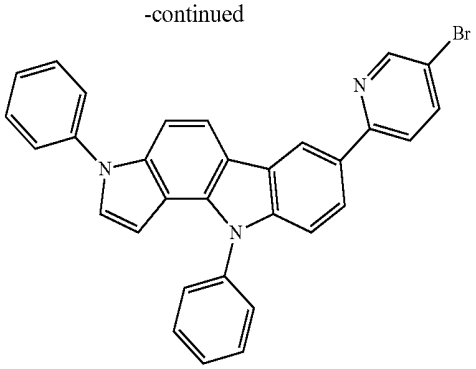
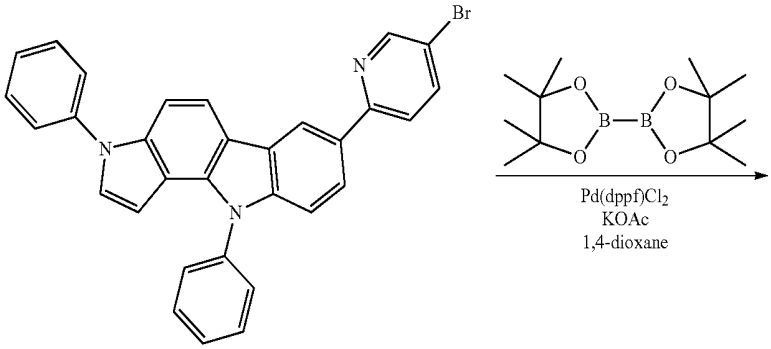
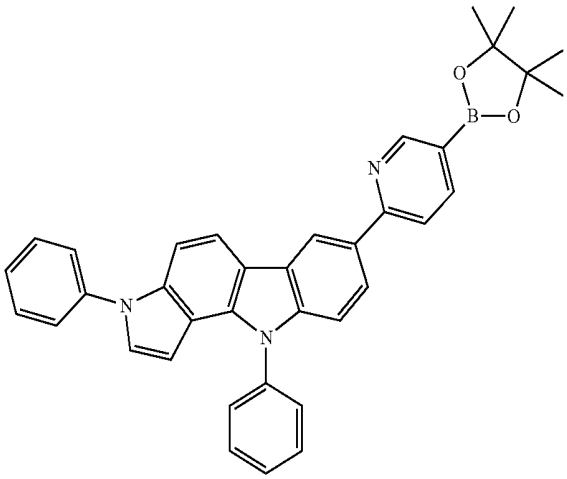


<Step 3> Synthesis of IC-15

[0167]





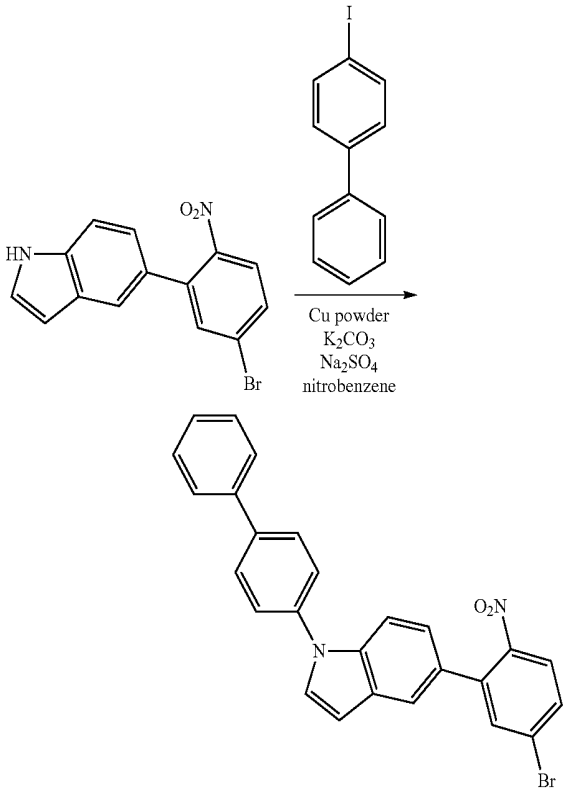
[0168] IC-15 was obtained by performing the same procedure as in Preparation Example 13, except that 5-bromo-2-iodopyridine was used instead of 1-bromo-4-iodobenzene.

Preparation Example 16

Synthesis of IC-16

<Step 1> Synthesis of 1-(biphenyl-4-yl)-5-(5-bromo-2-nitrophenyl)-1H-indole

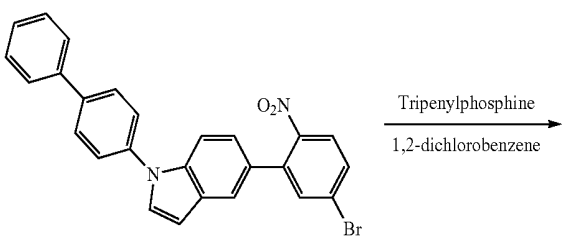
[0169]



[0170] 1-(biphenyl-4-yl)-5-(5-bromo-2-nitrophenyl)-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 1, except that 4-iodobiphenyl was used instead of iodobenzene.

<Step 2> Synthesis of 3-(biphenyl-4-yl)-7-bromo-3,10-dihydropyrrolo[3,2-a]carbazole

[0171]



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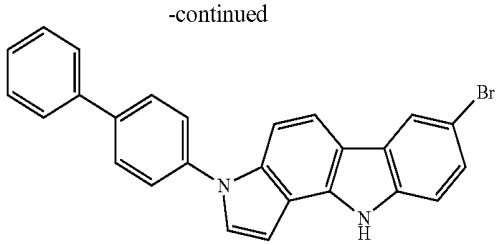
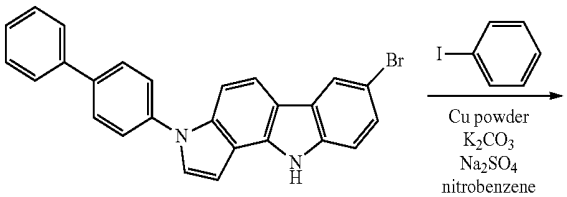
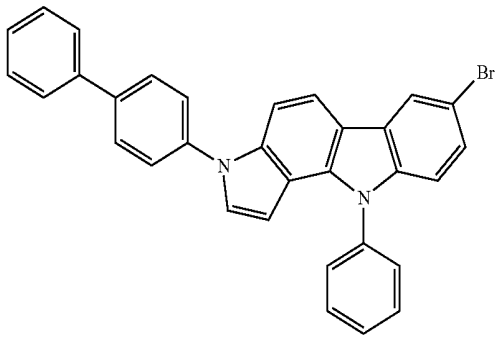


[0172] 3-(biphenyl-4-yl)-7-bromo-3,10-dihydropyrrolo[3,2-a]carbazole was obtained by performing the same procedure as in <Step 4> of Preparation Example 1, except that the product in <Step 1> was used instead of 5-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole.

<Step 3> Synthesis of 3-(biphenyl-4-yl)-7-bromo-10-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole

[0173]

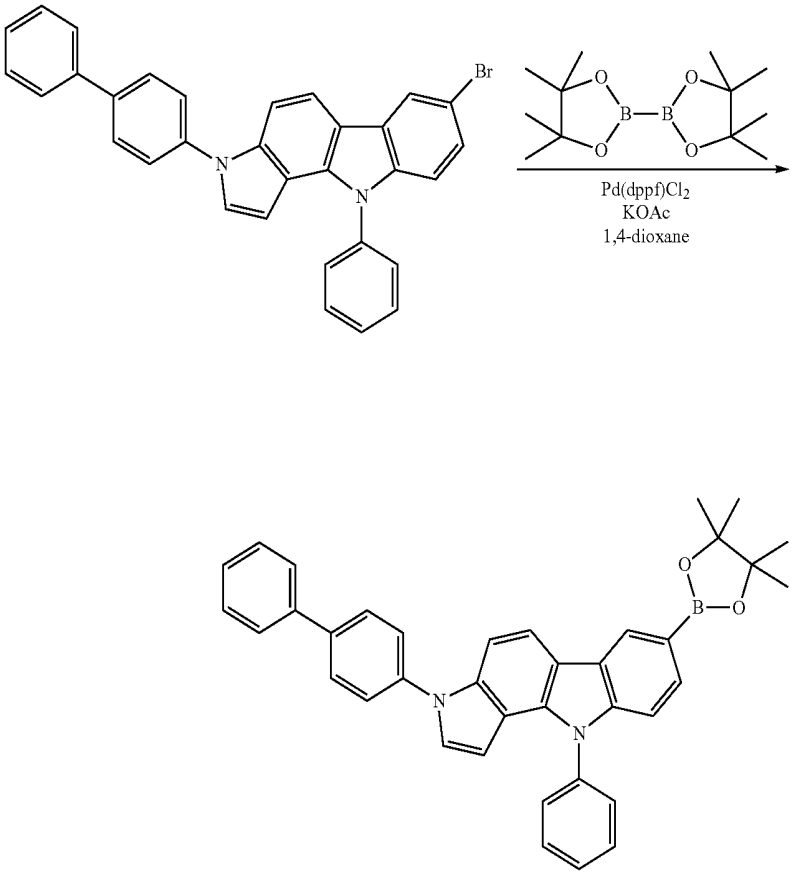




[0174] 3-(biphenyl-4-yl)-7-bromo-10-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole was obtained by performing the same procedure as in <Step 5> of Preparation Example 1, except that the product in <Step 2> was used instead of 7-bromo-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole.

<Step 4> Synthesis of IC-16

[0175]



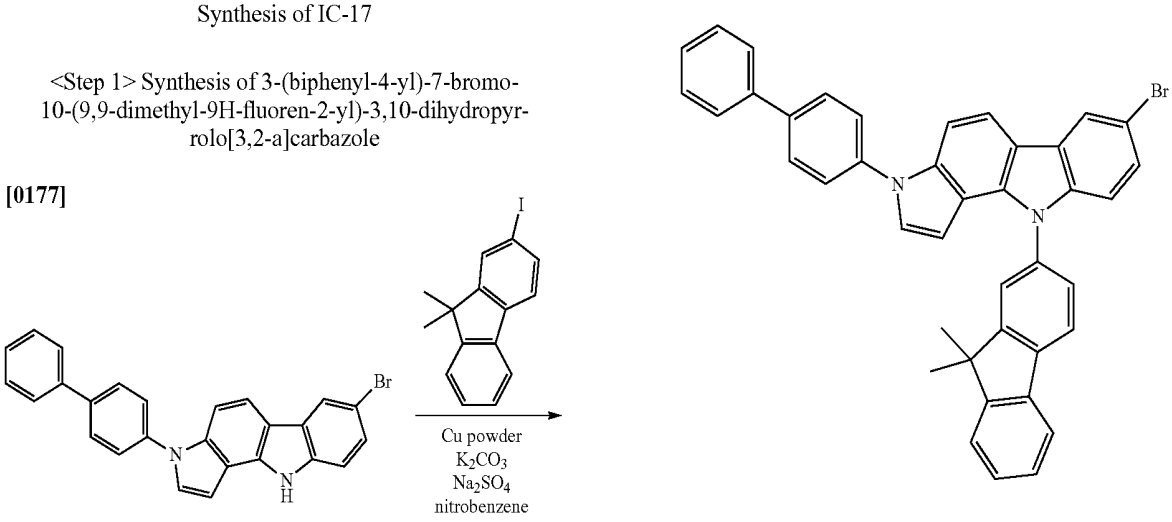
[0176] IC-16 was obtained by performing the same procedure as in <Step 6> of Preparation Example 1, except that the product in <Step 3> was used instead of 7-bromo-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole.

Preparation Example 17

Synthesis of IC-17

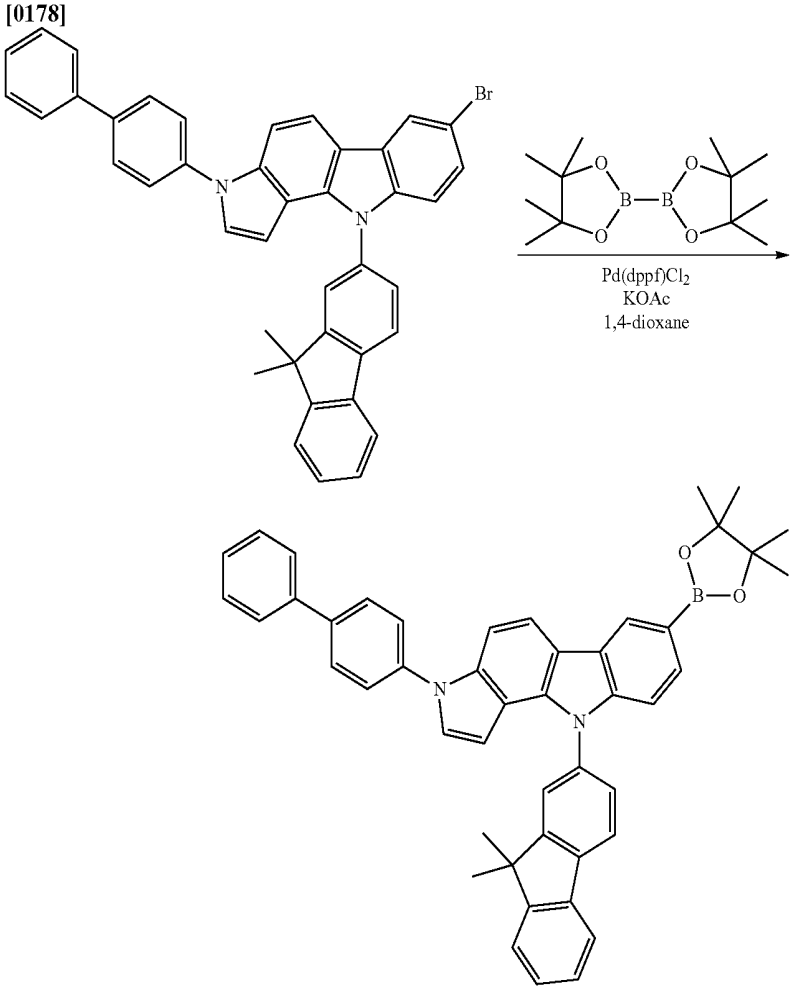
<Step 1> Synthesis of 3-(biphenyl-4-yl)-7-bromo-10-(9,9-dimethyl-9H-fluoren-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole

[0177]



<Step 2> Synthesis of IC-17

[0178]



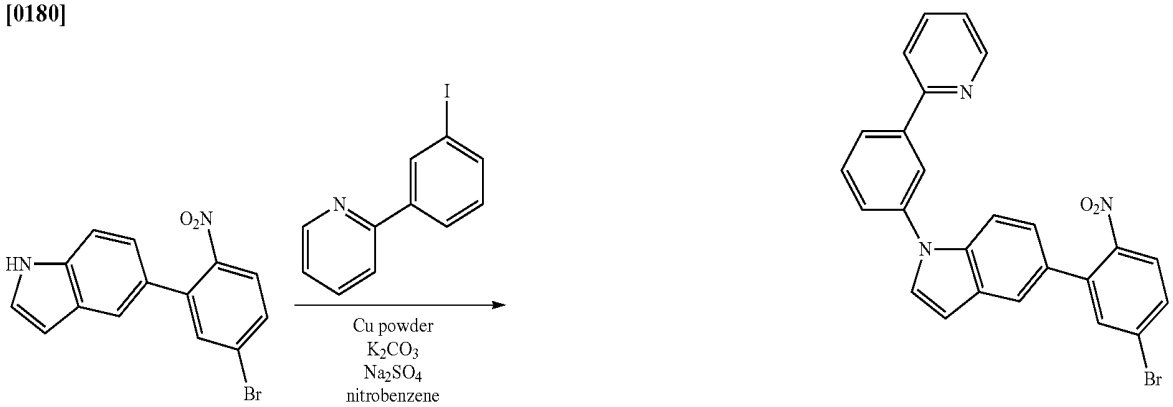
[0179] IC-17 was obtained by performing the same procedure as in Preparation Example 16, except that 2-iodo-9,9-dimethyl-9H-fluorene was used instead of iodobenzene.

Preparation Example 18

Synthesis of IC-18

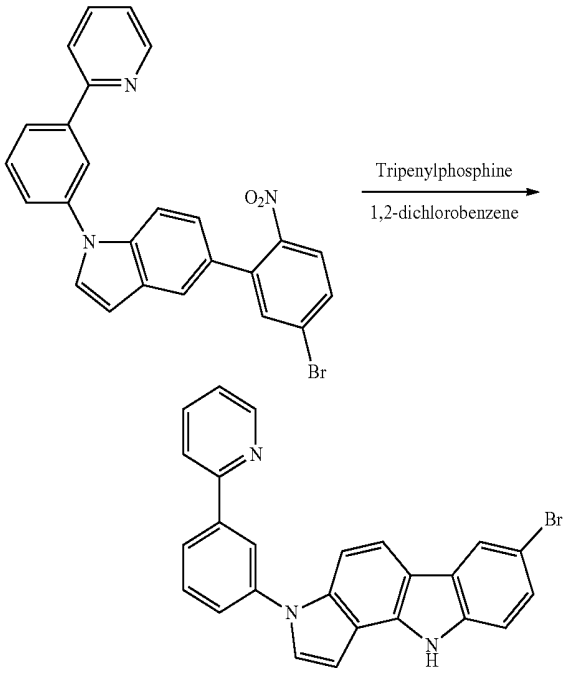
<Step 1> Synthesis of 5-(5-bromo-2-nitrophenyl)-1-(3-(pyridin-2-yl)phenyl)-1 H-indole

[0180]



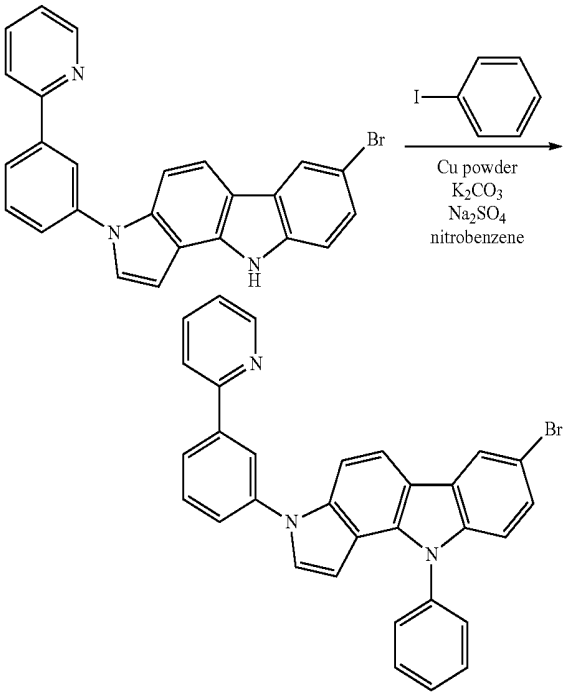
<Step 2> Synthesis of 7-bromo-3-(3-(pyridin-2-yl) phenyl)-3,10-dihydropyrrolo[3,2-a]carbazole

[0181]



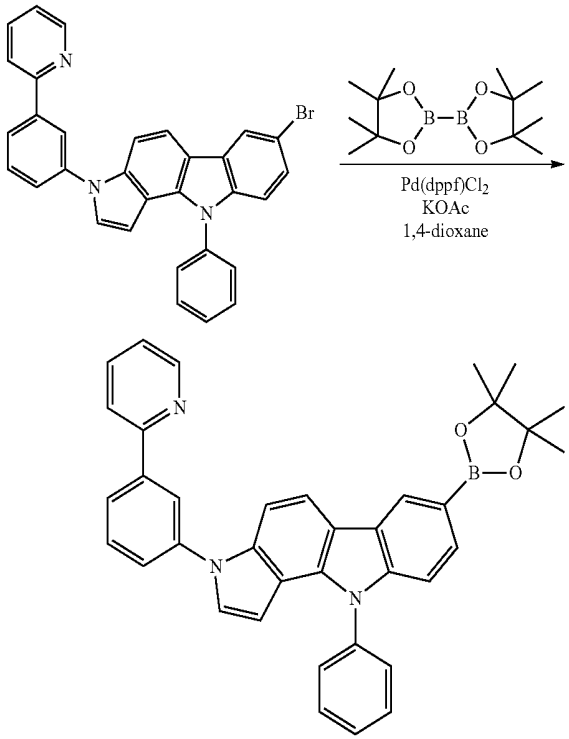
<Step 3> Synthesis of 7-bromo-10-phenyl-3-(3-(pyridin-2-yl)phenyl)-3,10-dihydropyrrolo[3,2-a]carbazole

[0182]



<Step 4> Synthesis of IC-18

[0183]



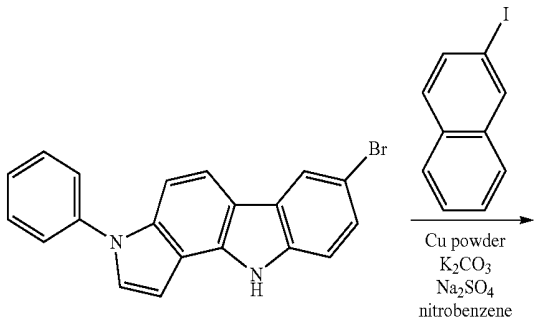
[0184] IC-18 was obtained by performing the same procedure as in Preparation Example 16, except that 2-(3-iodophenyl)pyridine was used instead of 4-iodobiphenyl.

Preparation Example 19

Synthesis of IC-19

<Step 1> Synthesis of 7-bromo-10-(naphthalen-2-yl)-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole

[0185]



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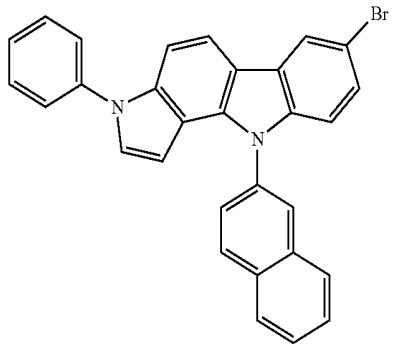
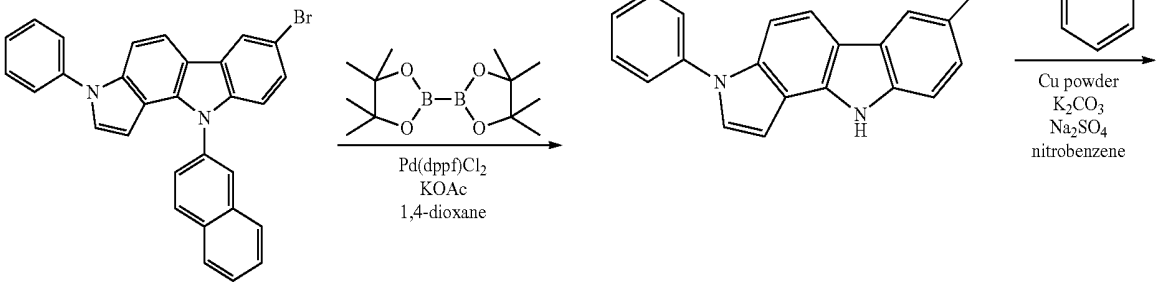
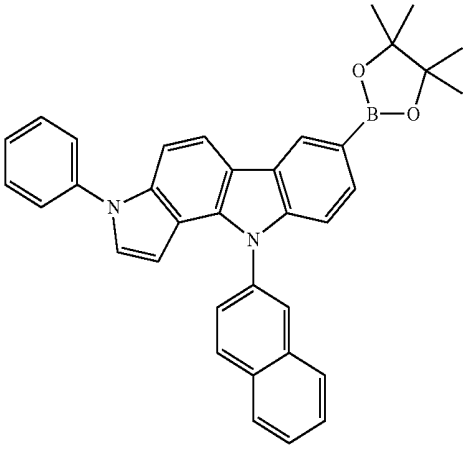
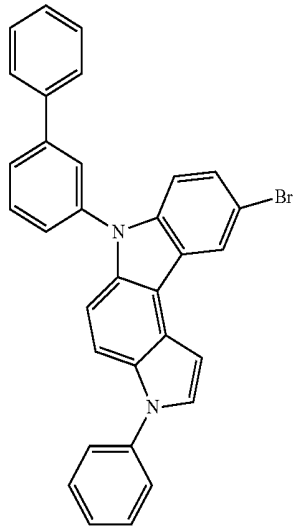


<Step 2> Synthesis of IC-19

[0186]







[0187] IC-19 was obtained by performing the same procedure as in Preparation Example 1, except that 2-iodonaphtalene was used instead of iodobenzene.

Preparation Example 20

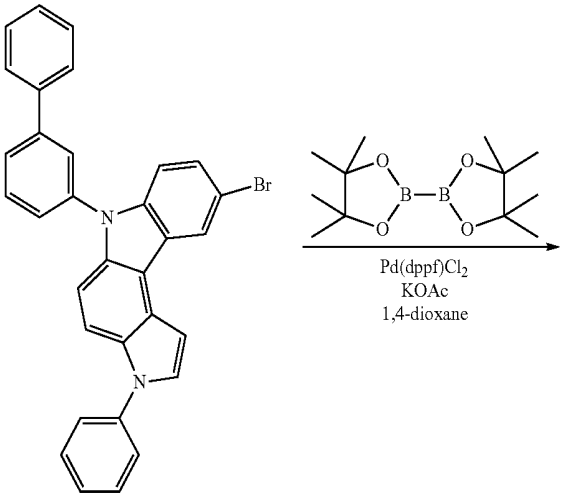
Synthesis of IC-20

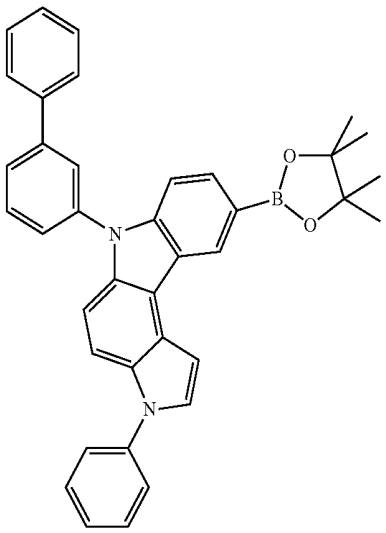
<Step 1> Synthesis of 6-(biphenyl-3-yl)-9-bromo-3-phenyl-3,6-dihydropyrrolo[2,3-c]carbazole

[0188]

<Step 2> Synthesis of IC-20

[0189]





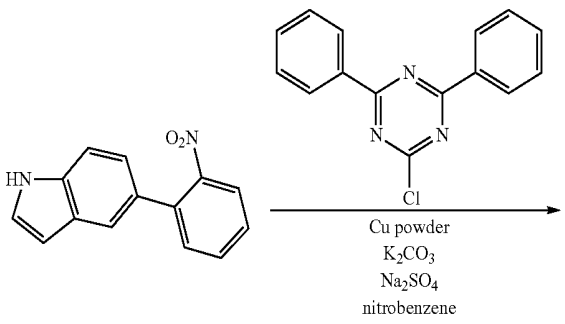
[0190] IC-20 was obtained by performing the same procedure as in Preparation Example 2, except that 3-iodobiphenyl was used instead of iodobenzene.

Preparation Example 21

Synthesis of IC-21

<Step 1> Synthesis of 1-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-(2-nitrophenyl)-1H-indole

[0191]



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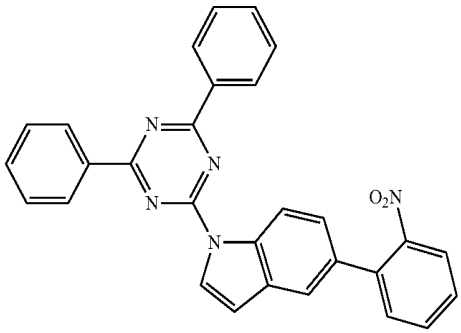
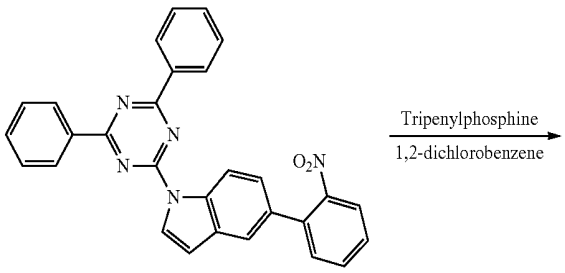
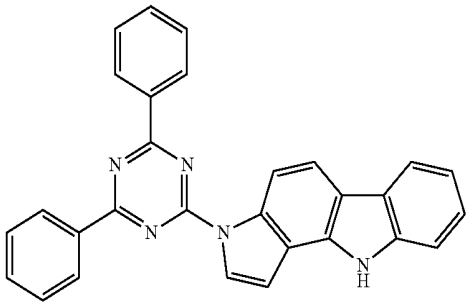


[0192] 1-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-(2-nitrophenyl)-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 7, except that 2-chloro-4,6-diphenyl-1,3,5-triazine was used instead of iodobenzene.

<Step 2> Synthesis of IC-21

[0193]





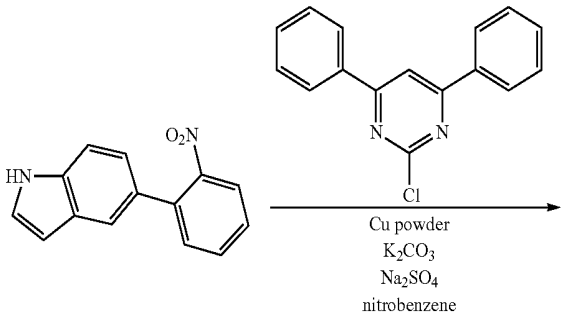
[0194] IC-21 was obtained by performing the same procedure as in <Step 4> of Preparation Example 7, except that the product in <Step 1> was used instead of 5-(2-nitrophenyl)-1-phenyl-1H-indole.

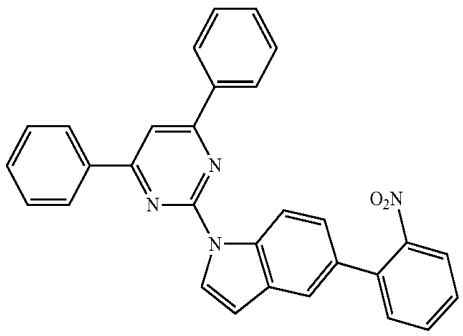
Preparation Example 22

Synthesis of IC-22

<Step 1> Synthesis of 1-(4,6-diphenylpyrimidine-2-yl)-5-(2-nitrophenyl)-1H-indole

[0195]

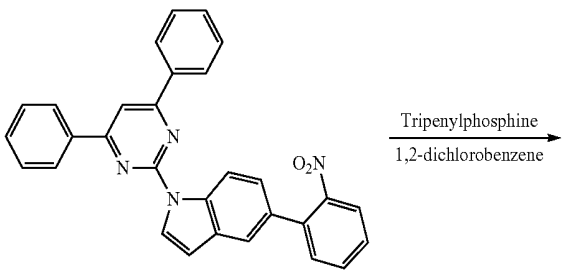




[0196] 1-(4,6-diphenylpyrimidine-2-yl)-5-(2-nitrophenyl)-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 7, except that 2-chloro-4,6-diphenylpyrimidine was used instead of iodobenzene.

<Step 2> Synthesis of IC-22

[0197]



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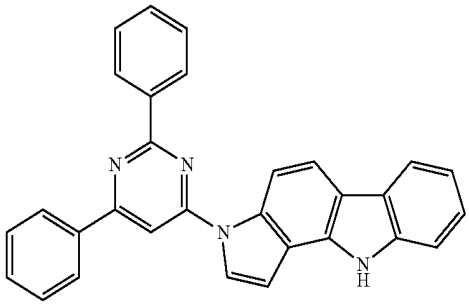


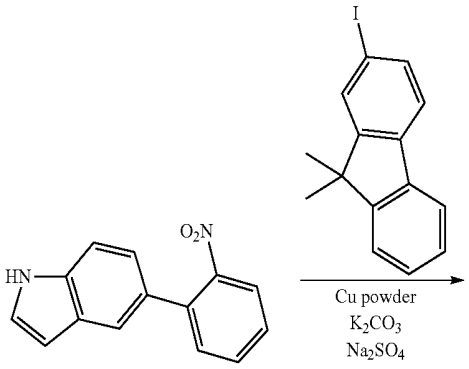
[0198] IC-22 was obtained by performing the same procedure as in <Step 4> of Preparation Example 7, except that the product in <Step 1> was used instead of 5-(2-nitrophenyl)-1-phenyl-1H-indole.

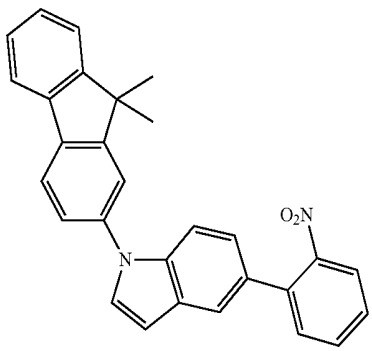
Preparation Example 23

Synthesis of IC-23

<Step 1> Synthesis of 1-(9,9-dimethyl-9H-fluoren-2-yl)-5-(2-nitrophenyl)-1H-indole

[0199]

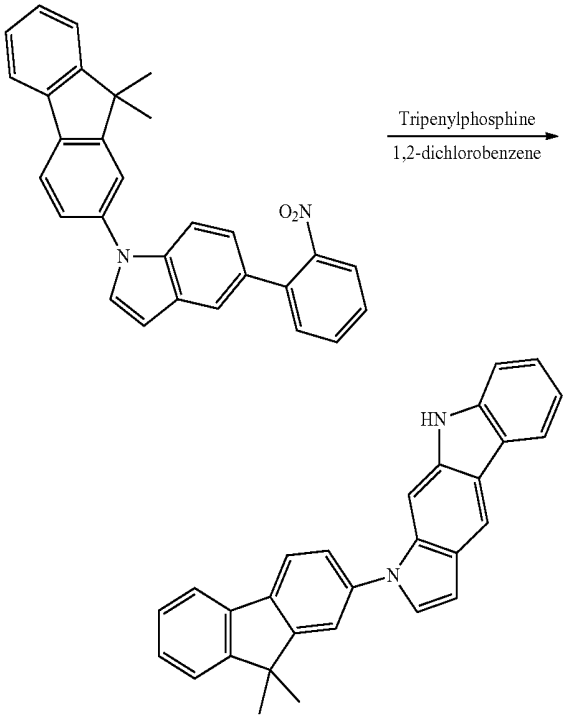




[0200] 1-(9,9-dimethyl-9H-fluoren-2-yl)-5-(2-nitrophenyl)-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 9, except that 2-iodo-9,9-dimethyl-9H-fluorene was used instead of iodobenzene.

