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

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
23 September 2010 (23.09.2010)

PCT

(10) International Publication Number
WO 2010/107244 A2

(51) International Patent Classification:
C09K 11/06 (2006.01)

(21) International Application Number:
PCT/KR2010/001647

(22) International Filing Date:
17 March 2010 (17.03.2010)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
10-2009-0023944 20 March 2009 (20.03.2009) KR

(71) Applicant *(for all designated States except US)*: **DOW ADVANCED DISPLAY MATERIALS, LTD.** [KR/KR]; 735-2, Baekseok-dong, Seobuk-gu, Cheonan-si, Chungcheongnam-do 331-980 (KR).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **KIM, Chi Sik** [KR/KR]; F3, 14-60, Seongsu1-ga, Seongdong-gu, Seoul 133-111 (KR). **CHO, Young Jun** [KR/KR]; #101-1111, Samsung Apt., 15-1, Donam-dong, Seongbuk-gu, Seoul 136-060 (KR). **KWON, Hyuck Joo** [KR/KR]; #224-2001, Samsung Raemian 2 Cha, Jangan-dong, Dongdaemun-gu, Seoul 130-100 (KR). **KIM, Bong Ok** [KR/KR]; #101-1108, Hansol Apt., 4, Samseong-dong, Gangnam-gu, Seoul 135-090 (KR). **KIM, Sung Min** [KR/KR]; #109-902, Mokdong Paragon, 917, Mok 1-dong, Yangcheon-gu, Seoul 158-761 (KR). **YOON, Seung Soo** [KR/KR]; #405-1409, Samik Apt., Suseo-dong, Gangnam-gu, Seoul 135-884 (KR).

(74) Agents: **KWON, Oh-Sig** et al.; 4F, Jooeunleaderstel, 921, Dunsan-dong, Seo-gu, Daejeon 302-120 (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, RO, RS, RU, 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, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (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, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— *without international search report and to be republished upon receipt of that report (Rule 48.2(g))*

WO 2010/107244 A2

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

(57) Abstract: Disclosed are a novel organic electroluminescent compound and an organic electroluminescent device comprising the same. When used as host material of organic electroluminescent material of an OLED device, the disclosed organic electroluminescent compound exhibits high luminous efficiency and excellent life property of the material as compared to conventional host material. Therefore, it can be used to manufacture OLEDs having very good operation life.

Description

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

Technical Field

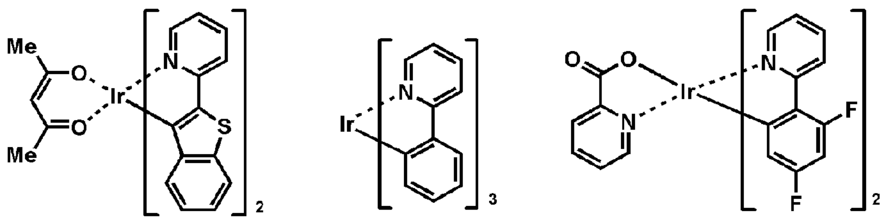
[1] The present invention relates to novel organic electroluminescent compounds and organic electroluminescent devices comprising the same. Specifically, it relates to novel organic electroluminescent compounds employed as electroluminescent material, and organic electroluminescent devices using them as a host.

Background Art

[2] The most important factor to determine luminous efficiency of an OLED (organic light-emitting diode) is the type of electroluminescent material. Though fluorescent materials has been widely used as an electroluminescent material up to the present, development of phosphorescent materials is one of the best methods to improve the luminous efficiency theoretically up to four(4) times, in view of electroluminescent mechanism.

[3] Up to now, iridium (III) complexes are widely known as phosphorescent material, including (acac)Ir(btp)$_2$, Ir(ppy)$_3$ and Firpic, as the red, green and blue one, respectively. In particular, a lot of phosphorescent materials have been recently investigated in Japan, Europe and America.

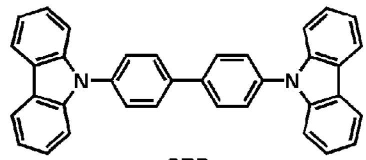
[4]

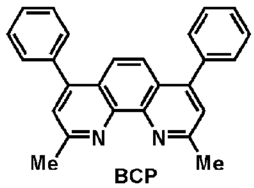


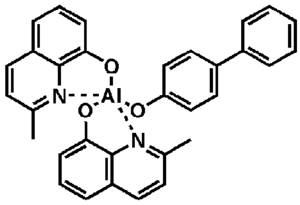
(acac)Ir(btp)$_2$ Ir(ppy)$_3$ Firpic

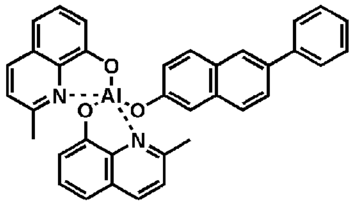
[5] As a host material for phosphorescent light emitting material, 4,4'-N,N'-dicarbazole-biphenyl (CBP) has been most widely known up to the present, and OLED's having high efficiency to which a hole blocking layer (such as BCP and BAlq) had been applied have been known. Pioneer (Japan) or the like reported OLED's of high performances which employs bis(2-methyl-8-quinolinato)(p-phenylphenolato)aluminum (III) (BAlq) derivatives as the host.

[6]


CBP


BCP


BAlq


BAlq derivative

[7] Though the materials in prior art are advantageous in view of light emitting property, they have low glass transition temperature and very poor thermal stability, so that the materials tend to be changed during the process vapor-deposition in vacuo at high temperature. In an OLED, it is defined that power efficiency = (π/voltage) x current efficiency. Thus, the power efficiency is inversely proportional to the voltage, and the power efficiency should be higher in order to obtain lower power consumption of an OLED. In practice, an OLED employing phosphorescent electroluminescent material shows significantly higher current efficiency (cd/A) than an OLED employing fluorescent EL material. However, in case that a conventional material such as BAlq and CBP as host material of the phosphorescent material is employed, no significant advantage can be obtained in terms of power efficiency (lm/w) because of higher operating voltage as compared to an OLED employing a fluorescent material. Moreover, such an OLED cannot result in satisfactory device life.

[8] Thus, development of host material having more improved stability and performances is required.

Disclosure of Invention

Technical Problem

[9] The present inventors endeavored to overcome the problems of conventional techniques, and consequently invented novel electroluminescent compounds to realize organic electroluminescent devices having excellent luminous efficiency and remarkably lengthened device life.

[10] Thus, the object of the invention is to overcome those problems and to provide organic electroluminescent compounds comprising a backbone to result in better luminous efficiency, improved device life, and appropriate color coordinate, as compared to conventional host materials.

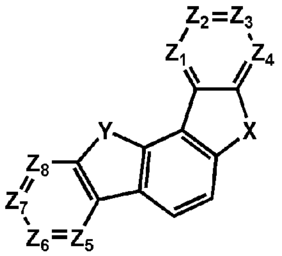
[11] Another object of the invention is to provide organic electroluminescent devices having high efficiency and long life, which employ such organic electroluminescent

compounds as electroluminescent material.

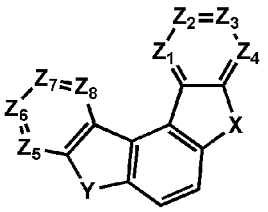
Solution to Problem

[12] Specifically, the present invention relates to organic electroluminescent compounds represented by one of Chemical Formulas (1) to (5), and organic electroluminescent devices comprising the same. Since the organic electroluminescent compounds according to the present invention provide better luminous efficiency and excellent life property as compared to conventional host material, OLED's having excellent operation life can be obtained therefrom.

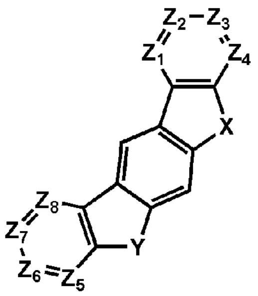
[13] [Chemical Formula 1]

[14] 

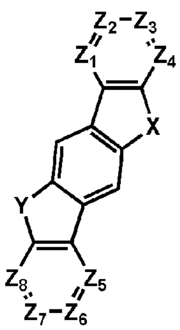
[15] [Chemical Formula 2]

[16] 

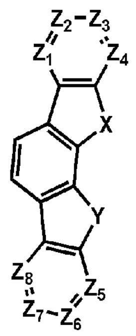
[17] [Chemical Formula 3]

[18] 

[19] [Chemical Formula 4]

[20] 

[21] [Chemical Formula 5]

[22] 

[23] wherein,

[24] X and Y are independently selected from N(Ar_1), O and S, wherein Ar_1 may be different from one another, and Ar_1 may be represented as Ar_1 or Ar_2 where there are two or more Ar_1 groups;

[25] Z_1 through Z_8 are independently selected from C(Ar_3) and N, wherein Ar_3 may be different from one another, and adjacent Ar_3 groups may be linked together to form a ring;

[26] Ar_1 and Ar_2 are independently selected from (C1-C60)alkyl, (C3-C60)cycloalkyl, 5- or 6-membered heterocycloalkyl containing one or more heteroatom(s) selected from N, O, S, Si and P, (C7-C60)bicycloalkyl, adamantyl, (C2-C60)alkenyl, (C2-C60)alkynyl, (C6-C60)aryl and (C3-C60)heteroaryl;

[27] Ar_3 are independently selected from hydrogen, (C1-C60)alkyl, halogen, cyano, (C3-C60)cycloalkyl, 5- or 6-membered heterocycloalkyl containing one or more heteroatom(s) selected from N, O, S, Si and P, (C7-C60)bicycloalkyl, adamantyl, (C2-C60)alkenyl, (C2-C60)alkynyl, (C6-C60)aryl, (C1-C60)alkoxy, (C6-C60)aryloxy, (C3-C60)heteroaryl, (C6-C60)arylthio, (C1-C60)alkylthio, mono- or di(C1-C30)alkylamino, mono- or di(C6-C30)arylamino, tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, mono- or di(C6-C30)arylboranyl, mono- or di(C1-C60)alkylboranyl, nitro and hydroxyl; and

[28] the alkyl, cycloalkyl, heterocycloalkyl, bicycloalkyl, adamantyl, alkenyl, alkynyl, aryl, alkoxy, aryloxy, heteroaryl, arylthio, alkylthio, alkylamino, arylamino, tri-alkylsilyl, dialkylarylsilyl, triarylsilyl, arylboranyl or alkylboranyl of Ar_1 through Ar_3 may be further substituted by one or more substituent(s) selected from a group consisting of (C1-C60)alkyl, halogen, cyano, (C3-C60)cycloalkyl, 5- or 6-membered heterocycloalkyl containing one or more heteroatom(s) selected from N, O, S, Si and P, (C7-C60)bicycloalkyl, adamantyl, (C2-C60)alkenyl, (C2-C60)alkynyl, (C6-C60)aryl, (C1-C60)alkoxy, (C6-C60)aryloxy, (C6-C60)aryl substituted by P(=O)R_aR_b [R_a and R_b independently represent (C1-C60)alkyl or (C6-C60)aryl], (C3-C60)heteroaryl, (C3-C60)heteroaryl subsitituted by (C6-C60)aryl, (C3-C60)heteroaryl substituted by (C1-C60)alkyl, (C6-C60)ar(C1-C60)alkyl,

(C6-C60)arylthio, (C1-C60)alkylthio, mono- or di(C1-C30)alkylamino, mono- or di(C6-C30)arylamino, tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, mono- or di(C6-C30)arylboranyl, mono- or di(C1-C60)alkylboranyl, nitro and hydroxyl,

[29] excluding the case where both X and Y are N(Ar_1) and all of Z_1 through Z_8 are C(Ar_3).

[30]

[31] The substituents, as described here, which comprises "(C1-C60)alkyl" moiety may contain from 1 to 60 carbon atoms, from 1 to 20 carbon atoms, or from 1 to 10 carbon atoms. The substituents comprising "(C6-C60)aryl" moiety may contain from 6 to 60 carbon atoms, from 6 to 20 carbon atoms, or from 6 to 12 carbon atoms. Those comprising "(C3-C60)heteroaryl" moiety may contain from 3 to 60 carbon atoms, from 4 to 20 carbon atoms, or from 4 to 12 carbon atoms. Those comprising "(C3-C60)cycloalkyl" moiety may contain from 3 to 60 carbon atoms, from 3 to 20 carbon atoms, or from 3 to 7 carbon atoms. The substituents comprising "(C2-C60)alkenyl or alkynyl" moiety may contain from 2 to 60 carbon atoms, from 2 to 20 carbon atoms, or from 2 to 10 carbon atoms.

[32] The term 'alkyl' of the present invention include linear or branched saturated monovalent hydrocarbon radicals or combinations thereof, which are composed only of carbon atoms and hydrogen atoms. The term 'alkoxy' means -O-alkyl group, in which alkyl is defined as above.

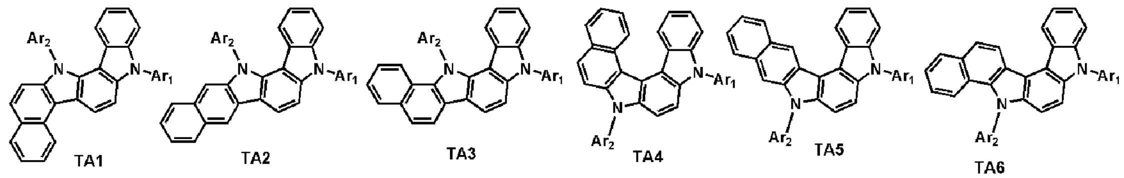
[33] The term "aryl" described herein represents an organic radical derived from aromatic hydrocarbon by deleting one hydrogen atom therefrom. Aryl groups include monocyclic and fused ring system, each ring of which suitably contains from 4 to 7, preferably from 5 or 6 cyclic atoms. Structures wherein two or more aryl groups are combined through chemical bond(s) are also included. Specific examples include phenyl, naphthyl, biphenyl, anthryl, indenyl, fluorenyl, phenanthryl, triphenylenyl, pyrenyl, perylenyl, chrysenyl, naphtacenyl, fluoranthenyl and the like, but are not restricted thereto.

