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(54) **NOVEL ORGANIC ELECTROLUMINESCENT COMPOUNDS, LAYERS AND ORGANIC ELECTROLUMINESCENT DEVICE USING THE SAME**

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(57) **ABSTRACT**

(22) Filed: **Aug. 13, 2015**

The present invention relates to a novel organic electroluminescent compound, layer and an organic electroluminescent device using the same. Said organic luminescent compound provides an organic light emitting layer and/or device which has high luminous efficiency and a long, operation lifetime and requires a low driving voltage improving power efficiency and power consumption.

Related U.S. Application Data

(63) Continuation-in-part of application No. 14/624,835, filed on Feb. 18, 2015, which is a continuation of application No. 14/004,089, filed on Nov. 25, 2013,

**NOVEL ORGANIC ELECTROLUMINESCENT
COMPOUNDS, LAYERS AND ORGANIC
ELECTROLUMINESCENT DEVICE USING
THE SAME**

CLAIM OF BENEFIT OF FILING DATE

[0001] The present application is a continuation-in-part of U.S. patent application Ser. No. 14/624,835 (filed Feb. 18, 2015), which is a continuation of U.S. patent application Ser. No. 14/004,089 (filed Nov. 25, 2013), which is a National application tiling based upon PCT Application No. PCT/KR12/01712 (filed Mar. 8, 2012), which claims the benefit of the filing date of Korean Patent Application No. 10-2011-0020492 (filed Mar. 8, 2011).

TECHNICAL FIELD

[0002] The present invention relates to novel combinations including organic electroluminescent compounds, and organic electroluminescent device using the same.

BACKGROUND

[0003] An electroluminescent (EL) device is a self-light-emitting device which has advantages over other types of display devices in that it provides a wider viewing angle, a greater contrast ratio, and has a faster response time. An organic EL device was first developed by Eastman Kodak, by using small molecules (aromatic diamines) and aluminum complexes in a light-emitting layer [Appl. Phys. Lett. 51, 913, 1987].

[0004] The most important factor to determine luminous efficiency in an organic EL device is a light-emitting materials. Until now, fluorescent materials have been widely used as light-emitting material. However, in view of electroluminescent mechanisms, phosphorescent materials theoretically show four (4) times higher luminous efficiency than fluorescent materials. Thus, recently, phosphorescent materials have been investigated.

[0005] Iridium(III) complexes have been widely known as phosphorescent material, including bis(2-(2'-benzothienyl)pyridinato-N,C3')iridium(acetylacetonate) ((acac)Ir(btp)₂), tris(2-phenylpyridine)iridium (Ir(ppy)₃) and bis(4,6-difluorophenylpyridinato-N,C2)picolinate iridium (Firpic) as red, green and blue materials, respectively.

[0006] In order to improve color purity, luminous efficiency and stability, light-emitting materials can be used as one prepared by mixing a dopant with a host material. in the host material/dopant system, the host material has a great influence on the efficiency and performance of an EL device, and thus is important.

[0007] At present, 4,4'-N,N'-dicarbazol-biphenyl (CBP) is the most widely known host material for phosphorescent materials. Further, Pioneer (Japan) developed a high performance organic EL device employing, as a host material, bathocuproine (BCP) or aluminum(III)bis(2-methyl-8-quinolinate)(4-phenylphenolate) (BALq) which had been a material used for a hole blocking layer.

[0008] Though these phosphorous host materials provide good light-emitting characteristics, they have the following

disadvantages: (1) Due to their low glass transition temperature and poor thermal stability, their degradation may occur during a high-temperature deposition process in a vacuum. (2) The power efficiency of an organic EL device is given by $[(\pi/\text{voltage}) \times \text{current efficiency}]$, and thus the power efficiency is inversely proportional to the voltage. Though an organic EL device comprising phosphorescent materials provides better current efficiency (cd/A) than one comprising fluorescent materials, a significantly high driving voltage is required to be applied to an organic EL device, thereby resulting in poor power efficiency (lm/W). (3) Further, the operation lifetime of an organic EL device is short and luminous efficiency is still required to be improved.

[0009] International Patent Application Publication No. WO 2006/049013 discloses compounds for organic electroluminescent materials whose backbone has a condensed bicycle group. However, it does not disclose compounds having a nitrogen-containing condensed bicyclic group, which is formed by condensing two 6-membered rings; a carbazolic group; and an aryl or heteroaryl group. Further, an organic EL device comprising said compounds fails to provide good luminous efficiency, operation lifetime and driving voltage.

[0010] An object of the present invention is to provide organic electroluminescent compounds imparting excellent luminous efficiency, long operation lifetime and low driving voltage to a device; improved layer combinations using said compounds; and an organic electroluminescent device using said compounds (e.g., in the form of a layer that includes at least one of said compounds as a host material, and also includes a metal complex dopant, specifically an iridium metal complex dopant).

SUMMARY OF THE INVENTION

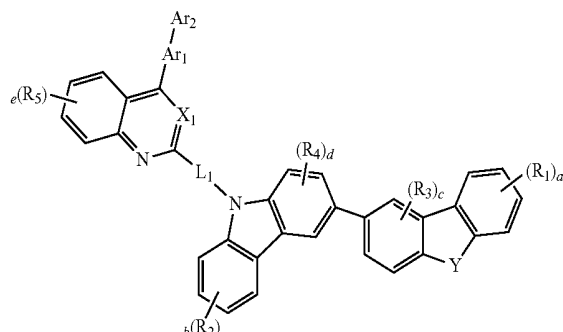
[0011] The present inventors found that the above object can be achieved by use of a unique combination of materials that are employed to provide an improved light emitting layer. Such layer may be disposed between an anode and a cathode. Thus, the layer may be such that an applied driving voltage causes electroluminescence by the layer. The layer may have therein (e.g., the layer may include or consist of) a host material and a metal complex (e.g., an iridium complex). The metal complex may be an iridium complex including an alkylated ligand. For instance it may be an iridium complex including an alkylated phenyl quinoline ligand. The alkyl group for the alkylated ligand may be to C1-C30 alkyl group. For example, it may be a C1 alkyl group, a C2 alkyl group, or any alkyl having a number of carbon atoms given by any other integer between 1 and 30. For a metal complex (e.g., an iridium complex) including an alkylated phenyl quinoline ligand, the alkylation may be of a phenyl moiety, a quinoline moiety or both.

[0012] Without limitation, an aspect of the invention may be described as a light emitting layer, including an organic electroluminescent compound as a host material in the layer; and

[0013] an iridium complex dopant,

[0014] wherein the organic electroluminescent compound is represented by the following Formula 1; and the iridium complex dopant is represented by the following Formula 2:

[Formula 1]



[0015] wherein:

[0016] L_1 represents a single bond;

[0017] X_1 represents N;

[0018] Y represents $-NR_{13}-$;

[0019] Ar_1 represents a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, a substituted or unsubstituted (C6-C30)arylene group;

[0020] Ar_2 represents hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group;

[0021] R_1 to R_5 each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted 5- to 7-membered heterocycloalkyl group, a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl group, to substituted or unsubstituted (C6-C30)aryl group fused with at least one (C3-C30)cycloalkyl group, a 5- or 7-membered heterocycloalkyl group fused with at least one substituted or unsubstituted (C6-C3) aromatic ring, (C3-C30)cycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, $-NR_{14}R_{15}$, $-SiR_{16}R_{17}R_{18}$, $-SR_{19}$, $-OR_{20}$, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C2-C30)alkynyl group, a cyano group, a nitro group, or a hydroxyl group; or are linked to an adjacent substituent via a substituted or unsubstituted (C3-C30)alkylene group or a substituted or unsubstituted (C3-C30)alkenylene group to form a mono- or polycyclic alicyclic ring or a mono- or polycyclic aromatic ring whose carbon atom(s) may be substituted by at least one hetero atom selected from nitrogen, oxygen and sulfur;

[0022] R_{13} to R_{20} have the same meaning as one of R_1 to R_5 ;

[0023] a, b and e each independently represent an integer of 1 to 4; where a, b or e is an integer of 2 or more, each of R_1 , each of R_2 or each of R_5 is the same or different;

[0024] c and d each independently represent an integer of 1 to 3; where c or d is an integer of 2 or more, each of R_3 or each of R_4 is the same or different; and

[0025] the heterocycloalkyl group and the heteroalkylene group contain at least one hetero atom selected from B, N, O, S, P(=O), Si and P, and

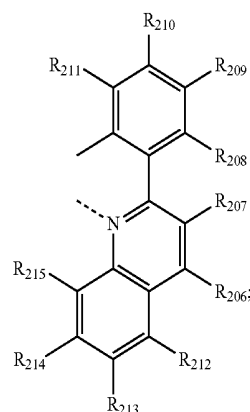
$M^1 L^{101} L^{102} L^{103}$

[Formula 2]

[0026] wherein

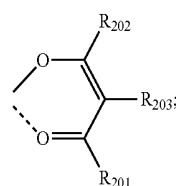
[0027] M^1 is Ir;

[0028] L^{101} and L^{102} are the same and represent



and

[0029] L^{103} represents



[0030] wherein R_{201} to R_{203} each independently represent hydrogen, deuterium, or a (C1-C30)alkyl group;

[0031] R_{206} to R_{208} , R_{210} , and R_{212} to R_{215} each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, or a substituted or unsubstituted (C6-C30)aryl group; and

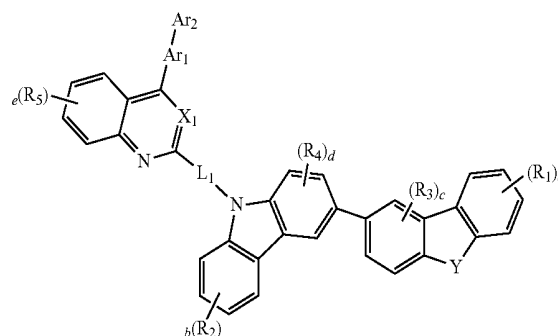
[0032] R_{209} and R_{211} each independently represent a substituted or unsubstituted (C1-C30)alkyl group.

DETAILED DESCRIPTION

[0033] With attention now to the general teachings herein, there are envisioned combinations of an organic electroluminescent host material and a complex dopant to form a light emitting layer.

[0034] The host material may be a compound represented by the following formula 1:

[Formula 1]



- [0035] wherein
- [0036] L_1 represents a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, at substituted or unsubstituted (C6-C30)arylene group, or a substituted or unsubstituted (C6-C30)cycloalkylene group;
- [0037] X_1 represents CH or N;
- [0038] Y represents $-\text{O}-$, $-\text{S}-$, $-\text{CR}_{11}\text{R}_{12}-$ or $-\text{NR}_{13}-$;
- [0039] Ar_1 represents a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, a substituted or unsubstituted (C6-C30)arylene group, or a substituted or unsubstituted (C1-C30)alkylene group;
- [0040] An represents hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group;
- [0041] R_1 to R_5 each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted 5- to 7-membered heterocycloalkyl group, a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group fused with at least one (C3-C30)cycloalkyl group, a 5- or 7-membered heterocycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, (C3-C30)cycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, $-\text{NR}_{14}\text{R}_{15}$, $-\text{SiR}_{16}\text{R}_{17}\text{R}_{18}$, $-\text{SR}_{19}$, $-\text{OR}_{20}$, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C2-C30)alkynyl group, a cyano group, as nitro group, or as hydroxyl group; or are linked to an adjacent substituent via a substituted or unsubstituted (C3-C30)alkylene group or a substituted or unsubstituted (C3-C30)alkenylene group to form a mono- or polycyclic acyclic ring or a mono- or polycyclic aromatic ring whose carbon atom(s) may be substituted by at least one hetero atom selected from nitrogen, oxygen and sulfur;
- [0042] R_{11} to R_{20} have the same meaning as one of R_1 to R_5 (or in the case in which Y represents NR_{13} , then R_{13} to R_{20} have the same meaning as one of R_1 to R_5);
- [0043] a, b and e each independently represent an integer of 1 to 4; where a, b or e is an integer of 2 or more, each of R_1 , each of R_2 or each of R_5 is the same or different;
- [0044] c and d each independently represent an integer of 1 to 3; where c or d is an integer of 2 or more, each of R_3 , or each of R_4 is the same or different; and
- [0045] the heterocycloalkyl group and the heteroaryl (ene) group contain at least one hetero atom selected from B, N, O, S, P(=O), Si and P.
- [0046] Herein, “(C1-C30)alkyl(ene)” is a linear or branched alkyl(ene) having 1 to 30, preferably 1 to 20, more preferably 1 to 10 carbon atoms and includes methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl, tert-butyl, etc.; “(C2-C30) alkenyl(ene)” is a linear or branched alkenyl(ene) having 2 to 30, preferably 2 to 20, more preferably 1 to 10 carbon atoms and includes vinyl, 1-propenyl, 2-propenyl, 1-butenyl, 2-butenyl, 3-butenyl, 2-methylbut-2-enyl, etc.; “(C2-C30) alkynyl” is a linear or branched alkynyl having 2 to 30, preferably 2 to 20, more preferably 1 to 10 carbon atoms and

includes ethynyl, 1-propynyl, 2-propynyl, 1-butylnyl, 2-butylnyl, 3-butylnyl, 1-methylpent-2-ynyl, etc.; “(C1-C30)alkoxy” is a linear or branched alkoxy having 1 to 30, preferably 2 to 20, more preferably 2 to 10 carbon atoms and includes methoxy, ethoxy, propoxy, isopropoxy, 1-ethylpropoxy, etc.; “(C3-C30)cycloalkyl” is a mono- or polycyclic hydrocarbon having 3 to 30, preferably 3 to 20, more preferably 3 to 7 carbon atoms and includes cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, etc.; “(C6-C30)cycloalkylene” is one formed by removing hydrogen from cycloalkyl having 6 to 30, preferably 6 to 20, more preferably 6 or 7 carbon atoms; and “5- to 7-membered heterocycloalkyl” is a cycloalkyl having at least one hetero atom selected from B, N, O, S, P(=O), Si and P, preferably N, O and S, and carbon atoms as remaining ring backbone atoms other than said hetero atom and includes tetrahydrofuran, pyrrolidine, tetrahydropyran, etc. Further, “(C6-C30)aryl(ene)” is a monocyclic ring or fused ring derived from an aromatic hydrocarbon and having preferably 6 to 20 ring backbone carbon atoms; and includes phenyl, biphenyl, terphenyl, naphthyl, fluorenyl, phenanthrenyl, anthracenyl, indenyl, triphenylenyl, pyrenyl, tetracenyl, perylenyl, chrysenyl, naphthacenyl, fluoranthenyl, etc. Further, “5- or 30-membered heteroaryl(ene)” is an aryl having at least one, preferably 1 to 4 hetero atom selected from the group consisting of B, N, O, S, P(=O), Si and P, and carbon atoms as remaining ring backbone atoms other than said hetero atom; is a monocyclic ring or fused ring condensed with at least benzene ring; has preferably 5 to 21 ring backbone atoms; may be partially saturated; may be one formed by linking at least one heteroaryl or aryl group to a heteroaryl group via a single bond(s); and includes a monocyclic ring-type heteroaryl including furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, etc., and a fused ring-type heteroaryl including benzofuranyl, benzothiophenyl, isobenzofuranyl, dibenzofuranyl, dibenzothiophenyl, benzoimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolyl, quinazolinyl, quinoxalinyl, carbazolyl, phenoxazinyl, phenanthridinyl, benzodioxolyl, etc.

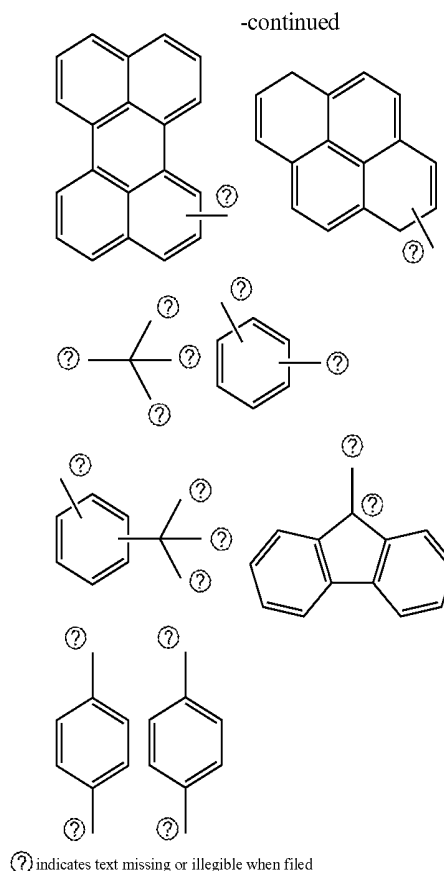
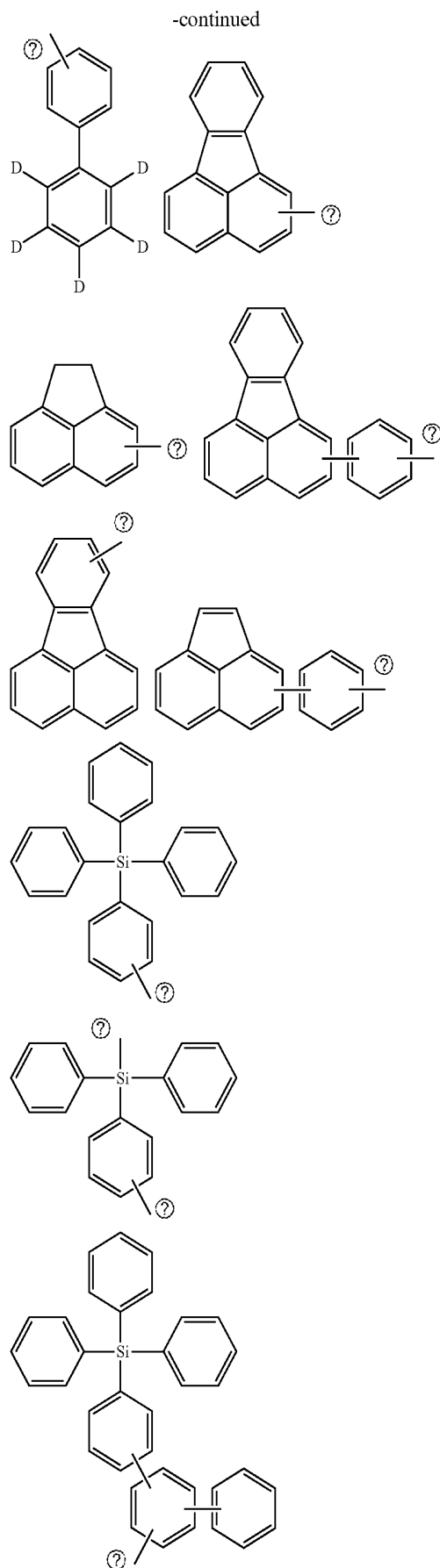
[0047] Preferably, substituents of formula 1 are as follows:

[0048] L_1 represents preferably a single bond, a substituted or unsubstituted 5- or 30-membered heteroarylene group or a substituted or unsubstituted (C6-C30)arylene group, more preferably a single bond or a substituted or unsubstituted (C6-C30)arylene group.

[0049] X represents preferably N.

[0050] Y represents preferably $-\text{O}-$, $-\text{S}-$, $-\text{CR}_{11}\text{R}_{12}-$ (wherein R_{11} and R_{12} each independently represent a substituted or unsubstituted (C1-C30)alkyl group) or $-\text{NR}_{13}-$ (wherein R_{13} represents a halogen, deuterium, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- or 30-membered heteroaryl group).

[0051] R_1 and R_2 each independently represent hydrogen, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- or 30-membered heteroaryl group, $-\text{NR}_{14}\text{R}_{15}$ (wherein R_{14} and R_{15} each independently represent a substituted or unsubstituted (C1-C30)alkyl group or a substituted or unsubstituted (C6-C30)aryl group) or a hydroxyl group, more preferably hydrogen or a substituted or unsubstituted (C6-C30)aryl group.

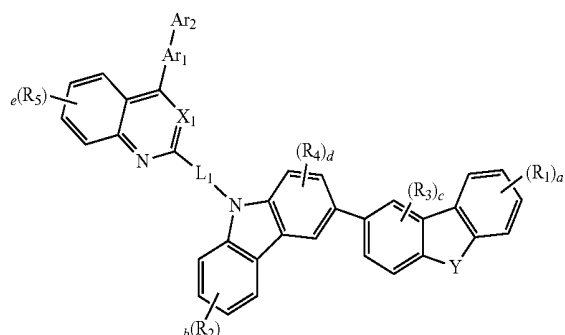


[0055] Herein, substituents of the substituted (C1-C30) alkyl group, the substituted (C2-C30)alkenyl group, the substituted (C2-C30)alkynyl group, the substituted (C6-C30) cycloalkylene group, the substituted (C3-C30)cycloalkyl group, the substituted 5- to 7-membered heterocycloalkyl group, the substituted (C6-C30)aryl(ene) group, the substituted 5- to 30-membered heteroaryl(ene) group and the substituted aromatic ring represented by said L₁, Ar₁, Ar₂, R₁ to R₅ and R₁₁ to R₂₀ each independently is at least one selected from the group consisting of deuterium, a halogen, a cyano group, a carboxyl group, a nitro group, a hydroxyl group, a (C1-C30)alkyl group, a halo(C1-C30)alkyl group, a (C2-C30)alkenyl group, a (C2-C30)alkynyl group, a (C1-C30)alkoxy group, a (C1-C30)alkylthio group, a (C3-C30)cycloalkyl group, a (C3-C30)cycloalkenyl group, a 5- to 7-membered heterocycloalkyl group, a (C6-C30)aryl group, a (C6-C30)aryloxy group, a (C6-C30)arylthio group, a 5- to 30-membered heteroaryl group, a 5- to 30-membered heteroaryl group substituted by a (C6-C30)aryl group, a (C6-C30)aryl group substituted by a 5- to 30-membered heteroaryl group, a tri(C1-C30)alkylsilyl group, a tri(C6-C30)arylsilyl group, a di(C1-C30)alkyl(C6-C30)arylsilyl group, a (C1-C30)alkyldi(C6-C30)arylsilyl group, an amino group, a mono or di(C1-30)alkylamino group, a mono or di(C6-C30)alkylamino group, a (C1-C30)alkyl(C6-C30)arylamino group, a (C1-C30)alkylcarbonyl group, a (C1-C30)alkoxycarbonyl group, a (C1-C30)arylcabonyl group, a di(C6-C30)arylbornyl group, a di(C6-C30)alkylbornyl group, a (C1-C30)alkyl(C6-C30)arylbornyl group, a (C6-30)aryl(C1-C30)alkyl group and a (C1-C30)alkyl(C6-C30)aryl group. Preferably, said substituents are at least one selected

from the group consisting of deuterium, a halogen, a (C1-C30)alkyl group, a halo(C1-C30)alkyl group, a (C6-30)aryl group, a 5- to 30-membered heteroaryl group, a tri(C1-C30)alkylsilyl group, a tri(C6-C30)arylsilyl group, a di(C1-C30)alkyl(C6-C30)arylsilyl group, a (C1-C30)alkyldi(C6-C30)arylsilyl group, a hydroxyl group and a (C1-C30)alkoxy group.

[0056] By way of more particular illustration, one preferred representation of Formula 1 is the following:

[Formula 1]



[0057] wherein:

[0058] L_1 represents a single bond;

[0059] X_1 represents N;

[0060] represents $-NR_{13}$;

[0061] Ar_1 represents a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, a substituted or unsubstituted (C6-C30)arylene group;

[0062] Ar_2 represents hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group;

[0063] R_1 to R_5 each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-30)aryl group, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted 5- to 7-membered heterocycloalkyl group, a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group fused with at least one (C3-(30)cycloalkyl group, a 5- or 7-membered heterocycloalkyl group

fused with at least one substituted or unsubstituted (C6-C30) aromatic ring, (C3-C30)cycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, $-NR_{14}R_{15}$, $-SiR_{16}R_{17}R_{18}$, $-SR_{19}$, $-OR_{20}$, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C2-C30)alkynyl group, a cyano group, a nitro group, or a hydroxyl group; or are linked to an adjacent substituent via a substituted or unsubstituted (C3-C30)alkylene group or a substituted or unsubstituted (C3-C30)alkerylene group to form a mono- or polycyclic alicyclic ring or a mono- or polycyclic aromatic ring whose carbon atom(s) may be substituted by at least one hetero atom selected from nitrogen, oxygen and sulfur;

[0064] R_{11} to R_{20} have the same meaning as one of R_1 to R_5 ,

[0065] a , b and e each independently represent an integer of 1 to 4; where a , b or e is an integer of 2 or more, each of R_2 or each of R_5 is the same or different

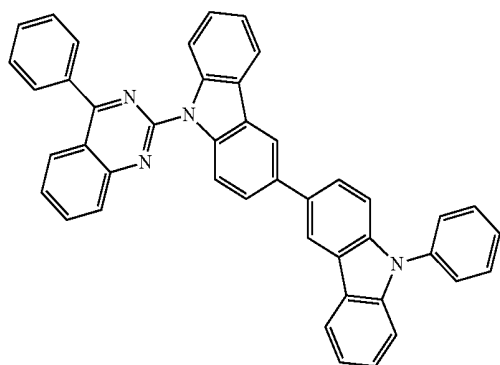
[0066] c and d each independently represent an integer of 1 to 3; where c or d is an integer of 2 or more, each of R_3 or each of R_4 is the same or different; and

[0067] the heterocycloalkyl group and the heteroaryl(ene) group contain at least one hetero atom selected from B, N, O, S, P(=O), Si and P.

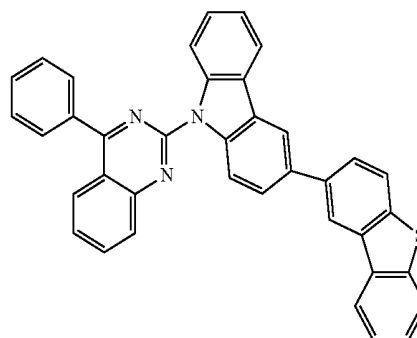
[0068] With more particularity, R_1 to R_5 may each independently represent hydrogen or a substituted or unsubstituted (C6-C30)aryl group. By way of illustration, either or both of R_3 or R_4 may represent a substituted or unsubstituted (C6-C30)aryl group.

