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(71) Applicant: **ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.** [KR/KR]; 736, Baekseok-dong, Seobuk-gu, Cheonan-si, Chungcheongnam-do 331-980 (KR).

(72) Inventors: **MOON, Doo-Hyeon;** 104-101, World Meridian 2 Cha Apt., Jinan-dong, Hwaseong-si, Gyeonggi-do 445-718 (KR). **AHN, Hee-Choon;** 105, Sinheung Villa, 355-1, Mangpo-dong, Yeongtong-gu, Suwon-si, Gyeonggi-do 443-400 (KR). **KU, Jong-Seok;** 109-204, Dongtan Yedang Maeul Daewoo Purgio Apt., Seoku-dong, Hwaseong-si, Gyeonggi-do 445-170 (KR). **KIM, Nam-Kyun;** 510-1601, Kumho Bestville Apt., 867, Sanghyeon-dong, Suji-gu, Yongin-si, Gyeonggi-do 448-130 (KR). **CHO, Young-Jun;** 204-701, EG The One Apt., Botdeulmaeul 2-danji, Sampyeong-dong Bundang-gu, Seongnam-si, Gyeonggi-do 463-892 (KR). **KWON, Hyuck-Joo;** 105-2003, Hillstate, Samseong-dong, Gangnam-gu, Seoul 135-877 (KR). **LEE, Kyung-Joo;** 210-1001, Hyundai Hometown, Dohwa-dong, Mapo-gu, Seoul 121-773 (KR). **KIM, Bong-Ok;** 208-401, Hillstate, 50, Samseong-dong, Gangnam-gu, Seoul 135-877 (KR).

(74) Agent: **CHANG, Hoon;** Central Intellectual Property & Law, Korean Re Bldg, 5F, #80, Soosong-dong, Chongro-ku, Seoul 110-733 (KR).

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

(57) **Abstract:** The present invention relates to novel organic electroluminescent compounds and an organic electroluminescent device comprising the same. The organic electroluminescent compounds according to the present invention have high luminescent efficiency and a long lifespan, and thus an organic electroluminescent device having a long operating lifespan can be prepared by using the organic electroluminescent compounds according to the present invention.

# Description

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

## Technical Field

[1] The present invention relates to novel organic electroluminescent compounds and organic electroluminescent device comprising the same.

## Background Art

[2] An electroluminescent (EL) device is a self-light-emitting device with the advantage of providing a wider viewing angle, a greater contrast ratio, and a faster response time. An organic EL device was first developed by Eastman Kodak, by using small aromatic diamine molecules and aluminum complexes as material for forming a light-emitting layer *[see* Appl. Phys. Lett. 51, 913, 1987].

[3] The most important factor determining luminescent efficiency in an organic EL device is the light-emitting material. Until now, fluorescent materials have been widely used as a light-emitting material. However, in view of electroluminescent mechanisms, developing phosphorescent materials is one of the best methods to theoretically enhance the luminescent efficiency by four (4) times compared to fluorescent materials. Iridium(III) complexes have been widely known as phosphorescent materials, including bis(2-(2'-benzothienyl)-pyridinato-N,C3')iridium(acetylacetonate) ((acac)Ir(btp)$_2$), tris(2-phenylpyridine)iridium (Ir(ppy)$_3$) and bis(4,6-difluorophenylpyridinato-N,C2)picolinato iridium (Firpic) as red, green and blue materials, respectively. Especially, many phosphorescent materials are being researched in Japan, Europe and U.S.A. recently.

[4] Until now, 4,4'-N,N'-dicarbazol-biphenyl (CBP) is the most widely known host material for phosphorescent substances. Further, high performance organic EL devices using bathocuproine (BCP), aluminum(III)bis(2-methyl-8-quinolinate)(4-phenylphenolate) (BAlq), etc., for a hole blocking layer are known, and Pioneer (Japan) et al. developed a high performance organic EL device employing a derivative of BAlq as a host material.

[5] Though these phosphorescent host materials provide good light-emitting characteristics, they have the following disadvantages: (1) Due to their low glass transition temperatures 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 [(π/voltage) x current efficiency], and thus the power efficiency is inversely proportional to voltage. An organic EL device comprising phosphorescent

host materials provides higher current efficiency (cd/A) but has a higher driving voltage than one comprising fluorescent host materials. Thus, the organic **EL** device using conventional phosphorescent materials has no advantage in terms of power efficiency (lm/W). (3) The operating lifespan and luminescent efficiency of the organic **EL** device using phosphorescent host materials are not satisfactory.

[6] International Publication No. WO 2006/049013 discloses a compound for an organic **EL** device, wherein the compound has a nitrogen-containing 3-membered heterocyclic ring to which a 2-membered heterocyclic ring is directly or via a linking group bonded. However, the device comprising the compound is not satisfactory in terms of an operating lifespan and luminescent efficiency.

## Disclosure of Invention

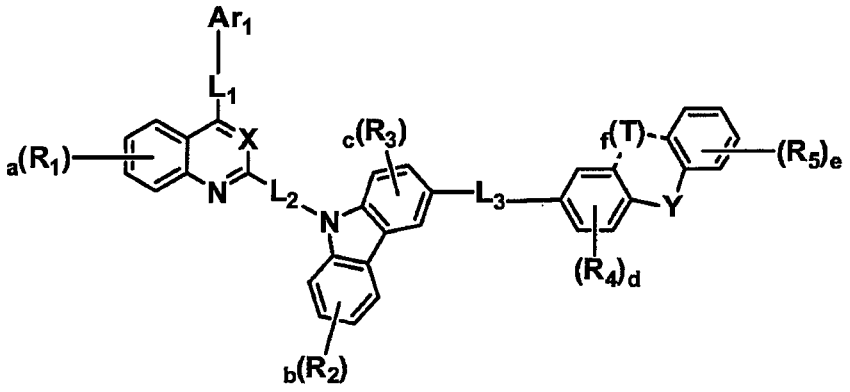
## Technical Problem

[7] The objective of the present invention is to provide an organic electroluminescenct compound imparting higher luminescent efficiency and a longer operating lifespan to a device over conventional materials in order to overcome said problems; and an organic electroluminescent device having high efficiency and a long lifespan, comprising the organic electroluminescent compound of the present invention as a light-emitting material.

## Solution to Problem

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

[9]




(1)

[10] wherein

[11] X represents CH or N;

[12] $L_1$ and $L_2$ each independently represent a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, or a substituted or unsubstituted (C6-C30)arylene group;

[13] $L_3$ represents a single bond, a substituted or unsubstituted (Cl-C30)alkylene group, a substituted or unsubstituted (C6-C30)arylene group, or a substituted or unsubstituted 3-

to 30-membered heteroarylene group;

[14] Y represents -0-, -S-, -CRnR$_{12}$- or -NR$_{13}$-;

[15] T represents a chemical bond;

[16] Ar$_1$ represents hydrogen, a halogen, deuterium, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted (Cl-C30)alkyl group;

[17] R$_i$ to R$_5$ each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- 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(Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group which is fused with at least one (C3-C30) aliphatic ring, a 5- to 7-membered heterocycloalkyl group which is fused with at least one substituted or unsubstituted (C6-C30) aromatic ring, a (C3-C30)cycloalkyl group which is fused with at least one substituted or unsubstituted (C6-C30) aromatic ring, -NR$_{14}$R$_{15}$, -SiRi$_6$RnRi8, -SR$_{19}$, -OR$_{2o}$, a (C2-C30)alkenyl group, a (C2-C30)alkynyl group, a cyano group, a nitro group, or a hydroxyl group;

[18] R$_{11}$ to R$_{2o}$ are as defined in R$_1$ to R$_5$;

[19] 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;

[20] 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;

[21] f represents an integer of 0 or 1; where f is 0, Y represents -NR$_{13}$-, wherein R$_{13}$ may be linked to R$_5$ to form a mono- or polycyclic, (C5-C30) alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur; and

[22] the heterocycloalkyl group and heteroaryl(ene) group contain at least one hetero atom selected from B, N, O, S, P(=0), Si and P.

## Advantageous Effects of Invention

[23] The organic electroluminescent compounds according to the present invention have high luminescent efficiency and a long lifespan. Therefore, an organic electroluminescent device comprising the compounds according to the present invention has a long operating lifespan.

## Mode for the Invention

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

the scope of the invention.

[25] The present invention relates to an organic electroluminescent compound represented by the formula 1, an organic electroluminescent material comprising the organic electroluminescent compound, and an organic electroluminescent device comprising the material.

[26] In formula 1, preferably, $L_1$ and $L_2$ each independently represent a single bond, a substituted or unsubstituted 5- to 15-membered heteroarylene group, or a substituted or unsubstituted (C6-C15)arylene group and more preferably a single bond, an unsubstituted 5- to 15-membered heteroarylene group, an unsubstituted (C6-C15)arylene group, or a (C6-C15)arylene group which is substituted with a (C1-C6) alkyl group. More specifically, $L_1$ and $L_2$ may be each independently selected from the group consisting of a single bond, phenylene, naphthylene, biphenylene, terphenylene, anthrylene, indenylene, fluorenylene, phenanthrylene, triphenylenylene, pyrenylene, perylenylene, chrysenylene, naphthacenylene, fluoranthenylene, furylene, thiophenylene, pyrrolylene, imidazolylene, pyrazolylene, thiazolylene, thiadiazolylene, isothiazolylene, isoxazolylene, oxazolylene, oxadiazolylene, triazinylene, tetrazinylene, triazolylene, tetrazolylene, furazanylene, pyridylene, pyrazinylene, pyrimidinylene, pyridazinylene, benzofuranylene, benzothiophenylene, isobenzofuranylene, benzoimidazolylene, benzothiazolylene, benzoisothiazolylene, benzoisoxazolylene, benzoxazolylene, isoindolylene, indolylene, indazolylene, benzothiadiazolylene, quinolylene, isoquinolylene, cinolynylene, quinazolinylene, quinoxalynylene, carbazolylene, phenanthrydinylene, benzodioxolylene, dibenzofuranylene and dibenzothiophenylene .

[27] In formula 1, $L_3$ preferably represents a single bond, or a substituted or unsubstituted (C6-C15)arylene group and more preferably a single bond or an unsubstituted (C6-C15)arylene group.

[28] In formula 1, Y represents -0-, -S-, -CRnRi $_2$- or -NRi $_3$-, in which preferably $R_{11}$ and $R_{12}$ each independently represent a substituted or unsubstituted (Cl-ClO)alkyl group and more preferably an unsubstituted (Cl-ClO)alkyl group, and $R_{13}$ preferably represents a substituted or unsubstituted (C6-C15)aryl group, or a substituted or unsubstituted 5- to 15-membered heteroaryl group and more preferably a (C6-C15)aryl group which is unsubstituted or substituted with deuterium, a halogen, a (Cl-C6)alkyl group or a (C6-C15)aryl group, or a 5- to 15-membered heteroaryl group which is substituted with a (C6-C15)aryl group.

[29] In formula 1, T preferably represents a single bond.

[30] In formula 1, $Ar_1$ preferably represents hydrogen, a substituted or unsubstituted 5- to 20-membered heteroaryl group, a substituted or unsubstituted (C6-C20)aryl group, or a substituted or unsubstituted (Cl-ClO)alkyl group and more preferably hydrogen; a 5-

to 20-membered heteroaryl group which is unsubstituted or substituted with a (C6-C15)aryl group; a (C6-C20)aryl group which is unsubstituted or substituted with deuterium, a halogen, a (Cl-C6)alkyl group, a (C6-C15)aryl group or a 5- to 15-membered heteroaryl group; or a (Cl-ClO)alkyl group which is unsubstituted or substituted with a (Cl-C6)alkyl group.

[31] In formula 1, preferably, ¾ to $R_5$ each independently represent hydrogen, a substituted or unsubstituted (C6-C15)aryl group, or a substituted or unsubstituted 5- to 15-membered heteroaryl group and more preferably hydrogen, an unsubstituted (C6-C15)aryl group or an unsubstituted 5- to 15-membered heteroaryl group.

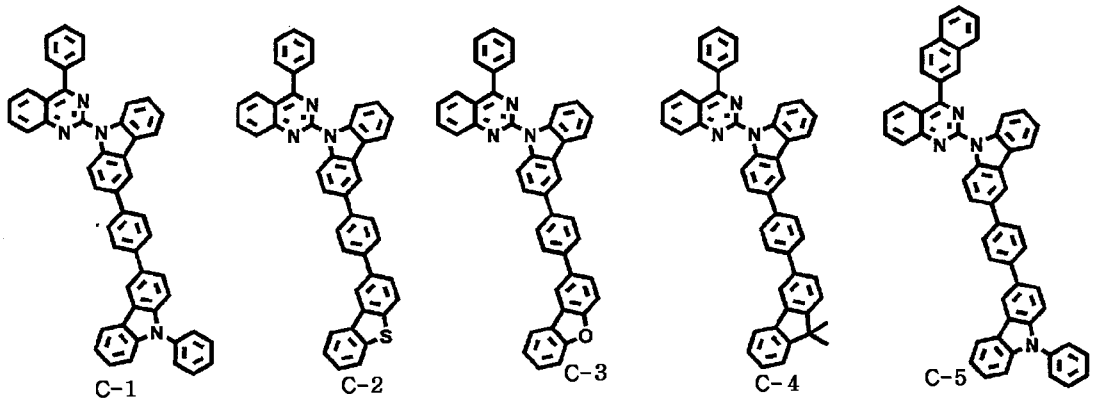
[32] Herein, "(Cl-C30)alkyl(ene)" is meant to be a linear or branched alkyl(ene) having 1 to 30 carbon atoms, in which the number of carbon atoms is preferably 1 to 20, more preferably 1 to 10, and includes methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl, tert-butyl, etc. "(C2-C30) alkenyl" is meant to be a linear or branched alkenyl having 2 to 30 carbon atoms, in which the number of carbon atoms is preferably 2 to 20, more preferably 2 to 10, 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 carbon atoms, in which the number of carbon atoms is preferably 2 to 20, more preferably 2 to 10, and includes ethynyl, 1-propynyl, 2-propynyl, 1-butynyl, 2-butynyl, 3-butynyl, l-methylpent-2-ynyl, etc. "(C3-C30)cycloalkyl" is a mono- or polycyclic hydrocarbon having 3 to 30 carbon atoms, in which the number of carbon atoms is preferably 3 to 20, more preferably 3 to 7, and includes cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, etc. "3- to 7-membered heterocycloalkyl" is a cycloalkyl having at least one heteroatom selected from B, N, O, S, P(=0), Si and P, preferably O, S and N, and 3 to 7 ring backbone atoms, and includes tetrahydrofurane, pyrrolidine, thiolan, tetrahydropyran, etc. "(C6-C30)aryl(ene)" is a monocyclic or fused ring derived from an aromatic hydrocarbon having 6 to 30 carbon atoms, in which the number of carbon atoms is preferably 6 to 20, more preferably 6 to 15, and includes phenyl, biphenyl, terphenyl, naphthyl, fluorenyl, phenanthrenyl, anthracenyl, indenyl, triphenylenyl, pyrenyl, tetracenyl, perylenyl, chrysenyl, naphthacenyl, fluoranthenyl, etc. "3- to 30-membered heteroaryl(ene)" is an aryl group having at least one, preferably 1 to 4 heteroatom selected from the group consisting of B, N, O, S, P(=0), Si and P, and 3 to 30 ring backbone atoms; is a monocyclic ring, or a fused ring condensed with at least one benzene ring; has preferably 5 to 20, more preferably 5 to 15 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, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenoxazinyl, phenanthridinyl, benzodioxolyl, etc. Further, "halogen" includes F, CI, Br and I.