[34] The term "heteroaryl" described herein means an aryl group containing from 1 to 4 heteroatom(s) selected from N, O and S for the aromatic cyclic backbone atoms, and carbon atom(s) for remaining aromatic cyclic backbone atoms. The heteroaryl may be a 5- or 6-membered monocyclic heteroaryl or a polycyclic heteroaryl which is fused with one or more benzene ring(s), and may be partially saturated. The structures having one or more heteroaryl groups bonded through chemical bond(s) are also included. The heteroaryl groups may include divalent aryl groups of which the heteroatoms are oxidized or quarternized to form N-oxides, quaternary salts, or the like. Specific examples include monocyclic heteroaryl groups such as furyl, thienyl,

pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl; polycyclic heteroaryl groups such as benzofuryl, benzothienyl, isobenzofuryl, benzimidazolyl, benzothiazolyl, benzisothiazolyl, benzisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinolizinyl, quinoxalinyl, carbazolyl, phenanthridinyl and benzodioxolyl; and corresponding N-oxides (for example, pyridyl N-oxide, quinolyl N-oxide) and quaternary salts thereof; but they are not restricted thereto.

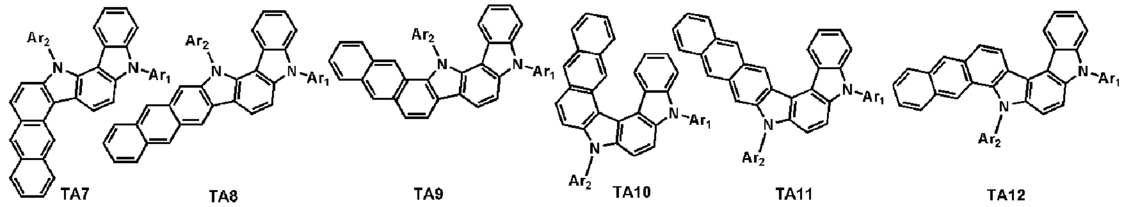
[35] The organic electroluminescent compounds according to the invention can be exemplified by the compounds represented by one of the following chemical formulas:

[36]



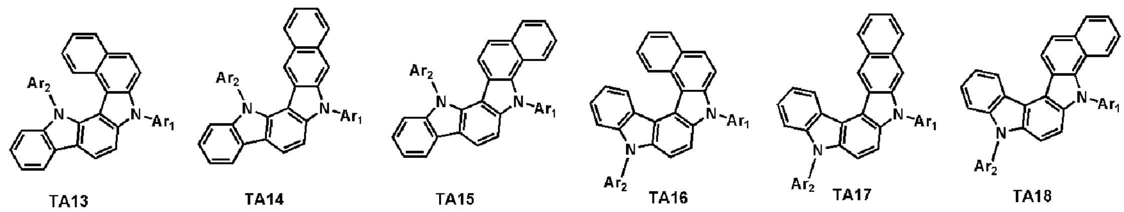
TA1 TA2 TA3 TA4 TA5 TA6

[37]



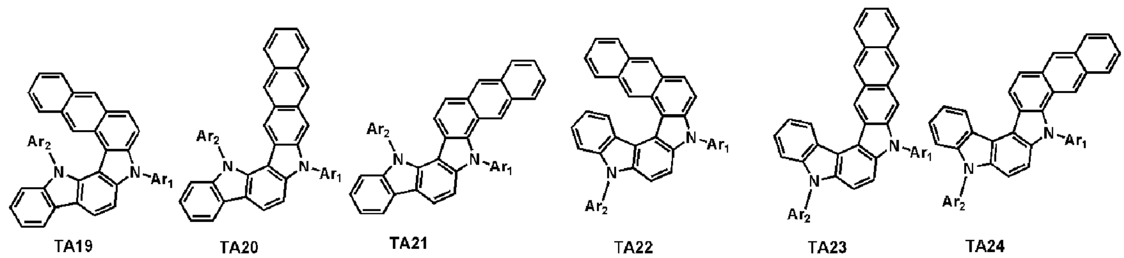
TA7 TA8 TA9 TA10 TA11 TA12

[38]



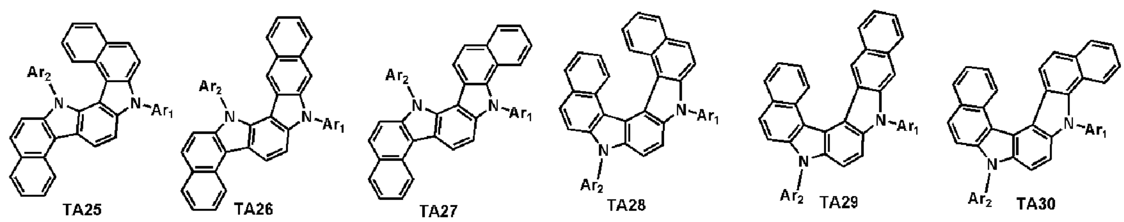
TA13 TA14 TA15 TA16 TA17 TA18

[39]



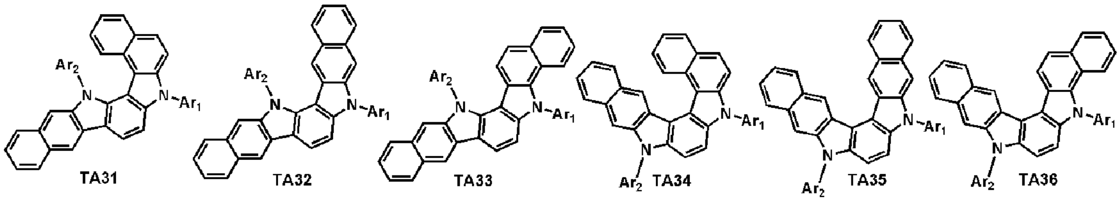
TA19 TA20 TA21 TA22 TA23 TA24

[40]



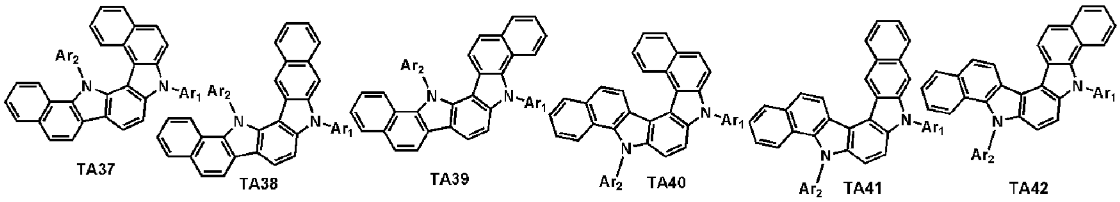
TA25 TA26 TA27 TA28 TA29 TA30

[41]



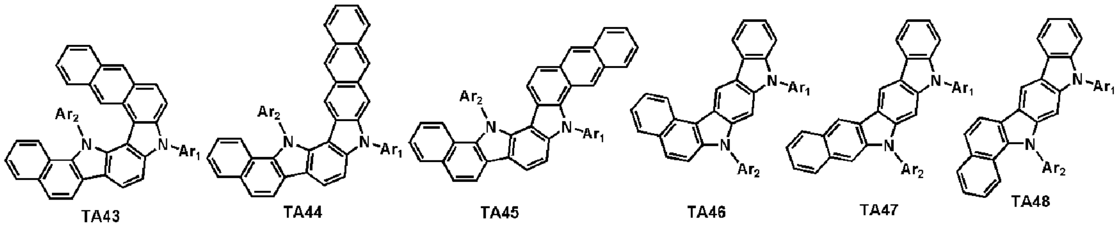
TA31 TA32 TA33 TA34 TA35 TA36

[42]



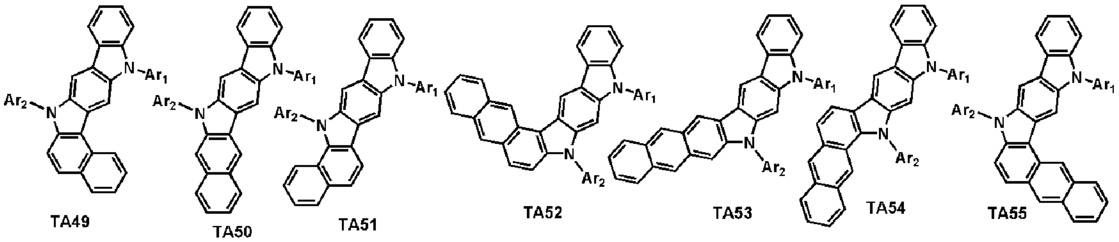
TA37 TA38 TA39 TA40 TA41 TA42

[43]



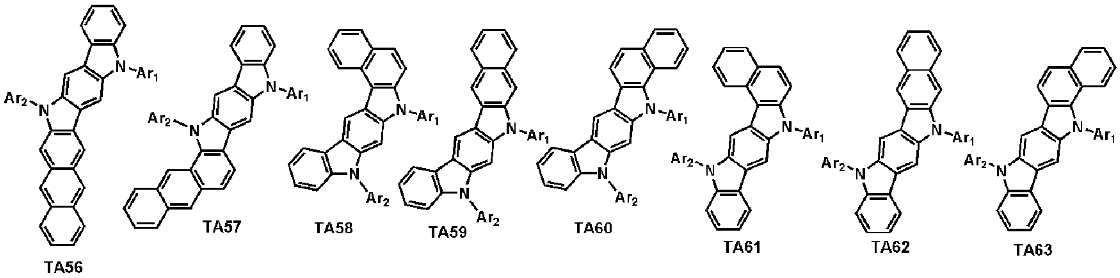
TA43 TA44 TA45 TA46 TA47 TA48

[44]



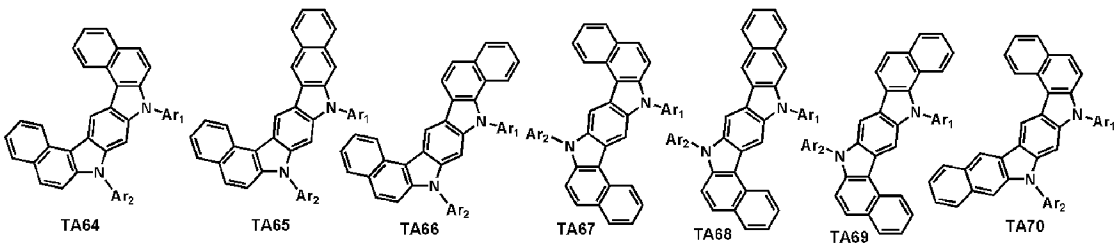
TA49 TA50 TA51 TA52 TA53 TA54 TA55

[45]



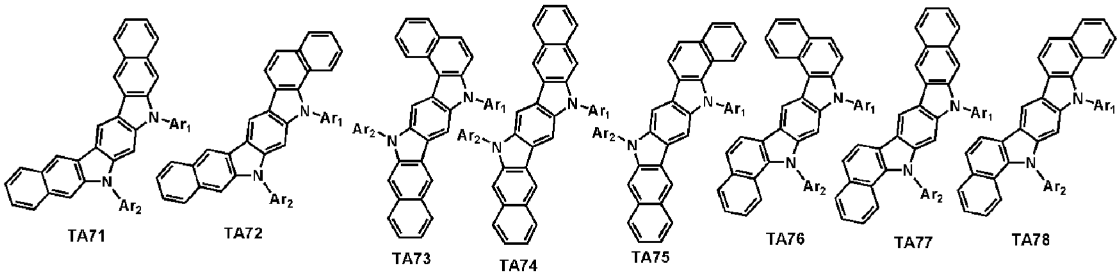
TA56 TA57 TA58 TA59 TA60 TA61 TA62 TA63

[46]



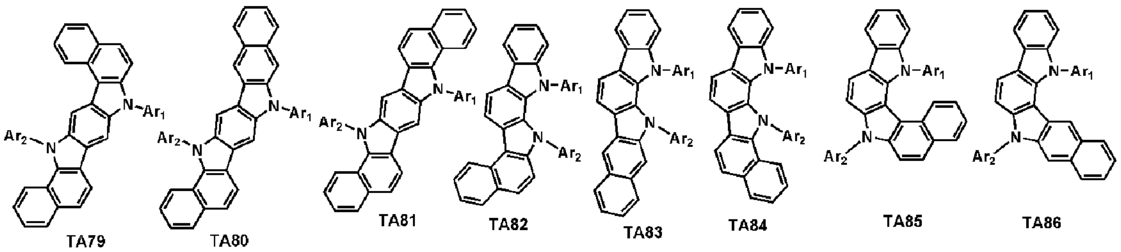
TA64 TA65 TA66 TA67 TA68 TA69 TA70

[47]



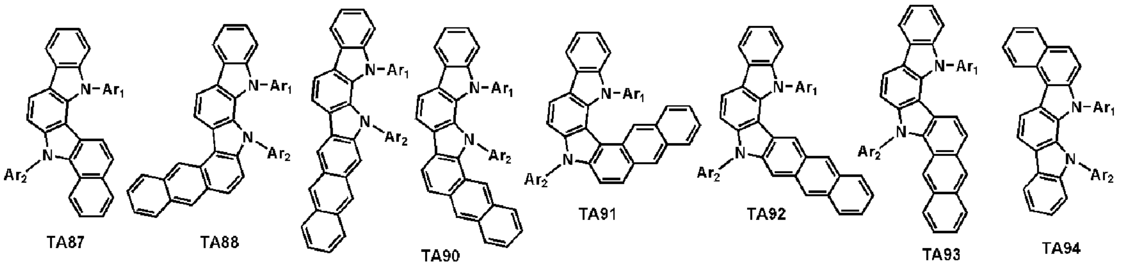
TA71 TA72 TA73 TA74 TA75 TA76 TA77 TA78

[48]



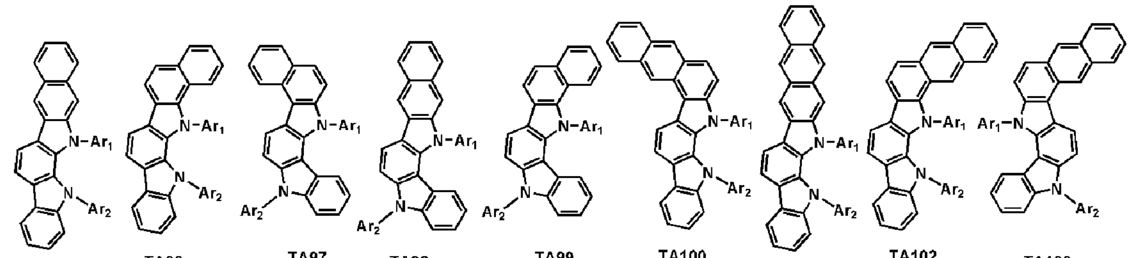
TA79 TA80 TA81 TA82 TA83 TA84 TA85 TA86

[49]