[0069] With more particularity, R_{13} may be a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C6-C30)aryl group fused with at least one (C3-C30)cycloalkyl group, a 5- or 7-membered heterocycloalkyl group fused with at least one substituted or unsubstituted (C6-C30) aromatic ring, or a (C3-C30)cycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring. For instance, R_{13} may be a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group. One particularly preferred approach contemplates that is substituted, or unsubstituted (C6-C30)aryl group.

[0070] Organic electroluminescent compounds according to the present invention include the following, but are not limited thereto:



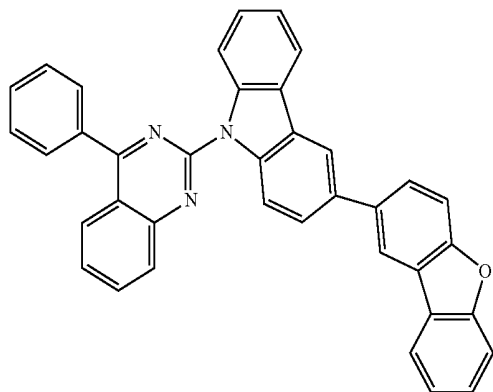
C-1



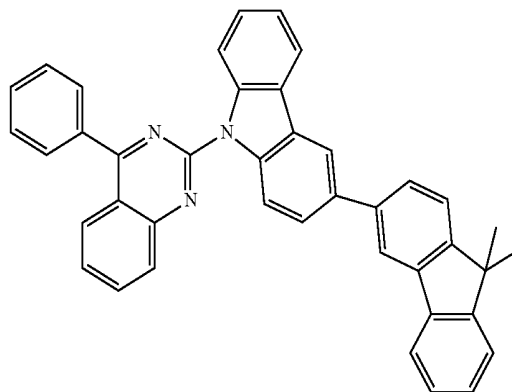
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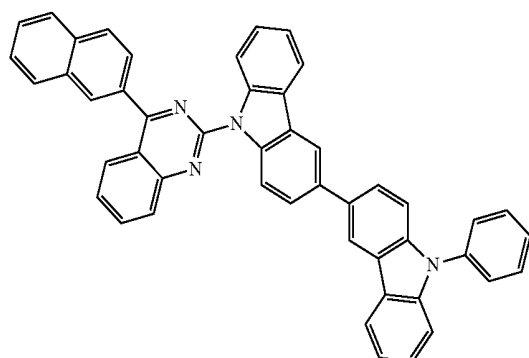
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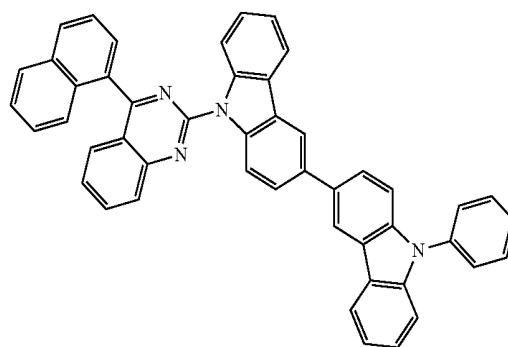
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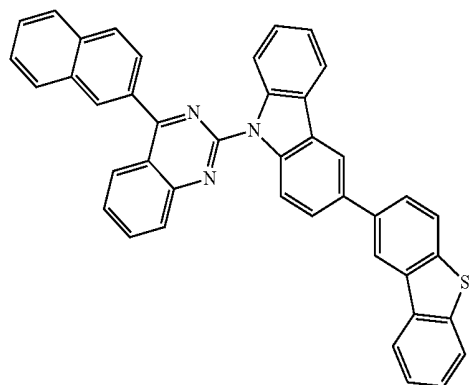
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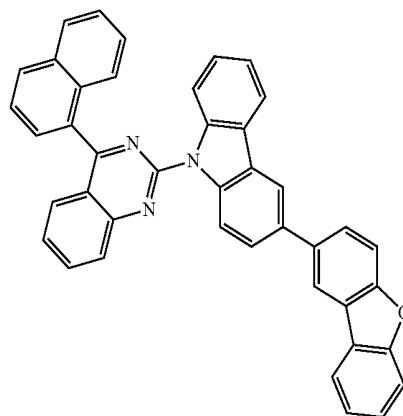
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C-7



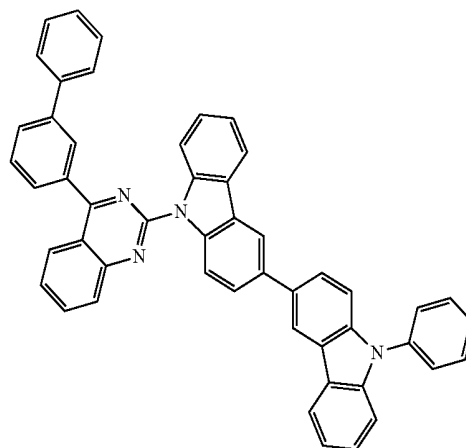
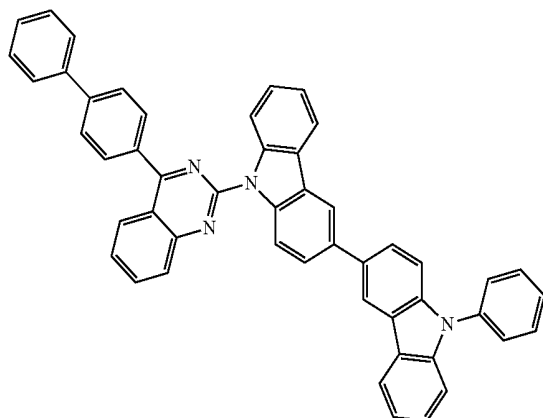
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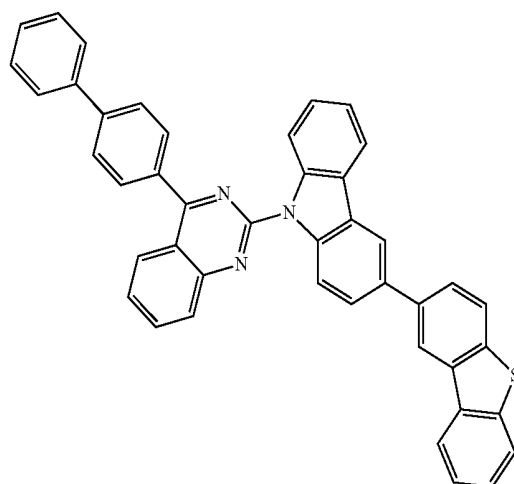
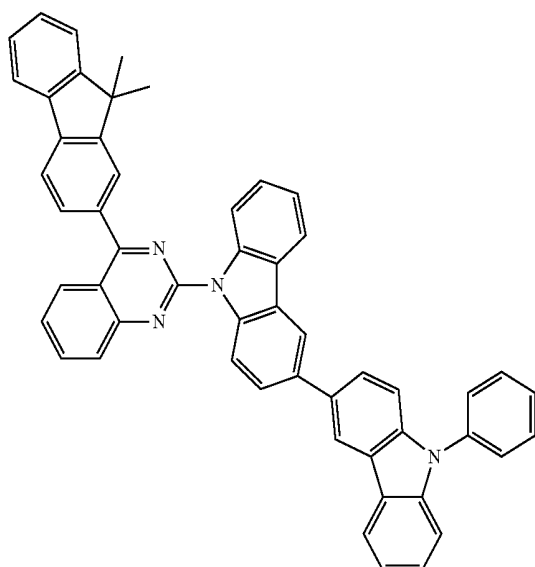
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C-10



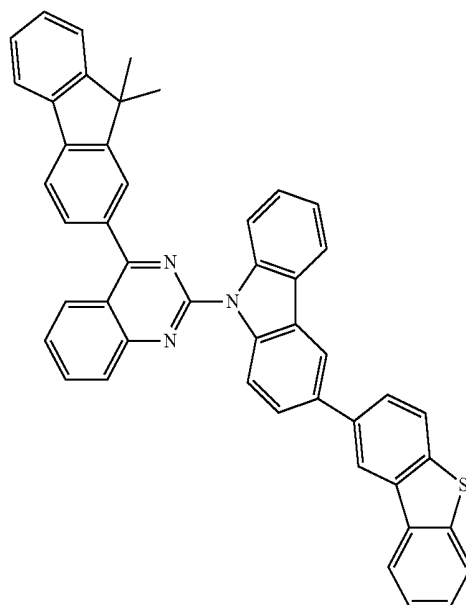
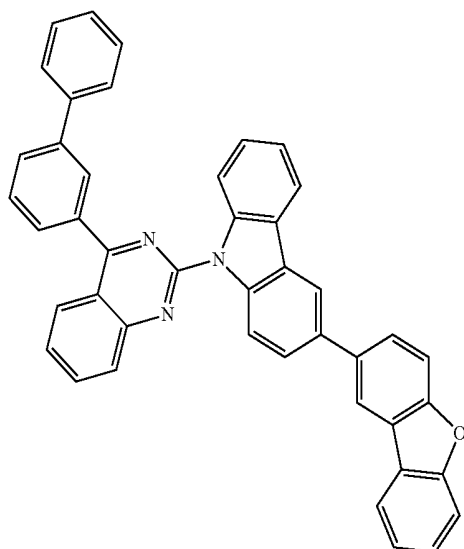
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C-12



C-13

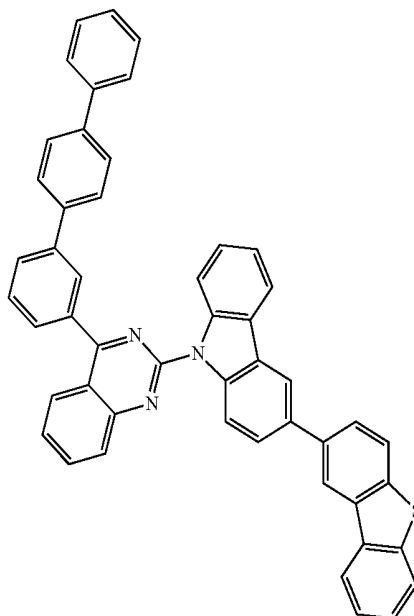
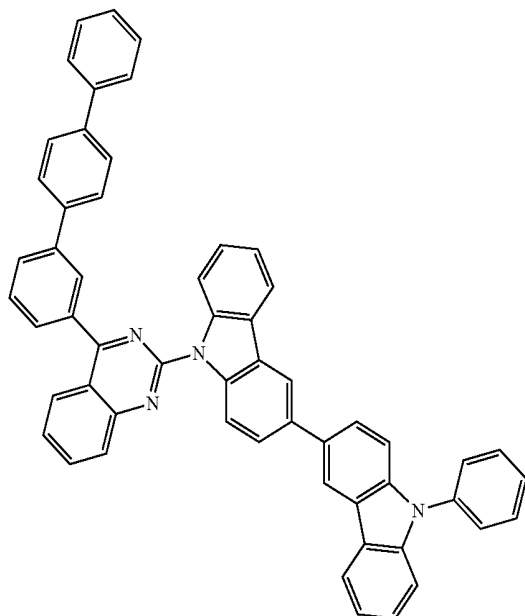
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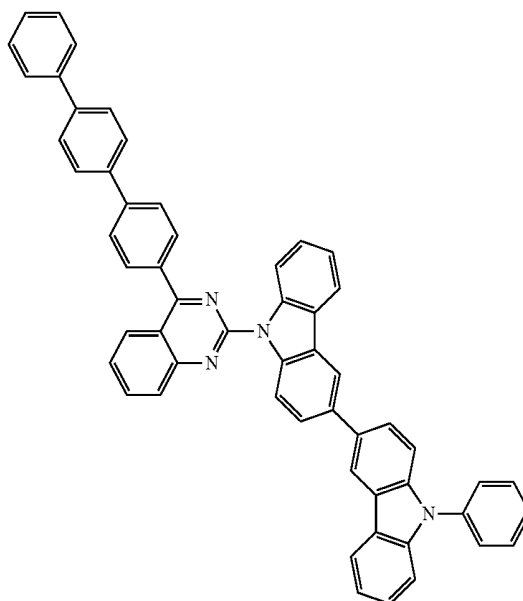
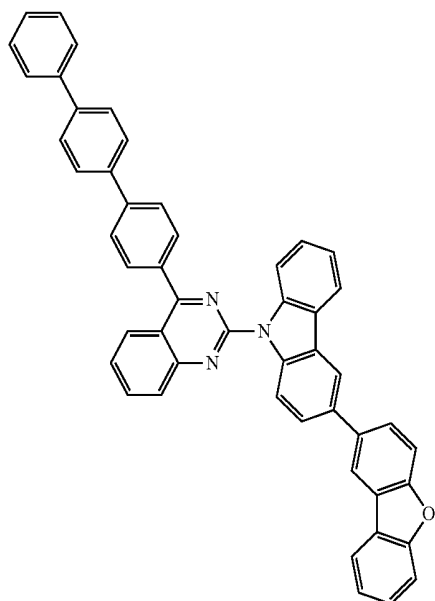
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C-16

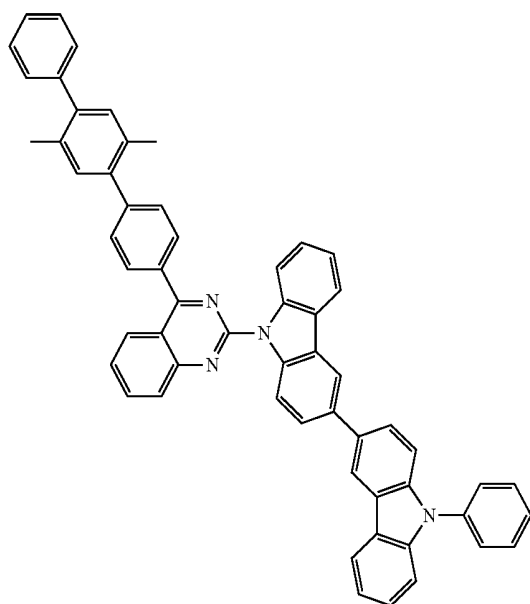


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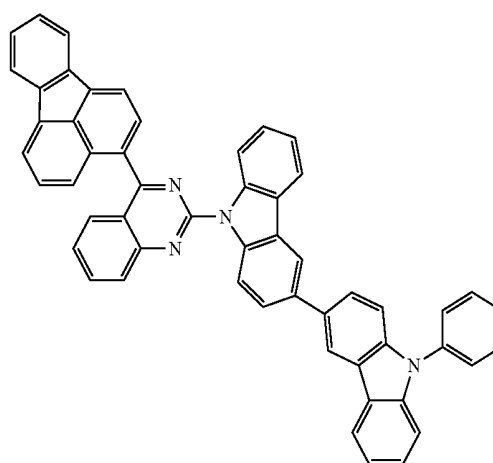
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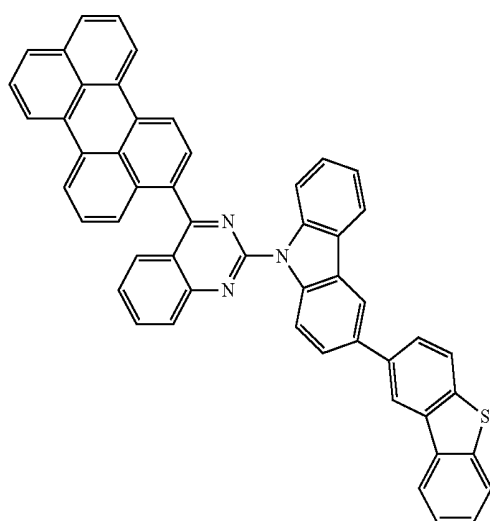
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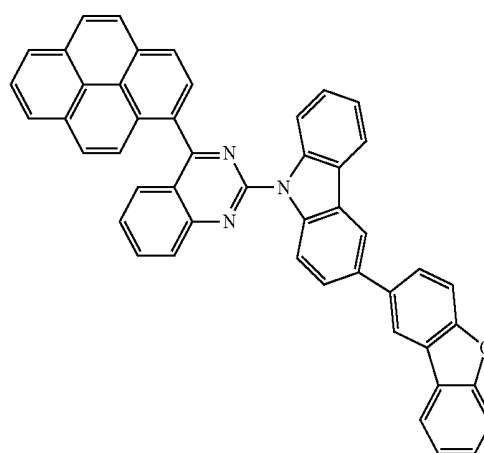
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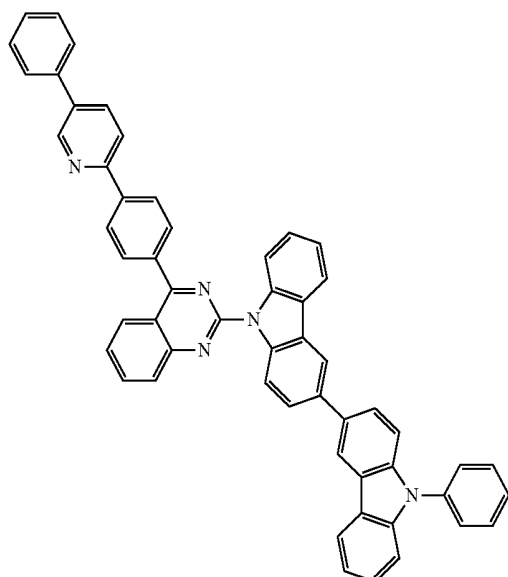
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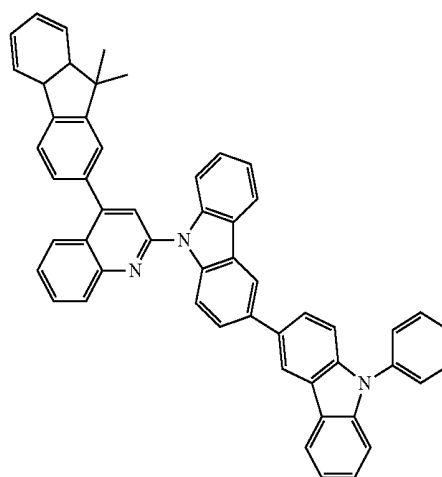
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C-23

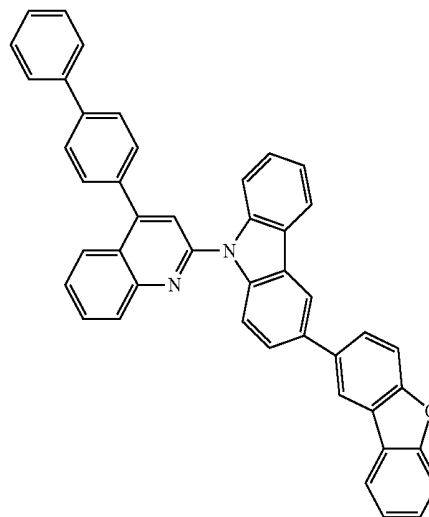
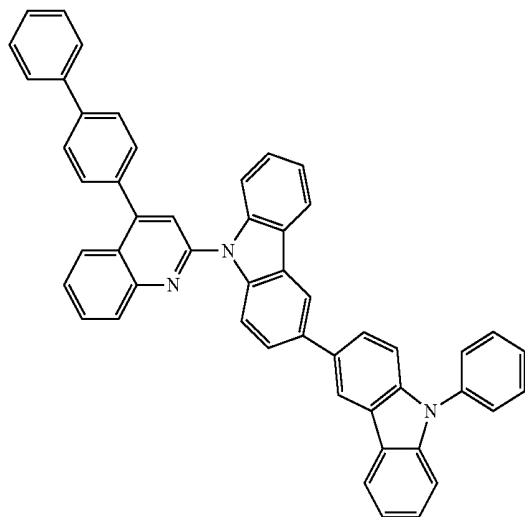


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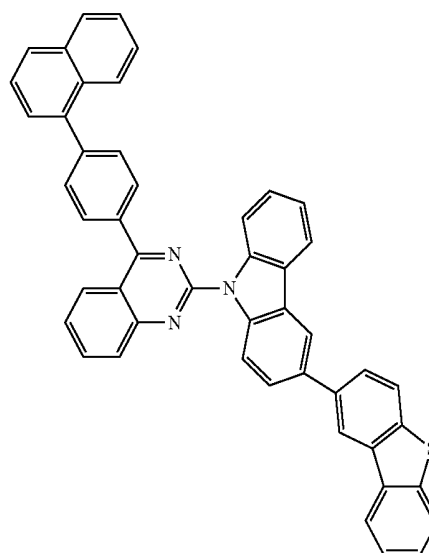
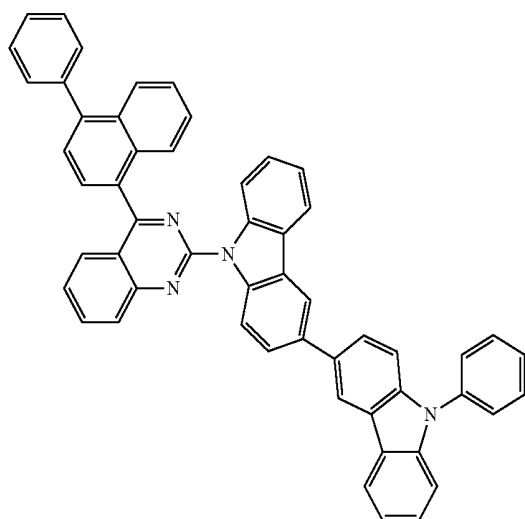
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C-26



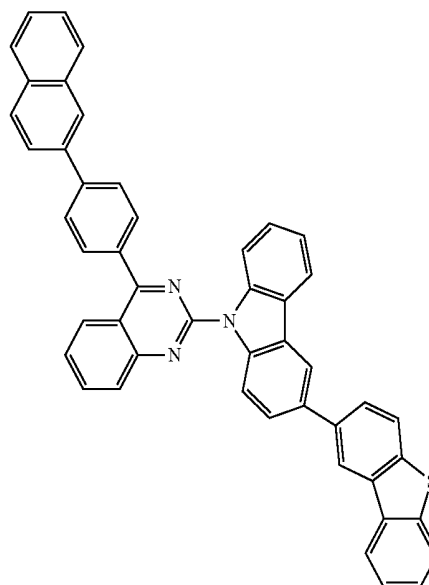
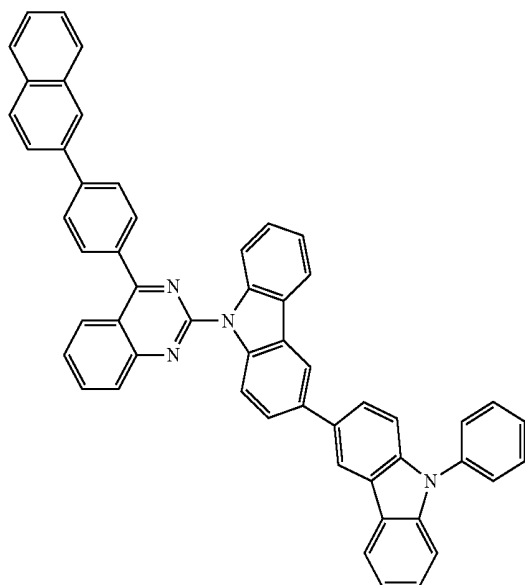
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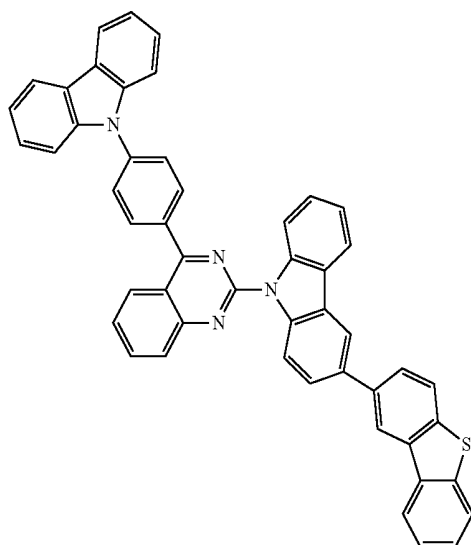
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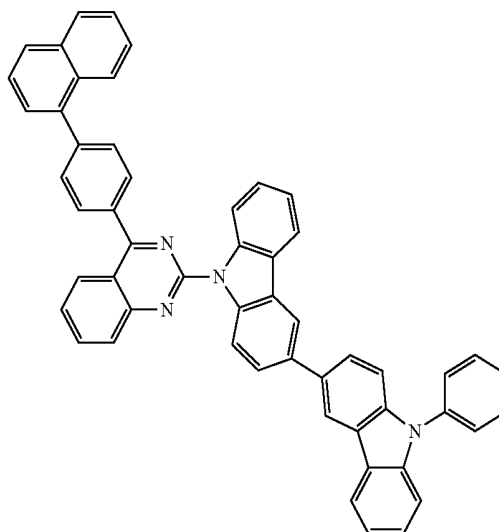
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C-30