[33] Herein, "substituted" in the expression "substituted or unsubstituted" means that a hydrogen atom in a certain functional group is replaced with another atom or group, i.e., a substituent. Substituents of the substituted alkyl(ene) group, the substituted aryl(ene) group, the substituted heteroaryl(ene) group, the substituted cycloalkyl group, and the substituted heterocycloalkyl group in formula 1 each independently are at least one selected from the group consisting of deuterium; a halogen; a (Cl-C30)alkyl group which is unsubstituted or substituted with a halogen; a (C6-C30)aryl group; a 3- to 30-membered heteroaryl group which is unsubstituted or substituted with a (C6-C30)aryl group; a 5- to 7-membered heterocycloalkyl group; a 5- to 7-membered heterocycloalkyl group which is fused with at least one (C6-C30) aromatic ring; a (C3-C30)cycloalkyl group; a (C6-C30)cycloalkyl group which is fused with at least one (C6-C30) aromatic ring; $R_aR_bR_cSi$-; a (C2-C30)alkenyl group; a (C2-C30)alkynyl group; a cyano group; a carbazolyl group; -$NR_dR_e$; -$BR_fR_g$; -$PR_hRi$; -$P(=0)R_jR_k$; a (C6-C30)aryl(Cl-C30)alkyl group; (Cl-C30)alkyl(C6-C30)aryl group; $R_lZ$-; $R_mC(=0)$-; $R_mC(=0)0$-; a carboxyl group; a nitro group; and a hydroxyl group, in which $R_a$ to $R_l$ each independently represent a (Cl-C30)alkyl group, a (C6-C30)aryl group or a 3- to 30-membered heteroaryl group, or are linked to an adjacent substituent(s) to form a mono- or polycyclic, (C5-C30) alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur, Z represents S or O, and $R_m$ represents a (Cl-C30)alkyl group, a (Cl-C30)alkoxy group, a (C6-C30)aryl group or a (C6-C30)aryloxy group.

[34] The organic electroluminescent compounds according to the present invention include the following compounds:

[35]



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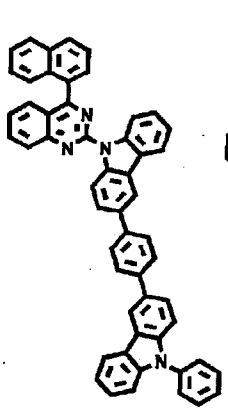
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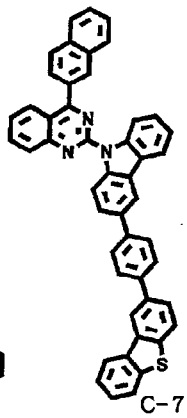
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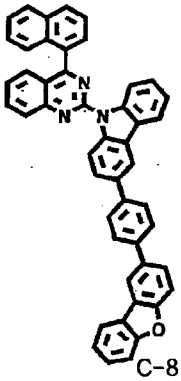
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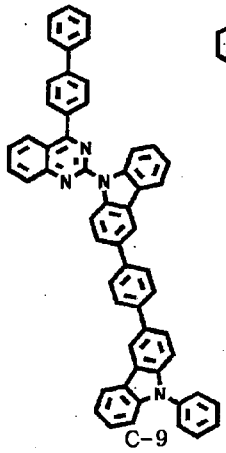
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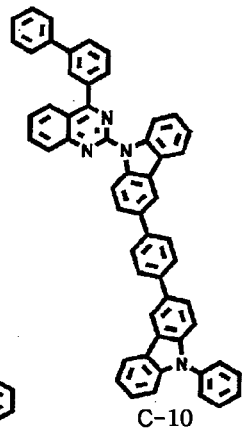
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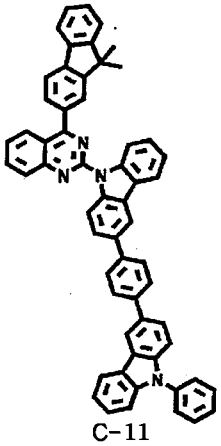
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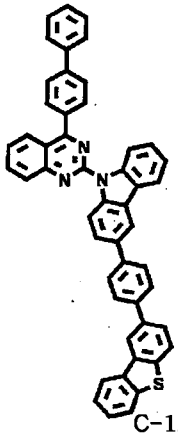
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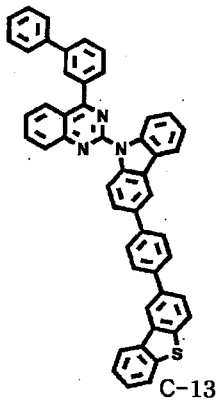
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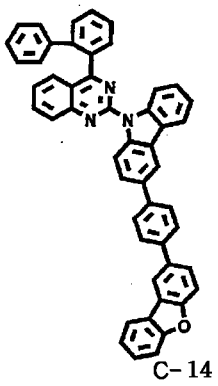
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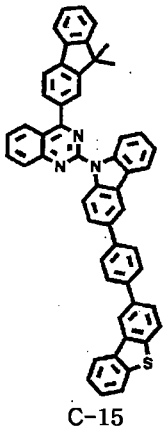
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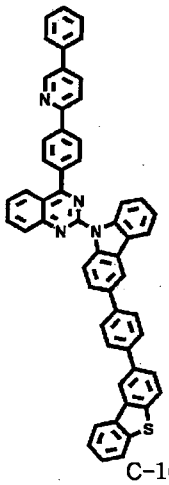
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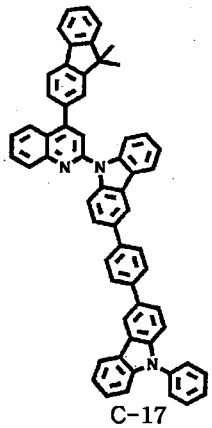
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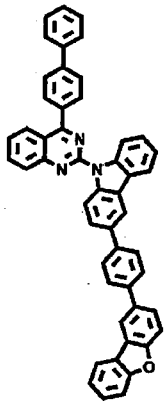
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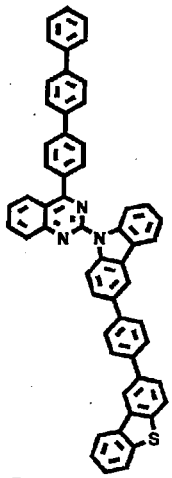

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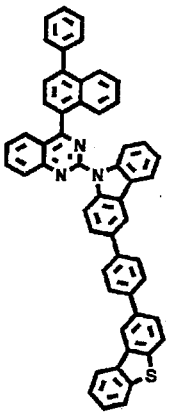

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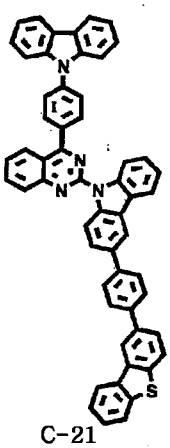

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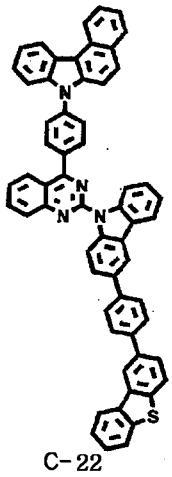

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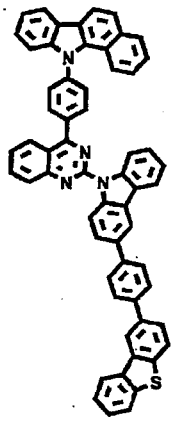

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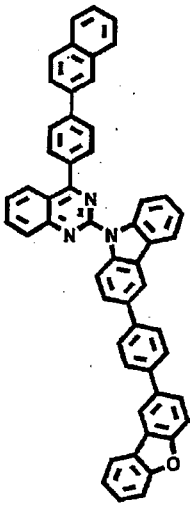

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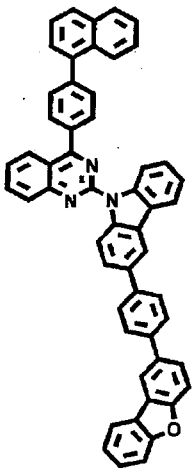

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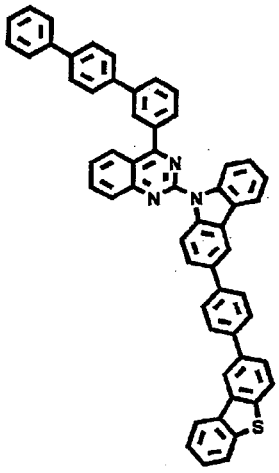

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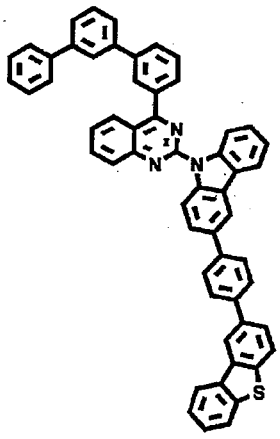

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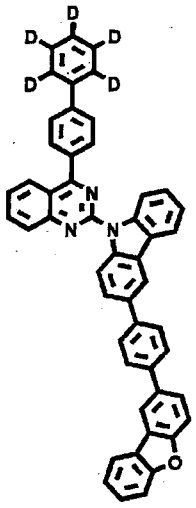

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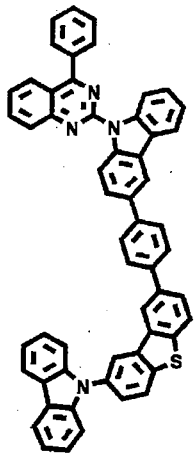

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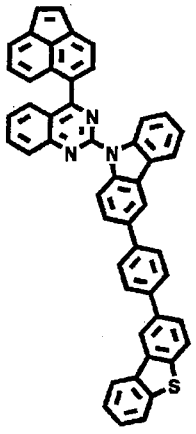

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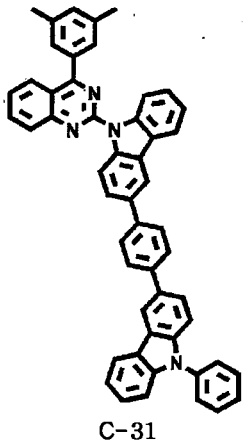

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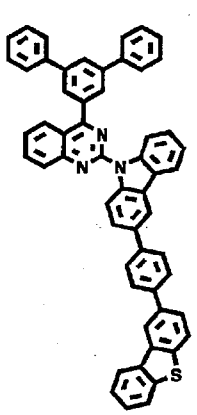

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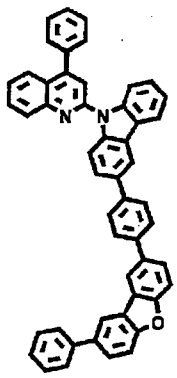

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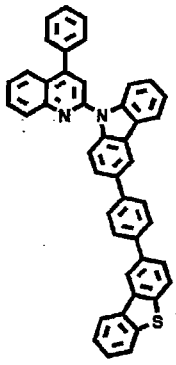

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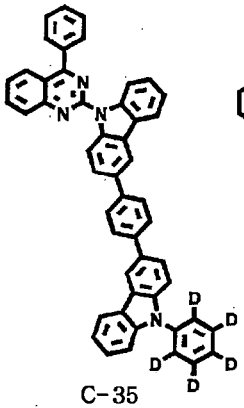

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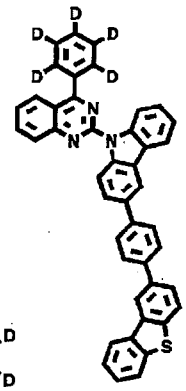

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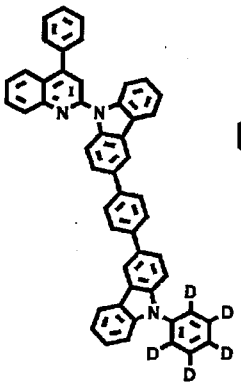

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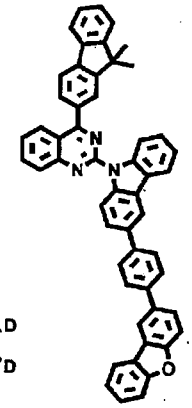

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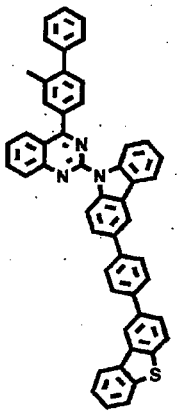

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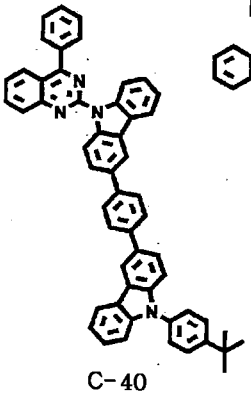

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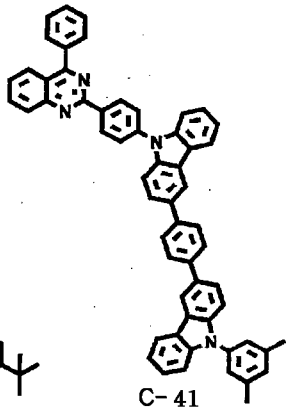

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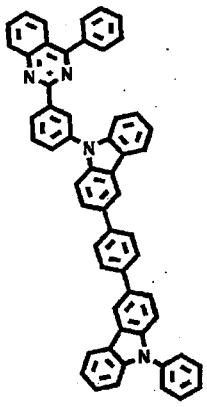

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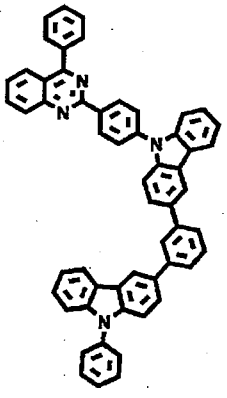

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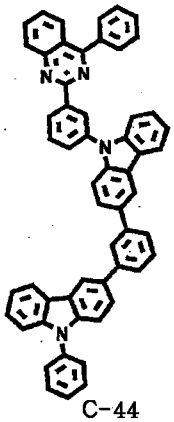

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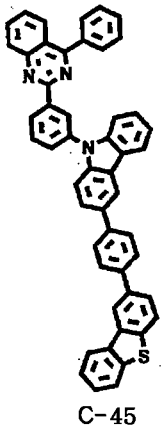

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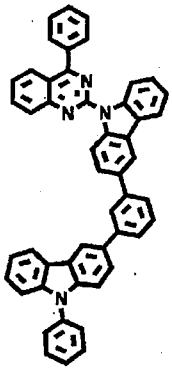

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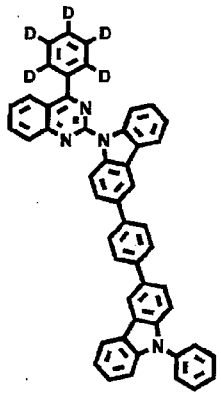
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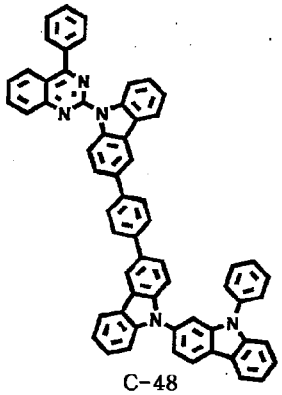
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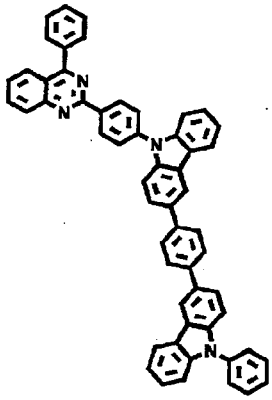
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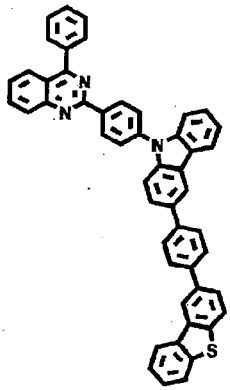
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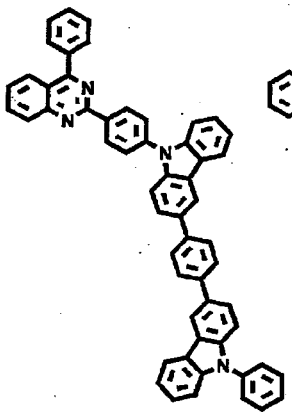
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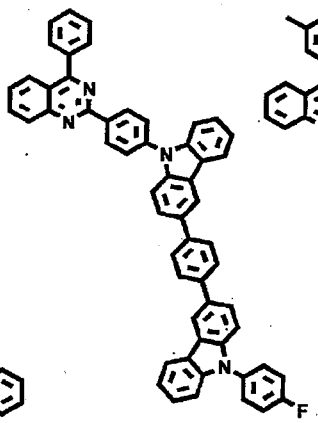
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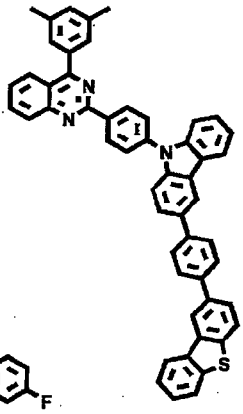
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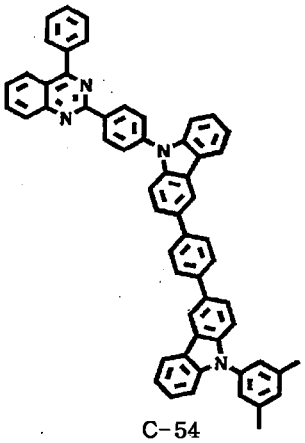
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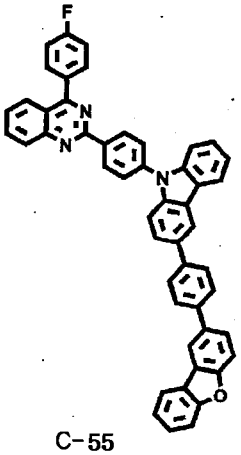
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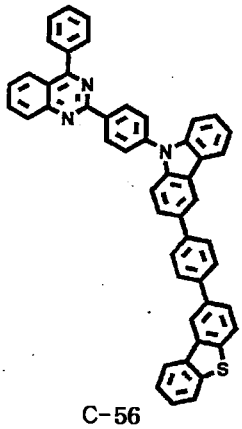
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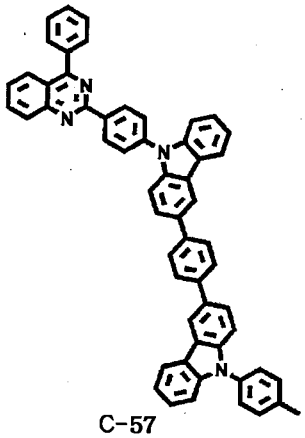
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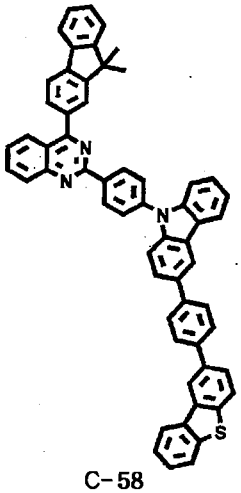
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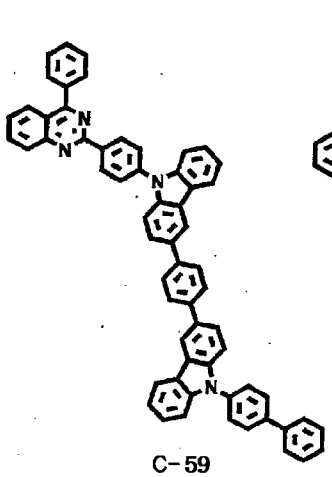

