

(10) International Publication Number
WO 2013/012297 A1(43) International Publication Date
24 January 2013 (24.01.2013)

(51) International Patent Classification:

C07D 487/04 (2006.01) **C07F 7/02** (2006.01)
C07D 495/04 (2006.01) **C09K 11/06** (2006.01)
C07D 491/04 (2006.01) **H01L 51/54** (2006.01)
C07D 403/04 (2006.01) **H01L 27/32** (2006.01)
C07D 409/14 (2006.01) **H05B 33/14** (2006.01)

(21) International Application Number:

PCT/KR2012/005840

(22) International Filing Date:

20 July 2012 (20.07.2012)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

10-2011-0072545 21 July 2011 (21.07.2011) KR

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

(72) **Inventors; and**

(75) **Inventors/Applicants** (for US only): **YANG, Soo-Jin** [KR/KR]; 811-1101, Supsok Maeul mayrouge Apt., Neung-dong, Hwaseong-si, Gyeonggi-do 445-794 (KR). **HWANG, Soo-Jin** [KR/KR]; 106-801, Samsung Raemian 1 Cha Apt., Gireum 1-dong, Seongbuk-gu, Seoul 136-770 (KR). **LEE, Seon-Woo** [KR/KR]; 104-108, KCC Switzen, Galgot-dong, Osan-si, Gyeonggi-do 447-310 (KR). **KIM, Chi-Sik** [KR/KR]; 441-1201, Solbit Maeul Ssangyong Yega Apt., Bansong-dong, Hwaseong-si, Gyeonggi-do 445-752 (KR). **LEE, Hyo-Jung** [KR/KR]; 117-1301, Ye-dang Maeul Umirin Jeil Punggyeongchae Apt., Seoku-

dong, Hwaseong-si, Gyeonggi-do 445-853 (KR). **PARK, Kyoung-Jin** [KR/KR]; A202, DongHyun Vila, 124-13 Hadaewon-dong, Jungwon-gu, Seongnam-si, Gyeonggi-do 462-838 (KR). **CHO, Young-Jun** [KR/KR]; 204-701, EG The one Apt., BotdulMaeul 2 Danji, Sampyeong-dong, Bundang-gu, Seongnam-si, Gyeonggi-do 463-892 (KR).

(74) **Agent:** **CHANG, Hoon**; Korean Re Bldg. 5F, #80, Soosong-dong, Chongro-ku, 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, 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, IS, JP, KE, KG, KM, KN, KP, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, 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, 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, ML, MR, NE, SN, TD, TG).

Published:

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

(54) **Title:** NOVEL ORGANIC ELECTROLUMINESCENCE COMPOUNDS AND ORGANIC ELECTROLUMINESCENCE DEVICE USING THE SAME

(57) **Abstract:** The present invention relates to a novel organic luminescent compound and an organic electroluminescence device containing the same. The compounds according to the present invention have high luminous efficiency and long operation lifetime. Therefore, they can produce an organic electroluminescent device which improves power consumption.



WO 2013/012297 A1

Description

Title of Invention: NOVEL ORGANIC ELECTROLUMINESCENCE COMPOUNDS AND ORGANIC ELECTROLUMINESCENCE DEVICE USING THE SAME

Technical Field

- [1] The present invention relates to novel organic electroluminescence compounds and organic electroluminescence device using the same.

Background Art

- [2] An electroluminescence (EL) device is a self-light-emitting device which has advantages over other types of display devices in that it provides a wider viewing angle, a greater contrast ratio, and has a faster response time. An organic EL device was first developed by Eastman Kodak, by using small molecules which are aromatic diamines, and aluminum complexes as a material for forming a light-emitting layer [Appl. Phys. Lett. 51, 913, 1987].
- [3] The most important factor to determine luminous efficiency in an organic EL device is a 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 luminous efficiency by four (4) times. 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)picolate 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, an organic EL device using bathocuproine (BCP) and aluminum(III)bis(2-methyl-8-quinolate)(4-phenylphenolate) (BALq) for a hole blocking layer is 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 materials provide good light-emitting characteristics, they have the following disadvantages. Due to their low glass transition temperature and poor thermal stability, their degradation may occur during a high-temperature deposition process in a vacuum. The power efficiency of an organic EL device is given by $[(\pi/\text{voltage}) \times \text{current efficiency}]$, and the power efficiency is inversely proportional to

voltage, and thus in order to lower the power consumption, the power efficiency should be raised. Although an organic EL device comprising phosphorescent materials provides much higher current efficiency (cd/A) than one comprising fluorescent materials, an organic EL device using conventional phosphorescent materials such as BAq or CBP has a higher driving voltage than that using fluorescent materials. Thus, the EL device using the conventional phosphorescent materials has no advantage in terms of power efficiency (lm/W). Further, the operation lifetime of the organic EL device is short.

- [6] Korean Patent No. KR 0948700 discloses as compounds for an organic EL device an arylcarbazole compound substituted with a heteroaryl group comprising a nitrogen atom. However, it does not disclose a fused carbazole compound which is, at the nitrogen position, directly or indirectly linked to a heteroaryl group substituted with a carbazole group.

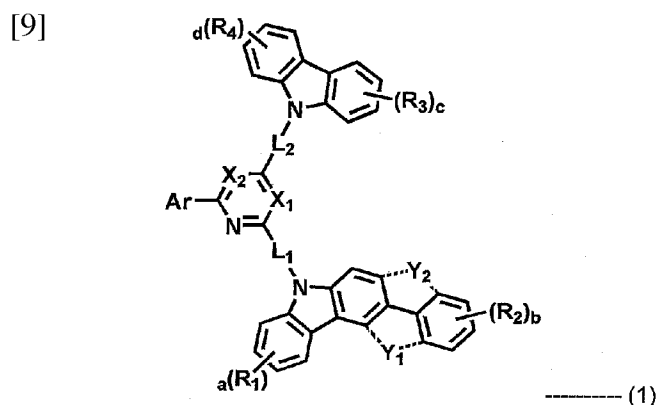
Disclosure of Invention

Technical Problem

- [7] The objective of the present invention is to provide an organic electroluminescence compound imparting high luminous efficiency and a long operation lifetime to a device, and having proper color coordination; and an organic electroluminescence device having high efficiency and a long lifetime, using said compound 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:



- [10] wherein

- [11] L_1 and L_2 each independently represent a single bond, a substituted or unsubstituted 3- to 30-membered heteroarylene group, a substituted or unsubstituted (C6-C30)arylene group, or a substituted or unsubstituted (C3-C30)cycloalkylene group;

- [12] X_1 and X_2 represent CH or N;
- [13] Y_1 and Y_2 each independently represent -O-, -S-, -CR₅R₆- or -NR₇-, provided that Y_1 and Y_2 do not simultaneously exist;
- [14] Ar represents hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- to 30-membered heteroaryl group, or an N-carbazolyl group;
- [15] R₁ to R₄ each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 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(C1-C30)alkyl group, -NR₁₁R₁₂, -SiR₁₃R₁₄R₁₅, -SR₁₆, -OR₁₇, a cyano group, a nitro group, or a hydroxyl 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;
- [16] R₅ to R₇ and R₁₁ to R₁₇ each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- to 30-membered heteroaryl group, a substituted or unsubstituted 5- to 7-membered heterocycloalkyl group, or a substituted or unsubstituted (C3-C30)cycloalkyl 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;
- [17] a, b, c and d each independently represent an integer of 1 to 4; where a, b, c or d is an integer of 2 or more, each of R₁, each of R₂, each of R₃ or each of R₄ is the same or different; and
- [18] the heterocycloalkyl group, the heteroarylene group and the heteroaryl group contain at least one hetero atom selected from B, N, O, S, P(=O), Si and P.

Advantageous Effects of Invention

- [19] The organic electroluminescence compounds according to the present invention can manufacture an organic electroluminescence device which has high luminous efficiency and a long operation lifetime.
- [20] In addition, since the compounds according to the present invention have high efficiency in transporting electrons, crystallization could be prevented when manufacturing a device. Further, the compounds have good layer formability and improve the current characteristic of the device. Therefore, they can produce an organic electro-

luminescence device having lowered driving voltages and enhanced power efficiency.

Mode for the Invention

- [21] 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.
- [22] The present invention relates to an organic electroluminescence compound represented by the above formula 1 and an organic electroluminescence device comprising the compound.
- [23] Herein, “(C1-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-butylnyl, 2-butylnyl, 3-butylnyl, 1-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(=O), Si and P, preferably O, S and N, and 3 to 7 ring backbone atoms, and includes tetrahydrofuran, 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(=O), 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, Cl, Br and I.

- [24] 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 alkyl group, the substituted aryl(ene) group, the substituted heteroaryl(ene) group, the substituted cycloalkyl(ene) group, the substituted heterocycloalkyl group, and the substituted aralkyl group in L_1 , L_2 , Ar, R_1 to R_7 and R_{11} to R_{17} groups each independently are at least one selected from the group consisting of deuterium; a halogen; a (C1-C30)alkyl group substituted or unsubstituted with a halogen; a (C6-C30)aryl group; a 3- to 30-membered heteroaryl group substituted or unsubstituted with a (C1-C30)alkyl or (C6-C30)aryl; a (C3-C30)cycloalkyl group; a 5- to 7-membered heterocycloalkyl group; a tri(C1-C30)alkylsilyl group; a tri(C6-C30)arylsilyl group; a di(C1-C30)alkyl(C6-C30)aryl silyl group; a (C1-C30)alkyldi(C6-C30)arylsilyl group; a (C2-C30)alkenyl group; a (C2-C30)alkynyl group; a cyano group; an N-carbazolyl group; a di(C1-C30)alkylamino group; a di(C6-C30)arylamino group; a (C1-C30)alkyl(C6-C30)arylamino group; a di(C6-C30)arylboronyl group; a di(C1-C30)alkylboronyl group; a (C1-C30)alkyl(C6-C30)arylboronyl group; a (C6-C30)aryl(C1-C30)alkyl group; a (C1-C30)alkyl(C6-C30)aryl group; a carboxyl group; a nitro group; and a hydroxyl group.