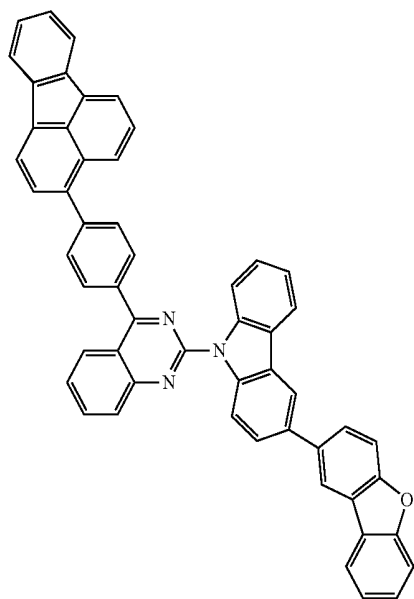


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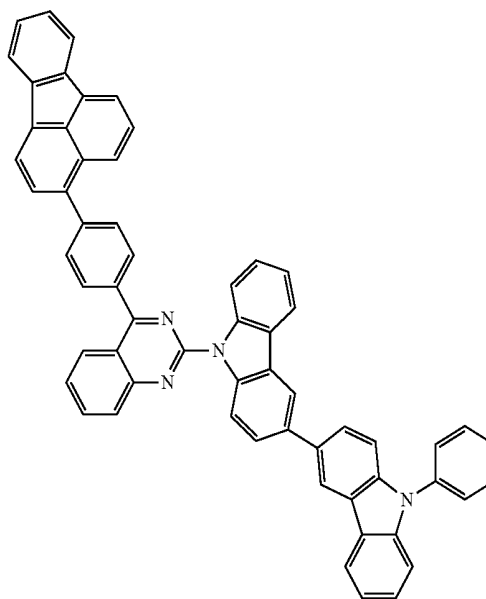
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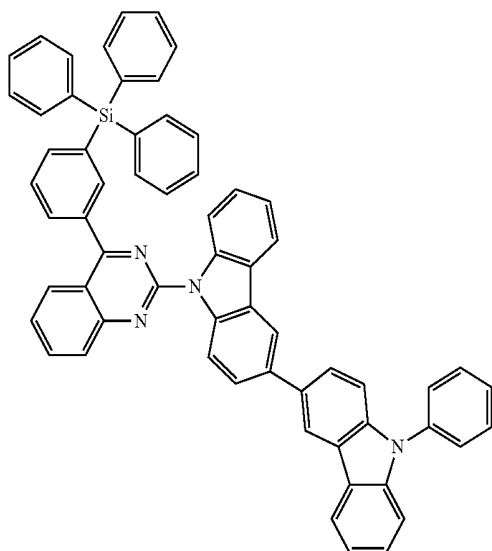
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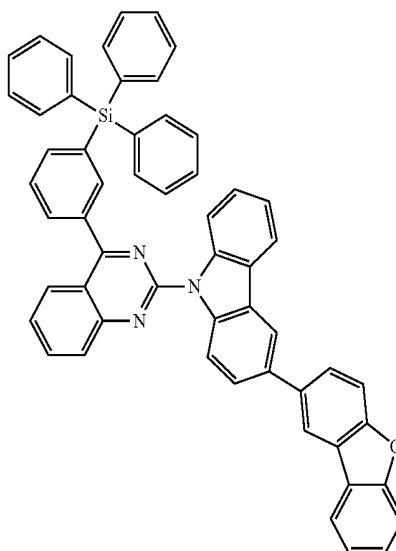
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C-35



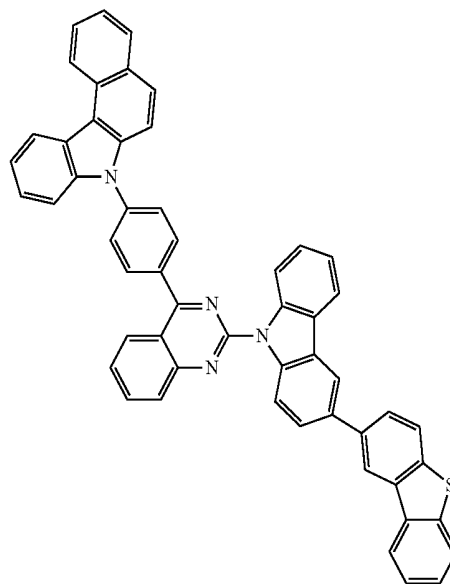
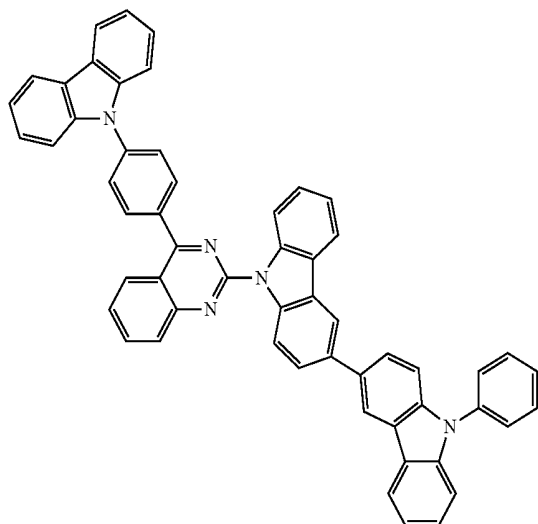
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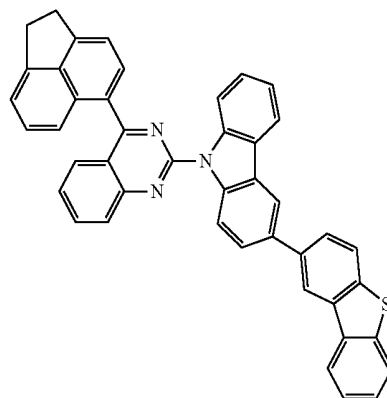
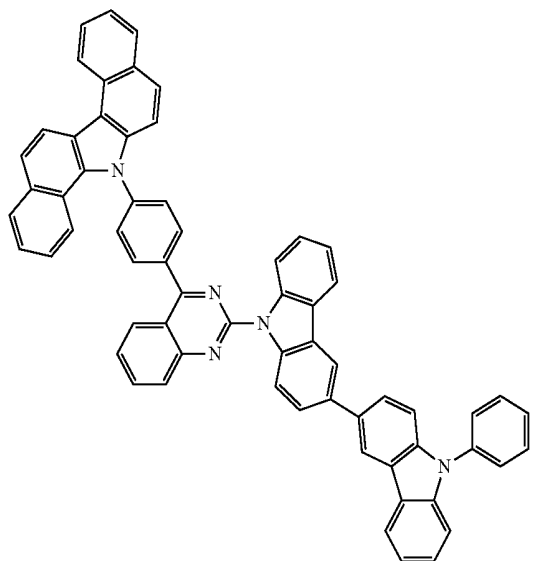
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C-38



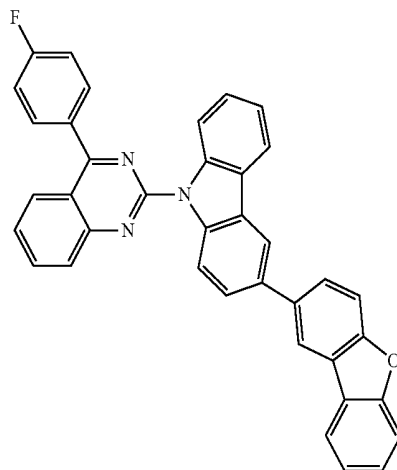
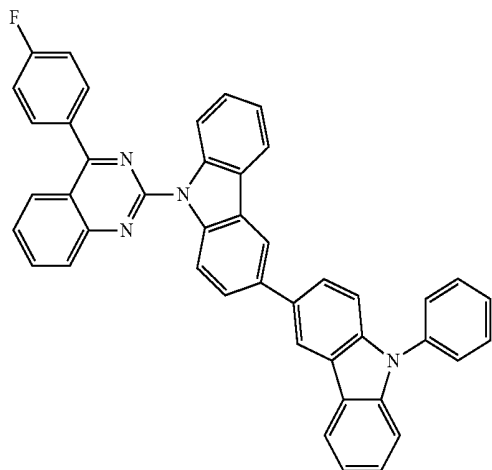
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C-40

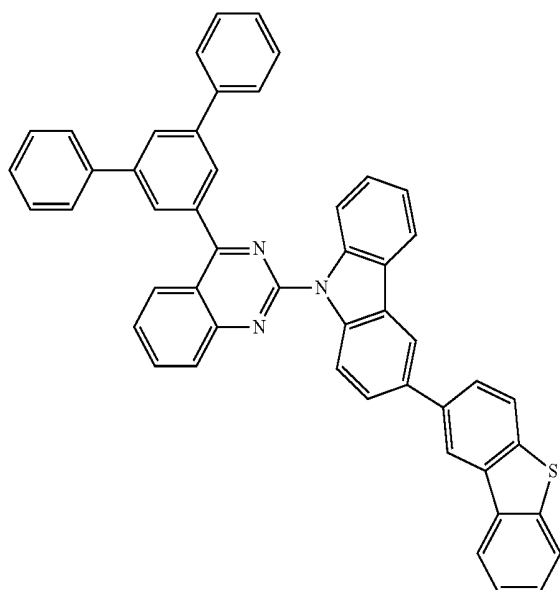
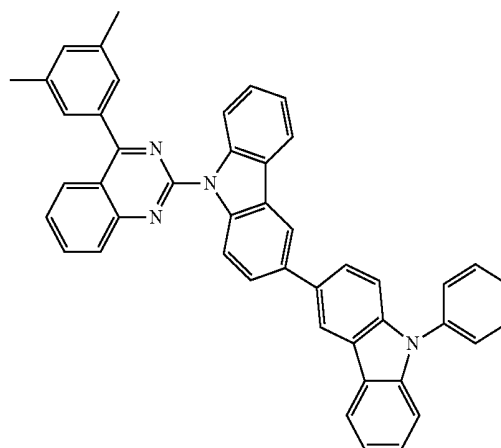
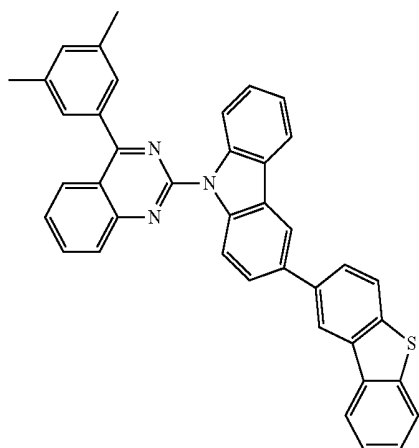
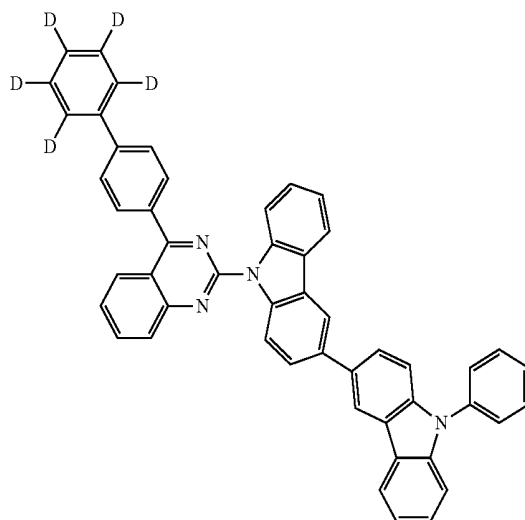
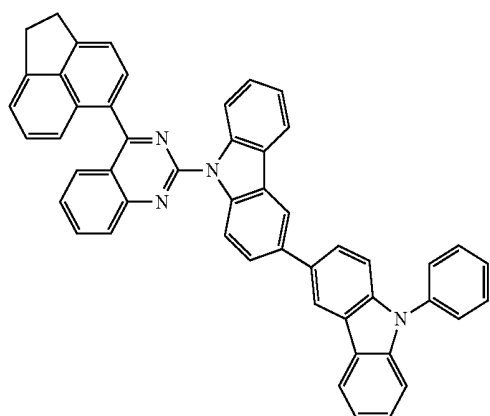


C-41

C-42

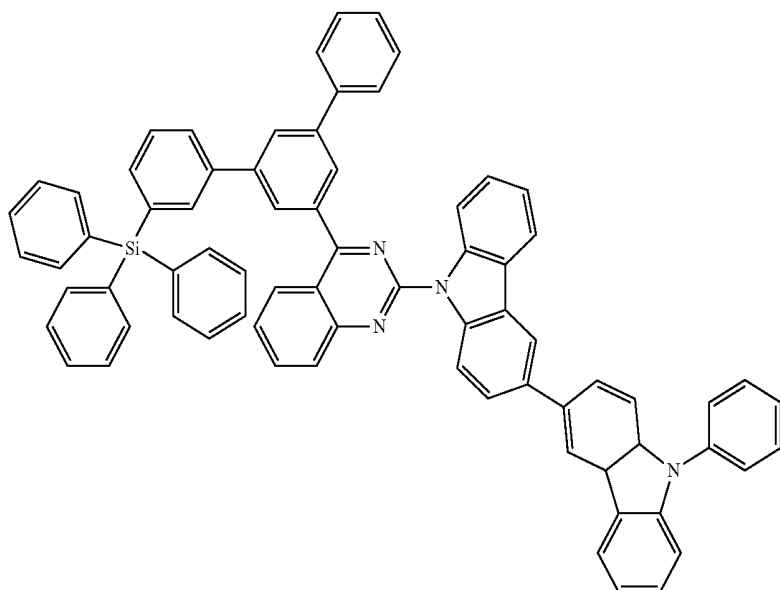


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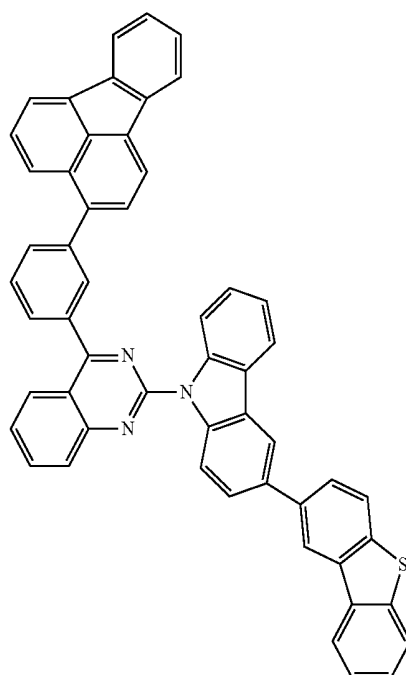
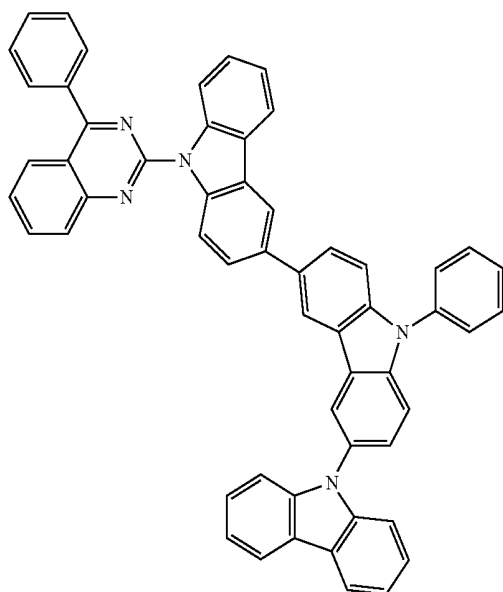
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C-49

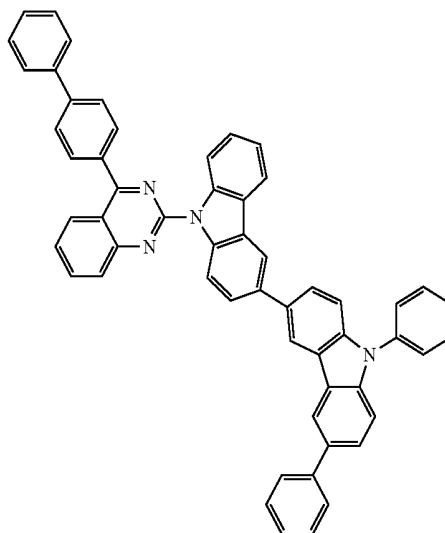
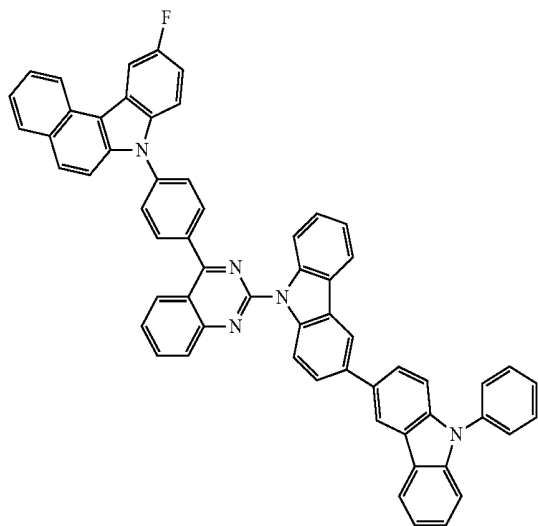
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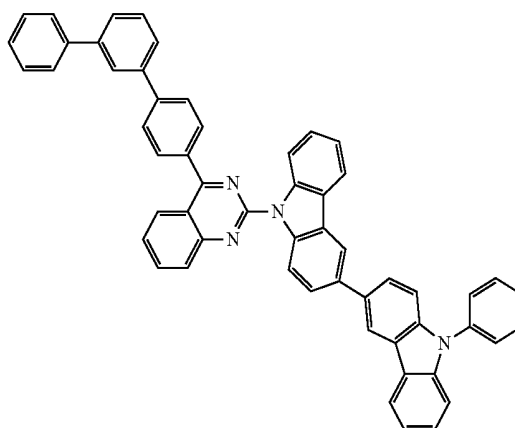
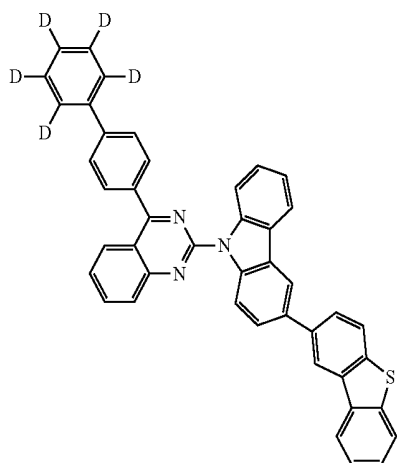
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C-52



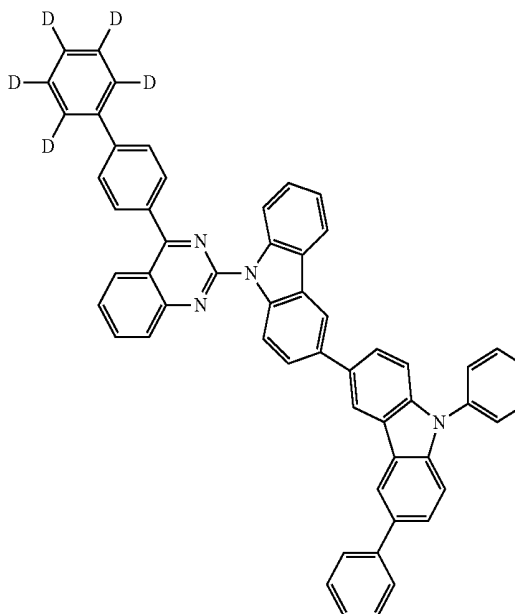
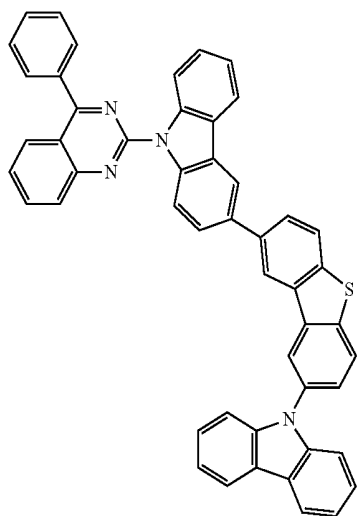
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C-54



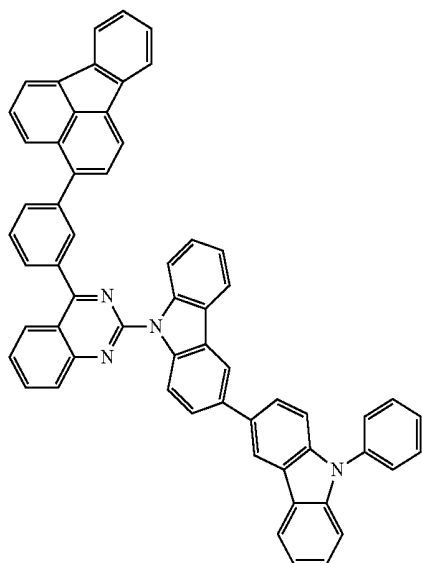
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C-56

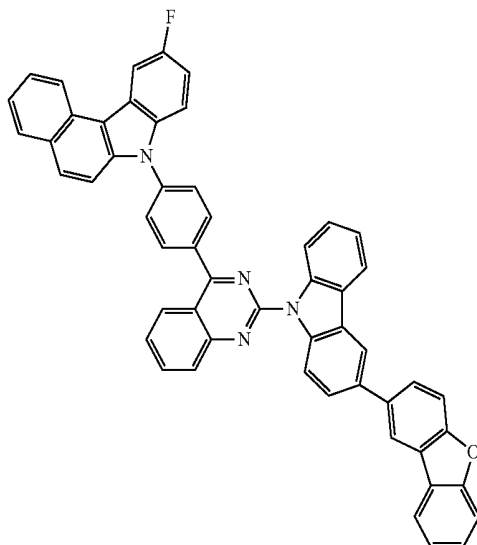


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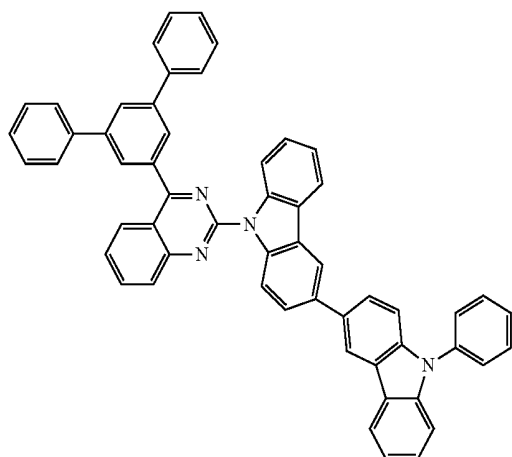
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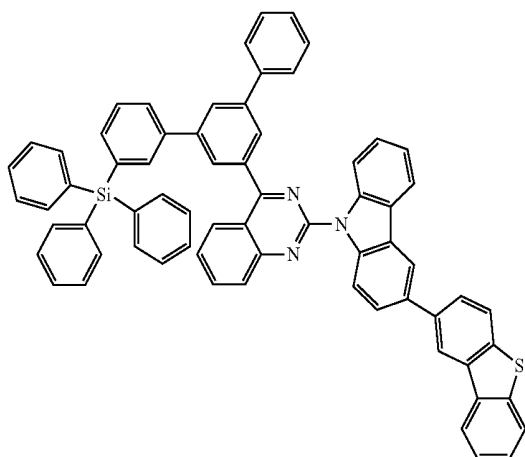
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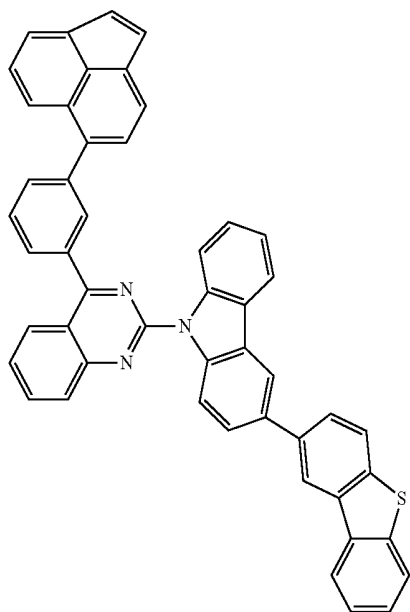
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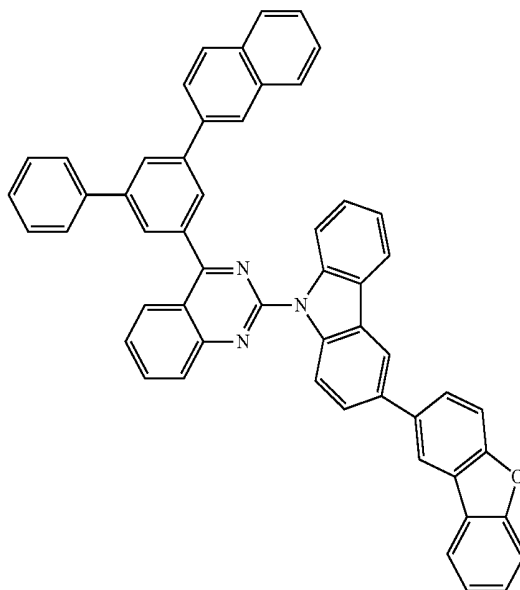
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C-61



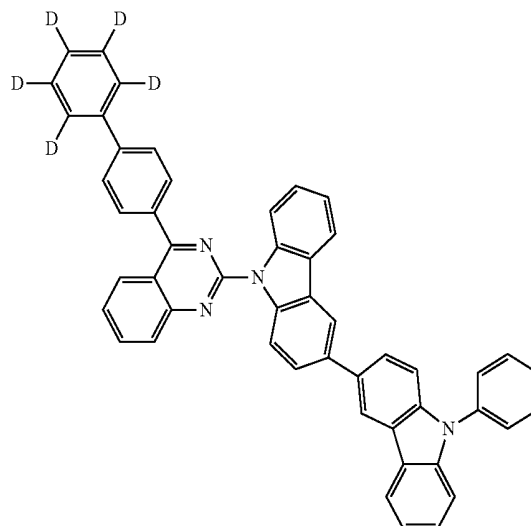
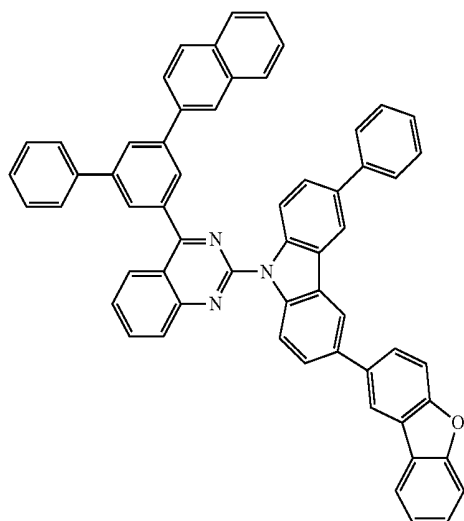
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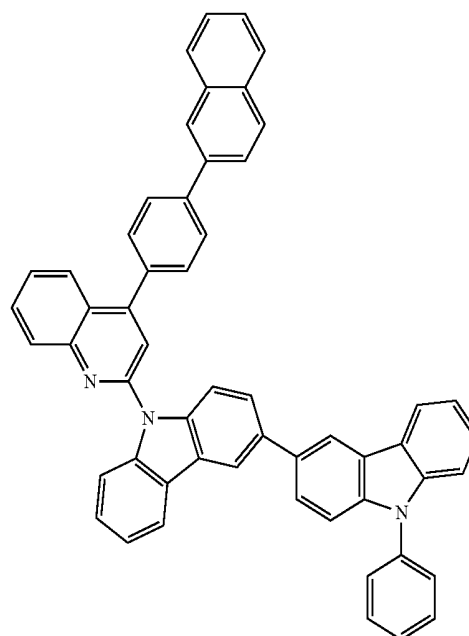
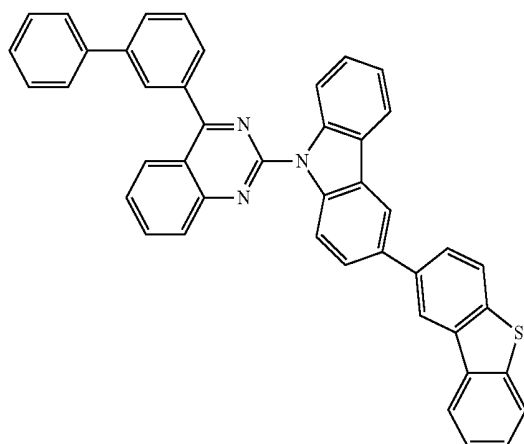
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C-64