<Step 2> Synthesis of IC-23

[0201]



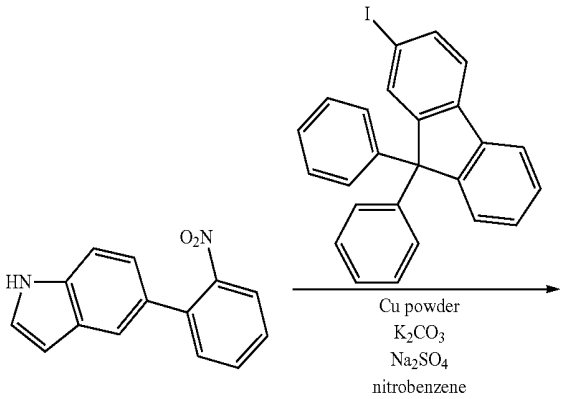
[0202] IC-23 was obtained by performing the same procedure as in <Step 4> of Preparation Example 9, except that the product in <Step 1> was used instead of 5-(2-nitrophenyl)-1-phenyl-1H-indole.

Preparation Example 24

Synthesis of IC-24

<Step 1> Synthesis of 1-(9,9-diphenyl-9H-fluoren-2-yl)-5-(2-nitrophenyl)-1H-indole

[0203]



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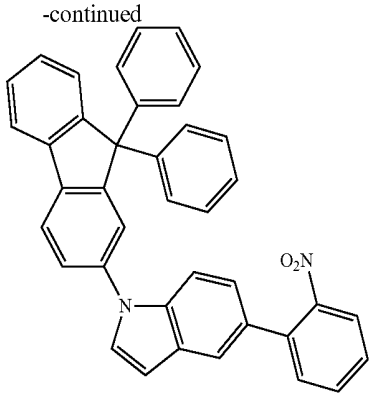
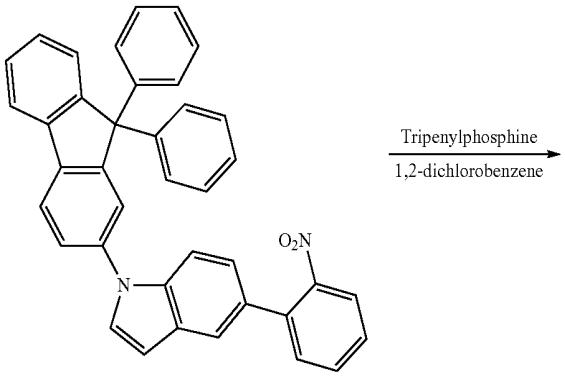
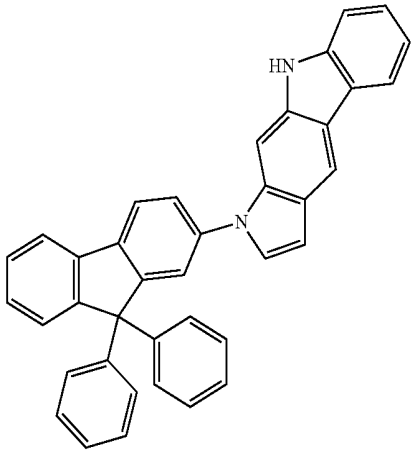


[0204] 1-(9,9-diphenyl-9H-fluoren-2-yl)-5-(2-nitrophenyl)-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 9, except that 2-iodo-9,9-diphenyl-9H-fluorene was used instead of iodobenzene.

<Step 2> Synthesis of IC-24

[0205]





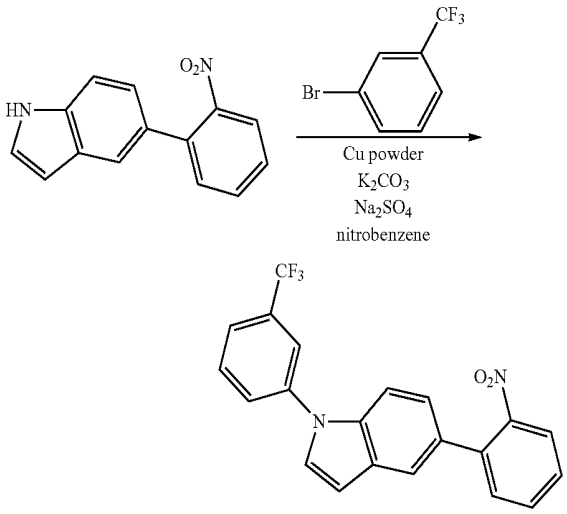
[0206] IC-24 was obtained by performing the same procedure as in <Step 4> of Preparation Example 9, except that the product in <Step 1> was used instead of 5-(2-nitrophenyl)-1-phenyl-1H-indole.

Preparation Example 25

Synthesis of IC-25

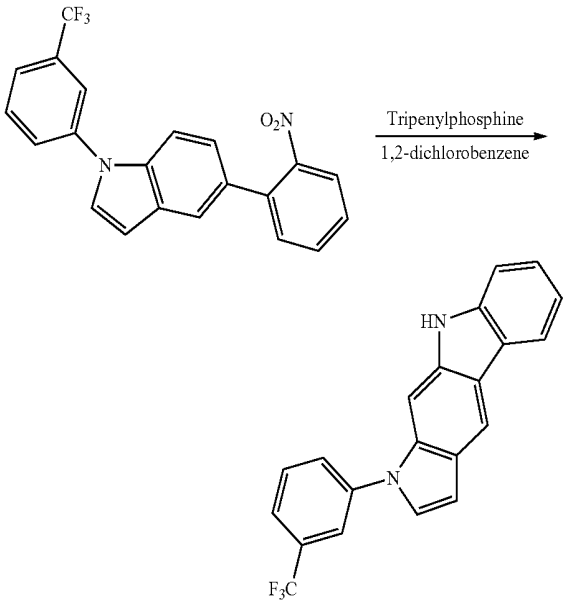
<Step 1> Synthesis of 5-(2-nitrophenyl)-1-(3-(trifluoromethyl)phenyl)-1H-indole

[0207]



<Step 2> Synthesis of IC-25

[0208]



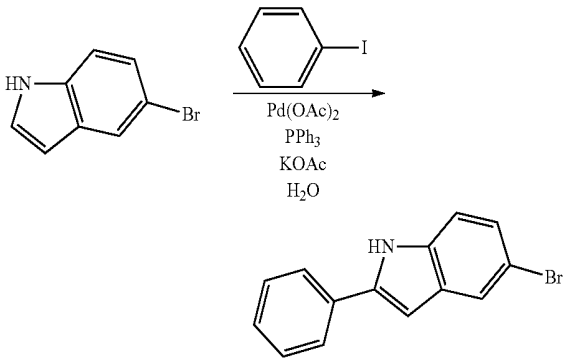
[0209] IC-25 was obtained by performing the same procedure as in Preparation Example 24, except that 1-bromo-3-(trifluoromethyl)benzene was used instead of 2-iodo-9,9-diphenyl-9H-fluorene.

Preparation Example 26

Synthesis of IC-26

<Step 1> Synthesis of 5-bromo-2-phenyl-1H-indole

[0210]

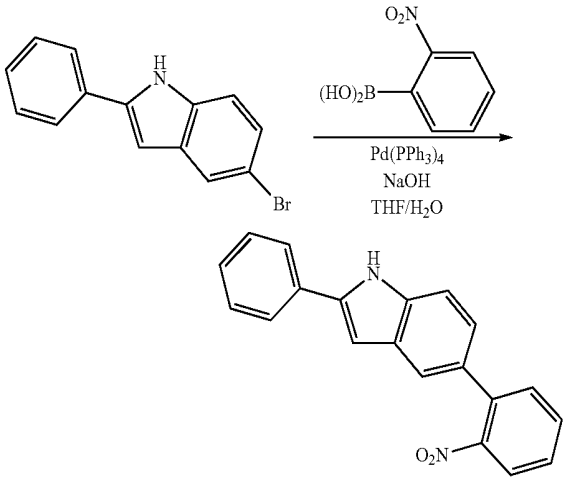


[0211] 5-bromo-1H-indole (25 g, 0.13 mol), iodobenzene (31.22 g, 0.15 mol), $Pd(OAc)_2$ (1.43 g, 5 mol %), triphenylphosphine (1.67 g, 5 mol %), KOAc (37.55 g, 0.38 mol), and H_2O (300 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 110° C. for 24 hours.

[0212] After the reaction was terminated, 5-bromo-2-phenyl-1H-indole (16.66 g, yield 48%) was obtained by performing extraction with ethyl acetate, removing moisture over $MgSO_4$, and refinement was performed by column chromatography (Hexane:EA=10:1 (v/v)).

<Step 2> Synthesis of 5-(2-nitrophenyl)-2-phenyl-1H-indole

[0213]

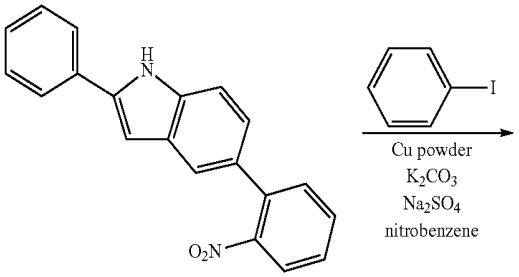


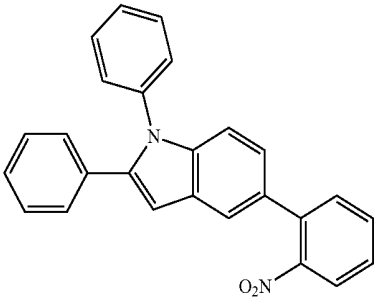
[0214] 2-nitrophenylboronic acid (11.04 g, 66.14 mmol), the 5-bromo-2-phenyl-1H-indole (15 g, 55.12 mmol) obtained in <Step 1>, NaOH (6.61 g, 165.36 mmol), and THF/H_2O (200 ml/100 ml) were mixed under nitrogen flow, $Pd(PPh_3)_4$ (3.18 g, 5 mol) was added thereto at 40° C., and the resulting mixture was stirred at 80° C. for 12 hours.

[0215] After the reaction was terminated, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 5-(2-nitrophenyl)-2-phenyl-1H-indole (10.74 g, yield 62%) was obtained by removing the solvent from the obtained organic layer, and refinement was performed by column chromatography (Hexane:EA=5:1 (v/v)).

<Step 3> Synthesis of 5-(2-nitrophenyl)-1,2-diphenyl-1H-indole

[0216]

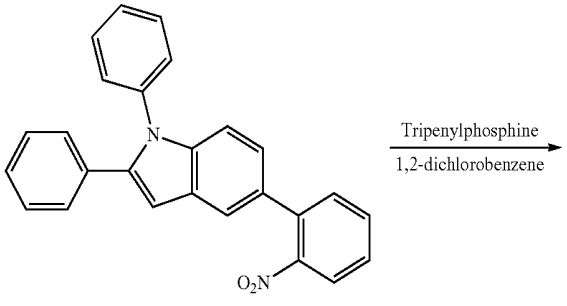




[0217] 5-(2-nitrophenyl)-1,2-diphenyl-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 7, except that the product in <Step 2> was used instead of 5-(2-nitrophenyl)-1H-indole.

<Step 4> Synthesis of IC-26

[0218]



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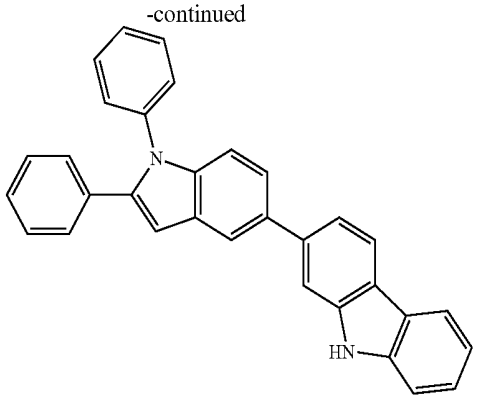


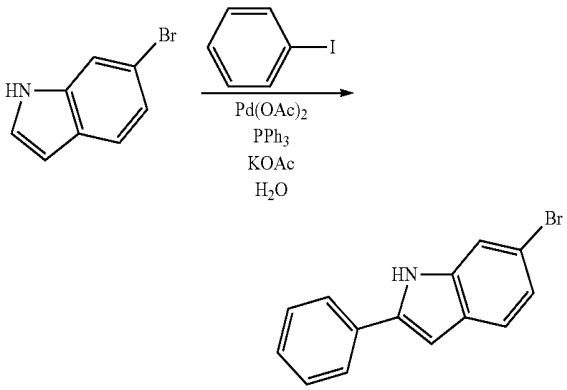
[0219] IC-26 was obtained by performing the same procedure as in <Step 4> of Preparation example 7, except that the product in <Step 3> was used instead of 5-(2-nitrophenyl)-1-phenyl-1H-indole.

Preparation Example 27

Synthesis of IC-27

<Step 1> Synthesis of 6-bromo-2-phenyl-1H-indole

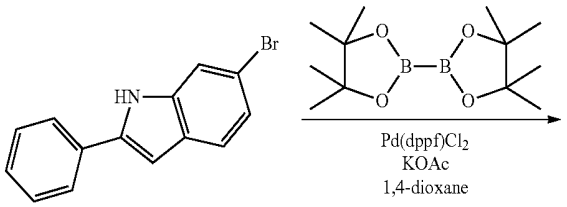
[0220]



[0221] 6-bromo-2-phenyl-1H-indole was obtained by performing the same procedure as in <Step 1> of Preparation Example 26, except that 6-bromo-1H-indole was used instead of 5-bromo-1H-indole.

<Step 2> Synthesis of 2-phenyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

[0222]



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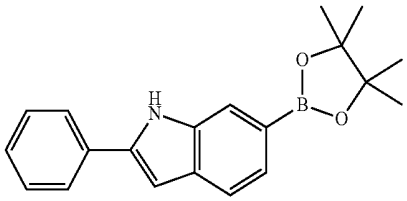
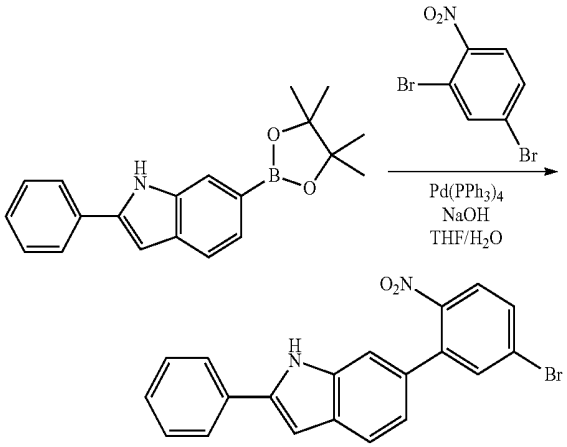


[0223] 2-phenyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole was obtained by performing the same procedure as in <Step 1> of Preparation Example 4, except that the product in <Step 1> was used instead of 6-bromo-1H-indole.

<Step 3> Synthesis of 6-(5-bromo-2-nitrophenyl)-2-phenyl-1H-indole

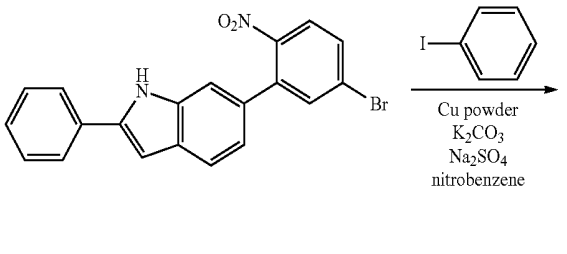
[0224]



[0225] 6-(5-bromo-2-nitrophenyl)-2-phenyl-1H-indole was obtained by performing the same procedure as in <Step 2> of Preparation Example 4, except that the product in <Step 2> was used instead of 6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole.

<Step 4> Synthesis of 6-(5-bromo-2-nitrophenyl)-1,2-diphenyl-1H-indole

[0226]



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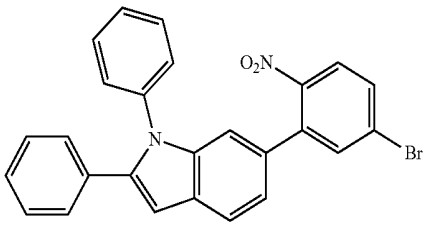
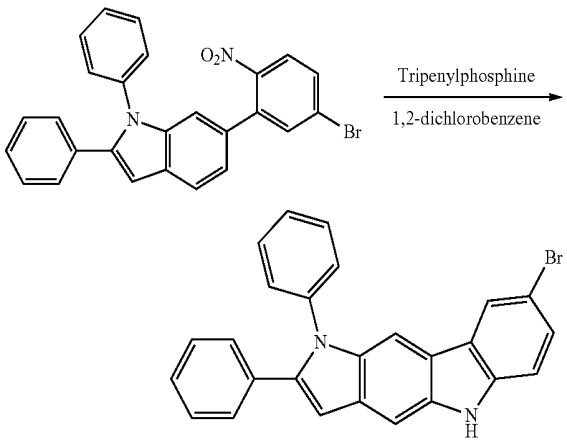


[0227] 6-(5-bromo-2-nitrophenyl)-1,2-diphenyl-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 4, except that the product in <Step 3> was used instead of 6-(5-bromo-2-nitrophenyl)-1H-indole.

<Step 5> Synthesis of 8-bromo-1,2-diphenyl-1,5-dihydropyrrolo[3,2-b]carbazole

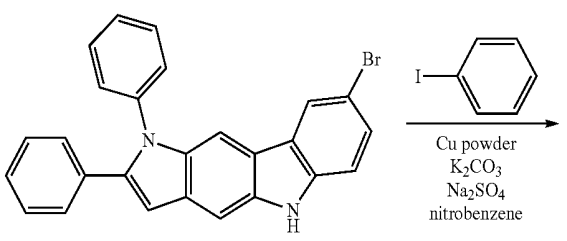
[0228]



[0229] 8-bromo-1,2-diphenyl-1,5-dihydropyrrolo[3,2-b]carbazole was obtained by performing the same procedure as in <Step 4> of Preparation Example 4, except that the product in <Step 4> was used instead of 6-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole.

<Step 6> Synthesis of 8-bromo-1,2,5-triphenyl-1,5-dihydropyrrolo[3,2-b]carbazole

[0230]



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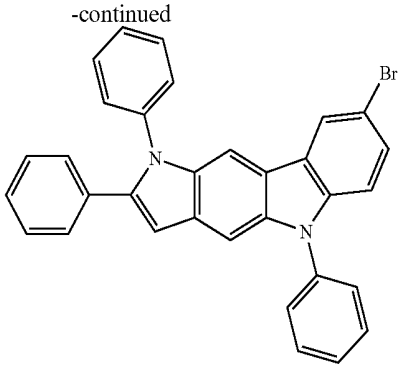
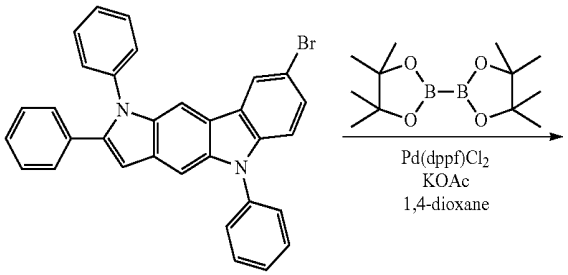
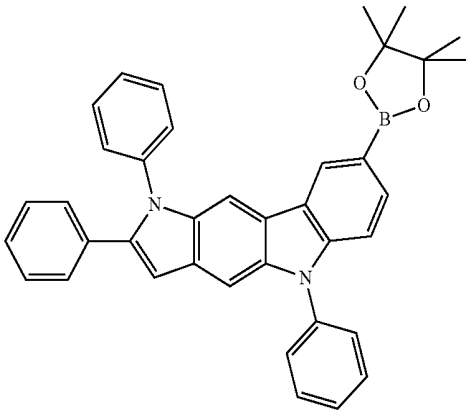


[0231] 8-bromo-1,2,5-triphenyl-1,5-dihydropyrrolo[3,2-b]carbazole was obtained by performing the same procedure as in <Step 5> of Preparation Example 4, except that the product in <Step 5> was used instead of 8-bromo-1-phenyl-1,5-dihydropyrrolo[3,2-b]carbazole.

<Step 7> Synthesis of IC-27

[0232]





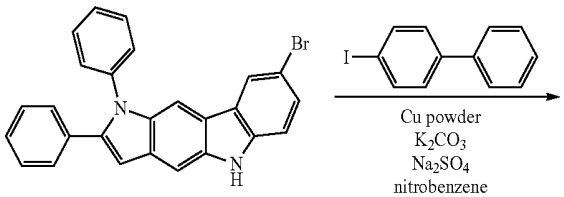
[0233] IC-27 was obtained by performing the same procedure as in <Step 6> of Preparation Example 4, except that the product in <Step 6> was used instead of 8-bromo-1,5-diphenyl-1,5-dihydropyrrolo[3,2-b]carbazole.

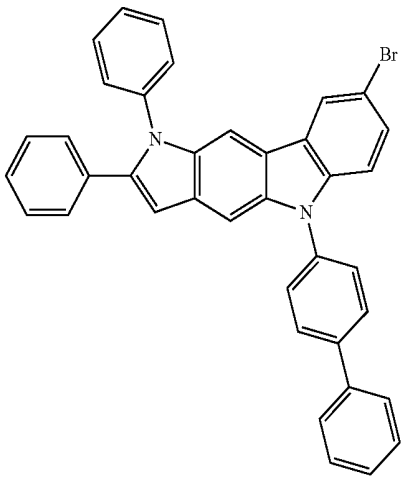
Preparation Example 28

Synthesis of IC-28

<Step 1> Synthesis of 5-(biphenyl-4-yl)-8-bromo-1,2-diphenyl-1,5-dihydropyrrolo[3,2-b]carbazole

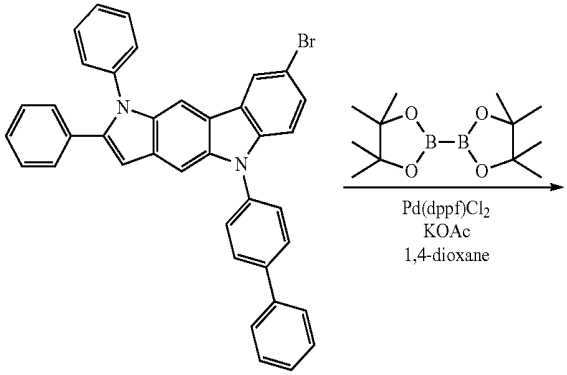
[0234]





<Step 2> Synthesis of IC-28

[0235]



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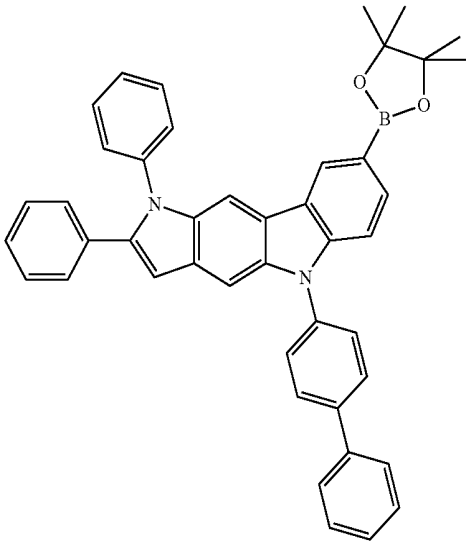


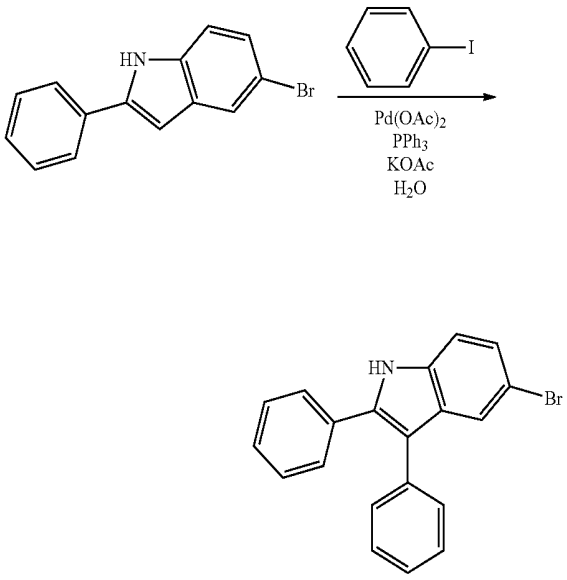
[0236] IC-28 was obtained by performing the same procedure as in Preparation Example 27, except that 4-iodobiphenyl was used instead of iodobenzene.

Preparation Example 29

Synthesis of IC-29

<Step 1> Synthesis of
5-bromo-2,3-diphenyl-1H-indole

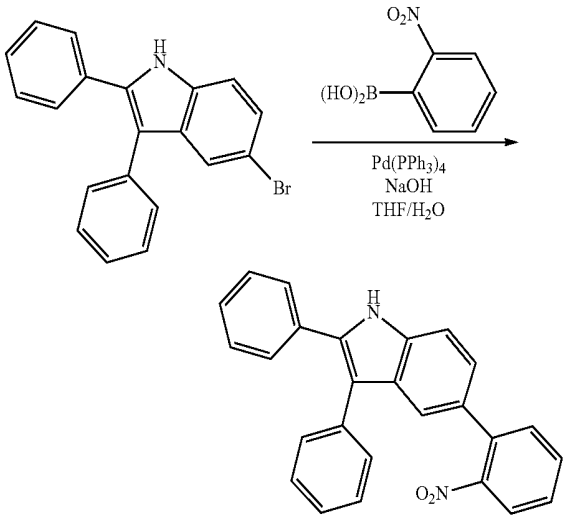
[0237]



[0238] 5-bromo-2,3-diphenyl-1H-indole was obtained by performing the same procedure as in <Step 1> of Preparation Example 26, except that 5-bromo-2-phenyl-1H-indole was used instead of 5-bromo-1H-indole.

<Step 2> Synthesis of
5-(2-nitrophenyl)-2,3-diphenyl-1H-indole

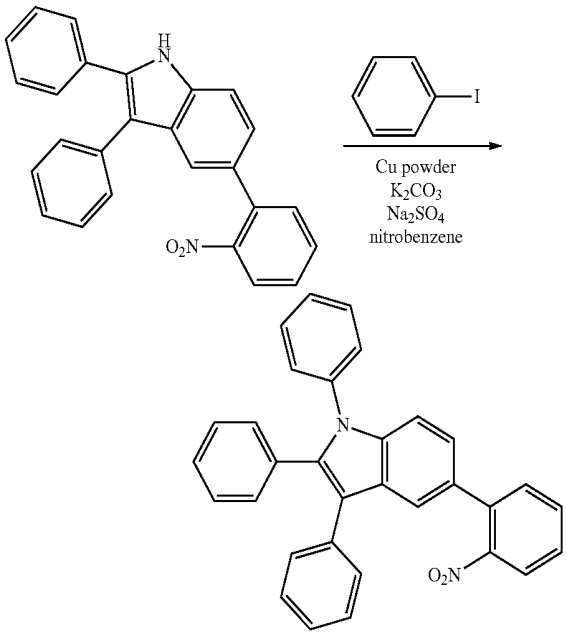
[0239]



[0240] 5-(2-nitrophenyl)-2,3-diphenyl-1H-indole was obtained by performing the same procedure as in <Step 2> of Preparation Example 26, except that the product in <Step 1> was used instead of 5-bromo-2-phenyl-1H-indole.

<Step 3> Synthesis of
5-(2-nitrophenyl)-1,2,3-triphenyl-1H-indole

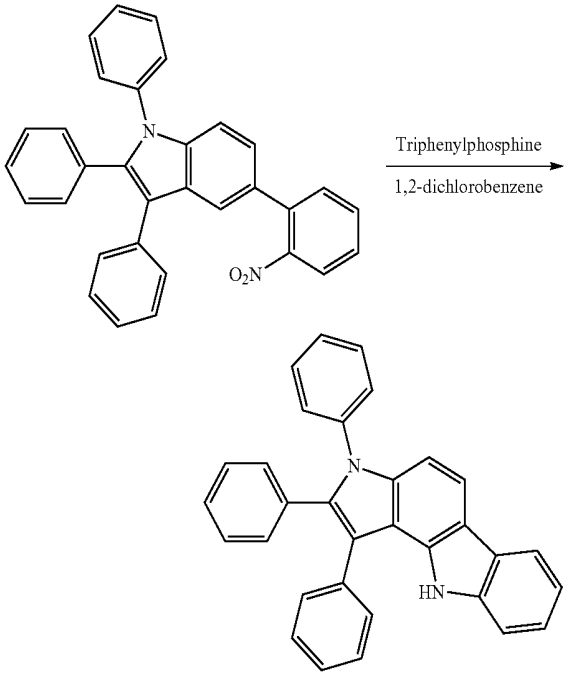
[0241]



[0242] 5-(2-nitrophenyl)-1,2,3-triphenyl-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 26, except that the product in <Step 2> was used instead of 5-(2-nitrophenyl)-2-phenyl-1H-indole.

<Step 4> Synthesis of IC-29

[0243]



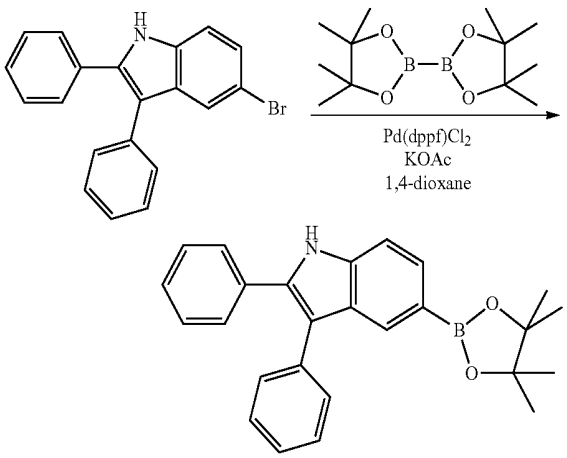
[0244] IC-29 was obtained by performing the same procedure as in <Step 4> of Preparation Example 26, except that the product in <Step 3> was used instead of 5-(2-nitrophenyl)-1,2-diphenyl-1H-indole.

Preparation Example 30

Synthesis of IC-30

<Step 1> Synthesis of 2,3-diphenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole

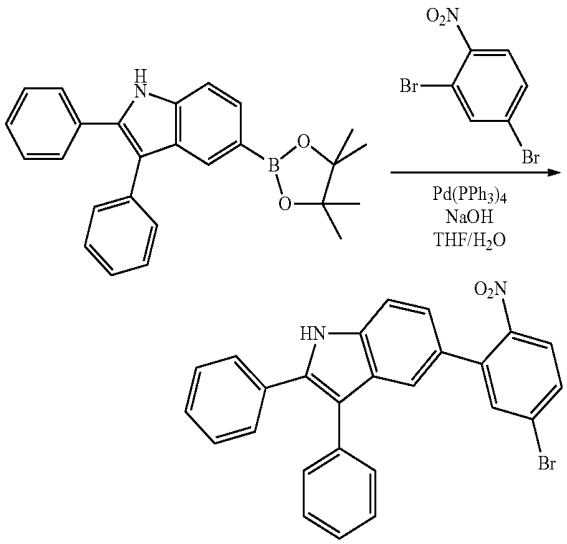
[0245]



[0246] 2,3-diphenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole was obtained by performing the same procedure as in <Step 1> of Preparation Example 1, except that 5-bromo-2,3-diphenyl-1H-indole was used instead of 5-bromo-1H-indole.

<Step 2> Synthesis of 5-(5-bromo-2-nitrophenyl)-2,3-diphenyl-1H-indole

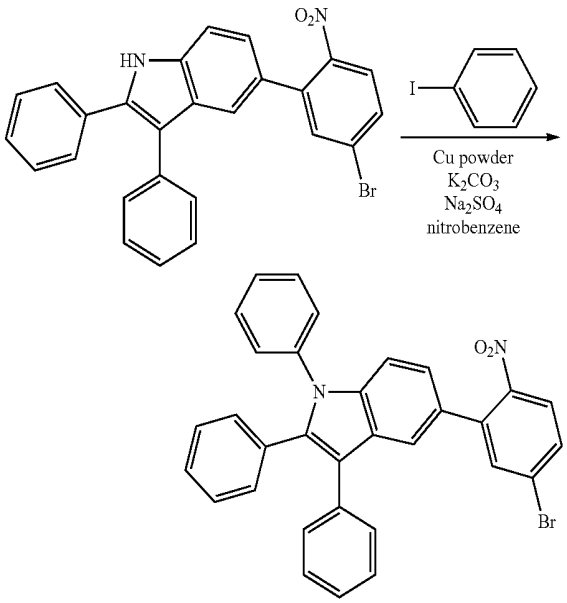
[0247]



[0248] 5-(5-bromo-2-nitrophenyl)-2,3-diphenyl-1H-indole was obtained by performing the same procedure as in <Step 2> of Preparation Example 1, except that the product in <Step 1> was used instead of 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole.