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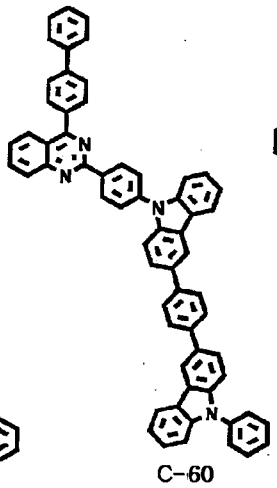

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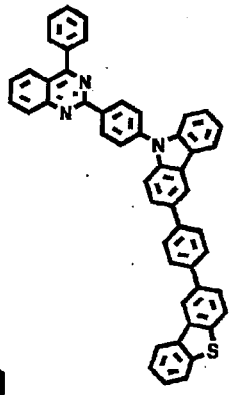

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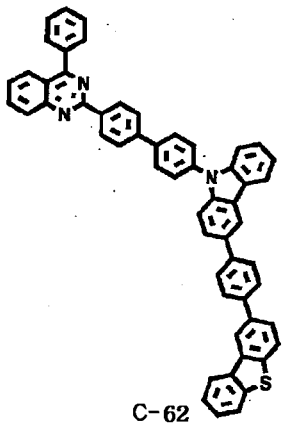

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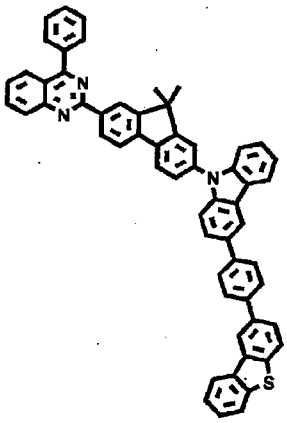

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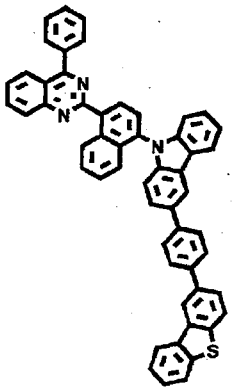

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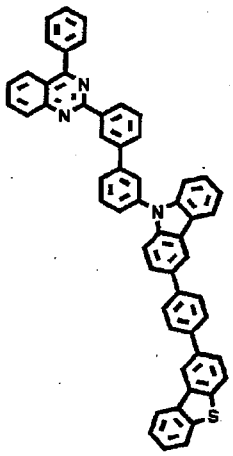

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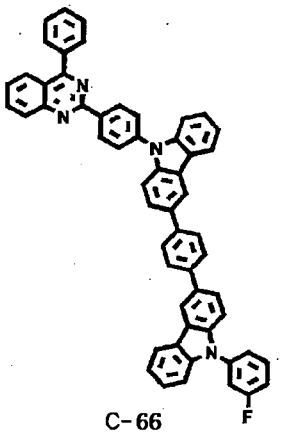

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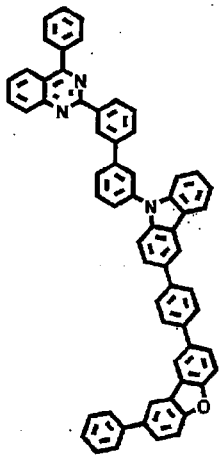

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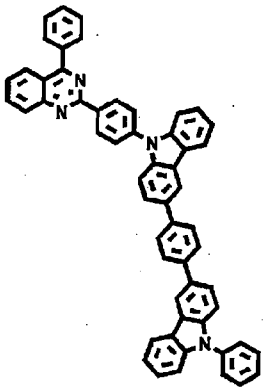

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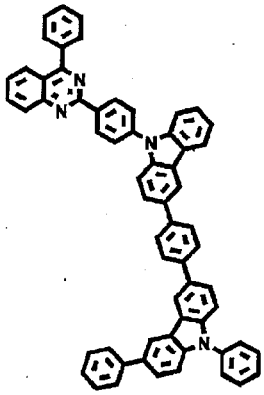

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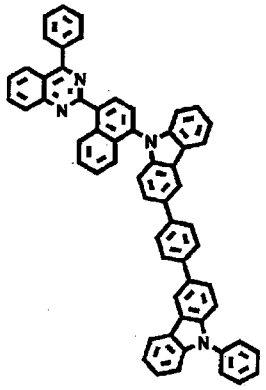

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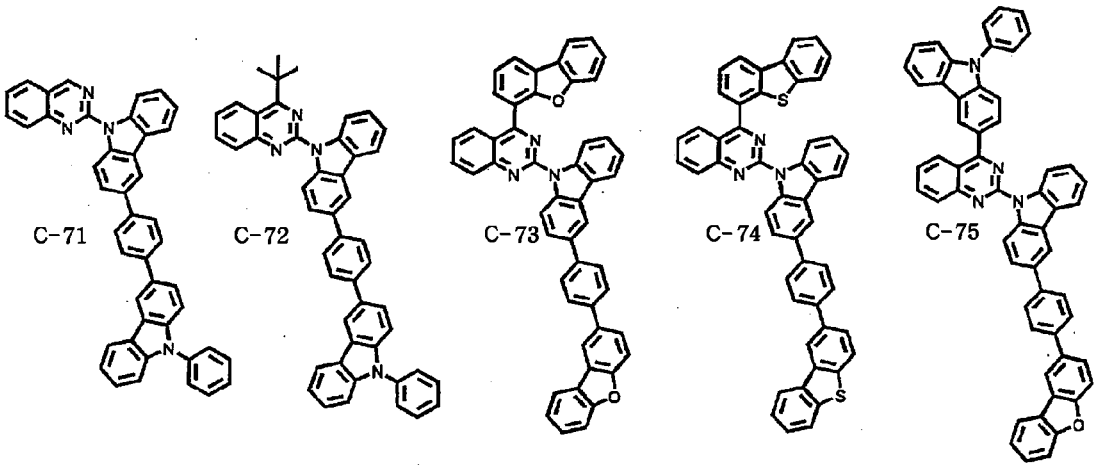


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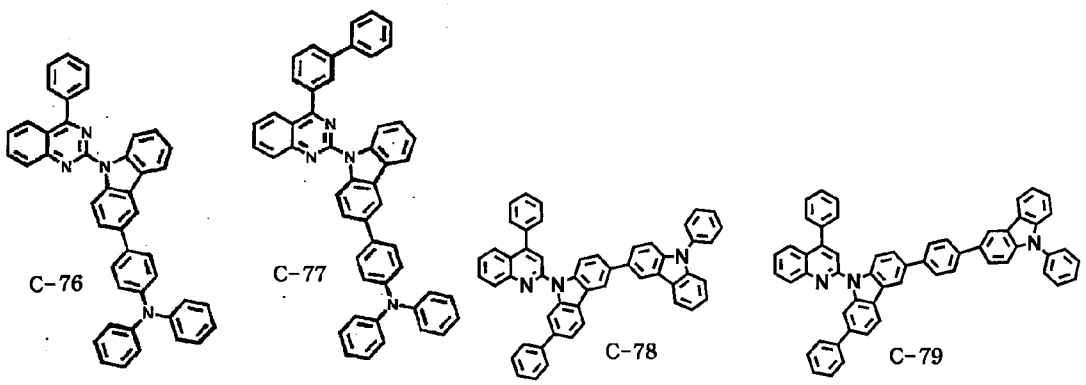


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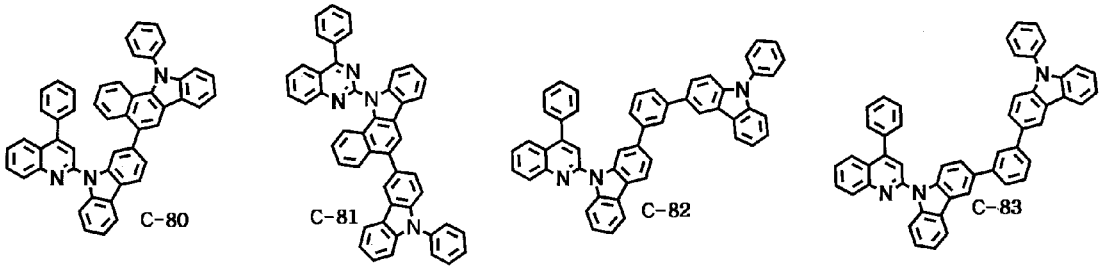


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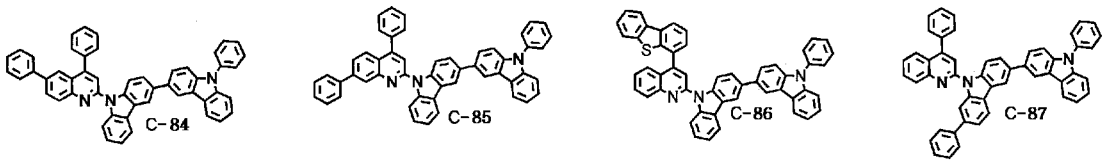


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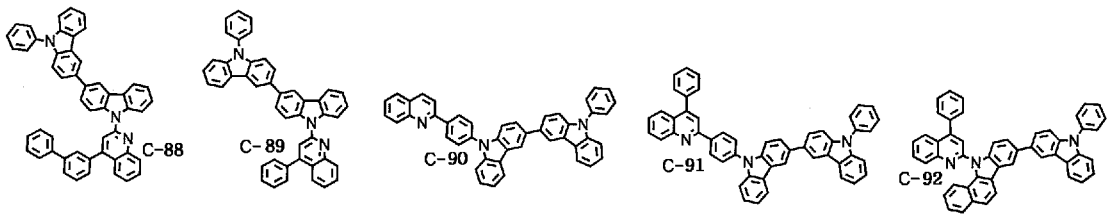
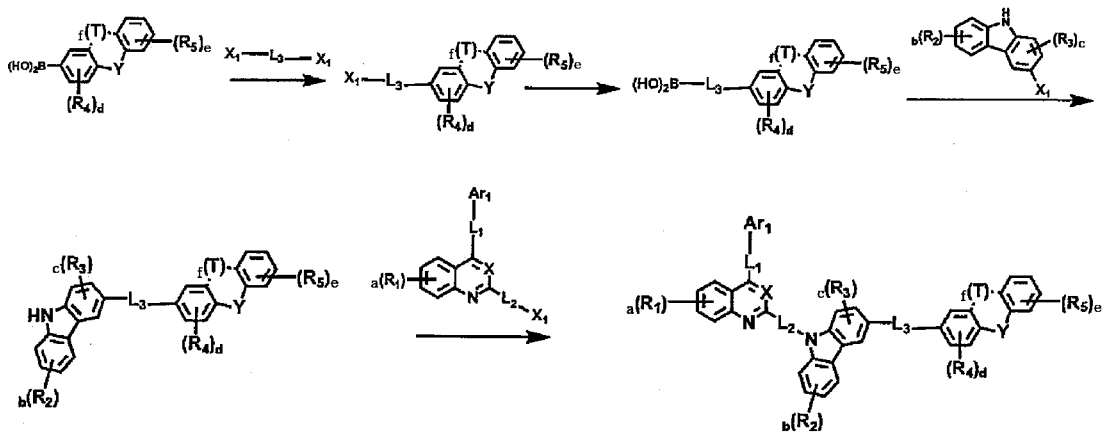



[56] The organic electroluminescent compounds according to the present invention can be prepared according to the following reaction scheme 1.

[57] [Reaction Scheme 1]

[58]

[59]



[60] wherein $Ar_1$, **Ri** to $\mathbf{R_5}$, Y, **X**, T, $L_1$, $L_2$, $L_3$, a, b, c, d, e and f are as defined in formula 1, and $\mathbf{X}_1$ represents a halogen.

[61] In addition, the present invention provides an organic electroluminescent material comprising the organic electroluminescent compound of formula 1, and an organic electroluminescent device comprising the material. The material can be comprised of the organic electroluminescent compound according to the present invention alone, or can further include conventional materials generally used in organic electroluminescent materials. The organic electroluminescent device according to the present invention comprises a first electrode, a second electrode, and at least one organic layer between said first and second electrodes. The organic layer comprises at least one compound of formula 1. Further, the organic layer comprises a light-emitting layer in which the organic electroluminescent compound of formula 1 may be used as a host material.