- [25] In the above formula 1, L_1 and L_2 each independently represent a single bond, a 3- to 30-membered heteroarylene group, or a (C6-C30)arylene group; X_1 and X_2 each independently represent CH or N; Y_1 and Y_2 each independently represent -O-, -S-, -CR₅R₆- or -NR₇-, provided that Y_1 and Y_2 do not simultaneously exist; Ar represents hydrogen, deuterium, a halogen, a (C1-C30)alkyl group, a (C6-C30)aryl group, a 3- to 30-membered heteroaryl group, or an N-carbazolyl group; R_1 to R_4 each independently represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl group, a (C6-C30)aryl group, a 3- to 30-membered heteroaryl group, an N-carbazolyl group, or -SiR₁₃R₁₄R₁₅; R_5 to R_7 each independently represent a (C1-C30)alkyl group, a (C6-C30)aryl group, or a 3- to 30-membered heteroaryl group; or R_5 and R_6 are linked to each other 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; R_{13} to R_{15} each independently represent a (C1-C30)alkyl group, a (C6-C30)aryl group, or a 3- to 30-membered heteroaryl group; and the arylene group and the heteroarylene

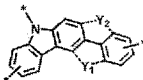
group in L_1 and L_2 , the alkyl group, the aryl group, the heteroaryl group and the N-carbazolyl group in Ar, the alkyl group, the aryl group, the heteroaryl group and the N-carbazolyl group in R_1 to R_4 , and the alkyl group, the aryl group and the heteroaryl group in R_5 to R_7 and R_{13} to R_{15} each independently can be substituted with at least one selected from the group consisting of deuterium; a halogen; a (C1-C30)alkyl group substituted or unsubstituted with a halogen; a (C6-C30)aryl group; a 3- to 30-membered heteroaryl group substituted or unsubstituted with a (C1-C30)alkyl or (C6-C30)aryl; a (C3-C30)cycloalkyl group; an N-carbazolyl group; a di(C1-C30)alkylamino group; a di(C6-C30)arylamino group; a (C1-C30)alkyl(C6-C30)aryl amino group; a (C6-C30)aryl(C1-C30)alkyl group; and a (C1-C30)alkyl(C6-C30)aryl group.

- [26] In the above formula 1, L_1 and L_2 each independently are preferably a single bond or a substituted or unsubstituted (C6-C20)arylene group, wherein the substituted arylene group can be substituted with a (C1-C6) alkyl or a (C6-C20)aryl.
- [27] Y_1 and Y_2 each independently represent -O-, -S-, -CR₅R₆- or -NR₇-, wherein R₅ and R₆ each independently are preferably a (C1-C6)alkyl group or a (C6-C20)aryl group, or are linked to each other to form a mono- or polycyclic, (C5-C30)alicyclic or aromatic ring, and R₇ is preferably a substituted or unsubstituted (C6-C20)aryl group, wherein the substituted aryl group can be substituted with deuterium, a halogen, a (C1-C6)alkyl, or a (C6-C12)arylamino.
- [28] Ar is preferably hydrogen, a substituted or unsubstituted (C6-C20)aryl group, or a substituted or unsubstituted 5- to 15-membered heteroaryl group, wherein the substituted aryl group and the substituted heteroaryl group can be substituted with deuterium, a halogen, a (C1-C6)alkyl, a (C6-C20)aryl or a 5- to 15-membered heteroaryl.
- [29] R_1 to R_4 each independently are preferably hydrogen, a substituted or unsubstituted (C1-C6)alkyl group, a substituted or unsubstituted (C6-C20)aryl group, a substituted or unsubstituted 5- to 15-membered heteroaryl group, or -SiR₁₃R₁₄R₁₅, wherein the substituted alkyl group, the substituted aryl group and the substituted heteroaryl group can be substituted with a (C1-C6)alkyl, and R_{13} to R_{15} each independently are preferably a (C1-C6)alkyl group or a (C6-C20)aryl group.
- [30] In the above formula 1, preferably, L_1 and L_2 each independently are a single bond or a substituted or unsubstituted (C6-C20)arylene group; Y_1 and Y_2 each independently represent -O-, -S-, -CR₅R₆- or -NR₇-, wherein R₅ and R₆ each independently are a (C1-C6)alkyl group or a (C6-C20)aryl group, or are linked to each other to form a mono- or polycyclic, (C5-C20)alicyclic or aromatic ring, and R₇ is a substituted or unsubstituted (C6-C20)aryl group; Ar is hydrogen, a substituted or unsubstituted (C6-C20)aryl group, or a substituted or unsubstituted 5- to 15-membered heteroaryl

group; R_1 to R_4 each independently are hydrogen, a substituted or unsubstituted (C1-C6)alkyl group, a substituted or unsubstituted (C6-C20)aryl group, a substituted or unsubstituted 5- to 15-membered heteroaryl group, or $-\text{SiR}_{13}\text{R}_{14}\text{R}_{15}$, wherein R_{13} to R_{15} each independently are a (C1-C6)alkyl group or a (C6-C20)aryl group.

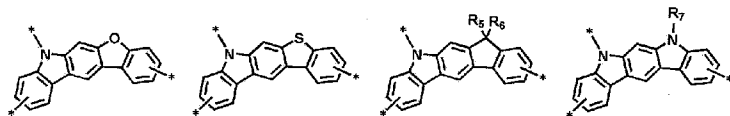
- [31] More specifically, L_1 and L_2 each independently represent a single bond, phenylene, biphenylene, terphenylene, indenylene, fluorenylene, triphenylenylene, pyrenylene, perylenylene, crysenylene, naphthacenylenylene, fluoranthenylenylene, thiophenylenylene, pyrrolylenylene, pyrazolylenylene, thiazolylenylene, oxazolylenylene, oxadiazolylenylene, triazinylene, tetrazinylenylene, triazolylenylene, furazanylenylene, pyridylene, benzofuranylenylene, benzothio-phenylene, indolylenylene, benzoimidazolylenylene, benzothiazolylenylene, benzoisothiazolylenylene, benzoisoxazolylenylene, benzoxazolylenylene, benzothiadiazolylenylene, dibenzofuranylenylene or dibenzothiophenylenylene; Ar represents hydrogen, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, biphenyl, fluorenyl, fluoranthenyl, terphenyl, pyrenyl, crysenyl, naphthacenyl, perylenyl, pyridyl, pyrrolyl, furanyl, thiophenyl, imidazolyl, benzoimidazolyl, quinolyl, triazinyl, benzofuranyl, dibenzofuranyl, benzothiophenyl, dibenzothiophenyl, pyrazolyl, indolyl, carbazolyl, thiazolyl, oxazolyl, benzothiazolyl, benzoxazolyl, phenanthrolinyl, quinoxalinyl, or N-carbazolyl; R_1 to R_4 each independently represent hydrogen, deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, naphthyl, anthryl, biphenyl, fluorenyl, fluoranthenyl, triphenylenyl, pyrenyl, crysenyl, naphthacenyl, perylenyl, pyridyl, pyrrolyl, furanyl, thiophenyl, imidazolyl, benzoimidazolyl, indenyl, pyrazinyl, pyrimidinyl, pyridazinyl, quinolyl, triazinyl, benzofuranyl, dibenzofuranyl, benzothiophenyl, dibenzothiophenyl, pyrazolyl, indolyl, carbazolyl, thiazolyl, oxazolyl, benzothiazolyl, benzoxazolyl, phenanthrolinyl, N-carbazolyl, trimethylsilyl, triethylsilyl, tripropylsilyl, tri(t-butyl)silyl, t-butyl dimethylsilyl, dimethylphenylsilyl, methyl diphenylsilyl or triphenylsilyl; the substituents in L_1 , L_2 , Ar and R_1 to R_4 each independently can be substituted with at least one selected from the group consisting of deuterium, chloro, fluoro, methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl, t-butyl, n-pentyl, i-pentyl, n-hexyl, n-heptyl, n-octyl, 2-ethylhexyl, n-nonyl, decyl, dodecyl, hexadecyl, trifluoromethyl, perfluoroethyl, trifluoroethyl, perfluoropropyl, perfluorobutyl, phenyl, naphthyl, biphenyl, 9,9-dimethylfluorenyl, 9,9-diphenylfluorenyl, fluoranthenyl, triphenylenyl, pyrenyl, crysenyl, naphthacenyl, perylenyl, dimethylamino, diethylamino, methylphenylamino, diphenylamino, trimethylsilyl, triethylsilyl, tripropylsilyl, tri(t-butyl)silyl, t-butyl dimethylsilyl, dimethylphenylsilyl,

methyldiphenylsilyl, triphenylsilyl, N-carbazolyl and N-phenylcarbazolyl.

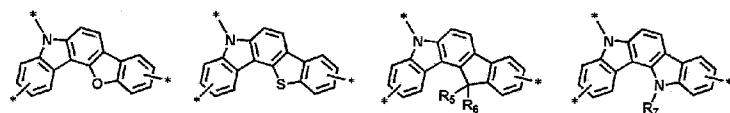
[32] In the above formula 1, the moiety,  is selected from the following

structures, but are not limited thereto:

[33]



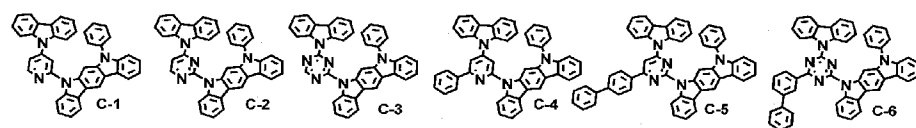
[34]



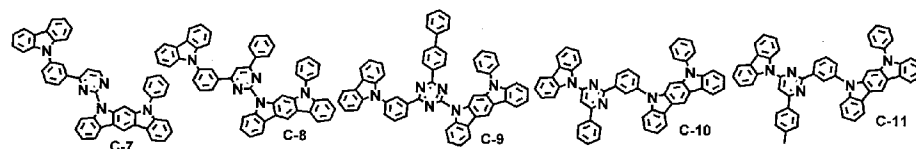
[35] wherein R₅, R₆ and R₇ are as defined in formula 1 above.

[36] The representative compounds of the present invention include the following compounds:

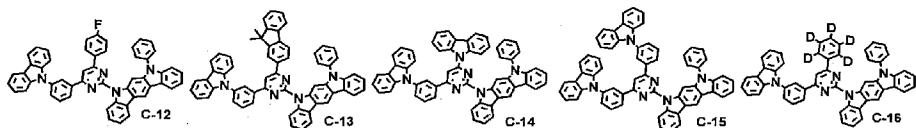
[37]



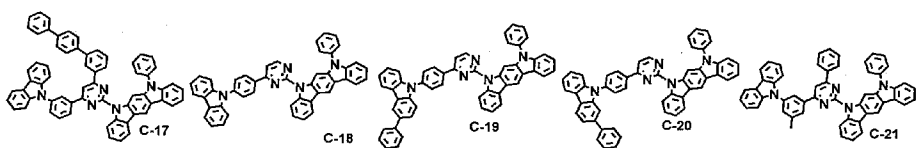
[38]



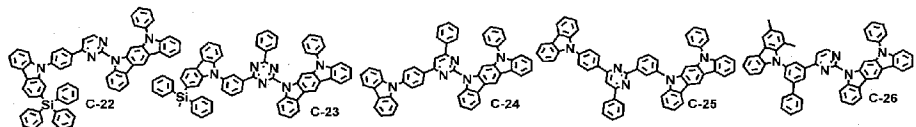
[39]



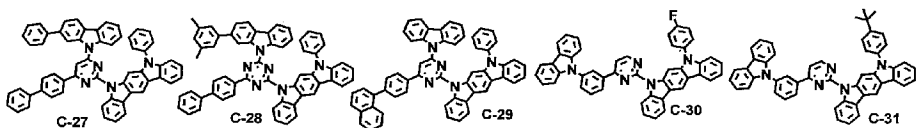
[40]