<Step 3> Synthesis of 5-(5-bromo-2-nitrophenyl)-1,2,3-triphenyl-1H-indole

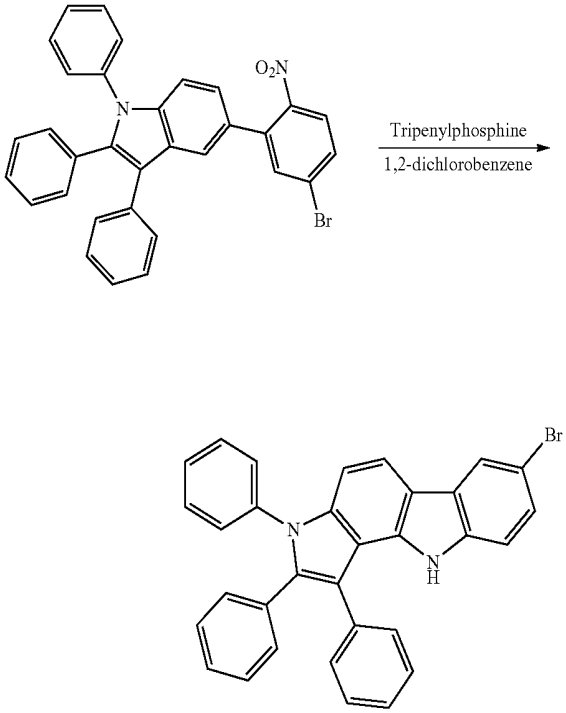
[0249]



[0250] 5-(5-bromo-2-nitrophenyl)-1,2,3-triphenyl-1H-indole was obtained by performing the same procedure as in <Step 3> of Preparation Example 1, except that the product in <Step 2> was used instead of 5-(5-bromo-2-nitrophenyl)-1H-indole.

<Step 4> Synthesis of 7-bromo-1,2,3-triphenyl-3,10-dihydropyrrolo[3,2-a]carbazole

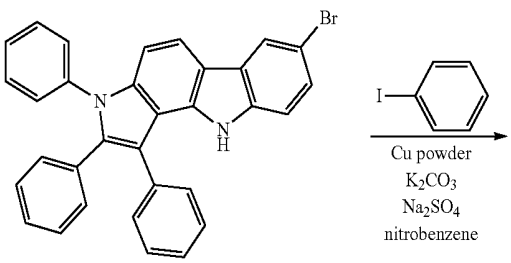
[0251]



[0252] 7-bromo-1,2,3-triphenyl-3,10-dihydropyrrolo[3,2-a]carbazole was obtained by performing the same procedure as in <Step 4> of Preparation Example 1, except that the product in <Step 3> was used instead of 5-(5-bromo-2-nitrophenyl)-1-phenyl-1H-indole.

<Step 5> Synthesis of 1,2,3,10-tetraphenyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole

[0253]



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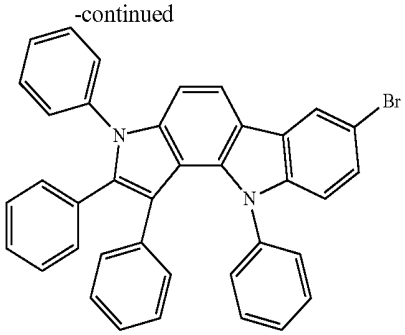
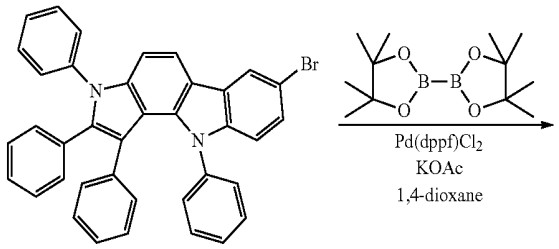
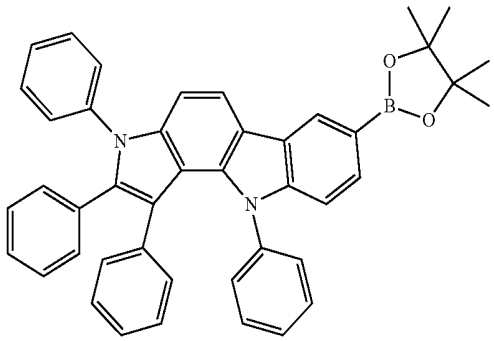


[0254] 1,2,3,10-tetraphenyl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3,10-dihydropyrrolo[3,2-a]carbazole was obtained by performing the same procedure as in <Step 5> of Preparation Example 1, except that the product in <Step 4> was used instead of 7-bromo-3-phenyl-3,10-dihydropyrrolo[3,2-a]carbazole.

<Step 6> Synthesis of IC-30

[0255]





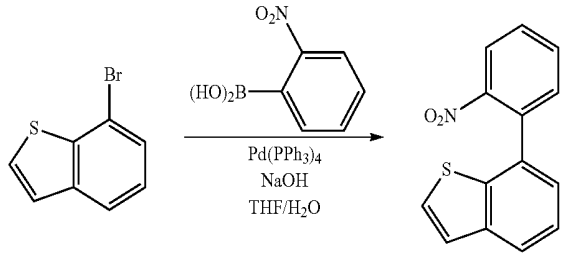
[0256] IC-30 was obtained by performing the same procedure as in <Step 6> of Preparation Example 1, except that the product in <Step 5> was used instead of 7-bromo-3,10-diphenyl-3,10-dihydropyrrolo[3,2-a]carbazole.

Preparation Example 31

Synthesis of IC-31

<Step 1> Synthesis of 7-(2-nitrophenyl)benzo[b]thiophene

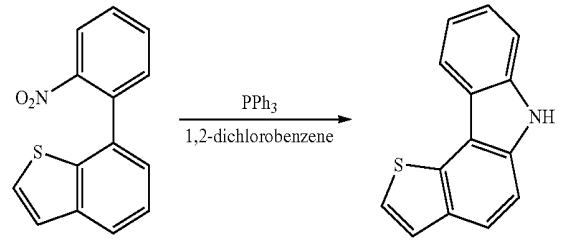
[0257]



[0258] 12.2 g (35.2 mmol) of 7-bromobenzo[b]thiophene, 6.44 g (38.7 mmol) of 2-nitrophenylboronic acid, 4.22 g (105.6 mmol) of NaOH, and 300 ml/150 ml of THF/H_2O were put thereinto under nitrogen flow, and the resulting mixture was stirred. 2.03 g (5 mol %) of $Pd(PPh_3)_4$ was added thereto at 40° C., and the resulting mixture was stirred at 80° C. for 12 hours. After the reaction was terminated, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 7.38 g (28.9 mmol, yield 82%) of 7-(2-nitrophenyl)benzo[b]thiophene was obtained by removing the solvent from the filtered organic layer, and then using column chromatography.

<Step 2> Synthesis of IC-31

[0259]



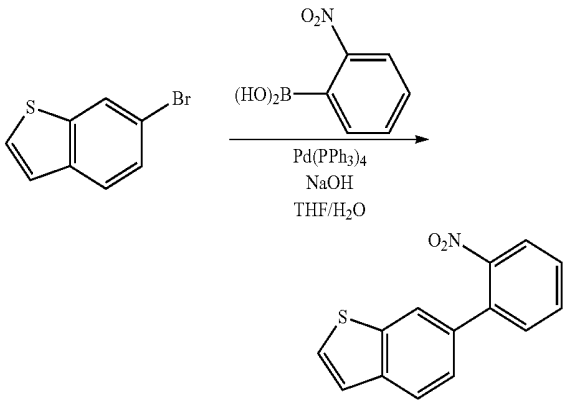
[0260] The product (5.53 g, 21.7 mmol) in <Step 1>, triphenylphosphine (14.2 g, 54.2 mmol), and 100 ml of 1,2-dichlorobenzene were put thereinto under nitrogen flow, and then the resulting mixture was stirred for 12 hours. After the reaction was terminated, 1,2-dichlorobenzene was removed, and extraction was performed with dichloromethane. 3.29 g (14.8 mmol, yield: 68%) of IC-31 was obtained by removing water from the extracted organic layer over $MgSO_4$ and using column chromatography.

Preparation Example 32

Synthesis of IC-32 and IC-33

<Step 1> Synthesis of 6-(2-nitrophenyl)benzo[b]thiophene

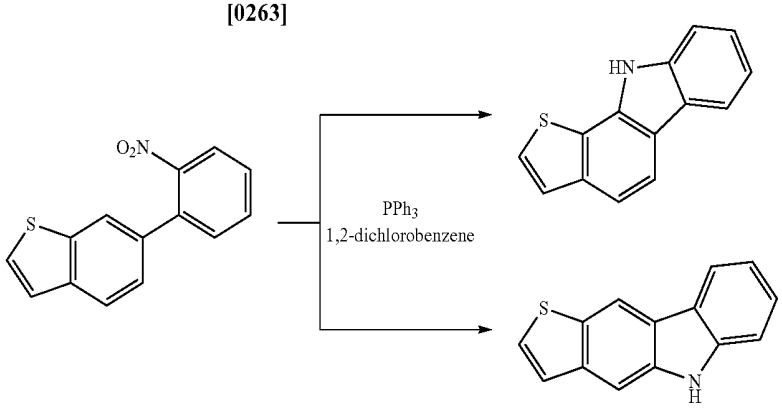
[0261]



[0262] 7.01 g (27.5 mmol, yield: 78%) of 6-(2-nitrophenyl) benzo[b]thiophene was obtained by performing the same procedure as in <Step 1> of Preparation Example 31, except that 6-bromobenzo[b]thiophene (12.2 g, 35.2 mmol) was used instead of 7-bromobenzo[b]thiophene.

<Step 2> Synthesis of IC-32 and IC-33

[0263]



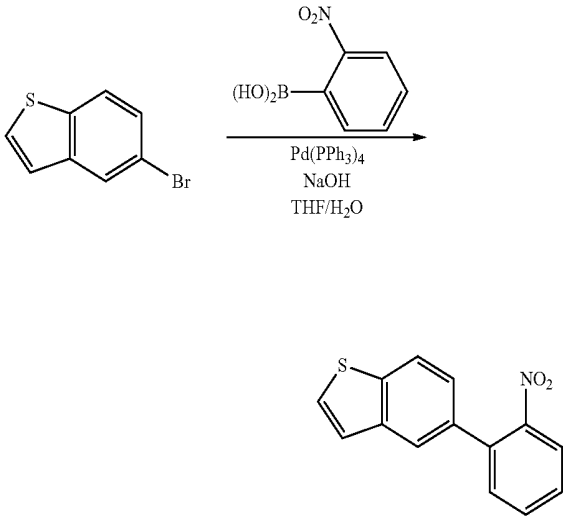
[0264] 1.60 g (7.16 mmol, yield: 33%) of IC-32 and 1.79 g (8.03 mmol, yield: 37%) of IC-33 were obtained by performing the same procedure as in <Step 2> of Preparation Example 31, except that 5.53 g (21.7 mmol) of the product in <Step 1> was used instead of 7-(2-nitrophenyl)benzo[b]thiophene.

Preparation Example 33

Synthesis of IC-34 and IC-35

<Step 1> Synthesis of 5-(2-nitrophenyl)benzo[b]thiophene

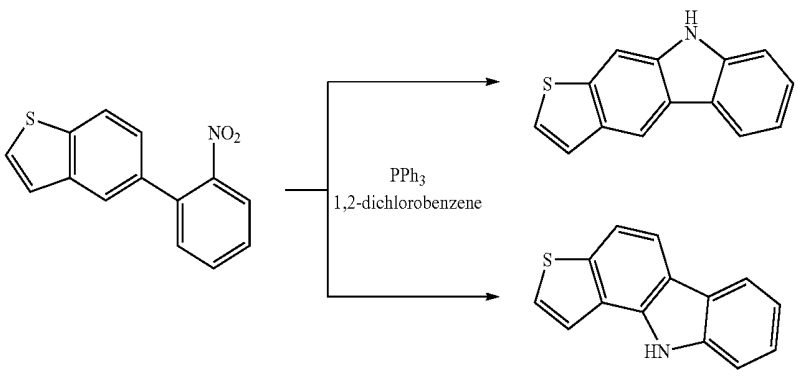
[0265]



[0266] 6.83 g (26.8 mmol, yield: 76%) of 5-(2-nitrophenyl) benzo[b]thiophene was obtained by performing the same procedure as in <Step 1> of Preparation Example 31, except that 5-bromobenzo[b]thiophene (12.2 g, 35.2 mmol) was used instead of 7-bromobenzo[b]thiophene.

<Step 2> Synthesis of IC-34 and IC-35

[0267]



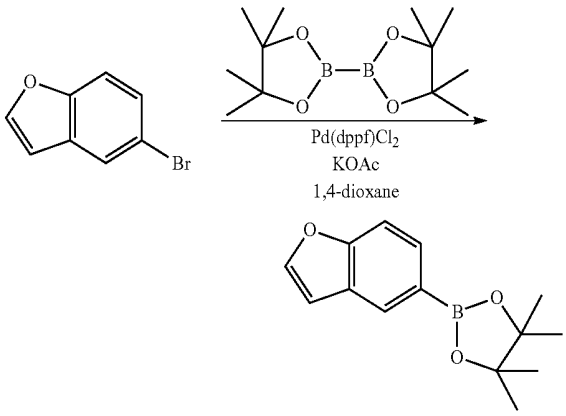
[0268] 1.70 g (7.60 mmol, yield: 35%) of IC-34 and 1.89 g (8.46 mmol, yield: 39%) of IC-35 were obtained by performing the same procedure as in <Step 2> of Preparation Example 31, except that the product (5.53 g, 21.7 mmol) in <Step 1> was used instead of 7-(2-nitrophenyl)benzo[b]thiophene.

Preparation Example 34

Synthesis of IC-36

<Step 1> Synthesis of 2-(benzofuran-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

[0269]

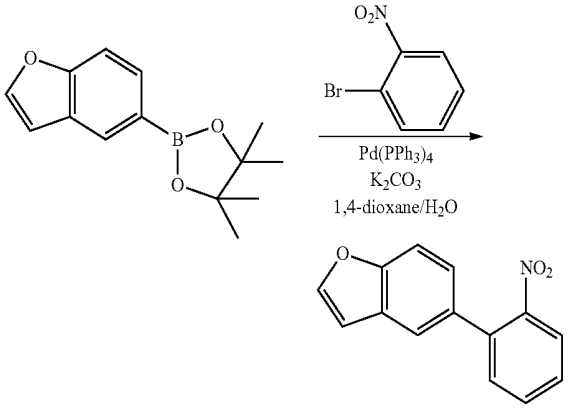


[0270] 5-bromobenzofuran (25 g, 0.126 mol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (38.67 g, 0.152 mol), $Pd(dppf)Cl_2$ (3.11 g, 3 mol %), KOAc (37.36 g, 0.381 mol), and 1,4-dioxane (500 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 130° C. for 12 hours.

[0271] After the reaction was terminated, 2-(benzofuran-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (23.23 g, yield 75%) was obtained by performing extraction with ethyl acetate, removing moisture over $MgSO_4$, and purifying the residue with column chromatography (Hexane:EA=10:1 (v/v)).

<Step 2> Synthesis of 5-(2-nitrophenyl)benzofuran

[0272]

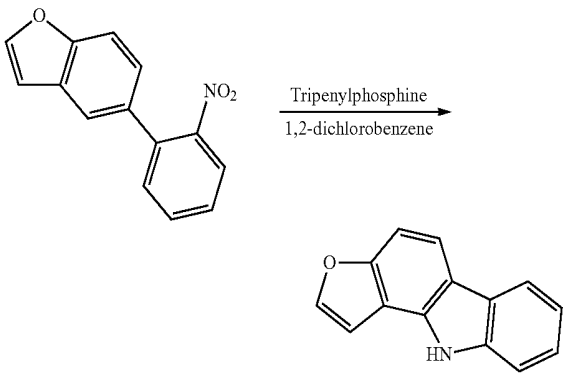


[0273] 1-bromo-2-nitrobenzene (15.86 g, 78.52 mmol), the product (23 g, 94.23 mmol) in <Step 1>, K_2CO_3 (32.56 g, 235.57 mmol), and 1,4-dioxane/H_2O (400 ml/200 ml) were mixed under nitrogen flow, $Pd(PPh_3)_4$ (4.54 g, 5 mol %) was added thereto at 40° C., and the resulting mixture was stirred at 110° C. for 12 hours.

[0274] After the reaction was terminated, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 5-(2-nitrophenyl)benzofuran (12.40 g, yield 66%) was obtained by removing the solvent from the obtained organic layer, and refinement was performed by column chromatography (Hexane:EA=3:1 (v/v)).

<Step 3> Synthesis of IC-36

[0275]



[0276] The product (10 g, 41.80 mmol) in <Step 2>, triphenylphosphine (27.41 g, 104.50 mmol), and 1,2-dichlorobenzene (150 ml) were mixed under nitrogen flow, and the resulting mixture was stirred for 12 hours.

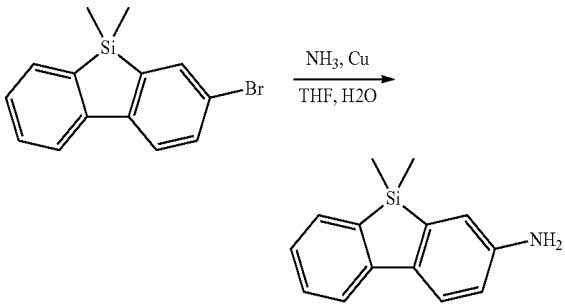
[0277] After the reaction was terminated, 1,2-dichlorobenzene was removed, and extraction was performed with dichloromethane. IC-36 (4.76 g, yield 55%) was obtained by removing water from the obtained organic layer over $MgSO_4$, and refinement was performed by column chromatography (Hexane:MC=3:1 (v/v)).

Preparation Example 35

Synthesis of IC-37

<Step 1> Synthesis of 5,5-dimethyl-5H-dibenzo[b,d]silole-3-amine

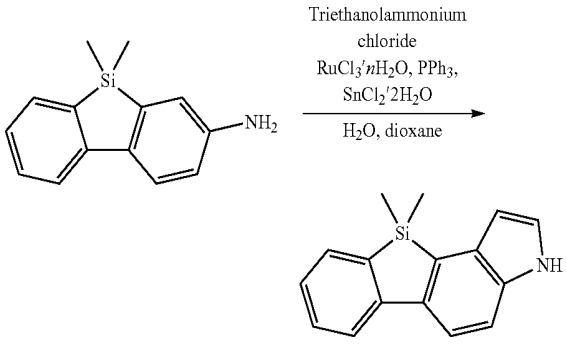
[0278]



[0279] After 3-bromo-5,5-dimethyl-5H-dibenzo[b,d]silole (7.41 g, 30.0 mmol) was dissolved in 100 ml of THF under nitrogen flow, 28% aqueous ammonia (10.2 ml, 150 mmol) and Cu (0.10 g, 5 mol %) were added thereto, and the resulting mixture was stirred at 110° C. for 12 hours. After the reaction was terminated, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 4.45 g (yield: 81%) of 5,5-dimethyl-5H-dibenzo[b,d]silole-3-amine was obtained by removing the solvent from the filtered organic layer, and refinement was performed by column chromatography (Hexane:EA=10:1 (v/v)).

<Step 2> Synthesis of IC-37

[0280]



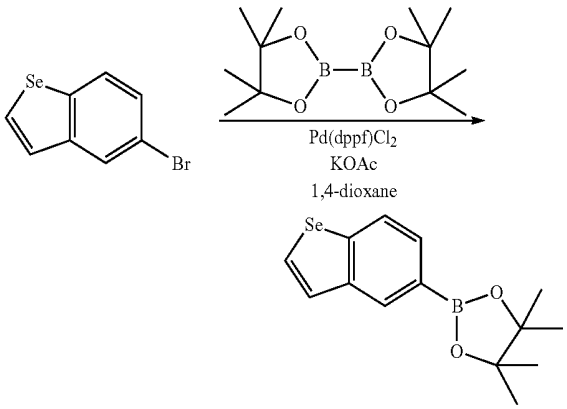
[0281] The product (4.45 g, 24.29 mmol) in <Step 1> was dissolved in H_2O/dioxane (10 ml/90 ml) under nitrogen flow, and then triethanolammonium chloride (0.45 g, 2.43 mmol), $RuCl_3.H_2O$ (0.055 g, 0.2 mmol), PPh_3 (0.191 g, 0.7 mmol), and $SnCl_2.2H_2O$ (0.548 g, 2.43 mmol) were added thereto, and the resulting mixture was stirred at 180° C. for 20 hours. After the reaction was terminated, the reactant was poured into aqueous 5% HCl, extraction was performed with methylene chloride, $MgSO_4$ was added thereto, and the resulting product was filtered. 2.7 g (yield: 53%) of IC-37 was obtained by removing the solvent from the filtered organic layer, and refinement was performed by column chromatography (Hexane:MC=1:1 (v/v)).

Preparation Example 36

Synthesis of IC-38

<Step 1> Synthesis of 2-(benzo[b]selenophen-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

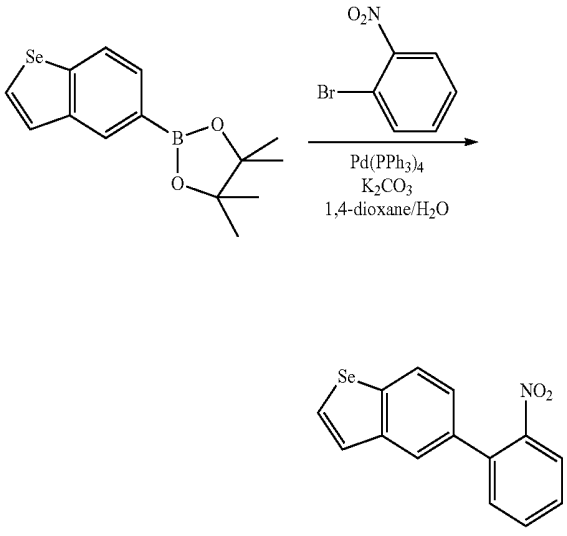
[0282]



[0283] 2-(benzo[b]selenophen-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane was obtained by performing the same procedure as in <Step 1> of Preparation Example 34, except that 5-bromobenzo[b]selenophene was used instead of 5-bromobenzofuran.

<Step 2> Synthesis of 5-(2-nitrophenyl)benzo[b]selenophene

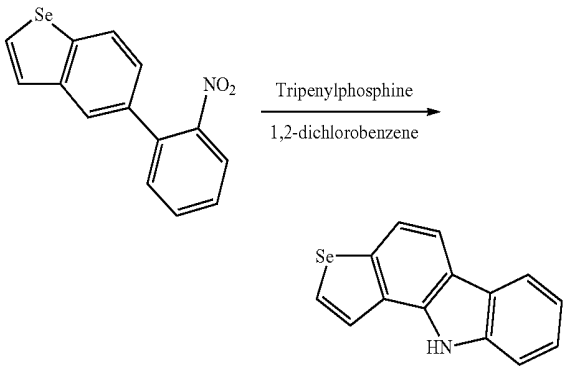
[0284]



[0285] 5-(2-nitrophenyl)benzo[b]selenophene was obtained by performing the same procedure as in <Step 2> of Preparation Example 34, except that the product in <Step 1> was used instead of 2-(benzofuran-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane.

<Step 3> Synthesis of IC-38

[0286]



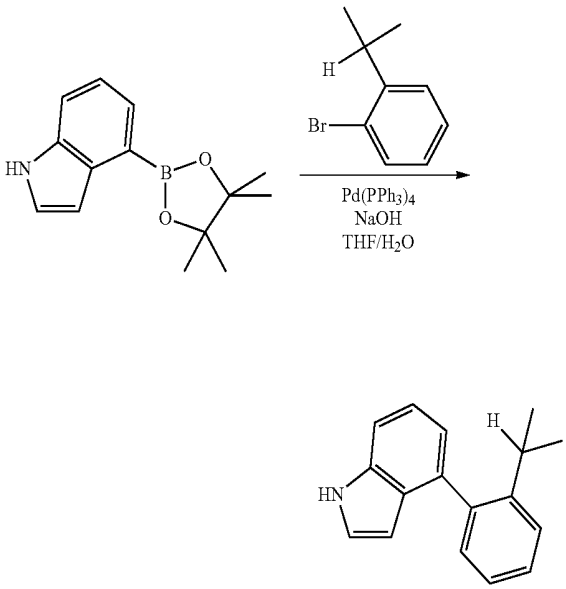
[0287] IC-38 was obtained by performing the same procedure as in <Step 3> of Preparation Example 34, except that the product in <Step 2> was used instead of 5-(2-nitrophenyl) benzofuran.

Preparation Example 37

Synthesis of IC-39

<Step 1> Synthesis of 4-(2-isopropylphenyl)-1H-indole

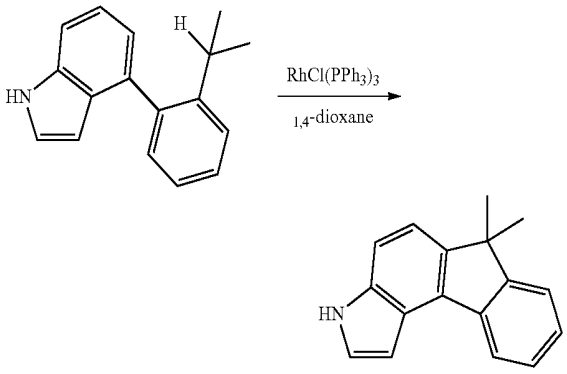
[0288]



[0289] 4-(2-isopropylphenyl)-1H-indole was obtained by performing the same procedure as in <Step 2> of Preparation Example 1, except that 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole was used instead of 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole and 1-bromo-2-isopropylbenzene was used instead of 2,4-dibromo-1-nitrobenzene.

<Step 2> Synthesis of IC-39

[0290]

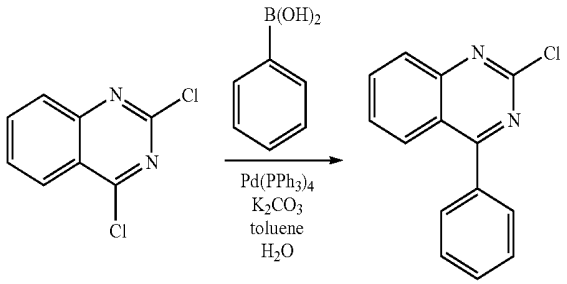


[0291] The product (5 g, 21.25 mmol) obtained in <Step 1> and $RhCl(PPh_3)_3$ (98.3 mg, 0.5 mol %) were dissolved in 50 ml of 1,4-dioxane under nitrogen flow, and then the resulting mixture was stirred at 135° C. for 1 hour. After the reaction was terminated, IC-39 (4 g, yield 81%) was obtained by removing the solvent and refinement was performed by column chromatography (Hexane:MC=3:1 (v:v)).

Preparation Example 38

Synthesis of Sub-1

[0292]



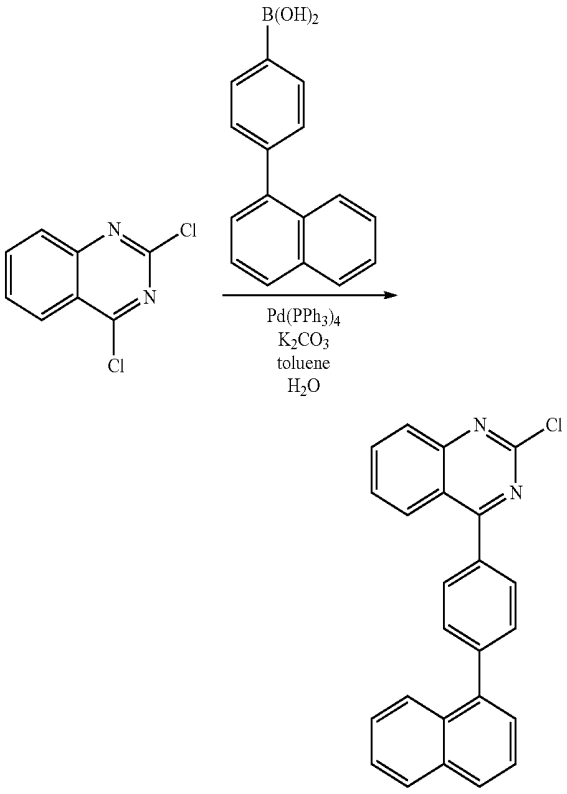
[0293] 2,4-dichloroquinazoline (10 g, 50.51 mmol), phenylboronic acid (6.16 g, 50.51 mmol), tetrakis (triphenylphosphine)palladium(0) (1.75 g, 1.515 mmol), and potassium carbonate (20.6 g, 151.53 mmol) were added thereto under nitrogen flow, and then the resulting mixture was stirred in 500 ml of toluene and 75 ml of H_2O.

[0294] After the reaction was terminated, the organic layer was separated by using ethyl acetate and water was removed by using $MgSO_4$. Sub-1 (4.8 g, yield 40%) was obtained by removing the solvent from the organic layer which water had been removed, and refinement was performed by recrystallization.

Preparation Example 39

Synthesis of Sub-2

[0295]

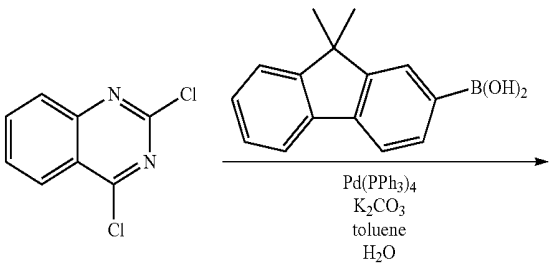


[0296] Sub-2 was obtained by performing the same procedure as in Preparation Example 38, except that 4-(naphthalen-1-yl)phenylboronic acid was used instead of phenylboronic acid.

Preparation Example 40

Synthesis of Sub-3

[0297]



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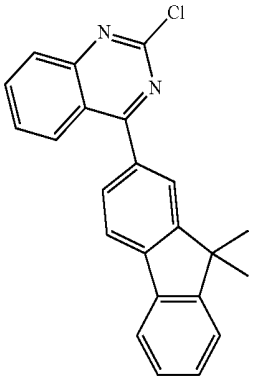
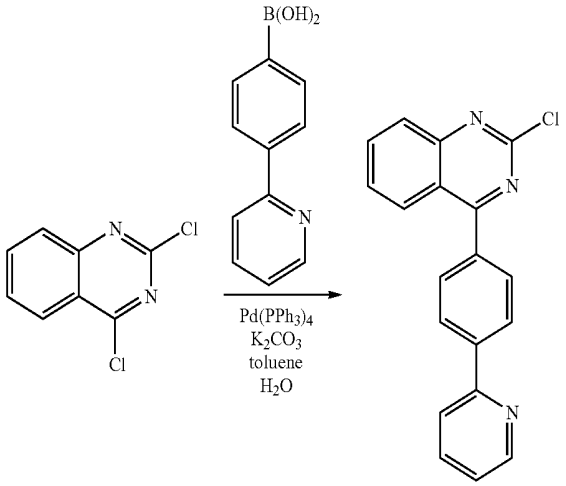


[0298] Sub-3 was obtained by performing the same procedure as in Preparation Example 38, except that 9,9-dimethyl-9H-fluoren-2-ylboronic acid was used instead of phenylboronic acid.

Preparation Example 41

Synthesis of Sub-4

[0299]

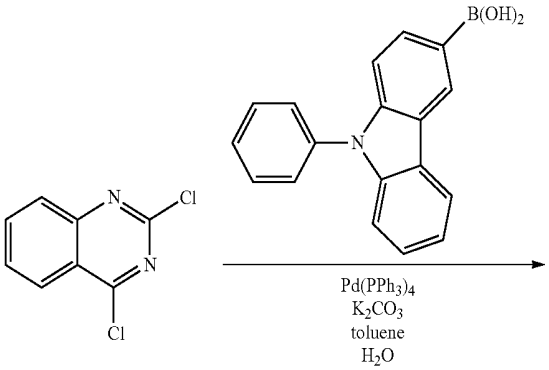


[0300] Sub-4 was obtained by performing the same procedure as in Preparation Example 38, except that 4-(pyridin-2-yl)phenylboronic acid was used instead of phenylboronic acid.

Preparation Example 42

Synthesis of Sub-5

[0301]



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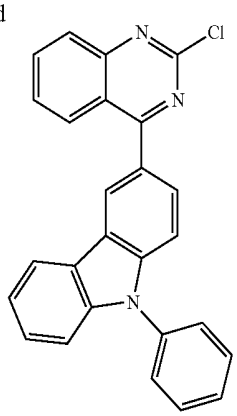
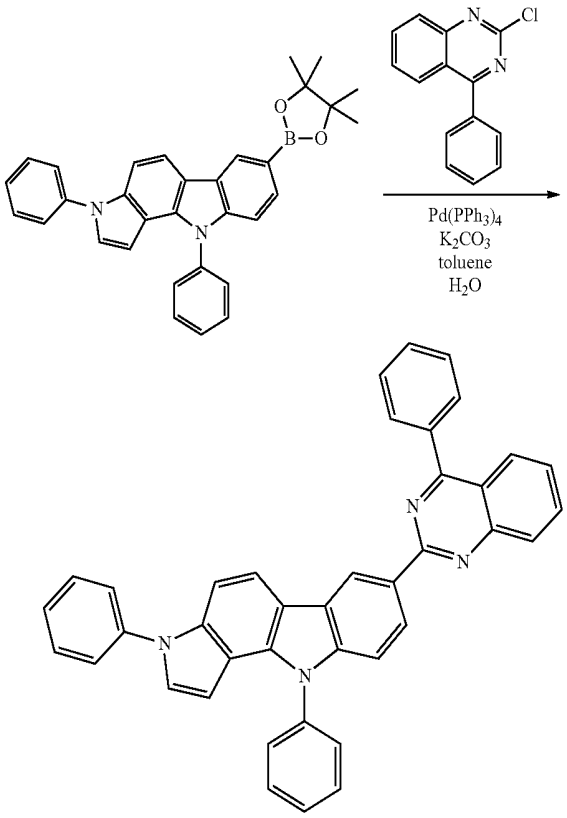


[0302] Sub-5 was obtained by performing the same procedure as in Preparation Example 38, except that 9-phenyl-9H-carbazol-3-ylboronic acid was used instead of phenylboronic acid.

Synthesis Example 1

Synthesis of Mat-1

[0303]



[0304] IC-1 (10 g, 20.65 mmol), sub-1 (5.9 g, 24.78 mmol), tetrakis (triphenylphosphine)palladium(0) (1.19 g, 1.03 mmol), and potassium carbonate (8.56 g, 61.95 mmol) were added thereto under nitrogen flow, and then the resulting mixture was stirred under reflux in 200 ml of toluene and 30 ml of H_2O.