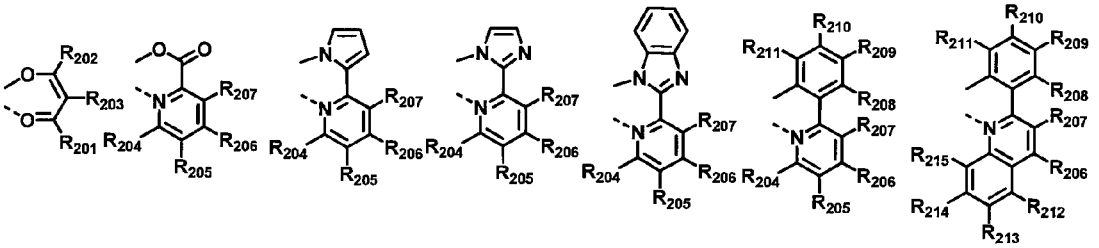
[62] When the organic electroluminescent compounds of formula 1 is used as a host in the light-emitting layer, the light-emitting layer may comprise at least one phosphorescent dopant. The phosphorescent dopant for an organic electroluminescent device of the present invention is not specifically limited, but is preferably selected from compounds represented by the following formula 2:

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

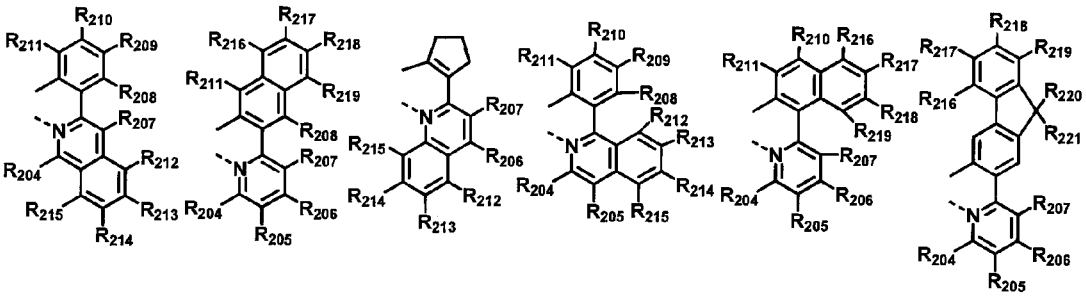
[64] wherein M'is selected from the group consisting of Ir, Pt, Pd and Os;

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

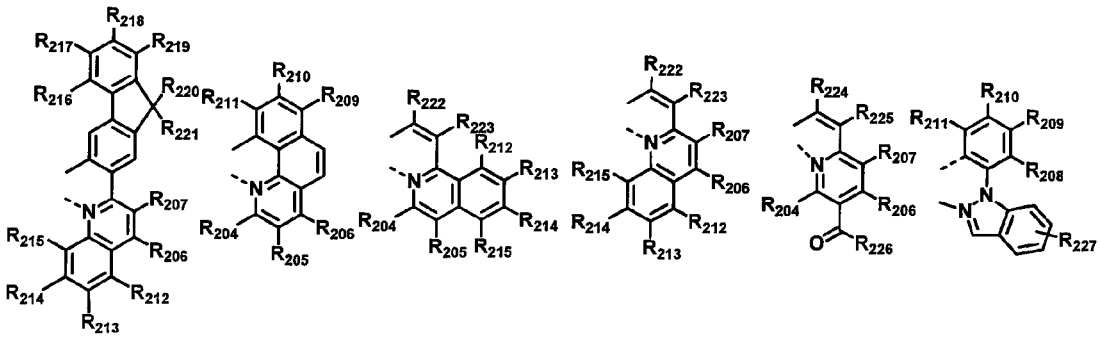
[66]



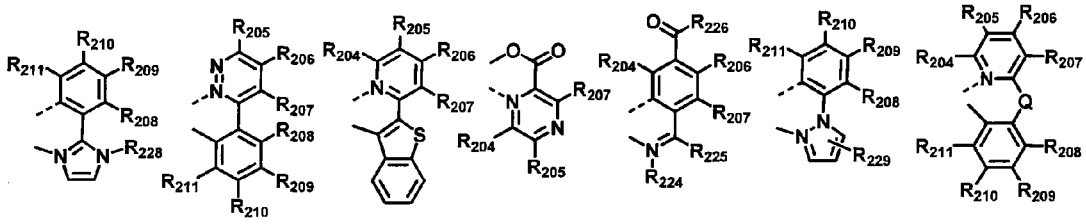
[67]



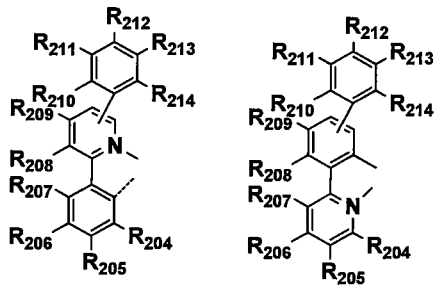
[68]



[69]



[70]



[71] $R_{20}i$ to $R_{203}$ each independently represent hydrogen, deuterium, a (Cl-C30)alkyl group which is unsubstituted or substituted with a halogen, a substituted or unsubstituted (C3-C30)cycloalkyl group, a (C6-C30)aryl group which is unsubstituted or substituted with a (Cl-C30)alkyl group, or a halogen;

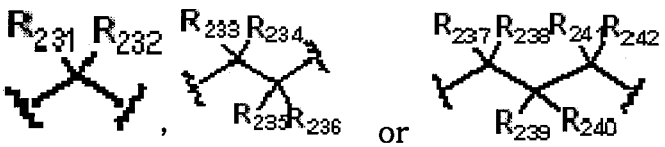
[72] $R_{204}$ to $R_{219}$ each independently represent hydrogen, deuterium, a substituted or unsubstituted (Cl-C30)alkyl group, a substituted or unsubstituted (Cl-C30)alkoxy group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted mono- or di-(Cl-C30)alkylamino group, a substituted or unsubstituted mono- or di-(C6-C30)arylamino group, $SF_5$, a substituted or unsubstituted tri(Cl-C30)alkylsilyl group, a substituted or unsubstituted di(Cl-C30)alkyl(C6-C30)arylsilyl group, a substituted or unsubstituted tri(C6-C30)arylsilyl group, a cyano group or a halogen;

[73] $R_{220}$ to $R_{223}$ each independently represent hydrogen, deuterium, a (Cl-C30)alkyl group which is unsubstituted or substituted with a halogen, or a (C6-C30)aryl group unsubstituted or substituted with a (Cl-C30)alkyl group;

[74] $R_{224}$ and $R_{225}$ each independently represent hydrogen, deuterium, a substituted or unsubstituted (Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a halogen, or $R_{224}$ and $R_{225}$ are linked to each other to form a mono- or polycyclic, (C5-C30)alicyclic or aromatic ring;

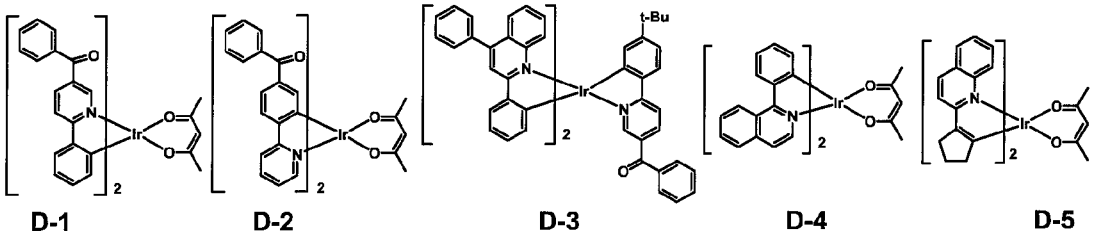
[75] $R_{226}$ represents a substituted or unsubstituted (Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- or 30-membered heteroaryl group or a halogen;

[76] $R_{227}$ to $R_{229}$ each independently represent hydrogen, deuterium, a substituted or unsubstituted (Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group or a halogen;

[77] Q represents  , wherein $R_{231}$ to $R_{242}$ each independently represent hydrogen, deuterium, a (Cl-C30)alkyl group which is unsubstituted or substituted with a halogen, a (Cl-C30)alkoxy group, a halogen, a substituted or unsubstituted (C6-C30)aryl group, a cyano group, or a substituted or unsubstituted (C5-C30)cycloalkyl group, or each of $R_{231}$ to $R_{242}$ may be linked to an adjacent substituent(s) to form a spiro ring or a fused ring or may be linked to $R_{207}$ or $R_{208}$ to form a saturated or unsaturated fused ring.

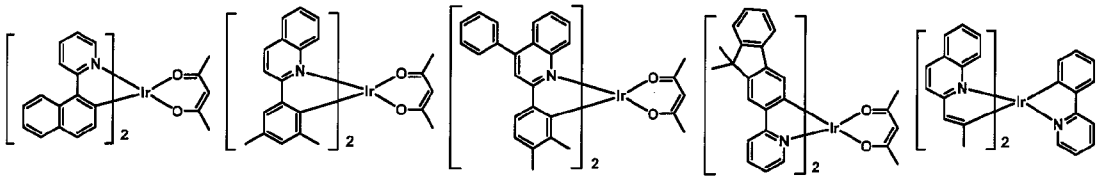
[78] The dopants of formula 2 include the following compounds, but are not limited thereto:

[79]



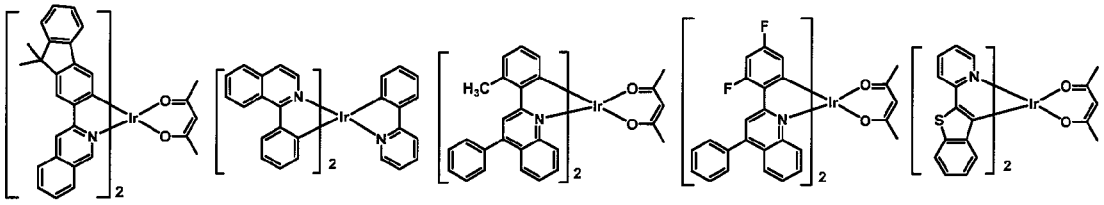
D-1 D-2 D-3 D-4 D-5

[80]



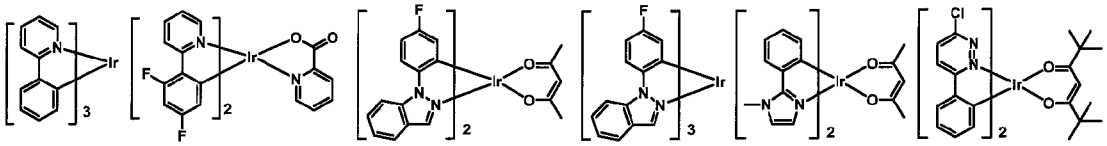
D-6 D-7 D-8 D-9 D-10

[81]



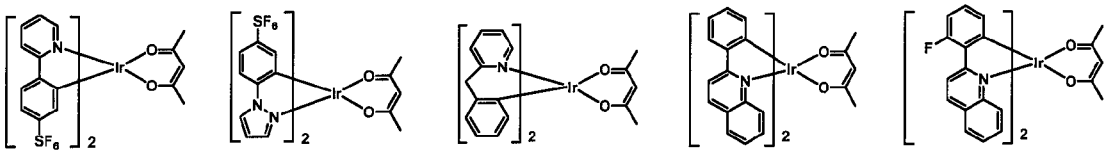
D-11 D-12 D-13 D-14 D-15

[82]



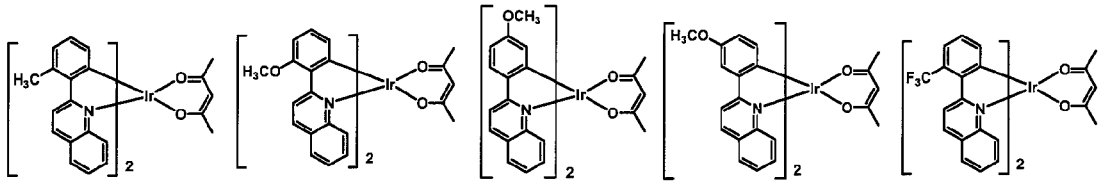
D-16 D-17 D-18 D-19 D-20 D-21

[83]



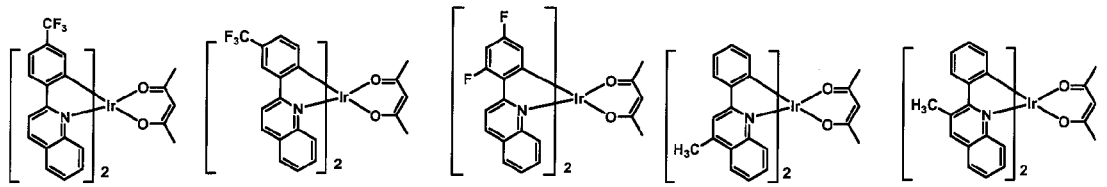
D-22 D-23 D-24 D-25 D-26

[84]



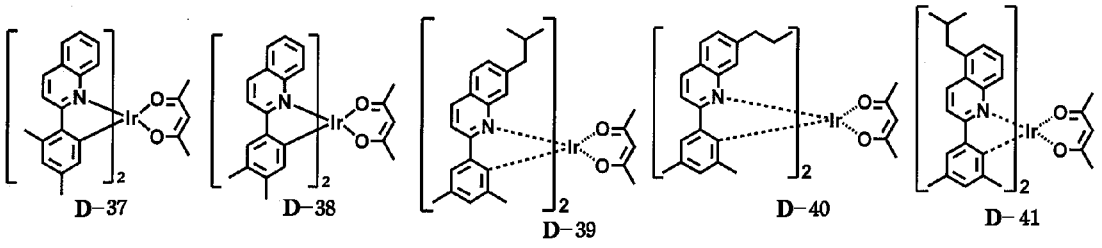
D-27 D-28 D-29 D-30 D-31

[85]



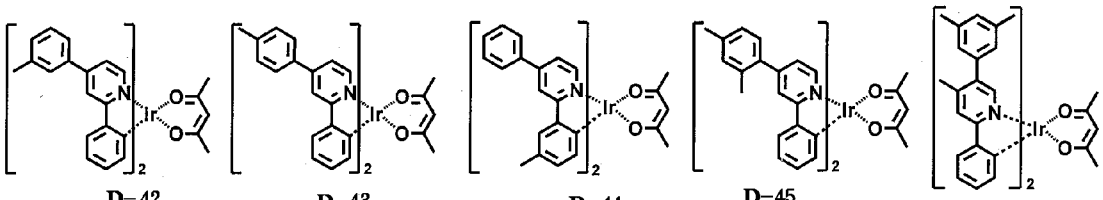
D-32 D-33 D-34 D-35 D-36

[86]



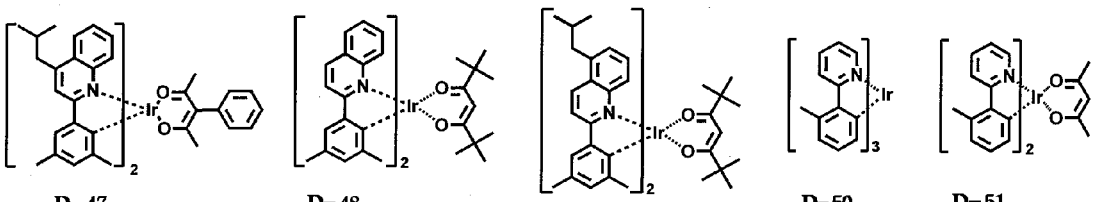
D-37 D-38 D-39 D-40 D-41

[87]



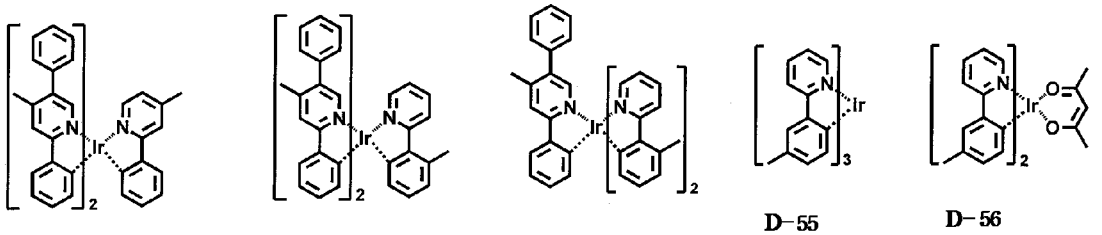
D-42 D-43 D-44 D-45 D-46

[88]



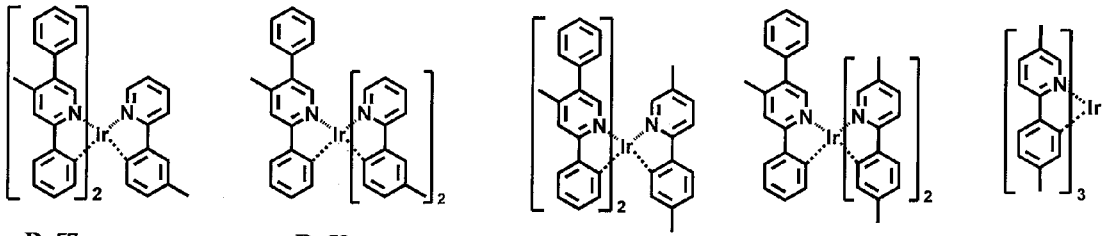
D-47 D-48 D-49 D-50 D-51

[89]



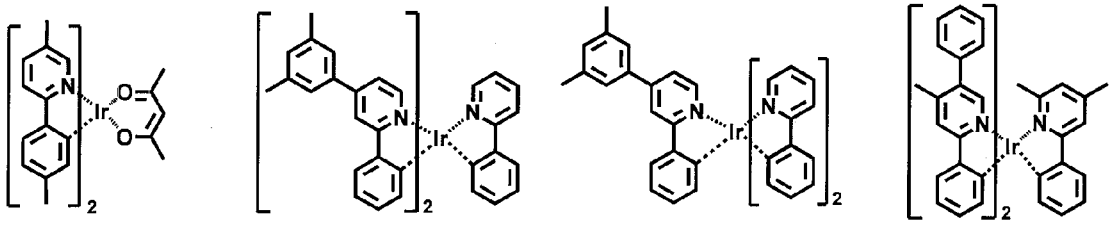
D-52 D-53 D-54 D-55 D-56

[90]



