(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
2 July 2015 (02.07.2015)

WIPO | PCT

(10) International Publication Number
WO 2015/099484 A1

(51) **International Patent Classification**:
C07D 209/86 (2006.01) ***C07D 409/14*** (2006.01)
C07D 403/02 (2006.01) ***H01L 51/50*** (2006.01)
C07D 405/02 (2006.01) ***C09K 11/06*** (2006.01)
C07D 405/14 (2006.01) ***H05B 33/14*** (2006.01)
C07D 409/02 (2006.01)

(21) **International Application Number**:
PCT/KR2014/012891

(22) **International Filing Date**:
26 December 2014 (26.12.2014)

(25) **Filing Language**: English

(26) **Publication Language**: English

(30) **Priority Data**:
10-2013-0165425
27 December 2013 (27.12.2013) KR

(71) **Applicant**: **ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.** [KR/KR]; 56, 3gongdan 1-ro, Seobuk-gu, Cheonan-si, Chungcheongnam-do 331-980 (KR).

(72) **Inventors**: **JUN, Ji-Song**; 97, Deogyeong-daero 1483beon-gil, Yeongtong-gu, Suwon-si, Gyeonggi-do 443-390 (KR). **MOON, Doo-Hyeon**; 906-1304, 117, Byeongjeom 3-ro, Hwaseong-si, Gyeonggi-do 445-768 (KR). **AHN, Hee-Choon**; 62, Yeongtong-ro 174beon-gil, Yeongtong-gu, Suwon-si, Gyeonggi-do 443-400 (KR). **LEE, Kyung-Joo**; 210-1001, 72, Saechang-ro 8-gil, Mapo-gu, Seoul 121-773 (KR). **LEE, Tae-Jin**; 10-1, Seongnam-daero 1148beon-gil, Jungwon-gu, Seongnam-si, Gyeonggi-do 462-827 (KR). **KIM, Chi-Sik**; 441-1201, 71, Dongtanbanseok-ro, Hwaseong-si, Gyeonggi-do 445-752 (KR). **CHO, Young-Jun**; 204-701, 393, Pangyo-ro, Bundang-gu, Seongnam-si, Gyeonggi-do 463-400 (KR).

(74) **Agent**: **CHANG, Hoon**; Central Intellectual Property & Law, Korean Re Bldg. 5F, 68, Jong-ro 5-gil, Jongno-gu, Seoul 110-733 (KR).

(81) **Designated States** *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JP, KE, KG, KN, KP, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) **Designated States** *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

Published:

— *with international search report (Art. 21(3))*

WO 2015/099484 A1

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

(57) **Abstract**: The present invention relates to a novel organic electroluminescent compound and an organic electroluminescent device comprising the same. By using the organic electroluminescent compound according to the present invention, an organic electroluminescent device can have a long lifespan and an improvement in current and power efficiencies.

Description

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

Technical Field

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

Background Art

[2] An electroluminescent device (EL device) is a self-light-emitting device which has advantages in that it provides a wider viewing angle, a greater contrast ratio, and a faster response time. An organic EL device was first developed by Eastman Kodak, by using small aromatic diamine molecules, and aluminum complexes as materials for forming a light-emitting layer [Appl. Phys. Lett. 51, 913, 1987].

[3] The most important factor determining luminous 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, since phosphorescent materials theoretically enhance luminous efficiency by four (4) times compared to fluorescent materials, development of phosphorescent light-emitting materials are widely being researched. Iridium(III) complexes have been widely known as phosphorescent materials, including bis(2-(2'-benzothienyl)-pyridinato-N,C3')iridium(acetylacetonate) ((acac)Ir(btp)$_2$), tris(2-phenylpyridine)iridium (Ir(ppy)$_3$) and bis(4,6-difluorophenylpyridinato-N,C2)picolinate iridium (Firpic) as red, green and blue materials, respectively.

[4] At present, 4,4'-N,N'-dicarbazol-biphenyl (CBP) is the most widely known phosphorescent host materials. Recently, Pioneer (Japan) et al. developed a high performance organic EL device using bathocuproine (BCP) and aluminum(III)bis(2-methyl-8-quinolinate)(4-phenylphenolate) (BAlq) etc. as host materials, which were known as hole blocking layer materials.

[5] Though these materials provide good light-emitting characteristics, they have the following disadvantages: (1) Due to their low glass transition temperature and poor thermal stability, their degradation may occur during a high-temperature deposition process in a vacuum, and the lifespan of the device decreases. (2) The power efficiency of an organic EL device is given by [(π/voltage) × current efficiency], and the power efficiency is inversely proportional to the voltage. Although an organic EL device comprising phosphorescent host materials provides higher current efficiency (cd/A)

than one comprising fluorescent materials, a significantly high driving voltage is necessary. Thus, there is no merit in terms of power efficiency (lm/W). (3) Further, the operational lifespan of an organic EL device is short and luminous efficiency is still required to be improved.

[6] Meanwhile, in order to enhance its efficiency and stability, an organic EL device has a structure of a multilayer comprising a hole injection layer, a hole transport layer, a light-emitting layer, an electron transport layer, and an electron injection layer. The selection of a compound comprised in the hole transport layer is known as a method for improving the characteristics of a device such as hole transport efficiency to the light-emitting layer, luminous efficiency, lifespan, etc.

[7] In this regard, copper phthalocyanine (CuPc), 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (NPB), N,N'-diphenyl-N,N'-bis(3-methylphenyl)-(1,1'-biphenyl)-4,4'-diamine (TPD), 4,4',4"-tris(3-methylphenylphenylamino)triphenylamine (MTDATA), etc. were used as a hole injection and transport material. However, an organic EL device using these materials is problematic in quantum efficiency and operational lifespan. It is because, when an organic EL device is driven under high current, thermal stress occurs between an anode and the hole injection layer. Thermal stress significantly reduces the operational lifespan of the device. Further, since the organic material used in the hole injection layer has very high hole mobility, the hole-electron charge balance may be broken and quantum yield (cd/A) may decrease. Therefore, a hole transport and injection layer for improving durability of an organic EL device still needs to be developed.

[8] Korean Patent Appln. Laying-Open No. 10-2012-025984 discloses a compound in which the 9-position of a fluorene is bonded to dibenzothiophene or dibenzofuran, as a hole injection material or a hole transport material. However, the above reference does not disclose a compound in which the 9-position of a fluorene is bonded to dibenzothiophene, dibenzofuran, or fluorene, and carbazole.

[9]

Disclosure of Invention

Technical Problem

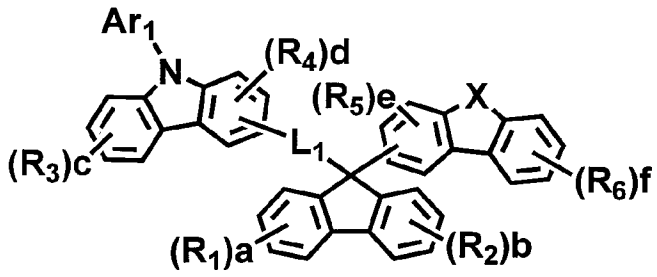
[10] The objective of the present invention is to provide i) an organic electroluminescent compound having high luminous efficiency, and ii) an organic electroluminescent device comprising the compound having long operational lifespan and improved power and current efficiencies.

Solution to Problem

[11] The present inventors found that the above objective can be achieved by an organic

electroluminescent compound represented by the following formula 1:

[12]



-------- (1)

[13] wherein

[14] Ar_1 represents a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent(s) to form a (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur;

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

[16] X represents -O-, -S-, or $-C(R_7)(R_8)-$;

[17] R_1 to R_6, each independently, represent hydrogen, deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, $-NR_9R_{10}$, $-SiR_{11}R_{12}R_{13}$, $-SR_{14}$, $-OR_{15}$, $-COR_{16}$, or $-B(OR_{17})(OR_{18})$; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;

[18] R_7 to R_{18}, each independently, represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C3-C30), mono- or polycyclic, alicyclic or aromatic ring;

[19] a, b, c, and f, each independently, represent an integer of 0 to 4; where a, b, c, or f represents an integer of 2 or more, each of R_1, R_2, R_3, or R_6 may be the same or different;

[20] d and e, each independently, represent an integer of 0 to 3; where d or e represents an integer of 2 or more, each of R_4 or R_5 may be the same or different; and

[21] the heterocycloalkyl and the heteroaryl(ene), each independently, contain at least one

hetero atom selected from B, N, O, S, P(=O), Si, and P.

[22]

Advantageous Effects of Invention

[23] By using the organic electroluminescent compound according to the present invention, it is possible to manufacture an organic electroluminescent device having excellent current and luminous efficiencies.

[24]

Mode for the Invention

[25] 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.

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

[27] The organic electroluminescent compound represented by the above formula 1 will be described in detail.

[28] Herein, "alkyl" includes methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl, tert-butyl, etc.; "alkenyl" includes vinyl, 1-propenyl, 2-propenyl, 1-butenyl, 2-butenyl, 3-butenyl, 2-methylbut-2-enyl, etc.; "alkynyl" includes ethynyl, 1-propynyl, 2-propynyl, 1-butynyl, 2-butynyl, 3-butynyl, 1-methylpent-2-ynyl, etc.; "cycloalkyl" includes cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, etc.; "(3- to 7-membered)heterocycloalkyl" is a cycloalkyl having 3 to 7 ring backbone atoms including at least one heteroatom selected from B, N, O, S, P(=O), Si, and P, preferably O, S, and N, and includes tetrahydrofuran, pyrrolidine, thiolan, tetrahydropyran, etc.; "aryl(ene)" is a monocyclic or fused ring derived from an aromatic hydrocarbon, and includes phenyl, biphenyl, terphenyl, naphthyl, binaphthyl, phenylnaphthyl, naphthylphenyl, fluorenyl, phenylfluorenyl, benzofluorenyl, dibenzofluorenyl, phenanthrenyl, phenylphenanthrenyl, anthracenyl, indenyl, triphenylenyl, pyrenyl, tetracenyl, perylenyl, chrysenyl, naphthacenyl, fluoranthenyl, etc.; "(3- to 30-membered)heteroaryl(ene)" is an aryl having 3 to 30 ring backbone atoms including at least one, preferably 1 to 4 heteroatom selected from the group consisting of B, N, O, S, P(=O), Si, and P; is a monocyclic ring, or a fused ring condensed with at least one benzene ring; may be partially saturated; may be one formed by linking at least one heteroaryl or aryl group to a heteroaryl group via a single bond(s); and includes a monocyclic ring-type heteroaryl including furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, bipyridyl, pyrazinyl,

pyrimidyl, pyridazinyl, etc., and a fused ring-type heteroaryl including benzofuranyl, benzothiophenyl, isobenzofuranyl, dibenzofuranyl, dibenzothiophenyl, naphthofuranyl, naphthothiophenyl, benzonaphthofuranyl, benzonaphthothiophenyl, benzimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indolinyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenoxazinyl, phenanthridinyl, benzodioxolyl, indolocarbazolyl, etc. Further, "halogen" includes F, Cl, Br, and I.

[29] Herein, "substituted" in the expression "substituted or unsubstituted" means that a hydrogen atom in a certain functional group is replaced with another atom or group, i.e., a substituent. The substituents of the substituted (C1-C30)alkyl, the substituted (C2-C30)alkenyl, the substituted (C2-C30)alkynyl, the substituted (C1-C30)alkoxy, the substituted (C3-C30)cycloalkyl, the substituted (C3-C30)cycloalkenyl, the substituted (3- to 7- membered)heterocycloalkyl, the substituted (C6-C30)aryl(ene), the substituted (3- to 30- membered)heteroaryl(ene), and the substituted (C3-C30), mono- or polycyclic, alicyclic or aromatic ring in Ar_1, L_1, and R_1 to R_{18} each independently are at least one selected from the group consisting of deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a (C1-C30)alkyl, a halo(C1-C30)alkyl, a (C2-C30)alkenyl, a (C2-C30)alkynyl, a (C1-C30)alkoxy, a (C1-C30)alkylthio, a (C3-C30)cycloalkyl, a (C3-C30)cycloalkenyl, a (3- to 7-membered)heterocycloalkyl, a (C6-C30)aryloxy, a (C6-C30)arylthio, a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl, a (C6-C30)aryl unsubstituted or substituted with a (3- to 30-membered)heteroaryl, a tri(C1-C30)alkylsilyl, a tri(C6-C30)arylsilyl, a di(C1-C30)alkyl(C6-C30)arylsilyl, a (C1-C30)alkyldi(C6-C30)arylsilyl, an amino, a mono- or di- (C1-C30)alkylamino, a mono- or di- (C6-C30)arylamino, a (C1-C30)alkyl(C6-C30)arylamino, a (C1-C30)alkylcarbonyl, a (C1-C30)alkoxycarbonyl, a (C6-C30)arylcarbonyl, a di(C6-C30)arylboronyl, a di(C1-C30)alkylboronyl, a (C1-C30)alkyl(C6-C30)arylboronyl, a (C6-C30)aryl(C1-C30)alkyl, and a (C1-C30)alkyl(C6-C30)aryl, and preferably each independently are at least one selected from the group consisting of a (C1-C30)alkyl and a (C6-C21)aryl.

[30] In formula 1 above, Ar_1 preferably represents a substituted or unsubstituted (C1-C20)alkyl, or a substituted or unsubstituted (C6-C21)aryl; more preferably represents a substituted or unsubstituted (C6-C18)aryl; and even more preferably represents a (C6-C18)aryl unsubstituted or substituted with a (C6-C18)aryl. Specifically, Ar_1 may represent phenyl, naphthyl, phenanthrenyl, or biphenyl, each may be substituted with phenyl or naphthyl; and more specifically, phenyl, naphthyl-substituted phenyl, naphthyl, phenyl-substituted naphthyl, phenanthrenyl, or biphenyl.