C-65

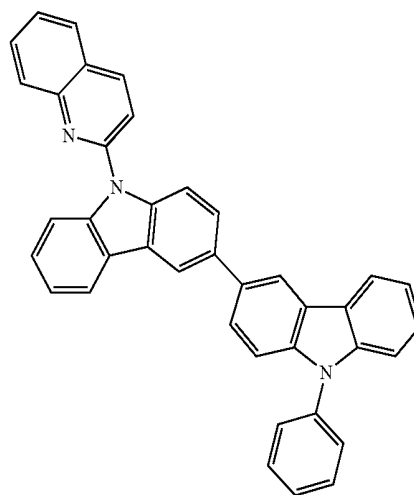
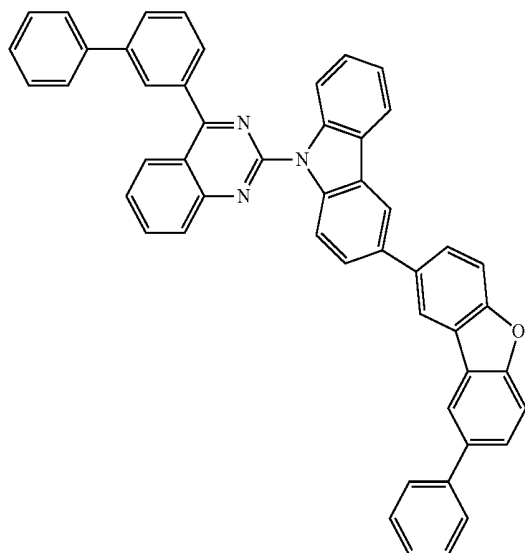
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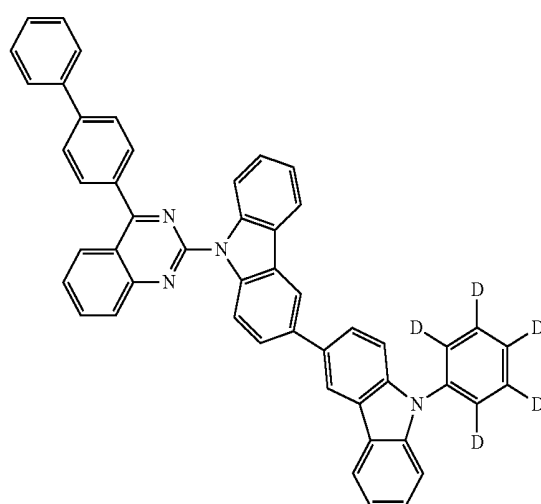
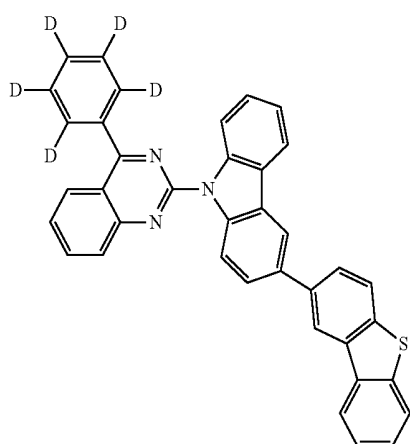
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C-68



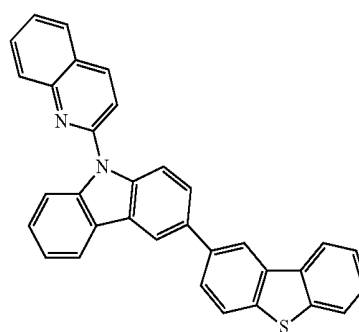
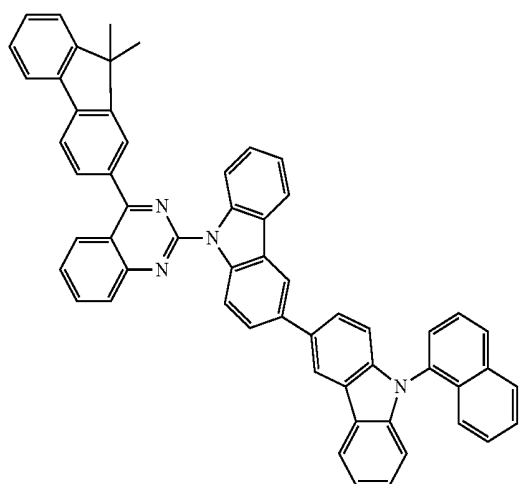
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C-70



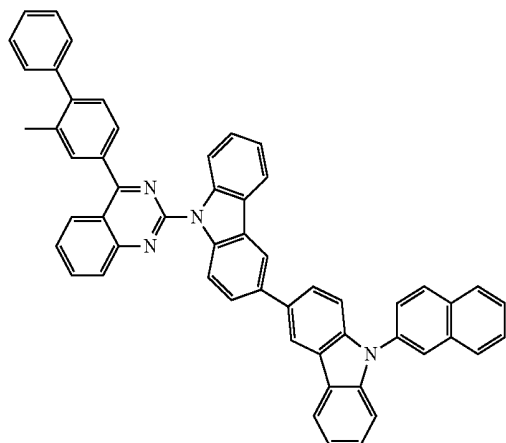
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C-72

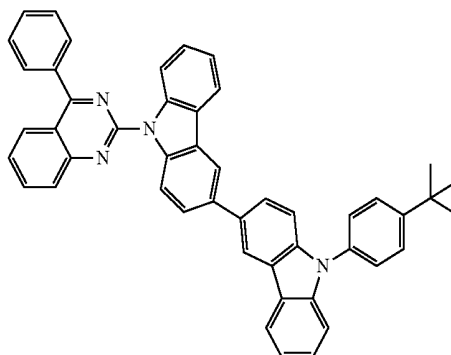


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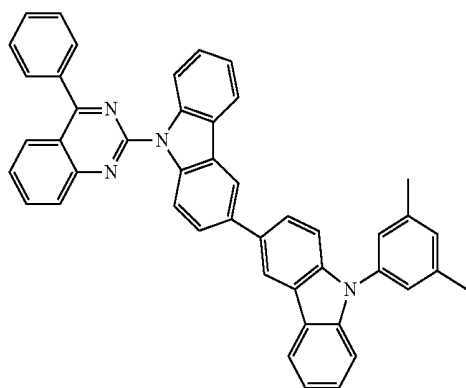
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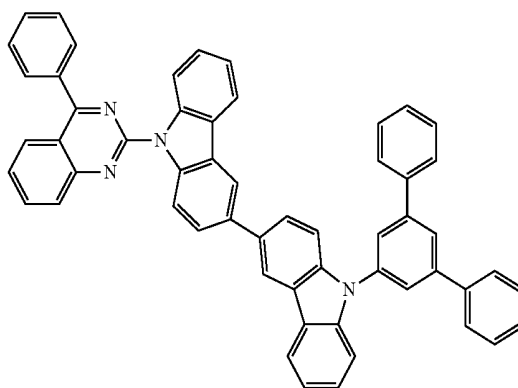
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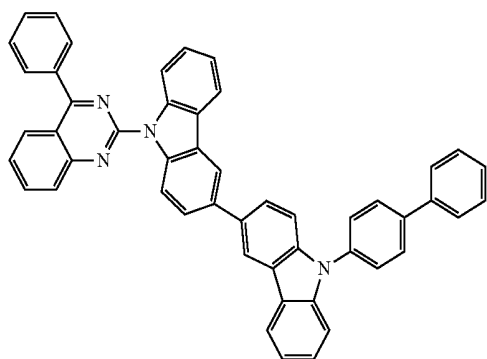
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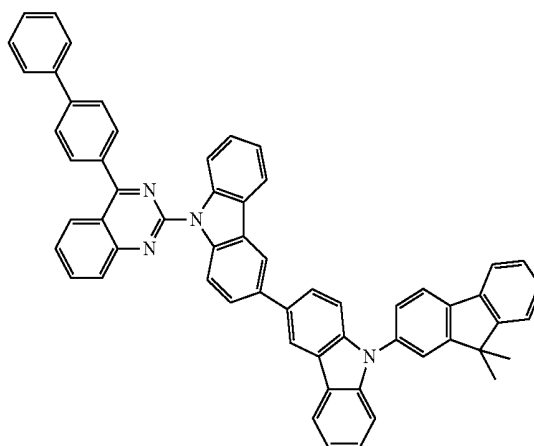
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C-77

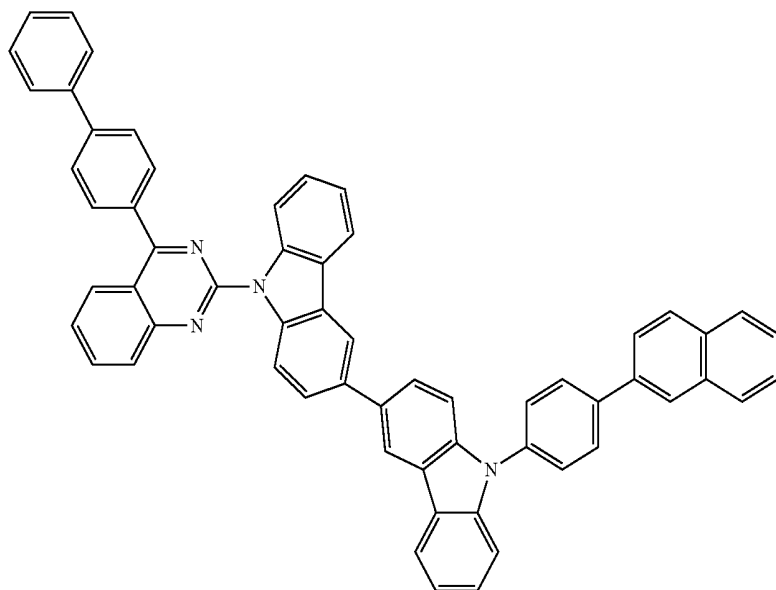


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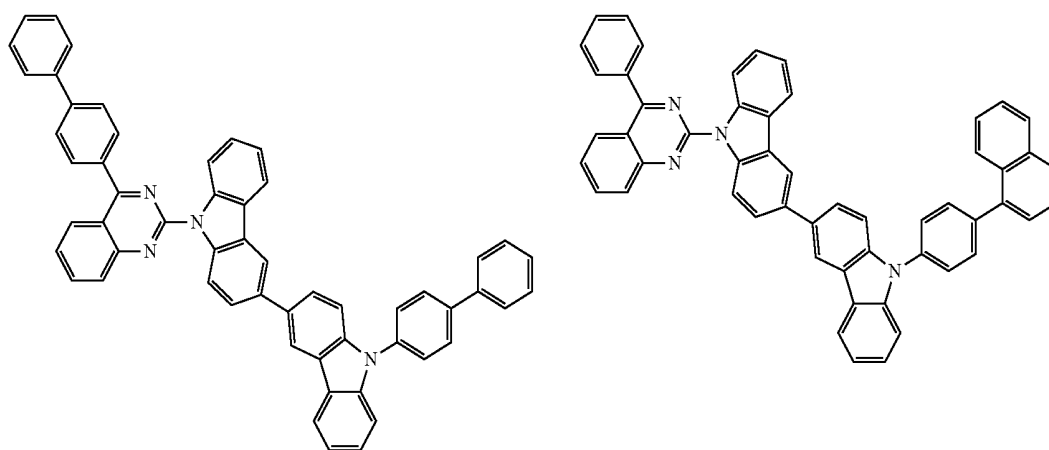
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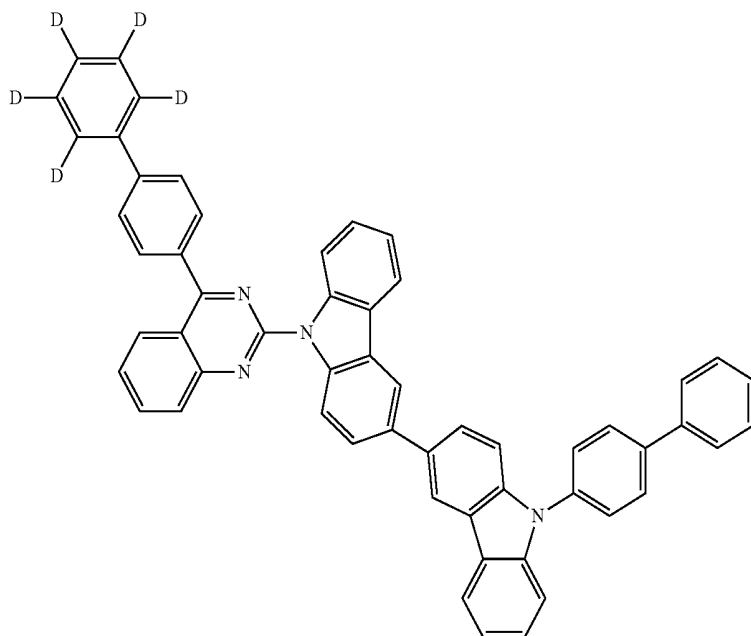


C-80

C-81

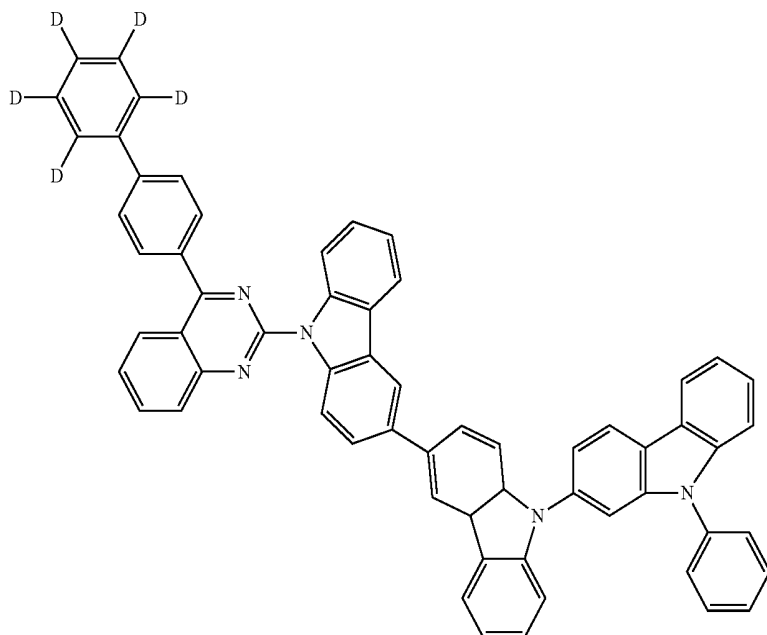


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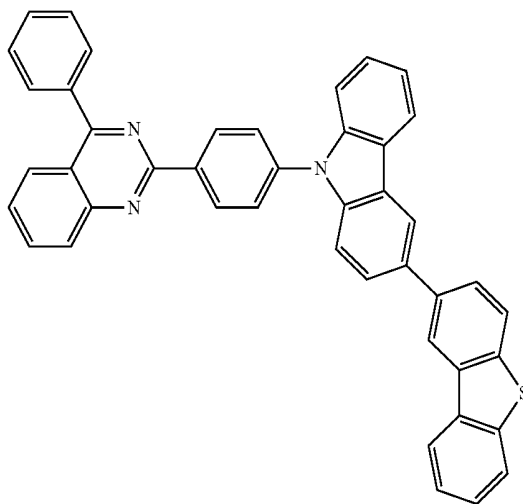
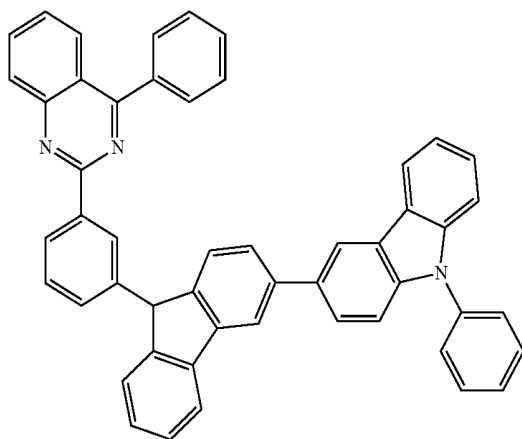
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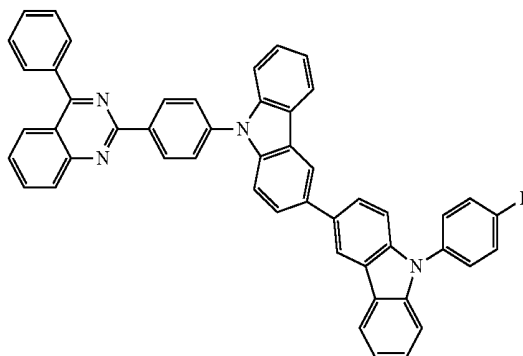
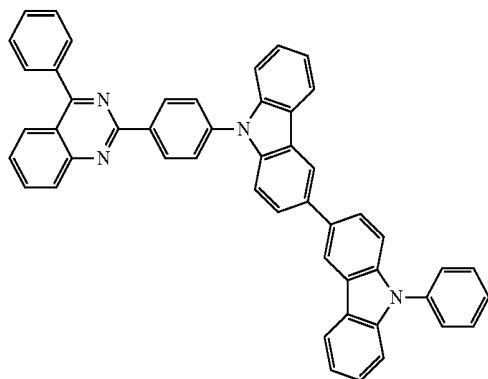
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C-85



C-86

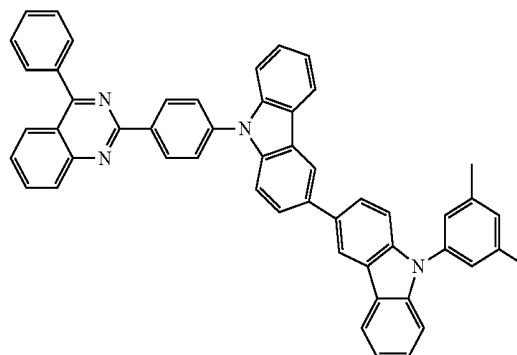
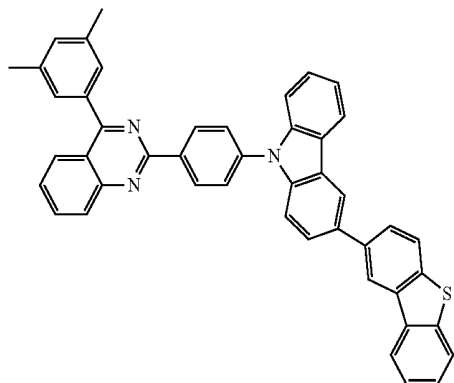
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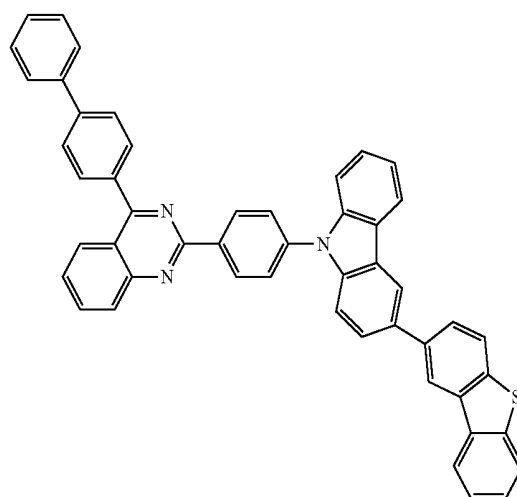
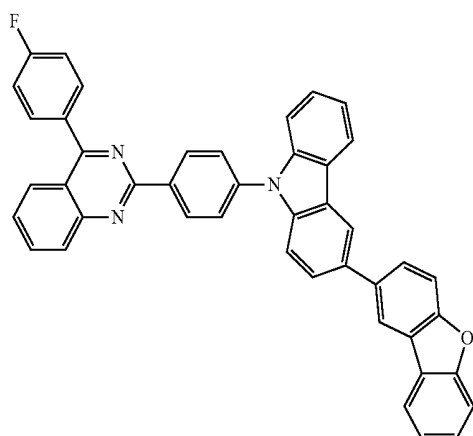
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C-89



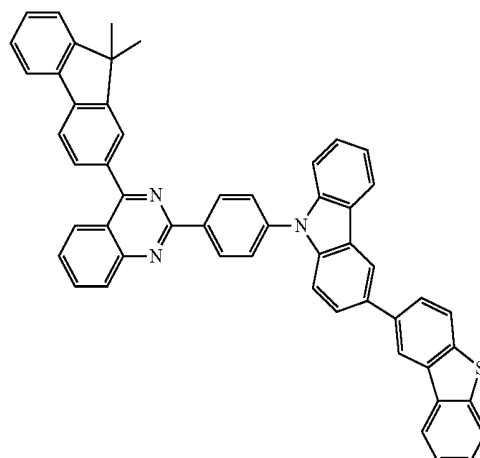
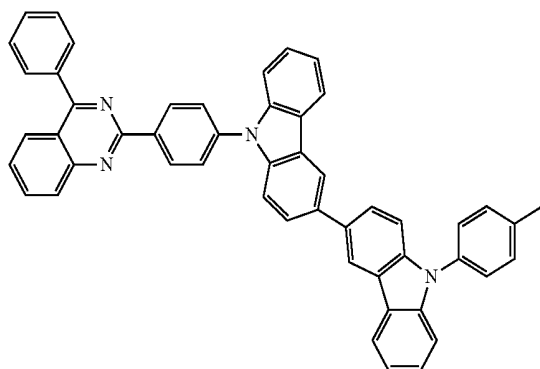
C-90

C-91



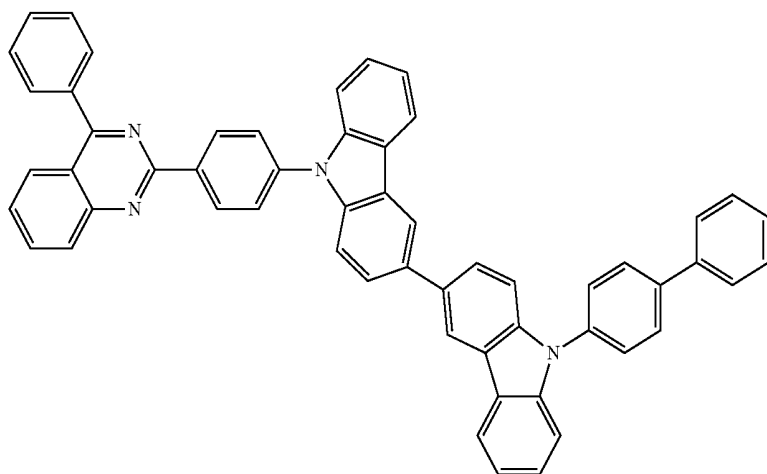
C-92

C-93



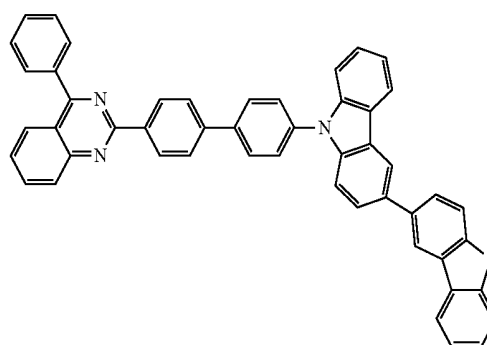
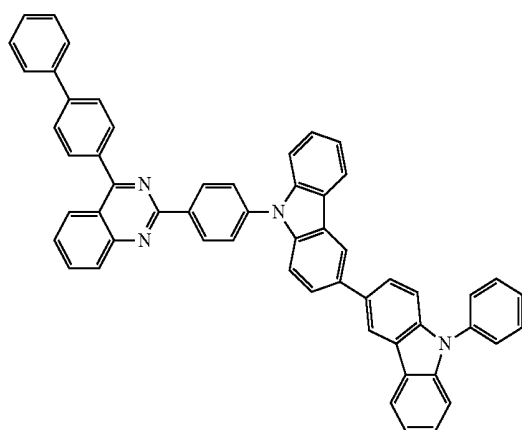
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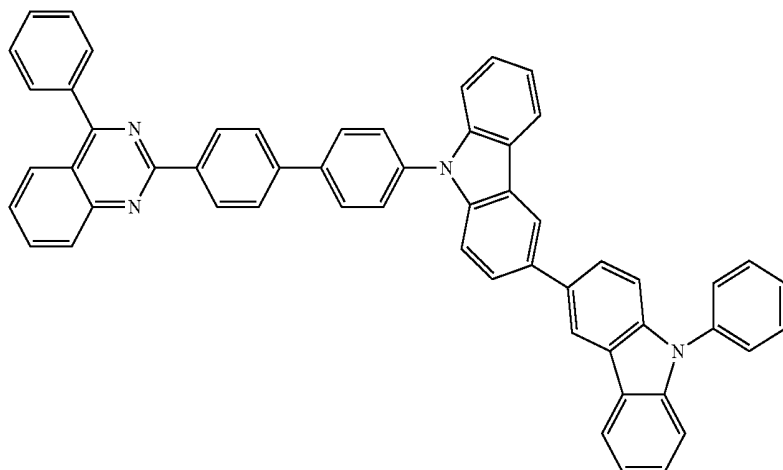