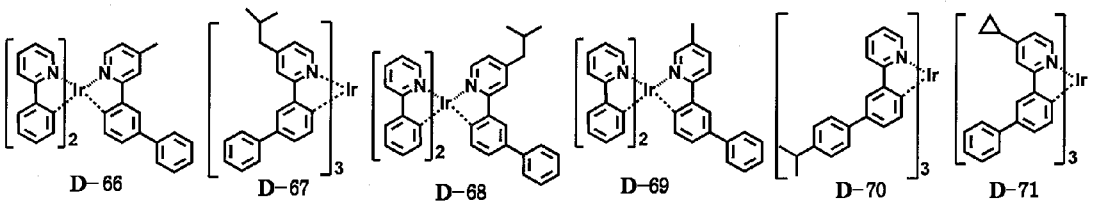
D-57 D-58 D-59 D-60 D-61

[91]



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

[92]

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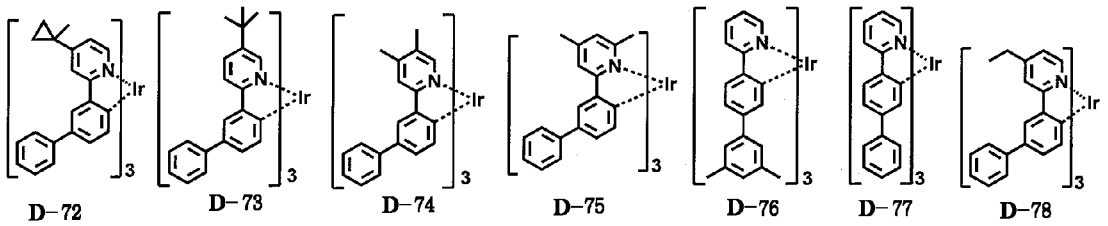


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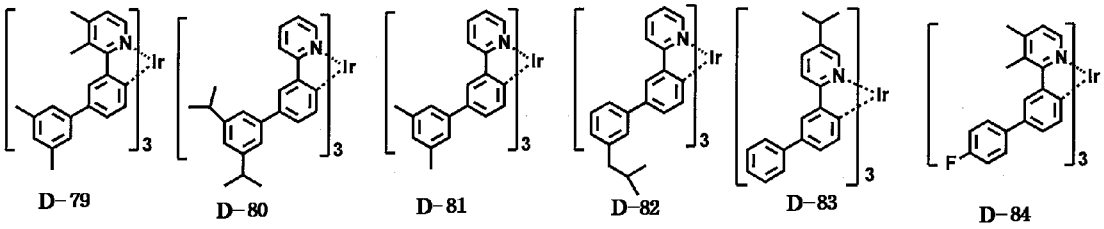


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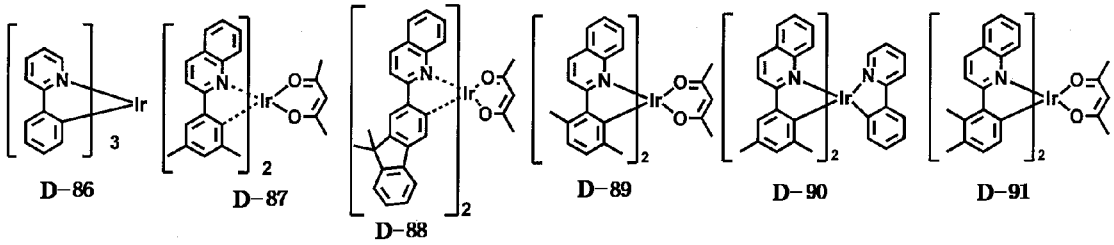


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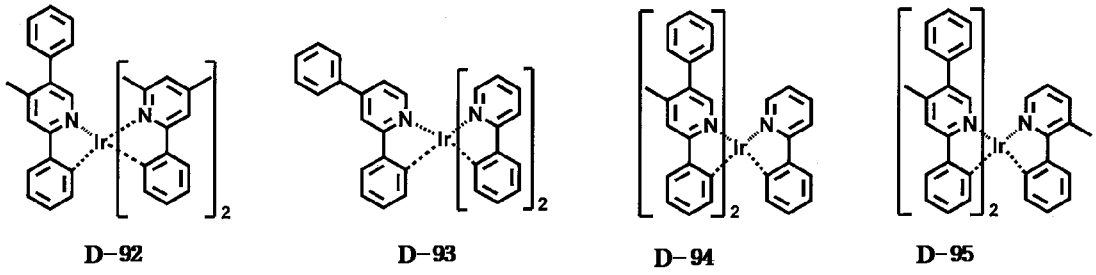


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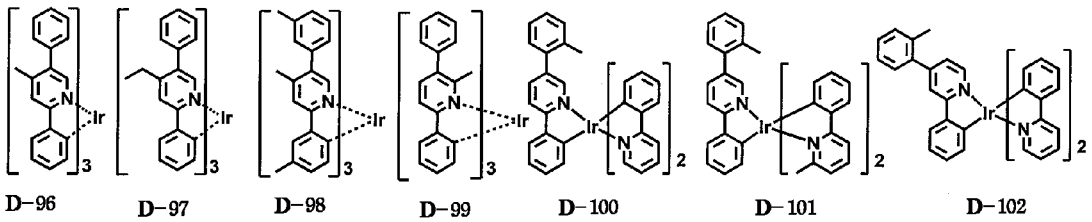


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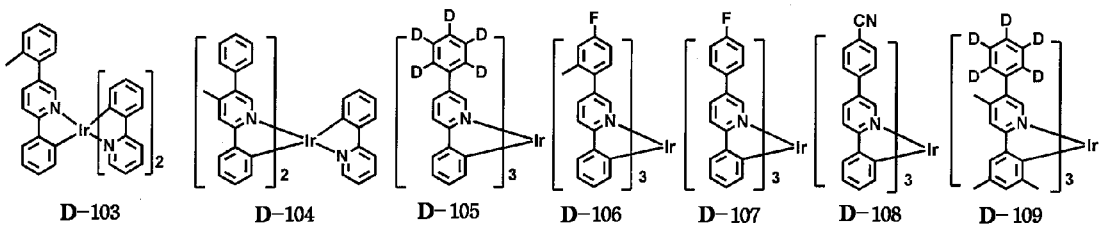

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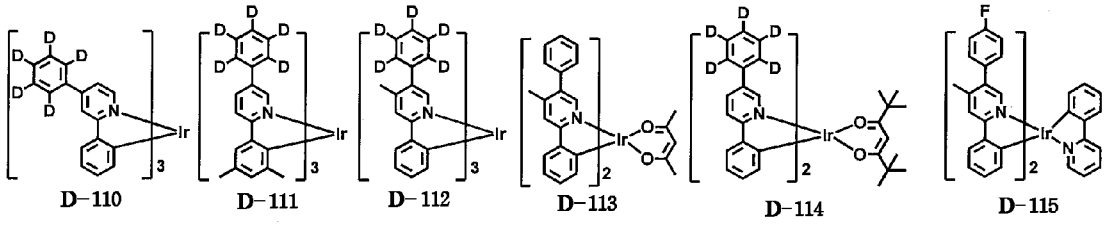


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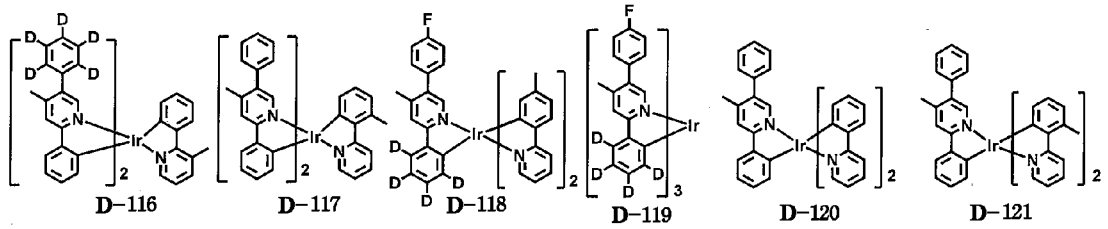


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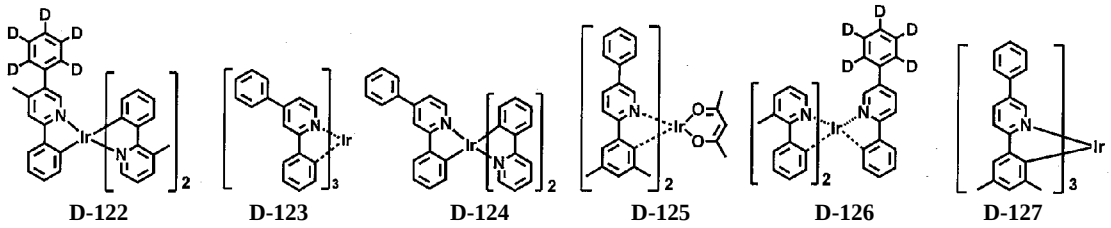


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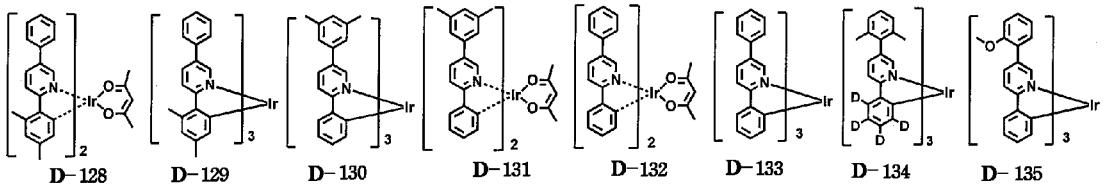


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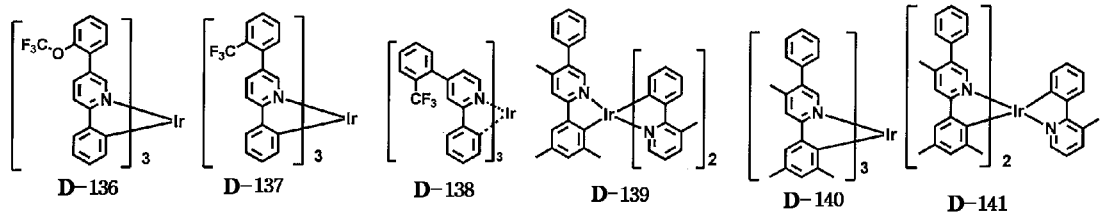
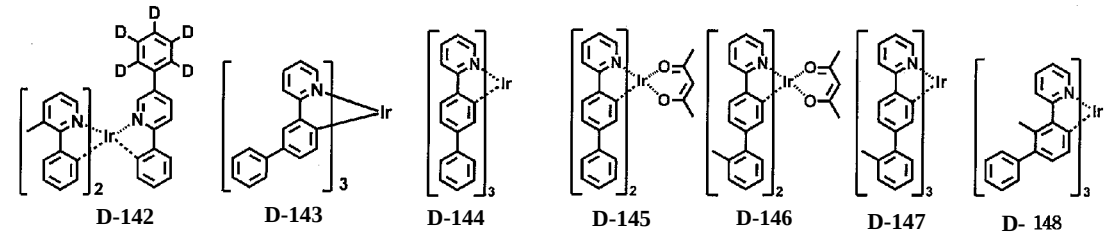



[104]

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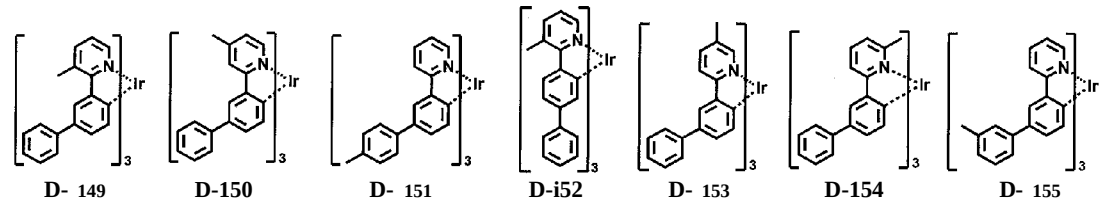


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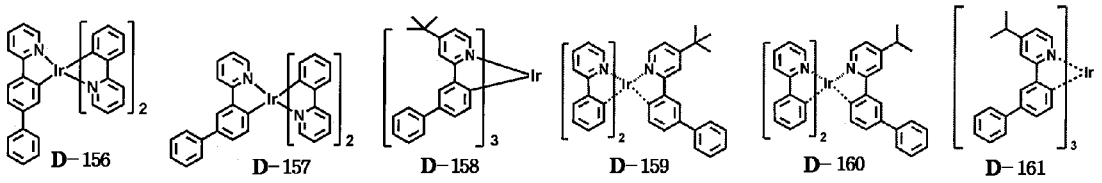


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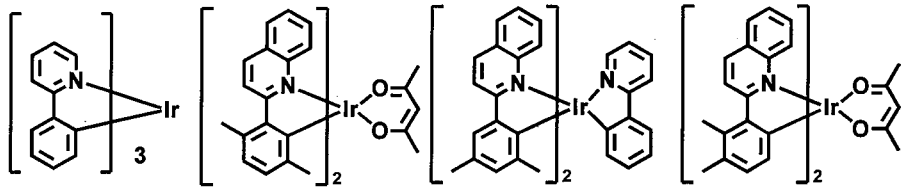



[108] The organic electroluminescent device of the present invention may further comprise, in addition to the organic electroluminescent compounds represented by formula 1, at least one compound selected from the group consisting of arylamine-based compounds and styrylarylamine-based compounds.

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

[110] In addition, the organic electroluminescent device of the present invention may emit white light by further comprising at least one light-emitting layer which comprises a blue electroluminescent compound, a red electroluminescent compound or a green electroluminescent compound which is known in the art, besides the organic electroluminescent compound of formula 1; and may further include a yellow or orange light-emitting layer, if necessary.

[Ill] 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 (includes oxides) 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. The surface layer provides operating stability for the organic electroluminescent device. Preferably, the chalcogenide includes $SiO_x$ ($1 \le X < 2$), $A10_X$ ($1 \le X < 1.5$), SiON, SiAlON, etc.; the metal halide includes LiF, $MgF_2$, $CaF_2$, a rare earth metal fluoride, etc.; and

the metal oxide includes $Cs_20$ , $Li_20$ , MgO, SrO, BaO, CaO, etc.

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

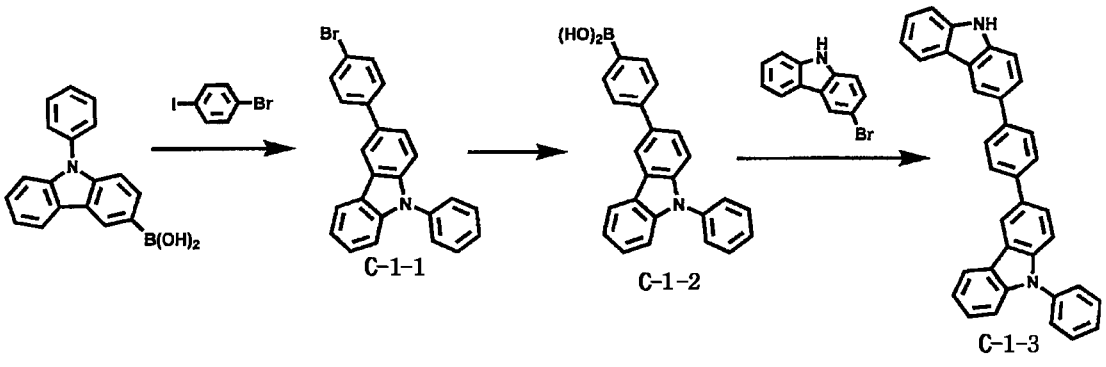
[113] In order to form each layer constituting the organic electroluminescent device according to the present invention, dry film-forming methods, such as vacuum evaporation, sputtering, plasma, ion plating methods, etc., or wet film-forming methods, such as spin coating, dip coating, flow coating methods, etc., can be used.

[114] When using a wet film-forming method, a thin film is formed by dissolving or dispersing the material constituting each layer in suitable solvents, such as ethanol, chloroform, tetrahydrofuran, dioxane, etc. The solvents are not specifically limited as long as the material constituting each layer is soluble or dispersible in the solvents, which do not cause any problems in forming a layer.