[31] L_1 preferably represents a single bond, a substituted or unsubstituted

(C6-C21)arylene, or a substituted or unsubstituted (3- to 21-membered)heteroarylene. Specifically, L_1 may represent a single bond.

[32] X preferably represents -O-, -S-, or -C(R_7)(R_8)-, wherein R_7 and R_8, each independently, may represent a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl; and more preferably, X represents -O-, -S-, or -C(R_7)(R_8)-, wherein R_7 and R_8, each independently, may represent an unsubstituted (C1-C10)alkyl, or an unsubstituted (C6-C18)aryl. Specifically, X may represent -O-, -S-, -C(CH_3)(CH_3)-, or -C(C_6H_5)(C_6H_5)-.

[33] R_1 to R_6, each independently, preferably represent hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, a substituted or unsubstituted (5- to 21-membered)heteroaryl, or a di(C6-C21)arylamino; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C5-C21), mono- or polycyclic aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur. More preferably, R_4 and R_5, each independently, represent a substituted or unsubstituted (C1-C10)alkyl; and R_1, R_2, R_3, and R_6, each independently, represent an unsubstituted (C6-C18)aryl, or a (6- to 18-membered)heteroaryl unsubstituted or substituted with a (C6-C12)aryl; or may be linked to an adjacent substituent(s) to form a (C6-C18), mono- or polycyclic aromatic ring unsubstituted or substituted with a (C6-C12)aryl, whose carbon atom may be replaced with one (1) nitrogen. Specifically, R_1, R_2, R_3, and R_6, each independently, may represent phenyl, or phenyl-substituted carbazole; or may be linked to an adjacent substituent(s) to form a phenyl- or naphthyl-substituted indole ring.

[34] a, b, c, d, e, and f, each independently, preferably represent an integer of 0 to 2; more preferably, a, b, c, and f, each independently, represent an integer of 0 to 2, and e and d, each independently, represent an integer of 0 or 1; and even more preferably, a, b, c, and f, each independently, represent an integer of 0 or 1, and e and d, each independently, represent 0. Specifically, a, b, d, e, and f may represent 0, and c may represent an integer of 0 or 1.

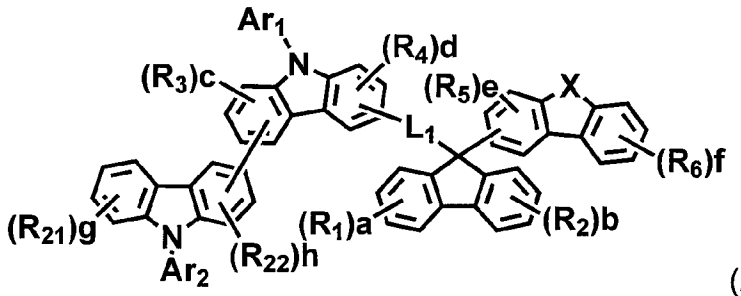
[35] According to one embodiment of the present invention, in formula 1 above, Ar_1 represents a substituted or unsubstituted (C1-C20)alkyl, or a substituted or unsubstituted (C6-C21)aryl; L_1 represents a single bond, a substituted or unsubstituted (C6-C21)arylene, or a substituted or unsubstituted (3- to 21-membered)heteroarylene; X represents -O-, -S-, or -C(R_7)(R_8)-, wherein R_7 and R_8, each independently, represent a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl; R_1 to R_6, each independently, represent hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, a substituted or unsub-

stituted (5- to 21-membered)heteroaryl, or a di(C6-C21)arylamino; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C5-C21), mono- or polycyclic aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur; a, b, c, d, e, and f, each independently, represent an integer of 0 to 2; where a, b, c, d, e, or f represents 2, each of R_1, R_2, R_3, R_4, R_5, or R_6 may be the same or different; and the heteroaryl(ene) contains at least one hetero atom selected from N, O, and S.

[36] According to another embodiment of the present invention, in formula 1 above, Ar_1 represents a substituted or unsubstituted (C6-C18)aryl; L_1 represents a single bond; X represents -O-, -S-, or $-C(R_7)(R_8)-$, wherein R_7 and R_8, each independently, represent a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl; R_1 to R_6, each independently, represent an unsubstituted (C6-C18)aryl, or a (6- to 18-membered)heteroaryl unsubstituted or substituted with a (C6-C12)aryl; or may be linked to an adjacent substituent(s) to form a (C6-C18), mono- or polycyclic aromatic ring unsubstituted or substituted with a (C6-C12)aryl, whose carbon atom may be replaced with one (1) nitrogen; a, b, c, and f, each independently, represent an integer of 0 to 2; e and d, each independently, represent an integer of 0 or 1; where a, b, c, or f represents 2, each of R_1, R_2, R_3, or R_6 may be the same or different; and the heteroaryl contains one or two hetero atom(s) selected from N, O, and S.

[37] According to another embodiment of the present invention, the compound of formula 1 can be represented by the following formula 2:

[38]



(2)

[39] wherein Ar_1, L_1, X, R_1 to R_6, a, b, d, e, and f are as defined in formula 1.

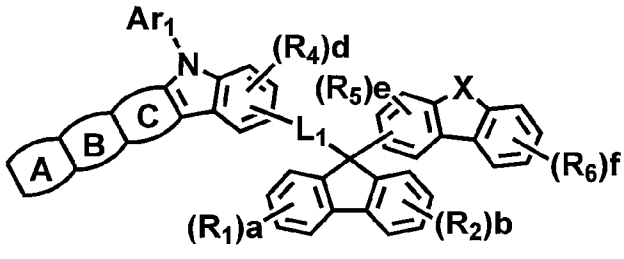
[40] In formula 2 above, Ar_2 represents a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent(s) to form a (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur. Ar_2 preferably represents a substituted or unsubstituted (C1-C20)alkyl, or a substituted or unsubstituted (C6-C21)aryl; more preferably represents a (C6-C18)aryl unsubstituted or substituted with a (C1-C10)alkyl; and even more preferably represents an unsubstituted (C6-C12)aryl. Specifically, Ar_2 may

represent phenyl or naphthyl.

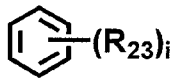
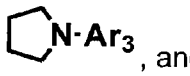
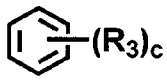
[41] In formula 2 above, R_{21} and R_{22}, each independently, represent hydrogen, deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, $-NR_9R_{10}$, $-SiR_{11}R_{12}R_{13}$, $-SR_{14}$, $-OR_{15}$, $-COR_{16}$, or $-B(OR_{17})(OR_{18})$; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur; and R_9 to R_{18}, each independently, represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl. R_{21} and R_{22}, each independently, preferably represent hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C5-C21), mono- or polycyclic, aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur; and more preferably represent a (C1-C10)alkyl unsubstituted or substituted with a (C6-C12)aryl, an unsubstituted (C6-C18)aryl, or a (6- to 18-membered)heteroaryl unsubstituted or substituted with a (C6-C12)aryl; or may be linked to an adjacent substituent(s) to form a (C6-C18), mono- or polycyclic, aromatic ring unsubstituted or substituted with a (C6-C12)aryl whose carbon atom(s) may be replaced with one (1) nitrogen.

[42] In formula 2 above, g represents an integer of 0 to 4; c and h, each independently, represent an integer of 0 to 3; where c, g, or h represents an integer of 2 or more, each of R_3, R_{21}, or R_{22} may be the same or different. Preferably, g represents an integer of 0 to 2, and c and h, each independently, represent 0 or 1. Specifically, c, g, and h may represent 0.

[43] According to another embodiment of the present invention, the compound of formula 1 can be represented by the following formula 3:

[44] 

(3)

[45] wherein L_1, X, Ar_1, R_1, R_2, R_4 to R_6, a, b, d, e, and f are as defined in formula 1; A represents  , B represents  , and C represents  .

[46] In formula 3 above, Ar_3 represents a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent(s) to form a (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur. Ar_3 preferably represents a substituted or unsubstituted (C1-C20)alkyl, or a substituted or unsubstituted (C6-C21)aryl; more preferably represents a (C6-C18)aryl unsubstituted or substituted with a (C1-C10)alkyl; and even more preferably represents an unsubstituted (C6-C12)aryl. Specifically, Ar_3 may represent phenyl or naphthyl.

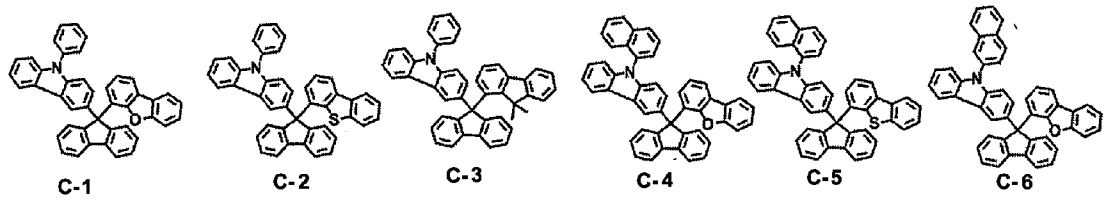
[47] In formula 3 above, R_{23} represents hydrogen, deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, $-NR_9R_{10}$, $-SiR_{11}R_{12}R_{13}$, $-SR_{14}$, $-OR_{15}$, $-COR_{16}$, or $-B(OR_{17})(OR_{18})$; and R_9 to R_{18}, each independently, represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl. R_{23} preferably represents hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl; and more preferably represent a (C1-C10)alkyl unsubstituted or substituted with a (C6-C12)aryl, an unsubstituted (C6-C18)aryl, or a (6- to 18-membered)heteroaryl unsubstituted or substituted with a (C6-C12)aryl.

[48] In formula 3 above, i represents an integer of 0 to 4; c represents an integer of 0 to 2; where c or i represents an integer of 2 or more, each of R_3 or R_{23} may be the same or

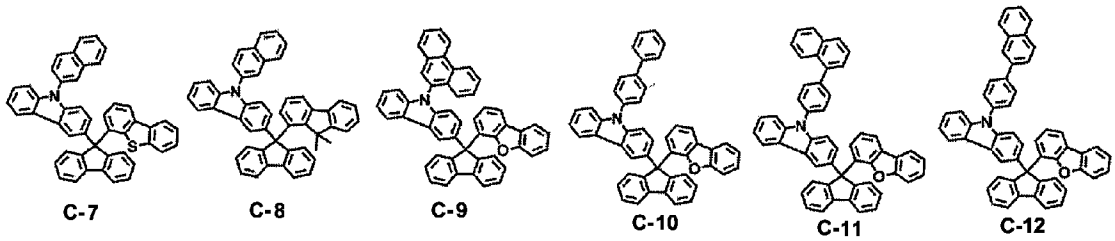
different. Preferably, i represents an integer of 0 to 2, and c represents 0 or 1. Specifically, i represents 0 or 1, and c represents 0.

[49] The specific compounds of the present invention include the following compounds, but are not limited thereto:

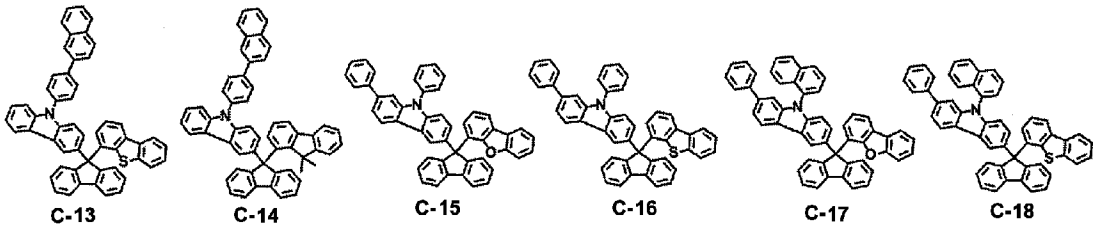
[50]



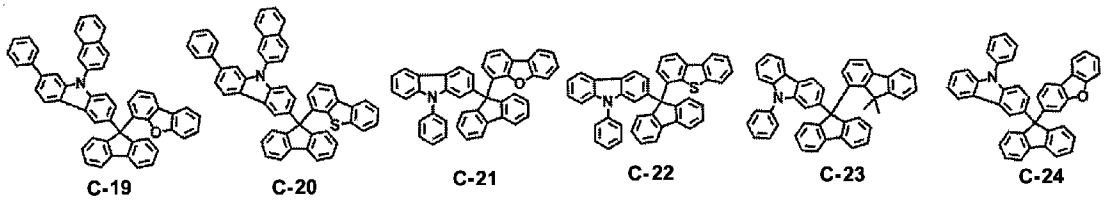
[51]



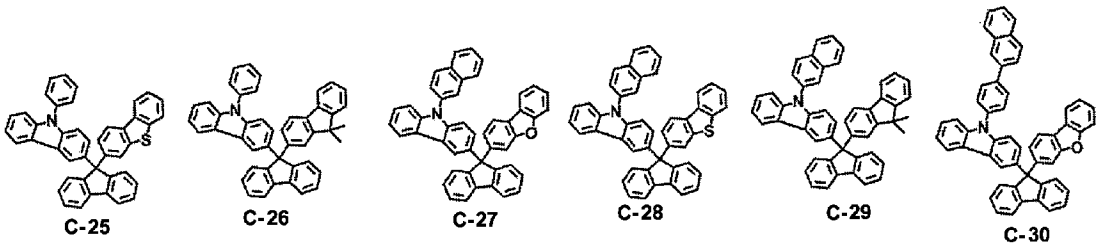
[52]