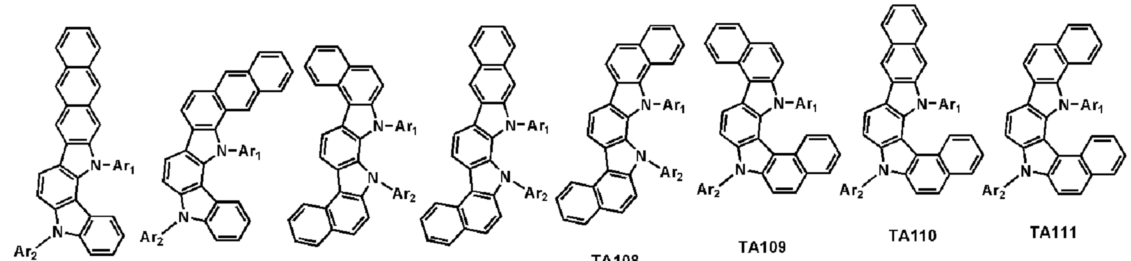
TA87 TA88 TA89 TA90 TA91 TA92 TA93 TA94

[50]



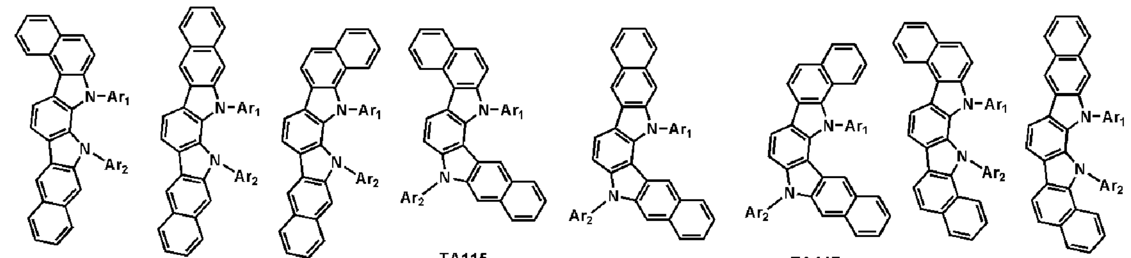
TA95 TA96 TA97 TA98 TA99 TA100 TA101 TA102 TA103

[51]



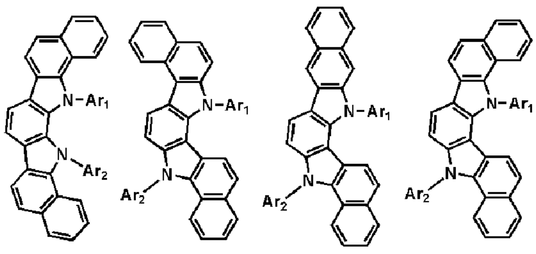
TA104 TA105 TA106 TA107 TA108 TA109 TA110 TA111

[52]



TA112 TA113 TA114 TA115 TA116 TA117 TA118 TA119

[53]

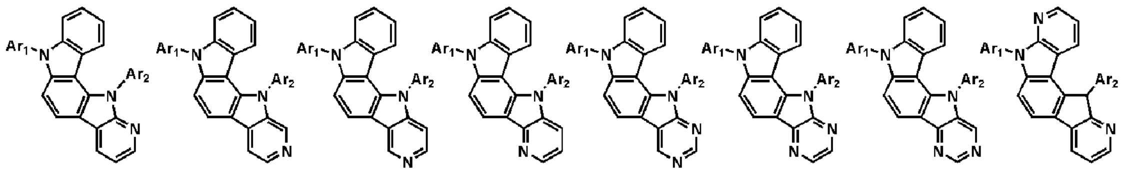


TA120 TA121 TA122 TA123

[54] wherein, Ar_1 and Ar_2 are defined as in Chemical Formulas (1) to (5).

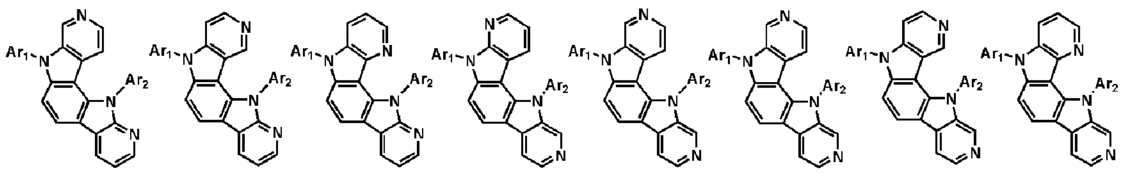
[55] Furthermore, the organic electroluminescent compounds according to the present invention can be exemplified by the compounds represented by one of the following chemical formulas:

[56]



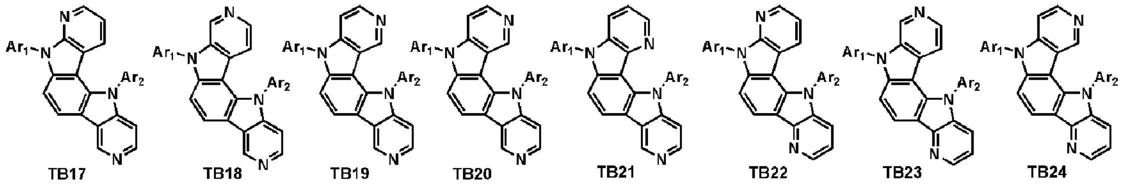
TB1 TB2 TB3 TB4 TB5 TB6 TB7 TB8

[57]



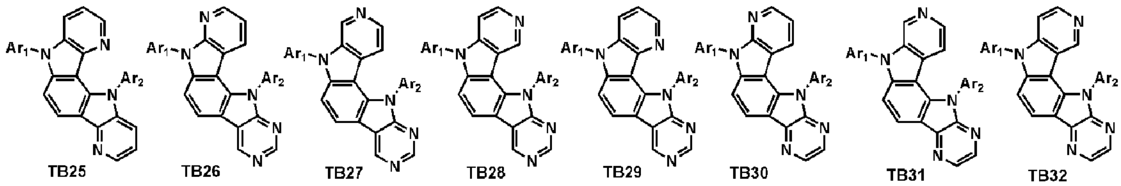
TB9 TB10 TB11 TB12 TB13 TB14 TB15 TB16

[58]



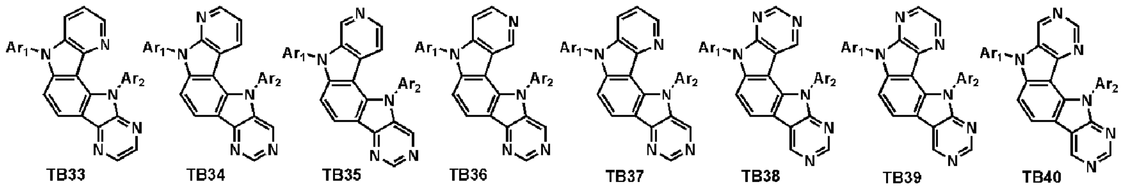
TB17 TB18 TB19 TB20 TB21 TB22 TB23 TB24

[59]



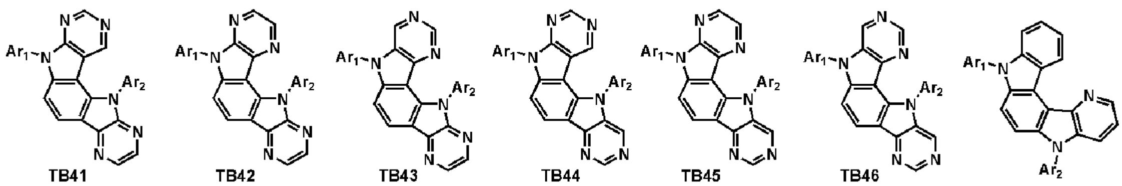
TB25 TB26 TB27 TB28 TB29 TB30 TB31 TB32

[60]



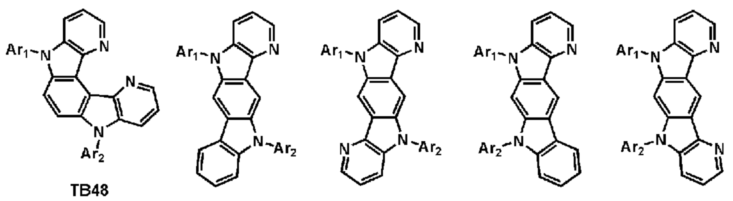
TB33 TB34 TB35 TB36 TB37 TB38 TB39 TB40

[61]



TB41 TB42 TB43 TB44 TB45 TB46 TB47

[62]

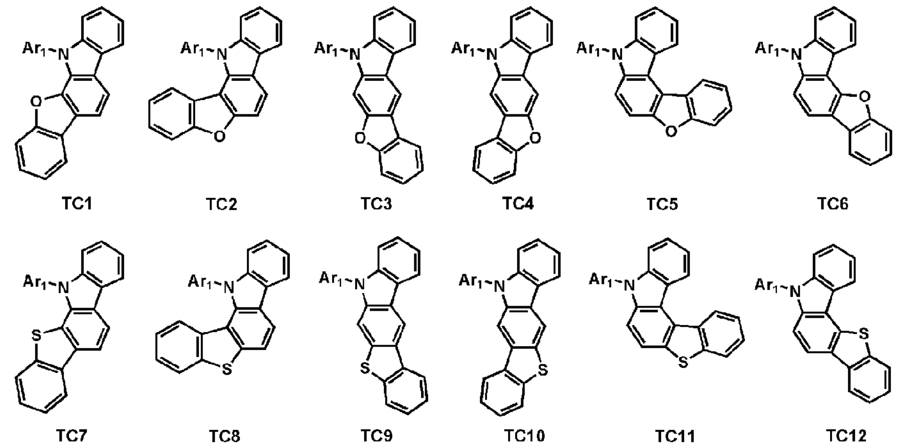


TB48 TB49 TB50 TB51 TB52

[63] wherein, Ar_1 and Ar_2 are defined as in Chemical Formulas (1) to (5).

[64] The organic electroluminescent compounds according to the present invention can be specifically exemplified by the compounds represented by one of the following chemical formulas:

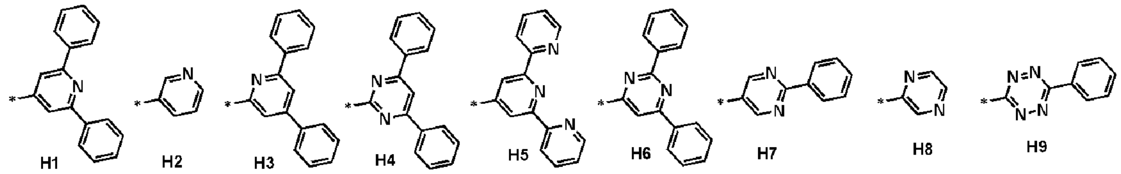
[65]


TC1 TC2 TC3 TC4 TC5 TC6 TC7 TC8 TC9 TC10 TC11 TC12

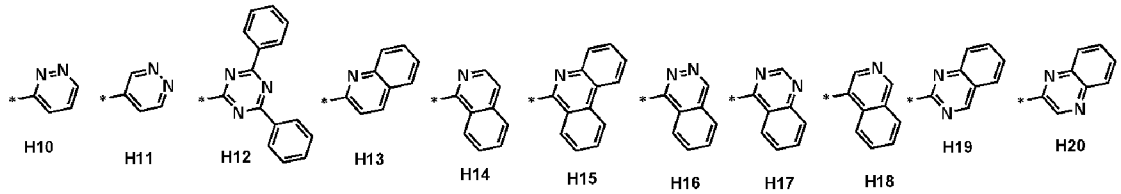
[66] wherein, Ar_1 is defined as in Chemical Formulas (1) to (5).

[67] More specifically, Ar_1 and Ar_2 independently represent phenyl, 1-naphthyl or 2-naphthyl, or a substituent represented by one of the following chemical formulas, but they are not restricted thereto.

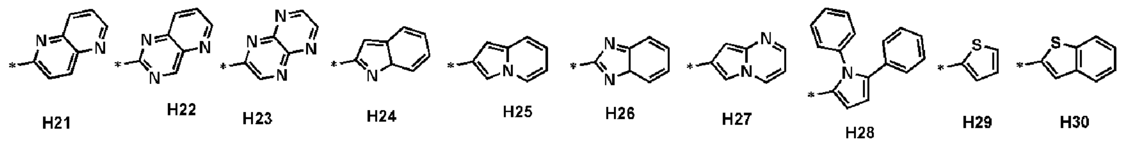
[68]


H1 H2 H3 H4 H5 H6 H7 H8 H9

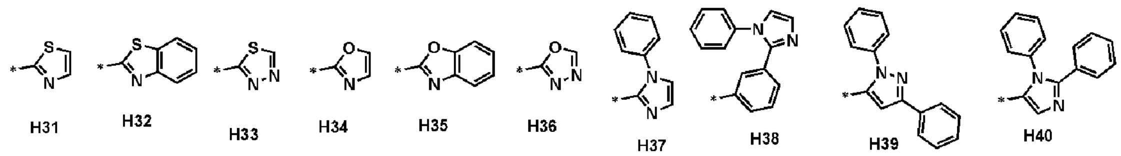
[69]


H10 H11 H12 H13 H14 H15 H16 H17 H18 H19 H20

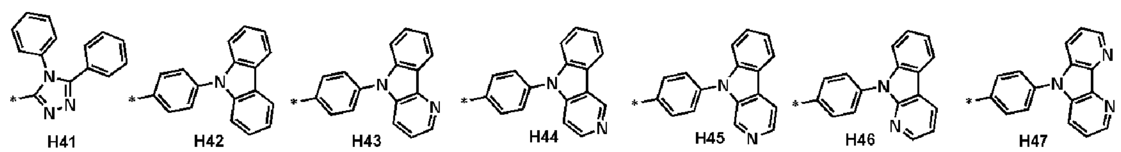
[70]


H21 H22 H23 H24 H25 H26 H27 H28 H29 H30

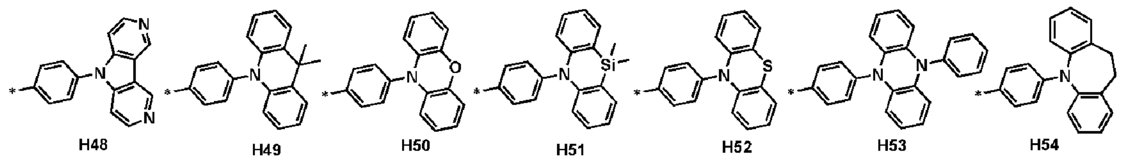
[71]