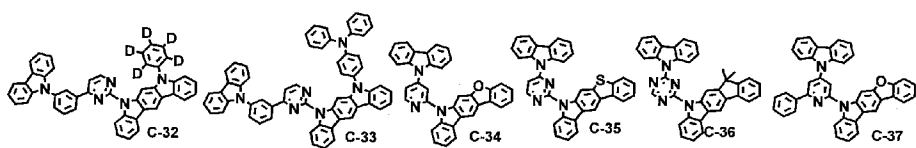
[41]



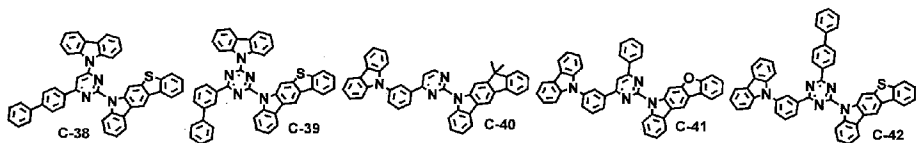
[42]

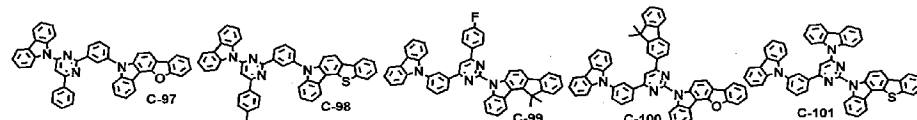


[43]

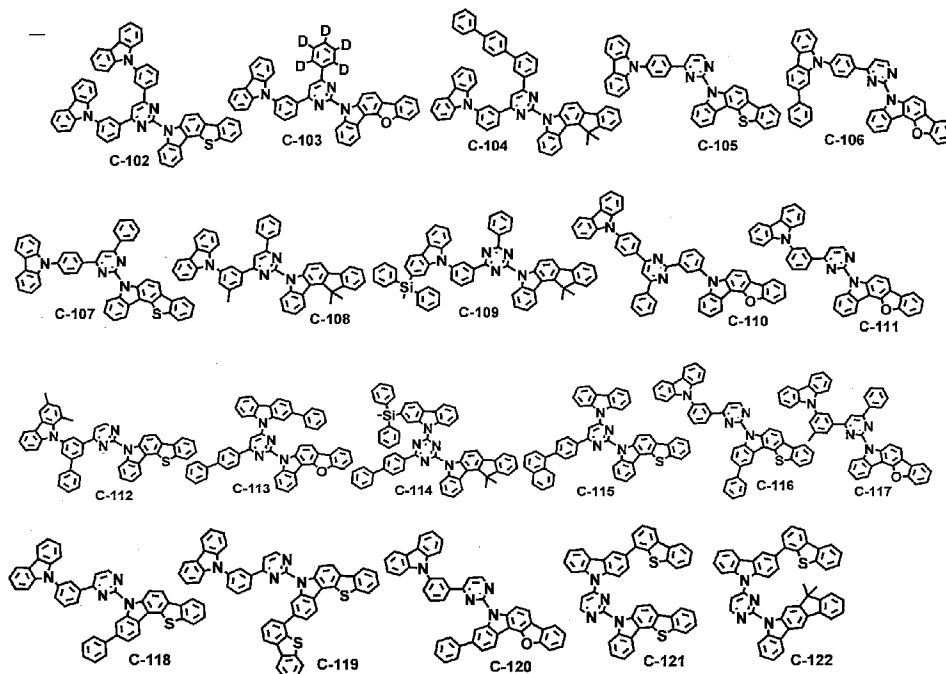


[44]





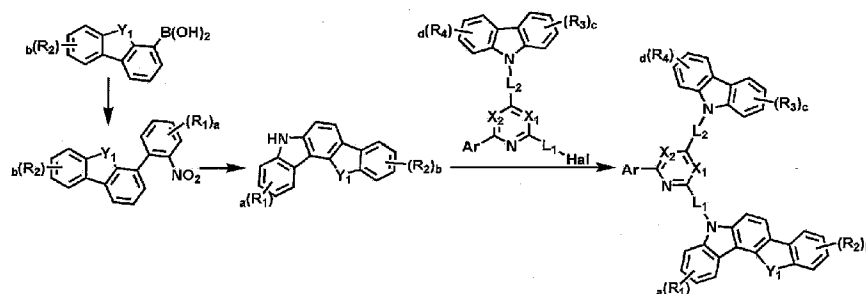
[51]



[52] The organic electroluminescence compounds according to the present invention can be prepared according to the following reaction scheme.

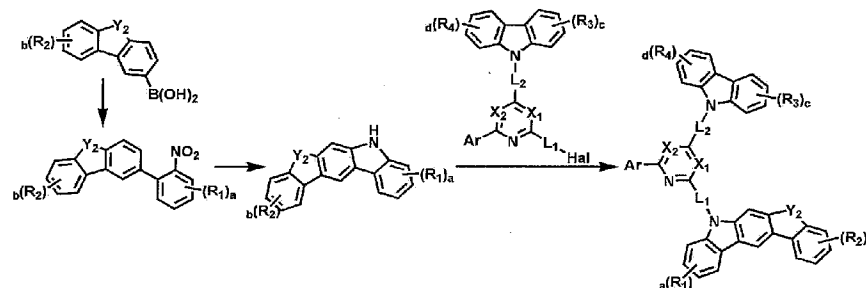
[53] [Reaction Scheme 1]

[54]



[55] [Reaction Scheme 2]

[56]



[57] wherein L_1 , L_2 , Ar, X_1 , X_2 , Y_1 , Y_2 , R_1 to R_4 , a, b, c and d are as defined in formula 1 above, and Hal represents a halogen.

[58] In addition, the present invention provides an organic electroluminescence device comprising the compound of formula 1. Said organic electroluminescence device comprises a first electrode, a second electrode, and at least one organic layer between said first and second electrodes. Said organic layer comprises at least one compound of

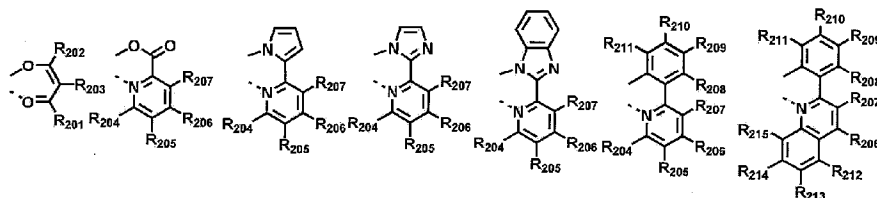
formula 1 according to the present invention. Further, said organic layer comprises a light-emitting layer in which the compound of formula 1 is comprised as a host material.

[59] In addition, a phosphorescent dopant, which is used for an organic electroluminescence device together with the host material according to the present invention, may be selected from compounds represented by the following formula 2:

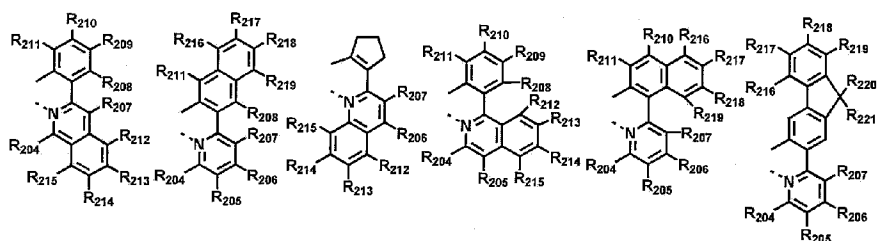
[60] $M^1 L^{101} L^{102} L^{103}$ ----- (2)

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

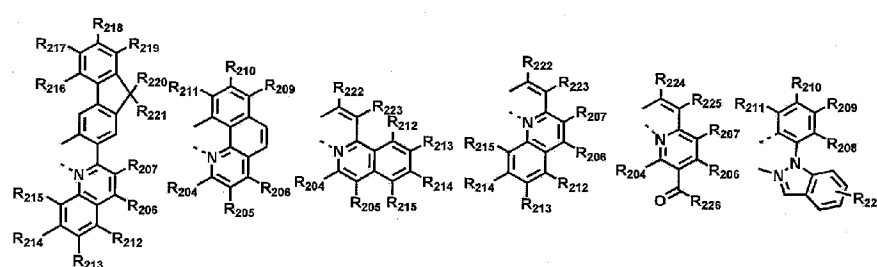
[62]



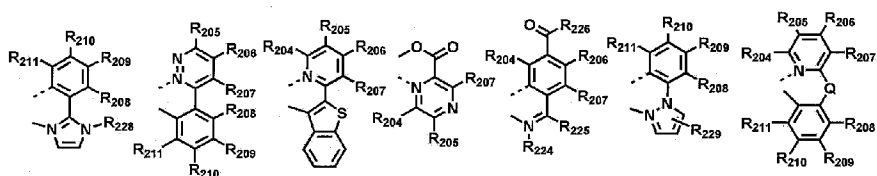
[63]



[64]



[65]



[66] R_{201} to R_{203} each independently represent hydrogen, deuterium, a (C1-C30)alkyl group unsubstituted or substituted with halogen(s), a (C6-C30)aryl group unsubstituted or substituted with (C1-C30)alkyl group(s), or a halogen;

[67] R_{204} to R_{219} each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C1-C30)alkoxy group, a substituted or unsubstituted (C3-C30)cycloalkyl group, a substituted or unsubstituted (C2-C30)alkenyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted mono- or di-(C1-C30)alkylamino group, a substituted or unsubstituted mono- or di-(C6-C30)arylamino group, SF_5 , a substituted or unsubstituted

tri(C1-C30)alkylsilyl group, a substituted or unsubstituted di(C1-C30)alkyl(C6-C30)arylsilyl group, a substituted or unsubstituted tri(C6-C30)arylsilyl group, a cyano group or a halogen;

[68] R_{220} to R_{223} each independently represent hydrogen, deuterium, a (C1-C30)alkyl group unsubstituted or substituted with halogen(s), or a (C6-C30)aryl group unsubstituted or substituted with (C1-C30)alkyl group(s);

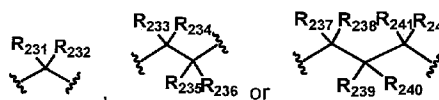
[69] R_{224} and R_{225} each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, or a halogen, or R_{224} and R_{225} are linked to an adjacent substituent(s) to form a mono- or polycyclic, (C5-C30)alicyclic or aromatic ring;

[70] R_{226} represents a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 5- or 30-membered heteroaryl group or a halogen;

[71] R_{227} to R_{229} each independently represent hydrogen, deuterium, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group or a halogen;

[72]

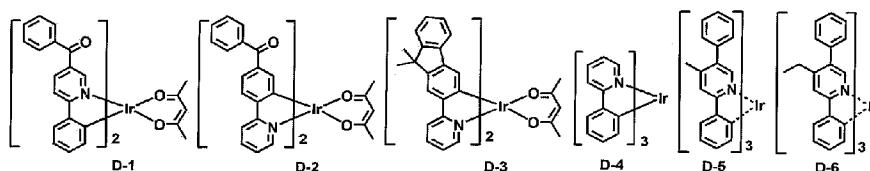
[73] Q represents



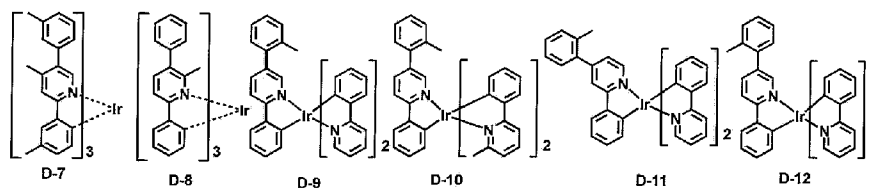
represent hydrogen, deuterium, a (C1-C30)alkyl group unsubstituted or substituted with halogen(s), a (C1-C30)alkoxy group, a halogen, a substituted or unsubstituted (C6-C30)aryl group, a cyano group, or a substituted or unsubstituted (C5-C30)cycloalkyl group, or each of R_{231} to R_{242} may be linked to an adjacent substituent via alkylene group or alkenylene group to form a spiro ring or a fused ring or may be linked to R_{207} or R_{208} via alkylene group or alkenylene group to form a saturated or unsaturated fused ring.