C-95

C-96



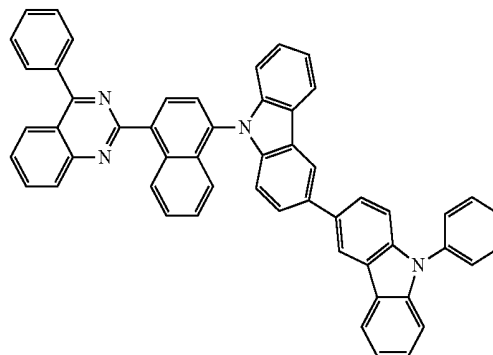
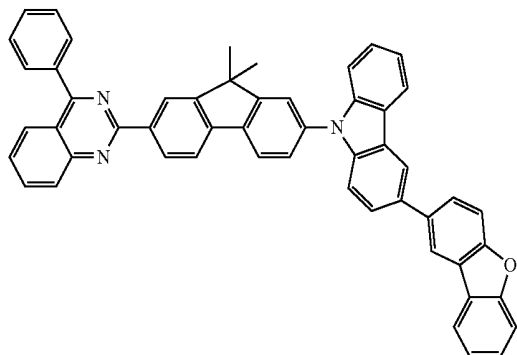
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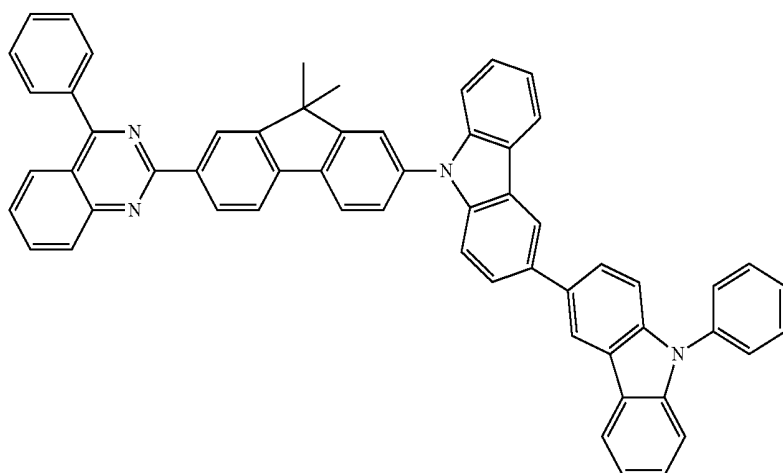
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C-98

C-99

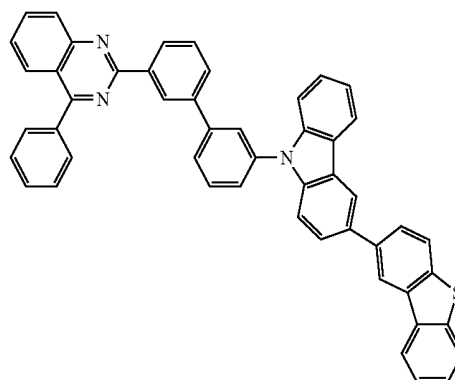
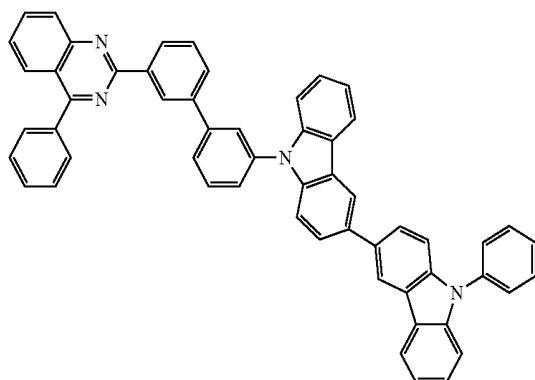


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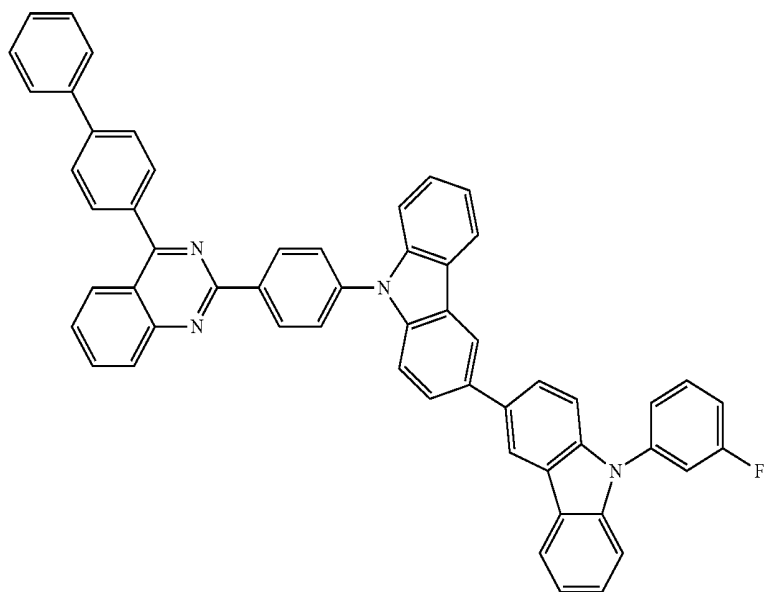
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C-102



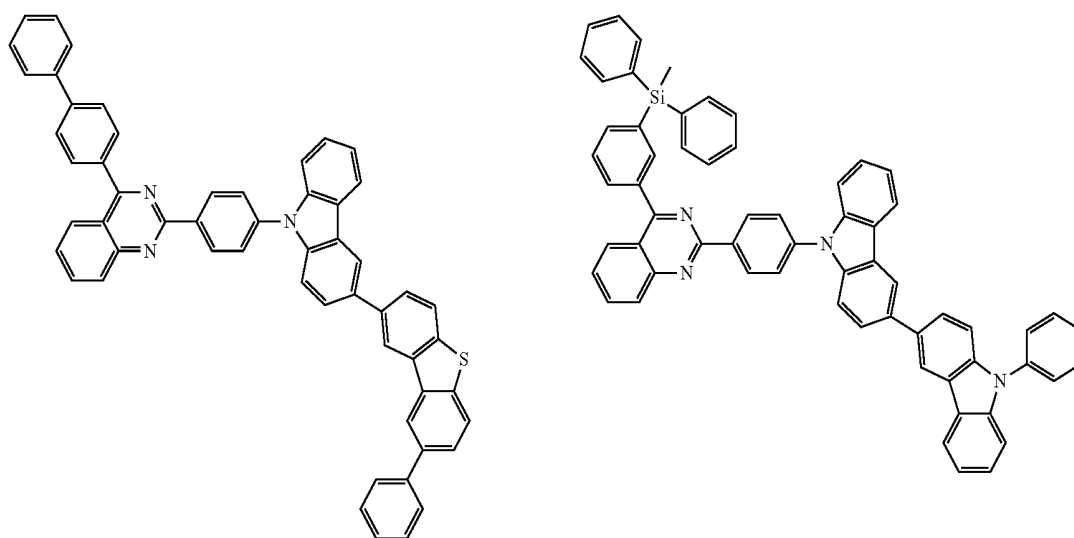
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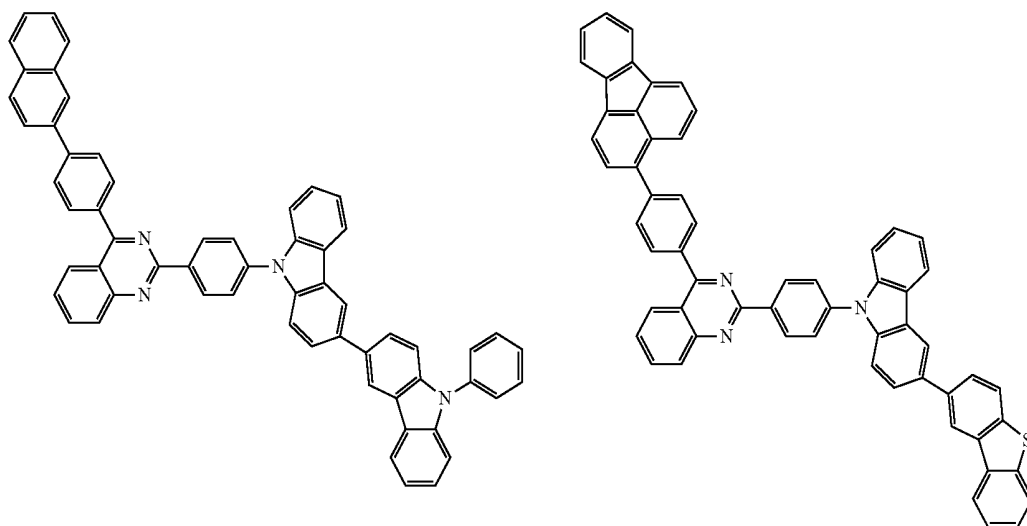
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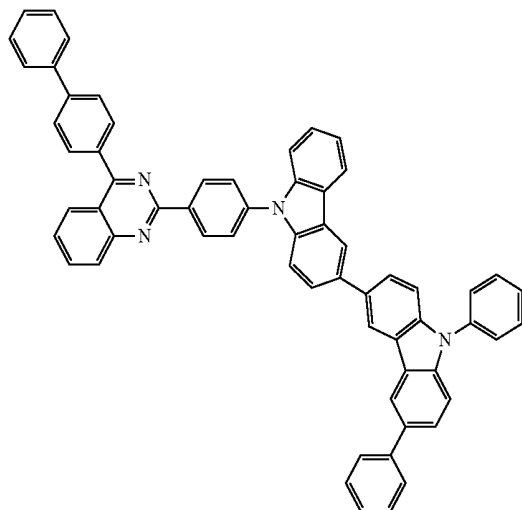
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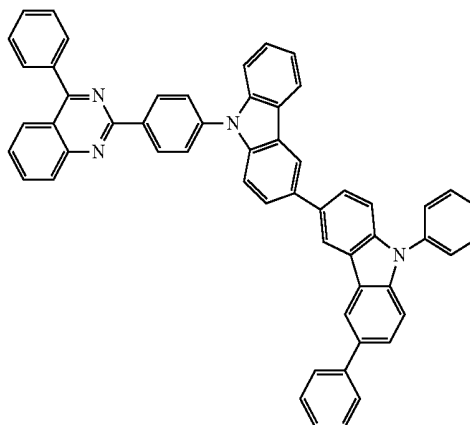


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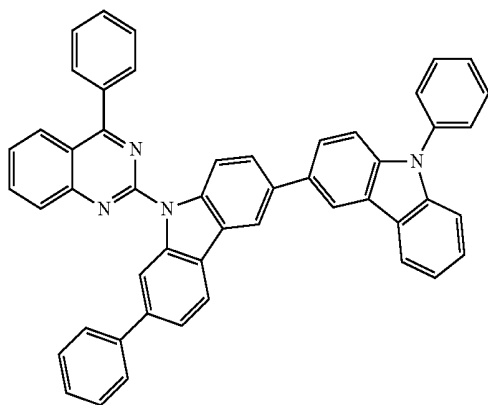
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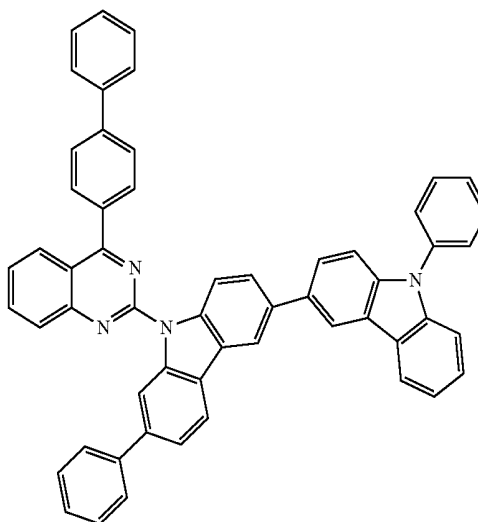
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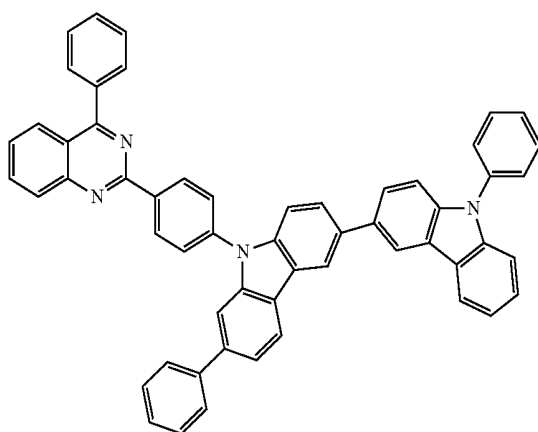
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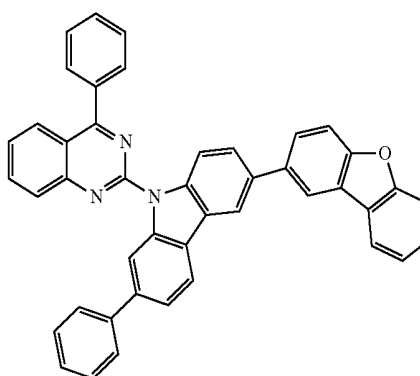
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C-112

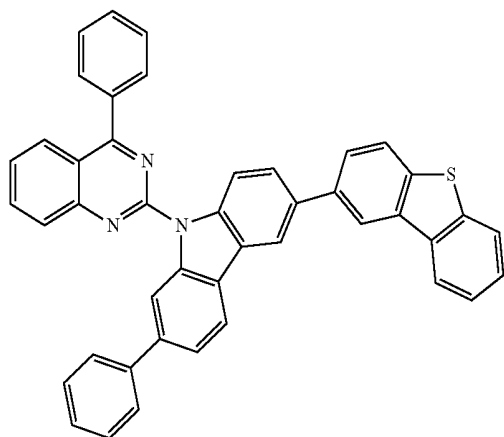


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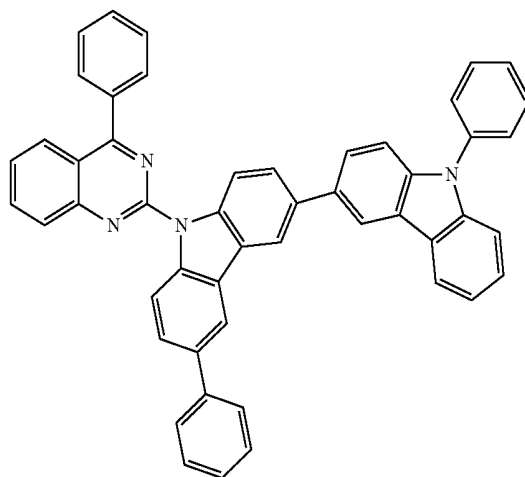


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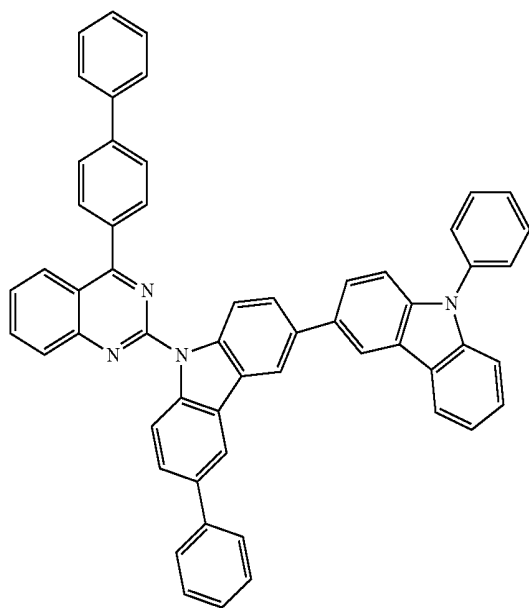
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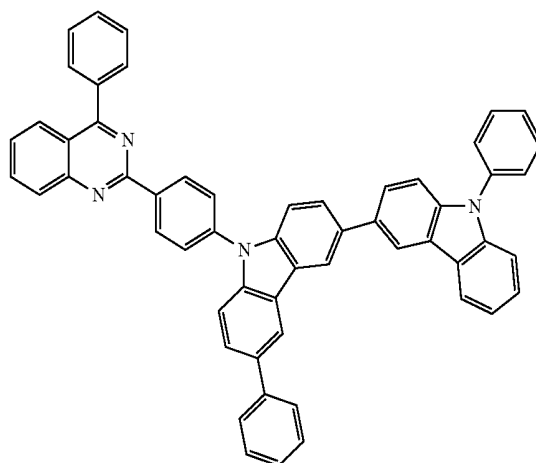
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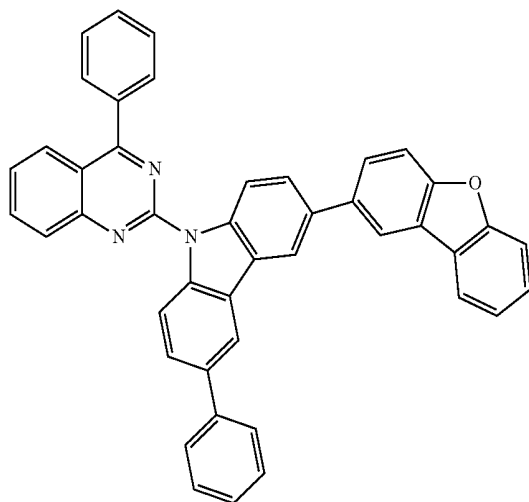
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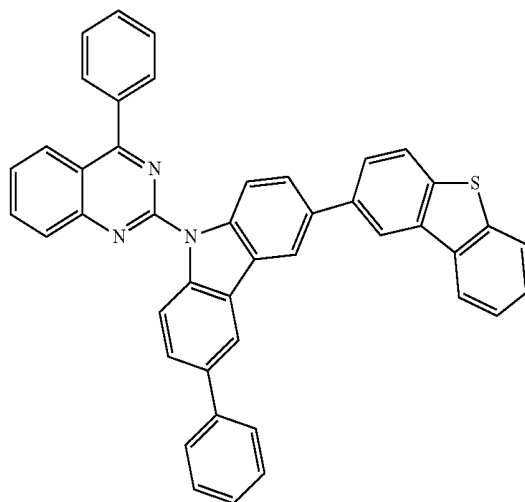
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C-118



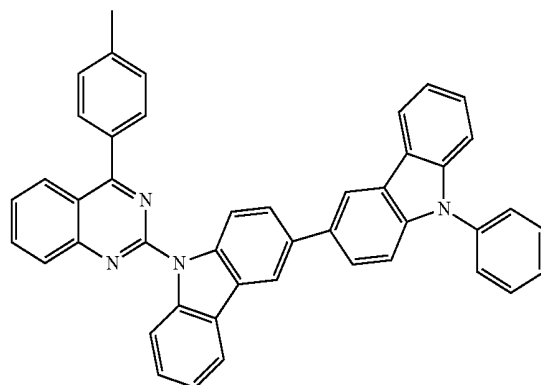
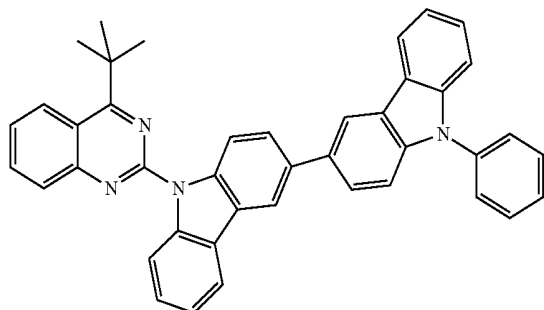
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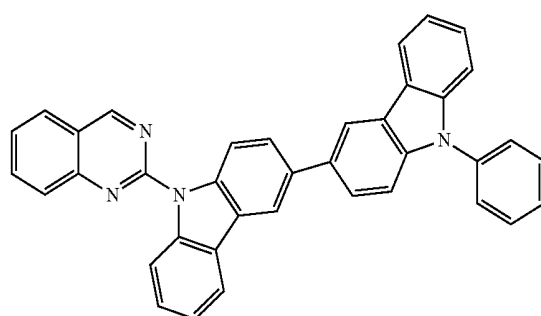
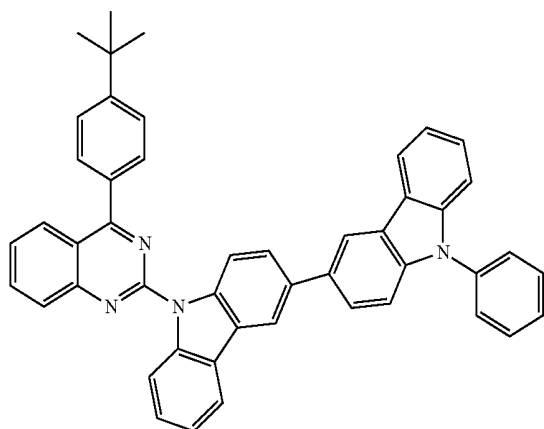
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C-121



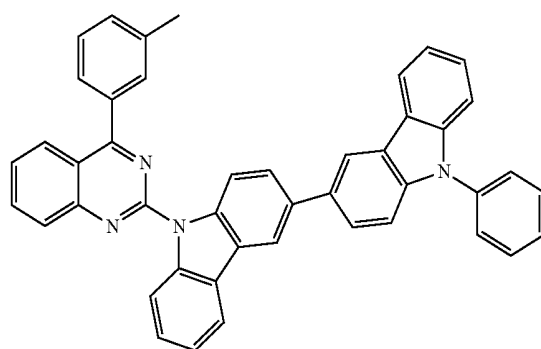
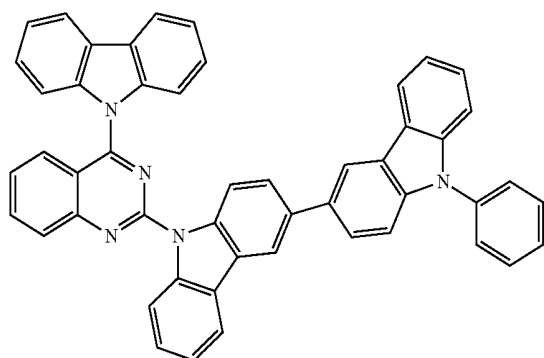
C-122

C-123

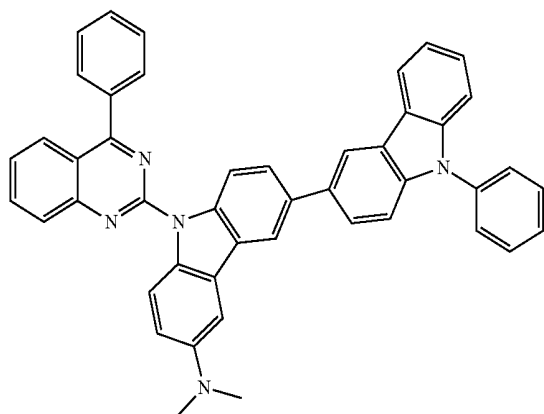


C-124

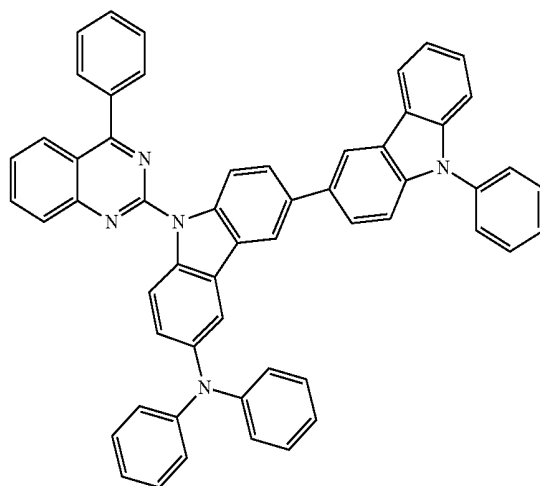
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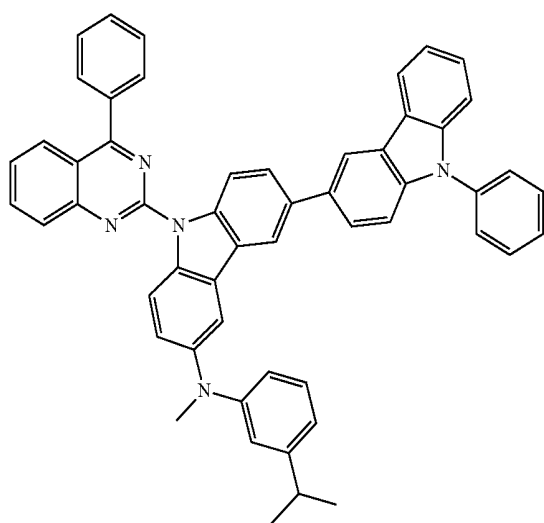
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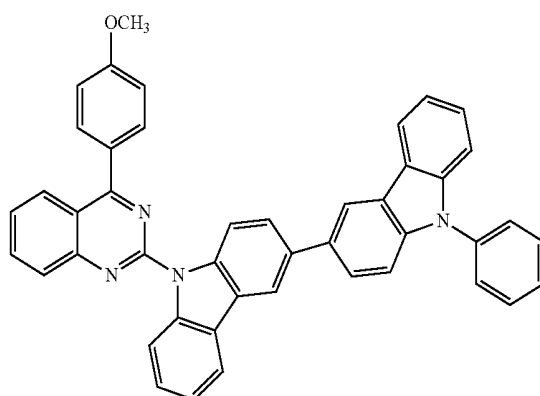
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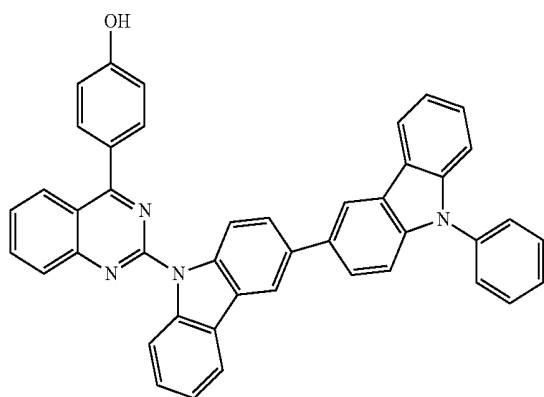
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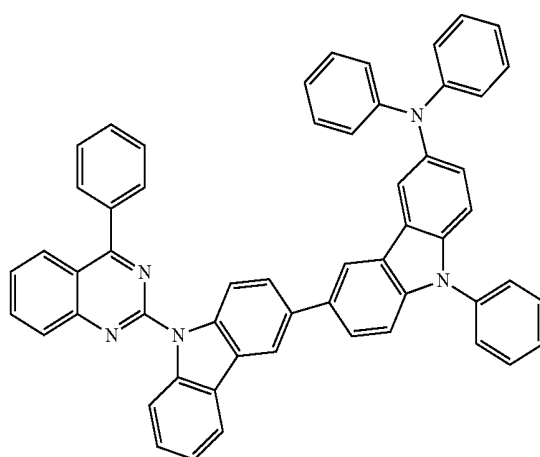
C-129