H31 H32 H33 H34 H35 H36 H37 H38 H39 H40

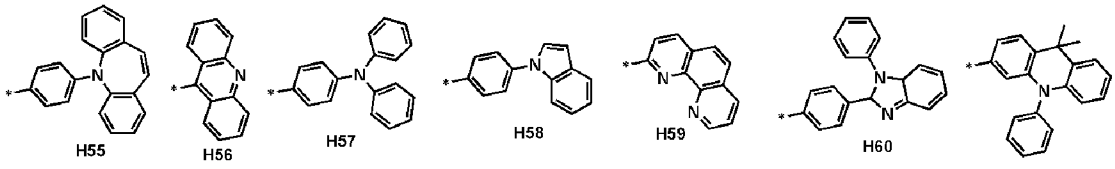
[72]


H41 H42 H43 H44 H45 H46 H47

[73]

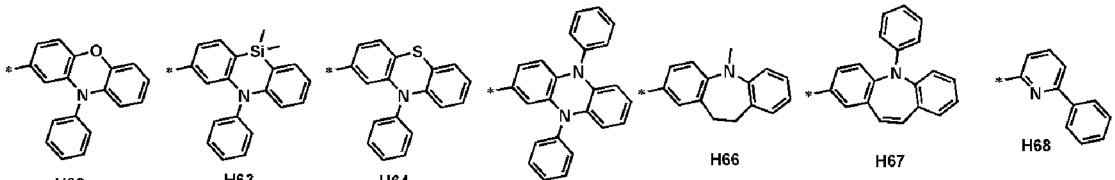

H48 H49 H50 H51 H52 H53 H54

[74]



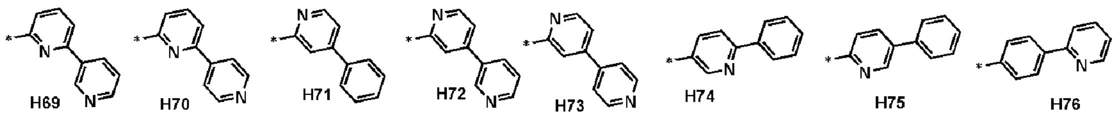
H55 H56 H57 H58 H59 H60 H61

[75]



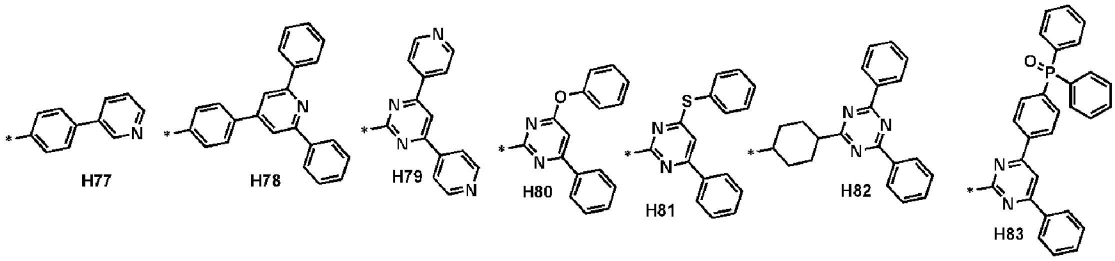
H62 H63 H64 H65 H66 H67 H68

[76]



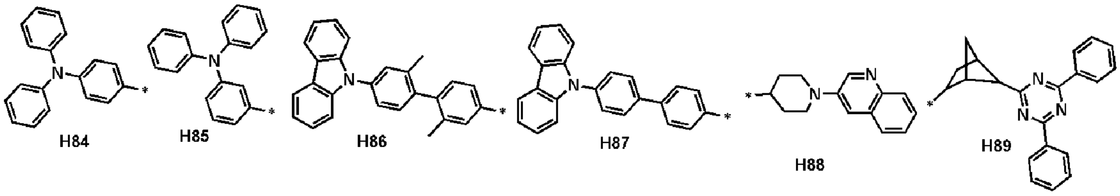
H69 H70 H71 H72 H73 H74 H75 H76

[77]



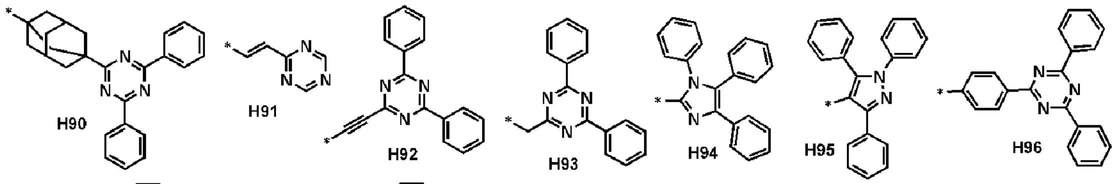
H77 H78 H79 H80 H81 H82 H83

[78]

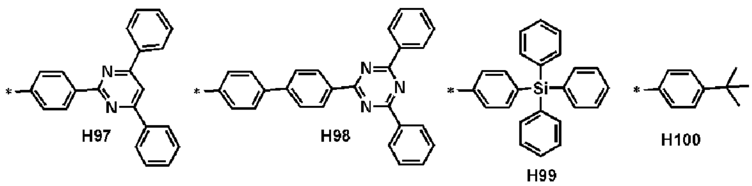


H84 H85 H86 H87 H88 H89

[79]



H90 H91 H92 H93 H94 H95 H96



H97 H98 H99 H100

[80] The present invention also provides an organic electroluminescent device which is comprised of a first electrode; a second electrode; and at least one organic layer(s) interposed between the first electrode and the second electrode; wherein the organic layer comprises one or more organic electroluminescent compound(s) represented by one of Chemical Formulas (1) to (5).

[81] The organic electroluminescent device according to the present invention is characterized in that the organic layer comprises an electroluminescent layer, which comprises one or more compound(s) represented by one of Chemical Formulas (1) to

(5) as electroluminescent host, and one or more phosphorescent dopant(s). The dopant is not particularly restricted.

[82] The organic electroluminescent device according to the invention may further comprise one or more compound(s) selected from a group consisting of arylamine compounds and styrylarylamine compounds, as well as one or more organic electroluminescent compound(s) represented by one of Chemical Formulas (1) to (5).

[83] In an organic electroluminescent device according to the present invention, the organic layer may further comprise one or more metal(s) selected from a group consisting of organic metals of Group 1, Group 2, 4^{th} period and 5^{th} period transition metals, lanthanide metals and d-transition elements, or complex(es) thereof, as well as one or more organic electroluminescent compound(s) represented by one of Chemical Formulas (1) to (5). The organic layer may comprise an electroluminescent layer and a charge generating layer.

[84] The organic electroluminescent device may also comprise one or more organic electroluminescent layer(s) emitting blue, green or red light, in addition to the organic electroluminescent compound(s) as described above, to form an organic electroluminescent device emitting white light.

Advantageous Effects of Invention

[85] The organic electroluminescent compounds according to the invention exhibit excellent luminous efficiency and very good life property of material when they are employed as host material of organic electroluminescent material of an OLED, so that OLED's having very good operation life can be manufactured therefrom.

Mode for the Invention

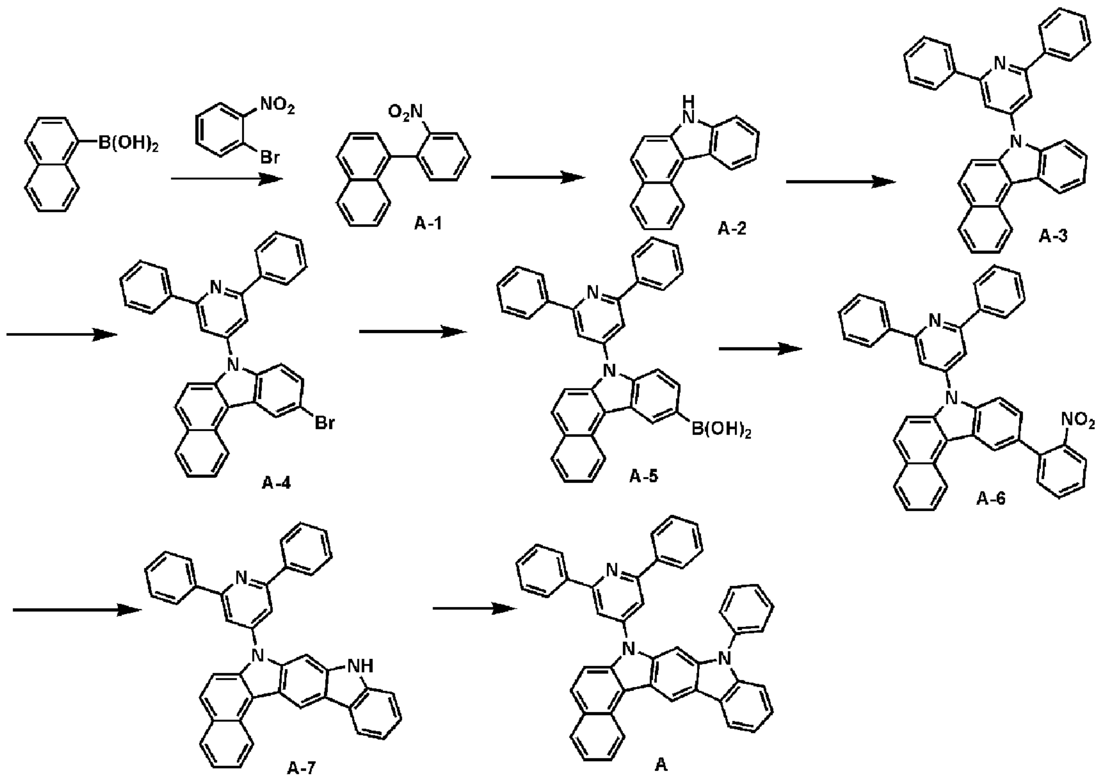
[86] The present invention is further described by referring to Preparation Examples and Examples in order to illustrate representative organic electroluminescent compounds, preparation thereof and luminescent properties of the electroluminescent devices according to the present invention, but those examples are provided for better understanding of the embodiments of the present invention only but are not intended to limit the scope of the invention by any means.

[87]

[88] [Preparation Examples]

[89] [Preparation Example 1] Preparation of Compound (A)

[90]



[91] Preparation of Compound (A-1)

[92] A mixture of bromo-2-nitrobenzene (30 g, 148.5 mmol), 1-naphtaleneboronic acid (30.6 g, 178.2 mmol), $Pd(PPh_3)_4$ (5.14 g, 4.45 mmol), aqueous 2M K_2CO_3 solution (297.01 mmol), toluene (500 mL) and ethanol (200 mL) was stirred under reflux for 4 hours. After cooling the mixture to ambient temperature, distilled water was added thereto. The resultant mixture was extracted with ethyl acetate, and the extract was dried over magnesium sulfate, and distilled under reduced pressure. Purification through a column gave Compound (A-1) (31 g, 124.3 mmol, 84.03%).

[93] Preparation of Compound (A-2)

[94] A mixture of Compound (A-1) (31 g, 124.3 mmol) and triethylphosphite (300 mL) was stirred under reflux for 10 hours. After cooling the mixture to ambient temperature, organic solvent was distilled off under reduced pressure. Distilled water was added thereto, and the mixture was extracted with ethyl acetate. The extract was dried over magnesium sulfate and distilled under reduced pressure. Purification through a column gave Compound (A-2) (18 g, 82.84 mmol, 66.81%).

[95] Preparation of Compound (A-3)

[96] A mixture of Compound (A-2) (18 g, 82.84 mmol), 1,5-diphenyl-3-chloropyridine (26.4 g, 99.41 mmol), $Pd(OAc)_2$ (1.85 g, 8.28 mmol), $P(t\text{-}bu)_3$ (8.17 ml, 16.5 mmol, 50% in xylene), NaOt-bu (23.8 g, 248.5 mmol) and toluene (500 mL) was stirred under reflux for 12 hours. After cooling the mixture to ambient temperature, distilled water was added thereto, and the mixture was extracted with ethyl acetate. The extract was

dried over magnesium sulfate and distilled under reduced pressure. Purification through a column gave Compound (A-3) (19 g, 42.54 mmol, 51.36%).

[97] Preparation of Compound (A-4)

[98] To a solution of Compound (A-3) (19 g, 42.54 mmol) dissolved in DMF (200 mL), added was NBS (8.33 g, 46.80 mmol). After 10 hours at ambient temperature, organic solvent was distilled off under reduced pressure. Distilled water was added thereto, and the mixture was extracted with ethyl acetate. The extract was dried over magnesium sulfate, and distilled under reduced pressure. Purification through a column gave Compound (A-4) (20 g, 38.06 mmol, 89.47%).

[99] Preparation of Compound (A-5)

[100] To a solution of Compound (A-4) (20 g, 38.06 mmol) dissolved in THF 200 mL, slowly added was n-buLi (15.22 mL, 38.06 mmol, 2.5 M in hexane) at -78℃. After stirring for an hour, trimethylborate (5.51 mL, 49.48 mmol) was added thereto. The mixture was slowly warmed to ambient temperature, and stirred for 12 hours. Distilled was added, and the mixture was extracted with ethyl acetate. The extract was dried over magnesium sulfate, and distilled under reduced pressure. Purification through a column gave Compound (A-5) (8 g, 16.31 mmol, 42.86%).

[101] Preparation of Compound (A-6)

[102] A mixture of Compound (A-5) (8 g, 16.31 mmol), bromo-2-nitrobenzene (3.95 g, 19.57 mmol), $Pd(PPh_3)_4$ (0.56 g, 0.48 mmol), aqueous 2M K_2CO_3 solution (16 mL, 32.62 mmol), toluene (70 mL) and ethanol (20 mL) was stirred under reflux. According to the same procedure as synthesis of Compound (A-1), obtained was Compound (A-6) (7 g, 12.33 mmol, 75.62%).

[103] Preparation of Compound (A-7)

[104] Compound (A-6) (7 g, 12.33 mmol) was mixed with triethylphosphite (100 mL), and the same procedure as for synthesis of Compound (A-2) was carried out to give Compound (A-7) (4 g, 7.46 mmol, 58.33%).