[74] The dopants of formula 2 include the following:

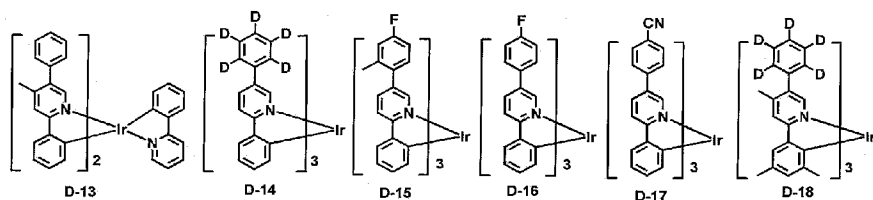
[75]



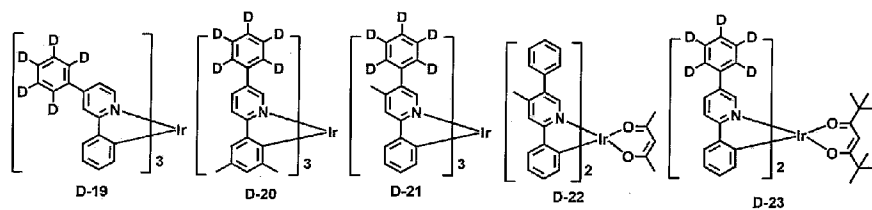
[76]



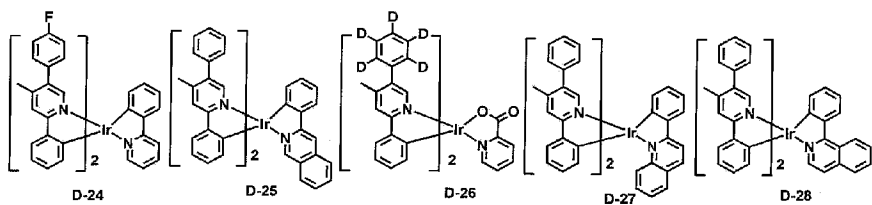
[77]



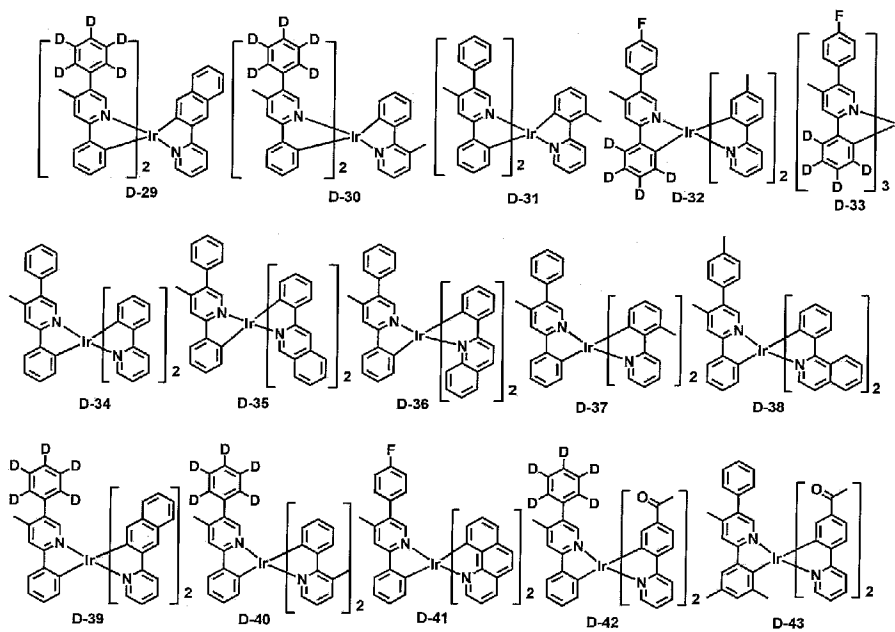
[78]



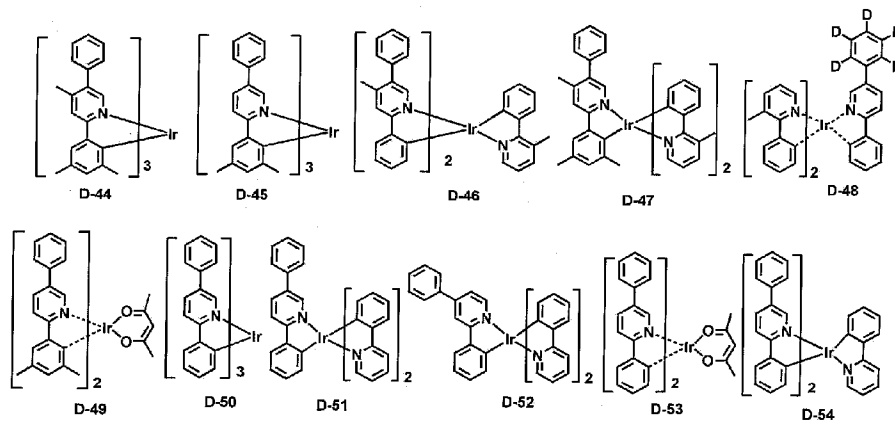
[79]



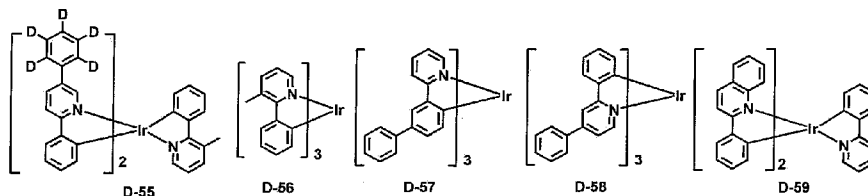
[80]



[81]



[82]

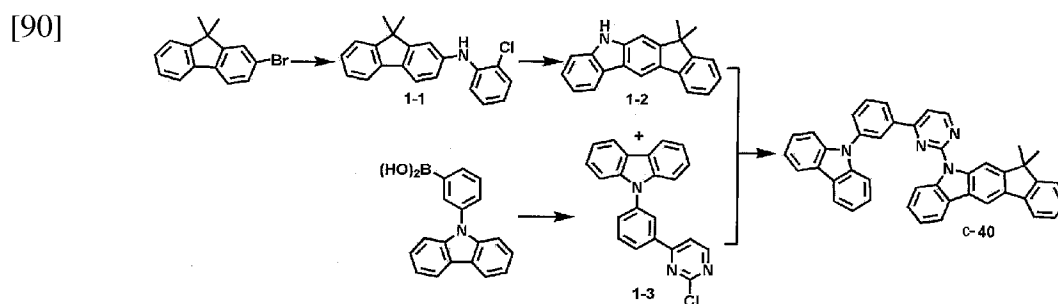


- [83] The organic electroluminescence device according to the present invention may further comprise, in addition to the compounds represented by formula 1, at least one compound selected from the group consisting of arylamine-based compounds and styrylarylamine-based compounds.
- [84] In the organic electroluminescence device according to the present invention, the organic layer may further comprise at least one metal selected from the group consisting of metals of Group 1, metals of Group 2, transition metals of the 4th period, transition metals of the 5th period, lanthanides and organic metals of d-transition elements of the Periodic Table, or at least one complex compound comprising said metal. The organic layer may comprise a light-emitting layer and a charge generating layer.
- [85] In addition, the organic electroluminescence device 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, besides the compound according to the present invention.
- [86] Preferably, in the organic electroluminescence 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. Such a surface layer provides operation stability for the organic electroluminescence 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.
- [87] Preferably, in the organic electroluminescence 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 electroluminescence device having two or more electroluminescent layers and emitting white light.

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

[89] **Example 1: Preparation of compound C-40**



[91] **Preparation of compound 1-1**

[92] After mixing 2-bromo-9,9-dimethyl-9H-fluorene (50 g, 183.0 mmol), 2-chloroaniline (38 mL, 366.1 mmol), Pd(OAc)₂ (1.2 g, 5.5 mmol), P(t-Bu)₃ (8.8 mL, 18.3 mmol), NaOt-Bu (35 g, 366.1 mmol) and toluene (180 mL), the reaction mixture was stirred for 2.5 hours under reflux. After terminating the reaction, the reaction mixture was filtered and the filtered cake was washed with dichloromethane. The obtained organic layer was washed with purified water and dried with MgSO₄, was concentrated under reduced pressure. And then, the crude oil was filtered through silica gel, and the remaining solution was concentrated under reduced pressure to obtain compound 1-1 (47 g, 80 %).

[93] **Preparation of compound 1-2**

[94] After mixing compound 1-1 (46 g, 143.8 mmol), Pd(OAc)₂ (968 mg, 4.3 mmol), di-t-butyl(methyl)phosphoniumtetrafluoroborate (2 g, 4.31 mmol) and DMAc (200 mL), the reaction mixture was stirred for 21 hours under reflux. After terminating the reaction, the reaction mixture was filtered, and the filtered cake was washed with dichloromethane. The obtained organic layer was washed with purified water and dried with MgSO₄, was concentrated under reduced pressure. And then, the crude oil was filtered through silica gel, and the remaining solution was concentrated under reduced pressure to obtain compound 1-2 (17 g, 53 %).

[95] **Preparation of compound 1-3**

[96] After mixing 3-(9H-carbazol-9-yl)phenyl boronic acid (7 g, 24.4 mmol), 2,4-dichloropyrimidine (3.9 g, 26.9 mmol), Pd(PPh₃)₄ (845 mg, 0.7 mmol), K₂CO₃ (6.7 g, 48.8 mmol), toluene (100 mL), EtOH (25 mL) and purified water (25 mL), the reaction mixture was stirred for 5 hours under reflux. After terminating the reaction, the reaction mixture was cooled to room temperature, was filtered, was dried with MgSO₄, was concentrated under reduced pressure, and was filtered through silica gel. The remaining solution was concentrated under reduced pressure to obtain compound 1-3 (6 g, 70 %).