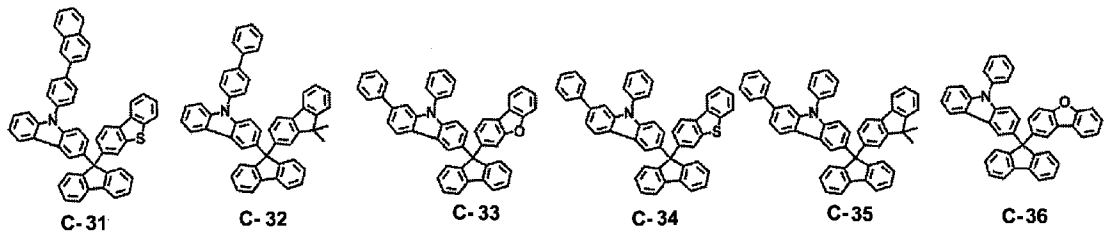
[53]



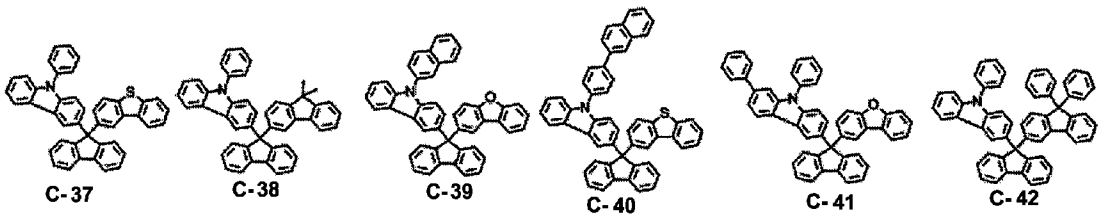
[54]



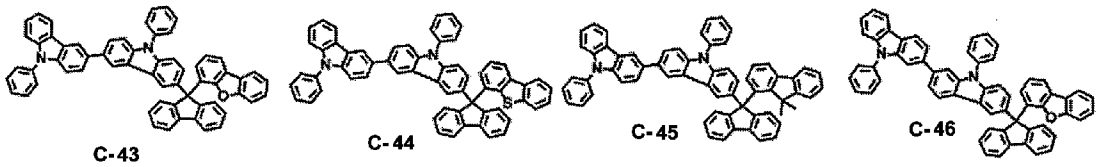
[55]



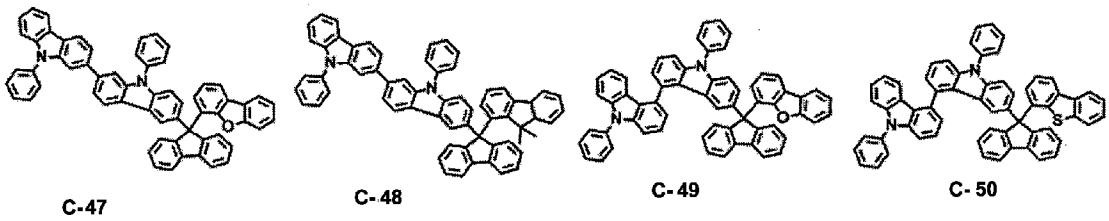
[56]



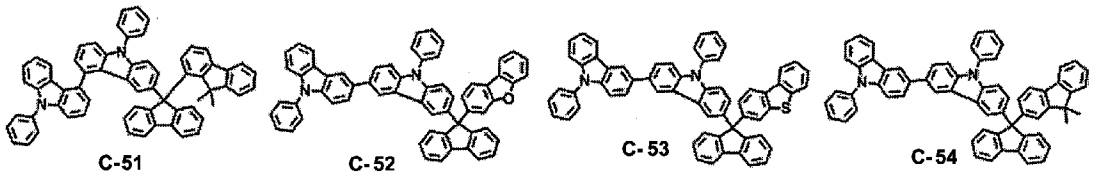
[57]



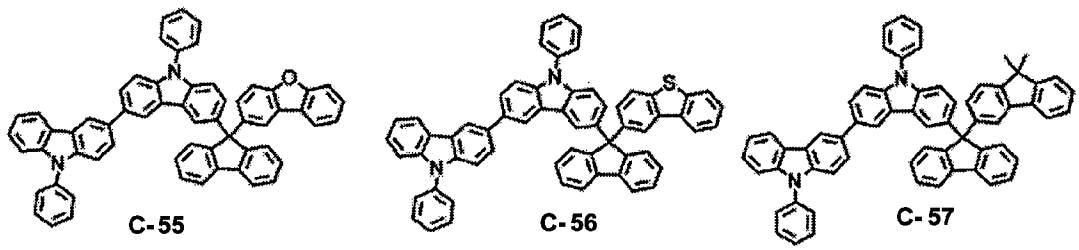
[58]



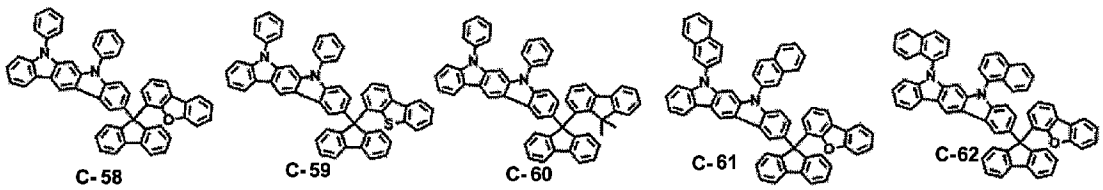
[59]



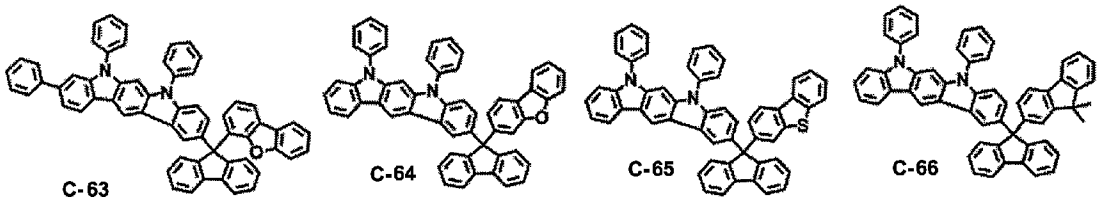
[60]



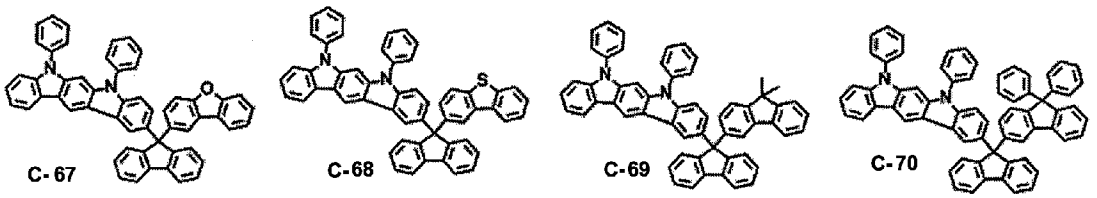
[61]



[62]



[63]



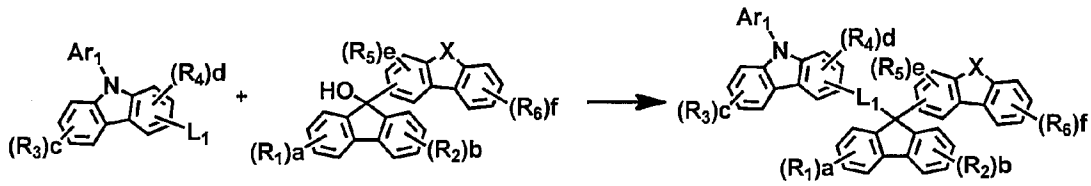
[64] The organic electroluminescent compound of the present invention preferably has a molecular weight of 1000 or less, more preferably 950 or less, more preferably 925 or less, and even more preferably 900 or less. By having the molecular weight as above, thermal decomposition of the compound during deposition by sublimation can be decreased or removed.

[65] In addition, the organic electroluminescent compound of the present invention preferably has a glass transition temperature of 90°C or more, and more preferably 110°C or more. By having the glass transition temperature as above, the compound can have excellent thermal stability.

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

[67] [Reaction Scheme 1]

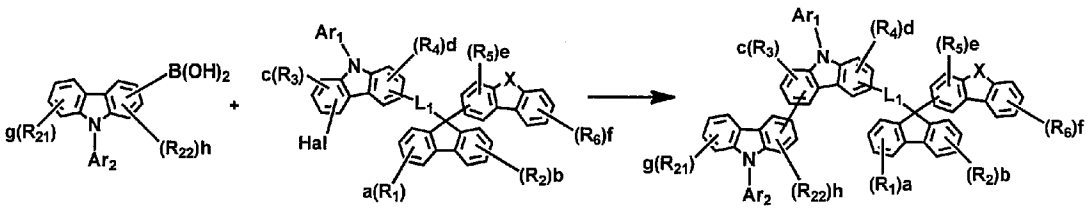
[68]



[69] wherein R_1 to R_6, X, Ar_1, L_1, and a to f are as defined in formula 1 above.

[70] [Reaction Scheme 2]

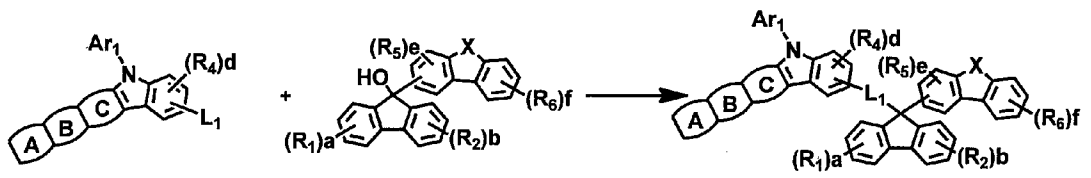
[71]



[72] wherein R_1 to R_6, R_{21}, R_{22}, X, Ar_1, Ar_2, L_1, and a to h are as defined in formula 2 above, and Hal represents a halogen.

[73] [Reaction Scheme 3]

[74]



[75] wherein A, B, C, R_1, R_2, R_4 to R_6, X, Ar_1, L_1, a, b, and d to f are as defined in formula 3 above.

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

[77] The above 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.

[78] The organic electroluminescent device comprises a first electrode; a second electrode; and at least one organic layer between the first and second electrodes. The organic layer may comprise at least one organic electroluminescent compound of formula 1.

[79] One of the first and second electrodes can be an anode, and the other can be a cathode. The organic layer comprises a light-emitting layer, and may further comprise at least one layer selected from the group consisting of a hole injection layer, a hole transport layer, an electron transport layer, an electron injection layer, an interlayer, a hole blocking layer, and an electron blocking layer.

[80] The organic electroluminescent compound according to the present invention can be comprised in at least one of the light-emitting layer and the hole transport layer. Where used in the hole transport layer, the organic electroluminescent compound of the present invention can be comprised as a hole transport material. Where used in the light-emitting layer, the organic electroluminescent compound of the present invention can be comprised as a host material.

[81] The organic electroluminescent device comprising the organic electroluminescent compound of the present invention can further comprise one or more compounds other than the organic electroluminescent compound according to the present invention as host materials, and can further comprise one or more dopants.

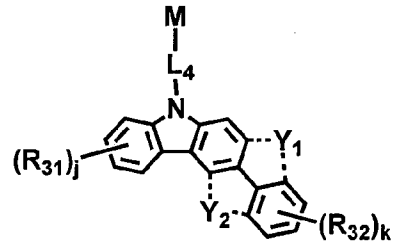
[82] Where the organic electroluminescent compound according to the present invention is comprised as a host material (first host material), the other compound may be comprised as a second host material. Herein, the weight ratio of the first host material to the second host material is in the range of 1:99 to 99:1.

[83] The host material other than the organic electroluminescent compound according to the present invention can be from any of the known fluorescent or phosphorescent hosts, preferably phosphorescent hosts in terms of luminous efficiency. Specifically, the phosphorescent host selected from the group consisting of the compounds of formulae 11 to 13 below is preferable in terms of luminous efficiency.

[84] $H\text{-}(Cz\text{-}L_4)_m\text{-}M$ ---------- (11)

[85] $H\text{-}(Cz)_n\text{-}L_4\text{-}M$ ---------- (12)

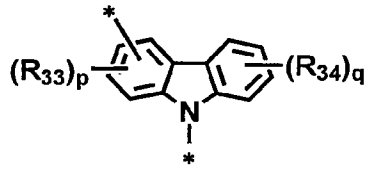
[86]



--------- (13)

[87] wherein Cz represents the following structure;

[88]



[89] R_{31} to R_{34} each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, a substituted of unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, or $-SiR_{35}R_{36}R_{37}$;

[90] R_{35} to R_{37} each independently represent a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl;

[91] L_4 represents a single bond, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (5- to 30-membered)heteroarylene;

[92] M represents a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl;

[93] Y_1 and Y_2 each independently represent -O-, -S-, $-N(R_{41})-$, or $-C(R_{42})(R_{43})-$, provided that Y_1 and Y_2 do not simultaneously exist;

[94] R_{41} to R_{43} each independently represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl, and R_{42} and R_{43} may be the same or different;

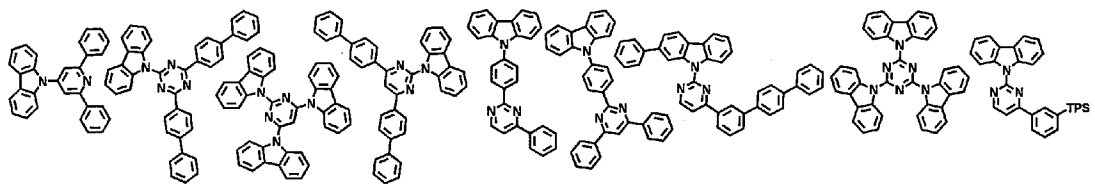
[95] m and n each independently represent an integer of 1 to 3;

[96] j, k, p, and q each independently represent an integer of 0 to 4; and

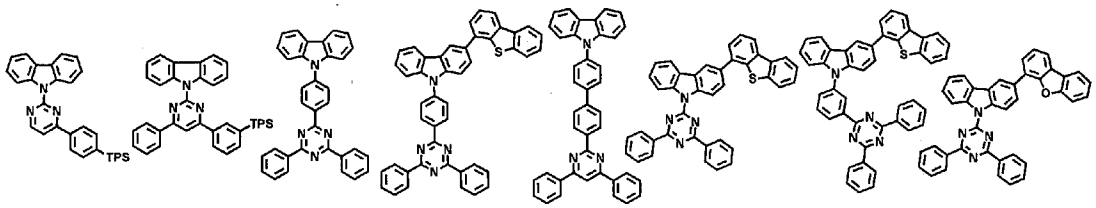
[97] where m, n, j, k, p or q is an integer of 2 or more, each of ($Cz-L_4$), each of (Cz), each of R_{31}, each of R_{32}, each of R_{33}, or each of R_{34} may be the same or different.