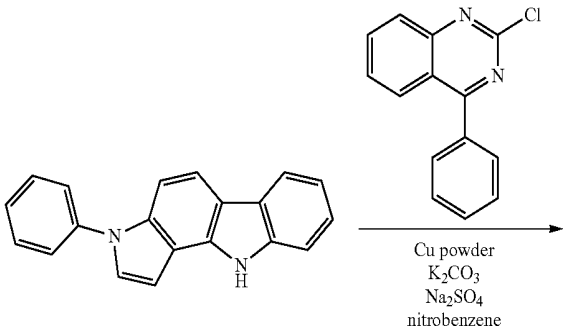
[0305] After the reaction was terminated, the organic layer was separated with methylene chloride and water was removed by using $MgSO_4$. Mat-1 (6.96 g, yield 60%) was obtained by removing the solvent from the organic layer which water had been removed, and refinement was performed by column chromatography (Hexane:MC=3:1 (v:v)).

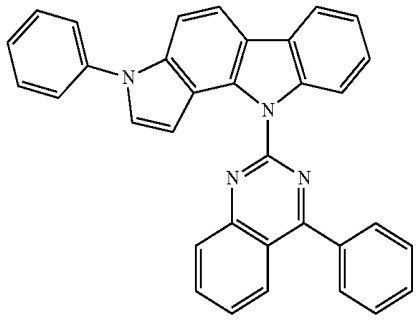
[0306] Elemental Analysis: C, 85.38; H, 4.66; N, 9.96/ HRMS $[M]^+$: 562

Synthesis Example 2

Synthesis of Mat-2

[0307]





[0308] IC-7 (10 g, 35.44 mmol), sub-1 (10.2 g, 42.53 mmol), Cu powder (0.22 g, 3.544 mmol), K_2CO_3 (9.8 g, 70.88 mmol), Na_2SO_4 (10 g, 70.88 mmol), and nitrobenzene (350 ml) were mixed under nitrogen flow, and the resulting mixture was stirred at 190° C. for 12 hours.

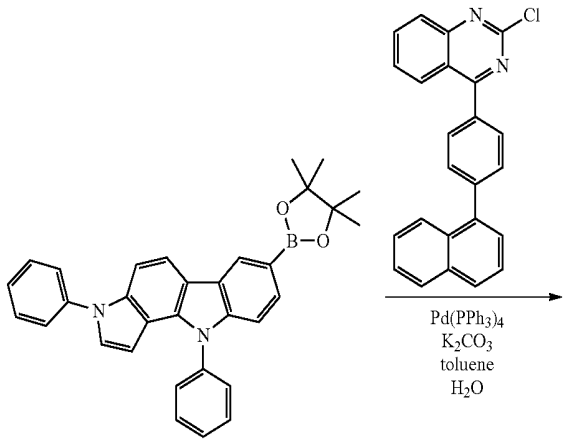
[0309] After the reaction was terminated, nitrobenzene was removed, the organic layer was separated by methylene chloride, and water was removed by using $MgSO_4$. Mat-2 (8.6 g, yield 50%) was obtained by removing the solvent from the organic layer from which water had been removed, and refinement was performed by column chromatography (Hexane:MC=3:1 (v:v)).

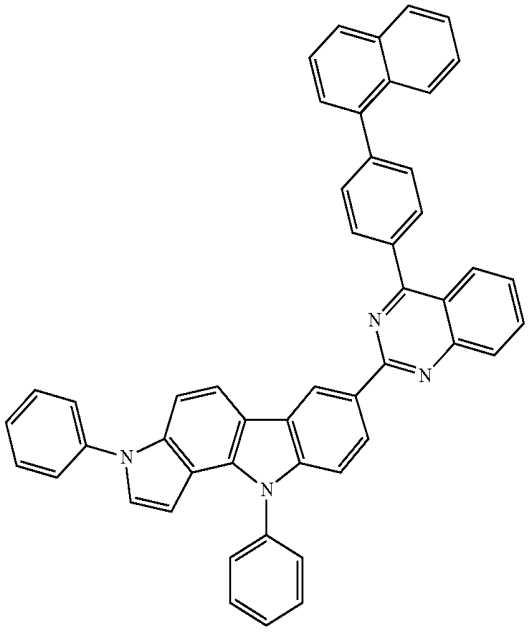
[0310] Elemental Analysis: C, 83.93; H, 4.56; N, 11.51/ HRMS $[M]^+$: 486

Synthesis Example 3

Synthesis of Mat-3

[0311]





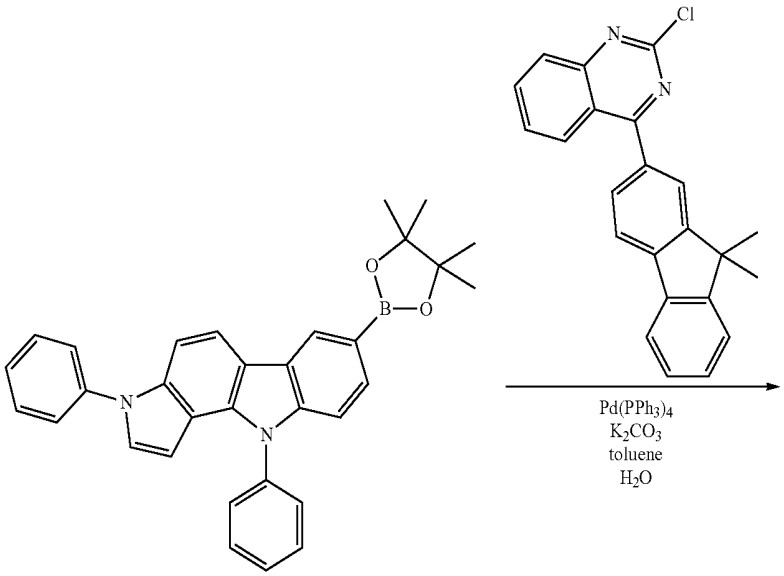
[0312] Mat-3 was obtained by performing the same procedure as in Synthesis Example 1, except that sub-2 was used instead of sub-1.

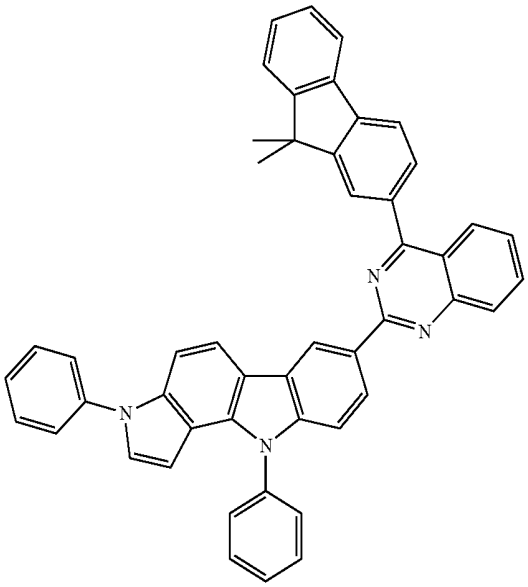
[0313] Elemental Analysis: C, 87.18; H, 4.68; N, 8.13/ HRMS $[M]^+$: 688

Synthesis Example 4

Synthesis of Mat-4

[0314]





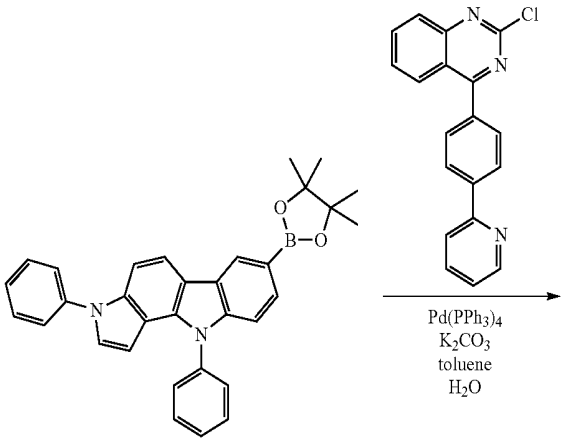
[0315] Mat-4 was obtained by performing the same procedure as in Synthesis Example 1, except that sub-3 was used instead of sub-1.

[0316] Elemental Analysis: C, 86.70; H, 5.05; N, 8.25/ HRMS $[M]^+$: 678

Synthesis Example 5

Synthesis of Mat-5

[0317]



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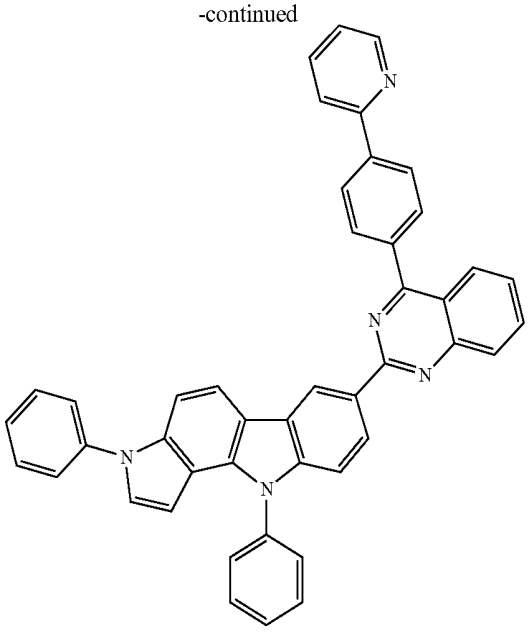


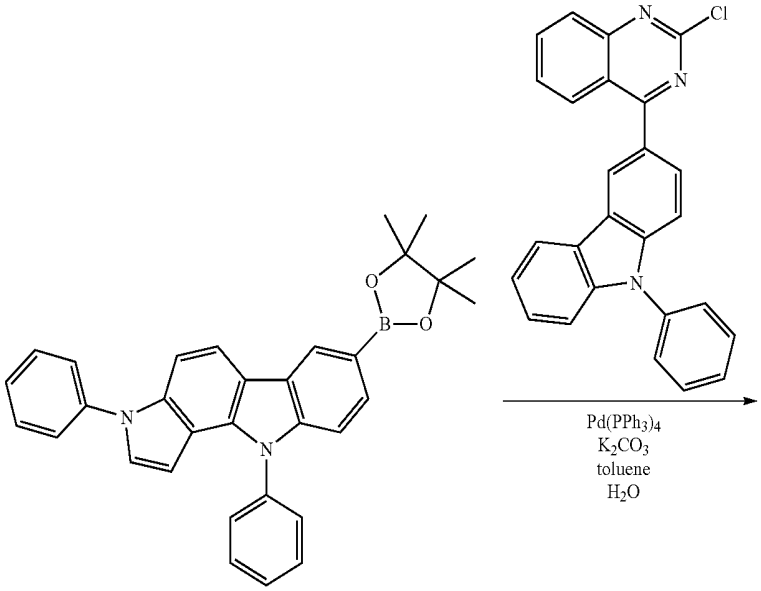
[0318] Mat-5 was obtained by performing the same procedure as in Synthesis Example 1, except that sub-4 was used instead of sub-1.

[0319] Elemental Analysis: C, 84.48; H, 4.57; N, 10.95/ HRMS $[M]^+$: 639

Synthesis Example 6

Synthesis of Mat-6

[0320]



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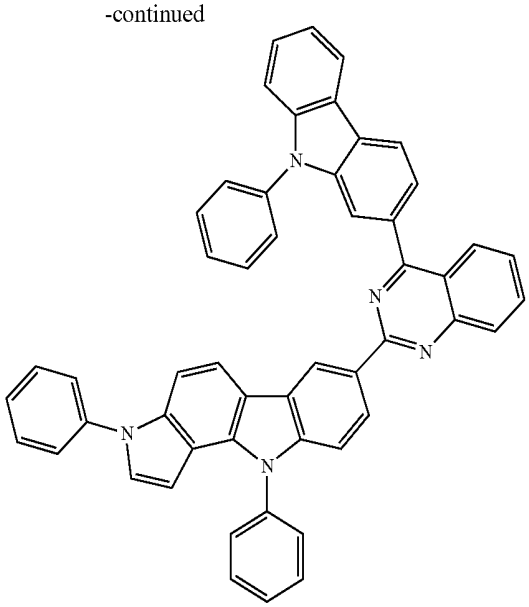


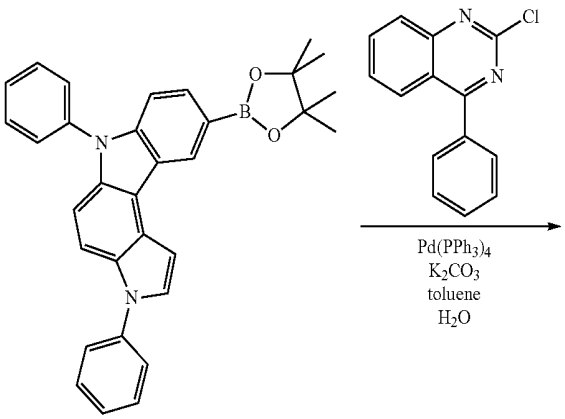
[0321] Mat-6 was obtained by performing the same procedure as in Synthesis Example 1, except that sub-5 was used instead of sub-1.

[0322] Elemental Analysis: C, 85.81; H, 4.57; N, 9.62/ HRMS $[M]^+$: 727

Synthesis Example 7

Synthesis of Mat-7

[0323]



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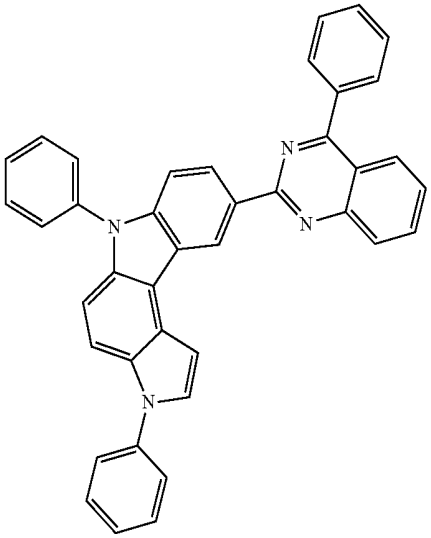


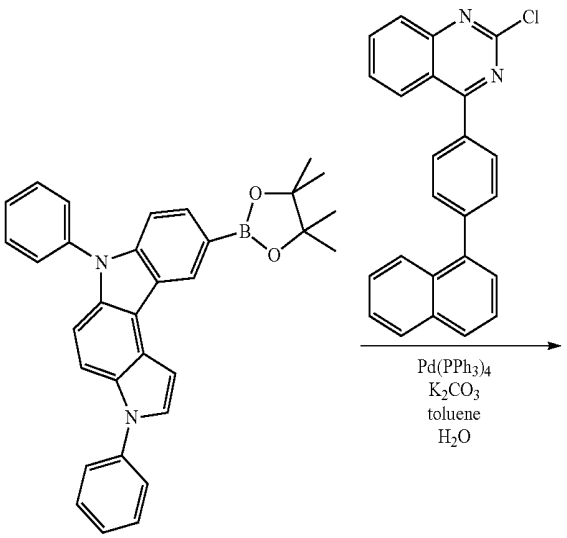
[0324] Mat-7 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-2 was used instead of IC-1.

[0325] Elemental Analysis: C, 85.38; H, 4.66; N, 9.96/ HRMS $[M]^+$: 562

Synthesis Example 8

Synthesis of Mat-8

[0326]



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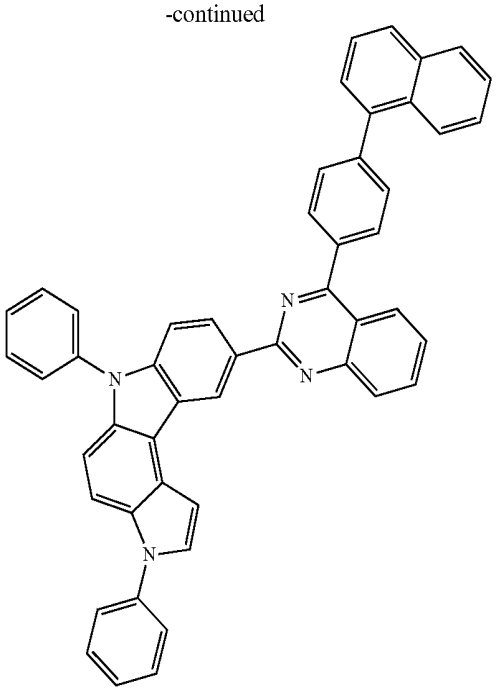


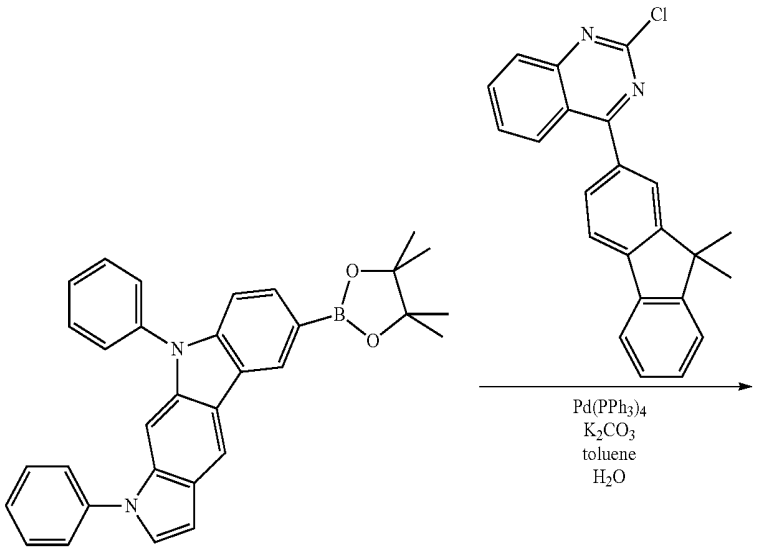
[0327] Mat-8 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-2 and sub-2 were used instead of IC-1 and sub-1, respectively.

[0328] Elemental Analysis: C, 87.18; H, 4.68; N, 8.13/ HRMS $[M]^+$: 688

Synthesis Example 9

Synthesis of Mat-9

[0329]



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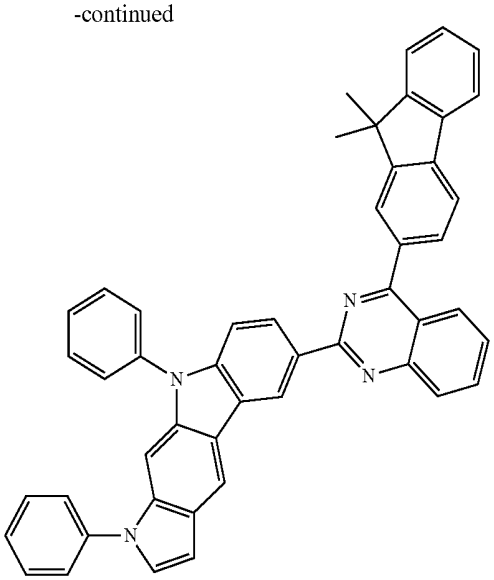


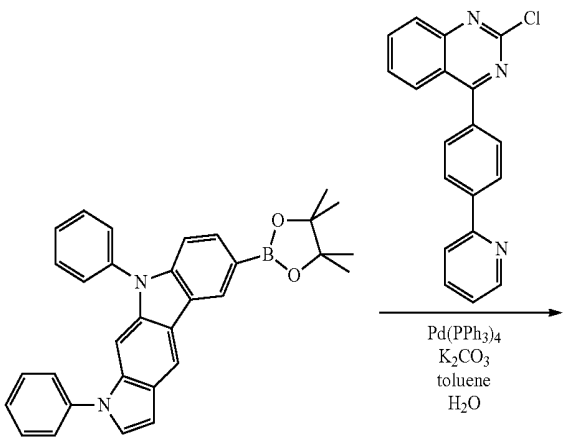
[0330] Mat-9 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-3 and sub-3 were used instead of IC-1 and sub-1, respectively.

[0331] Elemental Analysis: C, 86.70; H, 5.05; N, 8.25/ HRMS $[M]^+$: 678

Synthesis Example 10

Synthesis of Mat-10

[0332]



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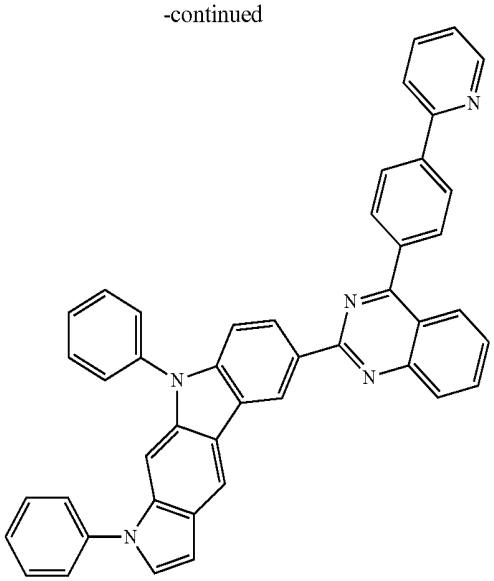


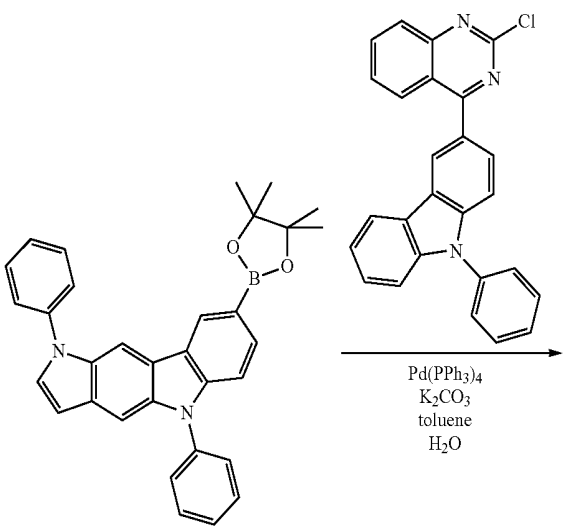
[0333] Mat-10 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-3 and sub-4 were used instead of IC-1 and sub-1, respectively.

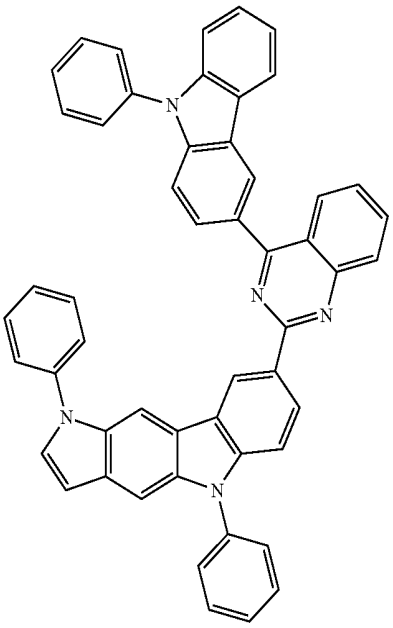
[0334] Elemental Analysis: C, 84.48; H, 4.57; N, 10.95/ HRMS $[M]^+$: 639

Synthesis Example 11

Synthesis of Mat-11

[0335]





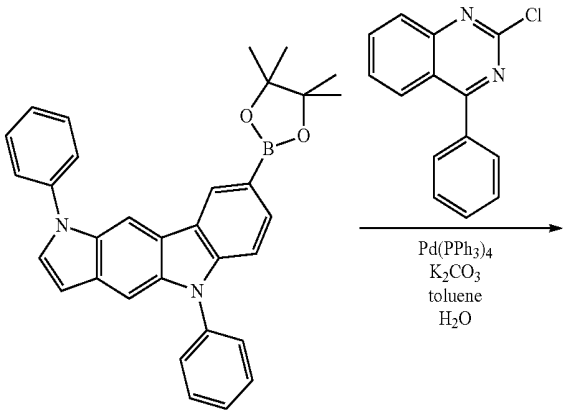
[0336] Mat-11 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-4 and sub-5 were used instead of IC-1 and sub-1, respectively.

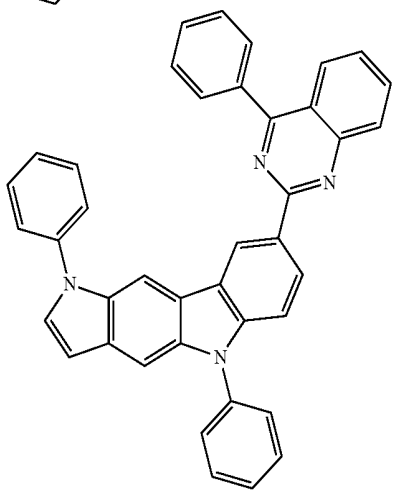
[0337] Elemental Analysis: C, 85.81; H, 4.57; N, 9.62/ HRMS $[M]^+$: 727

Synthesis Example 12

Synthesis of Mat-12

[0338]





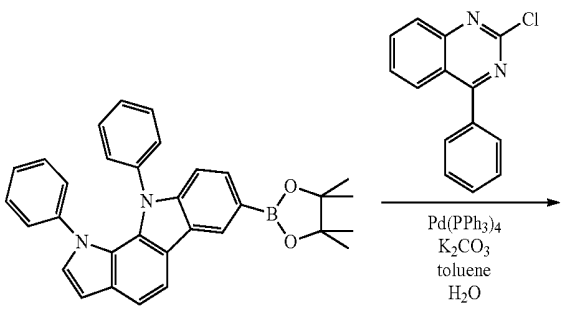
[0339] Mat-12 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-4 was used instead of IC-1.

[0340] Elemental Analysis: C, 85.38; H, 4.66; N, 9.96/ HRMS $[M]^+$: 562

Synthesis Example 13

Synthesis of Mat-13

[0341]



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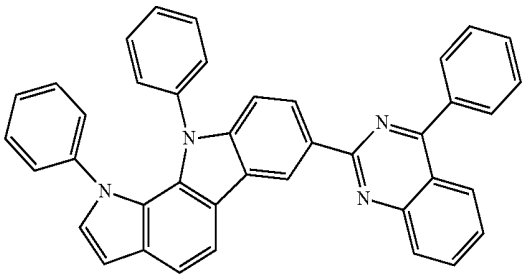


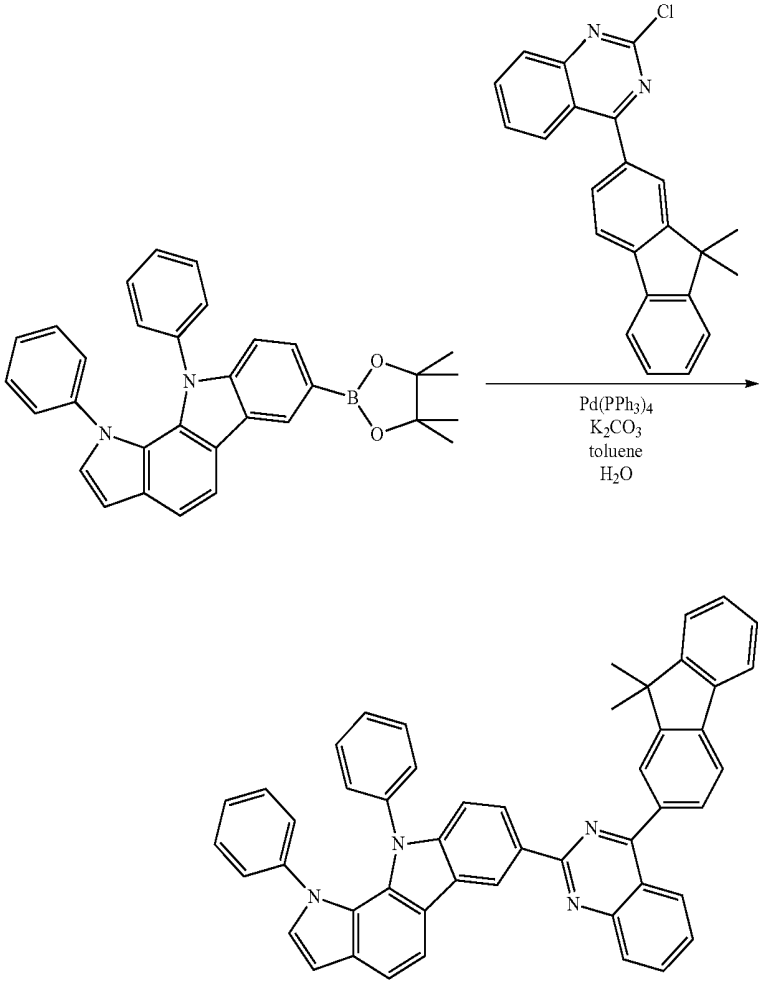
[0342] Mat-13 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-5 was used instead of IC-1.

[0343] Elemental Analysis: C, 85.38; H, 4.66; N, 9.96/ HRMS $[M]^+$: 562

Synthesis Example 14

Synthesis of Mat-14

[0344]



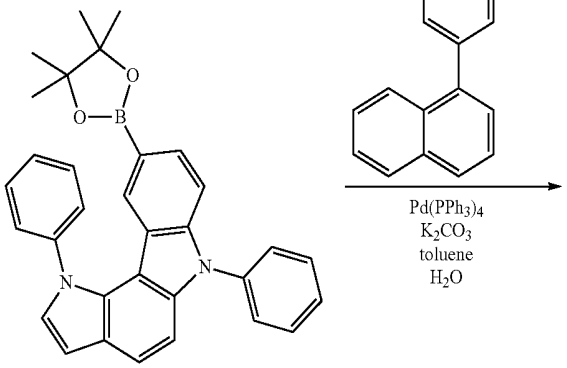
[0345] Mat-14 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-5 and sub-3 were used instead of IC-1 and sub-1, respectively.

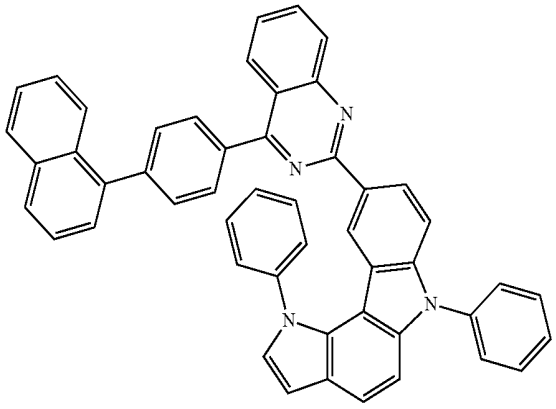
Elemental Analysis: C, 86.70; H, 5.05; N, 8.25/HRMS $[M]^+$: 678

Synthesis Example 15

Synthesis of Mat-15

[0346]





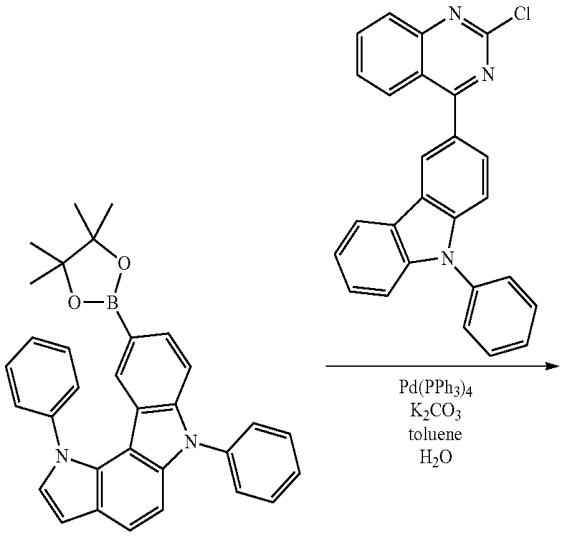
[0347] Mat-15 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-6 and sub-2 were used instead of IC-1 and sub-1, respectively.

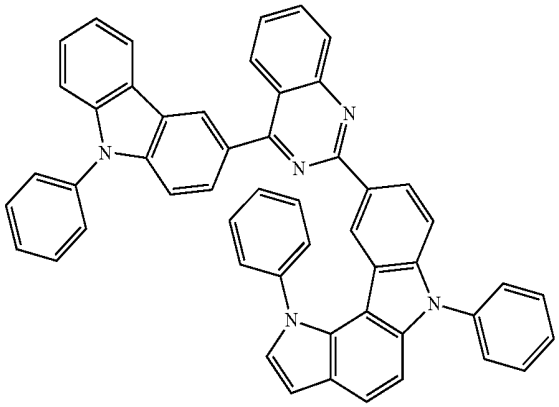
[0348] Elemental Analysis: C, 87.18; H, 4.68; N, 8.13/HRMS $[M]^+$: 688

Synthesis Example 16

Synthesis of Mat-16

[0349]





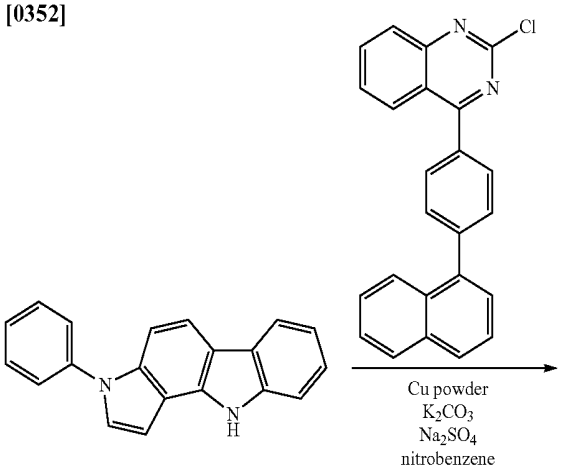
[0350] Ma-16 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-6 and sub-5 were used instead of IC-1 and sub-1, respectively.