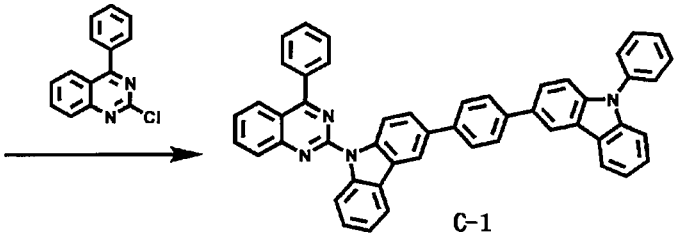
[115] Hereinafter, the organic electroluminescent compound of the present invention, the preparation method of the compound, and the luminescent properties of the device comprising the compound will be explained in detail with reference to the following examples:

[116] Example 1: Preparation of compound C-l

[117]




[118]



C-1

[119] Preparationof compound C-1-1

[120] After adding N-phenylcarbazole-3-boronic acid (30.0 g, 105.0 mmol), 4-bromoiodobenzene (44.0 g, 157.0 mmol), tetrakis(triphenylphosphine)palladium(0) [$Pd(PPh_3)_4$] (3.5 g, 3.14 mmol), $Na_2C0_3$ (33.0 g, 313.0 mmol), toluene (600 mL), ethanol (EtOH) (150 mL) and distilled water (150 mL) to a 2L round-bottom flask (RBF), the reaction mixture was stirred for 2 hours at 110°C. The reaction mixture was worked-up by using ethyl acetate (EA)/$H_20$, was dried over $MgS0_4$ to remove moisture, was distilled under reduced pressure, and was separated through column chromatography by using methylene chloride (MC) and hexane to obtain compound C-1-1 (30.0 g, 72%) as a yellow solid.

[121] Preparation of compound C-l-2

[122] After adding compound C-l-1 (30.0 g, 75.3 mmol) to a 1L RBF and substituting it with nitrogen, tetrahydrofuran (THF) (400.0 mL) was added to the flask. The solution was cooled to -78°C, n-BuLi (36 mL, 2.5 M in hexane, 90.4 mmol) was added to the solution, and the mixture was stirred for one hour. After adding triisopropyl borate (26.0 mL, 113 mmol) to the mixture, the mixture was stirred for 24 hours. The mixture was quenched with 2M HC1, was extracted with EA/$H_20$, was dried over $MgS0_4$ to remove moisture, was distilled under reduced pressure, and was recrystallized by using MC and hexane to obtain compound C-l-2 (22.0 g, 80%).

[123] Preparation of compound C-l-3

[124] After adding compound C-l-2 (20.0 g, 55.0 mmol), 3-bromocarbazole (11.0 g, 44.7 mmol), $Pd(PPh_3)_4$ (2.6 g, 2.2 mmol), $K_2C0_3$ (15.0 g, 107.0 mmol), toluene (150 mL), EtOH (50 mL) and distilled water (50 mL) to a 1L RBF, the reaction mixture was stirred for 24 hours at 110°C. The reaction mixture was extracted by using EA/$H_20$, was dried over $MgS0_4$ to remove moisture, was distilled under reduced pressure, and was separated through column chromatography by using MC and hexane to obtain compound C-l-3 (15.0 g, 69%) as a yellow solid.

[125] Preparation of compound C-1

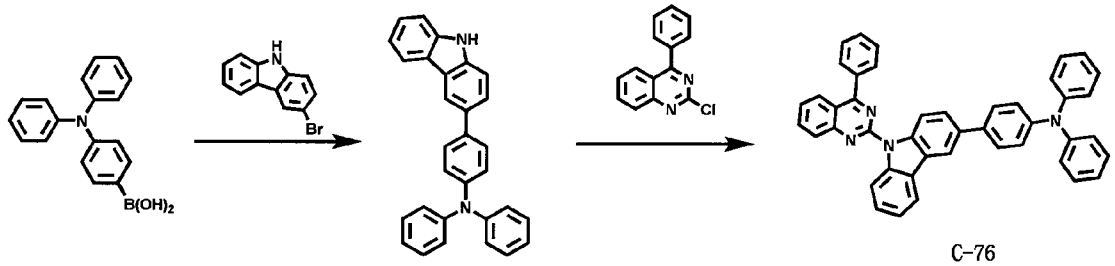
[126] After adding compound C-l-3 (8.0 g, 16.5 mmol) and dimethylformamide (DMF) (200 mL) to a 250 mL RBF and dissolving the mixture by stirring, NaH (0.85 g, 60% dispersion in a mineral oil, 21.5 mmol) was added to the mixture and the reaction mixture was stirred for 30 minutes. 2-Chloro-4-phenylquinazoline (4.0 g, 16.5 mmol)

was slowly added to the reaction mixture. After the addition, the reaction mixture was stirred for 2 hours at 50°C. The reaction mixture was quenched with methanol and was filtered to obtain a solid. The obtained solid was dried in a vacuum oven and was separated through column chromatography by using MC and hexane to obtain compound C-l (6.7 g, 60%) as a yellow solid.

[127]

[128] Example 2: Preparation of compound C-76

[129]




C-76-1

[130] Preparationofcompound C-76-1

[131] After adding 4-(diphenylamino)phenylboronic acid (14.0 g, 48.4 mmol), 3-bromocarbazole (10.0 g, 40.3 mmol), $Pd(PPh_3)_4$ (2.4 g, 2.0 mmol), $K_2C0_3$ (13.0 g, 96.8 mmol), toluene (200 mL), EtOH (50 mL) and distilled water (50 mL) to a 1L RBF, the reaction mixture was stirred for 24 hours at 110°C. The reaction mixture was extracted by using EA/$H_20$, was dried over $MgS0_4$ to remove moisture, was distilled under reduced pressure, and was separated through column chromatography by using MC and hexane to obtain compound C-76-1 (14.0 g, 84%) as a yellow solid.

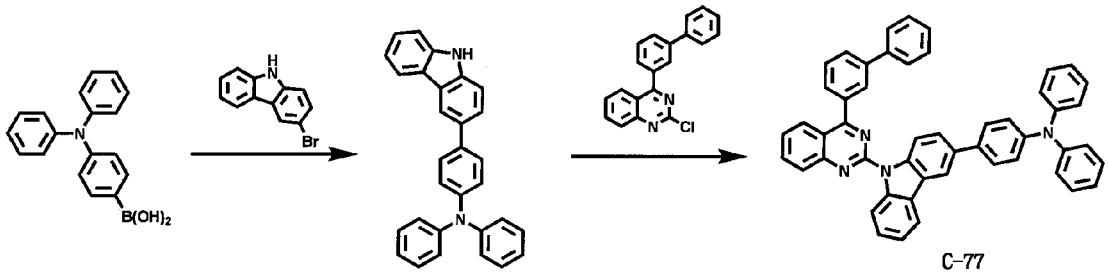
[132] Preparation of compound C-76

[133] Compound C-76-1 (6.0 g, 14.6 mmol) and DMF (75 mL) were added to a 250 mL RBF and were dissolved by stirring. NaH (0.9 g, 60% dispersion in a mineral oil, 21.9 mmol) was added to the mixture and the reaction mixture was stirred for 30 minutes. 2-Chloro-4-phenylquinazoline (4.0 g, 17.5 mmol) was slowly added to the reaction mixture, After the addition, the reaction mixture was stirred for 2 hours at 50°C. The reaction mixture was quenched with methanol and was filtered to obtain a solid. The obtained solid was dried in a vacuum oven and was separated through column chromatography by using MC and hexane to obtain compound C-76 (5.2 g, 58%) as a yellow solid.

[134]

[135] Example 3: Preparation of compound C-77

[136]




C-76-1

[137] Compound C-76-1 (4.0 g, 10.2 mmol) and DMF (50 mL) were added to a 250 mL RBF and were dissolved by stirring. NaH (0.6 g, 60% dispersion in a mineral oil, 15.4 mmol) was added to the mixture and then the reaction mixture was stirred for 30 minutes. 4-([l,l'-biphenyl]-3-yl)-2-chloroquinazoline (4.0 g, 12.3 mmol) was slowly added to the reaction mixture. After the addition, the reaction mixture was stirred for 2 hours at 50 °C. The reaction mixture was quenched with methanol and was filtered to obtain a solid. The obtained solid was dried in a vacuum oven, and was separated through column chromatography by using MC and hexane to obtain compound C-77 (2.1 g, 30%) as a yellow solid.

[138] The physical properties of the compounds of the present invention, which were prepared in Examples 1 to 3, are provided in the Table 1 below:

[139]

[140] Table 1

[141]

| Compound Nos. | Yield (%) | PL (in Tol, nm) | MP (°C) | MS/EIMS | |
|---|---|---|---|---|---|
| | | | | measured | calculated |
| C-1 | 60 | 489 | 257 | 688.20 | 719.26 |
| C-76 | 58 | 535 | 236 | 614.05 | 614.25 |
| C-77 | 30 | 543 | 200 | 690.04 | 690.28 |

[142]

[143] DeviceExample_1: ProductionofanOLEDdeviceusing

[144] theorganicelectroluminescentcompoundaccordingtothepresentinvention

[145] An OLED device was produced using the light-emitting material according to the present invention. A transparent electrode indium tin oxide (ITO) thin film (15 Ω/sq) on a glass substrate for an organic light-emitting diode (OLED) device (Samsung Corning, Republic of Korea) was subjected to an ultrasonic washing with

trichloroethylene, acetone, ethanol and distilled water, sequentially, and then was stored in isopropanol. Then, the ITO substrate was mounted on a substrate holder of a vacuum vapor depositing apparatus. N'^' '-iflJ'-biphenylJ^^'-diy^bisiN [1]-(naphthalen-l-yl)-N [4],N[4]-diphenylbenzene-l,4-diamine) was introduced into a cell of the vacuum vapor depositing apparatus, and then the pressure in the chamber of the apparatus was controlled to $10^{6}$ torr. Thereafter, an electric current was applied to the cell to evaporate the introduced material, thereby forming a hole injection layer having a thickness of 60 nm on the ITO substrate. Then, N,N'-di(4-biphenyl)-N,N'-di(4-biphenyl)-4,4'-diaminobiphenyl was introduced into another cell of the vacuum vapor depositing apparatus, and was evaporated by applying electric current to the cell, thereby forming a hole transport layer having a thickness of 20 nm on the hole injection layer. Thereafter, compound C-l of the present invention as a host was introduced into one cell of the vacuum vapor deposition apparatus, and compound D-l 1 as a dopant was introduced into another cell. The two materials were evaporated at different rates and deposited in a doping amount of 4 wt% of the dopant, based on the total weight of the host and dopant, to form a light-emitting layer having a thickness of 30 nm on the hole transport layer. Then, 2-(4-(9,10-di(naphthalen-2-yl)anthracen-2-yl)phenyl)-l-phenyl-lH-benzo[<i]imidazole was introduced into one cell and lithium quinolate (Liq) was introduced into another cell. The two materials were evaporated at the same rate and were respectively deposited in a doping amount of 50 wt% to form an electron transport layer having a thickness of 30nm on the light-emitting layer. Then, after depositing lithium quinolate as an electron injection layer having a thickness of 2 nm on the electron transport layer, an Al cathode having a thickness of 150 nm was deposited by another vacuum vapor deposition apparatus on the electron injection layer. Thus, an OLED device was produced. All the materials used for producing the OLED device were purified by vacuum sublimation at $10^{-6}$ torr prior to use.

[146] The produced OLED device showed red emission having a luminance of 1020 cd/$m^2$ and a current density of 11.8 mA/$cm^2$ at a driving voltage of 4.2 V. Further, the time taken to be reduced to 90 % of the luminance at a luminance of 5,000nit was at least 120 hours.

[147]

[148] DeviceExample 2: ProductionofanOLEDdeviceusing

[149] theorganicelectroluminescentcompoundaccordingtothepresentinvention

[150] An OLED device was produced in the same manner as in Device Example 1, except for using compound C-76 of the present invention as a host and compound D-7 as a dopant in a light-emitting material.

[151] The produced OLED device showed red emission having a luminance of 1040 cd/$m^2$

and a current density of 10.2 mA/cm$^2$ at a driving voltage of 4.5 V. Further, the time taken to be reduced to 90 % of the luminance at a luminance of 5,000nit was at least 80 hours.

[152]

[153] DeviceExample 3: ProductionofanOLEDdeviceusing

[154] theorganicelectroluminescentcompoundsaccordingtothepresentinvention

[155] An OLED device was produced in the same manner as in Device Example 1, except for using compound C-77 of the present invention as a host and compound D-l 1 as a dopant in a light-emitting material.

[156] The produced OLED device showed red emission having a luminance of 1050 cd/m$^2$ and a current density of 15.5 mA/cm$^2$ at a driving voltage of 4.7 V. Further, the time taken to be reduced to 90 % of the luminance at a luminance of 5,000nit was at least 50 hours.

[157]

[158] ComparativeExample _1: ProductionofanOLEDdevice

[159] using a conventionallight-emittingmaterial

[160] An OLED device was produced in the same manner as in Device Example 1, except that a light-emitting layer having a thickness of 30 nm was deposited on the hole transport layer by using 4,4'-N,N'-dicarbazol-biphenyl as a host and compound D-l 1 as a dopant in a light-emitting material and a hole blocking layer having a thickness of 10 nm was deposited on the light-emitting by using aluminum(III) bis(2-methyl-8-quinolinato)-4-phenyl phenolate.

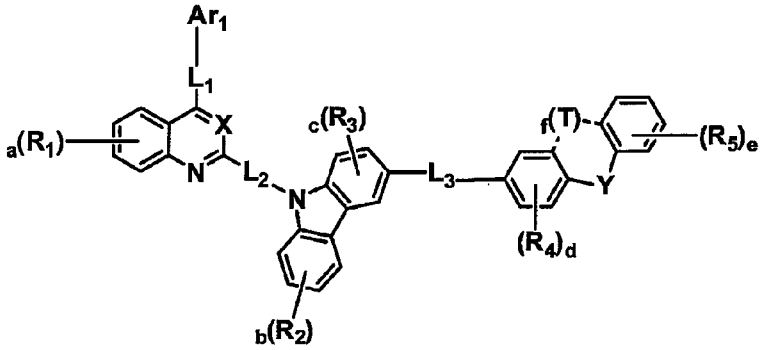
[161] The produced OLED device showed red emission having a luminance of 1000 cd/m$^2$ and a current density of 20.0 mA/cm$^2$ at a driving voltage of 8.2 V. Further, the time taken to be reduced to 90 % of the luminance at a luminance of 5,000nit was at least 10 hours.

[162]

[163] The organic electroluminescent compounds according to the present invention have high electron transmission efficiency, and thus can prevent crystallization in the production of a device; and are suitable for forming a layer, and thus can improve the current features of the device thereby reducing driving voltage of the device. The organic electroluminescent device having enhanced power efficiency can be prepared by using the organic electroluminescent compounds according to the present invention.

# Claims

[Claim 1] An organic electroluminescent compound represented by the following formula 1:



(1)

wherein

X represents CH or N;

Li and $L_2$ each independently represent a single bond, a substituted or unsubstituted 5- to 30-membered heteroarylene group, or a substituted or unsubstituted (C6-C30)arylene group;

$L_3$ represents a single bond, a substituted or unsubstituted (Cl-C30)alkylene group, a substituted or unsubstituted (C6-C30)arylene group, or a substituted or unsubstituted 3- to 30-membered heteroarylene group;

Y represents -0-, -S-, -CRnRi $_2$- or -NR $_{13}$-;

T represents a chemical bond;

$Ar_l$ represents hydrogen, a halogen, deuterium, a substituted or unsubstituted 5- to 30-membered heteroaryl group, a substituted or unsubstituted (C6-C30)aryl group, or a substituted or unsubstituted (Cl-C30)alkyl group;

Ri to $R_5$ each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- 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(Cl-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group which is fused with at least one (C3-C30) aliphatic ring, a 5- to 7-membered heterocycloalkyl group which is fused with at least one substituted or unsubstituted (C6-C30) aromatic ring, a (C3-C30)cycloalkyl group which is fused with at least one substituted

or unsubstituted (C6-C30) aromatic ring, -NR $_{14}$R $_{15}$, -SiRi $_6$Ri $_7$Ri $_8$, -SRi $_9$, -OR $_{20}$, a (C2-C30)alkenyl group, a (C2-C30)alkynyl group, a cyano group, a nitro group, or a hydroxy 1group;

$R_{11}$ to $R_{20}$ are as defined in Ri 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;

f represents an integer of 0 or 1; where f is 0, Y represents -NR $_{13}$-, wherein $R_{13}$ may be linked to $R_5$ to form a mono- or polycyclic, (C5-C30) alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur; and

the heterocycloalkyl group and heteroaryl(ene) group contain at least one hetero atom selected from B, N, O, S, P(=0), Si and P.