[98] Specifically, preferable examples of the host material are as follows:

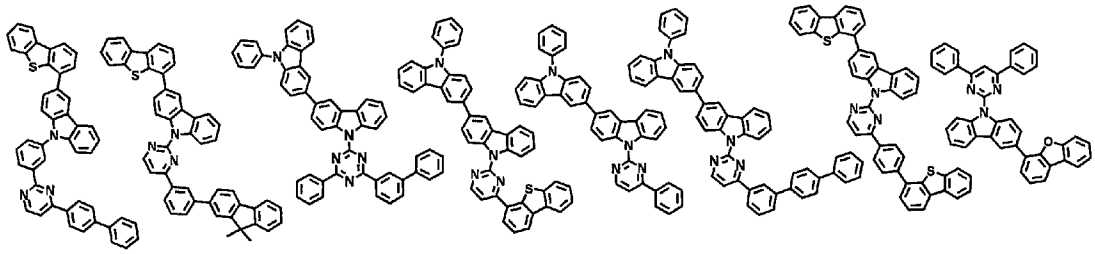
[99]



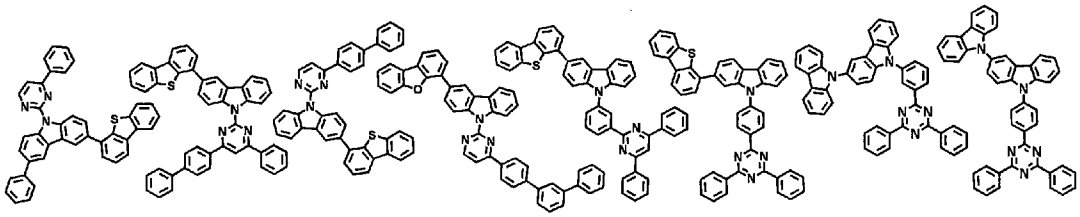
[100]



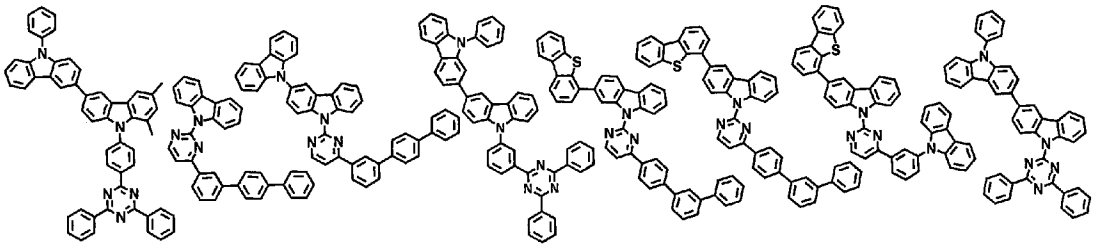
[101]



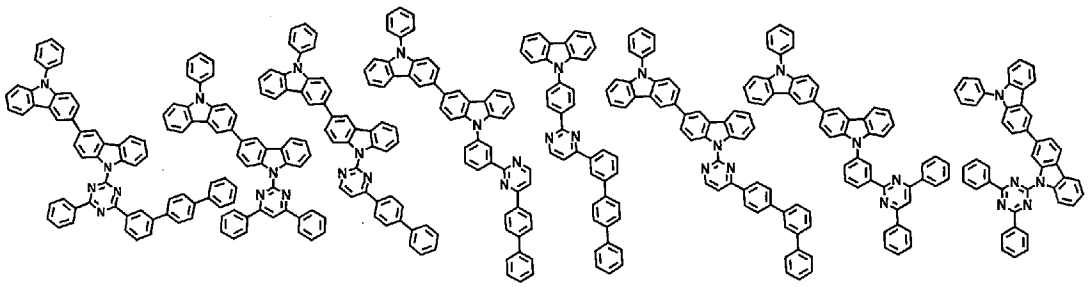
[102]



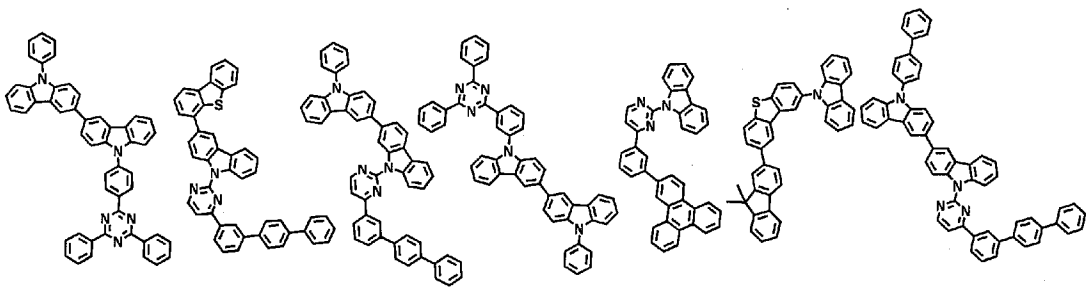
[103]



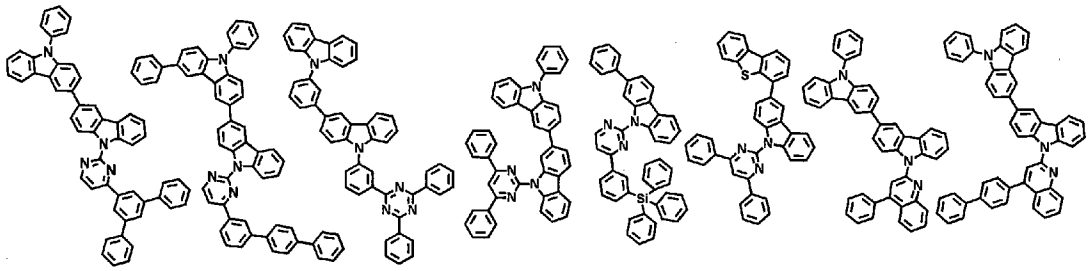
[104]



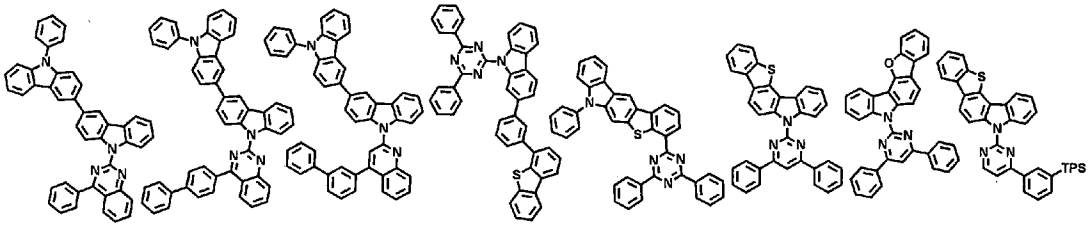
[105]



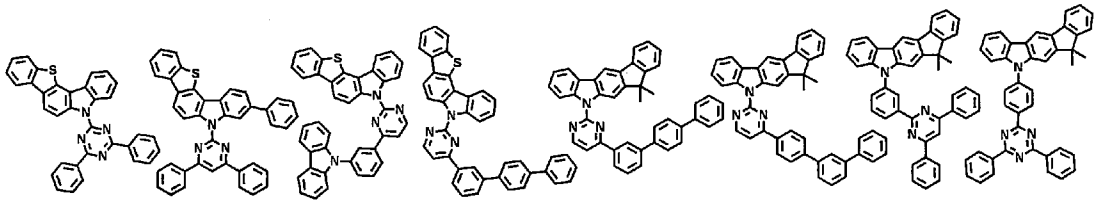
[106]



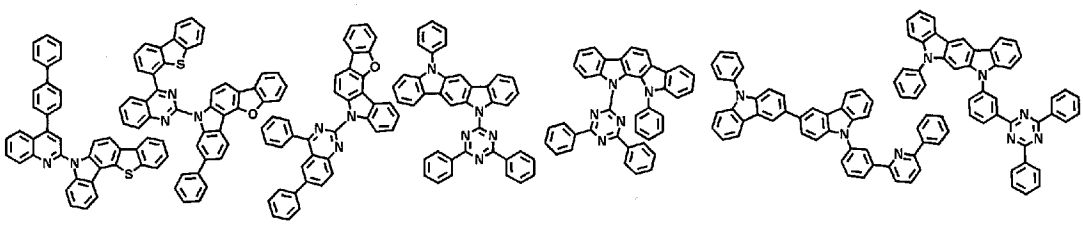
[107]



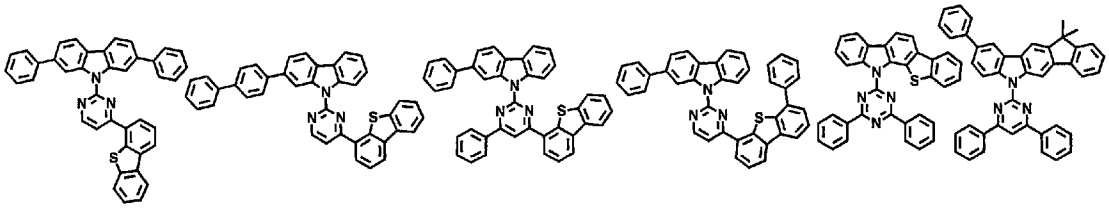
[108]



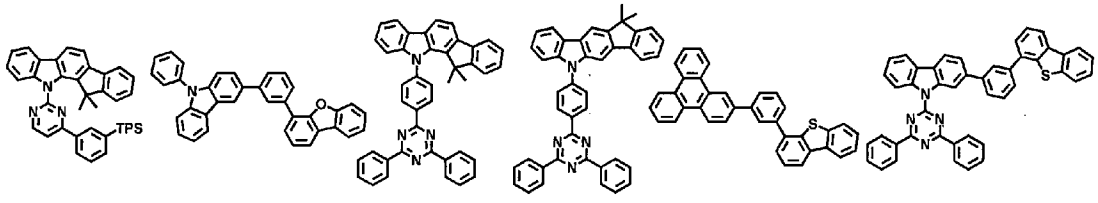
[109]



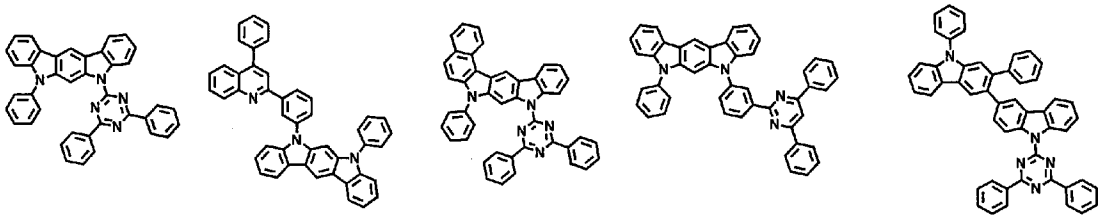
[110]



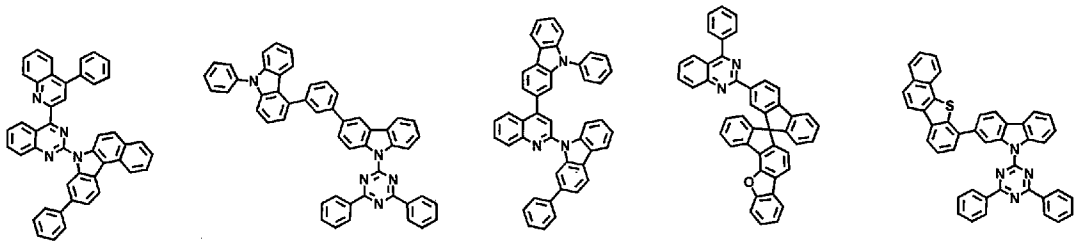
[111]



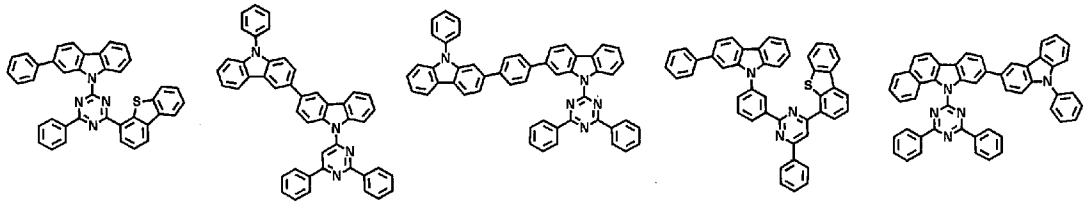
[112]