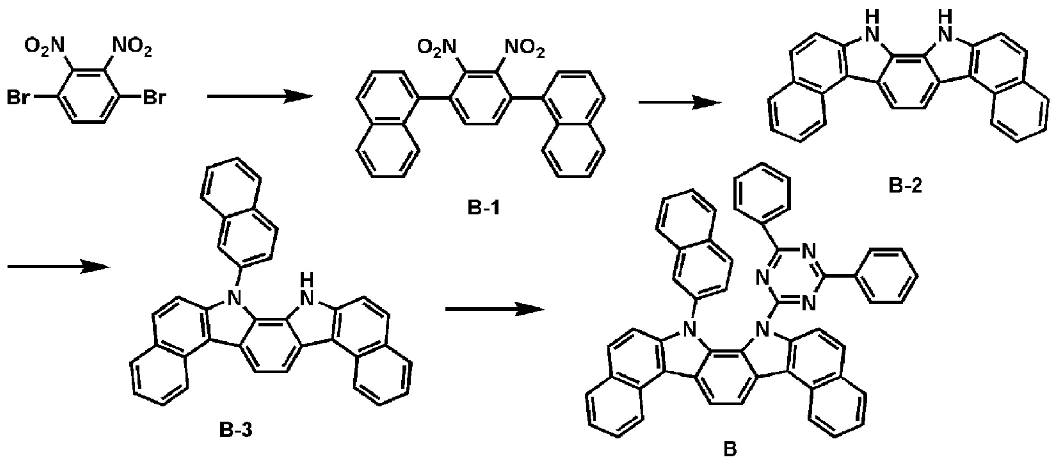
[105] Preparation of Compound (A)

[106] A mixture of Compound (A-7) (4 g, 7.46 mmol), iodobenzene (1.25 mL, 11.20 mmol), copper powder (0.71 g, 11.20 mmol), K_2CO_3 (3.09 g), 18-Crown-6 (0.15 g, 0.59 mmol) and 1,2-dichlorobenzene (100 mL) was stirred under reflux for 15 hours. After cooling the reaction mixture to ambient temperature, organic solvent was distilled off under reduced pressure. Distilled water was added thereto, and the mixture was extracted with ethyl acetate. The extract was purified through a column to obtain Compound (A) (3.6 g, 5.88 mmol, 78.88%).

[107]

[108] [Preparation Example 2] Preparation of Compound (B)

[109]



[110] Preparation of Compound (B-1)

[111] A mixture of 1,4-dibromo-2,3-dinitrobenzene (20 g, 61.36 mmol), 1-naphthaleneboronic acid (26 g, 153.42 mmol), $Pd(PPh_3)_4$ (3.54 g, 3.06 mmol), aqueous 2 M K_2CO_3 solution (90 mL), toluene (200 mL) and ethanol (100 mL) was stirred under reflux for 10 hours. After cooling the reaction mixture to ambient temperature, distilled water was added thereto, and the resultant mixture was extracted with ethyl acetate. The extract was dried over magnesium sulfate, and distilled under reduced pressure. Purification through a column gave Compound (B-1) (22 g, 52.32 mmol, 85.28%).

[112] Preparation of Compound (B-2)

[113] Compound (B-1) (22 g, 52.32 mmol) and triethylphosphite (200 mL) were mixed and stirred at 180°C. According to the same procedure as for synthesis of Compound (A-2), obtained was Compound (B-2) (10 g, 28.05 mmol, 53.95%).

[114] Preparation of Compound (B-3)

[115] A mixture of Compound (B-2) (10 g, 28.05 mmol), 2-iodonaphthalene (7.1 g, 28.05 mmol), copper powder (2.67 g, 42.08 mmol), K_2CO_3 (11.63 g, 84.17 mmol), 18-Crown-6 (0.59 g, 2.24 mmol) and 1,2-dichlorobenzene (100 mL) was stirred at 190°C for 20 hours. After cooling to ambient temperature, the organic solvent was distilled off under reduced pressure. Distilled water was added thereto, and the mixture was extracted with ethyl acetate. The extract was dried over magnesium sulfate and distilled under reduced pressure. Purification through a column gave Compound (B-3) (4 g, 8.28 mmol, 29.60%).

[116] Preparation of Compound (B)

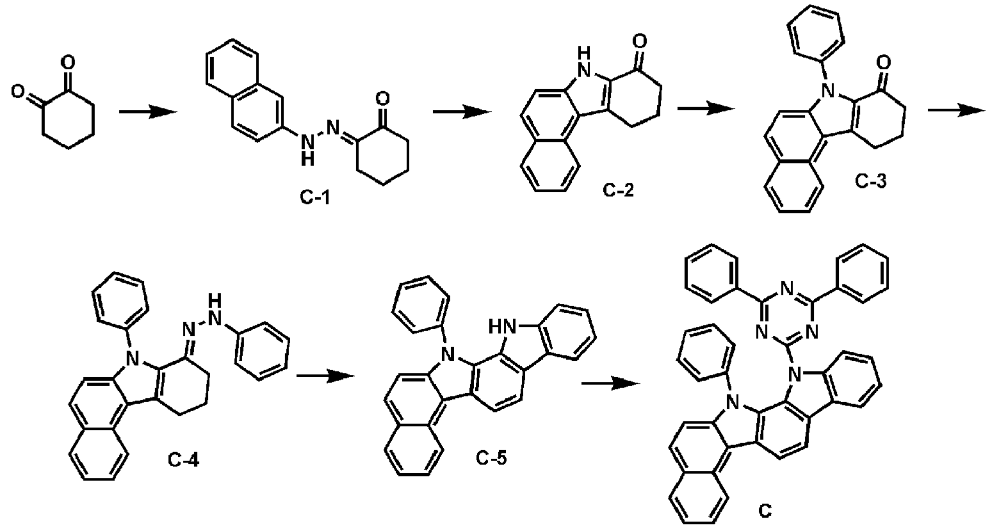
[117] To a reaction vessel containing a solution of NaH (0.49 g, 12.43 mmol, 60% dispersion in mineral oil) dissolved in DMF (20 mL), added was a solution of Compound (B-3) (4 g, 8.28 mmol) dissolved in DMF (20 mL). After one hour, a solution of 2-chloro-4,6-diphenyltriazine (2.66 g, 9.94 mmol) dissolved in DMF (20 mL) was added thereto. After stirring for 12 hours, distilled water was added, and the

solid produced was filtered under reduced pressure. Recrystallization from ethyl acetate and DMF gave Compound (B) (3.5 g, 4.90 mmol, 59.21%).

[118]

[119] [Preparation Example 3] Preparation of Compound (C)

[120]



[121] <u>Preparation of Compound (C-1)</u>

[122] To a solution of 1,2-cyclohexyldione (42.52 g, 379.26 mmol) dissolved in ethanol (1000 mL), slowly added was 2-naphthyl hydrazine (20 g, 126.42 mmol). Acetic acid (0.28 mL, 5.05 mmol) was added thereto, and the mixture was heated to 40℃. After 2 hours, the mixture was cooled and distilled water was added thereto. The solid produced was filtered under reduced pressure to obtain Compound (C-1) (17 g, 67.37 mmol, 53.47%).

[123] <u>Preparation of Compound (C-2)</u>

[124] To a solution of Compound (C-1) (17 g, 67.37 mmol) dissolved in acetic acid (100 mL), added was trifluoroacetic acid (10 mL). After stirring at ambient temperature for 2 hours, distilled water was added thereto. The mixture was neutralized by means of aqueous NaOH solution, and extracted with ethyl acetate. The extract was dried over magnesium sulfate, and distilled under reduced pressure. Purification through a column gave Compound (C-2) (11 g, 46.75 mmol, 69.39%).

[125] <u>Preparation of Compound (C-3)</u>

[126] According to the same procedure for synthesis of Compound (B-3), obtained was Compound (C-3) (10 g, 32.11 mmol, 68.69%).

[127] <u>Preparation of Compound (C-4)</u>

[128] According to the same procedure for synthesis of Compound (C-1), obtained was Compound (C-4) (12 g, 29.88 mmol, 93.07%).

[129] <u>Preparation of Compound (C-5)</u>

[130] According to the same procedure for synthesis of Compound (C-2), obtained was

Compound (C-5) (6 g, 15.68 mmol, 52.50%).

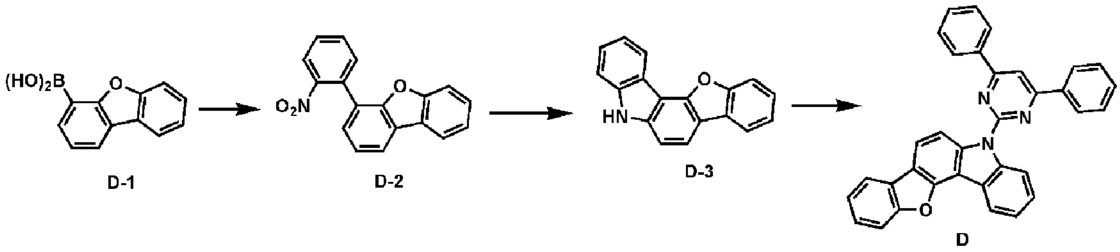
[131] Preparation of Compound (C)

[132] According to the same procedure for synthesis of Compound (B), obtained was Compound (C) (5 g, 8.14 mmol, 51.95%).

[133]

[134] [Preparation Example 4] Preparation of Compound (D)

[135]



[136] Preparation of Compound (D-2)

[137] According to the same procedure for synthesis of Compound (A-1) but using Compound (D-1), obtained was Compound (D-2) (11 g, 38.02 mmol, 89.22%).

[138] Preparation of Compound (D-3)

[139] According to the same procedure for synthesis of Compound (A-2), obtained was Compound (D-3) (8 g, 31.09 mmol, 81.78%).

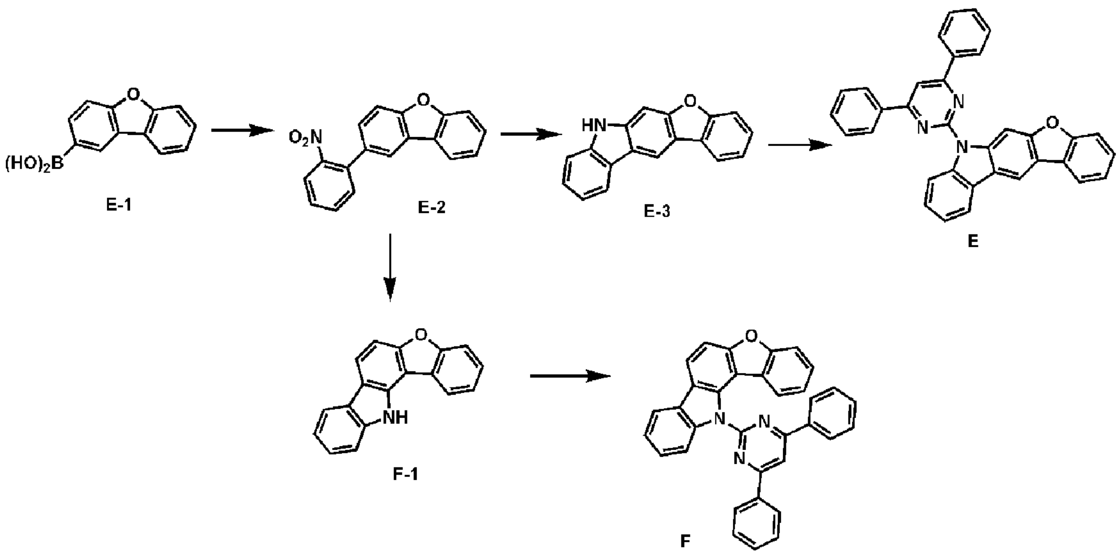
[140] Preparation of Compound (D)

[141] According to the same procedure for synthesis of Compound (B), obtained was Compound (D) (6 g, 12.30 mmol, 38.70%).

[142]

[143] [Preparation Example 5] Preparation of Compound E and F

[144]



[145] Preparation of Compound (E-2)

[146] According to the same procedure for synthesis of Compound (A-1) but using Compound (E-1), obtained was Compound (E-2) (15 g, 51.85 mmol, 86.51%).

[147] Preparation of Compound (E-3)

[148] According to the same procedure for synthesis of Compound (A-2), obtained was Compound (E-3) (6 g, 23.31 mmol, 44.97%).

[149] Preparation of Compound (E)

[150] According to the same procedure for synthesis of Compound (B), obtained was Compound (E) (5 g, 10.25 mmol, 43.99%).

[151] Preparation of Compound (F-1)

[152] According to the same procedure for synthesis of Compound (A-2), obtained was Compound (F-1) (3 g, 11.65 mmol, 22.48%).

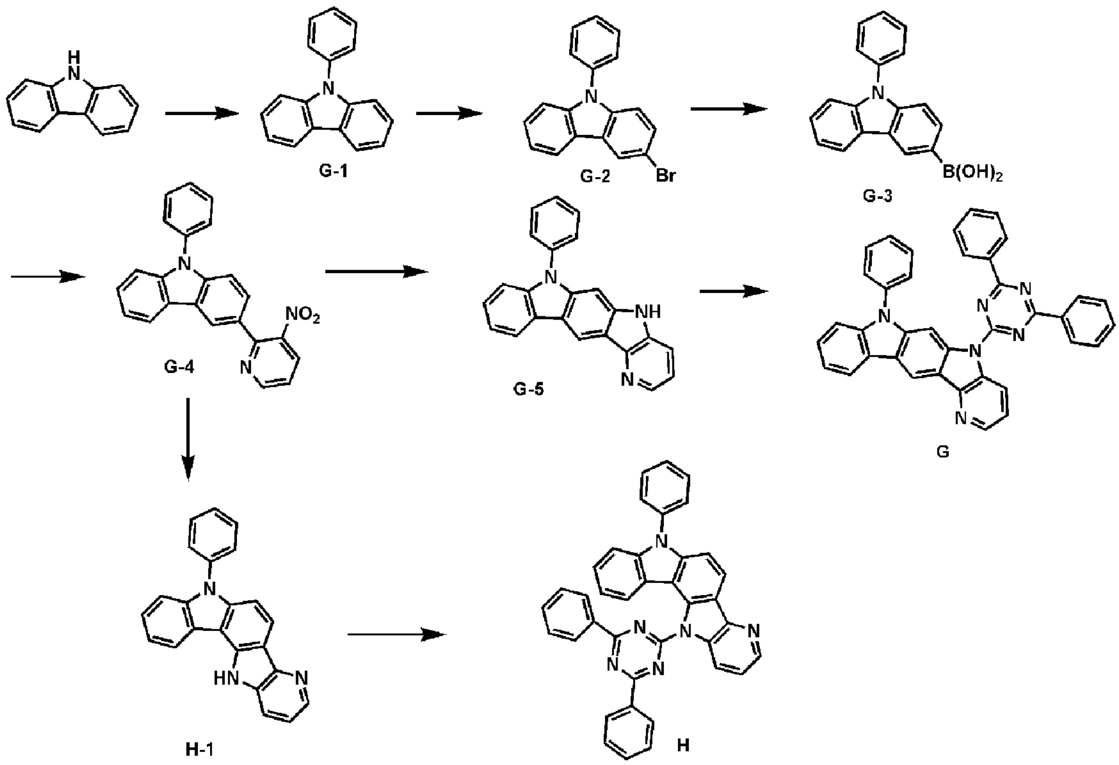
[153] Preparation of Compound (F)

[154] According to the same procedure for synthesis of Compound (B), obtained was Compound (F) (3 g, 6.15 mmol, 52.81%).