[Claim 2] The organic electroluminescent compound according to claim 1, wherein the substituents of the substituted alkyl(ene) group, the substituted aryl(ene) group,, the substituted heteroaryl(ene) group, the substituted cycloalkyl group, and the substituted heterocycloalkyl group in Li to $L_3$, Ar$_1$, $R_1$ to $R_5$, and $R_{11}$ to $R_{20}$ each independently are at least one selected from the group consisting of deuterium; a halogen; a (Cl-C30)alkyl group which is unsubstituted or substituted with a halogen; a (C6-C30)aryl group; a 3- to 30-membered heteroaryl group which is unsubstituted or substituted with a (C6-C30)aryl group; a 5- to 7-membered heterocycloalkyl group; a 5- to 7-membered heterocycloalkyl group which is fused with at least one (C6-C30) aromatic ring; a (C3-C30)cycloalkyl group; a (C6-C30)cycloalkyl group which is fused with at least one (C6-C30) aromatic ring; $R_aR_bR_c$Si-; a (C2-C30)alkenyl group; a (C2-C30)alkynyl group; a cyano group; a carbazolyl group; -NR $_d$R $_e$; -BR $_f$R $_g$; -PR $_h$Ri; -P(=0)R $_j$R $_k$; (C6-C30)aryl(Cl-C30)alkyl group; (Cl-C30)alkyl(C6-C30)aryl group; RiZ-; $R_m$C(=0)-; $R_m$C(=0)0-; a carboxyl group; a nitro group; and a hydroxyl group, in which $R_a$ to Ri each independently represent a (Cl-C30)alkyl group, a (C6-C30)aryl group or a 3- to 30-membered heteroaryl group, or are linked to an adjacent substituent(s) to form a mono- or polycyclic, (C5-C30) alicyclic or aromatic ring whose carbon

atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur, Z represents S or O, and $R_m$ represents a (Cl-C30)alkyl group, a (Cl-C30)alkoxy group, a (C6-C30)aryl group or a (C6-C30)aryloxy group.

[Claim 3] The organic electroluminescent compound according to claim 1, wherein $L_1$ and $L_2$ each independently represent a single bond, a substituted or unsubstituted 5- to 15-membered heteroarylene group, or a substituted or unsubstituted (C6-C15)arylene group;

$L_3$ represents a single bond, or a substituted or unsubstituted (C6-C15)arylene group;

Y represents -0-, -S-, -CRnRi $_2$- or -NRi $_3$-, in which $R_{11}$ and $R_{12}$ each independently represent a substituted or unsubstituted (Cl-ClO)alkyl group, $R_{13}$ represents a substituted or unsubstituted (C6-C15)aryl group, or a substituted or unsubstituted 5- to 15-membered heteroaryl group;

T represents a single bond;

Ari represents hydrogen, a substituted or unsubstituted 5- to 20-membered heteroaryl group, a substituted or unsubstituted (C6-C20)aryl group, or a substituted or unsubstituted (Cl-ClO)alkyl group; and

$R_1$ to $R_5$ each independently represent hydrogen, a substituted or unsubstituted (C6-C15)aryl group, or a substituted or unsubstituted 5- to 15-membered heteroaryl group.

[Claim 4] The organic electroluminescent compound according to claim 3, wherein $L_1$ and $L_2$ each independently represent a single bond, an unsubstituted 5- to 15-membered heteroarylene group, or a (C6-C15)arylene group which is unsubstituted or substituted with a (C1-C6) alkyl group;

$L_3$ represents a single bond or an unsubstituted (C6-C15)arylene group;

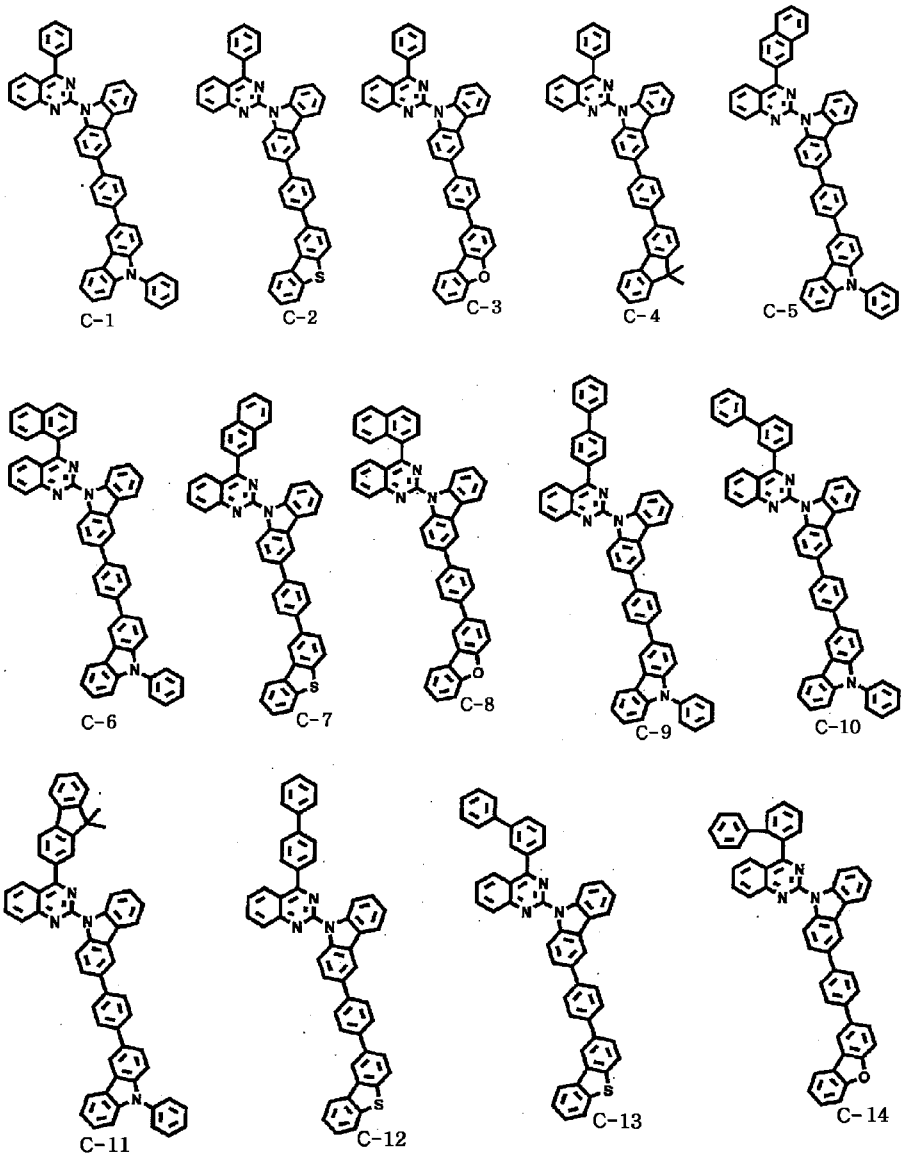
Y represents -0-, -S-, -CRnRi $_2$- or -NR $_{13}$-, in which $R_{11}$ and $R_{12}$ each independently represent an unsubstituted (Cl-ClO)alkyl group, $R_{13}$ represents a (C6-C15)aryl group which is unsubstituted or substituted with deuterium, a halogen, a (Cl-C6)alkyl group or a (C6-C15)aryl group, or a 5- to 15-membered heteroaryl group which is substituted with a (C6-C15)aryl group;

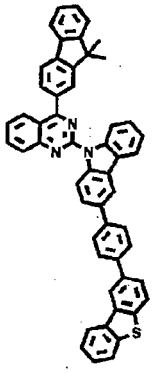
Ari represents hydrogen; a 5- to 20-membered heteroaryl group which is unsubstituted or substituted with a (C6-C15)aryl group; a (C6-C20)aryl group which is unsubstituted or substituted with deuterium, a halogen, a (Cl-C6)alkyl group, a (C6-C15)aryl group or a

5- to 15-membered heteroaryl group; or a (Cl-ClO)alkyl group which is unsubstituted or substituted with a (Cl-C6)alkyl group; and

Ri to $R_5$ each independently represent hydrogen, an unsubstituted (C6-C15)aryl group or an unsubstituted 5- to 15-membered heteroaryl group.

[Claim 5] The organic electroluminescent compound according to claim 1, wherein the compound represented by formula 1 is selected from the group consisting of the following compounds:





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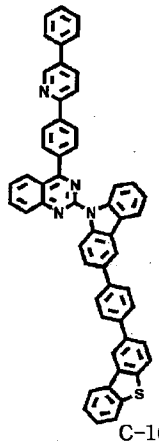

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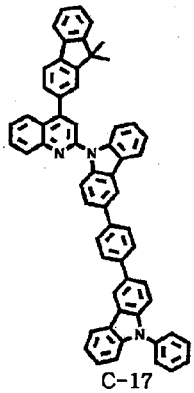

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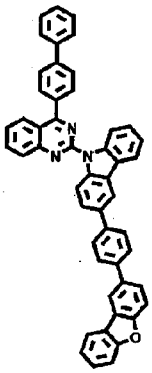

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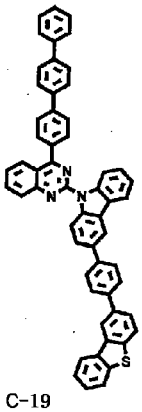

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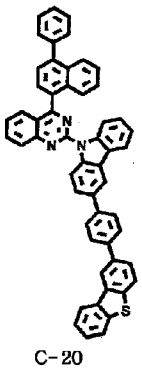

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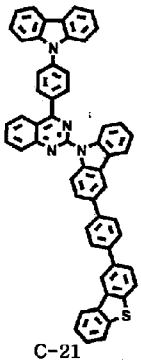

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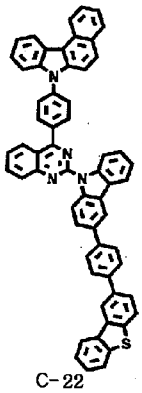

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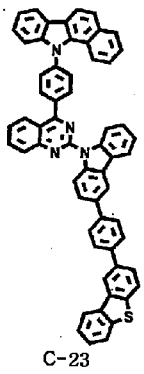

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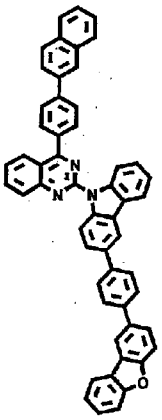

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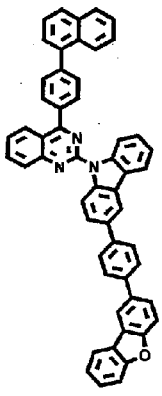

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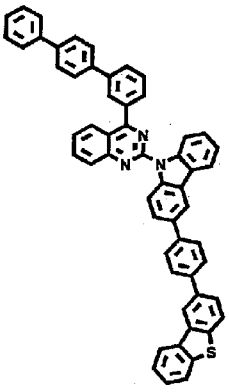

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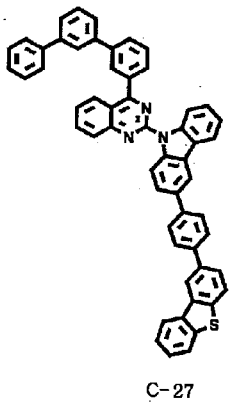

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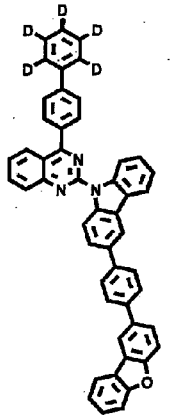

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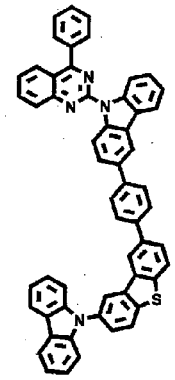

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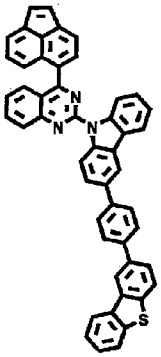

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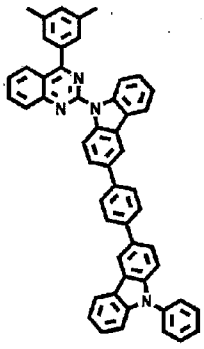

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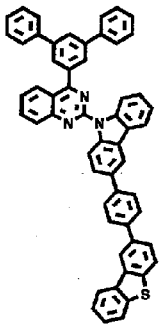

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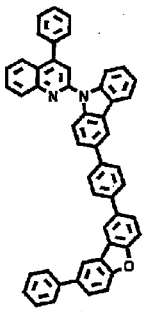

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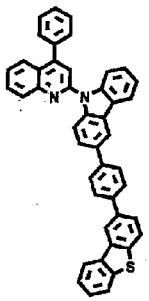

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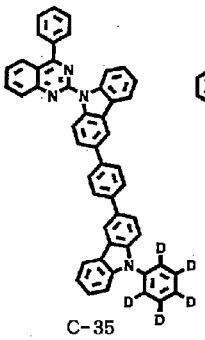

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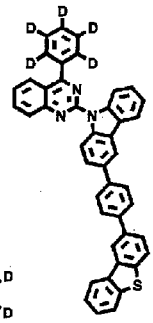

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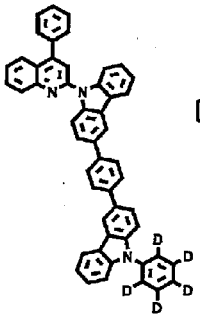

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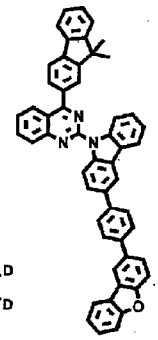

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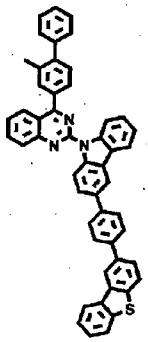

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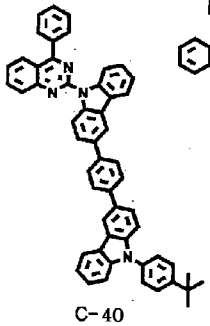

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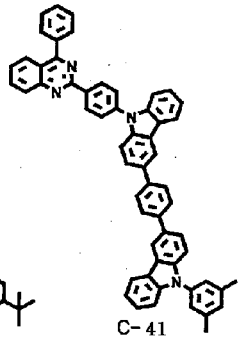

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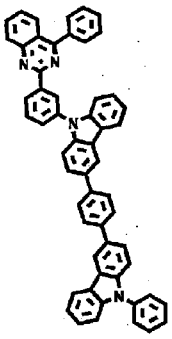

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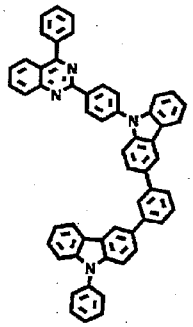

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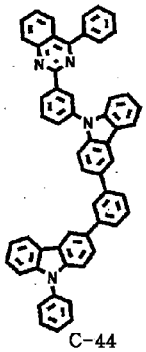

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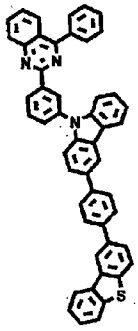

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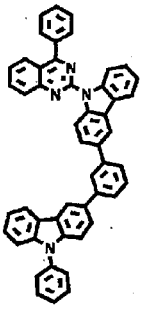