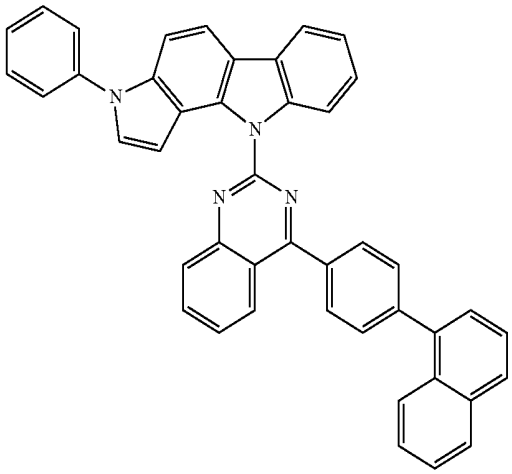
[0351] Elemental Analysis: C, 85.81; H, 4.57; N, 9.62/HRMS $[M]^+$: 727

Synthesis Example 17

Synthesis of Mat-17

[0352]





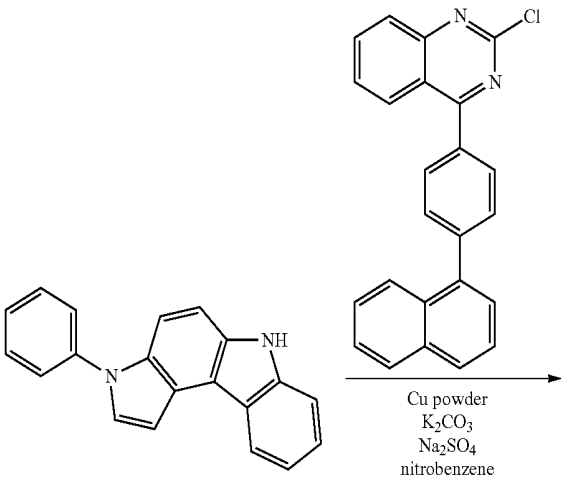
[0353] Mat-17 was obtained by performing the same procedure as in Synthesis Example 2, except that sub-2 was used instead of sub-1.

[0354] Elemental Analysis: C, 86.25; H, 4.61; N, 9.14/ HRMS $[M]^+$: 612

Synthesis Example 18

Synthesis of Mat-18

[0355]



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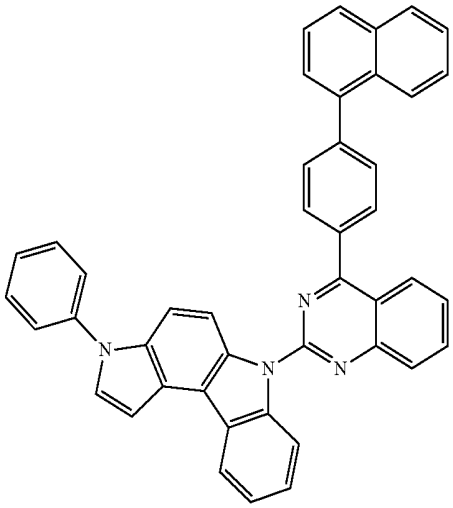


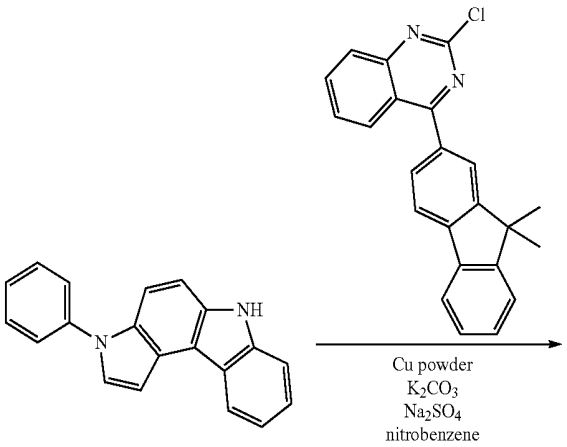
[0356] Mat-18 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-8 and sub-2 were used instead of IC-7 and sub-1, respectively.

[0357] Elemental Analysis: C, 86.25; H, 4.61; N, 9.14/ HRMS $[M]^+$: 612

Synthesis Example 19

Synthesis of Mat-19

[0358]



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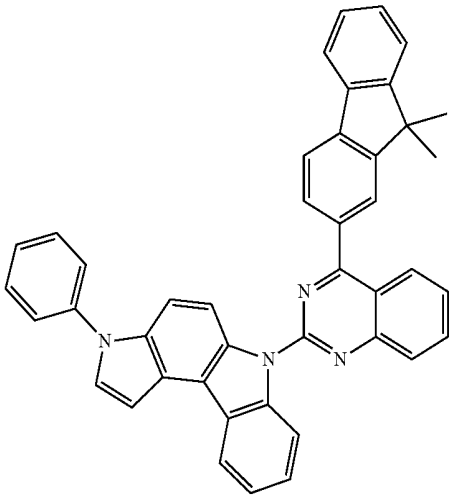


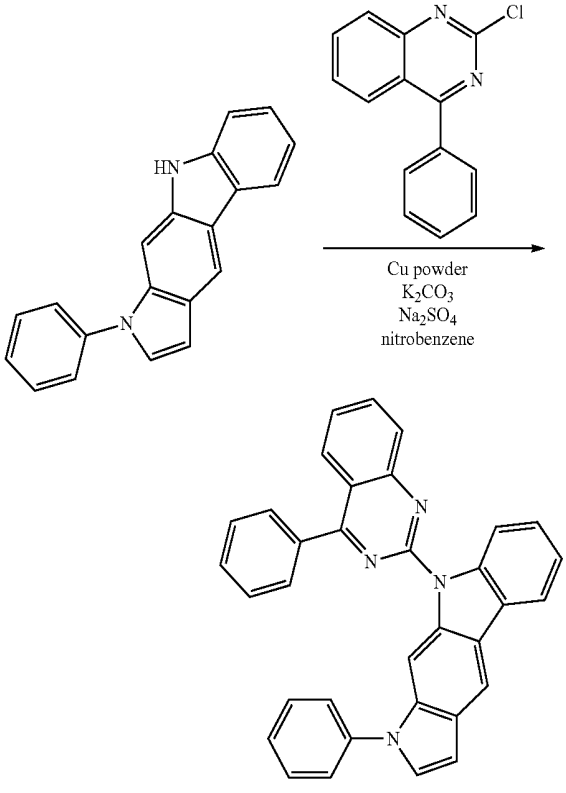
[0359] Mat-19 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-8 and sub-3 were used instead of IC-7 and sub-1, respectively.

[0360] Elemental Analysis: C, 85.69; H, 5.02; N, 9.30/ HRMS $[M]^+$: 602

Synthesis Example 20

Synthesis of Mat-20

[0361]



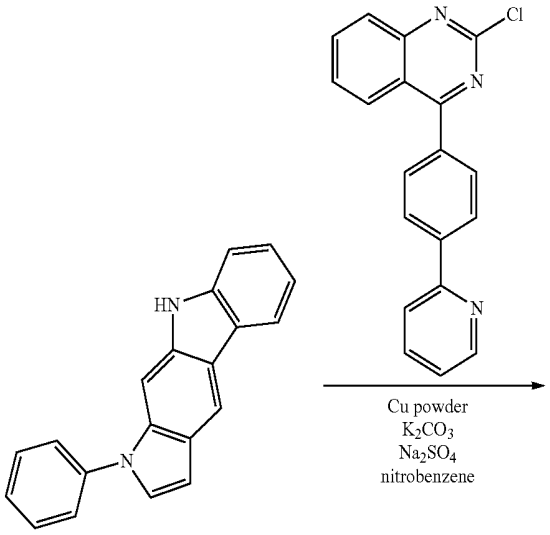
[0362] Mat-20 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-9 was used instead of IC-7.

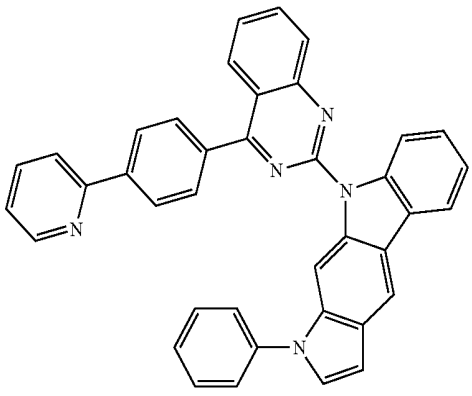
[0363] Elemental Analysis: C, 83.93; H, 4.56; N, 11.51/ HRMS $[M]^+$: 486

Synthesis Example 21

Synthesis of Mat-21

[0364]





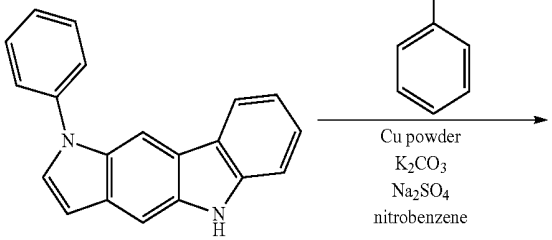
[0365] Mat-21 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-9 and sub-4 were used instead of IC-7 and sub-1, respectively.

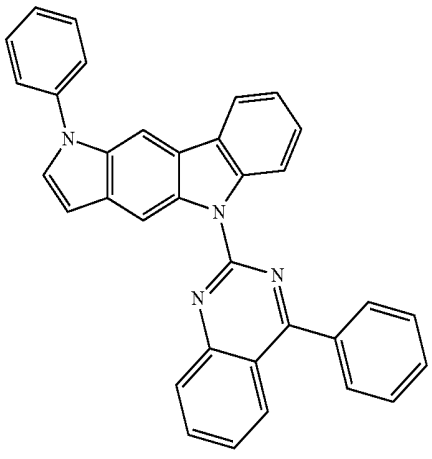
[0366] Elemental Analysis: C, 83.10; H, 4.47; N, 12.43/ HRMS $[M]^+$: 563

Synthesis Example 22

Synthesis of Mat-22

[0367]





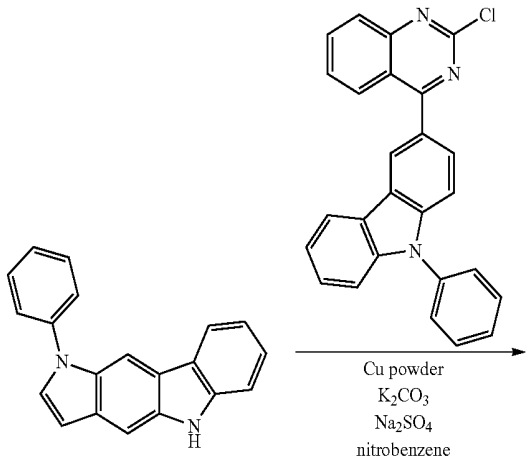
[0368] Mat-22 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-10 was used instead of IC-7.

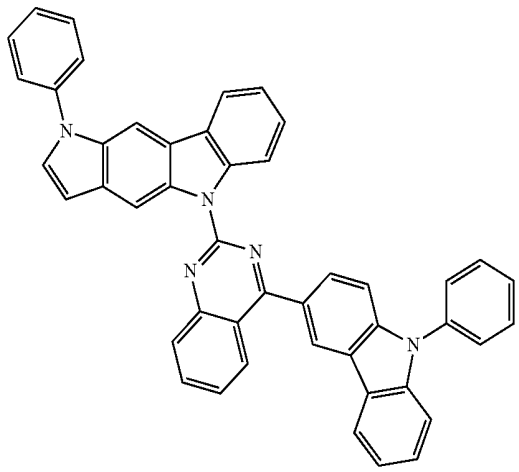
[0369] Elemental Analysis: C, 83.93; H, 4.56; N, 11.51/ HRMS $[M]^+$: 486

Synthesis Example 23

Synthesis of Mat-23

[0370]





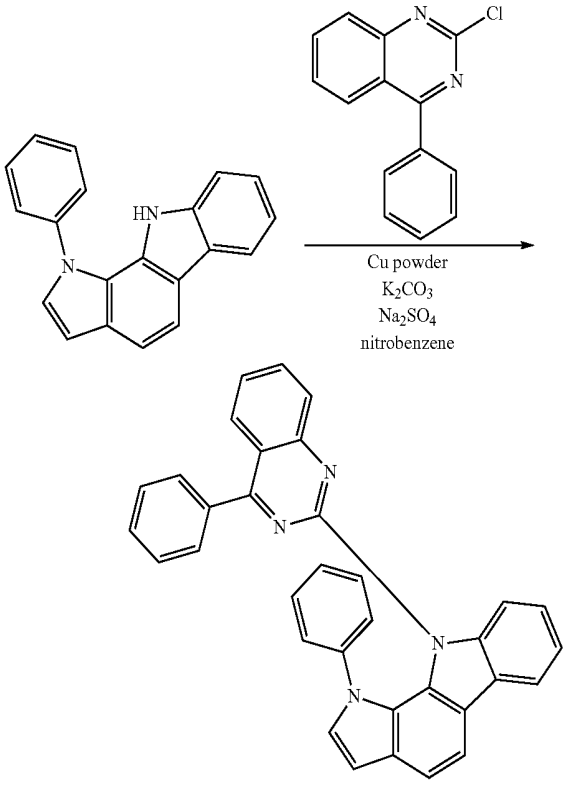
[0371] Mat-23 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-10 and sub-5 were used instead of IC-7 and sub-1, respectively.

[0372] Elemental Analysis: C, 84.77; H, 4.48; N, 10.75/ HRMS $[M]^+$: 651

Synthesis Example 24

Synthesis of Mat-24

[0373]



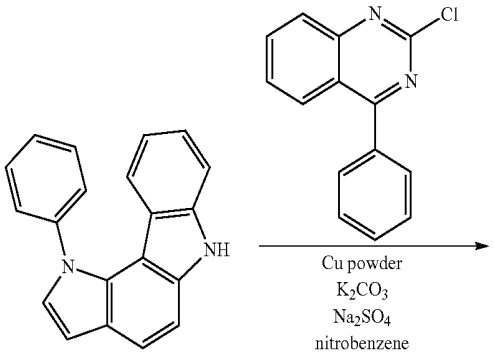
[0374] Mat-24 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-11 was used instead of IC-7.

[0375] Elemental Analysis: C, 83.93; H, 4.56; N, 11.51/ HRMS $[M]^+$: 486

Synthesis Example 25

Synthesis of Mat-25

[0376]



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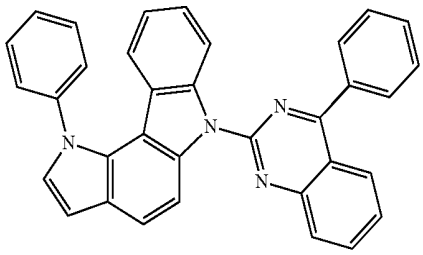


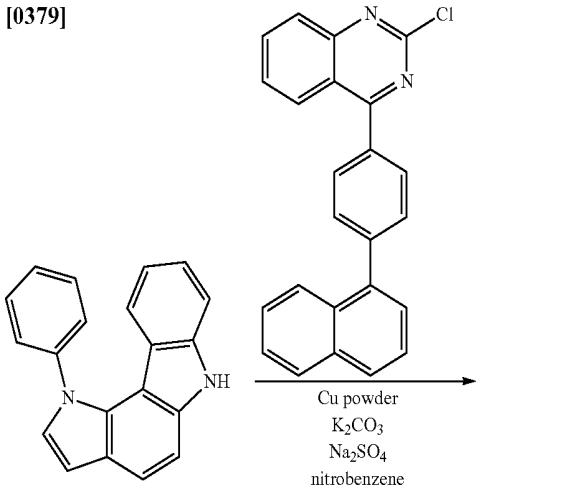
[0377] Mat-25 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-12 was used instead of IC-7.

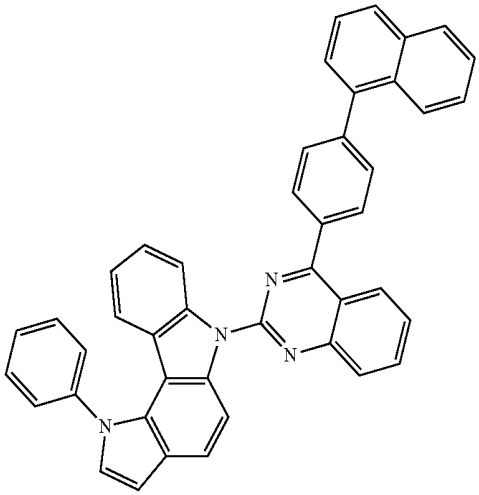
[0378] Elemental Analysis: C, 83.93; H, 4.56; N, 11.51/ HRMS $[M]^+$: 486

Synthesis Example 26

Synthesis of Mat-26

[0379]





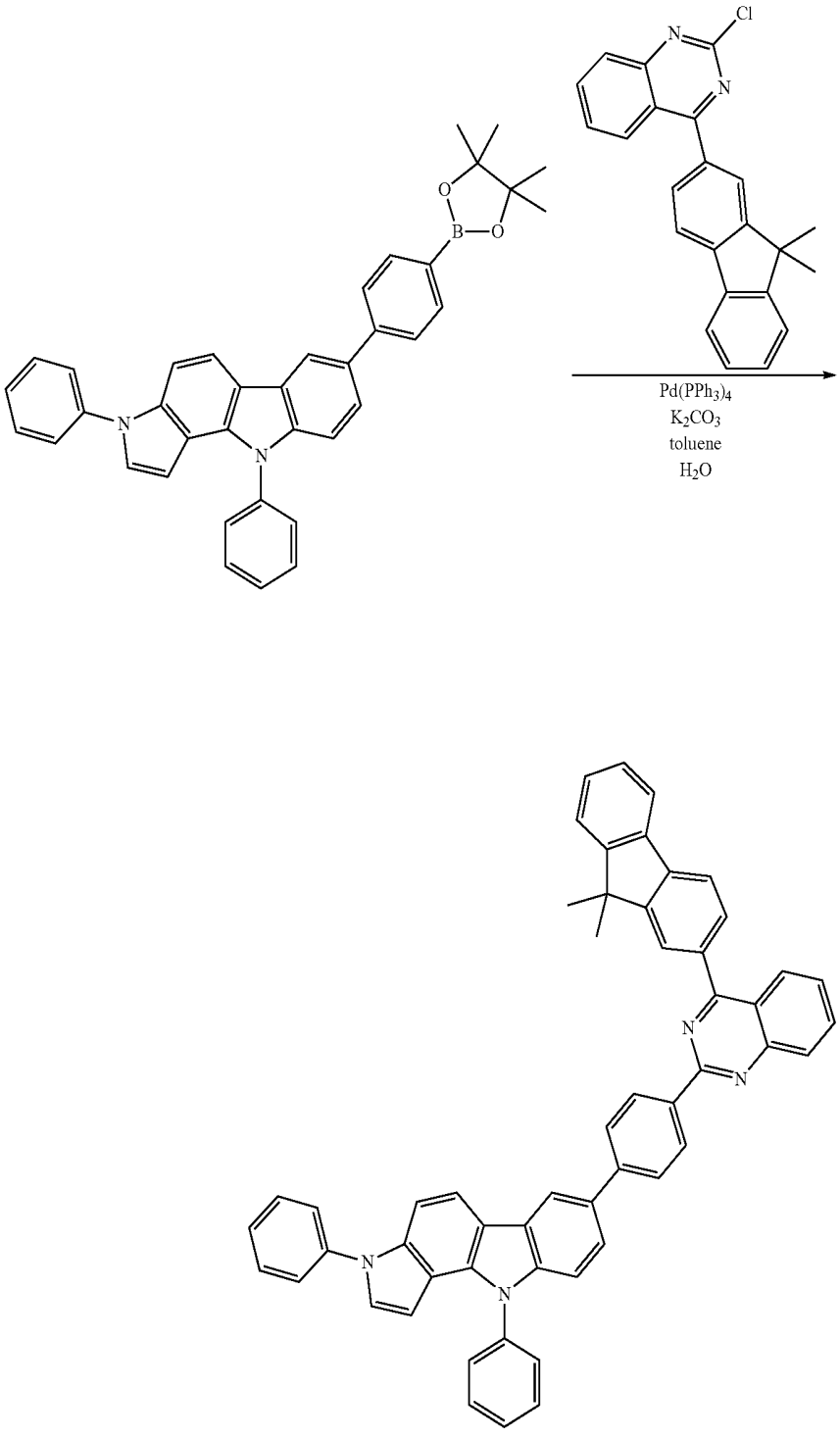
[0380] Mat-26 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-12 and sub-2 were used instead of IC-7 and sub-1, respectively.

[0381] Elemental Analysis: C, 86.25; H, 4.61; N, 9.14/ HRMS $[M]^+$: 616

Synthesis Example 27

Synthesis of Mat-27

[0382]



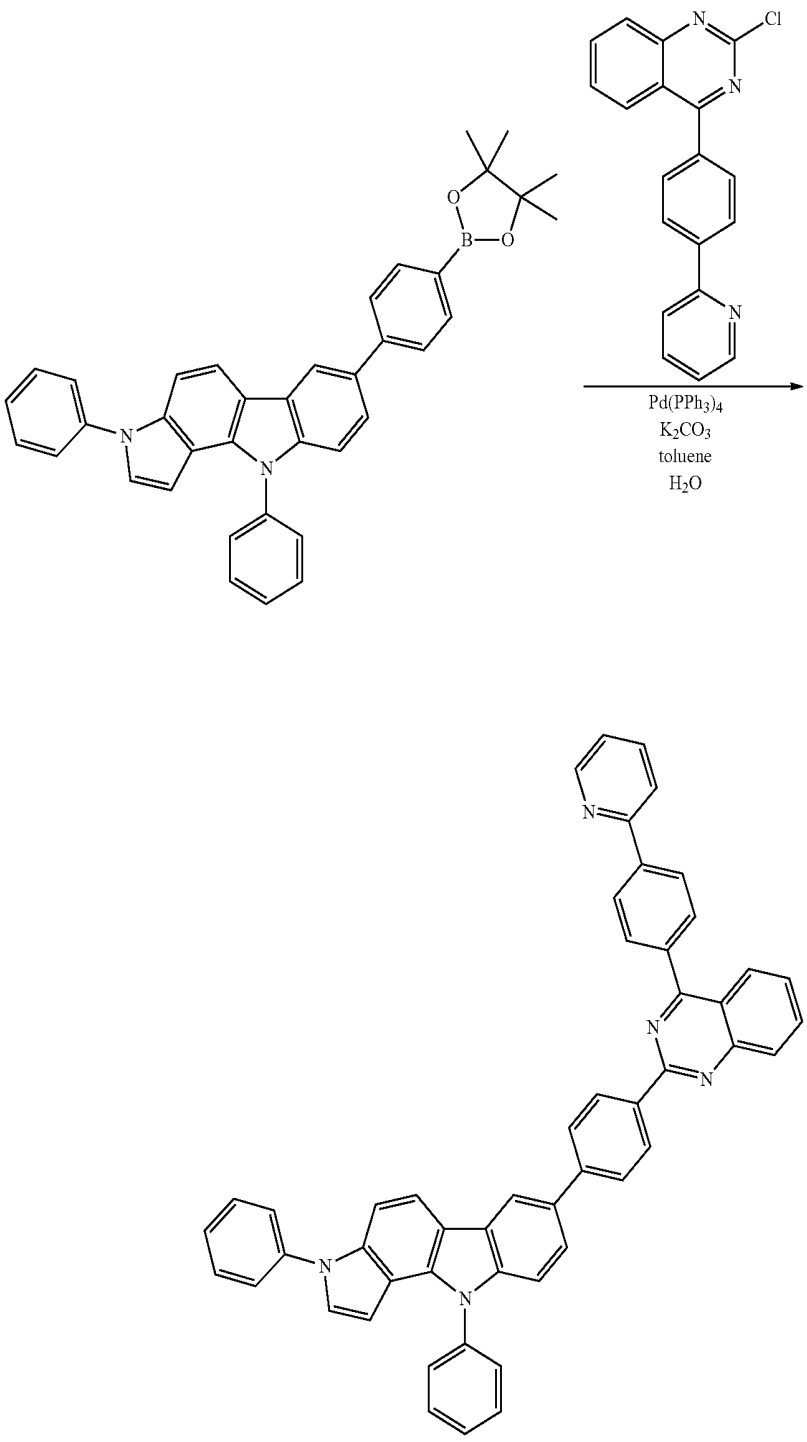
[0383] Mat-27 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-13 and sub-3 were used instead of IC-1 and sub-1, respectively.

[0384] Elemental Analysis: C, 87.50; H, 5.07; N, 7.42/ HRMS $[M]^+$: 754

Synthesis Example 28

Synthesis of Mat-28

[0385]



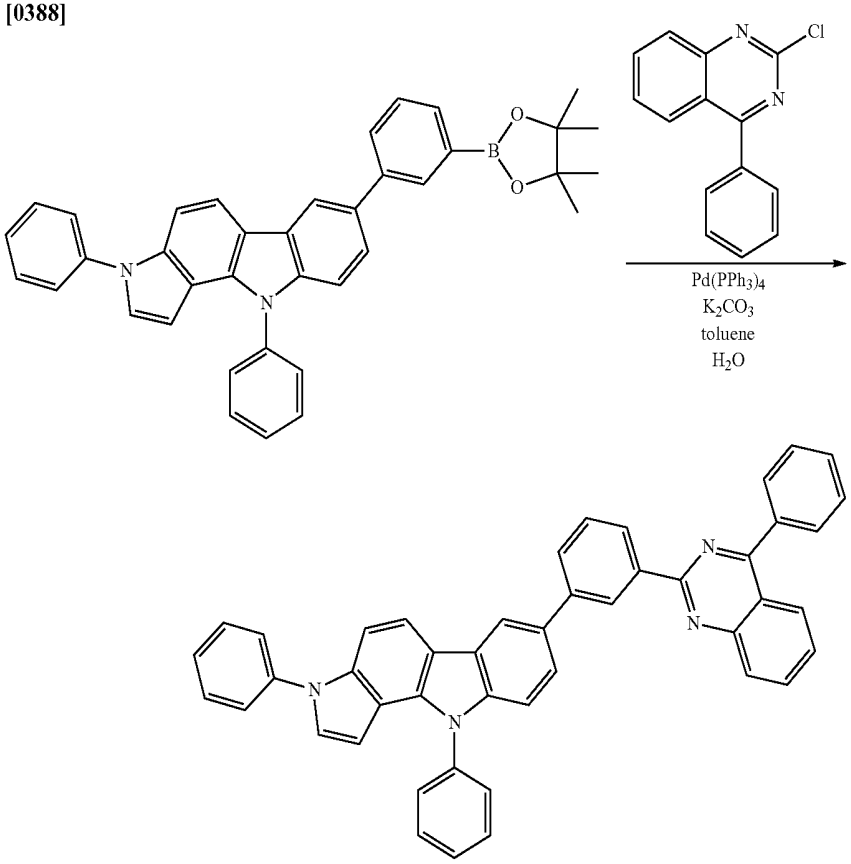
[0386] Mat-28 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-13 and sub-4 were used instead of IC-1 and sub-1, respectively.

[0387] Elemental Analysis: C, 85.57; H, 4.65; N, 9.78/ HRMS $[M]^+$: 715

Synthesis Example 29

Synthesis of Mat-29

[0388]



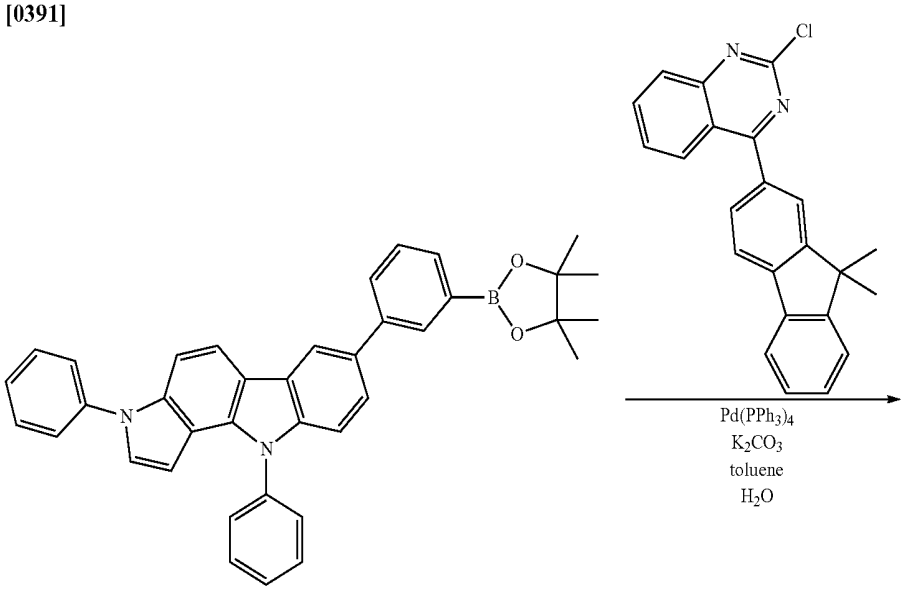
[0389] Mat-29 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-14 was used instead of IC-1.

[0390] Elemental Analysis: C, 86.49; H, 4.73; N, 8.77/ HRMS $[M]^+$: 638

Synthesis Example 30

Synthesis of Mat-30

[0391]



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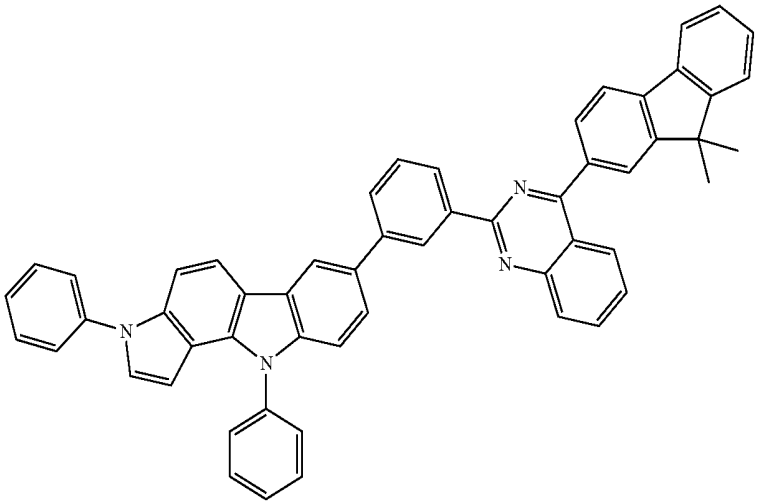


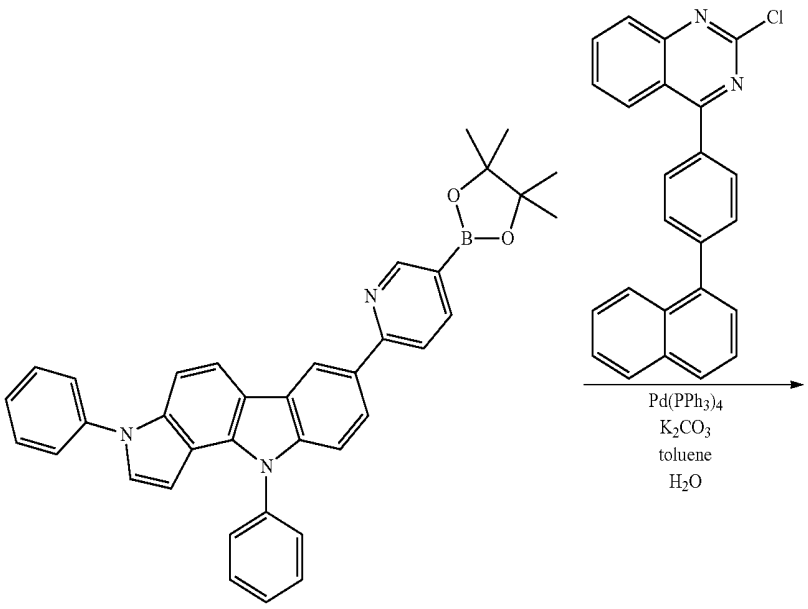
[0392] Mat-30 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-14 and sub-3 were used instead of IC-1 and sub-1, respectively.

[0393] Elemental Analysis: C, 87.50; H, 5.07; N, 7.42/ HRMS $[M]^+$: 754

Synthesis Example 31

Synthesis of Mat-31

[0394]



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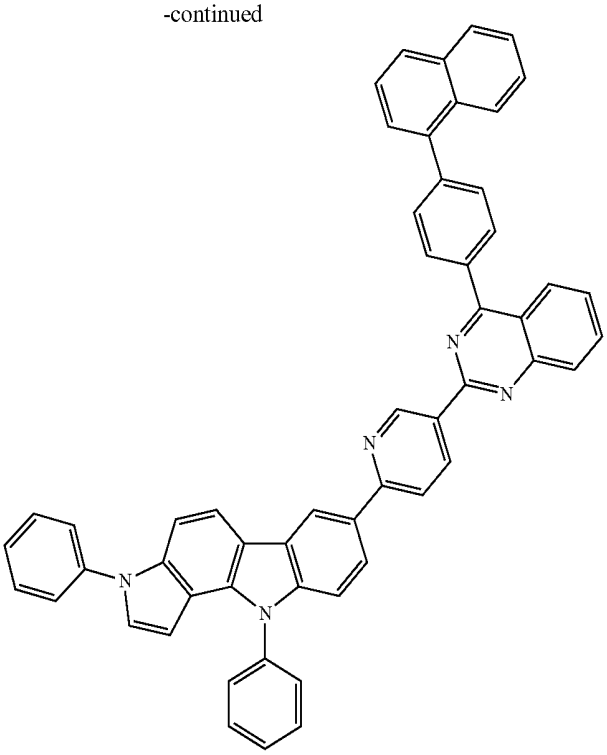


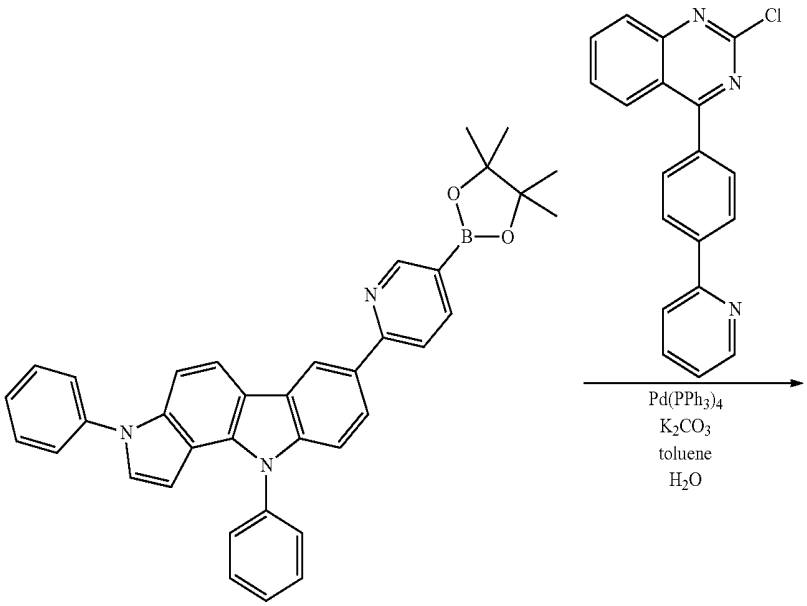
[0395] Mat-31 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-15 and sub-2 were used instead of IC-1 and sub-1, respectively.