[155]

[156] [Preparation Example 6] Preparation of Compound (G) and (H)

[157]



[158] Preparation of Compound (G-1)

[159] A mixture of carbazole (20 g, 119.6 mmol), iodobenzene (20 mL, 179.41 mmol), copper (11.4 g, 179.41 mmol), K_2CO_3 (49 g, 358.8 mmol), 18-Crown-6 (2.5 g, 9.56 mmol) and 1,2-dichlorobenzene was stirred at 190℃ for 12 hours. After cooling to ambient temperature, the reaction mixture was distilled under reduced pressure. Distilled water was added thereto, and the resultant mixture was extracted with ethyl acetate. The extract was dried over magnesium sulfate, and distilled under reduced

pressure. Purification through a column gave Compound (G-1) (22 g, 90.42 mmol, 75.60%).

[160] Preparation of Compound (G-2)

[161] According to the same procedure for synthesis of Compound (A-4), obtained was Compound (G-2) (25 g, 77.59 mmol, 85.81%).

[162] Preparation of Compound (G-3)

[163] According to the same procedure for synthesis of Compound (A-5), obtained was Compound (G-3) (11 g, 38.31 mmol, 49.37%).

[164] Preparation of Compound (G-4)

[165] According to the same procedure for synthesis of Compound (A-1), obtained was Compound (G-4) (12 g, 32.84 mmol, 85.72%).

[166] Preparation of Compound (G-5)

[167] According to the same procedure for synthesis of Compound (A-2), reaction was carried out for 4 hours to obtain Compound (G-5) (6 g, 17.99 mmol, 54.80%).

[168] Preparation of Compound (G)

[169] According to the same procedure for synthesis of Compound (B), obtained was Compound (G) (7 g, 12.39 mmol, 68.91%).

[170] Preparation of Compound (H-1)

[171] According to the same procedure for synthesis of Compound (A-2), the reaction was carried out for 4 hours to obtain Compound (H-1) (2 g, 5.99 mmol, 18.26%).

[172] Preparation of Compound (H)

[173] According to the same procedure for synthesis of Compound (B), obtained was Compound (H) (1.7 g, 3.01 mmol, 50.26%).

[174]

[175] Organic electroluminescent compounds (TA, TB and TC) were prepared according to the procedures of Preparation Examples (1)-(6). The substituents (Ar_1, Ar_2) of those organic electroluminescent compounds thus prepared, and ^1H NMR and MS/FAB data of the compounds are listed in Tables 1 and 2.

[176] [Table 1]

[177]

Compound	Ar_1	Ar_2	^1H NMR($CDCl_3$, 200 MHz)	MS/FAB	
				found	calculated
TA-1	phenyl	H1	δ = 7.05(2H, m), 7.29(1H, m), 7.45~7.67(15H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.3(4H, m), 8.54(1H, m)	611.73	611.24
	phenyl	H4	δ = 7.29(1H, m), 7.41~7.51(10H, m), 7.58~7.67(5H, m), 7.79(4H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.54(1H, m), 8.63(1H, s)	612.72	612.23
	phenyl	H12	δ = 7.29(1H, m), 7.41~7.51(10H, m), 7.58~7.67(5H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54(1H, m)	613.71	613.23
	phenyl	H19	δ = 7.29(1H, m), 7.45~7.5(4H, m), 7.58~7.67(5H, m), 7.8(1H, m), 7.94~7.96(4H, m), 8.05~8.16(5H, m), 8.54(1H, m), 9.74(1H, m)	510.59	510.18
	phenyl	H32	δ = 7.29(1H, m), 7.45~7.67(11H, m), 7.94~8.01(5H, m), 8.12~8.18(3H, m), 8.54(1H, m)	515.63	515.15
	phenyl	H42	δ = 7.25~7.33(4H, m), 7.45~7.5(5H, m), 7.58~7.67(10H, m), 7.94~7.96(5H, m), 8.12~8.16(3H, m), 8.54~8.55(2H, m)	623.74	623.24
	phenyl	H69	δ = 7.29~7.32(2H, m), 7.45~7.5(4H, m), 7.58~7.72(7H, m), 7.86(1H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.54(1H, m), 8.76(1H, m), 8.93(1H, m), 9.75(1H, m)	536.62	536.20
	phenyl	H78	δ = 7.29(1H, m), 7.45~7.54(17H, m), 7.79(2H, m), 7.94~7.96(4H, m), 8.12~8.2(4H, m), 8.3(4H, m), 8.54(1H, m)	687.83	687.27
	phenyl	H82	δ = 1.73(2H, m), 1.88(2H, m), 2.72(1H, m), 3.64(1H, m), 7.29(1H, m), 7.41~7.51(10H, m), 7.58~7.71(6H, m), 7.94~7.96(2H, m), 8.05(1H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54(1H, m)	695.85	695.30
	phenyl	H90	δ = 1.36(3H, m), 1.43(4H, m), 1.65(4H, m), 1.8(2H, m), 2.09(1H, s), 7.29(1H, m), 7.41~7.51(10H, m), 7.58~7.71(6H, m), 7.94~7.96(2H, m), 8.05(1H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54(1H, m)	747.93	747.34
	2-naphthyl	H92	δ = 7.29(1H, m), 7.36~7.41(3H, m), 7.5~7.51(5H, m), 7.59~7.67(5H, m), 7.83(1H, m), 7.94~8(7H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54(1H, m)	687.79	687.24
	1-naphthyl	H94	δ = 7.29(1H, m), 7.41(2H, m), 7.45(1H, m), 7.47~7.55(18H, m), 7.79(2H, m), 7.94~7.96(4H, m), 8.08~8.16(5H, m), 8.54(1H, m)	726.86	726.28
	H99	H98	δ = 7.25~7.29(3H, m), 7.36~7.41(3H, m), 7.5~7.51(5H, m), 7.59~7.68(7H, m), 7.79~7.85(5H, m), 7.94~8(7H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54(1H, m)	815.96	815.30

[178]

	H100	H1	δ = 1.35(9H, s), 7.05(2H, m), 7.28~7.29(3H, m), 7.46~7.54(9H, m), 7.63~7.67(3H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.3(4H, m), 8.54(1H, m)	667.84	667.30
	H1	H1	δ = 7.05(4H, m), 7.29(1H, m), 7.47~7.54(13H, m), 7.63~7.67(3H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.3(8H, m), 8.54(1H, m)	764.91	764.29
	H4	H4	δ = 7.29(1H, m), 7.41(4H, m), 7.5~7.51(9H, m), 7.63~7.67(3H, m), 7.79(8H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.54(1H, m), 8.63(2H, s)	766.89	766.28
	H12	H12	δ = 7.29(1H, m), 7.41(4H, m), 7.5~7.51(9H, m), 7.63~7.67(3H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.28(8H, m), 8.54(1H, m)	768.86	768.27
TA-7	phenyl	H1	δ = 7.05(2H, m), 7.29(1H, m), 7.39(3H, m), 7.45~7.63(13H, m), 7.91~7.96(5H, m), 8.12(1H, m), 8.3~8.31(6H, m)	661.79	661.25
	phenyl	H4	δ = 7.29(1H, m), 7.39~7.51(13H, m), 7.58~7.63(3H, m), 7.79(4H, m), 7.91~7.96(5H, m), 8.12(1H, m), 8.31(2H, m), 8.63(1H, s)	662.78	662.25
	phenyl	H12	δ = 7.29(1H, m), 7.39~7.51(13H, m), 7.58~7.63(3H, m), 7.91~7.96(5H, m), 8.12(1H, m), 8.28~8.31(6H, m)	663.77	663.24
	H2	H40	δ = 7.29~7.39(5H, m), 7.4(1H, s), 7.41~7.51(7H, m), 7.58~7.63(3H, m), 7.71(1H, m), 7.91~7.96(5H, m), 8.12(1H, m), 8.28~8.34(5H, m), 8.45(1H, m)	651.76	651.24
	H8	H91	δ = 5.6(1H, m), 6.9(1H, m), 7.29(1H, m), 7.39(3H, m), 7.5(1H, m), 7.63(1H, m), 7.91~7.96(5H, m), 8.12(1H, m), 8.31(2H, m), 8.76(2H, m), 8.82(3H, m)	539.59	539.19
TA-13	phenyl	H1	δ = 7.05(2H, m), 7.25(1H, m), 7.33(1H, m), 7.45~7.54(15H, m), 7.94~7.96(3H, m), 8.16(1H, m), 8.3(4H, m), 8.54~8.55(2H, m)	611.73	611.24
	phenyl	H4	δ = 7.25(1H, m), 7.33(1H, m), 7.41~7.51(9H, m), 7.58~7.67(6H, m), 7.79(4H, m), 7.94~7.96(3H, m), 8.16(1H, m), 8.54~8.55(2H, m), 8.63(1H, s)	612.72	612.23
	phenyl	H12	δ = 7.25(1H, m), 7.33(1H, m), 7.41~7.51(9H, m), 7.58~7.67(6H, m), 7.94~7.96(3H, m), 8.16(1H, m), 8.28(4H, m), 8.54~8.55(2H, m)	613.71	613.23
	H2	H87	δ = 7.25~7.34(6H, m), 7.5(1H, m), 7.63~7.71(10H, m), 7.79(4H, m), 7.94~7.96(4H, m), 8.12~8.16(2H, m), 8.34(1H, m), 8.45(1H, m), 8.54~8.55(3H, m)	700.83	700.26
	H11	H93	δ = 5.11(2H, m), 7.25(1H, m), 7.33(1H, m), 7.41(2H, m), 7.5~7.51(5H, m), 7.63~7.71(5H, m), 7.94(1H, m), 8.05(1H, m), 8.16(1H, m), 8.28(4H, m), 8.54~8.55(2H, m), 9.2(2H, m)	629.71	629.23

[179]

TA-25	phenyl	H1	δ = 7.05(2H, m), 7.45~7.54(17H, m), 7.94~7.96(4H, m), 8.16(2H, m), 8.3(4H, m), 8.54(2H, m)	661.79	661.25
	phenyl	H4	δ = 7.41~7.51(9H, m), 7.58~7.67(8H, m), 7.79(4H, m), 7.94~7.96(4H, m), 8.16(2H, m), 8.54(2H, m), 8.63(1H, s)	662.78	662.25
	phenyl	H12	δ = 7.41~7.51(9H, m), 7.58~7.67(8H, m), 7.94~7.96(4H, m), 8.16(2H, m), 8.28(4H, m), 8.54(2H, m)	663.77	663.24
	H7	H26	δ = 7.41~7.51(6H, m), 7.58~7.67(8H, m), 7.94~7.96(4H, m), 8.16(2H, m), 8.28(2H, m), 8.54(2H, m), 8.71(2H, m)	586.68	586.22
	H76	H96	δ = 7(1H, m), 7.26(1H, m), 7.45~7.51(4H, m), 7.58~7.71(10H, m), 7.94~7.96(4H, m), 8.16(2H, m), 8.3(2H, m), 8.5~8.54(3H, m)	585.69	585.22
TA-27	phenyl	H1	δ = 7.05(2H, m), 7.45~7.58(12H, m), 7.67(4H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.3(4H, m), 8.51~8.54(2H, m)	661.79	661.25
	phenyl	H4	δ = 7.41~7.51(9H, m), 7.57~7.58(3H, m), 7.67(4H, m), 7.79(4H, m), 7.94~7.96(4H, m), 8.12~8.16(3H,m), 8.51~8.54(2H, m),8.63(1H, s)	662.78	662.25
	phenyl	H12	δ = 7.41~7.51(9H, m), 7.57~7.58(3H, m), 7.67(4H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.28(4H, m), 8.51~8.54(2H, m)	663.77	663.24
	H24	H35	δ = 2.9(1H, m), 5.13(1H, m), 5.66(1H, m), 6.16(1H, m), 6.44(1H, m), 7.39(2H, m), 7.57(1H, m), 7.67(4H, m), 7.74(2H, m), 7.81(1H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.51~8.54(2H, m)	588.66	588.20
	H97	H97	δ = 7.41(4H, m), 7.51(8H, m), 7.57(1H, m), 7.67~7.68(8H, m), 7.79(12H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.23(2H, s), 8.51~8.54(2H, m)	969.14	968.36
TA-46	phenyl	H1	δ = 7.05(2H, m), 7.29(1H, m), 7.4(1H, s), 7.45~7.54(10H, m), 7.55(1H, s), 7.58~7.67(5H, m), 7.94~7.96(2H, m), 8.12~8.16(2H, m), 8.3(4H, m), 8.54(1H, m)	611.73	611.24
	phenyl	H4	δ = 7.29(1H, m), 7.4(1H, s), 7.41~7.51(10H, m), 7.55(1H, s), 7.58~7.67(5H, m), 7.79(4H, m), 7.94~7.96(2H, m), 8.12~8.16(2H, m), 8.54(1H, m), 8.63(1H, s)	612.72	612.23
	phenyl	H12	δ = 7.29(1H, m), 7.4(1H, s), 7.41~7.51(10H, m), 7.55(1H, s), 7.58~7.67(5H, m), 7.94~7.96(2H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54(1H, m)	613.71	613.23
	H2	H59	δ = 7.29~7.34(2H, m), 7.4(1H, s), 7.5(1H, m), 7.55(1H, s), 7.58~7.71(5H, m), 7.81(1H, m), 7.91~7.96(3H, m), 8.06~8.16(3H, m), 8.34~8.38(3H, m), 8.45(1H, m), 8.54(1H, m), 8.83(1H, m)	561.63	561.20