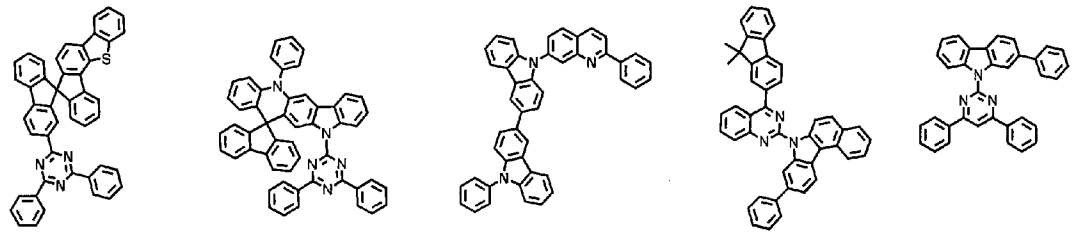
[113]



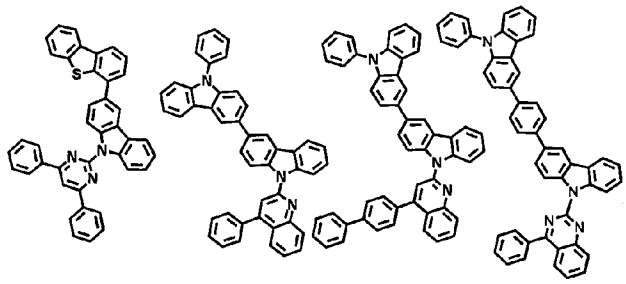
[114]



[115]



[116]

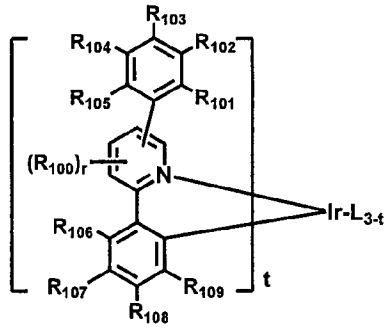


[117] [wherein TPS represents triphenylsilyl]

[118] The dopant comprised in the organic electroluminescent device according to the present invention is preferably at least one phosphorescent dopant. The dopant materials applied to the organic electroluminescent device according to the present invention are not limited, but may be preferably selected from metallated complex compounds of iridium, osmium, copper and platinum, more preferably selected from ortho-metallated complex compounds of iridium, osmium, copper and platinum, and even more preferably ortho-metallated iridium complex compounds.

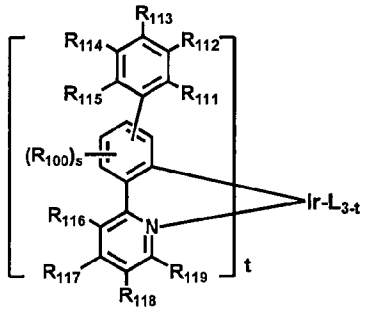
[119] The phosphorescent dopants may be preferably selected from compounds represented by the following formulae 101 to 103.

[120]



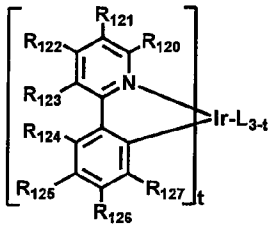
---------- (101)

[121]



---------- (102)

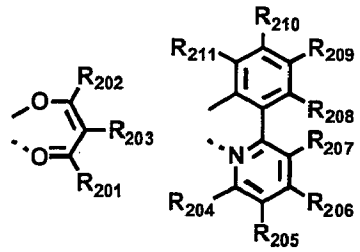
[122]



---------- (103)

[123] wherein L is selected from the following structures:

[124]



[125] R_{100} represents hydrogen, a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C3-C30)cycloalkyl;

[126] R_{101} to R_{109}, and R_{111} to R_{123} each independently represent hydrogen; deuterium; a halogen; a (C1-C30)alkyl unsubstituted or substituted with a halogen(s); a cyano; a substituted or unsubstituted (C1-C30)alkoxy; a substituted or unsubstituted (C6-C30)aryl; or a substituted or unsubstituted (C3-C30)cycloalkyl; R_{106} to R_{109} may be linked to an adjacent substituent(s) to form a substituted or unsubstituted fused ring, e.g. fluorene unsubstituted or substituted with alkyl, dibenzothiophene unsubstituted or substituted with alkyl, or dibenzofuran unsubstituted or substituted with alkyl; and R_{120}

to R_{123} may be linked to an adjacent substituent(s) to form a substituted or unsubstituted fused ring, e.g. quinoline unsubstituted or substituted with a halogen, alkyl, or aryl;

[127] R_{124} to R_{127} each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; and R_{124} to R_{127} may be linked to an adjacent substituent(s) to form a substituted or unsubstituted fused ring, e.g. fluorene unsubstituted or substituted with alkyl, dibenzothiophene unsubstituted or substituted with alkyl, or dibenzofuran unsubstituted or substituted with alkyl;

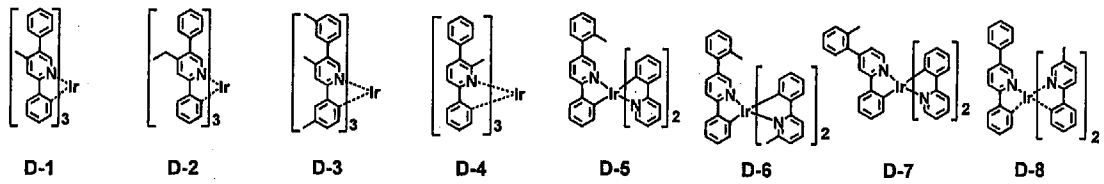
[128] R_{201} to R_{211} each independently represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl unsubstituted or substituted with a halogen(s), a substituted or unsubstituted (C3-C30)cycloalkyl, or a substituted or unsubstituted (C6-C30)aryl, and R_{208} to R_{211} may be linked to an adjacent substituent(s) to form a substituted or unsubstituted fused ring, e.g. fluorene unsubstituted or substituted with alkyl, dibenzothiophene unsubstituted or substituted with alkyl, or dibenzofuran unsubstituted or substituted with alkyl;

[129] r and s each independently represent an integer of 1 to 3; where r or s is an integer of 2 or more, each of R_{100} may be the same or different; and

[130] t represents an integer of 1 to 3.

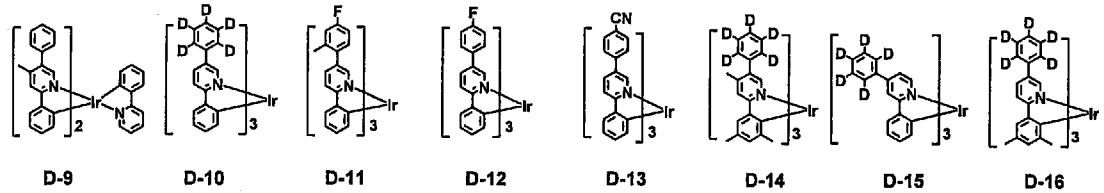
[131] Specifically, the phosphorescent dopant materials include the following:

[132]



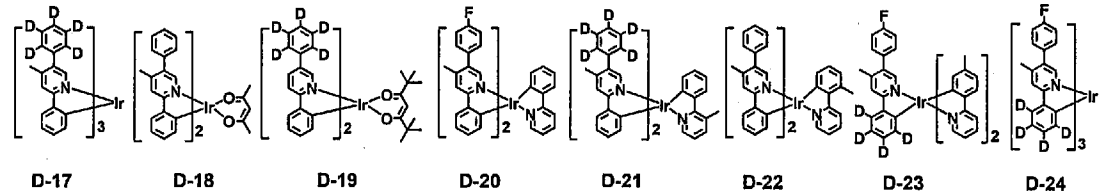
D-1 D-2 D-3 D-4 D-5 D-6 D-7 D-8

[133]



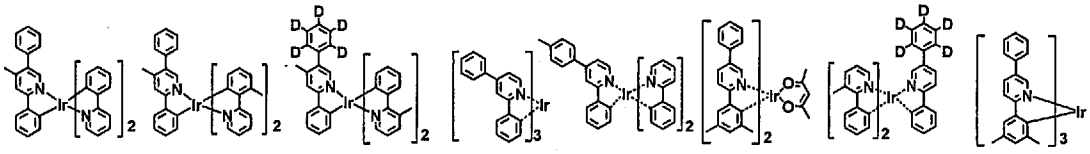
D-9 D-10 D-11 D-12 D-13 D-14 D-15 D-16

[134]



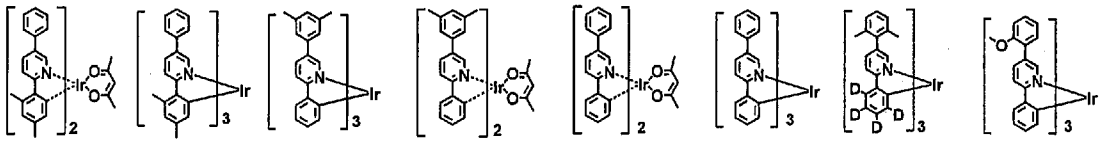
D-17 D-18 D-19 D-20 D-21 D-22 D-23 D-24

[135]



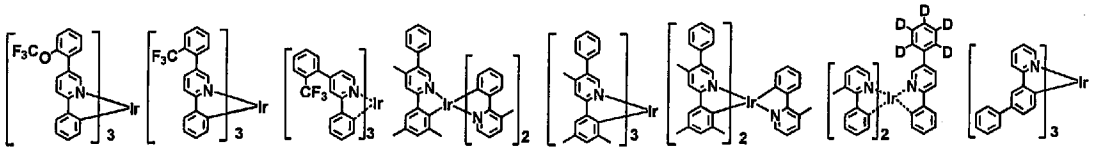
D-25 D-26 D-27 D-28 D-29 D-30 D-31 D-32

[136]



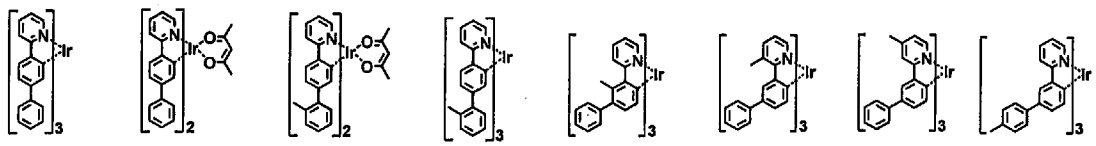
D-33 D-34 D-35 D-36 D-37 D-38 D-39 D-40

[137]



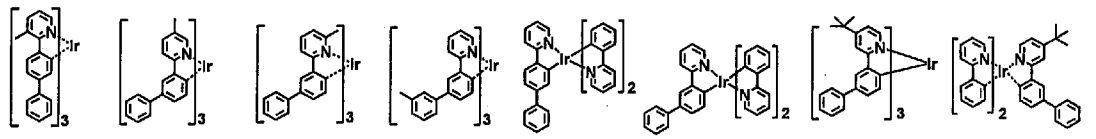
D-41 D-42 D-43 D-44 D-45 D-46 D-47 D-48

[138]



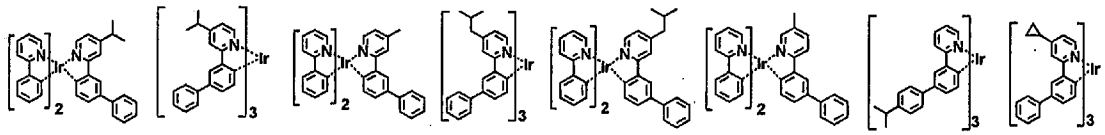
D-49 D-50 D-51 D-52 D-53 D-54 D-55 D-56

[139]



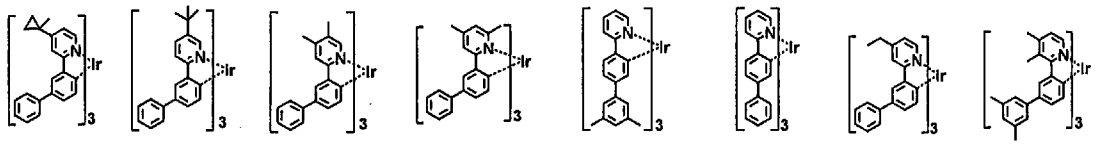
D-57 D-58 D-59 D-60 D-61 D-62 D-63 D-64

[140]



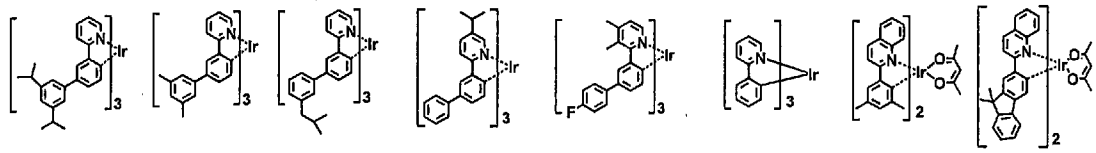
D-65 D-66 D-67 D-68 D-69 D-70 D-71 D-72

[141]



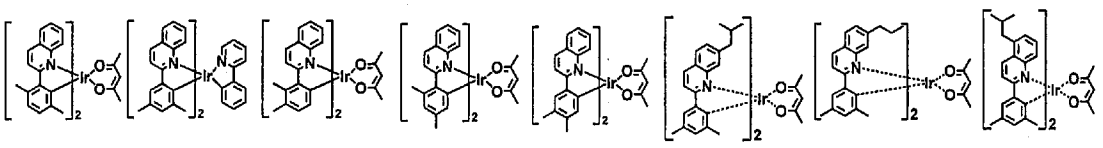
D-73 D-74 D-75 D-76 D-77 D-78 D-79 D-80

[142]