[97] Preparation of compound C-40

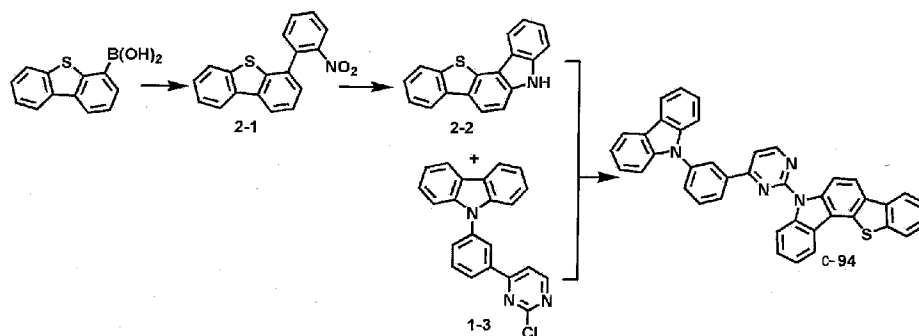
[98] After dissolving compound 1-2 (6.6 g, 18.6 mmol) in DMF (120 mL), NaH (813 mg, 20.3 mmol) was added at 0°C, and was stirred for 10 minutes. Compound 1-3 (4.8 g, 16.9 mmol) was added to the reaction mixture, and was stirred for 19 hours. After terminating the reaction, MeOH was added to the reaction mixture. The obtained solid was filtered through silica gel, was recrystallized with DMF to obtain compound C-40 (4 g, 36 %).

[99] MS/FAB found 603; calculated 602.73

[100]

[101] Example 2: Preparation of compound C-94

[102]



[103] Preparation of compound 2-1

[104] After mixing 1-bromo-2-nitrobenzene (85 g, 0.42 mol), dibenzo[b,d]thiophen-4-yl boronic acid (80 g, 0.35 mol), Pd(PPh₃)₄ (20 g, 0.018 mol), K₂CO₃ (116 g, 1.0 mol), toluene (1700 mL), EtOH (440 mL) and distilled water (440 mL), the reaction mixture was stirred for 12 hours at 120°C. After terminating the reaction, the reaction mixture was extracted with EA. The obtained organic layer was dried with MgSO₄, was filtered, was distilled under reduced pressure to remove the solvent, and was filtered through column to obtain compound 2-1 (93 g, 87 %).

[105] Preparation of compound 2-2

[106] After mixing compound 2-1 (88 g, 0.29 mol), P(OEt)₃ (960 mL, 0.4 M) and triethylphosphite (960 mL), the reaction mixture was stirred for 12 hours at 90°C. After terminating the reaction, the reaction mixture was distilled to remove triethylphosphite,

and was filtered through column to obtain compound 2-2 (40 g, 70 %)

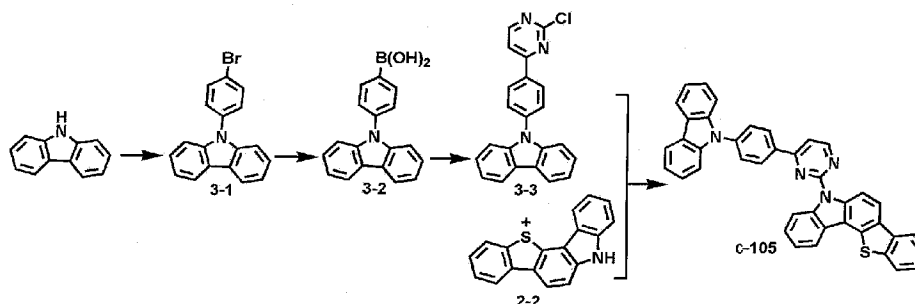
[107] Preparation of compound C-94

[108] After dissolving NaH 60 % (0.9 g, 0.02 mol) in DMF (50 mL), the solution was stirred. After dissolving compound 2-2 (4.69 g, 0.017 mol) in DMF (20 mL), the solution was added to the NaH solution, and was stirred for 1 hour. After dissolving compound 1-3 (6.1 g, 0.017 mol) in DMF (100 mL), the solution was stirred. And then, the mixed solution of compound 2-2 was added to the mixed solution of compound 1-3, and was stirred for 12 hours. After terminating the reaction, the obtained yellow solid was filtered, and was recrystallized to obtain compound C-94 (3 g, 30 %).

[109] MS/FAB found 593; calculated 592.71

[110] Example 3: Preparation of compound C-105

[111]



[112] Preparation of compound 3-1

[113] After mixing carbazole (26 g, 155.49 mmol), 4-bromoiodobenzene (87 g, 310.9 mmol), CuI (14.8 g, 77.74 mmol), ethylenediamine (9.3 g, 155.49 mmol), K₃PO₄ (99 g, 499.47 mmol), and toluene (1000 mL), the reaction mixture was stirred under reflux. After 15 hours, the reaction mixture was cooled to room temperature and was filtered under reduced pressure to remove CuI and K₃PO₄. The remaining solution was extracted with MC, was washed with distilled water, and then was filtered through column to obtain compound 3-1 (35 g, 70 %)

[114] Preparation of compound 3-2

[115] After dissolving compound 3-1 (35 g, 108.6 mmol) in THF (600 mL), and adding n-BuLi (52 mL, 130.35 mmol, 2.5 M in hexane) to the reaction mixture at -78°C, the reaction mixture was stirred for 1 hour. The reaction mixture was stirred for 12 hours at room temperature with adding B(Oi-Pr)₃ (37 mL, 162.9 mmol) slowly to the reaction mixture, and with slowly increasing the temperature. After extracting with EA, the obtained organic layer was dried with anhydrous MgSO₄ to remove the remaining moisture, was distilled under reduced pressure to remove the solvent, and was recrystallized with EA and hexane to obtain compound 3-2 (25 g, 81 %).

[116] Preparation of compound 3-3

[117] After mixing compound 3-2 (10 g, 34.82 mmol), 2,4-dichloropyrimidine (7.7 g,

52.24 mmol), $\text{Pd}(\text{PPh}_3)_4$ (1.6 g, 1.39 mmol), 2M Na_2CO_3 (45 mL), toluene (150 mL) and ethanol (45 mL), the reaction mixture was stirred under reduced pressure. After 12 hours, the reaction mixture was cooled to room temperature, distilled water was added, and the reaction mixture was extracted with EA. The obtained organic layer was dried with anhydrous MgSO_4 to remove the remaining moisture, was distilled under reduced pressure to remove the solvent, and was filtered through column to obtain compound 3-3 (11 g, 89 %).

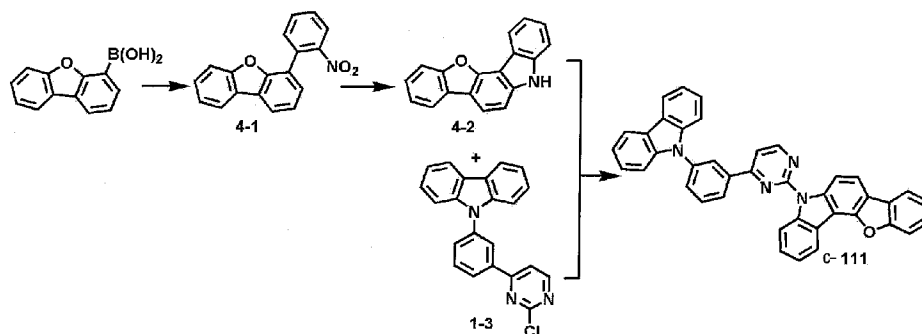
[118] Preparation of compound C-105

[119] After dissolving compound 2-2 (5 g, 18.29 mmol) and compound 3-3 (7.8 g, 21.94 mmol) in DMF (150 mL), NaH (1.09 g, 27.43 mmol, 60 % in mineral oil) was slowly added to the mixture, and was stirred for 12 hours at room temperature. And then, MeOH was added to the reaction mixture. The obtained solid was filtered under reduced pressure, and was recrystallized with EA and DMF to obtain compound C-105 (6.5 g, 60 %).

[120] MS/FAB found 593; calculated 592.71

[121] Example 4: Preparation of compound C-111

[122]



[123] Preparation of compound 4-1

[124] After mixing 1-bromo-2-nitrobenzene (44 g, 0.21 mol), dibenzo[b,d]furan-4-yl boronic acid (40 g, 0.18 mol), $\text{Pd}(\text{PPh}_3)_4$ (10.3 g, 0.008 mol), K_2CO_3 (72 g, 0.53 mol), toluene (880 mL), EtOH (300 mL) and distilled water (300 mL), the reaction mixture was stirred for 12 hours at 120°C. After terminating the reaction, the reaction mixture was extracted with EA. The obtained organic layer was dried with MgSO_4 , was filtered, was distilled under reduced pressure to remove the solvent, and was filtered through column to obtain compound 4-1 (43 g, 85 %).

[125] Preparation of compound 4-2

[126] After mixing compound 4-1 (43 g, 0.15 mol), $\text{P}(\text{OEt})_3$ (400 mL, 0.4 M) and triethylphosphite (400 mL), the reaction mixture was stirred for 12 hours at 90°C. After terminating the reaction, the reaction mixture was distilled to remove triethylphosphite, and was filtered through column to obtain compound 4-2 (30 g, 78 %).

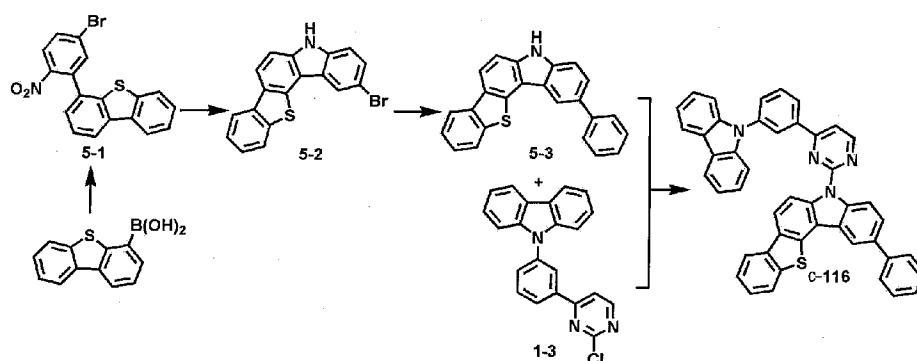
[127] Preparation of compound C-111

[128] After dissolving NaH 60 % (0.88 g, 0.022 mol) in DMF (100 mL), the solution was stirred. After dissolving compound 4-2 (4.34 g, 0.016 mol) in DMF (50 mL), the solution was added to the NaH solution, and was stirred for 1 hour. After dissolving compound 1-3 (6 g, 0.16 mol) in DMF (50 mL), the solution was stirred. And then, the mixed solution of compound 4-2 was added to the mixed solution of compound 1-3, and was stirred for 12 hours. After terminating the reaction, the obtained yellow solid was filtered, and was recrystallized to obtain compound C-111 (1.6 g, 18 %).