[0396] Elemental Analysis: C, 86.25; H, 4.61; N, 9.14/ HRMS $[M]^+$: 765

Synthesis Example 32

Synthesis of Mat-32

[0397]



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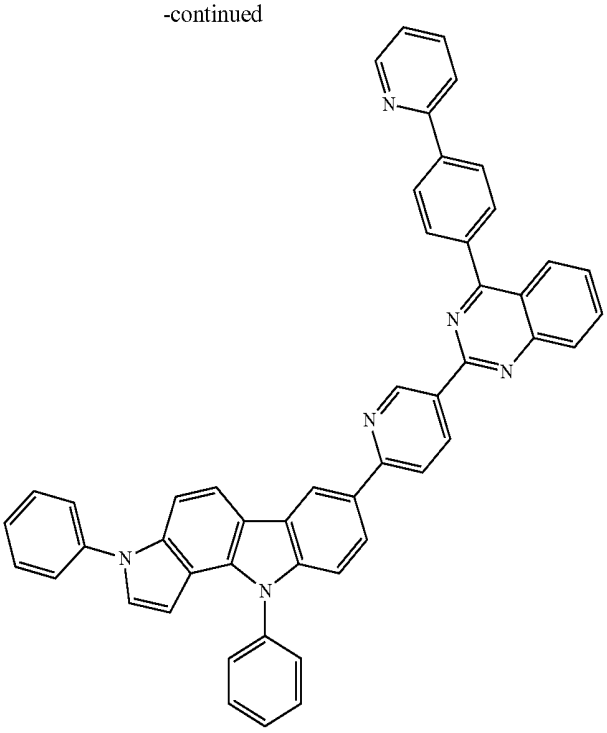


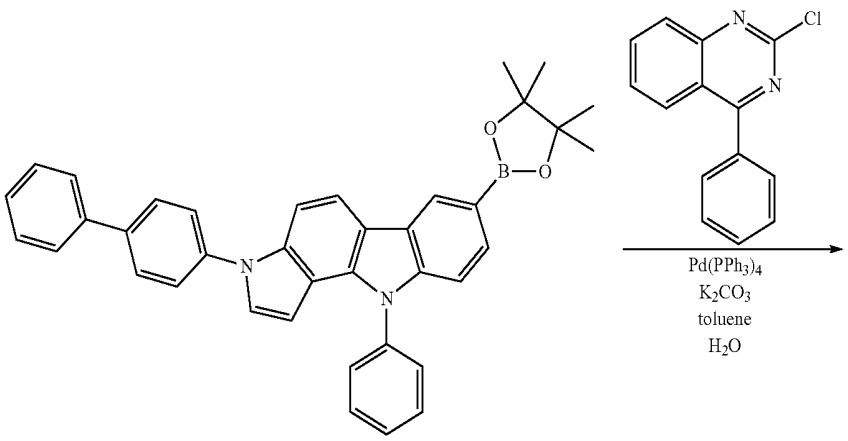
[0398] Mat-32 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-15 and sub-4 were used instead of IC-1 and sub-1, respectively.

[0399] Elemental Analysis: C, 83.78; H, 4.50; N, 11.72/ HRMS $[M]^+$: 716

Synthesis Example 33

Synthesis of Mat-33

[0400]



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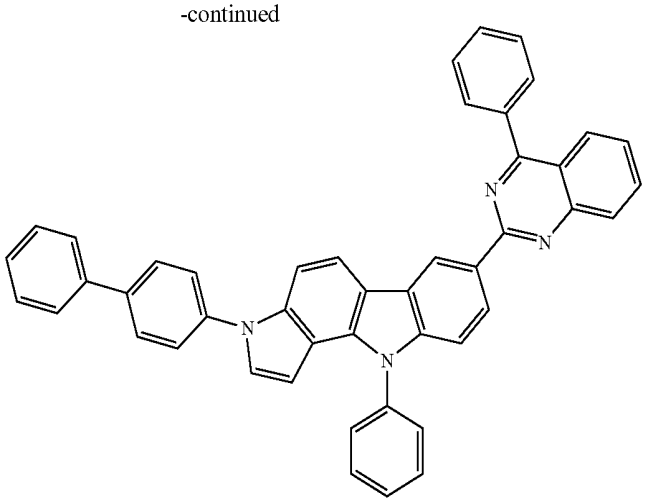


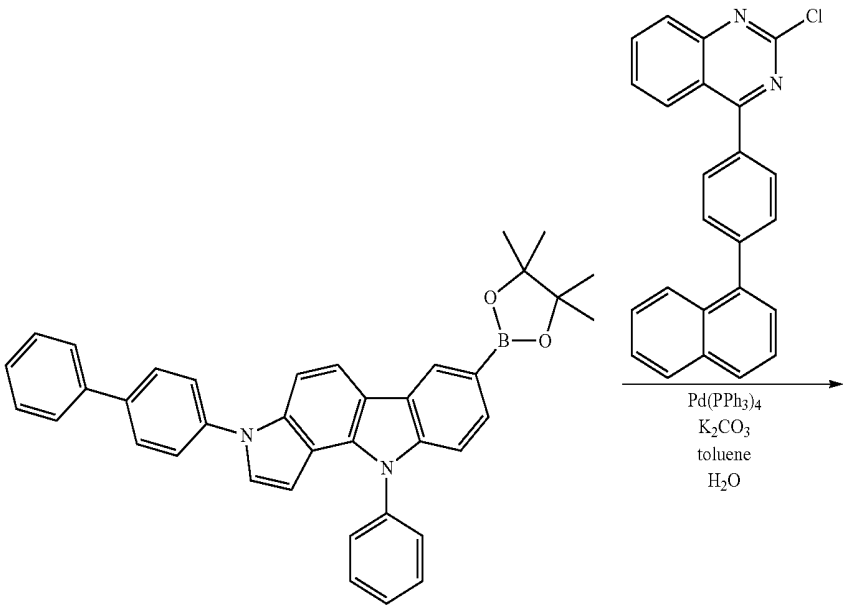
[0401] Mat-33 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-16 was used instead of IC-1.

[0402] Elemental Analysis: C, 86.49; H, 4.73; N, 8.77/ HRMS $[M]^+$: 638

Synthesis Example 34

Synthesis of Mat-34

[0403]



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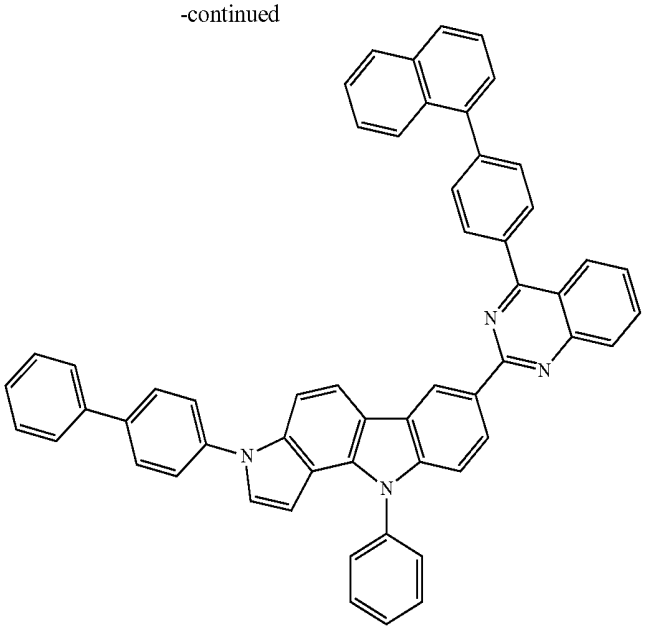


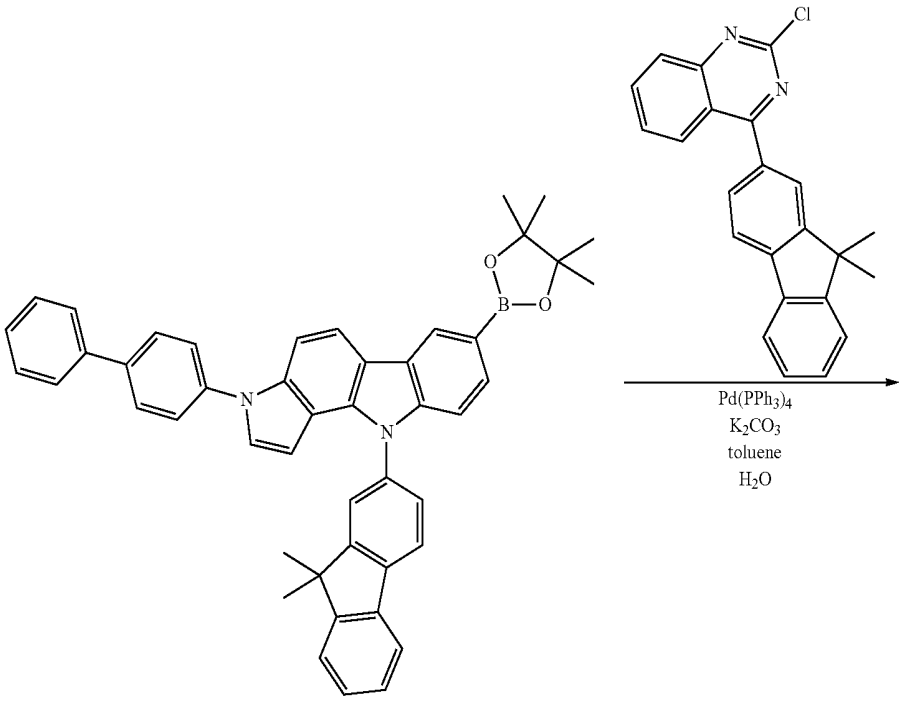
[0404] Mat-34 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-16 and sub-2 were used instead of IC-1 and sub-1, respectively.

[0405] Elemental Analysis: C, 87.93; H, 4.74; N, 7.32/ HRMS $[M]^+$: 764

Synthesis Example 35

Synthesis of Mat-35

[0406]



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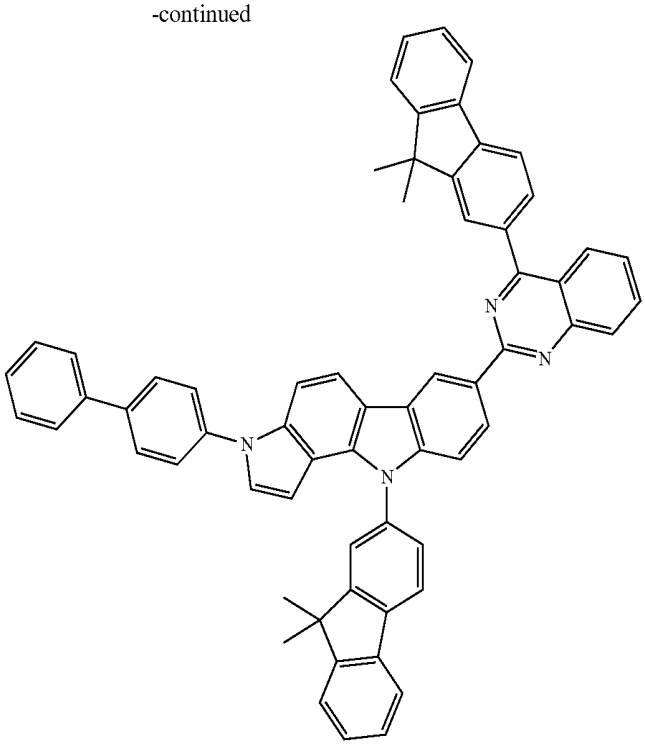


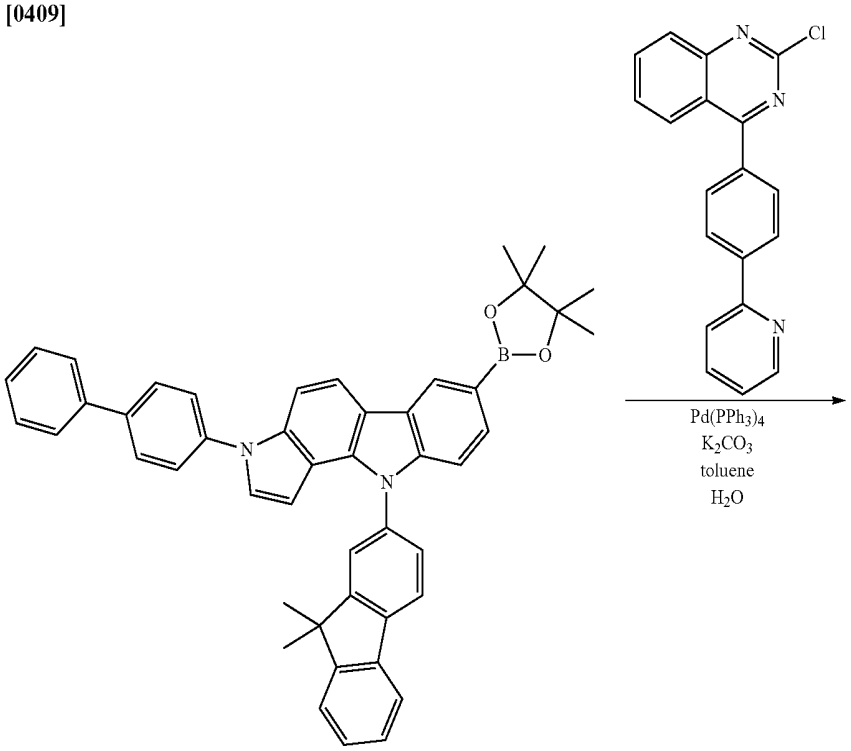
[0407] Mat-35 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-17 and sub-3 were used instead of IC-1 and sub-1, respectively.

[0408] Elemental Analysis: C, 88.25; H, 5.32; N, 6.43/ HRMS $[M]^+$: 870

Synthesis Example 36

Synthesis of Mat-36

[0409]



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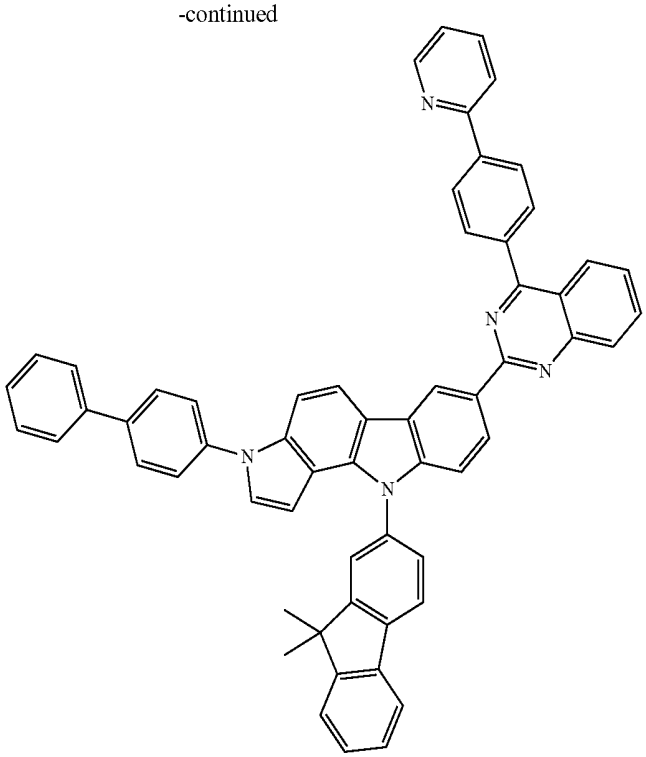


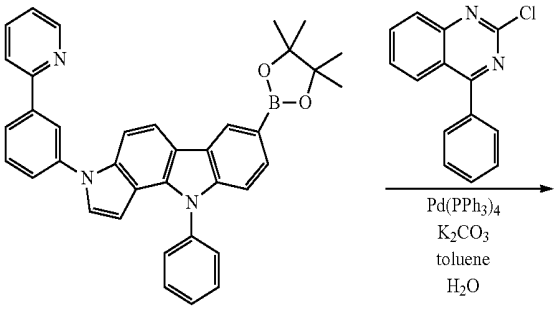
[0410] Mat-36 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-17 and sub-4 were used instead of IC-1 and sub-1, respectively.

[0411] Elemental Analysis: C, 86.62; H, 4.97; N, 8.42/ HRMS $[M]^+$: 831

Synthesis Example 37

Synthesis of Mat-37

[0412]



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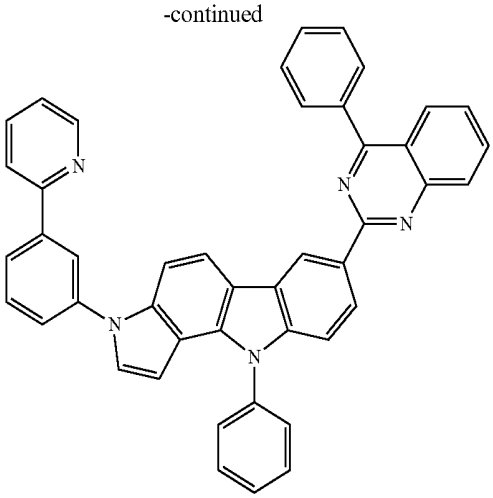


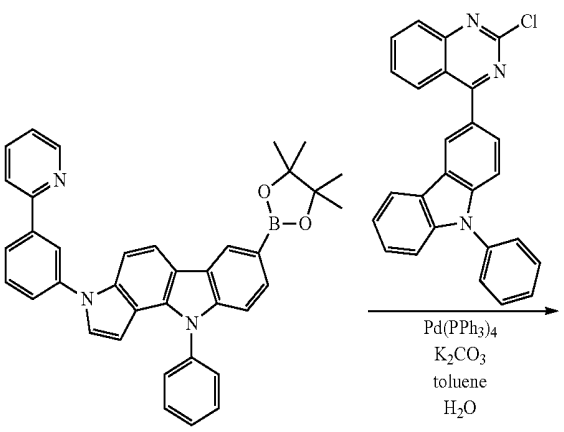
[0413] Mat-37 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-18 was used instead of IC-1.

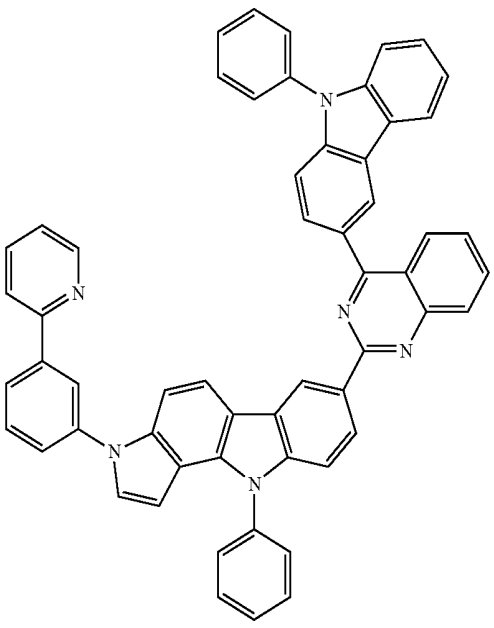
[0414] Elemental Analysis: C, 84.48; H, 4.57; N, 10.95/ HRMS $[M]^+$: 639

Synthesis Example 38

Synthesis of Mat-38

[0415]





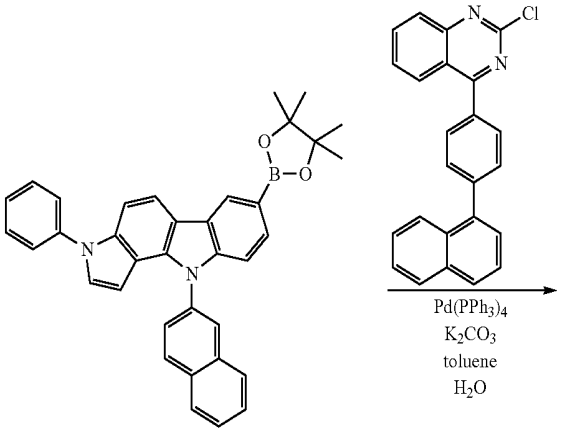
[0416] Mat-38 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-18 and sub-5 were used instead of IC-1 and sub-1, respectively.

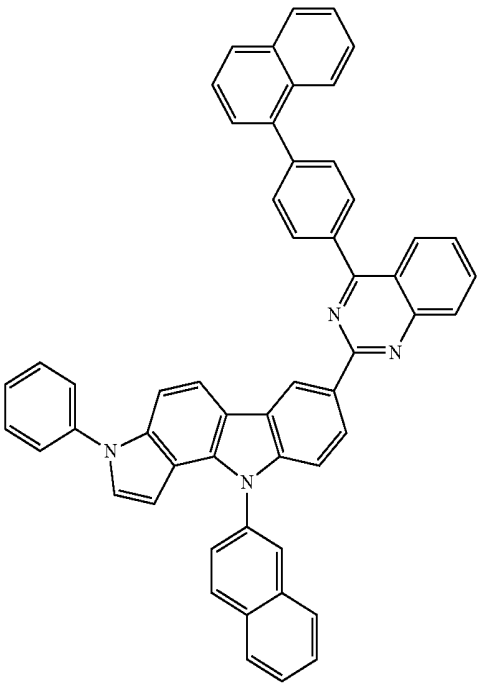
[0417] Elemental Analysis: C, 85.05; H, 4.51; N, 10.44/ HRMS $[M]^+$: 804

Synthesis Example 39

Synthesis of Mat-39

[0418]





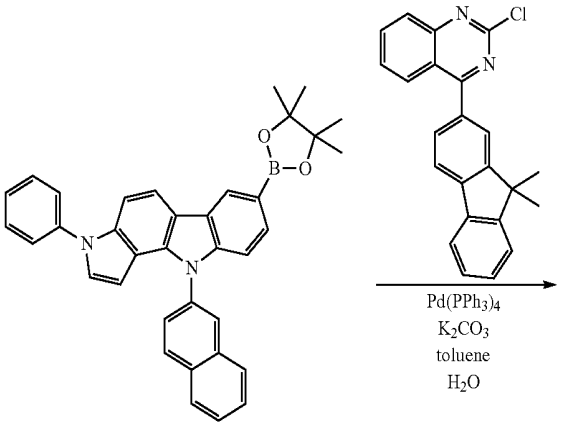
[0419] Mat-39 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-19 and sub-2 were used instead of IC-1 and sub-1, respectively.

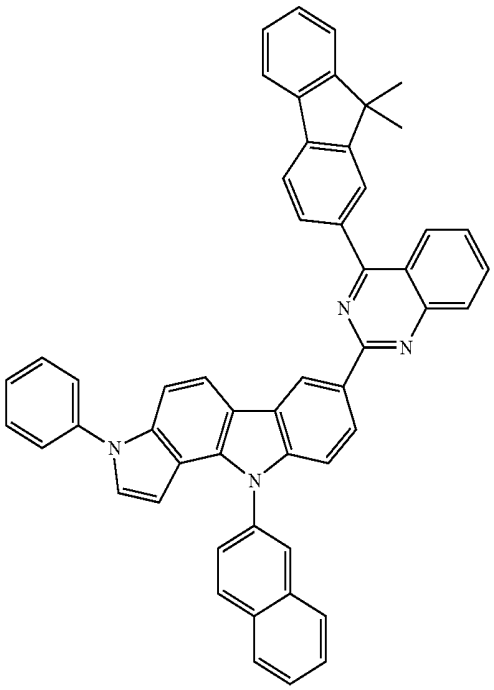
[0420] Elemental Analysis: C, 87.78; H, 4.64; N, 7.58/ HRMS $[M]^+$: 738

Synthesis Example 40

Synthesis of Mat-40

[0421]





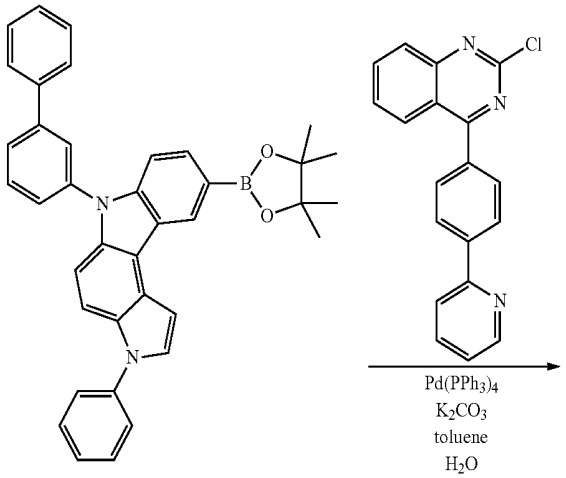
[0422] Mat-40 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-19 and sub-3 were used instead of IC-1 and sub-1, respectively.

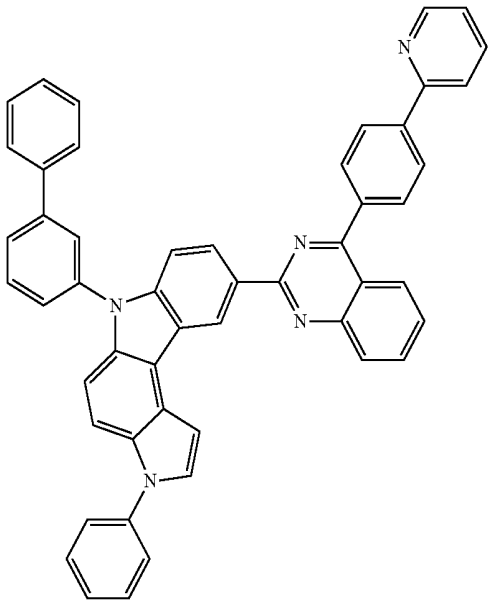
[0423] Elemental Analysis: C, 87.33; H, 4.98; N, 7.69/ HRMS $[M]^+$: 728

Synthesis Example 41

Synthesis of Mat-41

[0424]





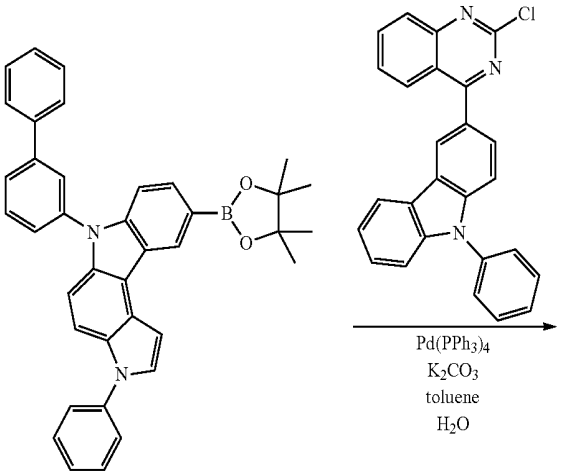
[0425] Mat-41 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-20 and sub-4 were used instead of IC-1 and sub-1, respectively.

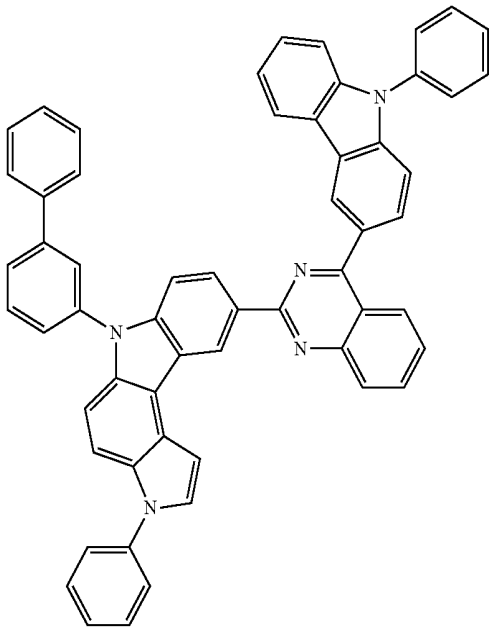
[0426] Elemental Analysis: C, 85.57; H, 4.65; N, 9.78/ HRMS $[M]^+$: 715

Synthesis Example 42

Synthesis of Mat-42

[0427]





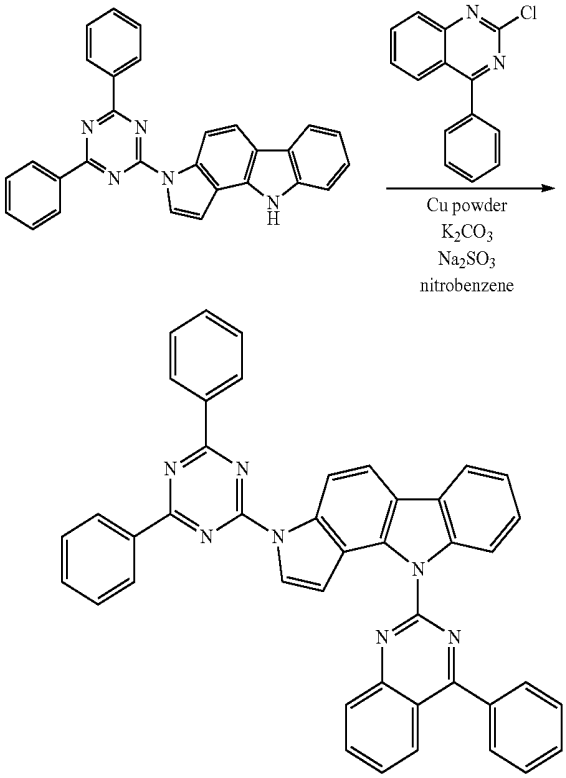
[0428] Mat-42 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-20 and sub-5 were used instead of IC-1 and sub-1, respectively.

[0429] Elemental Analysis: C, 86.65; H, 4.64; N, 8.71/ HRMS $[M]^+$: 803

Synthesis Example 43

Synthesis of Mat-43

[0430]



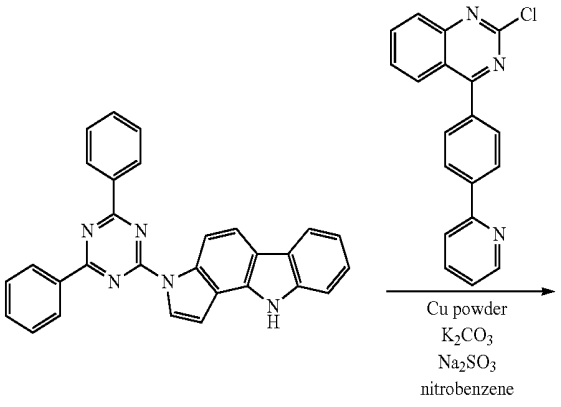
[0431] Mat-43 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-21 was used instead of IC-7.

[0432] Elemental Analysis: C, 80.48; H, 4.24; N, 15.28/ HRMS $[M]^+$: 641

Synthesis Example 44

Synthesis of Mat-44

[0433]



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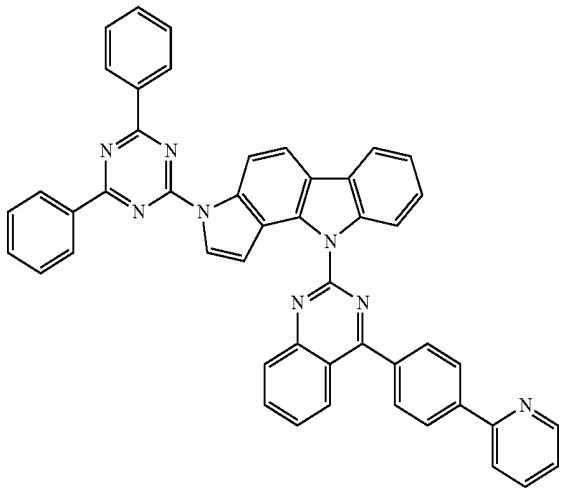

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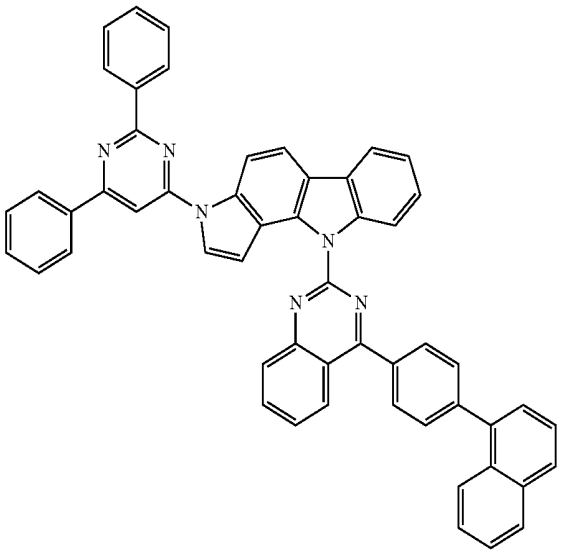


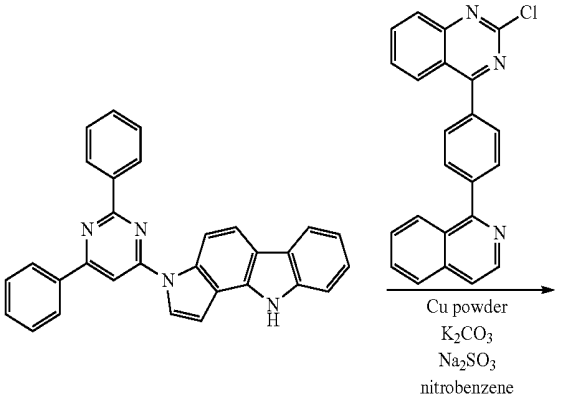
[0434] Mat-44 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-21 and sub-4 were used instead of IC-7 and sub-1, respectively.