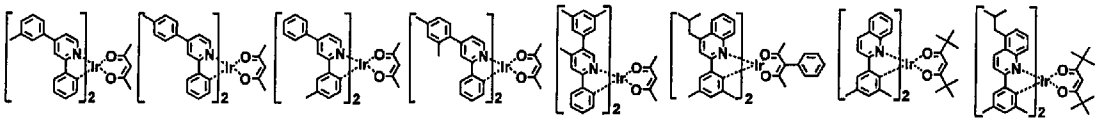
D-81 D-82 D-83 D-84 D-85 D-86 D-87 D-88

[143]



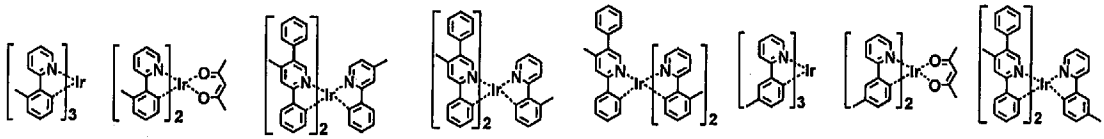
D-89 D-90 D-91 D-92 D-93 D-94 D-95 D-96

[144]



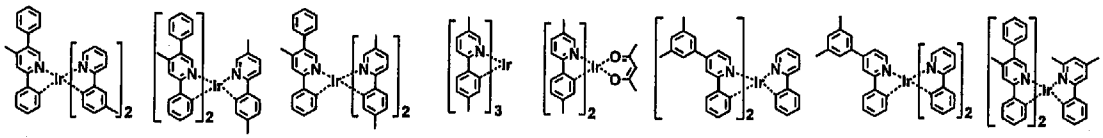
D-97 D-98 D-99 D-100 D-101 D-102 D-103 D-104

[145]



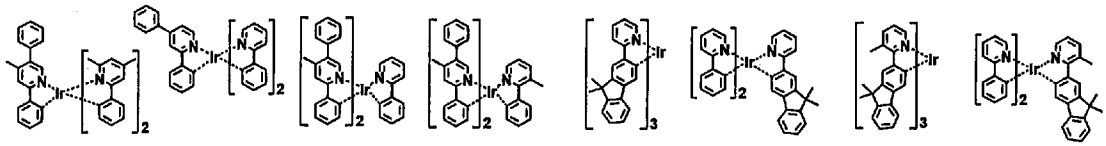
D-105 D-106 D-107 D-108 D-109 D-110 D-111 D-112

[146]



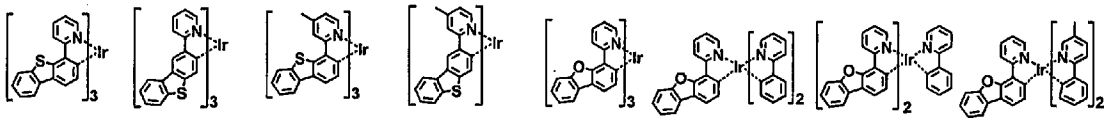
D-113 D-114 D-115 D-116 D-117 D-118 D-119 D-120

[147]



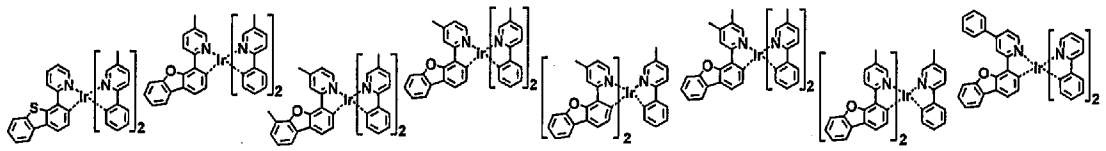
D-121 D-122 D-123 D-124 D-125 D-126 D-127 D-128

[148]



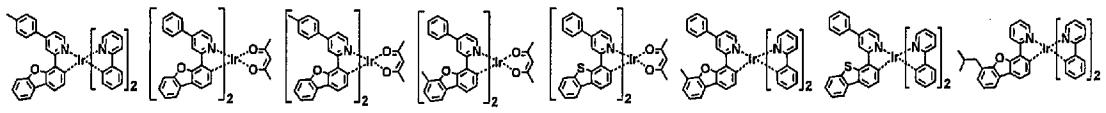
D-129 D-130 D-131 D-132 D-133 D-134 D-135 D-136

[149]



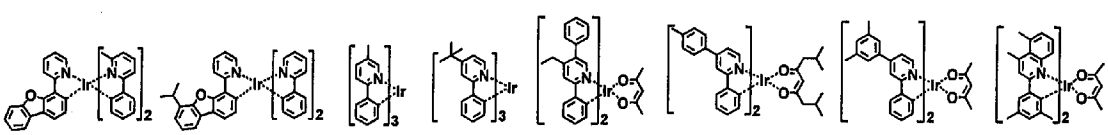
D-137 D-138 D-139 D-140 D-141 D-142 D-143 D-144

[150]



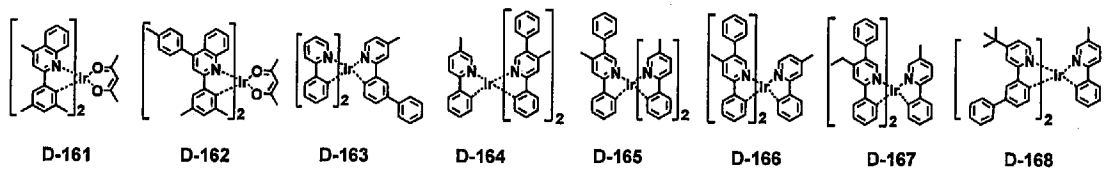
D-145 D-146 D-147 D-148 D-149 D-150 D-151 D-152

[151]



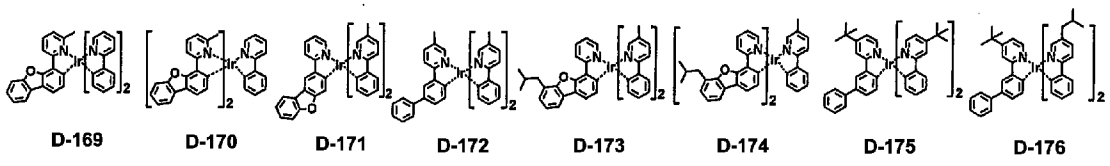
D-153 D-154 D-155 D-156 D-157 D-158 D-159 D-160

[152]



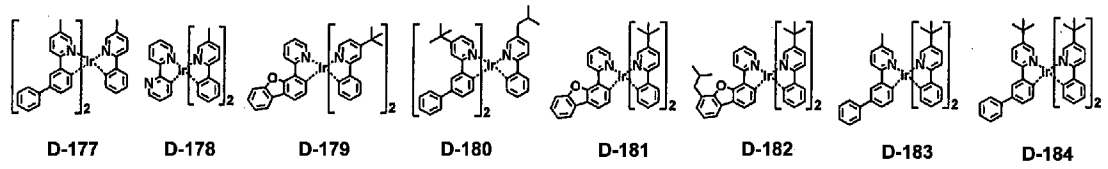
D-161 D-162 D-163 D-164 D-165 D-166 D-167 D-168

[153]



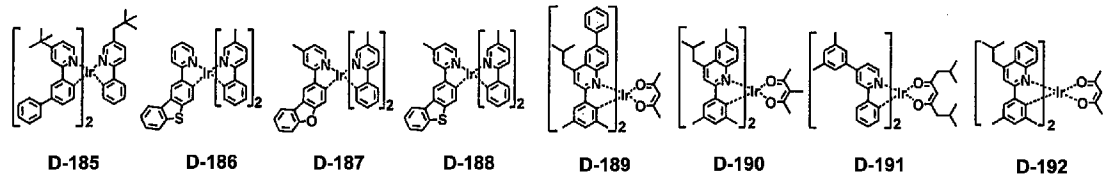
D-169 D-170 D-171 D-172 D-173 D-174 D-175 D-176

[154]



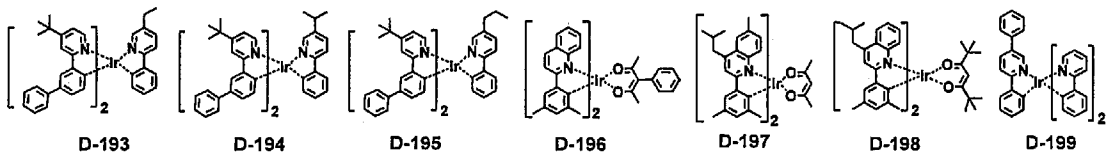
D-177 D-178 D-179 D-180 D-181 D-182 D-183 D-184

[155]



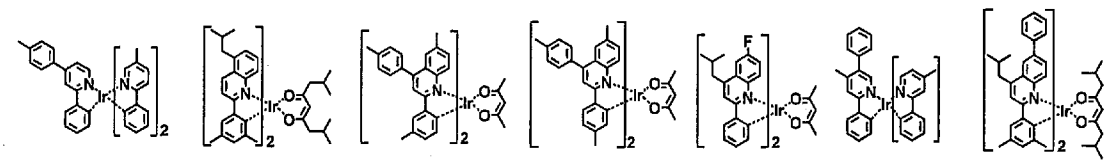
D-185 D-186 D-187 D-188 D-189 D-190 D-191 D-192

[156]



D-193 D-194 D-195 D-196 D-197 D-198 D-199

[157]



D-200 D-201 D-202 D-203 D-204 D-205 D-206

[158] In another embodiment of the present invention, a composition for preparing an organic electroluminescent device is provided. The composition comprises the compound according to the present invention as a host material or a hole transport material.

[159] In addition, the organic electroluminescent device according to the present invention comprises a first electrode; a second electrode; and at least one organic layer between the first and second electrodes. The organic layer comprises a light-emitting layer, and the light-emitting layer may comprise the composition for preparing the organic electroluminescent device according to the present invention.

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

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

[162] In addition, the organic electroluminescent device according to 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 known in the field, besides the compound according to the present invention. Also, if needed, a yellow or orange light-emitting layer can be comprised in the device.

[163] According to the present invention, at least one layer (hereinafter, "a surface layer") is preferably placed on an inner surface(s) of one or both electrode(s); selected from a chalcogenide layer, a metal halide layer and a metal oxide layer. Specifically, a chalcogenide(includes oxides) layer of silicon or aluminum is preferably placed on an anode surface of an electroluminescent medium layer, and a metal halide layer or a metal oxide layer is preferably placed on a cathode surface of an electroluminescent medium layer. Such a surface layer provides operation stability for the organic electroluminescent device. Preferably, said chalcogenide includes $SiO_X(1\leq X\leq 2)$, AlO_X $(1\leq X\leq 1.5)$, SiON, SiAlON, etc.; said metal halide includes LiF, MgF_2, CaF_2, a rare earth metal fluoride, etc.; and said metal oxide includes Cs_2O, Li_2O, MgO, SrO, BaO, CaO, etc.

[164] 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 is preferably 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 electroluminescent device having two or more electroluminescent layers and emitting white light.

[165] In order to form each layer of the organic electroluminescent device according to the

present invention, dry film-forming methods such as vacuum evaporation, sputtering, plasma and ion plating methods, or wet film-forming methods such as spin coating, dip coating, and flow coating methods can be used.

[166] When using a wet film-forming method, a thin film can be formed by dissolving or diffusing materials forming each layer into any suitable solvent such as ethanol, chloroform, tetrahydrofuran, dioxane, etc. The solvent can be any solvent where the materials forming each layer can be dissolved or diffused, and where there are no problems in film-formation capability.

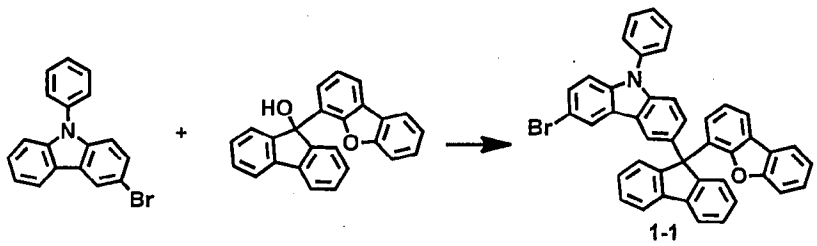
[167] Hereinafter, the organic electroluminescent compound, the preparation method of the compound, and the luminescent properties of the device will be explained in detail with reference to the following examples.

[168]

[169] **Example 1: Preparation of compound C-43**

[170] Preparation of compound 1-1

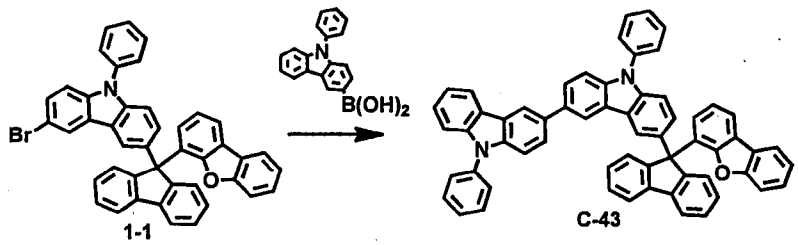
[171]



[172] After dissolving 3-bromo-N-phenylcarbazole 9.3 g (28.70 mmol) and 9-(dibenzo[b,d]furan-4-yl)-9H-fluoren-9-ol 10 g (28.70 mmol) in dichloromethane 150mL in a reaction container, Eaton's reagent 0.6 mL (0.9 M, 0.57 mmol) was slowly added dropwise to the mixture. After stirring the mixture for 30 minutes at room temperature, the reaction was completed with sodium hydrogen carbonate, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound 1-1 (17 g, 90%).