[180]

	H10	H95	δ = 7.29(1H, m), 7.4(1H, s), 7.41~7.51(8H, m), 7.55(1H, s), 7.58~7.68(8H, m), 7.79(4H, m), 7.94~7.96(2H, m), 8.12~8.16(2H, m), 8.35(1H, m), 8.54(1H, m), 9.38(1H, m)	678.78	678.25
TA-55	phenyl	H1	δ = 7.05(2H, m), 7.29(1H, m), 7.39(3H, m), 7.4(1H, s), 7.45~7.54(10H, m), 7.55(1H, s), 7.58~7.63(3H, m), 7.91(3H, m), 8.12(1H, m), 8.3~8.31(6H, m)	661.79	661.25
	phenyl	H4	δ = 7.29(1H, m), 7.39(3H, m), 7.4(1H, s), 7.41~7.51(10H, m), 7.55(1H, s), 7.58~7.63(3H, m), 7.79(4H, m), 7.91(3H, m), 8.12(1H, m), 8.31(2H, m), 8.63(1H, s)	662.78	662.25
	phenyl	H12	δ = 7.29(1H, m), 7.39(3H, m), 7.4(1H, s), 7.41~7.51(10H, m), 7.55(1H, s), 7.58~7.63(3H, m), 7.91(3H, m), 8.12(1H, m), 8.28~8.31(6H, m)	663.77	663.24
	H4	H43	δ = 7.22~7.39(7H, m), 7.4(1H, s), 7.41(2H, m), 7.5~7.51(5H, m), 7.55(1H, s), 7.62~7.63(5H, m), 7.79(4H, m), 7.91~7.97(5H, m), 8.12(1H, m), 8.31(2H, m), 8.43(1H, m), 8.63(1H, s), 8.74(1H, m)	828.96	828.30
	H12	H89	δ = 1.88~1.91(2H, m), 2.3~2.33(4H, m), 3.22(1H, m), 3.7(1H, m), 7.17(2H, s), 7.29(1H, m), 7.39~7.41(7H, m), 7.5~7.51(9H, m), 7.77(1H, m), 7.91(3H, m), 8.12(1H, m), 8.28~8.31(10H, m)	899.05	898.35
TA-66	phenyl	H1	δ = 7.05(2H, m), 7.4(1H, s), 7.45~7.54(9H, m), 7.55(1H, s), 7.57~7.58(3H, m), 7.67(4H, m), 7.94~7.96(2H, m), 8.12~8.16(3H, m), 8.3(4H, m), 8.51~8.54(2H, m)	661.79	661.25
	phenyl	H4	δ = 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.57~7.58(3H, m), 7.67(4H, m), 7.79(4H, m), 7.94~7.96(2H, m), 8.12~8.16(3H, m), 8.51~8.54(2H, m), 8.63(1H, s), (H,)	662.78	662.25
	phenyl	H12	δ = 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.57~7.58(3H, m), 7.67(4H, m), 7.94~7.96(2H, m), 8.12~8.16(3H, m), 8.28(4H, m), 8.51~8.54(2H, m)	663.77	663.24
	H7	H49	δ = 1.72(6H, s), 6.55(2H, m), 6.63(2H, m), 6.73(2H, m), 7.02~7.05(4H, m), 7.37(2H, m), 7.4(1H, s), 7.41(1H, m), 7.51(2H, m), 7.55(1H, s), 7.57(1H, m), 7.67(4H, m), 7.94~7.96(2H, m), 8.12~8.16(3H, m), 8.28(2H, m), 8.51~8.54(2H, m), 8.71(2H, m)	793.95	793.32
	H18	H88	δ = 1.94(4H, m), 2.96(4H, m), 3.7(1H, m), 7.1(1H, m), 7.17(2H, s), 7.42(1H, m), 7.49~7.57(4H, m), 7.67(4H, m), 7.76(1H, m), 7.86~7.96(5H, m), 8.12~8.21(4H, m), 8.48~8.54(3H, m), 8.91(1H, m)	693.84	693.29

[181]

TA-82	phenyl	H1	δ = 7.05(2H, m), 7.25(1H, m), 7.33(1H, m), 7.45~7.58(12H, m), 7.67(2H, m), 7.94~7.96(3H, m), 8.12~8.16(2H, m), 8.3(4H, m), 8.54~8.55(2H, m)	611.73	611.24
	phenyl	H4	δ = 7.25(1H, m), 7.33(1H, m), 7.41~7.51(9H, m), 7.57~7.58(3H, m), 7.67(2H, m), 7.79(4H, m), 7.94~7.96(3H, m), 8.12~8.16(2H, m), 8.54~8.55(2H, m), 8.63(1H, s)	612.72	612.23
	phenyl	H12	δ = 7.25(1H, m), 7.33(1H, m), 7.41~7.51(9H, m), 7.57~7.58(3H, m), 7.67(2H, m), 7.94~7.96(3H, m), 8.12~8.16(2H, m), 8.28(4H, m), 8.54~8.55(2H, m)	613.71	613.23
	H2	H76	δ = 7(1H, m), 7.25~7.26(2H, m), 7.33~7.34(2H, m), 7.51(1H, m), 7.57(1H, m), 7.67~7.71(5H, m), 7.94~7.96(3H, m), 8.12~8.16(2H, m), 8.3~8.34(3H, m), 8.45~8.55(4H, m)	536.62	536.20
	H31	H80	δ = 6.95~7.01(3H, m), 7.25~7.33(4H, m), 7.41(1H, m), 7.51(2H, m), 7.56(1H, s), 7.57~7.6(2H, m), 7.67(2H, m), 7.77~7.79(3H, m), 7.94~7.96(3H, m), 8.12~8.16(2H, m), 8.54~8.55(2H, m)	635.74	635.18
TA-106	phenyl	H1	δ = 7.05(2H, m), 7.45~7.58(12H, m), 7.67(4H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.3(4H, m), 8.54(2H, m)	661.79	661.25
	phenyl	H4	δ = 7.41~7.51(9H, m), 7.57~7.58(3H, m), 7.67(4H, m), 7.79(4H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.54(2H, m), 8.63(1H, s)	662.78	662.25
	phenyl	H12	δ = 7.41~7.51(9H, m), 7.57~7.58(3H, m), 7.67(4H, m), 7.94~7.96(4H, m), 8.12~8.16(3H, m), 8.28(4H, m), 8.54(2H, m)	663.77	663.24
	H2	H15	δ = 7.34(1H, m), 7.42(1H, m), 7.49(1H, m), 7.57~7.6(2H, m), 7.67~7.78(7H, m), 7.92~7.98(6H, m), 8.06~8.16(4H, m), 8.34(1H, m), 8.45(1H, m), 8.54(2H, m)	610.70	610.22
	H8	H88	δ = 1.94(4H, m), 2.96(4H, m), 3.7(1H, m), 7.1(1H, m), 7.52~7.57(3H, m), 7.67~7.71(5H, m), 7.86~7.96(4H, m), 8.05(1H, m), 8.12~8.16(3H, m), 8.48~8.54(3H, m), 8.76(2H, m), 8.82(1H, m)	644.77	644.27
TA-116	phenyl	H1	δ = 7.05(2H, m), 7.4~7.58(15H, m), 7.67(4H, m), 7.94~7.96(2H, m), 8.16(4H, m), 8.3(4H, m)	661.79	661.25
	phenyl	H4	δ = 7.4~7.58(15H, m), 7.67(4H, m), 7.79(4H, m), 7.94~7.96(2H, m), 8.16(4H, m), 8.63(1H, s)	662.78	662.25
	phenyl	H12	δ = 7.4~7.58(15H, m), 7.67(4H, m), 7.94~7.96(2H, m), 8.16(4H, m), 8.28(4H, m)	663.77	663.24
	H13	H13	δ = 7.4(2H, m), 7.55~7.6(4H, m), 7.67(4H, m), 7.78(2H, m), 7.91~7.98(6H, m), 8.06(2H, m), 8.16(4H, m), 8.38(2H, m)	610.70	610.22

[182]

	H12	H86	δ = 2.59(6H, s), 7.25~7.33(3H, m), 7.4~7.41(4H, m), 7.49~7.55(9H, m), 7.62~7.67(9H, m), 7.94~7.96(3H, m), 8.12~8.16(5H, m), 8.28(4H, m), 8.55(1H, m)	933.11	932.36
TB-4	H1	phenyl	δ = 7.05(2H, m), 7.22(1H, m), 7.29(1H, m), 7.45~7.63(14H, m), 7.97(1H, m), 8.12(1H, m), 8.3(4H, m), 8.43(2H, m)	562.66	562.22
	H4	phenyl	δ = 7.22(1H, m), 7.29(1H, m), 7.41~7.63(14H, m), 7.79(4H, m), 7.97(1H, m), 8.12(1H, m), 8.43(2H, m), 8.63(1H, s), (H,)	563.65	563.21
	H5	phenyl	δ = 7.14(2H, m), 7.22(1H, m), 7.29(1H, m), 7.45~7.63(8H, m), 7.7(2H, m), 7.97(1H, m), 8.12~8.15(3H, m), 8.43(2H, m), 8.53(2H, m), 9.3(2H, m)	564.64	564.21
	H12	phenyl	δ = 7.22(1H, m), 7.29(1H, m), 7.41~7.63(14H, m), 7.97(1H, m), 8.12(1H, m), 8.28(4H, m), 8.43(2H, m)	564.64	564.21
	H24	phenyl	δ = 2.9(1H, m), 5.13(1H, m), 5.66(1H, m), 6.16(1H, m), 6.44(1H, m), 7.22(1H, m), 7.29(1H, m), 7.45~7.5(4H, m), 7.58~7.63(3H, m), 7.81(1H, m), 7.94~7.97(3H, m), 8.12(1H, m), 8.43(1H, m)	448.52	448.17
	H38	phenyl	δ = 7.16~7.22(2H, m), 7.29(1H, m), 7.45~7.51(16H, m), 7.97(1H, m), 8.09~8.12(2H, m), 8.28(1H, m), 8.43(2H, m)	551.64	551.21
	H49	phenyl	δ = 1.72(6H, s), 6.55(2H, m), 6.63(2H, m), 6.73(2H, m), 7.02~7.05(4H, m), 7.22(1H, m), 7.29(1H, m), 7.37(2H, m), 7.45~7.63(8H, m), 7.97(1H, m), 8.12(1H, m), 8.43(2H, m)	616.75	616.26
	H56	phenyl	δ = 7.22(1H, m), 7.29(1H, m), 7.45~7.63(10H, m), 7.78(2H, m), 7.97~7.98(3H, m), 8.12(1H, m), 8.22(2H, m), 8.43(2H, m)	510.59	510.18
	H72	phenyl	δ = 7.22(1H, m), 7.29(1H, m), 7.45~7.63(10H, m), 7.97(1H, m), 8.12(1H, m), 8.4~8.47(5H, m), 8.7(1H, m), 9.24(1H, m)	487.55	487.18
	H81	phenyl	δ = 7.22~7.29(5H, m), 7.39~7.5(13H, m), 7.66(1H, s), 7.79(2H, m), 7.97(1H, m), 8.12(1H, m), 8.43(2H, m)	595.71	595.18
TB-7	H1	phenyl	δ = 7.05(2H, m), 7.29(1H, m), 7.45~7.63(14H, m), 8.12(1H, m), 8.3(4H, m), 8.43(1H, m), 8.63(2H, m)	563.65	563.21
	H4	phenyl	δ = 7.29(1H, m), 7.41~7.63(14H, m), 7.79(4H, m), 8.12(1H, m), 8.43(1H, m), 8.63(3H, m)	564.64	564.21
	H12	phenyl	δ = 7.29(1H, m), 7.41~7.63(14H, m), 8.12(1H, m), 8.28(4H, m), 8.43(1H, m), 8.63(2H, m)	565.63	565.20
	H23	phenyl	δ = 7.29(1H, m), 7.45~7.63(8H, m), 8.12(1H, m), 8.43(1H, m), 8.63(4H, m), 8.82(1H, s)	464.48	464.15
	H97	phenyl	δ = 7.29(1H, m), 7.41~7.51(16H, m), 7.79(6H, m), 8.12(1H, m), 8.23(1H, s), 8.43(1H, m), 8.63(2H, m)	640.73	640.24

[183]