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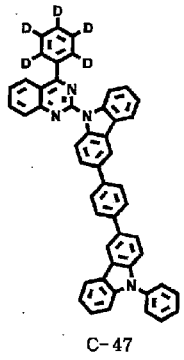
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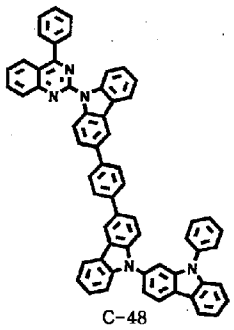
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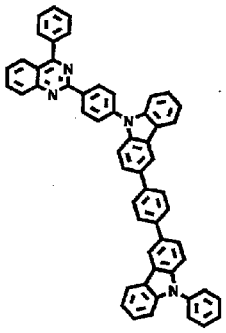
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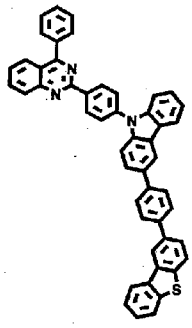
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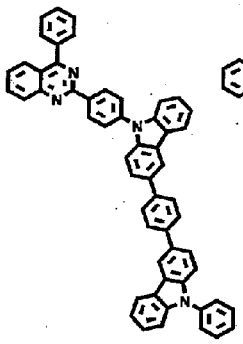
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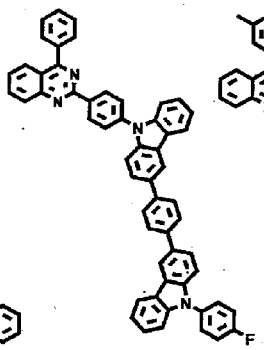
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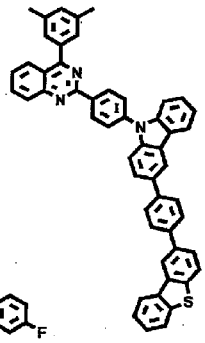
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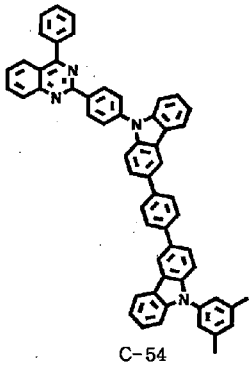
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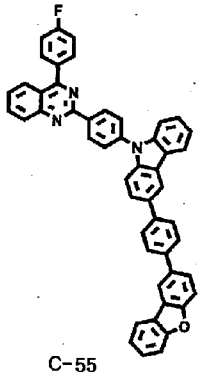
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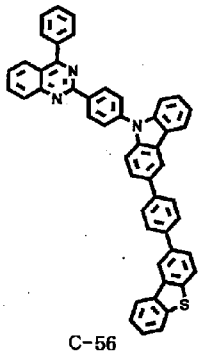
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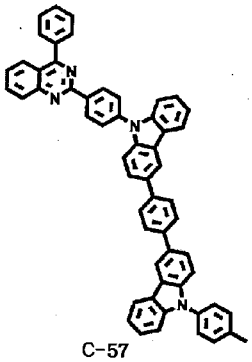
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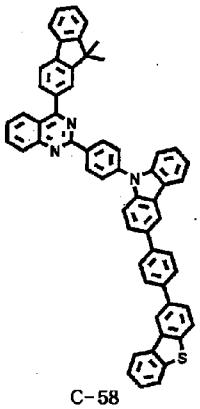
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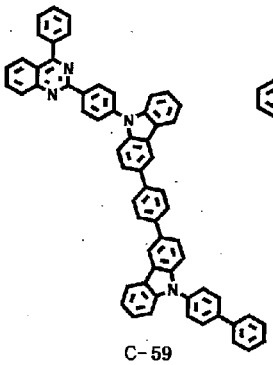
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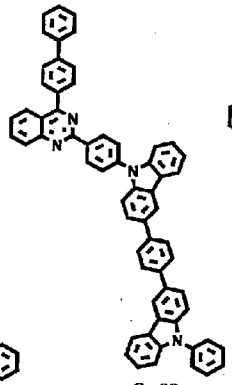
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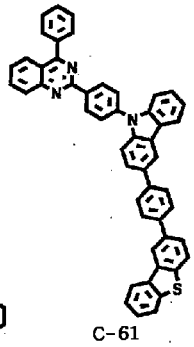
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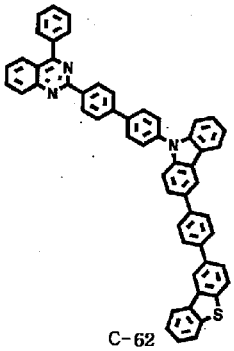
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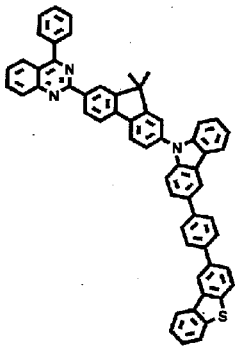

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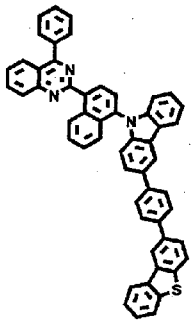

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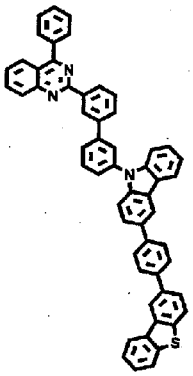

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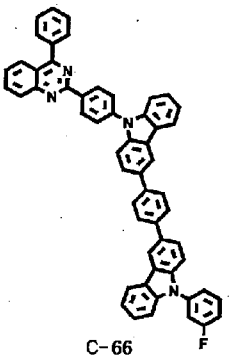

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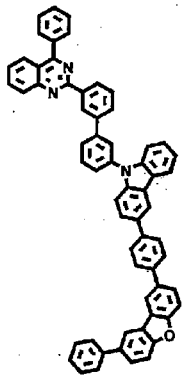

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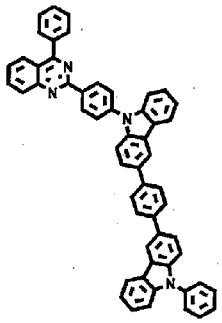

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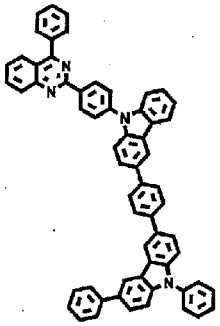

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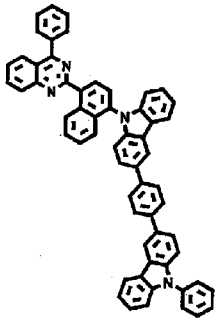

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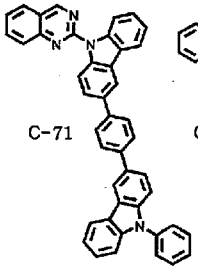

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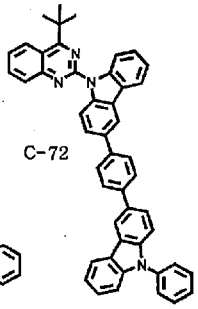

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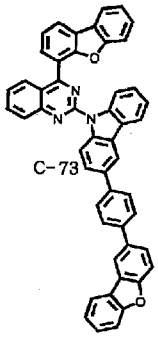

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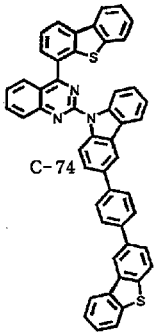

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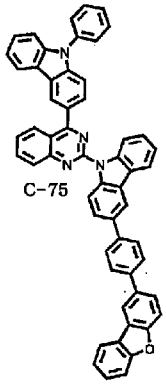

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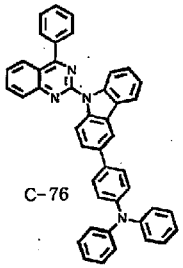

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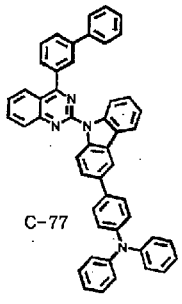

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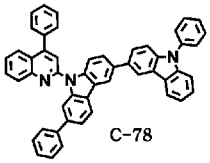

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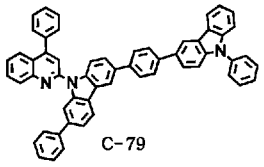

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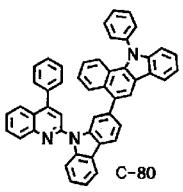

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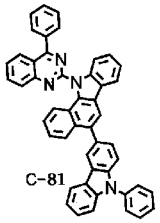

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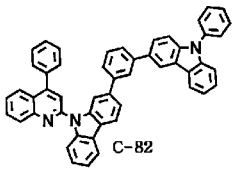

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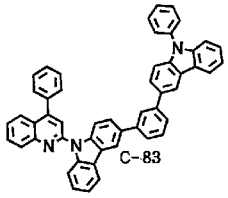

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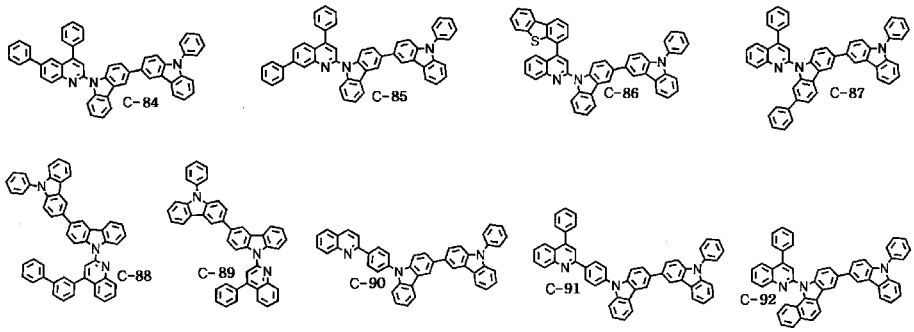


[Claim 6] An organic electroluminescent device comprising the organic electroluminescent compound according to claim 1.

**INTERNATIONAL SEARCH REPORT**

International application No.
**PCT/KR2013/005171**

A. CLASSIFICATION OF SUBJECT MATTER

***C09K 11/06 (2006.01) C07D 403/14 (2006.01) C07D 401/14 (2006.01) C07D 405/14 (2006.01) C07D 409/14 (2006.01) H01L 51/54 (2006.01) C07D 403/04 (2006.01) H01L 27/32 (2006.01) H05B 33/14 (2006.01)***

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

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

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

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

Databases - STN: Chemical Abstracts Registry and CAPLUS. Substructure search of Chemical Formula 1.

C. DOCUMENTS CONSIDERED TO BE RELEVANT

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

[X] Further documents are listed in the continuation of Box C [X] See patent family annex

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

| Date of the actual completion of the international search | Date of mailing of the international search report |
|---|---|
| 19 August 2013 | 19 August 2013 |

**Name and mailing address of the ISA/All**

AUSTRALIAN PATENT OFFICE
PO BOX 200, WODEN ACT 2606, AUSTRALIA
Email address: pct@ipaustralia.gov.au
Facsimile No.: +61 2 6283 7999

**Authorised officer**

Scott Makin
AUSTRALIAN PATENT OFFICE
(ISO 9001 Quality Certified Service)
Telephone No. +61262837971

| INTERNATIONAL SEARCH REPORT | | International application No. |
|---|---|---|
| C (Continuation). | DOCUMENTS CONSIDERED TO BE RELEVANT | **PCT/KR2013/005171** |

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|---|---|---|
| X | EP 2423209 A1 (IDEMITSU KOSAN CO., LTD.) 29 February 2012<br>Abstract; Fig. 1; Chemical Formulae 34 (p. 30) and 38 (p. 32); Examples, pp. 127-138; Claims | 1-6 |
| X | WO 2011/019156 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 17 February 2011<br>Abstract; Examples, pp. 22-24; Claims; Cpd 8 (p. 7) | 1-6 |
| X | KR 10-2012-0013173 A (CHEIL INDUSTRIES INC.) 14 February 2012<br>Abstract; Cpd 11b (para. [0079]-[0080], pp. 26-27); Cpd 11c (para. [0100], p. 29) | 1-4 and 6 |
| P,X | WO 2012/121561 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 13 September 2012<br>Abstract; Examples, pp. 29-31; Claims; Compounds on pp. 7-12 | 1-4 and 6 |
| P,X | WO 2012/134124 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 04 October 2012<br>Abstract; Examples, pp. 16-18; Claims; Cpd C-96 (p. 10 and claim 5) | 1, 2 and 6 |
| P,X | WO 2012/141499 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 18 October 2012<br>Abstract; Examples, pp. 24-26; Claims; Compounds on pp. 7-9 | 1-4 and 6 |
| E | WO 2013/085243 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 13 June 2013<br>Abstract; Examples, pp. 20-22; Claims; Cpds C-20 and C-49 (p. 8) | 1, 3, 4 and 6 |

| INTERNATIONAL SEARCH REPORT<br>Information on patent family members | International application No.<br>**PCT/KR2013/005171** |
|---|---|

This Annex lists known patent family members relating to the patent documents cited in the above-mentioned international search report. The Australian Patent Office is in no way liable for these particulars which are merely given for the purpose of information.

| Patent Document/s Cited in Search Report | | Patent Family Member/s | |
|---|---|---|---|
| **Publication Number** | **Publication Date** | **Publication Number** | **Publication Date** |
| EP 2423209 A1 | 29 Feb 2012 | CN 102439004 A | 02 May 2012 |
| | | EP 2415769 A1 | 08 Feb 2012 |
| | | EP 2423209 A1 | 29 Feb 2012 |
| | | JP 5074627 B2 | 14 Nov 2012 |
| | | JP 2013030781 A | 07 Feb 2013 |
| | | KR 20120034648 A | 12 Apr 2012 |
| | | KR 20120057561 A | 05 Jun2012 |
| | | KR 20120127746 A | 23 Nov 2012 |
| | | TW 201141989 A | 01 Dec 2011 |
| | | TW 201141990 A | 01 Dec 2011 |
| | | US 2011278555 A1 | 17 Nov 2011 |
| | | US 2011279020 A1 | 17 Nov 2011 |
| | | US 2012138911 A1 | 07 Jun2012 |
| | | US 2012138912 A1 | 07 Jun2012 |
| | | WO 2011132683 A1 | 27 Oct 2011 |
| | | WO 2011132684 A1 | 27 Oct 2011 |
| WO 2011/019156 A1 | 17 Feb 2011 | KR 20110015836 A | 17 Feb 2011 |
| | | TW 201120186 A | 16 Jun2011 |
| | | US 2012235123 A1 | 20 Sep 2012 |
| | | WO 2011019156 A1 | 17 Feb 2011 |
| KR 10-2012-0013173 A | 14 Feb 2012 | None | |
| WO 2012/121561 A1 | 13 Sep 2012 | TW 201238962 A | 01 Oct 2012 |
| | | WO 2012121561 A1 | 13 Sep 2012 |
| WO 2012/134124 A1 | 04 Oct 2012 | TW 201245406 A | 16 Nov 2012 |
| | | WO 2012134124 A1 | 04 Oct 2012 |
| WO 2012/141499 A1 | 18 Oct 2012 | TW 201249960 A | 16 Dec 2012 |
| | | WO 2012141499 A1 | 18 Oct 2012 |
| WO 2013/085243 A1 | 13 Jun2013 | WO 2013085243 A1 | 13 Jun2013 |

**End of Annex**

Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001.

| | | | |
|---|---|---|---|
| 专利名称(译) | 新型有机电致发光化合物和包含该化合物的有机电致发光装置 | | |
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| [标]申请(专利权)人(译) | 罗门哈斯电子材料有限公司 | | |
| 申请(专利权)人(译) | 罗门哈斯电子材料KOREA LTD. | | |
| 当前申请(专利权)人(译) | 罗门哈斯电子材料KOREA LTD. | | |
| [标]发明人 | MOON DOO HYEON<br>AHN HEE CHOON<br>KU JONG SEOK<br>KIM NAM KYUN<br>CHO YOUNG JUN<br>KWON HYUCK JOO<br>LEE KYUNG JOO<br>KIM BONG OK | | |
| 发明人 | MOON, DOO-HYEON<br>AHN, HEE-CHOON<br>KU, JONG-SEOK<br>KIM, NAM-KYUN<br>CHO, YOUNG-JUN<br>KWON, HYUCK-JOO<br>LEE, KYUNG-JOO<br>KIM, BONG-OK | | |
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| 代理机构(译) | 霍顿MARK PHILLIP | | |
| 优先权 | 1020120063068 2012-06-13 KR | | |
| 外部链接 | Espacenet | | |


摘要(译)

本发明涉及新型有机电致发光化合物和包含该化合物的有机电致发光器件。根据本发明的有机电致发光化合物具有高发光效率和长寿命，因此通过使用根据本发明的有机电致发光化合物可以制备具有长使用寿命的有机电致发光器件。