[0435] Elemental Analysis: C, 80.20; H, 4.21; N, 15.59/ HRMS $[M]^+$: 718

Synthesis Example 45

Synthesis of Mat-45

[0436]



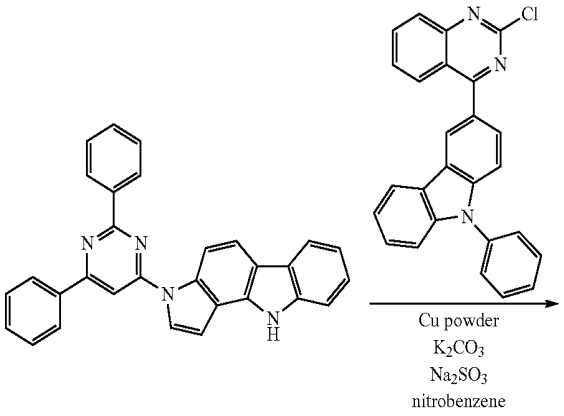
[0437] Mat-45 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-22 and sub-2 were used instead of IC-7 and sub-1, respectively.

[0438] Elemental Analysis: C, 84.57; H, 4.47; N, 10.96/ HRMS $[M]^+$: 766

Synthesis Example 46

Synthesis of Mat-46

[0439]



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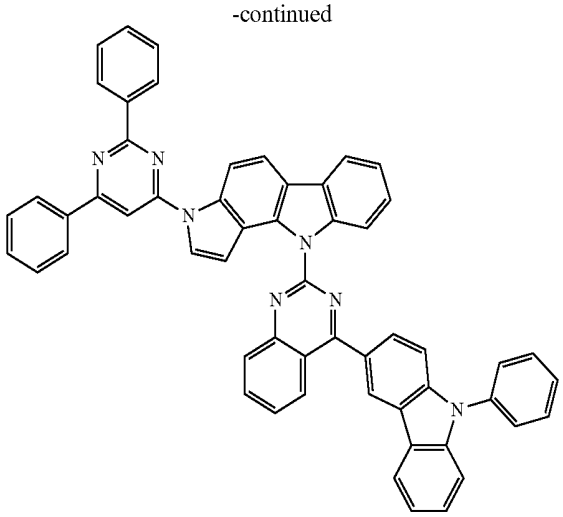


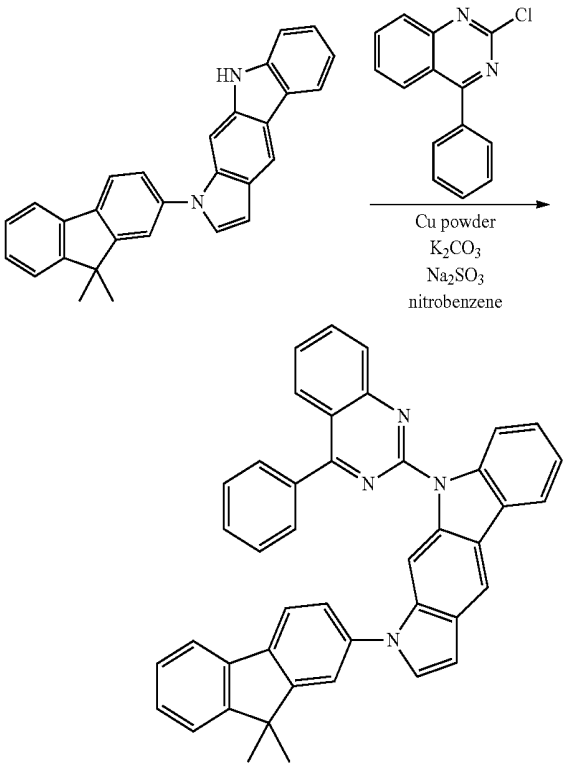
[0440] Mat-46 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-22 and sub-5 were used instead of IC-7 and sub-1, respectively.

[0441] Elemental Analysis: C, 83.46; H, 4.38; N, 12.17/ HRMS $[M]^+$: 805

Synthesis Example 47

Synthesis of Mat-47

[0442]



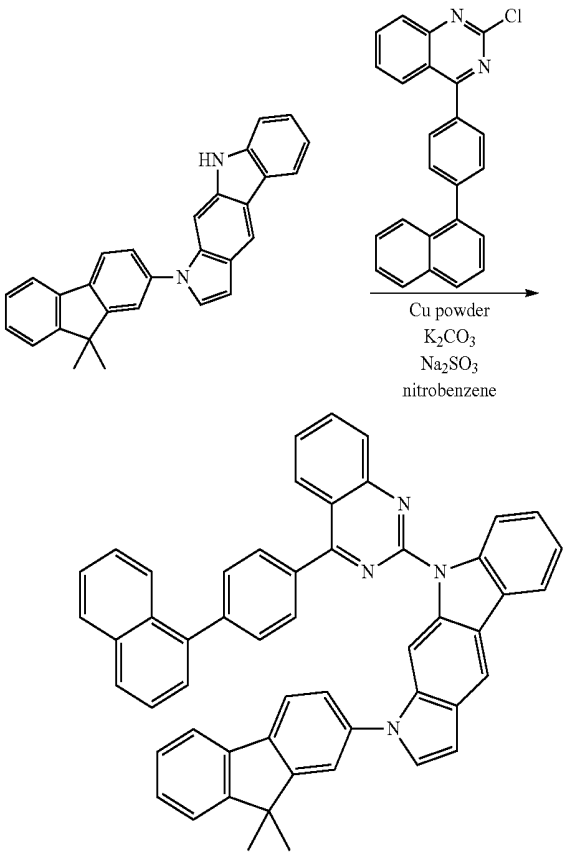
[0443] Mat-47 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-23 was used instead of IC-7.

[0444] Elemental Analysis: C, 85.69; H, 5.02; N, 9.30/ HRMS $[M]^+$: 602

Synthesis Example 48

Synthesis of Mat-48

[0445]



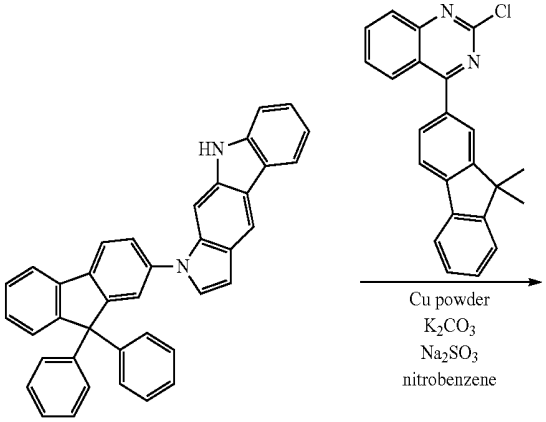
[0446] Mat-48 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-23 and sub-2 were used instead of IC-7 and sub-1, respectively.

[0447] Elemental Analysis: C, 87.33; H, 4.98; N, 7.69/ HRMS $[M]^+$: 728

Synthesis Example 49

Synthesis of Mat-49

[0448]



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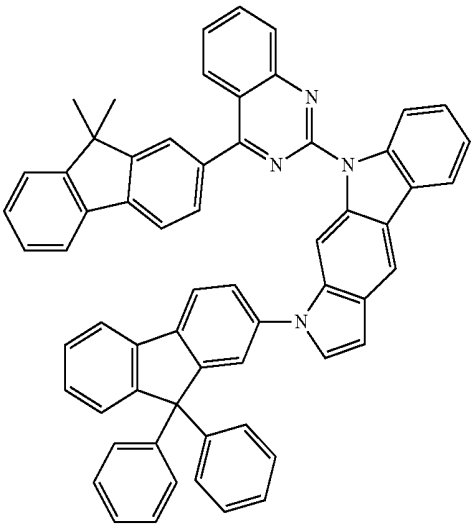


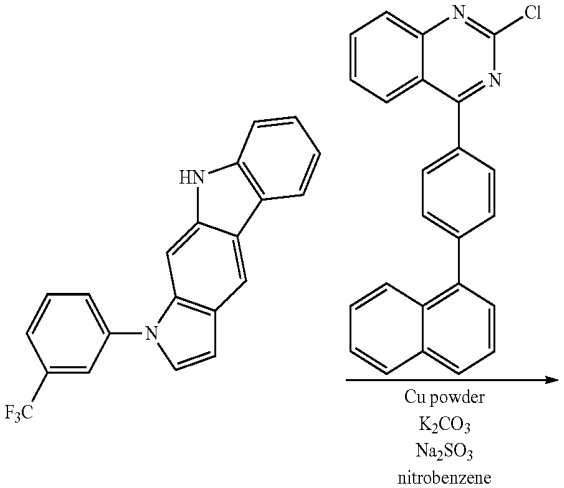
[0449] Mat-49 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-24 and sub-3 were used instead of IC-7 and sub-1, respectively.

[0450] Elemental Analysis: C, 88.33; H, 5.02; N, 6.65/ HRMS $[M]^+$: 842

Synthesis Example 50

Synthesis of Mat-50

[0451]



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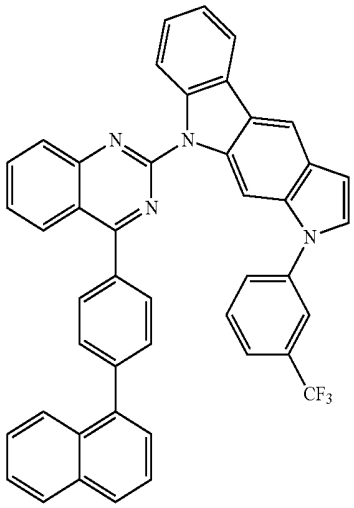


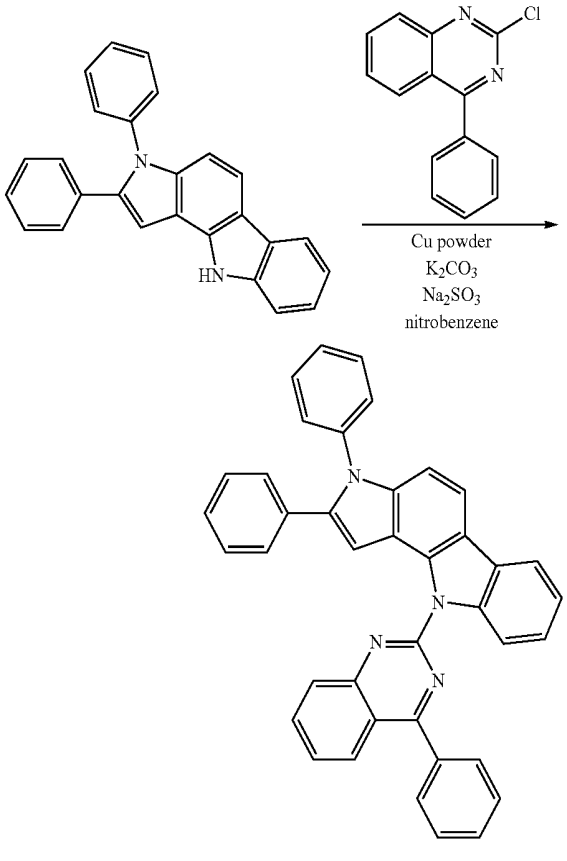
[0452] Mat-50 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-25 and sub-2 were used instead of IC-7 and sub-1, respectively.

[0453] Elemental Analysis: C, 79.40; H, 4.00; N, 8.23/ HRMS $[M]^+$: 680

Synthesis Example 51

Synthesis of Mat-51

[0454]



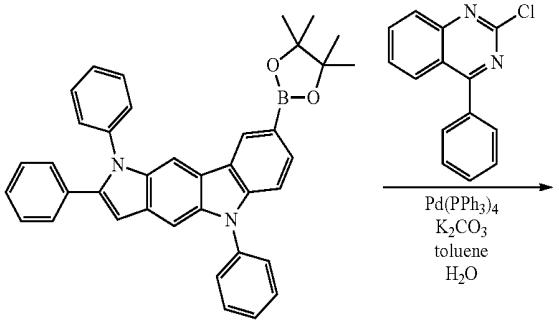
[0455] Mat-51 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-26 was used instead of IC-7.

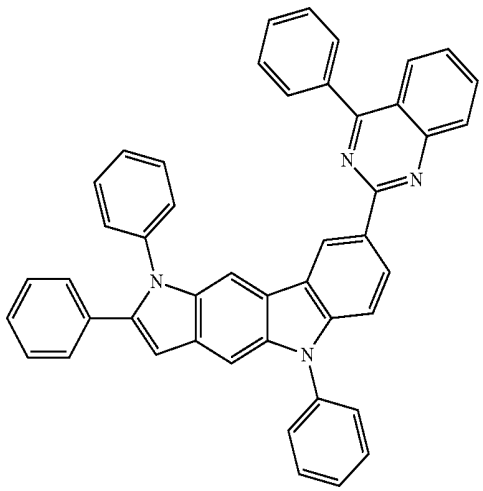
[0456] Elemental Analysis: C, 85.38; H, 4.66; N, 9.96/ HRMS $[M]^+$: 562

Synthesis Example 52

Synthesis of Mat-52

[0457]





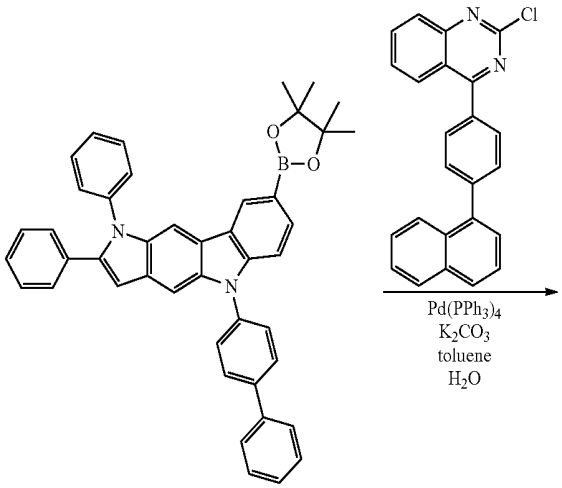
[0458] Mat-52 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-27 was used instead of IC-1.

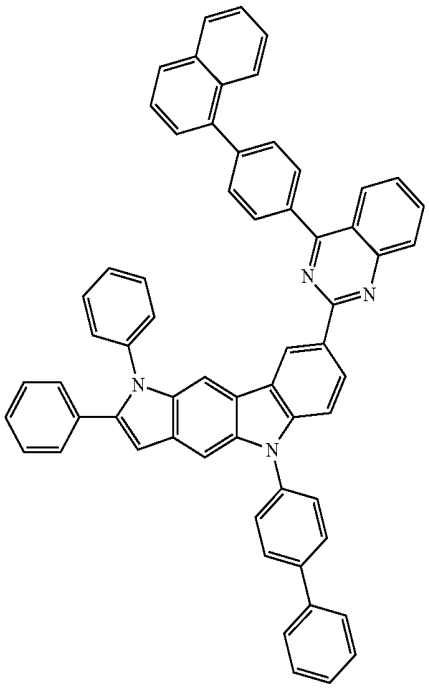
[0459] Elemental Analysis: C, 86.49; H, 4.73; N, 8.77/ HRMS $[M]^+$: 638

Synthesis Example 53

Synthesis of Mat-53

[0460]





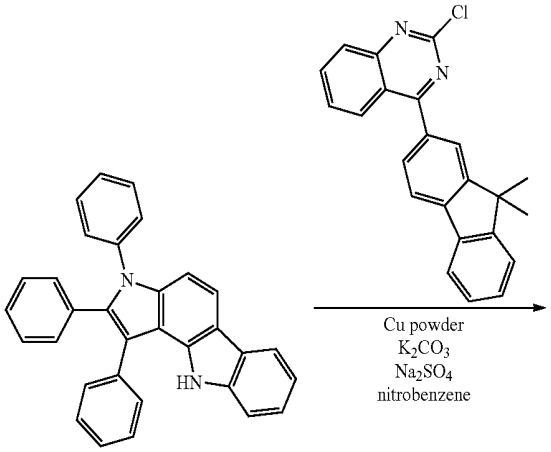
[0461] Mat-53 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-28 and sub-2 were used instead of IC-1 and sub-1, respectively.

[0462] Elemental Analysis: C, 88.54; H, 4.79; N, 6.66/ HRMS $[M]^+$: 840

Synthesis Example 54

Synthesis of Mat-54

[0463]



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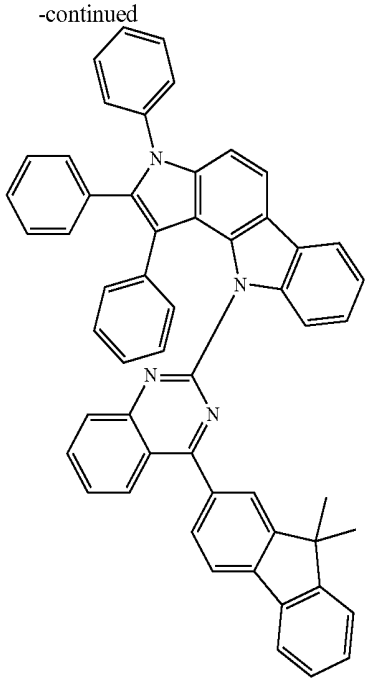


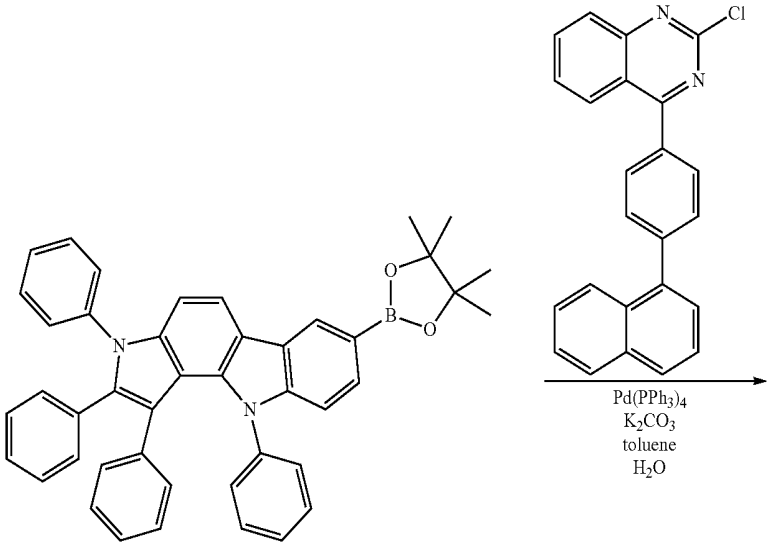
[0464] Mat-54 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-29 and sub-3 were used instead of IC-7 and sub-1, respectively.

[0465] Elemental Analysis: C, 87.50; H, 5.07; N, 7.42/ HRMS $[M]^+$: 754

Synthesis Example 55

Synthesis of Mat-55

[0466]



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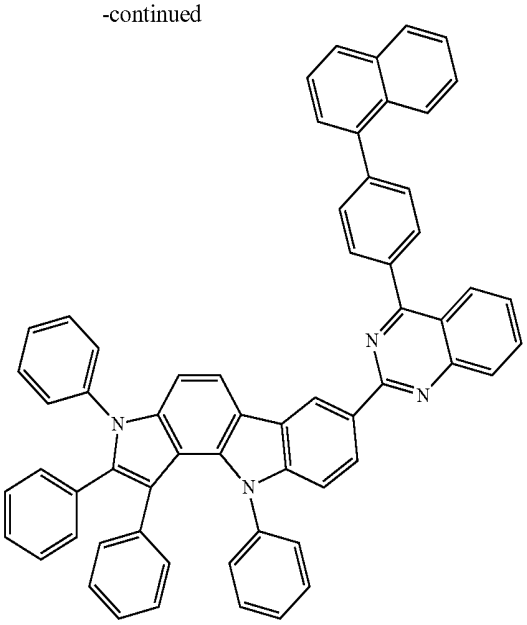


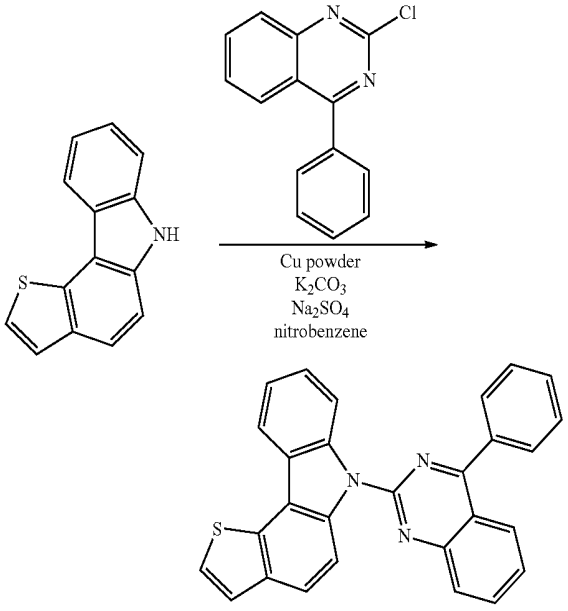
[0467] Mat-55 was obtained by performing the same procedure as in Synthesis Example 1, except that IC-30 and sub-2 were used instead of IC-1 and sub-1, respectively.

[0468] Elemental Analysis: C, 88.54; H, 4.79; N, 6.66/HRMS $[M]^+$: 840

Synthesis Example 56

Synthesis of Mat-56

[0469]



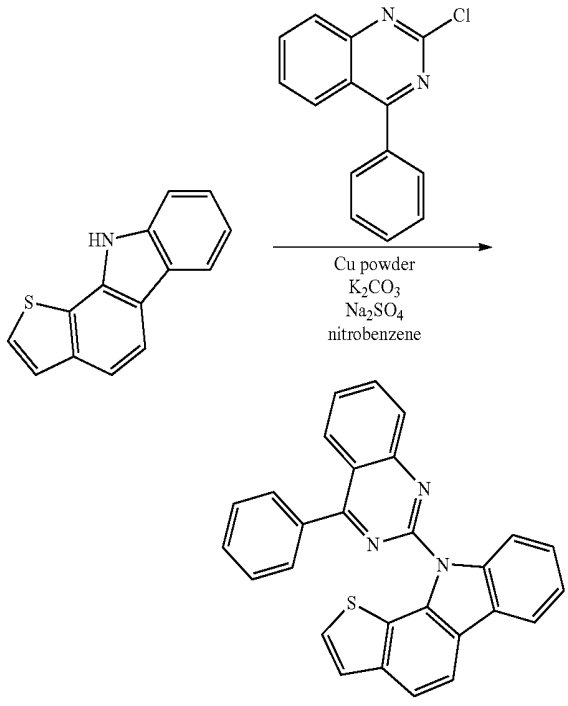
[0470] Mat-56 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-31 was used instead of IC-7.

[0471] Elemental Analysis: C, 78.66; H, 4.01; N, 9.83; S, 7.50/HRMS $[M]^+$: 427

Synthesis Example 57

Synthesis of Mat-57

[0472]



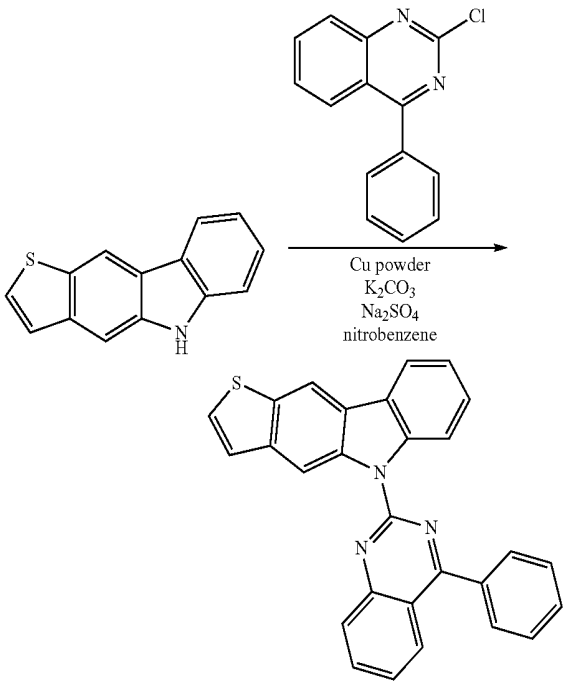
[0473] Mat-57 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-32 was used instead of IC-7.

[0474] Elemental Analysis: C, 78.66; H, 4.01; N, 9.83; S, 7.50/HRMS $[M]^+$: 427

Synthesis Example 58

Synthesis of Mat-58

[0475]



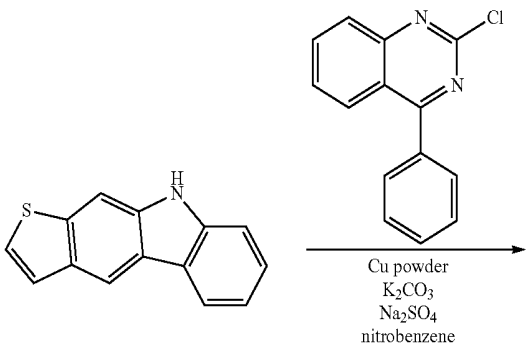
[0476] Mat-58 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-33 was used instead of IC-7.

[0477] Elemental Analysis: C, 78.66; H, 4.01; N, 9.83; S, 7.50/HRMS $[M]^+$: 427

Synthesis Example 59

Synthesis of Mat-59

[0478]



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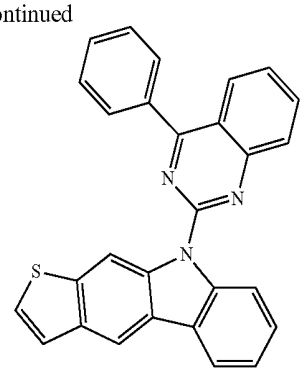


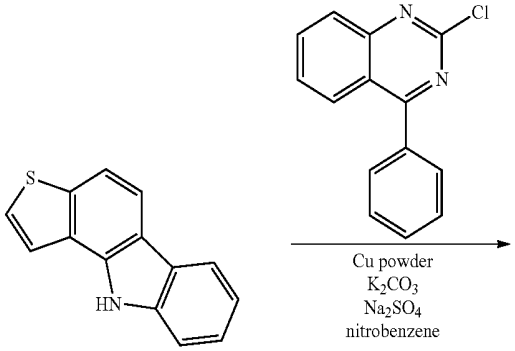
[0479] Mat-59 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-34 was used instead of IC-7.

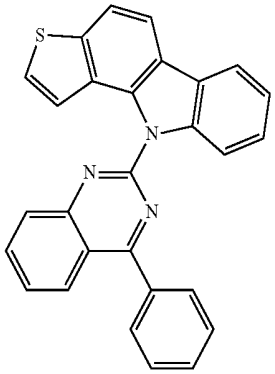
[0480] Elemental Analysis: C, 78.66; H, 4.01; N, 9.83; S, 7.50/HRMS $[M]^+$: 427

Synthesis Example 60

Synthesis of Mat-60

[0481]





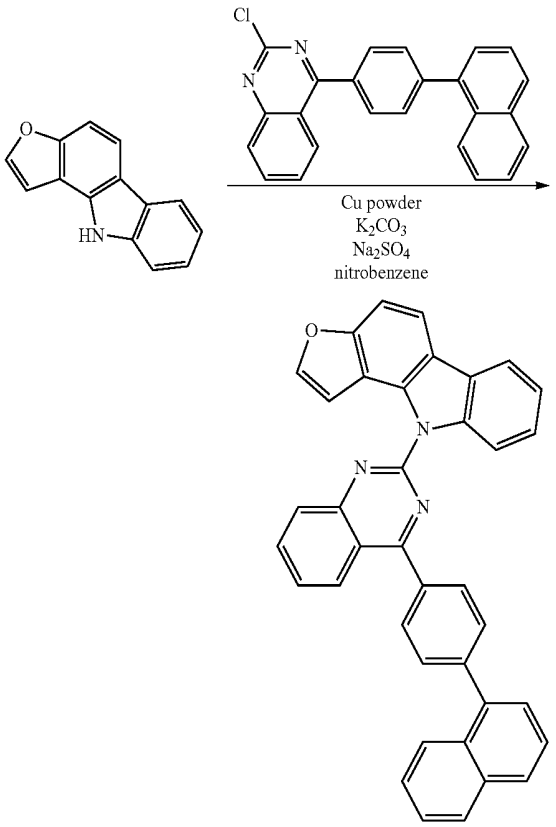
[0482] Mat-60 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-35 was used instead of IC-7.

[0483] Elemental Analysis: C, 78.66; H, 4.01; N, 9.83; S, 7.50/HRMS $[M]^+$: 427

Synthesis Example 61

Synthesis of Mat-61

[0484]



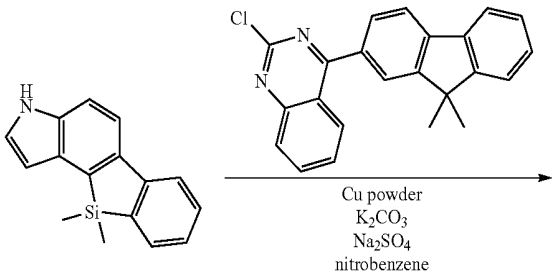
[0485] Mat-61 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-36 and sub-2 were used instead of IC-7 and sub-1, respectively.

[0486] Elemental Analysis: C, 84.90; H, 4.31; N, 7.82; 0, 2.98/HRMS $[M]^+$: 537

Synthesis Example 62

Synthesis of Mat-62

[0487]



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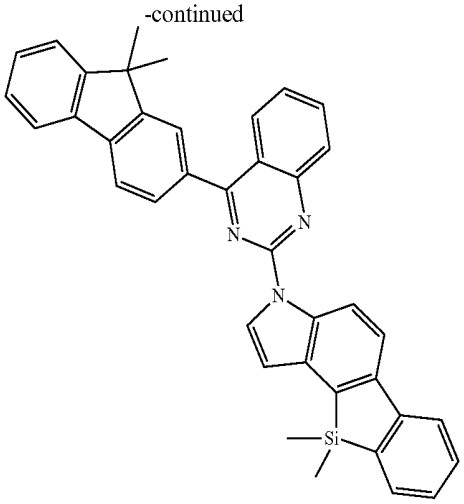


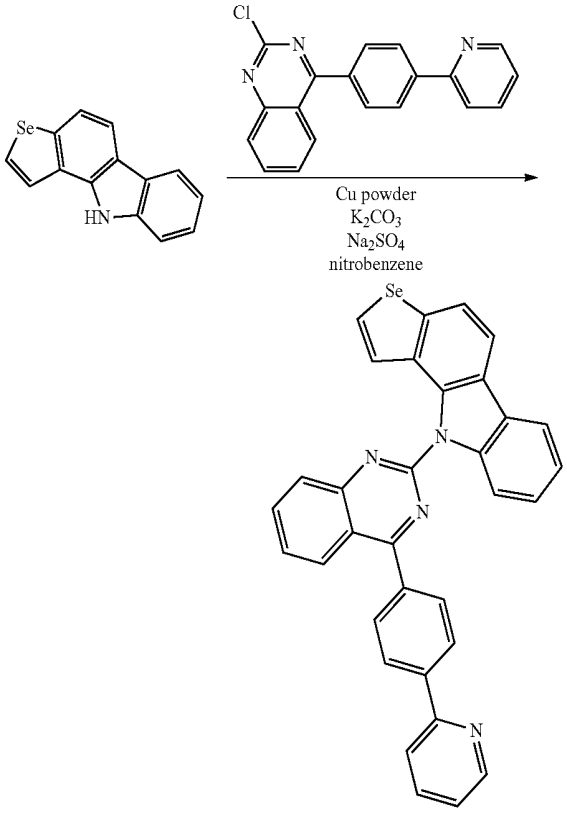
[0488] Mat-62 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-37 and sub-3 were used instead of IC-7 and sub-1, respectively.

[0489] Elemental Analysis: C, 82.21; H, 5.48; N, 7.37; Si, 4.93 HRMS $[M]^+$: 569

Synthesis Example 63

Synthesis of Mat-63

[0490]



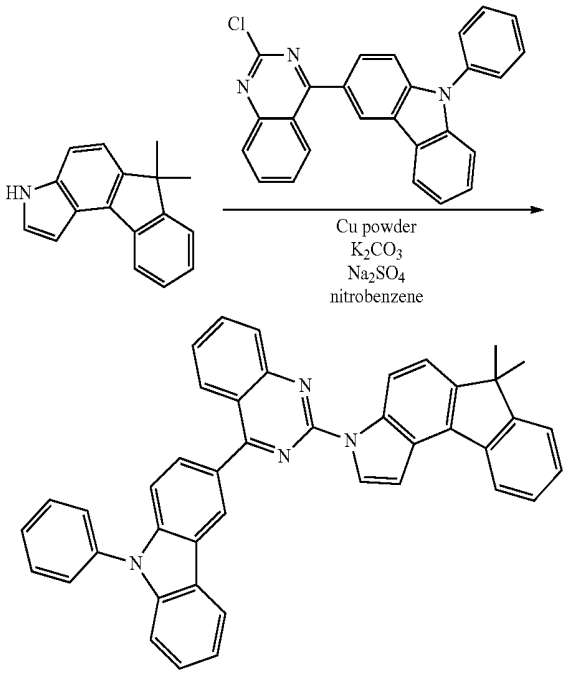
[0491] Mat-63 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-38 and sub-4 were used instead of IC-7 and sub-1, respectively.

[0492] Elemental Analysis: C, 71.87; H, 3.66; N, 10.16; Se, 14.3 HRMS $[M]^+$: 552

Synthesis Example 64

Synthesis of Mat-64

[0493]



[0494] Mat-64 was obtained by performing the same procedure as in Synthesis Example 2, except that IC-39 and sub-5 were used instead of IC-7 and sub-1, respectively.