C-130

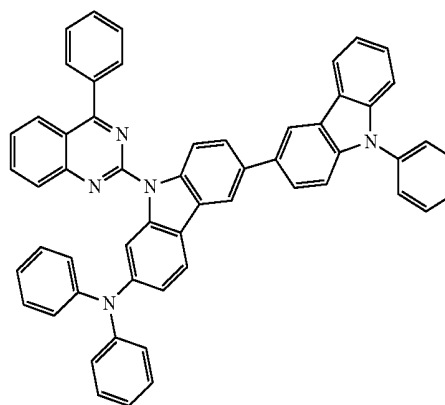
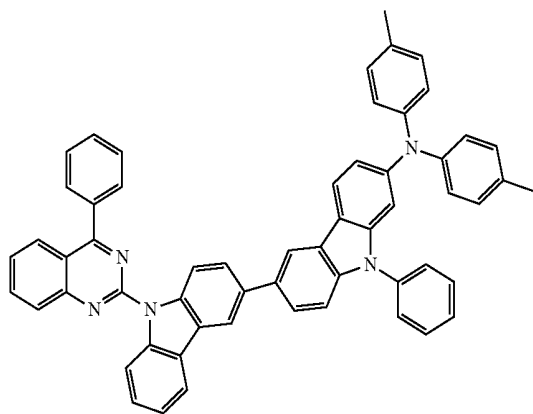


C-131



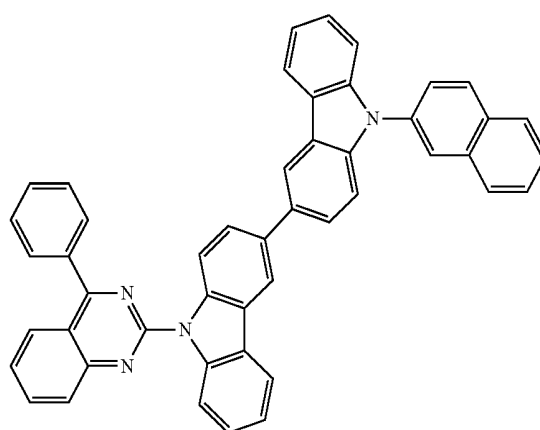
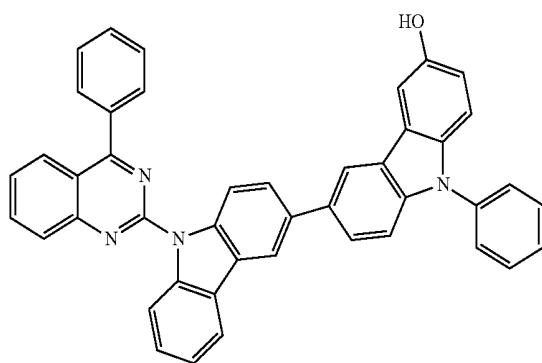
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C-132

C-133



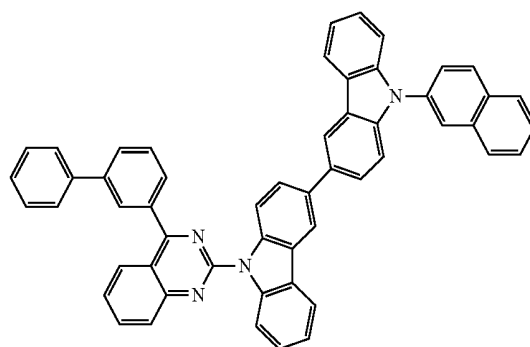
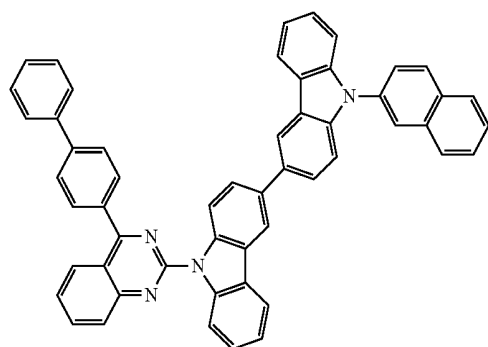
C-134

C-135



C-136

C-137



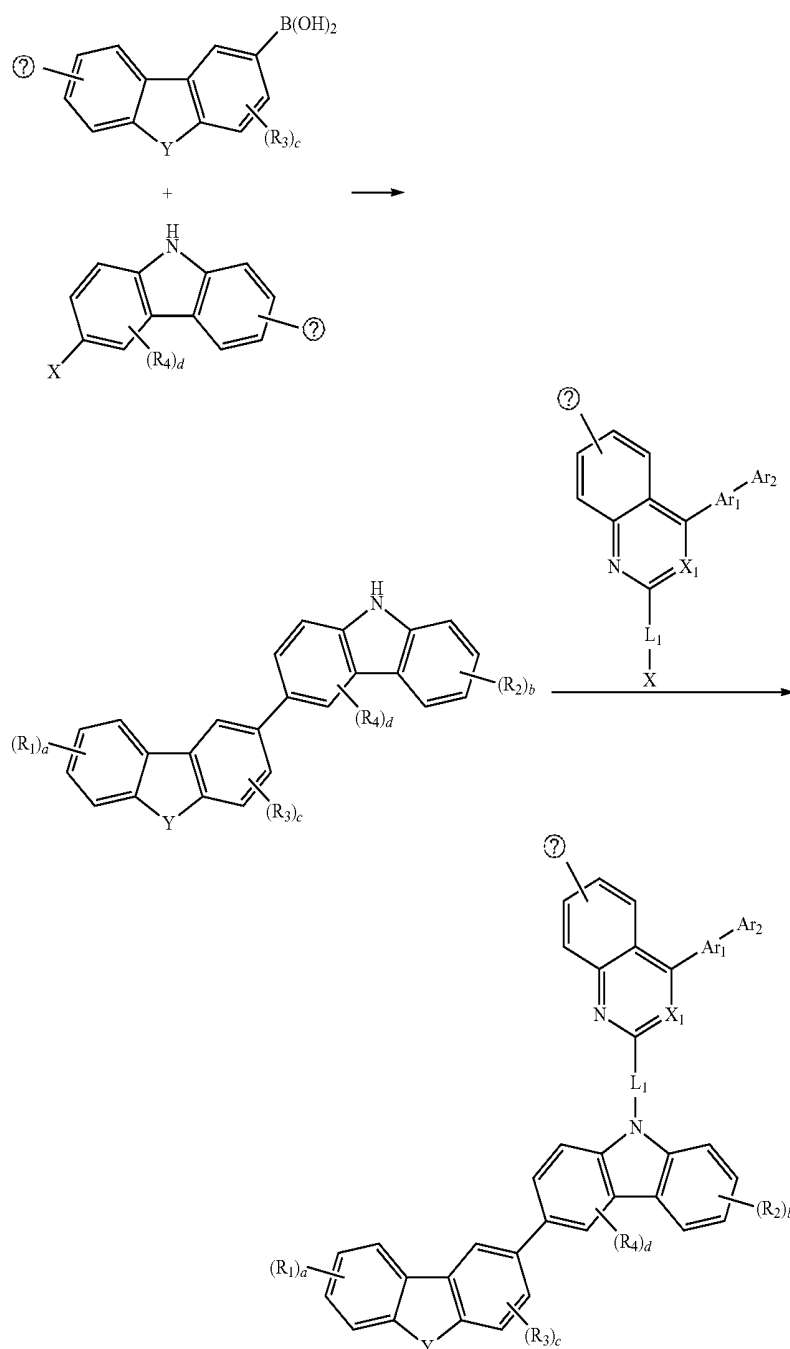
[0071] Of the above, without intending to be limited thereby, particularly preferred compounds are one or more of those depicted as compound C-1, C-5, C-9, C-77, C-135, C-136 or C-137. Particularly preferred compounds may be selected from C-1, C-5, C-9, or C-77. Particularly preferred compounds may be selected, from C-135, C-136 or C-137.

[0072] Another feature of the present teachings is the possibility to realize a glass transition temperature (T_g) (as measured by differential scanning calorimetry) for the compound

of Formula 1 (namely, the host material of a light emitting layer of the invention) in excess of about 80° C., about 90° C., or about 100° C. The glass transition temperature for the host material may be below about 350° C., below about 325° C., or below about 300° C.

[0073] Organic electroluminescent compounds according to the present invention (e.g., for use as a host material) can be prepared by well-known methods in the art, for example, according to the following scheme 1.

[Scheme 1]



⑦ indicates text missing or illegible when filed

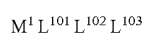
[0074] wherein, R_1 to R_5 , Ar_1 , Ar_2 , Y , X_1 , L_1 , a , h , c , d and e are as defined in formula 1 above. and X represents a halogen.

[0075] Further, the present invention provides a light emitting layer, and/or an organic electroluminescent device comprising the organic electroluminescent compound of formula 1.

[0076] Said organic electroluminescent device comprises a first electrode, a second electrode and at least one organic layer, namely a light emitting layer, between said first elec-

trode and said second electrode. Said organic layer comprises at least one organic electroluminescent compound of formula 1. Further, said organic layer comprises a light-emitting layer in which the organic electroluminescent compound of formula 1 is comprised as a host material, Where the organic electroluminescent compound of formula 1 is comprised as a host material in the light-emitting layer, said light-emitting layer further comprises at least one phosphorescent dopant. In the organic electroluminescent device of the present invention, said phosphorescent dopant is not particularly limited,

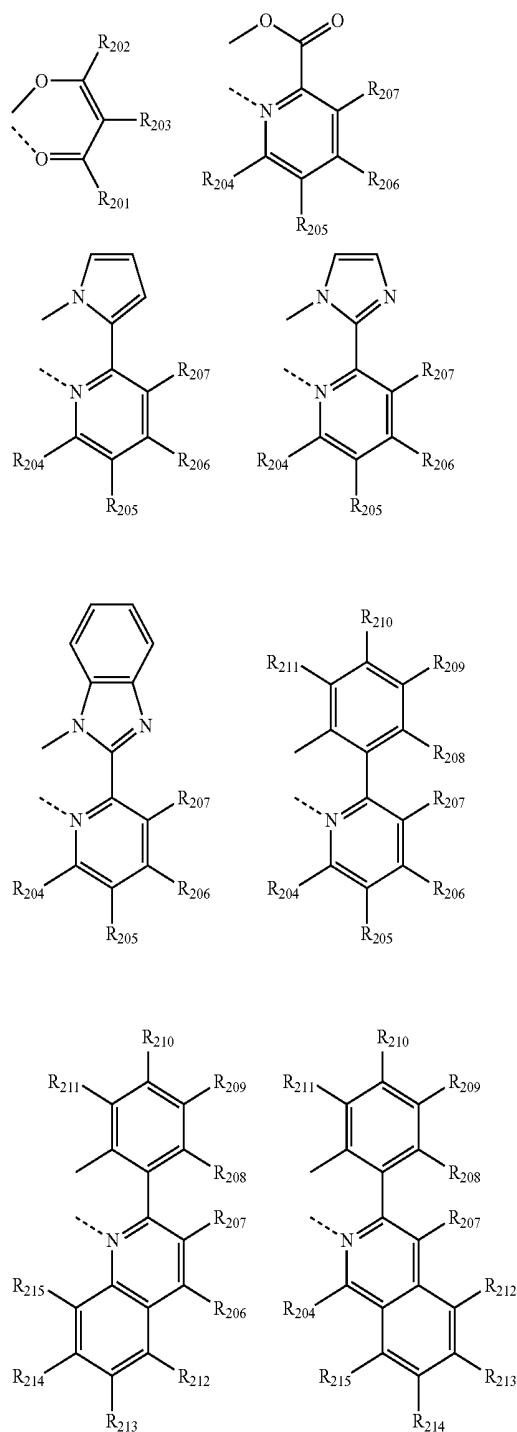
but may be selected from compounds represented by the following formula 2:



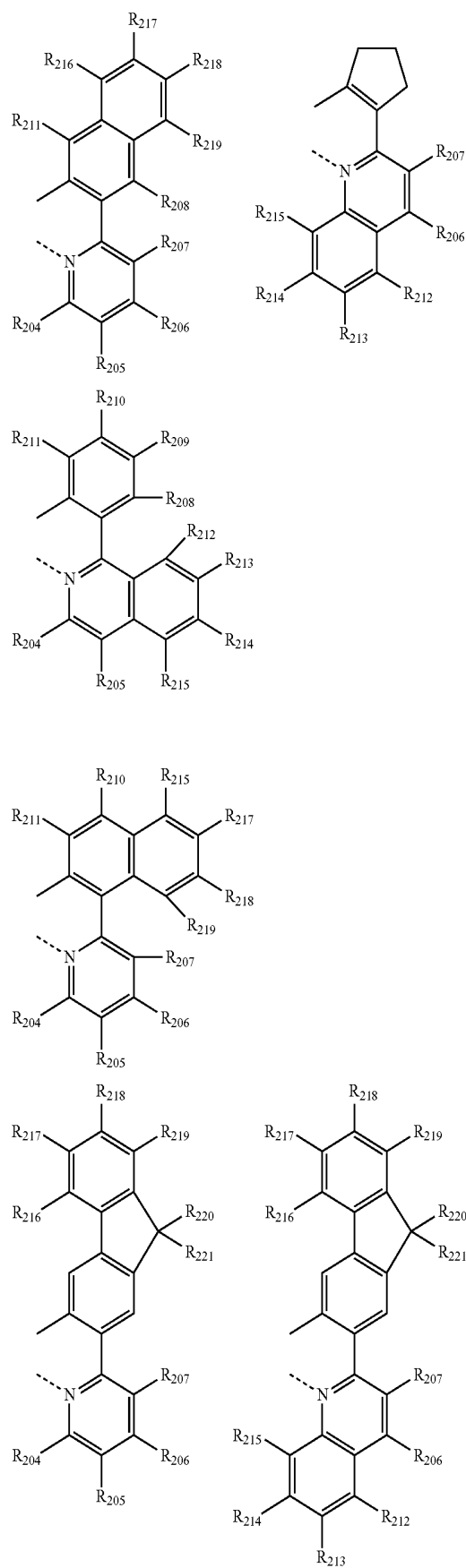
[Formula 2]

[0077] wherein

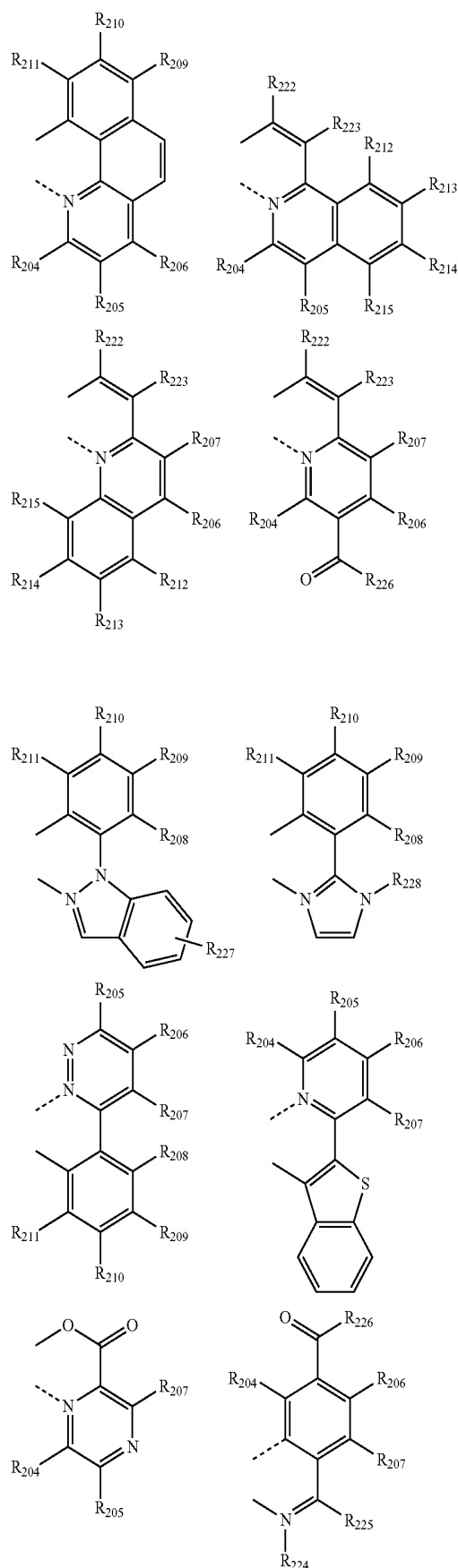
[0078] M^1 is selected from the group consisting of Ir, Pt, Pd and Os; L^{101} , L^{102} and L^{103} each independently are selected from the following structures:



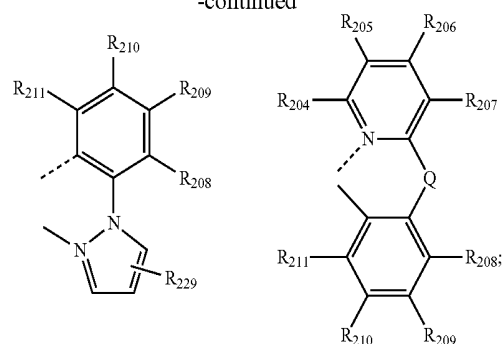
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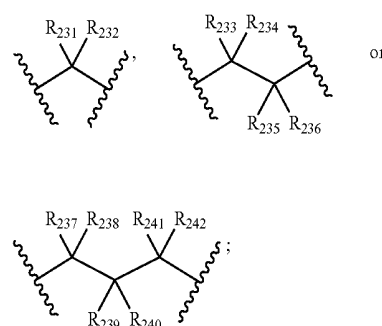
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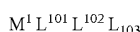


[0079] R₂₀₁ to R₂₀₃ each independently represent hydrogen, deuterium, a (C1-C30)alkyl group unsubstituted or substituted by a halogen(s), a (C6-C30)aryl group unsubstituted or substituted by a (C1-C30)alkyl group(s), or a halogen; R₂₀₄ to R₂₁₉ each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C1-C30)alkoxy group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted mono- or di-(C1-C30)alkylamino group, a substituted or unsubstituted mono- or di-(C6-C30)arylamino group, SF₅, a substituted or unsubstituted tri(C1-C30)alkylsilyl group, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)atylsilyl group, a substituted or unsubstituted tri(C6-C30)arylsilyl group, a cyano group or a halogen; R₂₂₀ to R₂₂₃ each independently represent hydrogen, deuterium, a (C1-C30)alkyl group unsubstituted or substituted by a halogen(s), or a (C6-C30)aryl group unsubstituted or substituted by a (C1-C30)alkyl group(s); R₂₂₄ and R₂₂₅ each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a halogen, or R₂₂₄ and R₂₂₅ may be linked to each other via a (C3-C12)alkylene group or (C3-C12)alkenylene group with or without a fused ring, to form a mono- or polycyclic alicyclic ring or a mono- or polycyclic aromatic ring; R₂₂₆ represents a substituted or unsubstituted (C1-C30)alkyl group, a substituted, or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- or 30-membered heteroaryl group or a halogen; R₂₂₇ to R₂₂₉ each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group or a halogen; Q represents



R231 to R242 each independently represent hydrogen, deuterium, a (C1-C30)alkyl group unsubstituted or substituted by a halogen(s), a (C1-C30)alkoxy group, a halogen, a substituted or unsubstituted (C6-C30)aryl group, a cyano group, a substituted or unsubstituted (C5-C30)cycloalkyl group, or each of R₂₃₁ to R₂₄₂ may be linked to an adjacent substituent via (C2-C30)alkylene group or (C2-C30)alkenylene group to form a spiro ring or a fused ring, or may be linked to R₂₀₇ or R₂₀₈ via (C2-C30)alkylene group or (C2-C30)alkenylene group to form a saturated or unsaturated fused ring.

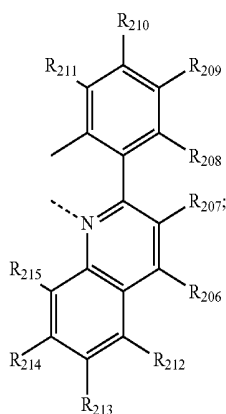
[0080] With more particularity, Formula 2 may be represented by the following:



[Formula 2]

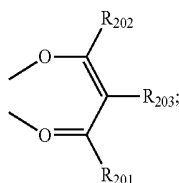
[0081] wherein M¹ is Ir;

[0082] L¹⁰¹ and L¹⁰² are the same and represent



and

[0083] L¹⁰³ represents



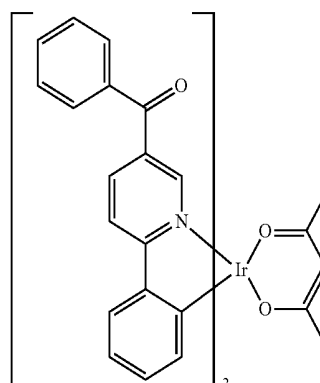
[0084] wherein R₂₀₁ to R₂₀₃ each independently represent hydrogen, deuterium, or a C1-C30alkyl group;

[0085] R₂₀₆ to R₂₀₈, R₂₁₀, and R₂₁₂ to R₂₁₅ each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, or a substituted or unsubstituted (C6-C30)aryl group; and

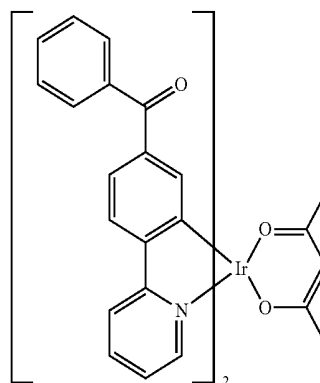
[0086] R₂₀₉ and R₂₁₁ each independently represent a substituted or unsubstituted (C1-C30)alkyl group.

[0087] For example, in Formula 2, R₂₀₉ and R₂₁₁ may each independently represent unsubstituted (C1-C10)alkyl group. By way of further example, R₂₀₇, R₂₀₈, R₂₁₀, R₂₁₄ and R₂₁₅ may each independently represent hydrogen or deuterium.