[173] Preparation of compound C-43

[174]



[175] After introducing compound 1-1 10 g (15.32 mmol), N-phenylcarbazol-3-boronic

acid 4.8 g (16.86 mmol), tetrakis(triphenylphosphine)palladium 0.5 g (0.46 mmol), sodium carbonate 4.1 g (38.30 mmol), toluene 76 mL, and ethanol 19 mL in a reaction container, distilled water 19 mL was added to the mixture, and the mixture was stirred at 120°C for 4 hours. After the reaction, the mixture was washed with distilled water, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound C-43 (2.7 g, 22%).

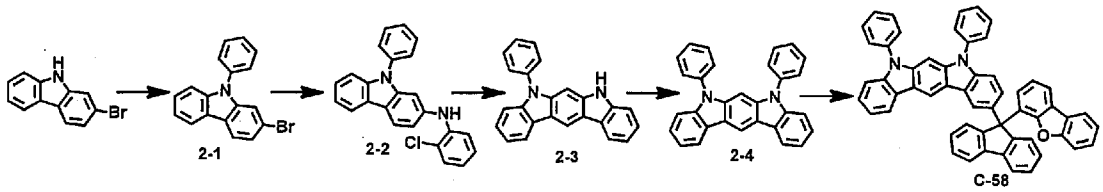
[176] UV=364 nm, PL=409 nm, melting point (MP)=236°C

[177] molecular weight (MW)=814.97, glass transition temperature (Tg)=195°C

[178]

[179] **Example 2: Preparation of compound C-58**

[180]



[181] Preparation of compound 2-1

[182] After introducing 2-bromocarbazole 100 g (0.406 mol), iodobenzene 166 g (0.813 mol), copper iodide 38.7 g (0.203 mol), ethylenediamine 27 mL (0.406 mol), cesium carbonate 265 g (0.813 mol), and toluene 1.3 L in a reaction container, the mixture was stirred under reflux for 3 hours. After the reaction, the mixture was washed with distilled water, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound 2-1 (116 g, 90%).

[183] Preparation of compound 2-2

[184] After introducing compound 2-1 116 g (0.362 mol), 2-chloroaniline 56 mL (0.542 mol), palladium(II)acetate 3.4 g (0.015 mol), tri-t-butyl phosphine 15 mL (50%, 0.030 mol), sodium tert-butoxide 87 g (0.905 mol), and toluene 1 L in a reaction container, the mixture was stirred under reflux for 5 hours. After the reaction, the mixture was washed with distilled water, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound 2-2 (75 g, 56%).

[185] Preparation of compound 2-3

[186] After introducing compound 2-2 75 g (203.33 mmol), palladium(II)acetate 2.3 g (10.17 mmol), tricyclohexylphosphine tetrafluoroborate 7.5 g (20.33 mmol), cesium

carbonate 199 g (609.99 mmol), and N,N-dimethylacetamide 1 L in a reaction container, the mixture was stirred for 5 hours at 190°C. After the reaction, the mixture was washed with distilled water, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound 2-3 (30 g, 44%).

[187] Preparation of compound 2-4

[188] After introducing compound 2-3 10 g (30.08 mmol), iodobenzene 5 mL (45.12 mmol), copper iodide 2.8 g (15.04 mmol), diaminocyclohexane 7.2 mL (60.16 mmol), cesium carbonate 19.6 g (60.16 mmol), and xylene 150 mL in a reaction container, the mixture was stirred under reflux for 4 hours. After the reaction, the mixture was washed with distilled water, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound 2-4 (11 g, 89%).

[189] Preparation of compound C-58

[190] After dissolving compound 2-4 8 g (19.58 mmol), 9-(dibenzo[b,d]furan-4-yl)-9H-fluoren-9-ol 4.2 g (12.03 mmol) in dichloromethane 60mL in a reaction container, Eaton's reagent 0.3 mL (0.9 M, 0.24 mmol) was slowly added dropwise to the mixture. After stirring the mixture for 30 minutes at room temperature, the reaction was completed with sodium hydrogen carbonate, and an organic layer was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed using a rotary evaporator. The remaining substance was then purified with column chromatography to obtain compound C-58 (2.7 g, 30%).

[191] UV=344 nm, PL=393 nm, MP=305°C, MW=738.87, Tg=208°C

[192]

[193] **Device Example 1: Production of an OLED device comprising the organic**

[194] **electroluminescent compound according to the present invention**

[195] An OLED device was produced using the organic electroluminescent compound according to the present invention. A transparent electrode indium tin oxide (ITO) thin film (10 Ω/sq) on a glass substrate for an organic light-emitting diode (OLED) device (Geomatec, Japan) was subjected to an ultrasonic washing with acetone and isopropan alcohol, sequentially, and then was stored in isopropan alcohol. Then, the ITO substrate was mounted on a substrate holder of a vacuum vapor depositing apparatus. $N^1,N^{1'}$-([1,1'-biphenyl]-4,4'-diyl)bis(N^1-(naphthalen-1-yl)-N^4,N^4-diphenylbenzen-1,4-diamine) was introduced into a cell of said vacuum vapor depositing apparatus, and then the pressure in the chamber of said apparatus was controlled to 10^{-6} torr. Thereafter, an

electric current was applied to the cell to evaporate the above introduced material, thereby forming a hole injection layer having a thickness of 60 nm on the ITO substrate. Then, compound **C-58** was introduced into another cell of said vacuum vapor depositing apparatus, and was evaporated by applying an electric current to the cell, thereby forming a hole transport layer having a thickness of 20 nm on the hole injection layer. Thereafter, 9-(3-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9'-phenyl-9H,9'H-3,3'-bicarbazole was introduced into one cell of the vacuum vapor depositing apparatus, as a host material, and compound **D-1** was introduced into another cell as a dopant. The two materials were evaporated at different rates and were deposited in a doping amount of 15 wt% based on the total amount of the host and dopant to form a light-emitting layer having a thickness of 30 nm on the hole transport layer. Then, 2-(4-(9,10-di(naphthalene-2-yl)anthracen-2-yl)phenyl)-1-phenyl-1H-benzo[d]imidazol e was introduced into one cell and lithium quinolate was introduced into another cell. The two materials were evaporated at the same rate and were deposited in a doping amount of 50 wt% each to form an electron transport layer having a thickness of 30 nm 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.

[196] The produced OLED device showed a green emission having a luminance of 1000 cd/m^2 and a current density of 2.0 mA/cm^2.

[197]

[198] **Device Example 2: Production of an OLED device comprising the organic**

[199] **electroluminescent compound according to the present invention**

[200] An OLED device was produced in the same manner as in Device Example 1, except for evaporating compound **C-43** to form a hole transport layer in a thickness of 20 nm; and introducing 9-(4-([1,1'-biphenyl]-4-yl)quinazolin-2-yl)-9'-phenyl-9H,9'H-3,3'-bicarbazole into one cell of the vacuum vapor depositing apparatus as a host, introducing compound **D-87** into another cell as a dopant, and evaporating the two materials at different rates and depositing them in a doping amount of 3 wt% based on the total amount of the host and dopant to form a light-emitting layer having a thickness of 30 nm on the hole transport layer.

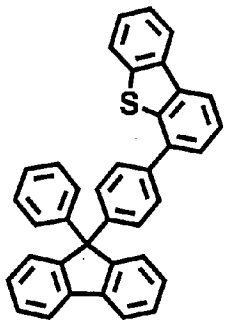
[201] The produced OLED device showed a red emission having a luminance of 2100 cd/m^2 and a current density of 14.4 mA/cm^2.

[202]

[203] **Comparative Example 1: Production of an OLED device comprising a**

[204] **conventional organic electroluminescent compound**

[205]



R-1

[206] An OLED device was produced in the same manner as in Device Example 1, except for evaporating compound **R-1** as above to form a hole transport layer in a thickness of 20 nm.

[207] The produced OLED device showed a green emission having a luminance of 2200 cd/m^2 and a current density of 27.5 mA/cm^2.

[208]

[209] **Comparative Example 2: Production of an OLED device comprising a**

[210] **conventional organic electroluminescent compound**

[211] An OLED device was produced in the same manner as in Device Example 2, except for evaporating compound **R-1** as above to form a hole transport layer in a thickness of 20 nm.

[212] The produced OLED device showed a red emission having a luminance of 100 cd/m^2 and a current density of 2.0 mA/cm^2.

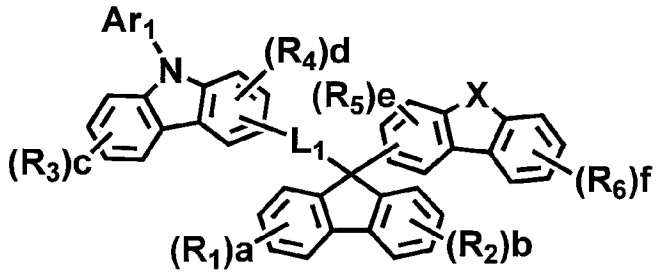
[213]

[214] It is verified that the luminous characteristics of the organic electroluminescent compound according to the present invention is superior to the conventional materials. In addition, an organic electroluminescent device using the organic electroluminescent compound according to the present invention has excellent luminous and lifespan characteristics.

[215]

Claims

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



-------- (1)

wherein

Ar_1 represents a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent(s) to form a (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur;

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

X represents -O-, -S-, or $-C(R_7)(R_8)-$;

R_1 to R_6, each independently, represent hydrogen, deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, $-NR_9R_{10}$, $-SiR_{11}R_{12}R_{13}$, $-SR_{14}$, $-OR_{15}$, $-COR_{16}$, or $-B(OR_{17})(OR_{18})$; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;

R_7 to R_{18}, each independently, represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl; or may be

linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C3-C30), mono- or polycyclic, alicyclic or aromatic ring;
a, b, c, and f, each independently, represent an integer of 0 to 4; where a, b, c, or f represents an integer of 2 or more, each of R_1, R_2, R_3, or R_6 may be the same or different;
d and e, each independently, represent an integer of 0 to 3; where d or e represents an integer of 2 or more, each of R_4 or R_5 may be the same or different; and
the heterocycloalkyl and the heteroaryl(ene), each independently, contain at least one hetero atom selected from B, N, O, S, P(=O), Si, and P.

[Claim 2] The organic electroluminescent compound according to claim 1, wherein the substituents of the substituted (C1-C30)alkyl, the substituted (C2-C30)alkenyl, the substituted (C2-C30)alkynyl, the substituted (C1-C30)alkoxy, the substituted (C3-C30)cycloalkyl, the substituted (C3-C30)cycloalkenyl, the substituted (3- to 7-membered)heterocycloalkyl, the substituted (C6-C30)aryl(ene), the substituted (3- to 30-membered)heteroaryl(ene), and the substituted (C3-C30), mono- or polycyclic, alicyclic or aromatic ring in Ar_1, L_1, and R_1 to R_{18}, each independently, are at least one selected from the group consisting of deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a (C1-C30)alkyl, a halo(C1-C30)alkyl, a (C2-C30)alkenyl, a (C2-C30)alkynyl, a (C1-C30)alkoxy, a (C1-C30)alkylthio, a (C3-C30)cycloalkyl, a (C3-C30)cycloalkenyl, a (3- to 7-membered)heterocycloalkyl, a (C6-C30)aryloxy, a (C6-C30)arylthio, a (3- to 30-membered)heteroaryl unsubstituted or substituted with a (C6-C30)aryl, a (C6-C30)aryl unsubstituted or substituted with a (3- to 30-membered)heteroaryl, a tri(C1-C30)alkylsilyl, a tri(C6-C30)arylsilyl, a di(C1-C30)alkyl(C6-C30)arylsilyl, a (C1-C30)alkyldi(C6-C30)arylsilyl, an amino, a mono- or di-(C1-C30)alkylamino, a mono- or di- (C6-C30)arylamino, a (C1-C30)alkyl(C6-C30)arylamino, a (C1-C30)alkylcarbonyl, a (C1-C30)alkoxycarbonyl, a (C6-C30)arylcarbonyl, a di(C6-C30)arylboronyl, a di(C1-C30)alkylboronyl, a (C1-C30)alkyl(C6-C30)arylboronyl, a (C6-C30)aryl(C1-C30)alkyl, and a (C1-C30)alkyl(C6-C30)aryl.

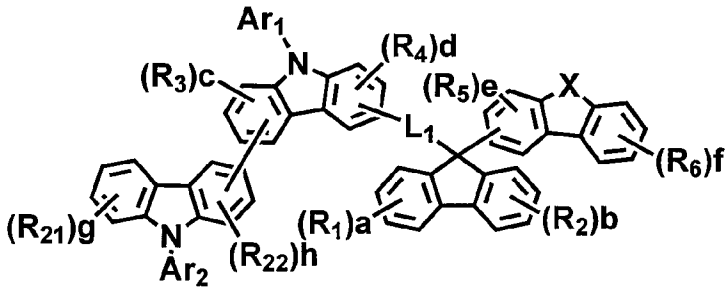
[Claim 3] The organic electroluminescent compound according to claim 1, wherein

Ar_1 represents a substituted or unsubstituted (C1-C20)alkyl, or a substituted or unsubstituted (C6-C21)aryl;
L_1 represents a single bond, a substituted or unsubstituted (C6-C21)arylene, or a substituted or unsubstituted (3- to 21-membered)heteroarylene;
X represents -O-, -S-, or $-C(R_7)(R_8)-$, wherein R_7 and R_8, each independently, represent a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl;
R_1 to R_6, each independently, represent hydrogen, a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, a substituted or unsubstituted (5- to 21-membered)heteroaryl, or a di(C6-C21)arylamino; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C5-C21), mono- or polycyclic aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;
a, b, c, d, e, and f, each independently, represent an integer of 0 to 2; where a, b, c, d, e, or f represents 2, each of R_1, R_2, R_3, R_4, R_5, or R_6 may be the same or different; and
the heteroaryl(ene) contains at least one hetero atom selected from N, O, and S.