[129] MS/FAB found 577; calculated 576.64

[130] Example 5: Preparation of compound C-116

[131]



[132] Preparation of compound 5-1

[133] After mixing dibenzo[b,d]thiophen-4-yl boronic acid (41 g, 181 mmol), 1,3-dibromnitrobenzene (71 g, 254.5 mmol), 2 M Na₂CO₃ aqueous solution (270 mL), toluene (900 mL) and ethanol (300 mL), the reaction mixture was stirred under reflux. After 5 hours, the reaction mixture was cooled to room temperature, distilled water was added, and the reaction mixture was extracted with EA. The organic layer was dried with anhydrous MgSO₄ to remove the remaining moisture, was distilled under reduced pressure to remove the solvent, and was filtered through column to obtain compound 5-1 (34 g, 35 %)

[134] Preparation of compound 5-2

[135] After mixing compound 5-1 (34 g, 89.52 mmol), triethylphosphite (350 mL) and 1,2-dichlorobenzene (350 mL), the reaction mixture was stirred for 12 hours at 150°C. After terminating the reaction, the reaction mixture was cooled to room temperature, was distilled under reduced pressure to remove the solvent, and was recrystallized with EA to obtain compound 5-2 (11 g, 35 %).

[136] Preparation of compound 5-3

[137] After mixing compound 5-2 (7 g, 25.60 mmol), iodobenzene (10.44 g, 51.21 mmol), CuI (2.5 g, 12.80 mmol), K₃PO₄ (16.30 g, 76.82 mmol), and toluene (200 mL), the reaction mixture was heated to 50°C, ethylenediamine (1.72 mL, 25.60 mmol) was added, and was stirred under reflux for 12 hours. The reaction mixture was cooled to room temperature, was extracted with EA, was washed with aqueous solution of

NaHCO₃, was dried with MgSO₄, was filtered, was distilled under reduced pressure to remove the solvent, and was filtered through column to obtain compound 5-3 (8 g, 89 %).

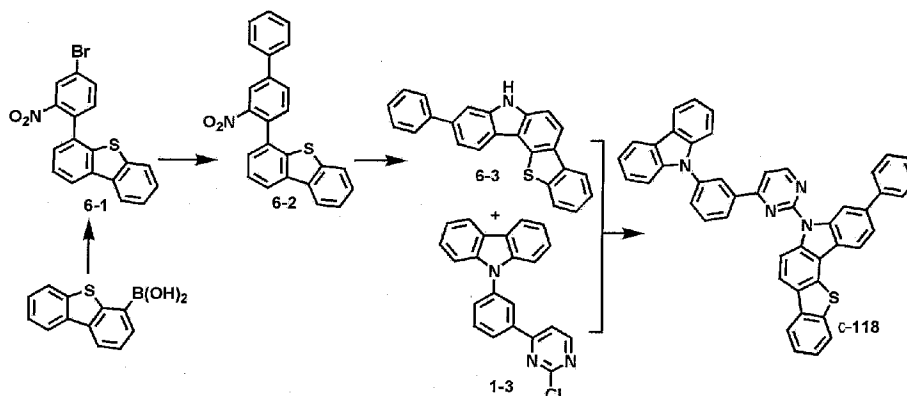
[138] Preparation of compound C-116

[139] After dissolving NaH (216 mg) in DMF (30 mL), the solution was stirred. After dissolving compound 5-3 (3.5 g, 10.015 mmol) in DMF (20 mL), the solution was added to the above NaH solution, and was stirred for 1 hour. After dissolving compound 1-3 (4.3 g, 12.0189 mmol) in DMF (20 mL), the solution was stirred. And then, the mixed solution of compound 5-3 was added to the mixed solution of compound 1-3, and was stirred for 12 hours. After terminating the reaction, the obtained yellow solid was filtered, and was recrystallized to obtain compound C-116 (12 g, 60 %).

[140] MS/FAB found 669; calculated 668.81

[141] Example 6: Preparation of compound C-118

[142]



[143] Preparation of compound 6-1

[144] After mixing 2,5-dibromonitrobenzene (30 g, 106.8 mmol), dibenzothiophen-4-ylboronic acid (20.3 g, 88.9 mmol), Pd(PPh₃)₄ (5.1 g, 4.45 mmol), Na₂CO₃ (27.9 g, 267 mmol), toluene (600 mL) and EtOH (100 mL), the reaction mixture was stirred for 3 hours at 90°C. After stirring, purified water was added, and the reaction mixture was extracted with EA. The obtained organic layer was dried with MgSO₄ to remove the remaining moisture, was distilled under reduced pressure to remove the solvent, and was filtered through column to obtain compound 6-1 (24 g, 59 %).

[145] Preparation of compound 6-2

[146] After mixing compound 6-1 (23 g, 59.85 mmol), phenylboronic acid (8.8 g, 71.83 mmol), Pd(PPh₃)₄ (3.46 g, 2.99 mmol), Na₂CO₃ (19 g, 179.5 mmol), toluene (180 mL) and EtOH (90 mL), the reaction mixture was stirred for 3 hours at 120°C. After stirring, purified water was added, and the reaction mixture was extracted with EA. The obtained organic layer was dried with MgSO₄ to remove the remaining moisture, was distilled under reduced pressure to remove the solvent, and was filtered through

column to obtain compound 6-2 (22 g, 96 %).

[147] Preparation of compound 6-3

[148] After mixing compound 6-2 (15 g, 39.3 mmol), and triethylphosphite (150 mL), the reaction mixture was stirred for 24 hours at 150°C. After stirring, the remaining solvent was removed using distillation device, and the reaction mixture was filtered through column to obtain compound 6-3 (6 g, 46 %).

[149] Preparation of compound C-118

[150] After dissolving NaH (600 mg, 18.1 mmol) in DMF (30 mL), the solution was stirred. After dissolving compound 6-3 (5 g, 14.3 mmol) in DMF (30 mL), the solution was added to the above NaH solution, and was stirred for 1 hour. After dissolving compound 1-3 (4.3 g, 11.9 mmol) in DMF (30 mL), the solution was stirred. And then, the mixed solution of compound 6-3 was added to the mixed solution of compound 1-3, and was stirred for 24 hours at room temperature. After terminating the reaction, the obtained solid was filtered, was washed with EA, and was filtered through column to obtain compound C-118 (1.8 g, 23 %).

[151] MS/FAB found 669; calculated 668.81

[152] Experimental Example 1: Production of an OLED device using the compound according to the present invention

[153] An OLED device was produced using the compound 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. N¹,N^{1'}-([1,1'-biphenyl]-4,4'-diyl)bis(N¹-(naphthalen-1-yl)-N⁴,N^{4'}-diphenylbenzene-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, N,N'-di(4-biphenyl)-N,N'-di(4-biphenyl)-4,4'-diaminobiphenyl was introduced into another cell of said 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-40 was introduced into one cell of the vacuum vapor depositing apparatus, as a host material, and compound D-5 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% 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)-1-phenyl-1H-benzo[d]imidazole was introduced into one cell and lithium quinolate was introduced into another cell. The two materials were evaporated at same rates and were 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 material used for producing the OLED device were purified by vacuum sublimation at 10^{-6} torr prior to use.

[154] The produced OLED device showed green emission having a luminance of 1110 cd/m² and a current density of 2.33 mA/cm² at a driving voltage of 3.9 V.

[155] Experimental Example 2: Production of an OLED device using the compound according to the present invention

[156] An OLED device was produced in the same manner as in Example 1, except for using compound C-94 as a host material, and compound D-5 as a dopant. The produced OLED device showed green emission having a luminance of 1110 cd/m² and a current density of 2.08 mA/cm² at a driving voltage of 3.9 V.

[157] Experimental Example 3: Production of an OLED device using the compound according to the present invention

[158] An OLED device was produced in the same manner as in Example 1, except for using compound C-105 as a host material, and compound D-34 as a dopant. The produced OLED device showed green emission having a luminance of 1170 cd/m² and a current density of 2.53 mA/cm² at a driving voltage of 4.0 V.

[159] Experimental Example 4: Production of an OLED device using the compound according to the present invention

[160] An OLED device was produced in the same manner as in Example 1, except for using compound C-111 as a host material, and compound D-5 as a dopant. The produced OLED device showed green emission having a luminance of 1150 cd/m² and a current density of 2.12 mA/cm² at a driving voltage of 4.2 V.

[161] Experimental Example 5: Production of an OLED device using the compound according to the present invention

[162] An OLED device was produced in the same manner as in Example 1, except for using compound C-118 as a host material, and compound D-5 as a dopant. The produced OLED device showed orange emission having a luminance of 1090 cd/m² and a current density of 2.22 mA/cm² at a driving voltage of 3.8 V.

[163] Comparative Example 1: Production of an OLED device using conventional electro-

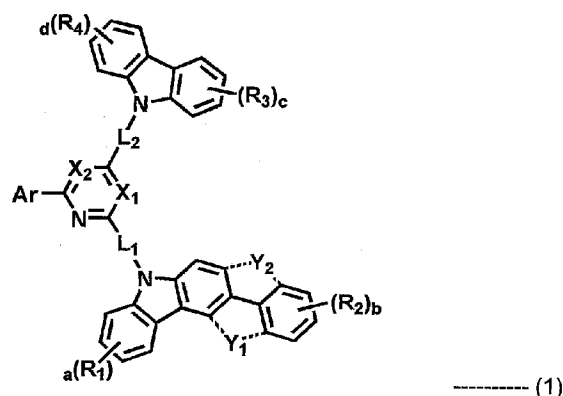
luminescent compounds

- [164] An OLED device was produced in the same manner as that of 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 material and compound D-5 as a dopant and that a hole blocking layer having a thickness of 10 nm was deposited by using aluminum(III) bis(2-methyl-8-quinolinato)-4-phenylphenolate.
- [165] The produced OLED device showed green emission having a luminance of 1000 cd/m² and a current density of 2.86 mA/cm² at a driving voltage of 4.9 V.
- [166] The organic electroluminescence compounds of the present invention have superior luminous characteristics than the conventional materials. In addition, a device using the compounds according to the present invention as a green or orange light emitting host material not only has excellent luminous characteristics, but also induces an increase in power efficiency by reducing the driving voltage.