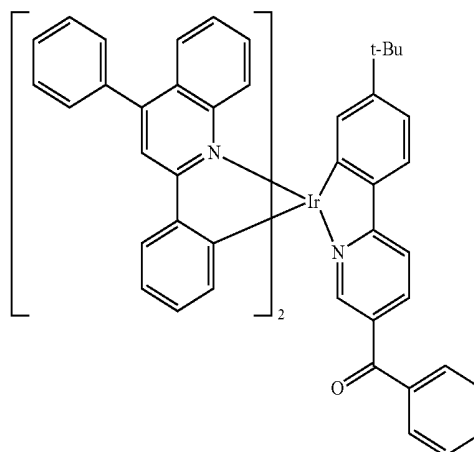
[0088] Examples of the iridium complex dopants of formula 2 include the following, but are not limited thereto:



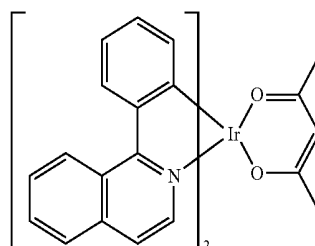
D-1



D-2

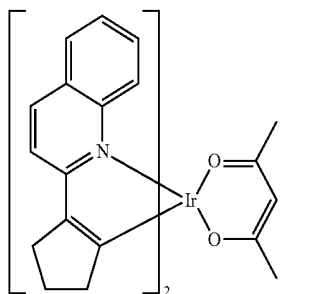


D-3



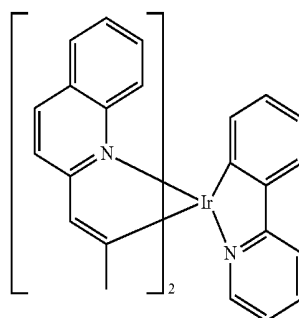
D-4

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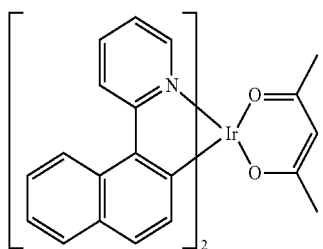


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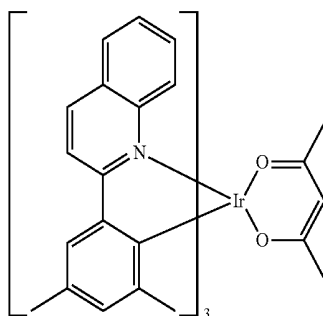
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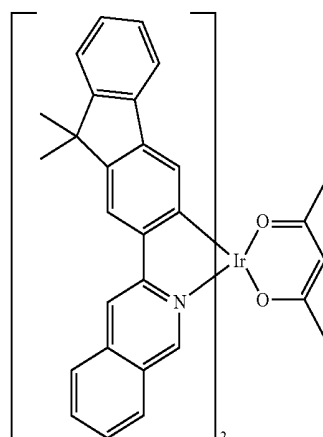
D-10



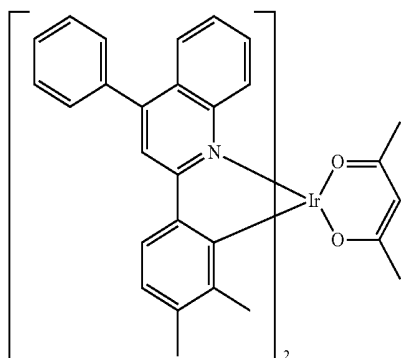
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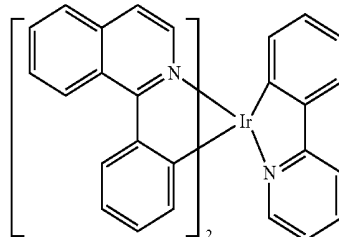
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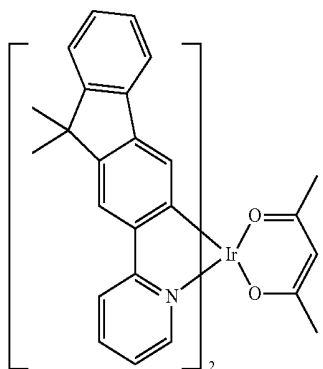
D-8



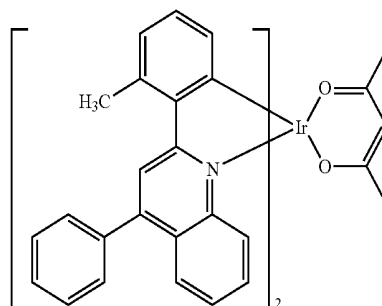
D-11



D-12

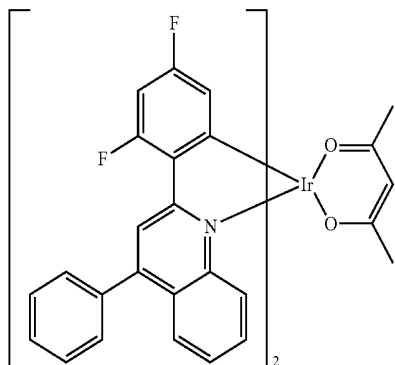


D-9



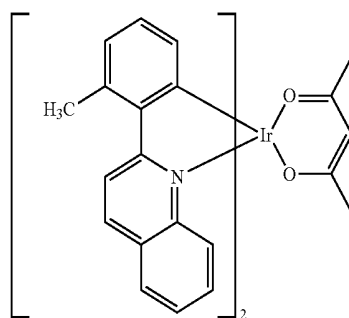
D-13

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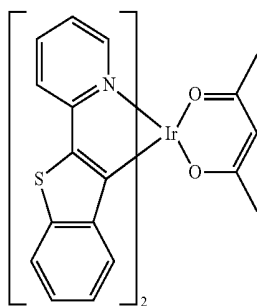


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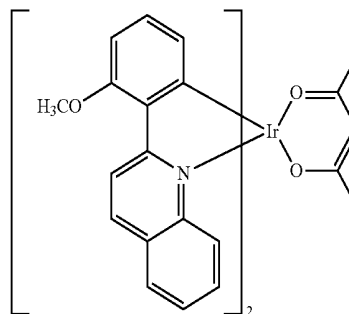
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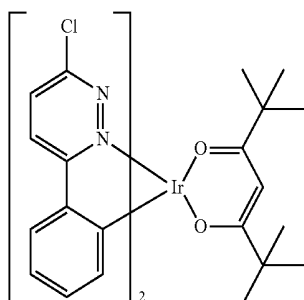
D-19



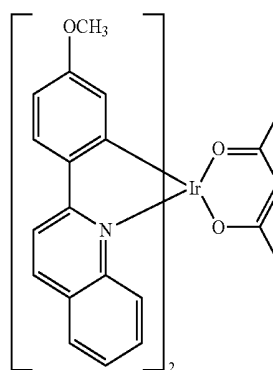
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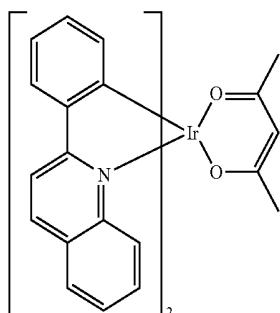
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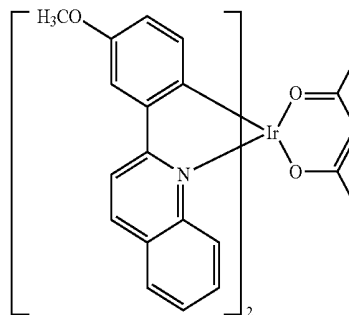
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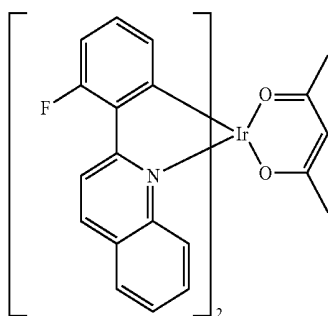
D-21



D-17

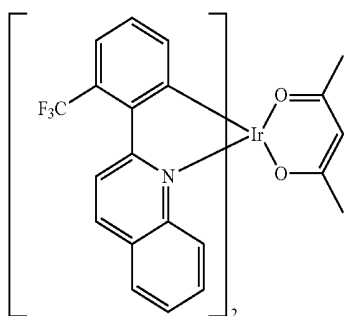


D-22



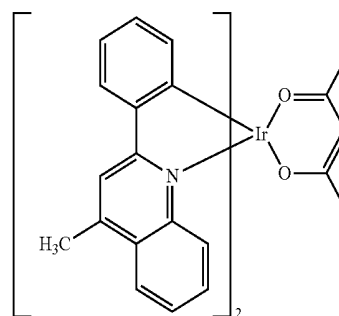
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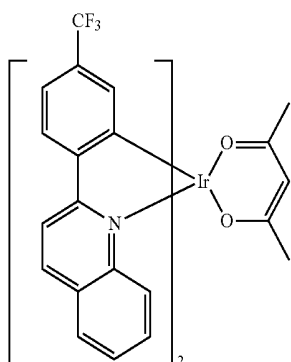


D-23

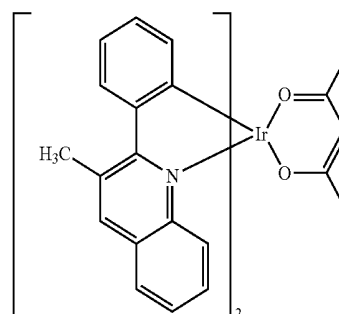
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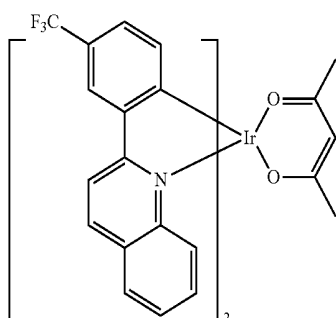
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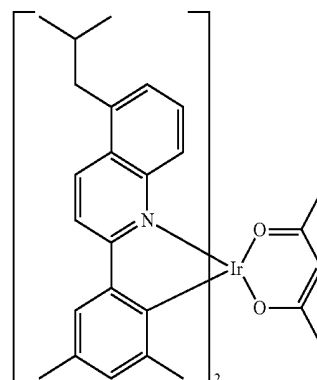
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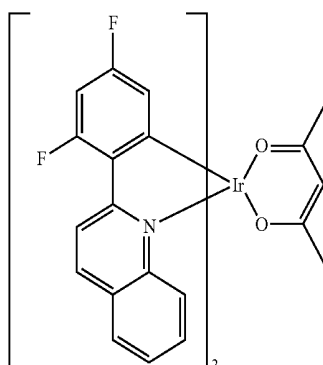
D-28



D-25



D-29



D-26

[0089] Of the above, without intending to be limited thereby, particularly preferred complexes are one or both of those depicted as complex D-7 or D-29.

[0090] For the light emitting layer herein, the amount by weight of the host material to the metal complex (e.g., iridium complex) may be below about 100:1, 90:1, 80:1, 70:1, or 60:1. The amount by weight of the host material to the metal complex (e.g., iridium complex as described herein) may be above about 10:1, 20:1, or 30:1. For example, the amount by weight of the host material to the metal complex (e.g., iridium complex as described herein) may range from about 100:1 to about 10:1.

[0091] A possible approach to manufacture a layer is to deposit each of the host material and the metal complex dopant in their respective amounts by a suitable deposition (e.g., vapor deposition) process. The relative amounts can be varied as desired, for example, by selecting different deposition rates for each. The layers are deposited to a desired thickness. For example the thickness may be greater than about 1 nm, greater than about 5 nm, or greater than about 10 nm. The thickness may be less than about 300 nm, less than about 200 nm, or less than about 100 nm.

[0092] With more particularity, for a light emitting layer having a combination of a host of formula 1 and a metal complex of formula 2, the Ar_1 may be a single bond or it can be a substituted or unsubstituted C6-C30 arylene (e.g., a substituted or unsubstituted C6 arylene). For such combination, Ar_2 may be a substituted or unsubstituted C6-C30 aryl (e.g., a C6 aryl). For such combination, R_{212} may be hydrogen, deuterium, a substituted or unsubstituted C1-C30 alkyl or a substituted or unsubstituted C6-C30 aryl (e.g., R_{212} may be hydrogen or a substituted or unsubstituted C1-C30 alkyl). For such a combination, R_{13} may be a substituted or unsubstituted C5-C20 aryl (e.g., R_{13} may be a substituted or unsubstituted C6, C10, C12, C16 or other aryl).

[0093] The organic electroluminescent device according to the present invention may further comprise, in addition to the organic electroluminescent compound according to the present invention, at least one amine-based compound selected from the group consisting of arylamine-based compounds and styrylamine-based compounds.

[0094] In the organic electroluminescent device according to the present invention, the organic layer, may further comprise at least one metal selected from the group consisting of metals of Group 1, metals of Group 2, transition metals of the 4th period, transition metals of the 5th period, lanthanides and organic metals of d-transition elements of the Periodic Table, or at least one complex compound comprising said metal. The organic layer may comprise a light-emitting layer and a charge generating layer.

[0095] The organic electroluminescent device according to the present invention may emit a white light by further comprising in addition to the organic electroluminescent compound according to the present invention, at least one light-emitting layer which comprises a blue electroluminescent compound, a red electroluminescent compound or a green electroluminescent compound. If necessary, the organic electroluminescent device may further comprise a yellow light-emitting layer or an orange light-emitting layer.

[0096] Preferred combinations of host and metal complex are such that they provide an organic layer, namely a light emitting layer, which exhibits a peak intensity at a wavelength within a range of about 600 nm to about 700 nm as measured by spectrophotometry (e.g., using a Varian brand Carry Eclipse Fluorescence spectrophotometer according to its standard operating parameters). A light emitting layer that includes a host material and a metal complex (e.g., an iridium complex as described herein) of the present teachings may exhibit red upon application of a driving voltage. The driving voltage may be a voltage of at least about 2 volts (V), at least about 4V, at least about 6V, or at least about 8V. The driving voltage may be a voltage below about 20V, below about 18V, below about 16V or below about 14V.

[0097] Preferably, in the organic electroluminescent device according to the present invention, at least one layer (hereinafter, "a surface layer") selected from a chalcogenide layer, a metal halide layer and a metal oxide layer may be placed on an inner surface(s) of one or both electrode(s). Specifically, it is preferred that a Chalcogenide layer of silicon or aluminum is placed on an anode surface of an electroluminescent medium layer, and a metal halide layer or metal oxide layer is placed on a cathode surface of an electroluminescent medium

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

[0098] Preferably, in the organic electroluminescent device according to the present invention, a mixed region of an electron transport compound or a mixed region of a hole transport compound and an oxidative dopant may be placed on at least one surface of a pair of electrodes, in that case, the electron transport compound is reduced to an anion, and thus facilitates injecting and transporting electrons to an electroluminescent medium. Further, the hole transport compound is oxidized to a cation, and thus facilitates injecting and transporting holes to an electroluminescent medium. Preferably, the oxidative dopant includes various Lewis acids and acceptor compounds; and the reductive dopant includes alkali metals, alkali metal compounds, alkaline earth metals, rare-earth metals, and mixtures thereof. A reductive dopant layer may be employed as a charge generating layer to prepare an electroluminescent device having two or more light emitting layers and emitting a white light.

[0099] The organic electroluminescent compound according to the present invention provides an organic light emitting layer and device, which has high luminous efficiency and a long operation lifetime and requires a low driving voltage improving power efficiency and power consumption.

[0100] For instance, a light emitting layer of the present invention, which may be employed for an OLED device, may show red emission. The red emission may have a luminance of at least 1,000 cd/m^2 at a driving voltage of 3.8 V and as current density of 3.4 mA/cm^2 . For instance, the layer may show red emission (with a peak intensity at a wavelength within a range of about 600 nm to about 700 nm as measured by spectrophotometry as described) having a luminance of at least about 800, at least about 900, or at least about 1,000 cd/m^2 at a driving voltage of below about 8V, below about 6V, or below about 4V (e.g., about 3.8V) and a current density of about 1 to about 10, about 2 to about 6, or about 3 to about 4 mA/cm^2 . Further, the minimum time for a luminance of 5,000 nit to be reduced to 97% of the luminance may be at least 170 hours.

[0101] It is also possible that by use of the combination of the compounds of the invention and the metal complexes of the invention (e.g., an iridium complex, and particularly one as described, in the present teachings, such as an alkylated complex as described), that operational lifetime (e.g., at about a 5000 nit level) can be surprisingly substantially higher than other combinations that have been employed. For example, it is believed possible that alkylated metal complex dopants of formula 2 as described in the teachings) when used in combination with an organic electroluminescent compound (e.g., those of Formula 1 of the teachings) as a host material may be able to achieve at least about 1.3 times, about 1.5 times, about 1.8 times or about 2 times the operational lifetime as compared with a similar combination, but where the metal complex dopant is not alkylated.

[0102] In general, other aspects of the invention are that either or both of the metal complex or the host material of the organic layer (namely the light emitting layer) may be free of

any halogen (e.g., in the form of a substituent), as may also be the situation for the light emitting layer as a whole. The organic electroluminescent compounds according to the present invention have superior properties than those of conventional electroluminescent compounds, and thus provide an organic electroluminescent device which has high luminous efficiency and a long operation lifetime and requires a low driving voltage improving power efficiency and power consumption.

[0103] Hereinafter, examples are provided for preparing the organic electroluminescent compounds, and properties of the organic electroluminescent devices using them.

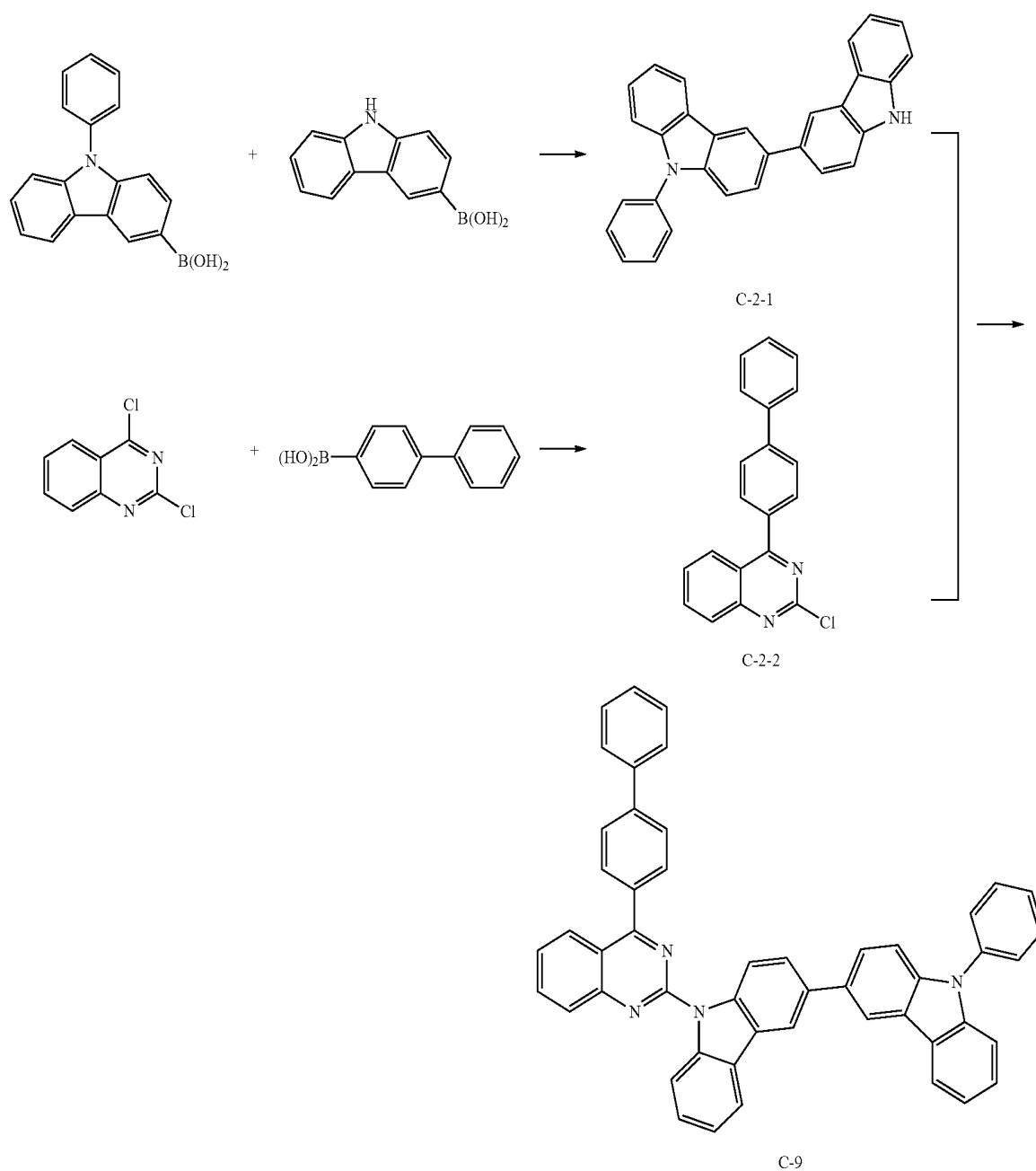
[0104] The abbreviations used in the examples have the following meanings:

[0105] Ph: phenyl, MeOH: methanol, EtOH: ethanol, MC: methylene chloride, EA: ethyl acetate,

[0106] DMF: dimethylformamide, n-Bu: normal-butyl, i-Pr: isopropyl, Me: methyl, THF: tetrahydrofuran, FDA: ethylene diamine, NBS: N-bromosuccinimide it is believed that the resulting Compounds C-9 of the preparation examples could exhibit a T_g of from about 140° C. to about 150° C.

[Preparation Example 1] Preparation of Compound C-9

[0107]



Preparation of Compound C-2-1

[0108] 9-phenyl-9H-carbazol-3-yl boronic acid (14 g, 48.76 mmol), 3-bromo-9H-carbazole (10 g, 40.63 mmol), K_2CO_3 (13.5 g, 97.52 mmol) and $Pd(PPh_3)_4$ (2.35 g, 2.03 mmol) were added to toluene 200 mL, EtOH 50 mL and purified water 50 mL. After stirring the reaction mixture for 3 hours at 90 to 100° C. the mixture was cooled to room temperature. An aqueous layer was removed from the mixture by a gravity separation. The obtained organic layer was concentrated, was triturated with MC, and then was filtered to obtain compound C-2-1 (12 g, 72%).

Preparation of Compound C-2-2

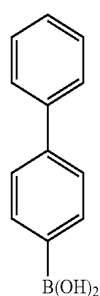
[0109] 2,4-dichloroquinazoline (20 g, 0.1 mol), biphenyl-4-yl boronic acid (18.9 g, 0.1 mol), $Pd(PPh_3)_4$ (3.5 g, 3.01 mmol) and Na_2CO_3 (31.9 g, 0.3 mol) were added to toluene 800 mL, EtOH 200 mL, and petrified water 200 mL. After stirring the reaction mixture for 3 hours at 70 to 80° C., an aqueous layer was removed from the mixture by a gravity separation. The obtained organic layer was concentrated, and then was purified by silica column chromatography to obtain compound C-2-2 (15 g, 47%).

Preparation of Compound C-9

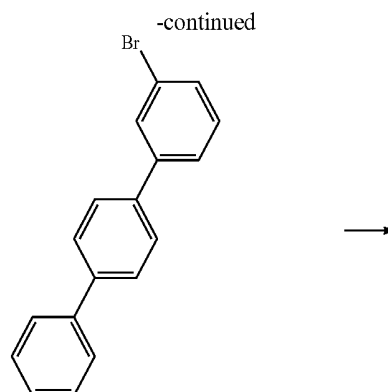
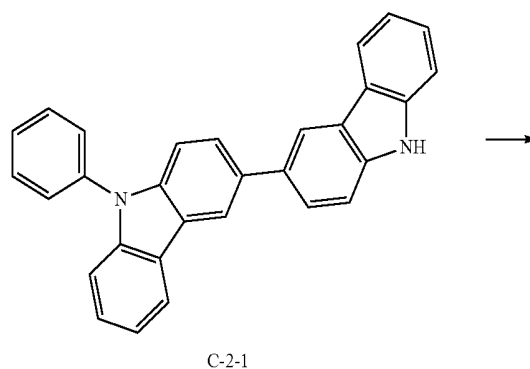
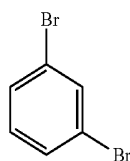
[0110] After suspending compound C-2-2 (4.6 g, 14.7 mmol) and compound C-2-1 (5 g, 12.2 mmol) in DMF 80 mL, 60% NaH (881 g, 22 mmol) was added to the mixture at room temperature. The obtained reaction mixture was stirred for 12 hours. After adding purified Water (1 L), the mixture was filtered under reduced pressure. The obtained solid was triturated with Me.OH/EA, was dissolved in MC, was filtered through silica, and then was triturated with MC/n-hexane to obtain compound C-9 (4 g, 47.4%).

[Preparation Example 2] Preparation of Compound C-15

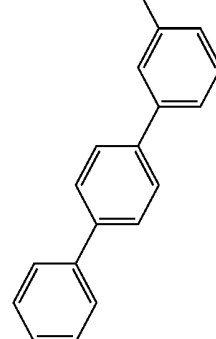
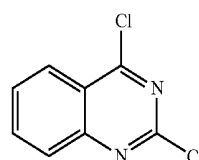
[0111]



+



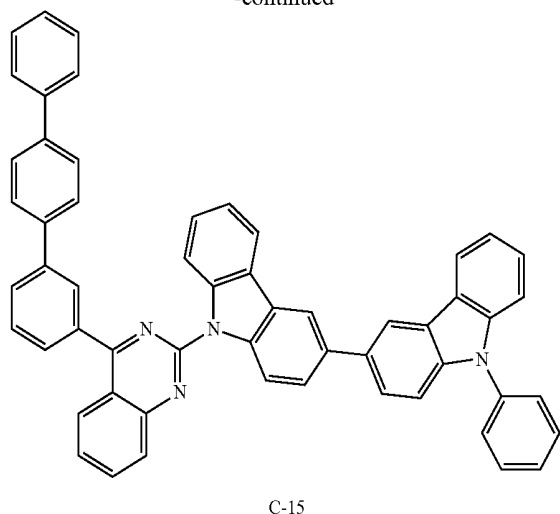
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C-4-1
(HO)₂BC-4-2
Cl

C-4-3

+

-continued



Preparation of Compound C-4-1

[0112] After dissolving biphenyl-4-yl boronic acid (157 g, 554 mmol), 1,3-dibromobenzene (100 g, 581.7 mmol), Pd(PPhhd **3**)₄ (13 g, 11.08 mmol) and NaCO₃ (150 g, 1.385 mol) in toluene (3.5 L), EtOH (0.7 L) and distilled water (0.7 L), the reaction mixture was stirred for 3 hours at 90° C. The mixture was extracted with EA and distilled water, was dissolved in chloroform (10 L) by heat, and then was filtered through silica. After triturating the resultant with EA and hexane, the resultant was triturated with EA and MeOH to obtain compound C-4-1 (94 g, 60%).

Preparation of Compound C-4-2

[0113] After dissolving compound C-4-1 (55 g, 178 mmol) in THF (800 mL), 2.5 M n-BuLi in hexane (106 mL, 267 mmol) was added to the reaction mixture at -78° C., and then the mixture was stirred for 1 hour. B(Oi-Pr)₃ (82 mL, 356 mmol) was added slowly to the mixture, and then the mixture was stirred for 2 hours. The mixture was quenched by adding 2 M HCl, was extracted with distilled water and EA, and then was recrystallized with hexane and acetone, Compound C-4-2 (43 g, 88.0%) was obtained.

Preparation of Compound C-4-3

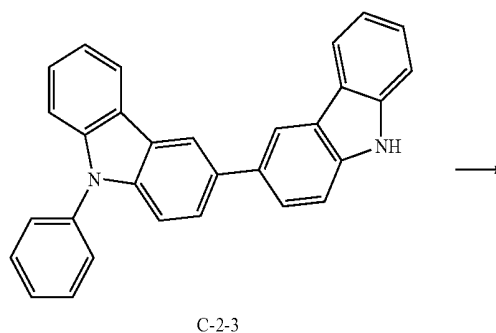
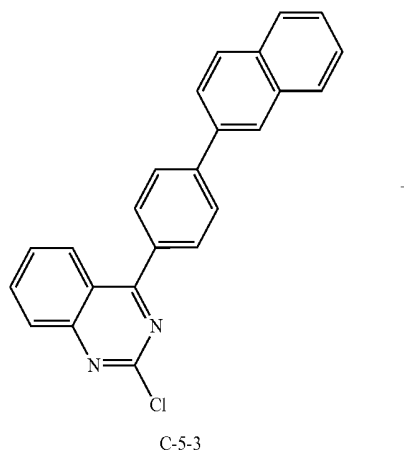
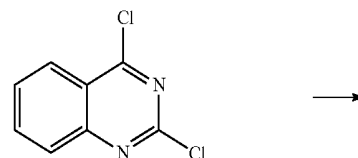
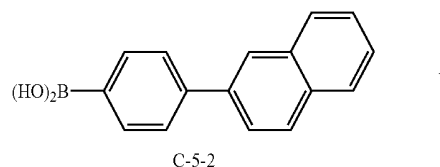
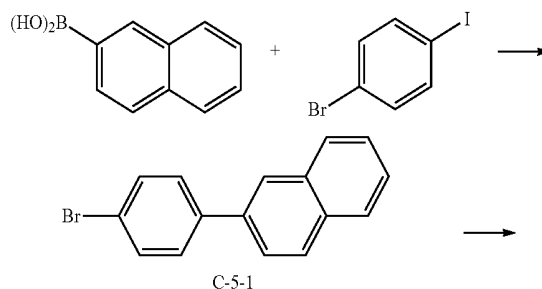
[0114] 2,4-dichloroquinazoline (20 g, 73 mmol), compound C-4-2 (15 g, 73 mmol), Pd(PPh₃)₄ (2.5 g, 2.2 mmol) and Na₂CO₃ (23 g, 241 mmol) were dissolved in toluene (500 mL), EtOH (100 mL) and distilled water (100 mL), and then was stirred for 5 hours at 100° C. The reaction mixture was distilled under reduced pressure to obtain an organic layer, and then was triturated with MeOH. The obtained solid was dissolved in MC, was filtered through silica, and then was triturated with MC and hexane to obtain compound C-4-3 (19.5 g, 68%).