[Claim 4] The organic electroluminescent compound according to claim 1, wherein
Ar_1 represents a substituted or unsubstituted (C6-C18)aryl;
L_1 represents a single bond;
X represents -O-, -S-, or $-C(R_7)(R_8)-$, wherein R_7 and R_8, each independently, represent a substituted or unsubstituted (C1-C20)alkyl, a substituted or unsubstituted (C6-C21)aryl, or a substituted or unsubstituted (5- to 21-membered)heteroaryl;
R_1 to R_6, each independently, represent an unsubstituted (C6-C18)aryl, or a (6- to 18-membered)heteroaryl unsubstituted or substituted with a (C6-C12)aryl; or may be linked to an adjacent substituent(s) to form a (C6-C18), mono- or polycyclic aromatic ring unsubstituted or substituted with a (C6-C12)aryl, whose carbon atom may be replaced with one (1) nitrogen;
a, b, c, and f, each independently, represent an integer of 0 to 2; e and d, each independently, represent an integer of 0 or 1; where a, b, c, or f represents 2, each of R_1, R_2, R_3, or R_6 may be the same or different; and

the heteroaryl contains one or two hetero atom(s) selected from N, O, and S.

[Claim 5] The organic electroluminescent compound according to claim 1, wherein the compound of formula 1 is represented by the following formula 2:



(2)

wherein

Ar_1, L_1, X, R_1 to R_6, a, b, d, e, and f are as defined in claim 1;

Ar_2 represents a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent(s) to form a (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;

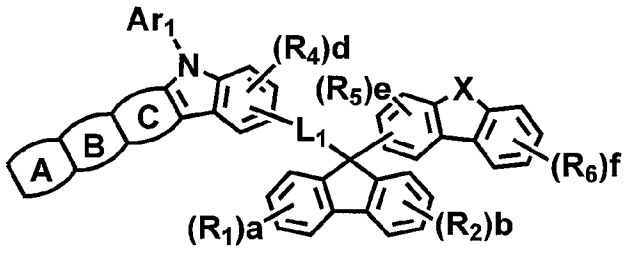
R_{21} and R_{22}, each independently, represent hydrogen, deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, $-NR_9R_{10}$, $-SiR_{11}R_{12}R_{13}$, $-SR_{14}$, $-OR_{15}$, $-COR_{16}$, or $-B(OR_{17})(OR_{18})$; or may be linked to an adjacent substituent(s) to form a substituted or unsubstituted, (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;

R_9 to R_{18}, each independently, represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl;

g represents an integer of 0 to 4; c and h, each independently, represent an integer of 0 to 3; where c, g, or h represents an integer of 2 or more,

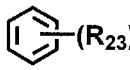
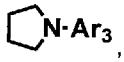
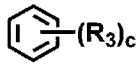
each of R_3, R_{21}, or R_{22} may be the same or different; and
the heterocycloalkyl and the heteroaryl(ene), each independently, contain at least one hetero atom selected from N, O, and S.

[Claim 6] The organic electroluminescent compound according to claim 1, wherein the compound of formula 1 is represented by the following formula 3:



(3)

wherein

L_1, X, Ar_1, R_1, R_2, R_4 to R_6, a, b, d, e, and f are as defined in claim 1; A represents  , B represents  , and C represents  ;

Ar_3 represents a substituted or unsubstituted (C1-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; or may be linked to an adjacent substituent(s) to form a (C3-C30), mono- or polycyclic, alicyclic or aromatic ring whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;

R_{23} represents hydrogen, deuterium, a halogen, a cyano, a carboxyl, a nitro, a hydroxyl, a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C2-C30)alkenyl, a substituted or unsubstituted (C2-C30)alkynyl, a substituted or unsubstituted (C1-C30)alkoxy, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (3- to 30-membered)heteroaryl, $-NR_9R_{10}$, $-SiR_{11}R_{12}R_{13}$, $-SR_{14}$, $-OR_{15}$, $-COR_{16}$, or $-B(OR_{17})(OR_{18})$;

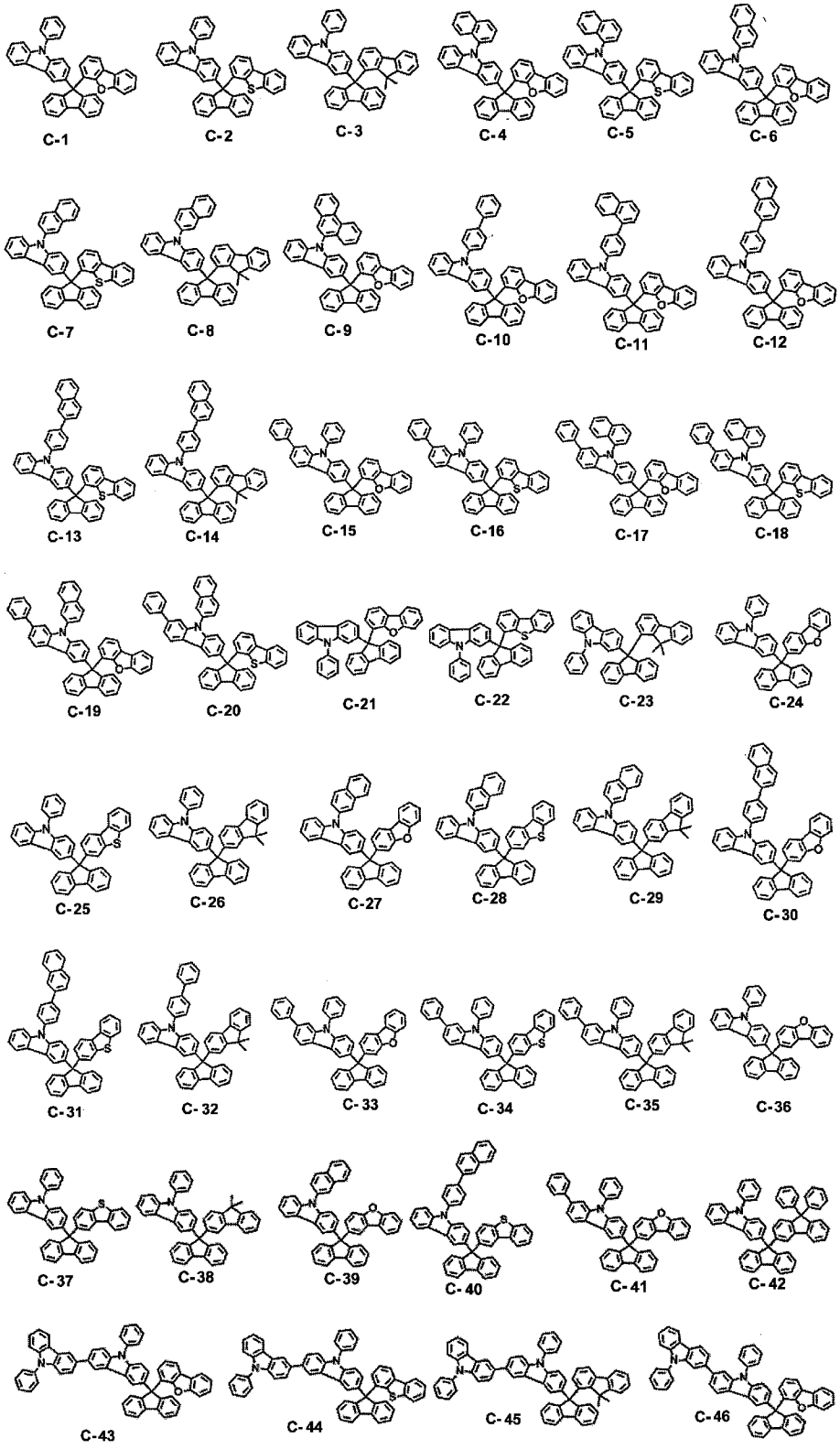
R_9 to R_{18}, each independently, represent a substituted or unsubstituted (C1-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (3- to 30-membered)heteroaryl;

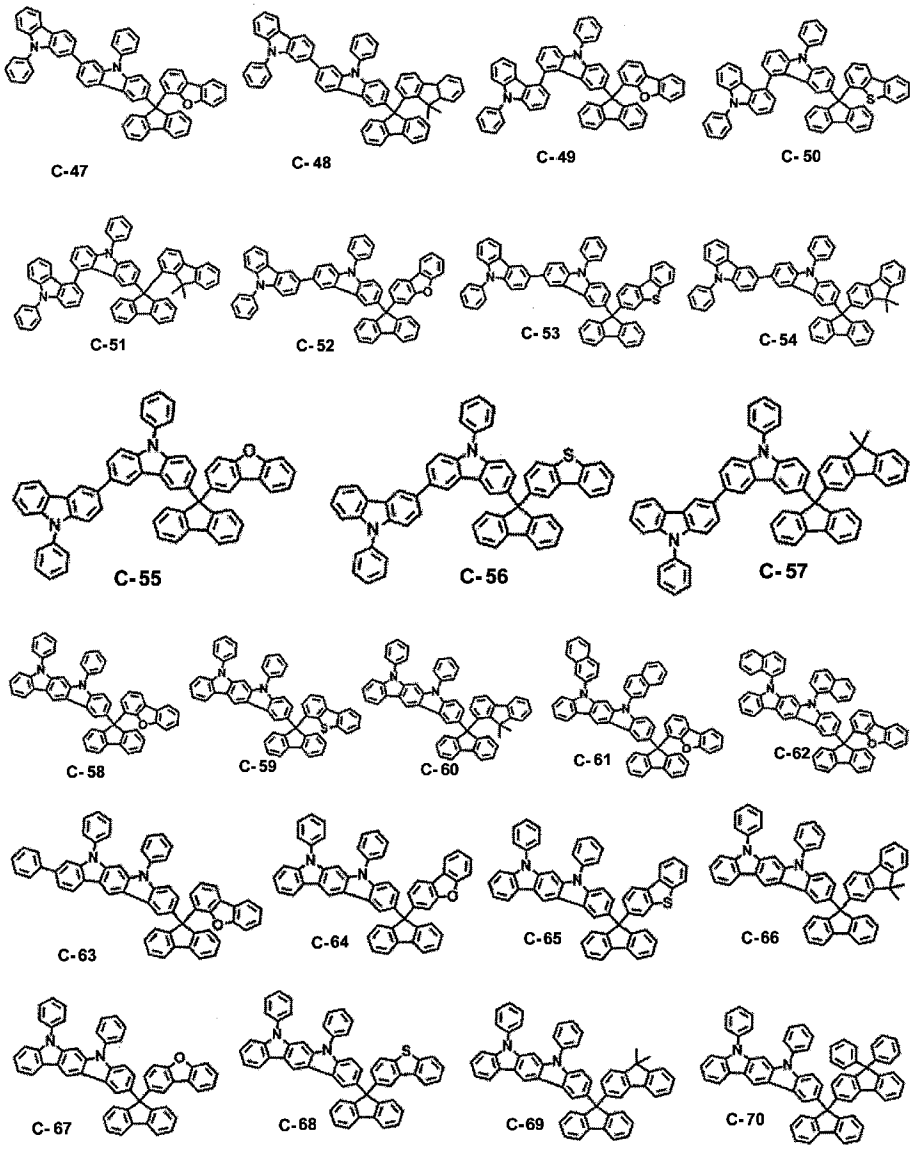
i represents an integer of 0 to 4; c represents an integer of 0 to 2; where c or i represents an integer of 2 or more, each of R_3 or R_{23} may be the

same or different; and

the heterocycloalkyl and the heteroaryl(ene), each independently, represent at least one hetero atom selected from N, O, and S.

[Claim 7] The organic electroluminescent compound according to claim 1, wherein the compound is selected from the group consisting of:





[Claim 8] An organic electroluminescent device comprising the organic electroluminescent compound according to claim 1.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2014/012891

A. CLASSIFICATION OF SUBJECT MATTER

C07D 209/86 (2006.01) ***C07D 403/02 (2006.01)*** ***C07D 405/02 (2006.01)*** ***C07D 405/14 (2006.01)*** ***C07D 409/02 (2006.01)*** ***C07D 409/14 (2006.01)*** ***H01L 51/50 (2006.01)*** ***C09K 11/06 (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)

STN: CAPLUS, REGISTRY: Substructure search of compound of instant formula 1

Espacenet: Author/Inventor, Electroluminescent, Rohm and Haas

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
23 March 2015	23 March 2015
Name and mailing address of the ISA/AU	**Authorised officer**
AUSTRALIAN PATENT OFFICE PO BOX 200, WODEN ACT 2606, AUSTRALIA Email address: pct@ipaustralia.gov.au	Marica Nikac AUSTRALIAN PATENT OFFICE (ISO 9001 Quality Certified Service) Telephone No. 0262832087

INTERNATIONAL SEARCH REPORT C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT		International application No. **PCT/KR2014/012891**
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 2013/157495 A1 (KONICA MINOLTA, INC.) 24 October 2013 Abstract; Table 16, page 40	1-8
A	MONDAL, E. et al., "Molecular topology tuning of bipolar host materials composed of fluorene-bridged benzimidazole and carbazole for highly efficient electrophosphorescence', Chemistry - A European Journal, 2013, Vol. 19, No. 32, pages 10563-10572. Abstract; also see "Introduction", page 10563; Scheme 1, page 10564	1-8
A	US 2011/0042654 A1 (JUNG et al) 24 February 2011 Abstract; Examples 12-13, pages 64-66	1-8

INTERNATIONAL SEARCH REPORT Information on patent family members	International application No. **PCT/KR2014/012891**

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**
WO 2013/157495 A1	24 October 2013		
US 2011/0042654 A1	24 February 2011	US 8586200 B2	19 Nov 2013
		KR 20090028357 A	18 Mar 2009
		KR 101002733 B1	21 Dec 2010
		WO 2009035296 A2	19 Mar 2009

End of Annex

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