Claims

[Claim 1]

A compound represented by the following formula 1:



wherein

L_1 and L_2 each independently represent a single bond, a substituted or unsubstituted 3- to 30-membered heteroarylene group, a substituted or unsubstituted (C6-C30)arylene group, or a substituted or unsubstituted (C3-C30)cycloalkylene group;

X_1 and X_2 represent CH or N;

Y_1 and Y_2 each independently represent -O-, -S-, -CR₅R₆- or -NR₇-, provided that Y_1 and Y_2 do not simultaneously exist;

Ar represents hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- to 30-membered heteroaryl group, or an N-carbazolyl group;

R_1 to R_4 each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 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(C1-C30)alkyl group, -NR₁₁R₁₂, -SiR₁₃R₁₄R₁₅, -SR₁₆, -OR₁₇, a cyano group, a nitro group, or a hydroxyl 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;

R_5 to R_7 and R_{11} to R_{17} each independently represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (C1-C30)alkyl

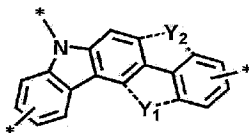
group, a substituted or unsubstituted (C6-C30)aryl group, a substituted or unsubstituted 3- to 30-membered heteroaryl group, a substituted or unsubstituted 5- to 7-membered heterocycloalkyl group, or a substituted or unsubstituted (C3-C30)cycloalkyl group; or are linked to an adjacent substituent(s) 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;

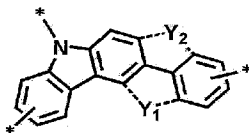
a, b, c and d each independently represent an integer of 1 to 4; where a, b, c or d is an integer of 2 or more, each of R₁, each of R₂, each of R₃ or each of R₄ is the same or different; and the heterocycloalkyl group, the heteroarylene group and the heteroaryl group contain at least one hetero atom selected from B, N, O, S, P(=O), Si and P.

[Claim 2]

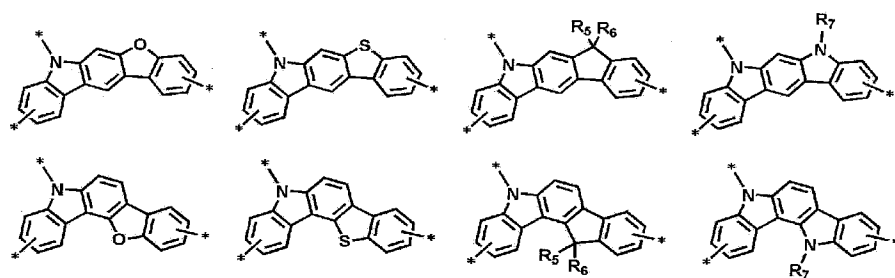
The compound according to claim 1, wherein the substituents of the substituted alkyl group, the substituted aryl(ene) group, the substituted heteroaryl(ene) group, the substituted cycloalkyl(ene) group, the substituted heterocycloalkyl group, and the substituted aralkyl group in L₁, L₂, Ar, R₁ to R₇ and R₁₁ to R₁₇ groups each independently are at least one selected from the group consisting of deuterium; a halogen; a (C1-C30)alkyl group substituted or unsubstituted with a halogen; a (C6-C30)aryl group; a 3- to 30-membered heteroaryl group substituted or unsubstituted with a (C1-C30)alkyl or (C6-C30)aryl; a (C3-C30)cycloalkyl group; a 5- to 7-membered heterocycloalkyl group; a tri(C1-C30)alkylsilyl group; a tri(C6-C30)arylsilyl group; a di(C1-C30)alkyl(C6-C30)aryl silyl group; a (C1-C30)alkyldi(C6-C30)arylsilyl group; a (C2-C30)alkenyl group; a (C2-C30)alkynyl group; a cyano group; an N-carbazolyl group; a di(C1-C30)alkylamino group; a di(C6-C30)arylamino group; a (C1-C30)alkyl(C6-C30)arylamino group; a di(C6-C30)arylboronyl group; a di(C1-C30)alkylboronyl group; a (C6-C30)aryl(C1-C30)alkyl group; a (C1-C30)alkyl(C6-C30)arylboronyl group; a (C1-C30)alkyl(C6-C30)aryl group; a carboxyl group; a nitro group; and a hydroxyl group.

[Claim 3]

The compound according to claim 1, wherein the moiety,  in formula 1 is selected from the



following structures:



wherein R5, R6 and R7 are as defined in claim 1.

[Claim 4]

The compound according to claim 1, wherein

L_1 and L_2 each independently represent a single bond, a 3- to 30-membered heteroarylene group, or a (C6-C30)arylene group;

X_1 and X_2 each independently represent CH or N;

Y_1 and Y_2 each independently represent -O-, -S-, -CR₅R₆- or -NR₇-, provided that Y_1 and Y_2 do not simultaneously exist;

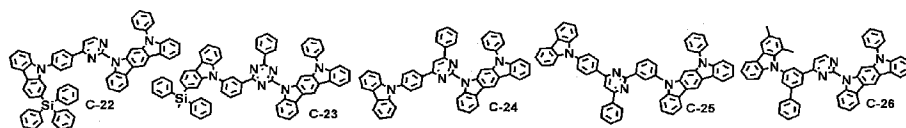
Ar represents hydrogen, deuterium, a halogen, a (C1-C30)alkyl group, a (C6-C30)aryl group, a 3- to 30-membered heteroaryl group, or an N-carbazolyl group;

R_1 to R_4 each independently represent hydrogen, deuterium, a halogen, a (C1-C30)alkyl group, a (C6-C30)aryl group, a 3- to 30-membered heteroaryl group, an N-carbazolyl group, or -SiR₁₃R₁₄R₁₅;

R_5 to R_7 each independently represent a (C1-C30)alkyl group, a (C6-C30)aryl group, or a 3- to 30-membered heteroaryl group; or R_5 and R_6 are linked to each other 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;

R_{13} to R_{15} each independently represent a (C1-C30)alkyl group, a (C6-C30)aryl group, or a 3- to 30-membered heteroaryl group; and the arylene group and the heteroarylene group in L_1 and L_2 , the alkyl group, the aryl group, the heteroaryl group and the N-carbazolyl group in Ar, the alkyl group, the aryl group, the heteroaryl group and the N-carbazolyl group in R_1 to R_4 , and the alkyl group, the aryl group and the heteroaryl group in R_5 to R_7 and R_{13} to R_{15} each independently can be substituted with at least one selected from the group consisting of deuterium; a halogen; a (C1-C30)alkyl group substituted or unsubstituted with a halogen; a (C6-C30)aryl group; a 3- to 30-membered heteroaryl group substituted or unsubstituted with a (C1-C30)alkyl or (C6-C30)aryl; a (C3-C30)cycloalkyl group; an N-carbazolyl group; a

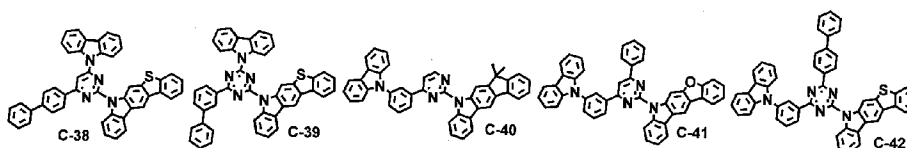
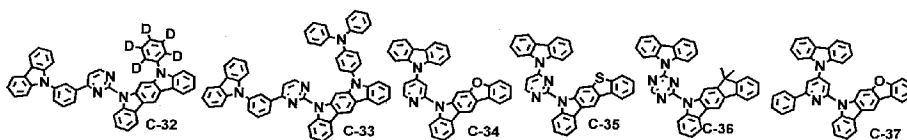
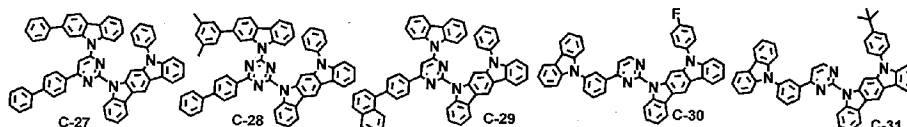
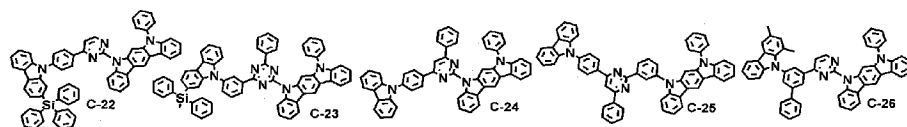
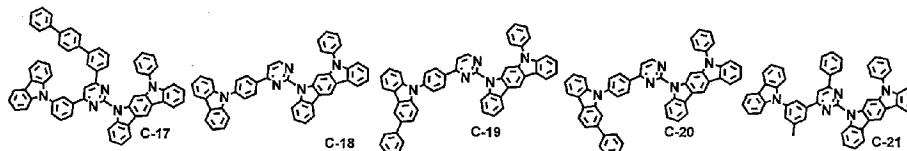
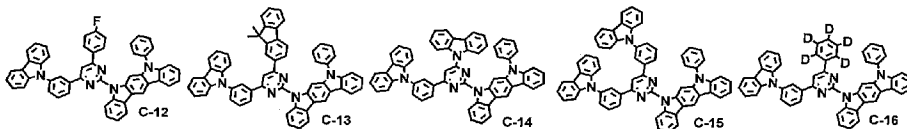
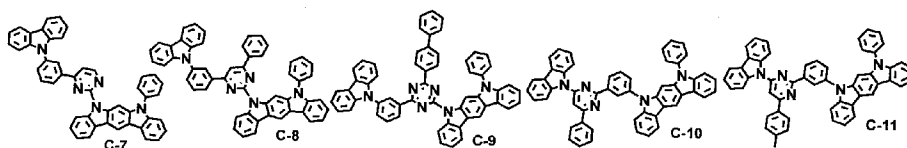
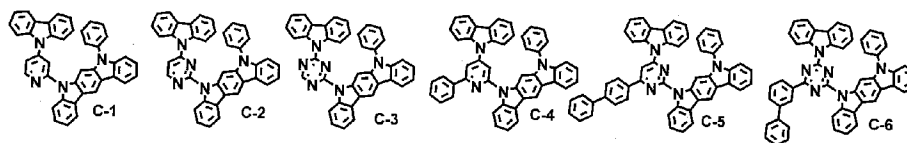
di(C1-C30)alkylamino group; a di(C6-C30)arylamino group; a
(C1-C30)alkyl(C6-C30)aryl amino group; a
(C6-C30)aryl(C1-C30)alkyl group; and a