Preparation of Compound C-15

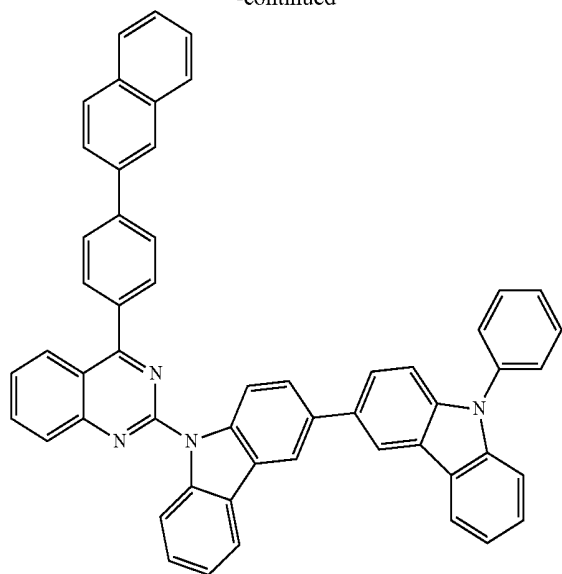
[0115] After suspending compound C-2-1 (5 g, 12.2 mmol) and compound C-4-3 (4.6 g, 11.6 mmol) in DMF 80 mL, 60% NaH (881 mg, 22 mmol) was added to the mixture at room temperature. The obtained reaction mixture was stirred for 12 hours. After adding purified water (1 L), the mixture was

filtered under reduced pressure. The obtained solid was triturated with MeOH/EA, was triturated with DMF, and then was triturated with EA/THF. The resultant was dissolved in MC, was filtered through silica, and then was triturated with MeOH/EA. Compound C-15 (5.1 g, 57%) was obtained.

[Preparation Example 3] Preparation of Compound C-29

[0116]

-continued



C-29

Preparation of Compound C-5-1

[0117] After dissolving 2-naphthylboronic acid (157 g, 554 mmol), 1-bromo-4-iodobenzene (100 g, 581.7 mmol), $\text{Pd}(\text{PPh}_3)_4$ (13 g, 11.08 mmol) and Na_2CO_3 (150 g, 1.385 mol) in toluene (3.5 L), EtOH (0.7 L) and distilled water (0.7 L), the reaction mixture was stirred for 3 hours at 90° C. The mixture was extracted with EA and distilled water, was dissolved in chloroform (10 L) by heat, and then was filtered through silica. After triturating the resultant with EA and hexane, the resultant was triturated with EA and MeOH to obtain compound C-5-1 (94 g, 60%).

Preparation of Compound C-5-2

[0118] After dissolving compound C-5-1 (94 g, 332 mmol) in THF (800 mL), 2.5 M n-BuLi in hexane (80 mL, 386.4 mmol) was added to the reaction mixture at -78° C., and then the mixture was stirred for 1 hour. $\text{B}(\text{OMe})_3$ (28 mL, 498 mmol) was added slowly to the mixture, and then the mixture was stirred for 2 hours. The mixture was quenched by adding 2 M HCl, was extracted with distilled water and EA, and then was recrystallized with hexane and acetone. Compound C-5-2 (57 g, 67.0%) was obtained.

Preparation of Compound C-5-3

[0119] 2,4-dichloroquinazoline (46 g, 230 mmol), compound C-5-2 (57 g, 230 mmol), $\text{Pd}(\text{PPh}_3)_4$ (10.6 g, 9.2 mmol) and Na_2CO_3 (73 g, 690 mmol) were dissolved in toluene (1.1 L), EtOH (230 mL) and distilled water (350 mL), and then was stirred for 5 hours at 100° C. The reaction mixture was distilled under reduced pressure to obtain an organic layer, and then was triturated with MeOH. The obtained solid was dissolved in MC, was filtered through silica, and then was triturated with MC and hexane to obtain compound C-5-3 (51 g, 99.9%).

Preparation of Compound C-29

[0120] After suspending compound C-2-1 (5 g, 12.2 mmol) and compound C-5-3 (4.5 g, 12.2 mmol) in DMF 80 mL, 60%

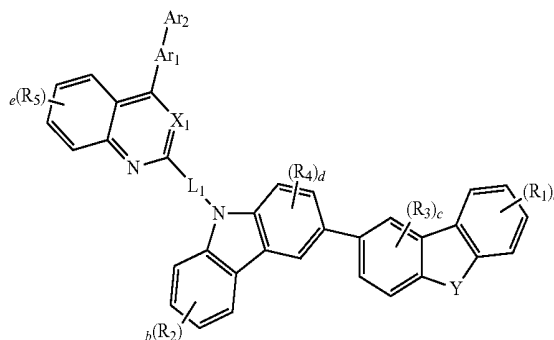
NaR (881 mg, 22 mmol) was added to the mixture at room temperature. The obtained reaction mixture was stirred for 12 hours. After adding purified water (1 L), the mixture was filtered under reduced pressure. The obtained solid was triturated with MeOH/EA, was triturated with DME, and then was triturated with EA/THF. The resultant was dissolved in MC, was filtered through silica, and then was triturated with MeOH/EA. Compound C-29 (1.8 g, 20%) was obtained.

[0121] In general, as to all teachings herein, the use of the terms “comprising” or “including” to describe combinations of elements, ingredients, components or steps herein also contemplates embodiments that consist essentially of, or even consist of the elements, ingredients, components or steps. Many embodiments, as well as many applications besides the examples provided, will be apparent to those of skill in the art upon reading the above description. The scope of the invention should, therefore, be determined not with reference to the above description, but should instead be determined with reference to the appended claims, along with the full scope of equivalents to which such claims are entitled.

What is claimed is:

1. A light emitting layer, comprising:
an organic electroluminescent compound as a host material M the layer; and
an iridium complex dopant,
wherein the organic electroluminescent compound is represented by the following Formula 1; and the iridium complex dopant is represented by the following Formula 2:

[Formula 1]



wherein:

L_1 represents a single bond;

X_1 represents N;

Y represents $-\text{NR}_{13}-$;

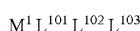
Ar_1 represents a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, a substituted or unsubstituted (C6-C30)arylene group;

Ar_2 represents hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group;

R_1 to R_5 each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted 5- to 7-membered heterocycloalkyl group,

a substituted or unsubstituted (C6-C30)aryl(C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group fused with at least one (C3-C30)cycloalkyl group, a 5- or 7-membered heterocycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, (C3-C30)cycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, $-\text{NR}_{14}\text{R}_{15}$, $-\text{SiR}_{16}\text{R}_{17}\text{R}_{18}$, $-\text{SR}_{19}$, $-\text{OR}_{20}$, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C2-C30)alkynyl group, a cyano group, a nitro group, or a hydroxyl group; or are linked to an adjacent substituent via a substituted or unsubstituted (C3-C30)alkylene group or a substituted or unsubstituted (C3-C30)alkenylerte group to form a mono- or polycyclic alicyclic ring or a mono- or polycyclic aromatic ring whose carbon atoints) may be substituted by at least one hetero atom selected from nitrogen, oxygen and sulfur;

R_{13} to R_{20} have the same meaning as one of R_1 to R_5 ,
 a , b and e each independently represent an integer of 1 to 4;
 where a , b or e is an integer of 2 or more, each of R_1 , each of R_2 or each of R_5 is the same or different;
 c and d each independently represent an integer of 1 to 3;
 where c or d is an integer of 2 or more, each of R_3 or each of R_4 is the same or different; and
 the heterocycloalkyl group and the heteroaryl(ene) group contain at least one hetero atom selected from B, N, O, S, P(=O), Si and P, and

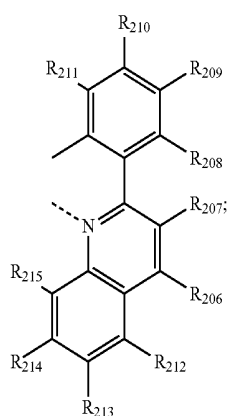


[Formula 2]

wherein

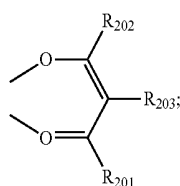
M^1 is Ir;

L^{101} and L^{102} are the same and represent



and

L^{103} represents



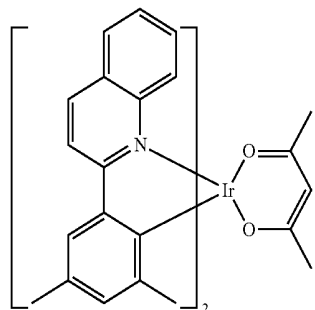
wherein R_{201} to R_{203} each independently represent hydrogen, deuterium, or a (C1-C30)alkyl group;

R_{206} to R_{208} , R_{210} , and R_{212} to R_{215} each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, or a substituted or unsubstituted (C6-C30)aryl group, and

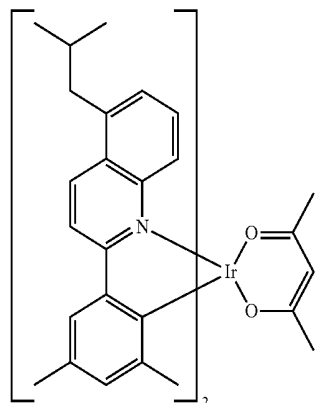
R_{209} and R_{211} each independently represent a substituted or unsubstituted (C1-C30)aryl group.

2. The light emitting layer of claim 1, wherein R_{209} and R_{211} each independently represent unsubstituted (C1-C10)alkyl group, and wherein R_{207} , R_{208} , R^{210} , R^{214} and R_{215} each independently represent hydrogen or deuterium.

3. The light emitting layer of claim 1, wherein the iridium complex dopant is selected from:



4. The light emitting layer of claim 1, wherein the iridium complex dopant is:

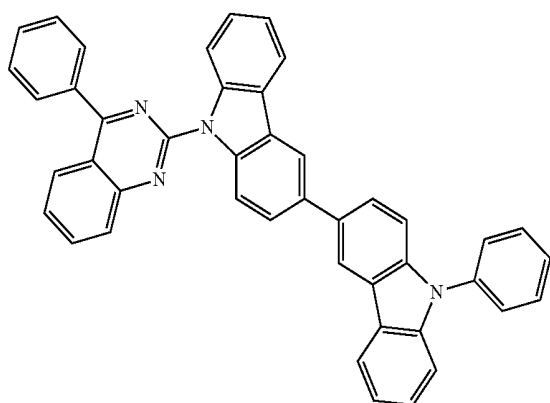


5. The light emitting layer of claim 1, wherein R_{13} is a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C6-C30)aryl group fused with at least one (C3-C30)cycloalkyl group, a 5- or 7-membered heterocycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring, or a (C3-C30)cycloalkyl group fused with at least one substituted or unsubstituted (C6-C30)aromatic ring.

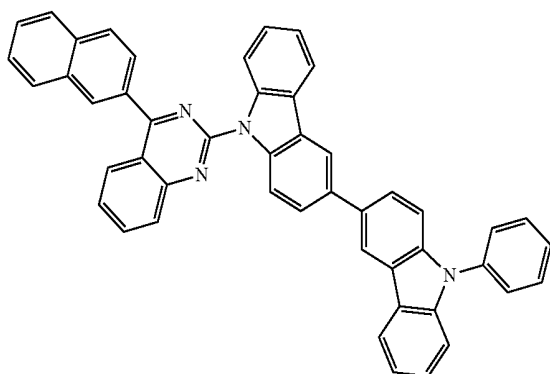
6. The light emitting layer of claim 2, wherein R_{13} is a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted 5- to 30-membered heteroaryl group.

7. The light emitting layer of claim 2, wherein R_{13} is substituted or unsubstituted (C6-C30)aryl group.

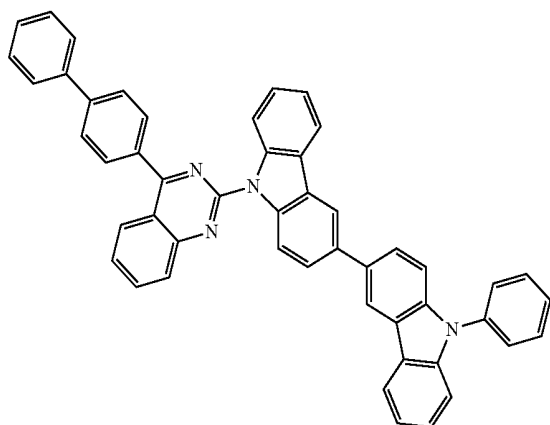
8. The light emitting layer of claim 1, wherein the organic electroluminescent compound as a host material is selected from the following compounds C-1, C-5, C-9, or C-77;



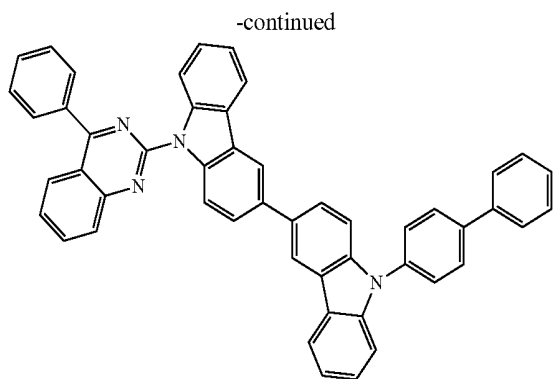
C-1



C-5

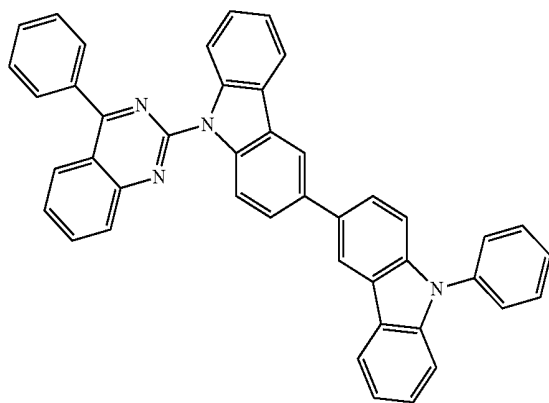


C-9

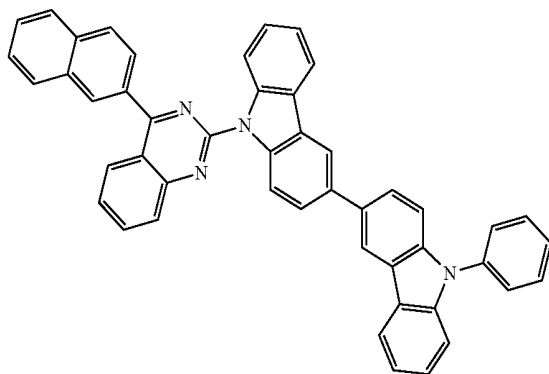


C-77

9. The light emitting layer of claim 3, wherein the organic electroluminescent compound as a host material is selected from the following compounds C-1, C-5, C-9, or C-77;

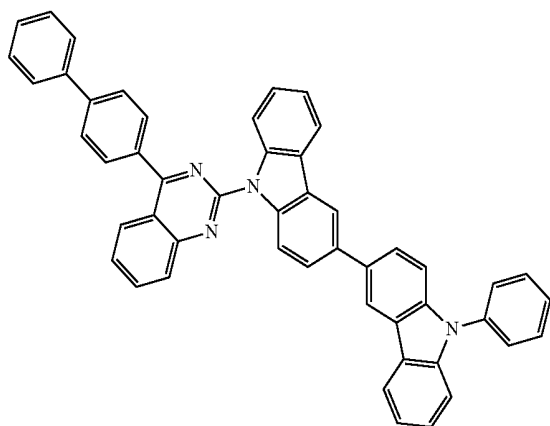


C-1



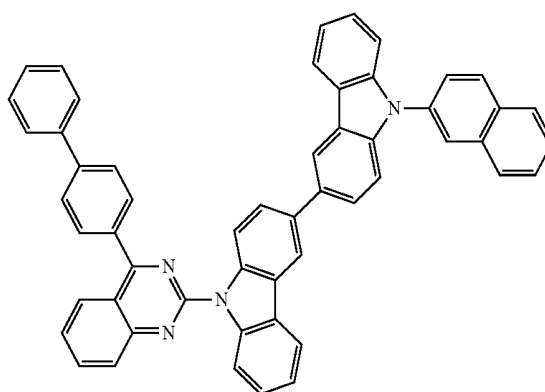
C-5

-continued

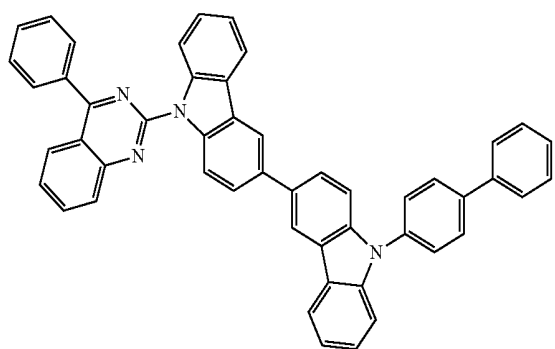


C-9

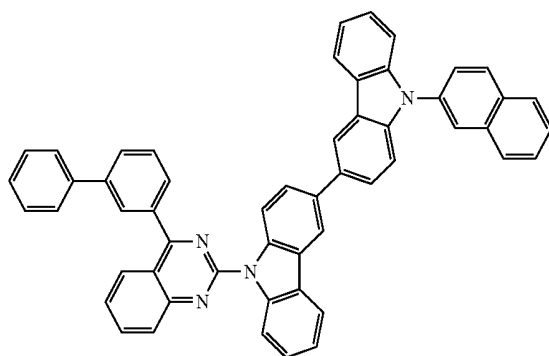
-continued



C-136



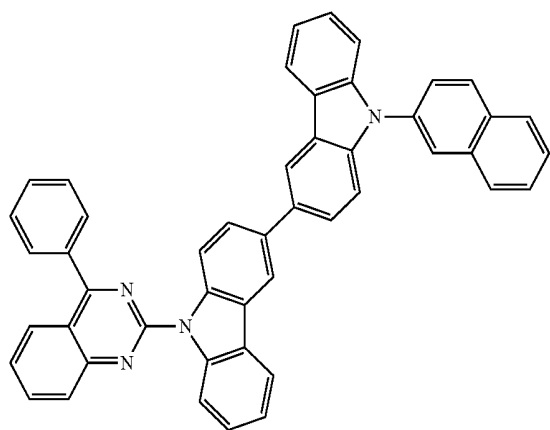
C-77



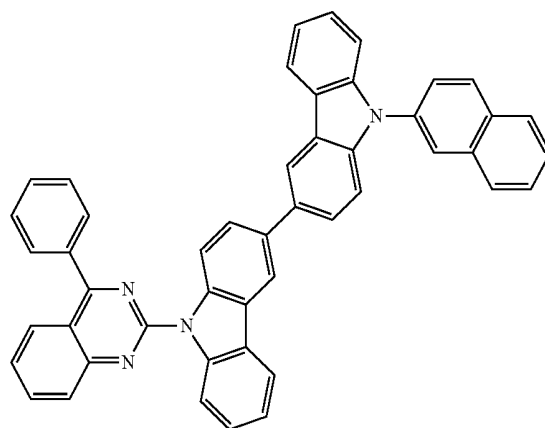
C-137

10. The light emitting layer of claim 1, wherein the organic electroluminescent compound as a host material is selected from the following compounds C-135, C-136 or C-137;

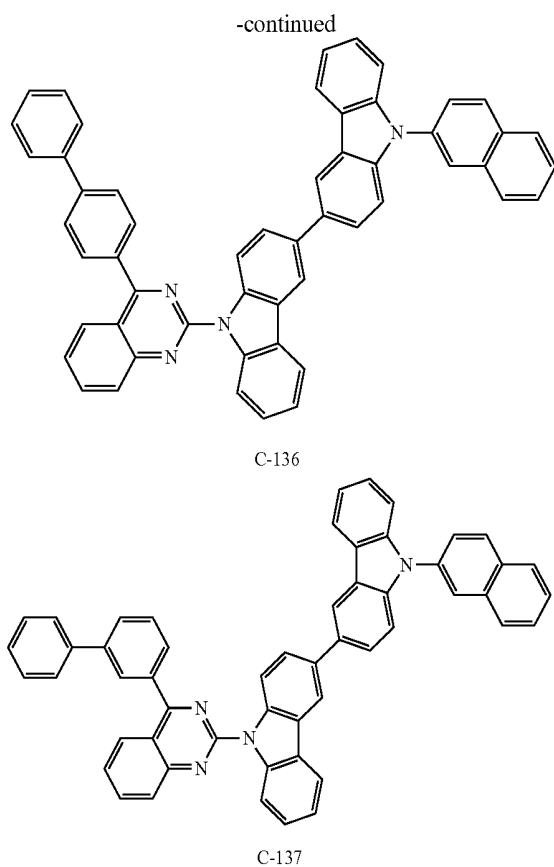
11. The light emitting layer of claim 4, wherein the organic electroluminescent compound as a host material is selected from the following compounds C-135, C-136 or C-137;



C-135



C-135



12. The light emitting layer of claim 3, wherein one of (a) R_1 to R_5 each independently represent hydrogen or a substituted or unsubstituted (C6-C30)aryl group; (b) R_3 represents a

substituted or unsubstituted (C6-C30)aryl group; or (c) R_4 represents a substituted or unsubstituted (C6-C30)aryl group.

13. The light emitting layer of claim 4, wherein one of (a) R_1 to R_5 each independently represent hydrogen or a substituted or unsubstituted (C6-C30)aryl group; (b) R_3 represents a substituted or unsubstituted (C6-C30)aryl group; or (e) R_4 represents a substituted or unsubstituted (C6-C30)aryl group.

14. The light emitting layer of claim 3, wherein a ratio of an amount by weight of the host material to the iridium complex ranges from about 100:1 to about 10:1.

15. The light emitting layer of claim 14, wherein the layer luminesces red upon application of a driving voltage, and wherein the light emitting layer exhibits a peak intensity at a wavelength within a range of about 600 nm to about 700 nm and the host exhibits a glass transition temperature (T_g) of at least about 80° C.

16. The light emitting layer of claim 4, wherein a ratio of an amount by weight of the host material to the iridium complex ranges from about 100:1 to about 10:1.

17. The light emitting layer of claim 16, wherein the layer luminesces red upon application of a driving voltage, and wherein the light emitting layer exhibits a peak intensity at a wavelength within a range of about 600 nm to about 700 nm and the host exhibits a glass transition temperature (T_g) of at least about 80° C.

18. An organic electroluminescent device comprising an anode, a cathode, and the light emitting layer according to claim 3 disposed between the anode and the cathode.

19. An organic electroluminescent device comprising an anode, a cathode, and the light emitting layer according to claim 4 disposed between the anode and the cathode.

20. An organic electroluminescent device comprising an anode, a cathode, and the light emitting layer according to claim 9 disposed between the anode and the cathode.

* * * * *

专利名称(译)	新型机电致发光化合物，层和使用它们的机电致发光器件		
公开(公告)号	US20150357583A1	公开(公告)日	2015-12-10
申请号	US14/825517	申请日	2015-08-13
[标]申请(专利权)人(译)	罗门哈斯电子材料KOREA		
申请(专利权)人(译)	罗门哈斯电子材料公司		
当前申请(专利权)人(译)	罗门哈斯电子材料KOREA LTD.		
[标]发明人	AHN HEE CHOON YOON SEOK KEUN MOON DOO HYEON KIM HEE SOOK LEE SU HYUN SHIN HYO NIM LEE KYUNG JOO PARK KYOUNG JIN KIM NAM KYUN CHO YOUNG JUN KWON HYUCK JOO KIM BONG OK		
发明人	AHN, HEE-CHOON YOON, SEOK-KEUN MOON, DOO-HYEON KIM, HEE-SOOK LEE, SU-HYUN SHIN, HYO-NIM LEE, KYUNG-JOO PARK, KYOUNG-JIN KIM, NAM-KYUN CHO, YOUNG-JUN KWON, HYUCK-JOO KIM, BONG-OK		
IPC分类号	H01L51/00 C09K11/06		
CPC分类号	H01L51/0072 C09K2211/185 H01L51/0074 H01L51/0073 H01L51/0052 H01L51/0054 H01L51/0055 H01L51/0067 H01L51/0094 C09K11/06 H01L51/5012 C09K2211/1044 C09K2211/1029 C09K2211 /1092 C09K2211/1088 C09K2211/1011 H01L51/0085 C07D401/04 C07D403/04 C07D403/14 C07D405 /14 C07D409/14 C09K2211/1007 H01L51/5016 H05B33/14		
优先权	1020110020492 2011-03-08 KR 14/004089 2013-11-25 US PCT/KR2012/001712 2012-03-08 WO		
其他公开文献	US9287512		
外部链接	Espacenet USPTO		

摘要(译)

本发明涉及新型机电致发光化合物，层和使用其的机电致发光器件。所述有机发光化合物提供有机发光层和/或器件，其具有高发光效率和长的工作寿命，并且需要低驱动电压，从而提高功率效率和功耗。