[0495] Elemental Analysis: C, 85.69; H, 5.02; N, 9.30 HRMS $[M]^+$: 602

Examples 1 to 64

Manufacture of Red Organic Electroluminescence Device

[0496] Mat-1 to Mat-64, which are the compounds synthesized in Synthesis Examples 1 to 64, were subjected to highly-pure sublimation purification by a typically known method, and then red organic electroluminescence devices were manufactured according to the following procedure.

[0497] First, a glass substrate thinly coated with indium tin oxide (ITO) to have a thickness of 1,500 Å was ultrasonically washed with distilled water. When the ultrasonic washing with distilled water was completed, the substrate was ultrasonically washed with a solvent such as isopropyl alcohol, acetone, and methanol, dried, transferred to a UV ozone cleaner (Power sonic 405, manufactured by Hwashin Tech), washed for 5 minutes by using UV, and then transferred to a vacuum evaporator.

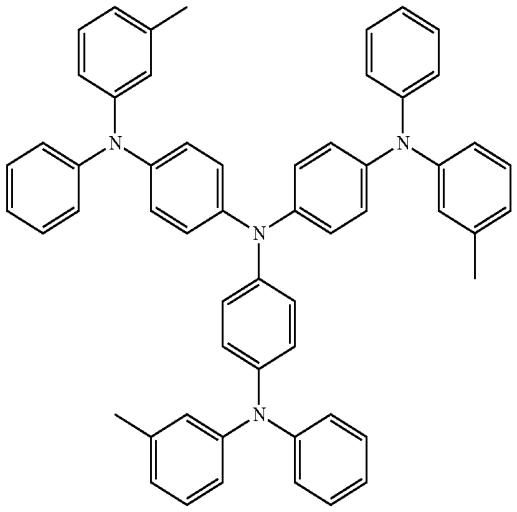
[0498] A red organic electroluminescence device was manufactured by laminating m-MTDATA (60 nm)/NPB (20 nm)/each compound of Mat-1 to Mat-64+10% $(piq)_2Ir(acac)$ (30 nm)/BCP (10 nm)/Alq_3 (30 nm)/LiF (1 nm)/A1 (200 nm) on the ITO transparent substrate (electrode).

Comparative Example

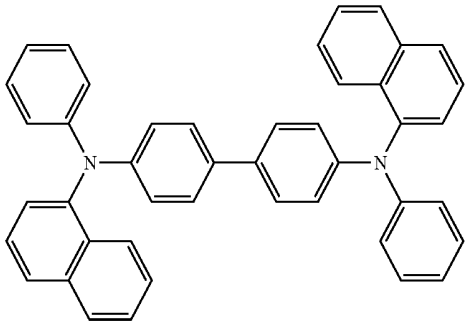
Manufacture of Red Organic Electroluminescence Device

[0499] A red organic electroluminescence device was manufactured by the same procedure as in Example 1, except that when a light-emitting layer is formed, CBP was used as a light-emitting host material instead of Compound Mat-1.

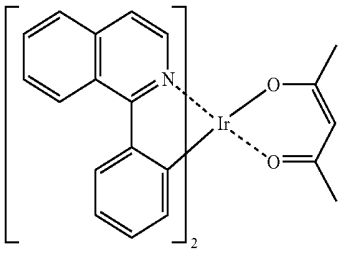
[0500] The structures of m-MTDATA, NPB, $(piq)_2Ir(acac)$, BCP, and CBP used in Examples 1 to 64 and the Comparative Example are as follows.



m-MTDATA



NPB



(piq)2Ir(acac)

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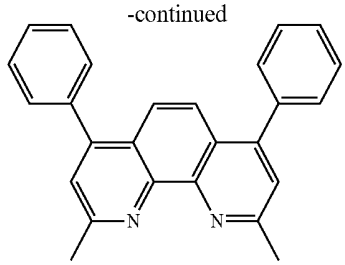
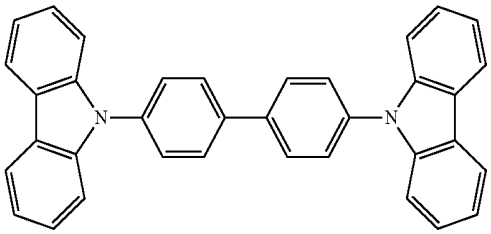


BCP



CBP

Evaluation Example

[0501] For each of the organic electroluminescence devices manufactured in Examples 1 to 64 and the Comparative Example, the driving voltage, current efficiency, and light-emitting peaks thereof were measured at a current density of 10 mA/cm^2, and the results are shown in the following Table 1.

TABLE 1

Sample	Host	Driving voltage (V)	Current efficiency (cd/A)
Example 1	Mat-1	4.65	13.5
Example 2	Mat-2	4.57	13.3
Example 3	Mat-3	4.60	12.5
Example 4	Mat-4	4.65	13.0
Example 5	Mat-5	4.70	12.6
Example 6	Mat-6	4.66	13.1
Example 7	Mat-7	4.72	13.5
Example 8	Mat-8	4.62	13.2
Example 9	Mat-9	4.70	13.3
Example 10	Mat-10	4.65	14.2
Example 11	Mat-11	4.71	13.1
Example 12	Mat-12	4.75	13.3
Example 13	Mat-13	4.60	14.2
Example 14	Mat-14	4.70	13.5
Example 15	Mat-15	4.80	13.2
Example 16	Mat-16	4.75	14.3
Example 17	Mat-17	4.70	13.5
Example 18	Mat-18	4.50	12.6
Example 19	Mat-19	4.55	13.3
Example 20	Mat-20	4.60	12.8
Example 21	Mat-21	4.64	14.2
Example 22	Mat-22	4.66	13.5
Example 23	Mat-23	4.71	13.2
Example 24	Mat-24	4.65	14.1
Example 25	Mat-25	4.70	13.9
Example 26	Mat-26	4.70	13.1
Example 27	Mat-27	4.65	14.5
Example 28	Mat-28	4.80	13.9
Example 29	Mat-29	4.72	13.4
Example 30	Mat-30	4.65	13.4
Example 31	Mat-31	4.71	12.9
Example 32	Mat-32	4.75	14.0
Comparative Example	CBP	5.25	8.2

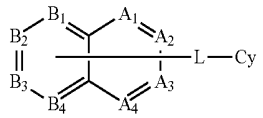
TABLE 1-continued

Sample	Host	Driving voltage (V)	Current efficiency (cd/A)
Example 33	Mat-33	4.69	13.5
Example 34	Mat-34	4.70	13.3
Example 35	Mat-35	4.75	13.1
Example 36	Mat-36	4.70	14.6
Example 37	Mat-37	4.80	13.9
Example 38	Mat-38	4.64	12.9
Example 39	Mat-39	4.59	13.8
Example 40	Mat-40	4.55	13.3
Example 41	Mat-41	4.50	14.0
Example 42	Mat-42	4.70	13.5
Example 43	Mat-43	4.65	13.0
Example 44	Mat-44	4.60	14.0
Example 45	Mat-45	4.70	13.5
Example 46	Mat-46	4.64	13.8
Example 47	Mat-47	4.69	12.9
Example 48	Mat-48	4.70	13.8
Example 49	Mat-49	4.72	13.9
Example 50	Mat-50	4.70	13.3
Example 51	Mat-51	4.74	13.6
Example 52	Mat-52	4.60	14.1
Example 53	Mat-53	4.65	13.7
Example 54	Mat-54	4.70	13.5
Example 55	Mat-55	4.65	14.5
Example 56	Mat-56	4.60	14.0
Example 57	Mat-57	4.65	13.3
Example 58	Mat-58	4.66	13.9
Example 59	Mat-59	4.70	13.4
Example 60	Mat-60	4.75	13.5
Example 61	Mat-61	4.65	13.9
Example 62	Mat-62	4.60	14.3
Example 63	Mat-63	4.64	14.0
Example 64	Mat-64	4.71	13.9

[0502] As shown in Table 1, it can be seen that the cases where the compounds (Mat-1 to Mat-64) according to the present invention are used in a light-emitting layer of a red organic electroluminescence device (Examples 1 to 64) are excellent in efficiency and driving voltage as compared to the case (Comparative Example) where the CBP in the related art is used.

1. A compound represented by the following Formula 1:

[Formula 1]



in Formula 1,

A_1 to A_4 are each independently CR_1 or N, and here, at least one or more thereof are N,

B_1 to B_4 are each independently CR_2 or N,

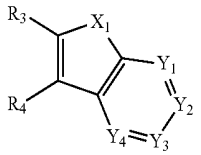
R_1 and R_2 are each independently selected from the group consisting of hydrogen, deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 60 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphos-

phine oxide group and a C_6 to C_{60} arylamine group, or adjacent group form a fused ring,

L is a single bond, or a C_6 to C_{30} arylene group or a heteroarylene group having 5 to 30 nuclear atoms,

Cy is a compound represented by the following Formula 2, and

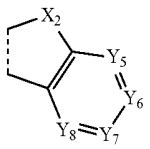
Formula 2



in Formula 2,

Y_1 to Y_4 are each independently CR_5 or N, and one of Y_1 and Y_2, Y_2 and Y_3 or Y_3 and Y_4 forms a fused ring represented by the following Formula 3,

[Formula 3]



in Formula 3,

the dotted line means a site where a fusion with the compound of Formula 2 occurs,

Y_5 to Y_8 are each independently CR_6 or N,

X_1 and X_2 are each independently selected from the group consisting of O, S, Se, $N(Ar_1)$, $C(Ar_2)(Ar_3)$ and $Si(Ar_4)(Ar_5)$, and here, at least one of X_1 and X_2 is $N(Ar_1)$,

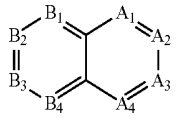
R_3 to R_6 are each independently selected from the group consisting of hydrogen, deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 60 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphosphine oxide group and a C_6 to C_{60} arylamine group, or adjacent group form a fused ring,

Ar_1 to Ar_5 are each independently selected from the group consisting of hydrogen, deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 60 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphosphine oxide group and a C_6 to C_{60} arylamine group,

the alkyl group, the alkenyl group, the alkynyl group, the cycloalkyl group, the heterocycloalkyl group, the aryl group, the heteroaryl group, the alkyloxy group, the aryloxy group, the alkylsilyl group, the arylsilyl group, the alkylboron group, the arylboron group, the arylphosphine group, the arylphosphine oxide group and the arylamine group of R_1 to R_6 and Ar_1 to Ar_5 are each independently unsubstituted or substituted with one or more selected from the group consisting of deuterium, halogen, a cyano group, a nitro group, an amino group, a C_1 to C_{40} alkyl group, a C_2 to C_{40} alkenyl group, a C_2 to C_{40} alkynyl group, a C_3 to C_{40} cycloalkyl group, a heterocycloalkyl group having 3 to 40 nuclear atoms, a C_6 to C_{40} aryl group, a heteroaryl group having 5 to 40 nuclear atoms, a C_1 to C_{40} alkyloxy group, a C_6 to C_{60} aryloxy group, a C_1 to C_{40} alkylsilyl group, a C_6 to C_{60} arylsilyl group, a C_1 to C_{40} alkylboron group, a C_6 to C_{60} arylboron group, a C_6 to C_{60} arylphosphine group, a C_6 to C_{60} arylphosphine oxide group and a C_6 to C_{60} arylamine group, and

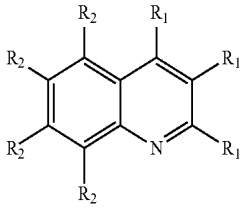
L is linked to any one of X_1, X_2, R_3, R_4 and Y_1 to Y_8 of Formula 2.

2. The compound of claim **1**, wherein

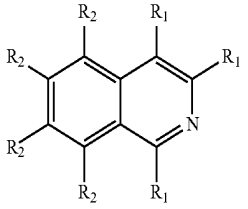


of Formula 1 is selected from the group consisting of structures represented by the following S-1 to S-30:

S-1



S-2



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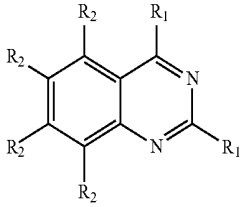

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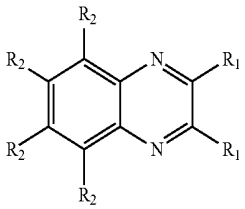

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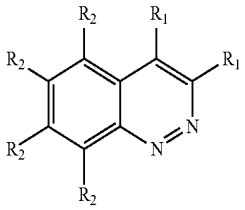

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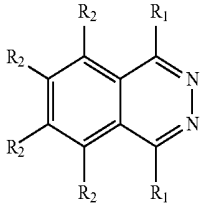

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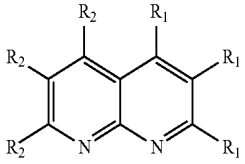

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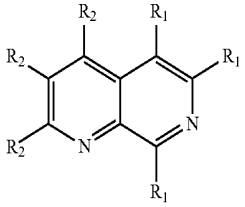

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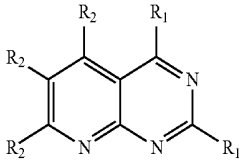

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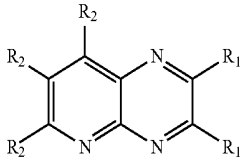

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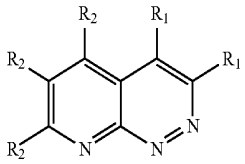

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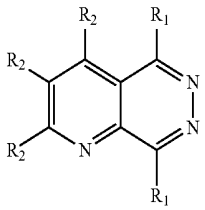

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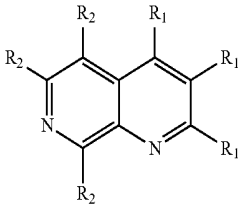

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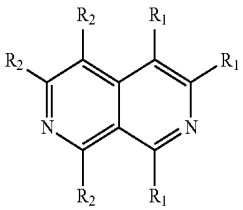

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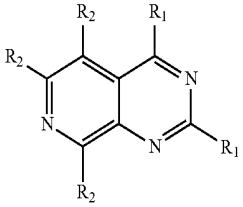

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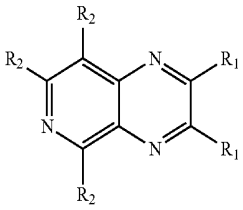

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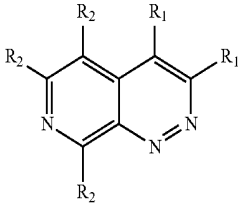

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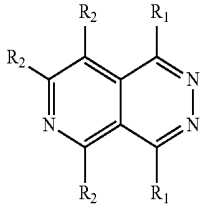

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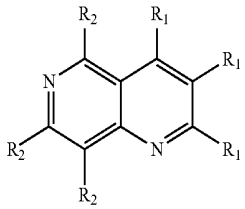

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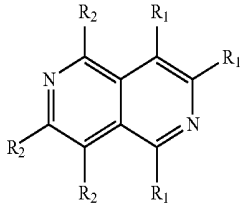

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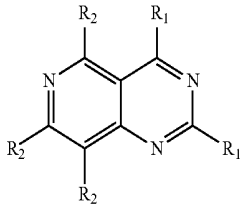

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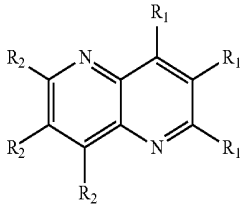

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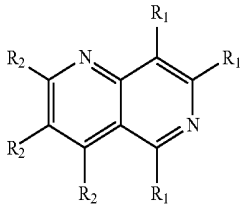

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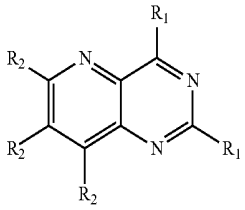

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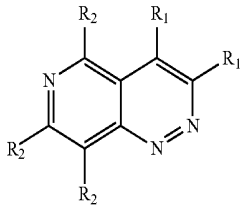

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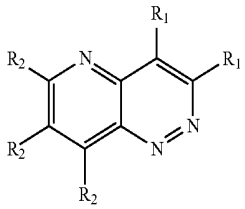
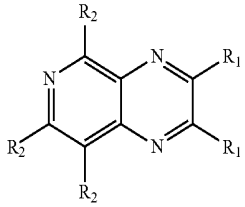
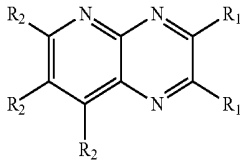
S-26



S-27



S-28



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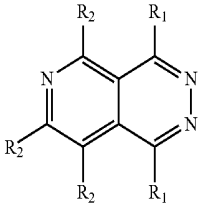

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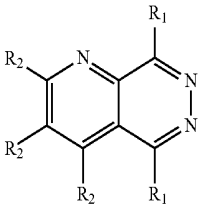


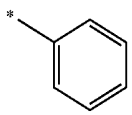
in the structures represented by S-1 to S-30,

R_1 and R_2 are the same as those defined in claim **1**, and a plurality of R_1's is the same as or different from each other, and a plurality of R_2's is the same as or different from each other.

3. The compound of claim **1**, wherein R_1 and R_2 are each independently selected from the group consisting of hydrogen, a C_6 to C_{60} aryl group, a heteroaryl group having 5 to 40 nuclear atoms and a C_6 to C_{60} arylamine group.

4. The compound of claim **1**, wherein R_1 and R_2 are each independently selected from the group consisting of hydrogen, or structures represented by the following A1 to A70:

A1



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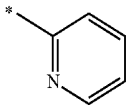

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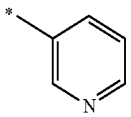

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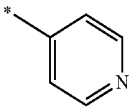

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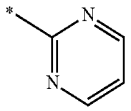

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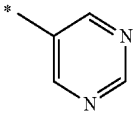

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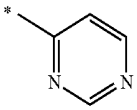

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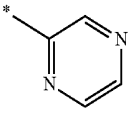

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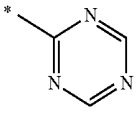

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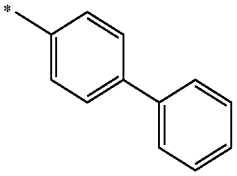

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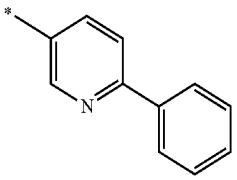

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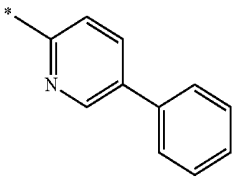

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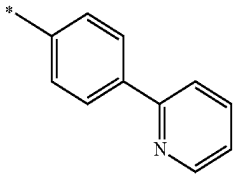

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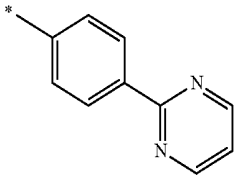

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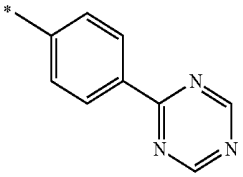

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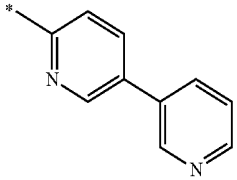

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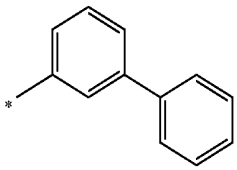

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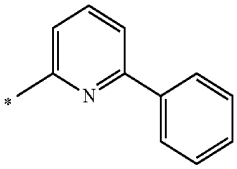

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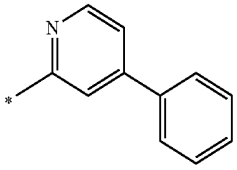

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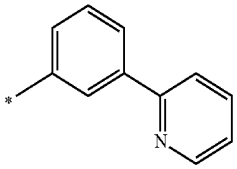

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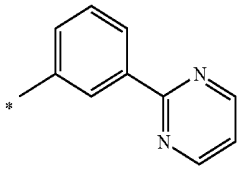

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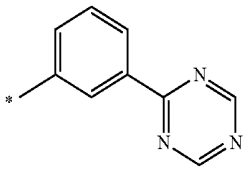

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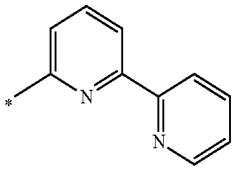

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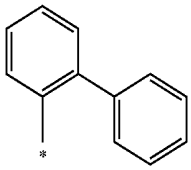

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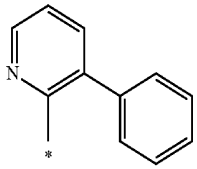

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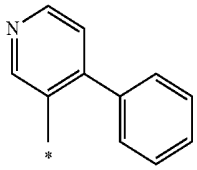

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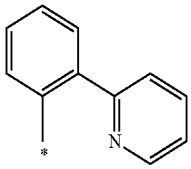

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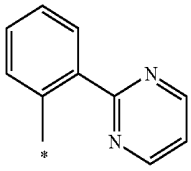

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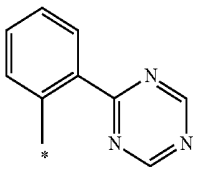

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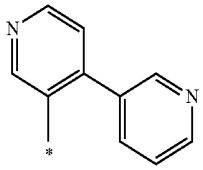

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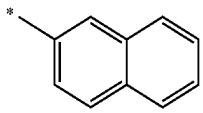

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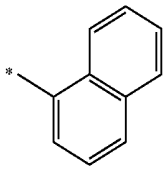

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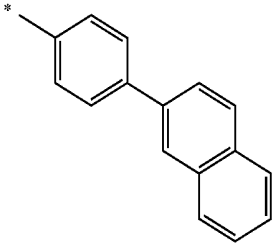

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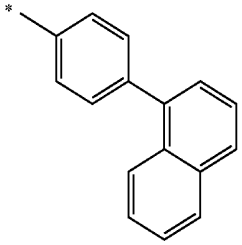

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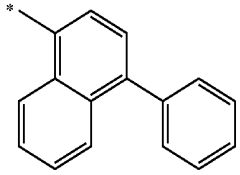

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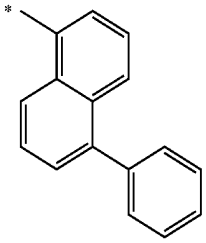

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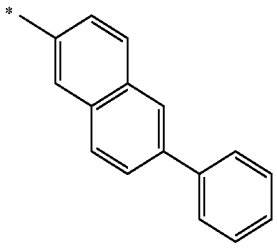

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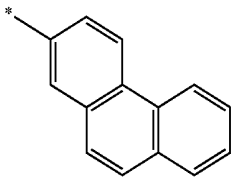

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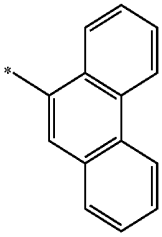

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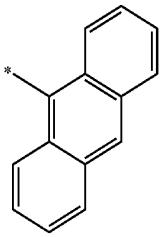

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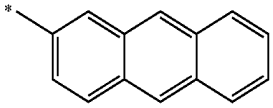

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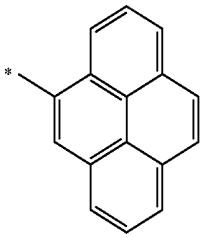

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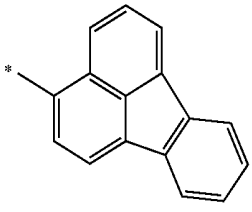

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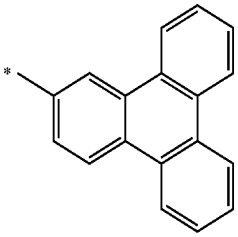

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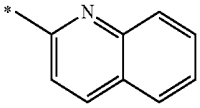

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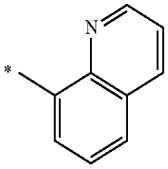

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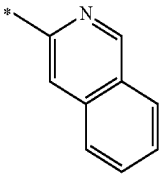

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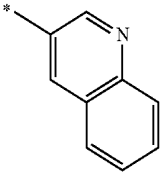

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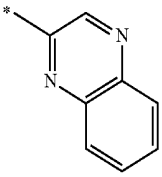

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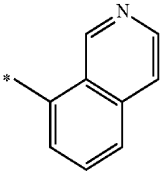

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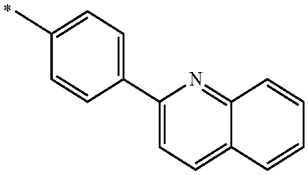

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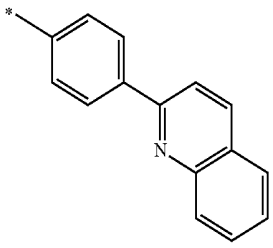

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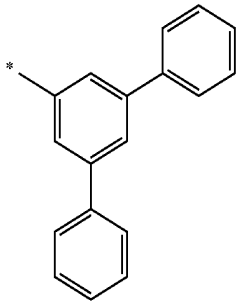

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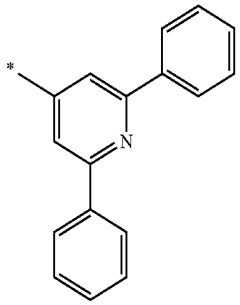

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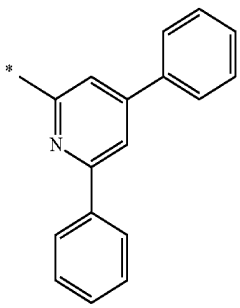

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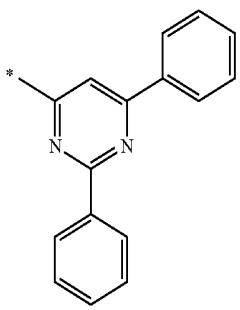

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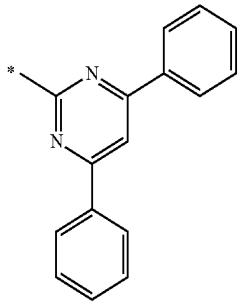

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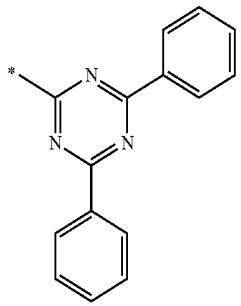

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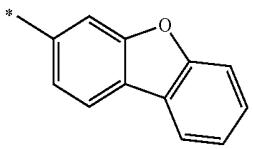

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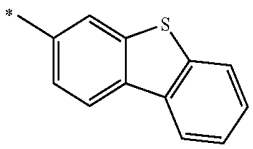

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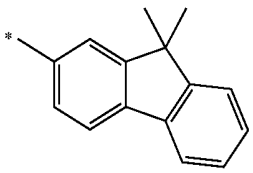

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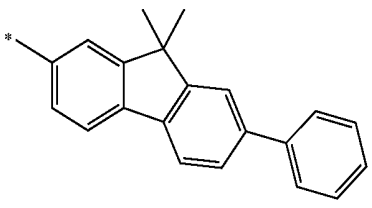

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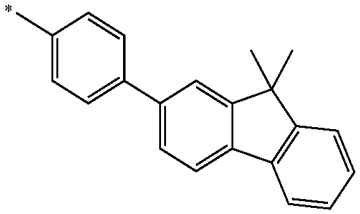

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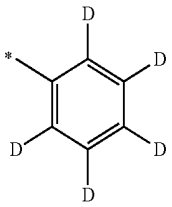

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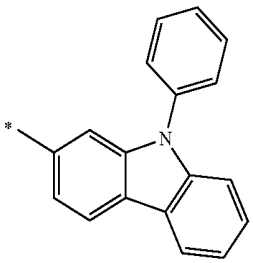

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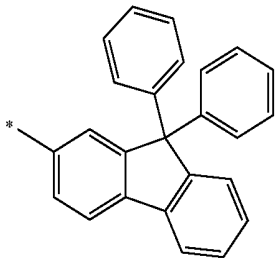

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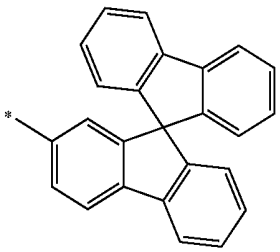

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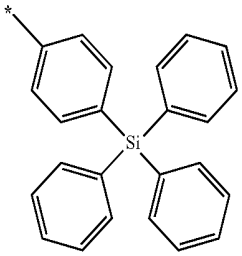

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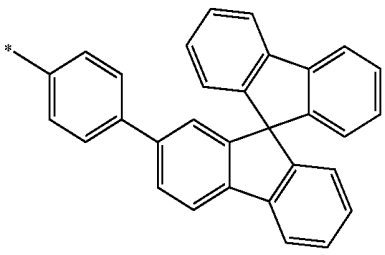

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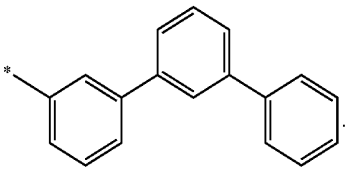
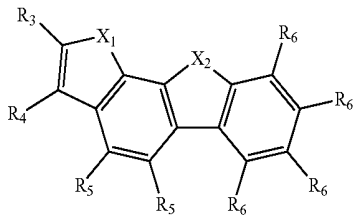
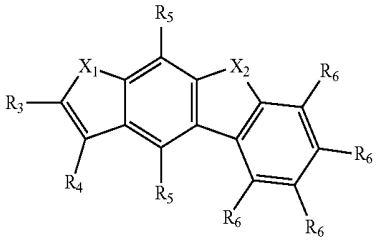


5. The compound of claim **1**, wherein the compound represented by Formula 2 is selected from the group consisting of compounds represented by the following Formulae 2a to 2f:

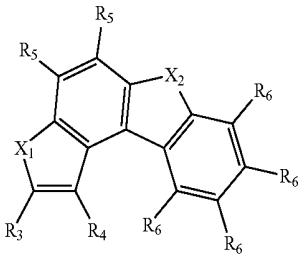
Formula 2a



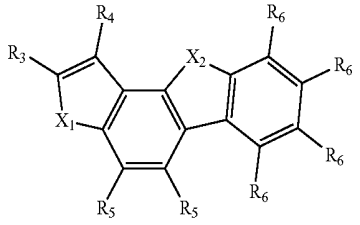
Formula 2b



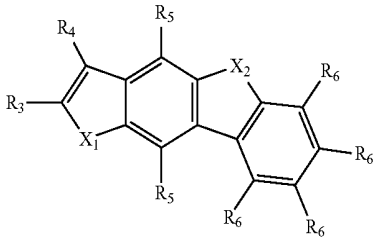
Formula 2c



Formula 2d



Formula 2e



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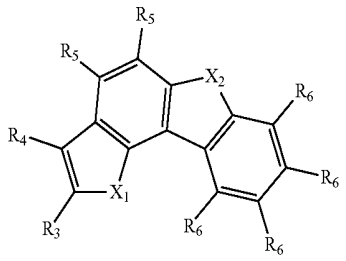
Formula 2f



in Formulae 2a to 2f,

X_1, X_2, and R_3 to R_6 are the same as those defined in claim **1**, and a plurality of R_5's is the same as or different from each other, and a plurality of R_6's is the same as or different from each other.

6. The compound of claim **5**, wherein L of Formula 1 is a single bond or phenylene,

X_1 and X_2 are $N(Ar_1)$, and here, Ar_1 is the same as or different from each other, and

Ar_1 is selected from the group consisting of hydrogen, a C_6 to C_{60} aryl group, and a heteroaryl group having 5 to 40 nuclear atoms.

7. The compound of claim **1**, wherein L is linked to any one of X_1 and Y_5 to Y_8 of Formula 2.

8. An organic electroluminescence device comprising:

an anode;

a cathode; and

an organic material layer having one or more layers interposed between the anode and the cathode,

wherein at least one of the organic material layer having one or more layers comprises the compound of claim **1**.

9. The organic electroluminescence device of claim **8**, wherein the organic material layer comprising the compound is selected from the group consisting of a hole injection layer, a hole transporting layer and a light-emitting layer.

10. The organic electroluminescence device of claim **8**, wherein the organic material layer comprising the compound is a light-emitting layer, and the compound is a phosphorescent host material of the light-emitting layer.

* * * * *

专利名称(译)	新型化合物和包含其的有机电致发光器件		
公开(公告)号	US20150236271A1	公开(公告)日	2015-08-20
申请号	US14/420539	申请日	2013-08-07
[标]申请(专利权)人(译)	株式会社斗山		
申请(专利权)人(译)	斗山公司		
当前申请(专利权)人(译)	斗山公司		
[标]发明人	KIM TAE HYUNG LEE IN HYUK KIM HOE MOON SHIN JIN YONG PARK HO CHEOL LEE CHANG JUN BEAK YOUNG MI LEE EUN JUNG		
发明人	KIM, TAE HYUNG LEE, IN HYUK KIM, HOE MOON SHIN, JIN YONG PARK, HO CHEOL LEE, CHANG JUN BEAK, YOUNG MI LEE, EUN JUNG		
IPC分类号	H01L51/00 C07D495/04 C09K11/06 C07F7/08 C07D517/04 C07D403/14 C07D487/04 C07D491/048		
CPC分类号	H01L51/0072 H01L2251/308 C07D495/04 C07D491/048 C07F7/0816 C07D517/04 C07D403/14 C09K11/06 H01L51/0052 H01L51/0067 H01L51/0058 H01L51/0094 C09K2211/1074 C09K2211/1066 C09K2211/1062 C09K2211/107 H01L51/5206 H01L51/5221 H01L51/5016 H01L51/5088 H01L51/5056 C07D487/04 C07D401/04 C07D401/14 C07D403/04 C07D403/10 C07D471/04 C07D519/00 C09B57/00 C09K2211/1007 C09K2211/1011 C09K2211/1029 C09K2211/1033 C09K2211/1037 C09K2211/104 C09K2211/1044 C09K2211/1059 H01L51/5012 H05B33/14		
优先权	1020120088004 2012-08-10 KR 1020120103947 2012-09-19 KR		
其他公开文献	US9905777		
外部链接	Espacenet USPTO		

摘要(译)

本发明涉及新化合物和包含其的有机电致发光器件，并且根据本发明的化合物可以用于有机材料层，优选有机电致发光器件的发光层，从而增强光 - 有机电致发光器件的发光效率，驱动电压，寿命等。

[Formula 1]