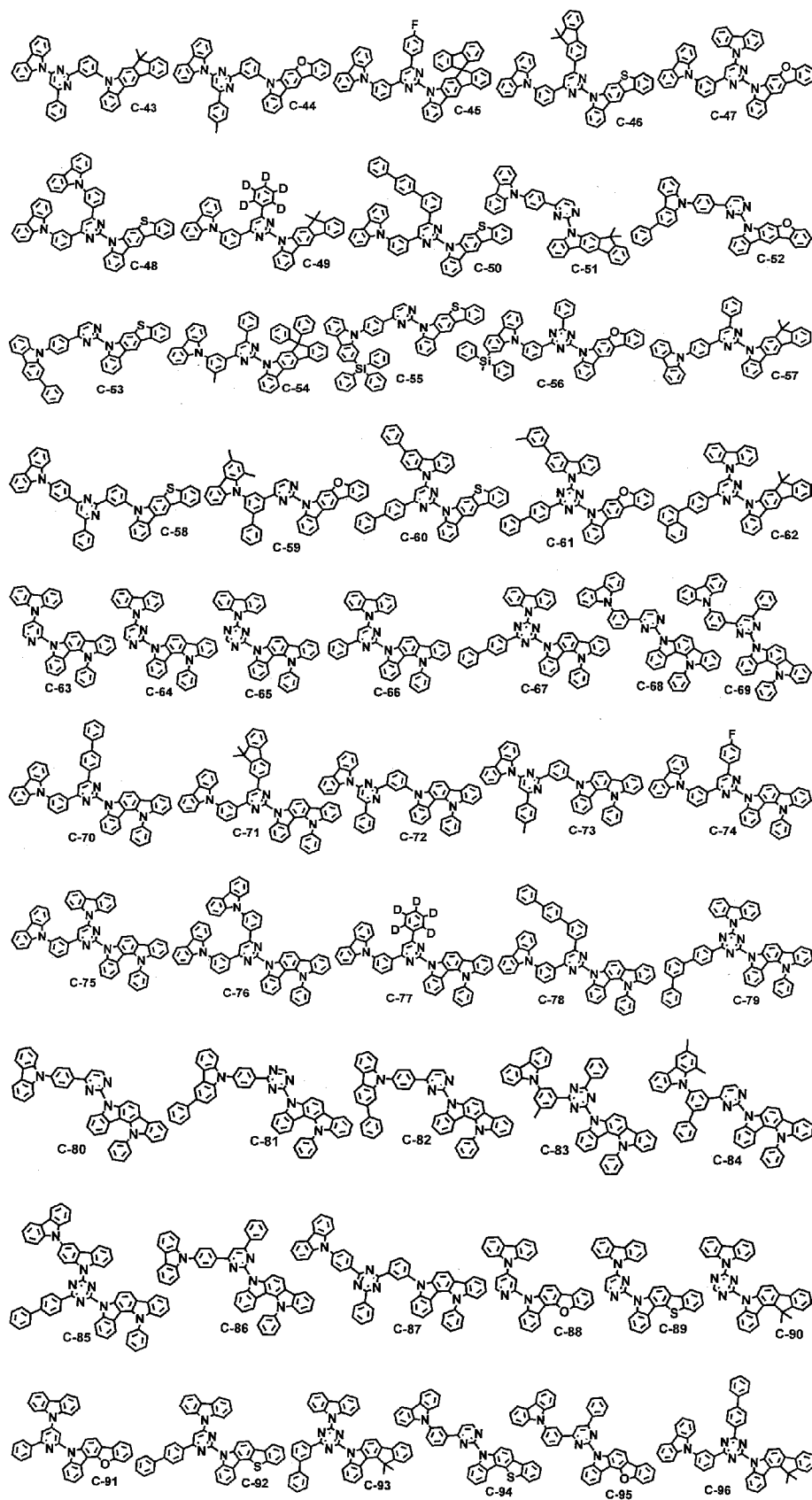


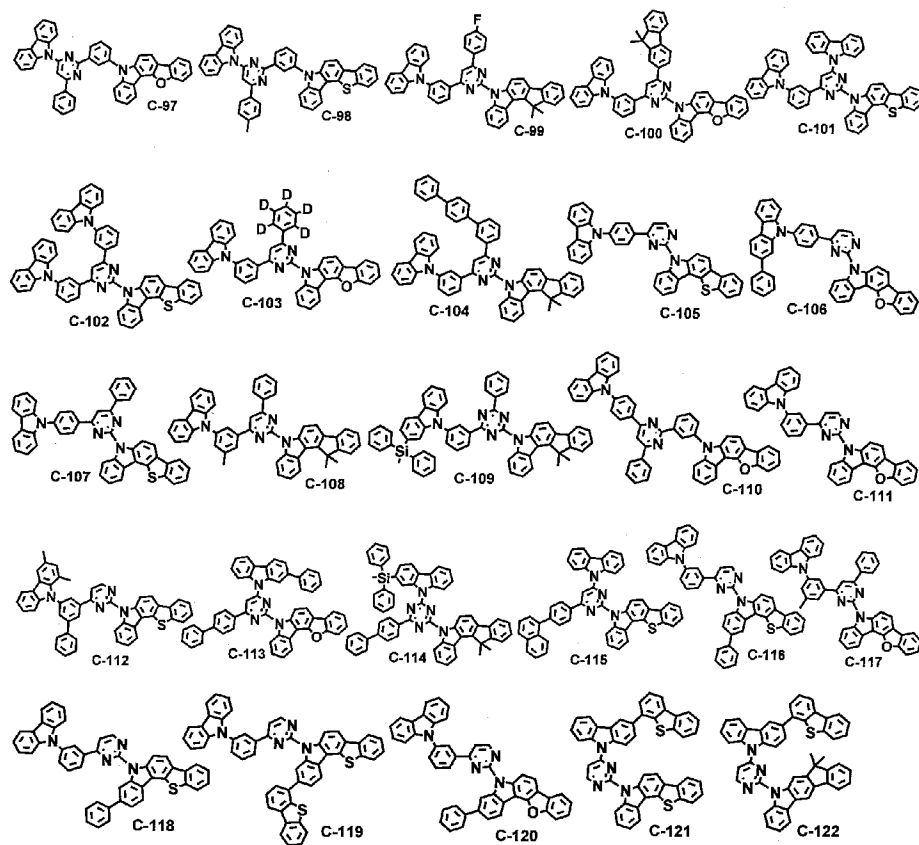
(C1-C30)alkyl(C6-C30)aryl group.

[Claim 5]

The compound according to claim 1, wherein the compound represented by formula 1 is selected from the group consisting of:







[Claim 6]

An organic electroluminescent device comprising the compound according to claim 1.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/KR2012/005840

A. CLASSIFICATION OF SUBJECT MATTER

C07D 487/04 (2006.01) C07D 495/04 (2006.01) C07D 491/04 (2006.01) C07D 403/04 (2006.01) C07D 409/14 (2006.01)
 C07F 7/02 (2006.01) C09K 11/06 (2006.01) H01L 51/54 (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)

Registry, CAPLUS: substructure search based on claim 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	

☒ Further documents are listed in the continuation of Box C☒ See patent family annex

* Special categories of cited documents:	
"A" document defining the general state of the art which is not considered to be of particular relevance	"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
"E" earlier application or patent but published on or after the international filing date	"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
"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)	"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
"O" document referring to an oral disclosure, use, exhibition or other means	"&" document member of the same patent family
"P" document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search
 28 September 2012

Date of mailing of the international search report
 28 September 2012

Name and mailing address of the ISA/AU

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

Authorised officer

Alica Daly
 AUSTRALIAN PATENT OFFICE
 (ISO 9001 Quality Certified Service)
 Telephone No. 0399359606

INTERNATIONAL SEARCH REPORT		International application No.
C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT		PCT/KR2012/005840
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	KR 10-2010-0094415 A (SFC LTD.) 26 August 2010 See abstract; compounds 67 & 69; p10.	1, 3, 6
X	WO 2010/136109 A1 (MERCK PATENT GMBH) 02 December 2010 See abstract; examples 21, 43 & 53b; compounds H18, H21 & H47; pp32, 50 & 52.	1, 3, 6
X	WO 2010/151084 A2 (CHEIL INDUSTRIES INC.) 29 December 2010 See abstract; compounds 15, 16, 30 & 31; pp12-14.	1, 3, 6
X	WO 2011/010844 A1 (ROHM AND HAAS ELECTRONIC MATERIALS KOREA LTD.) 27 January 2011 See abstract; chemical formulae 3, 6, TA3, TA6, TC3 & TC6; pp3-9 & 26; claim 1.	1-6
P,X	WO 2011/108902 A2 (DUKSAN HIGH METAL CO., LTD.) 09 September 2011 See abstract; compounds 33-64; intermediate C; pp7-8 & 13.	1-3, 6
P,X	KR 10-2011-0110508 A (SFC LTD.) 07 October 2011 See abstract; compounds 291, 292 & 300; p41.	1, 3, 6
P,X	WO 2011/136755 A1 (UNIVERSAL DISPLAY CORPORATION et al.) 03 November 2011 See abstract; paragraph [0001]; compound H235; p23.	1, 3, 4, 6

INTERNATIONAL SEARCH REPORT		International application No.	
Information on patent family members		PCT/KR2012/005840	
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
KR 10-2010-0094415 A	26 Aug 2010	None	
WO 2010/136109 A1	02 Dec 2010	CN 102448946 A	09 May 2012
		CN 102498120 A	13 Jun 2012
		CN 102498121 A	13 Jun 2012
		DE 102009023155 A1	02 Dec 2010
		DE 102009041414 A1	17 Mar 2011
		DE 102009053644 A1	19 May 2011
		DE 102009053645 A1	19 May 2011
		EP 2477999 A1	25 Jul 2012
		KR 20100129101 A	08 Dec 2010
		KR 20100130197 A	10 Dec 2010
		KR 20120081155 A	18 Jul 2012
		KR 20120081603 A	19 Jul 2012
		TW 201114742 A	01 May 2011
		TW 201124422 A	16 Jul 2011
		TW 201134786 A	16 Oct 2011
		US 2012068170 A1	22 Mar 2012
		US 2012175561 A1	12 Jul 2012
		US 2012228552 A1	13 Sep 2012
		US 2012228554 A1	13 Sep 2012
		US 2012238105 A1	20 Sep 2012
		WO 2010136109 A1	02 Dec 2010
		WO 2011032626 A1	24 Mar 2011
		WO 2011032686 A1	24 Mar 2011
		WO 2011060859 A1	26 May 2011
		WO 2011060877 A2	26 May 2011
		WO 2011137922 A1	10 Nov 2011
		WO 2011157339 A1	22 Dec 2011
WO 2010/151084 A2	29 Dec 2010	CN 102459506 A	16 May 2012
		EP 2447335 A2	02 May 2012
		KR 20100138631 A	31 Dec 2010
		US 2012091445 A1	19 Apr 2012
		WO 2010151084 A2	29 Dec 2010
WO 2011/010844 A1	27 Jan 2011	CN 102625819 A	01 Aug 2012

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

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

Form PCT/ISA/210 (Family Annex)(July 2009)

INTERNATIONAL SEARCH REPORT Information on patent family members		International application No. PCT/KR2012/005840	
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
		KR 20110009920 A	31 Jan 2011
		TW 201109305 A	16 Mar 2011
		US 2012206037 A1	16 Aug 2012
		WO 2011010844 A1	27 Jan 2011
WO 2011/108902 A2	09 Sep 2011	KR 20110100877 A	15 Sep 2011
		WO 2011108902 A2	09 Sep 2011
KR 10-2011-0110508 A	07 Oct 2011	None	
WO 2011/136755 A1	03 Nov 2011	TW 201209047 A	01 Mar 2012
		WO 2011136755 A1	03 Nov 2011
End of Annex			

Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001.
 Form PCT/ISA/210 (Family Annex)(July 2009)