TB-25	H1	phenyl	δ = 7.05(2H, m), 7.22(2H, m), 7.45~7.58(12H, m), 7.97(2H, m), 8.3(4H, m), 8.43(3H, m)	563.65	563.21
	H4	phenyl	δ = 7.22(2H, m), 7.41~7.58(12H, m), 7.79(4H, m), 7.97(2H, m), 8.43(3H, m), 8.63(1H, s)	564.64	564.21
	H9	phenyl	δ = 7.22(2H, m), 7.41~7.58(9H, m), 7.97(2H, m), 8.28(2H, m), 8.43(3H, m)	490.52	490.17
	H12	phenyl	δ = 7.22(2H, m), 7.41~7.58(12H, m), 7.97(2H, m), 8.28(4H, m), 8.43(3H, m)	565.63	565.20
	H16	phenyl	δ = 7.22(2H, m), 7.45~7.58(6H, m), 7.97(2H, m), 8.43(3H, m), 8.66(2H, m), 8.74(2H, m), 9.4(1H, m)	462.50	462.16
TB-33	H1	phenyl	δ = 7.05(2H, m), 7.22(1H, m), 7.45~7.58(12H, m), 7.97(1H, m), 8.3(4H, m), 8.43(2H, m), 8.63(2H, m)	564.64	564.21
	H4	phenyl	δ = 7.22(1H, m), 7.41~7.58(12H, m), 7.79(4H, m), 7.97(1H, m), 8.43(2H, m), 8.63(3H, m)	565.63	565.20
	H12	phenyl	δ = 7.22(1H, m), 7.41~7.58(12H, m), 7.97(1H, m), 8.28(4H, m), 8.43(2H, m), 8.63(2H, m)	566.61	566.20
	H39	phenyl	δ = 7.05(1H, s), 7.22(1H, m), 7.41~7.51(7H, m), 7.58(4H, m), 7.94~7.97(3H, m), 8.05(2H, m), 8.24(2H, m), 8.43(1H, m), 8.63(2H, m)	533.61	533.20
	H89	phenyl	δ = 1.88~1.91(2H, m), 2.3~2.33(2H, m), 3.22(1H, m), 3.7(1H, m), 7.22(1H, m), 7.41~7.51(9H, m), 7.58(2H, m), 7.71(1H, m), 7.97(1H, m), 8.05(1H, m), 8.28(4H, m), 8.43(1H, m), 8.63(2H, m)	646.74	646.26
TB-47	H1	phenyl	δ = 7.05(2H, m), 7.22(1H, m), 7.29(1H, m), 7.45~7.63(14H, m), 7.94~7.97(2H, m), 8.12(1H, m), 8.3(4H, m), 8.43(1H, m)	562.66	562.22
	H4	phenyl	δ = 7.22(1H, m), 7.29(1H, m), 7.41~7.51(10H, m), 7.58~7.63(4H, m), 7.79(4H, m), 7.94~7.97(2H, m), 8.12(1H, m), 8.43(1H, m), 8.63(1H, s)	563.65	563.21
	H83	phenyl	δ = 7.22(1H, m), 7.29(1H, m), 7.41~7.51(13H, m), 7.58~7.63(4H, m), 7.77~7.83(10H, m), 7.94~7.97(2H, m), 8.12(1H, m), 8.43(1H, m), 8.63(1H, s)	763.82	763.25
TB-48	H1	phenyl	δ = 7.05(2H, m), 7.22(2H, m), 7.45~7.62(12H, m), 7.94~7.97(3H, m), 8.3(4H, m), 8.43(2H, m)	563.65	563.21
	H4	phenyl	δ = 7.22(2H, m), 7.41~7.51(9H, m), 7.58~7.62(3H, m), 7.79(4H, m), 7.94~7.97(3H, m), 8.43(2H, m), 8.63(1H, s)	564.64	564.21
	H58	phenyl	δ = 6.52(1H, m), 6.87(1H, m), 7.22(2H, m), 7.33(1H, m), 7.45~7.5(3H, m), 7.58~7.62(8H, m), 7.93~7.97(5H, m), 8.43(2H, m)	525.60	525.20
TB-49	H1	phenyl	δ = 7.05(2H, m), 7.22~7.25(2H, m), 7.33(1H, m), 7.4(1H, s), 7.45~7.54(9H, m), 7.55(1H, s), 7.58(2H, m), 7.94~7.97(2H, m), 8.3(4H, m), 8.43(1H, m), 8.55(1H, m)	562.66	562.22

[184]

	H4	phenyl	δ = 7.22~7.25(2H, m), 7.33(1H, m), 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.58(2H, m), 7.79(4H, m), 7.94~7.97(2H, m), 8.43(1H, m), 8.55(1H, m), 8.63(1H, s)	563.65	563.21
	H47	phenyl	δ = 7.22~7.25(4H, m), 7.33(1H, m), 7.4(1H, s), 7.45~7.5(3H, m), 7.55(1H, s), 7.58~7.62(6H, m), 7.94~7.97(4H, m), 8.43(3H, m), 8.55(1H, m)	576.65	576.21
TB-50	H1	phenyl	δ = 7.05(2H, m), 7.22(2H, m), 7.4(1H, s), 7.45~7.54(9H, m), 7.55(1H, s), 7.58(2H, m), 7.97(2H, m), 8.3(4H, m), 8.43(2H, m)	563.65	563.21
	H4	phenyl	δ = 7.22(2H, m), 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.58(2H, m), 7.79(4H, m), 7.97(2H, m), 8.43(2H, m), 8.63(1H, s)	564.64	564.21
	H62	phenyl	δ = 6.59~6.63(4H, m), 6.77~6.81(2H, m), 6.89~6.94(4H, m), 7.2~7.22(4H, m), 7.4(1H, s), 7.45~7.5(3H, m), 7.55(1H, s), 7.58(2H, m), 7.97(2H, m), 8.43(2H, m)	591.66	591.21
TB-51	H1	phenyl	δ = 7.05(2H, m), 7.22~7.25(2H, m), 7.33(1H, m), 7.4(1H, s), 7.45~7.54(9H, m), 7.55(1H, s), 7.58(2H, m), 7.94~7.97(2H, m), 8.3(4H, m), 8.43(1H, m), 8.55(1H, m)	562.66	562.22
	H4	phenyl	δ = 7.22~7.25(2H, m), 7.33(1H, m), 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.58(2H, m), 7.79(4H, m), 7.94~7.97(2H, m), 8.43(1H, m), 8.55(1H, m), 8.63(1H, s)	563.65	563.21
	H33	phenyl	δ = 7.22~7.25(2H, m), 7.33(1H, m), 7.4(1H, s), 7.45~7.5(3H, m), 7.55(1H, s), 7.58(2H, m), 7.94~7.97(2H, m), 8.43(1H, m), 8.55(1H, m), 9(1H, s)	417.49	417.10
TB-52	H1	phenyl	δ = 7.05(2H, m), 7.22(2H, m), 7.4(1H, s), 7.45~7.54(9H, m), 7.55(1H, s), 7.58(2H, m), 7.97(2H, m), 8.3(4H, m), 8.43(2H, m)	563.65	563.21
	H4	phenyl	δ = 7.22(2H, m), 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.58(2H, m), 7.79(4H, m), 7.97(2H, m), 8.43(2H, m), 8.63(1H, s)	564.64	564.21
	H79	H12	δ = 7.22(2H, m), 7.4(1H, s), 7.41~7.51(9H, m), 7.55(1H, s), 7.58(2H, m), 7.97(2H, m), 8.28(4H, m), 8.43(2H, m)	565.63	565.20

[185]

[186] [Table 2]

[187]

Compound	Ar_1	^1H NMR($CDCl_3$, 200 MHz)	MS/FAB	
			found	calculated
TC-1	H1	δ = 7.05(2H, m), 7.25(1H, m), 7.32~7.38(3H, m), 7.47(2H, m), 7.53~7.54(5H, m), 7.66(1H, m), 7.89~7.94(3H, m), 8.3(4H, m), 8.55(1H, m)	486.56	486.17
	H9	δ = 7.25(1H, m), 7.32~7.41(4H, m), 7.51~7.53(3H, m), 7.66(1H, m), 7.89~7.94(3H, m), 8.28(2H, m), 8.55(1H, m)	413.43	413.13
	H12	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.51~7.53(5H, m), 7.66(1H, m), 7.89~7.94(3H, m), 8.28(4H, m), 8.55(1H, m)	488.54	488.16
TC-2	H4	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.51(4H, m), 7.59(1H, m), 7.66(2H, m), 7.79(4H, m), 7.89~7.94(2H, m), 8.55(1H, m), 8.63(1H, s)	487.55	487.17
	H12	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.51(4H, m), 7.59(1H, m), 7.66(2H, m), 7.89~7.94(2H, m), 8.28(4H, m), 8.55(1H, m)	488.54	488.16
	H20	δ = 7.25(1H, m), 7.32~7.38(3H, m), 7.59(1H, m), 7.66~7.67(4H, m), 7.8(2H, m), 7.89~7.94(2H, m), 8.55(1H, m), 8.7(1H, s)	385.42	385.12
TC-3	H4	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.42(1H, s), 7.49(1H, s), 7.51(4H, m), 7.66(1H, m), 7.79(4H, m), 7.89~7.94(2H, m), 8.55(1H, m), 8.63(1H, s)	487.55	487.17
	H12	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.42(1H, s), 7.49(1H, s), 7.51(4H, m), 7.66(1H, m), 7.89~7.94(2H, m), 8.28(4H, m), 8.55(1H, m)	488.54	488.16
	H94	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.42(1H, s), 7.45~7.47(3H, m), 7.49(1H, s), 7.5~7.51(6H, m), 7.58(2H, m), 7.66(1H, m), 7.79(2H, m), 7.89~7.94(2H, m), 8.55(1H, m)	551.64	551.20
TC-4	H1	δ = 7.05(2H, m), 7.25(1H, m), 7.32~7.38(3H, m), 7.42(1H, s), 7.47(2H, m), 7.49(1H, s), 7.54(4H, m), 7.66(1H, m), 7.89~7.94(2H, m), 8.3(4H, m), 8.55(1H, m)	486.56	486.17
	H4	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.42(1H, s), 7.49(1H, s), 7.51(4H, m), 7.66(1H, m), 7.79(4H, m), 7.89~7.94(2H, m), 8.55(1H, m), 8.63(1H, s)	487.55	487.17
	H95	δ = 7.25(1H, m), 7.32~7.41(5H, m), 7.42(1H, s), 7.45(1H, m), 7.49(1H, s), 7.51(4H, m), 7.58~7.66(5H, m), 7.79(4H, m), 7.89~7.94(2H, m), 8.55(1H, m)	551.64	551.20
TC-5	H1	δ = 7.05(2H, m), 7.19~7.25(2H, m), 7.32~7.38(3H, m), 7.47(2H, m), 7.54(4H, m), 7.66(2H, m), 7.89~7.94(2H, m), 8.3(4H, m), 8.55(1H, m)	486.56	486.17
	H12	δ = 7.19~7.25(2H, m), 7.32~7.41(5H, m), 7.51(4H, m), 7.66(2H, m), 7.89~7.94(2H, m), 8.28(4H, m), 8.55(1H, m)	488.54	488.16
	H50	δ = 6.59~6.63(4H, m), 6.77(2H, m), 6.89~6.92(4H, m), 7.19~7.25(2H, m), 7.32~7.38(5H, m), 7.66(2H, m), 7.89~7.94(2H, m), 8.55(1H, m)	514.57	514.17
	H70	δ = 7.19~7.25(2H, m), 7.32~7.38(4H, m), 7.66~7.72(3H, m), 7.86~7.94(3H, m), 8.5~8.55(3H, m), 8.78(2H, m)	411.45	411.14

[188]

TC-6	H4	δ = 7.13(1H, m), 7.25(1H, m), 7.32~7.41(5H, m), 7.51(4H, m), 7.66(1H, m), 7.79(4H, m), 7.89~7.94(3H, m), 8.55(1H, m), 8.63(1H, s), . .	487.55	487.17
	H14	δ = 7.13(1H, m), 7.25(1H, m), 7.32~7.42(5H, m), 7.49(1H, m), 7.63~7.66(2H, m), 7.89~7.94(4H, m), 8.21(1H, m), 8.55(1H, m)	384.43	384.13
	H48	δ = 7.13(1H, m), 7.25(1H, m), 7.32~7.38(3H, m), 7.51(2H, m), 7.62~7.66(5H, m), 7.89~7.94(3H, m), 8.43(2H, m), 8.55(1H, m), 9.34(2H, m)	500.55	500.16
TC-7	H12	δ = 7.25(1H, m), 7.33(1H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.6(1H, m), 7.94~7.98(2H, m), 8.05(1H, m), 8.28(4H, m), 8.45(1H, m), 8.55(1H, m)	504.60	504.14
	H30	δ = 7.25(1H, m), 7.33(1H, m), 7.5~7.52(4H, m), 7.6(1H, m), 7.7(1H, m), 7.79(1H, m), 7.94~7.98(3H, m), 8.05(1H, m), 8.45(1H, m), 8.55(1H, m)	405.53	405.06
	H73	δ = 7.25(1H, m), 7.33(1H, m), 7.5~7.52(3H, m), 7.6(1H, m), 7.94~7.99(4H, m), 8.05(1H, m), 8.4~8.47(3H, m), 8.55(1H, m), 8.75(2H, m)	427.52	427.11
TC-8	H1	δ = 7.05(2H, m), 7.25(1H, m), 7.33(1H, m), 7.47~7.54(8H, m), 7.8(1H, m), 7.94~7.98(2H, m), 8.08(1H, m), 8.3(4H, m), 8.45(1H, m), 8.55(1H, m)	502.63	502.15
	H4	δ = 7.25(1H, m), 7.33(1H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.79~7.8(5H, m), 7.94~7.98(2H, m), 8.08(1H, m), 8.45(1H, m), 8.55(1H, m), 8.63(1H, s)	503.62	503.15
	H96	δ = 7.25(1H, m), 7.33(1H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.68(2H, m), 7.79~7.8(3H, m), 7.94~7.98(2H, m), 8.08(1H, m), 8.28(4H, m), 8.45(1H, m), 8.55(1H, m)	580.70	580.17
TC-9	H4	δ = 7.25(1H, m), 7.33(1H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.78(1H, s), 7.79(4H, m), 7.86(1H, s), 7.94~7.98(2H, m), 8.45(1H, m), 8.55(1H, m), 8.63(1H, s)	503.15	503.62
	H52	δ = 6.63(2H, m), 6.97(2H, m), 7.16~7.25(7H, m), 7.33~7.37(3H, m), 7.5~7.52(2H, m), 7.78(1H, s), 7.86(1H, s), 7.94~7.98(2H, m), 8.45(1H, m), 8.55(1H, m)	546.70	546.12
	H65	δ = 6.38~6.39(4H, m), 6.56(2H, m), 6.63(4H, m), 6.73(1H, m), 6.81(2H, m), 7.2~7.25(5H, m), 7.33(1H, m), 7.5~7.52(2H, m), 7.78(1H, s), 7.86(1H, s), 7.94~7.98(2H, m), 8.45(1H, m), 8.55(1H, m)	605.75	605.19
TC-10	H4	δ = 7.25(1H, m), 7.33(1H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.78(1H, s), 7.79(4H, m), 7.86(1H, s), 7.94~7.98(2H, m), 8.45(1H, m), 8.55(1H, m), 8.63(1H, s)	503.62	503.15
	H6	δ = 7.25(1H, m), 7.32(1H, s), 7.33(1H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.78(1H, s), 7.79(2H, m), 7.86(1H, s), 7.94~7.98(2H, m), 8.28(2H, m), 8.45(1H, m), 8.55(1H, m)	503.62	503.15
	H55	δ = 6.63(4H, m), 6.81(2H, m), 6.99~7.05(4H, m), 7.25(3H, m), 7.33~7.37(3H, m), 7.5~7.52(2H, m), 7.78(1H, s), 7.86(1H, s), 7.94~7.98(2H, m), 8.45(1H, m), 8.55(1H, m)	540.68	540.17

[189]

TC-11	H4	δ = 7.25~7.33(3H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.79(4H, m), 7.94~7.98(3H, m), 8.45(1H, m), 8.55(1H, m), 8.63(1H, s)	503.62	503.15
	H12	δ = 7.25~7.33(3H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.94~7.98(3H, m), 8.28(4H, m), 8.45(1H, m), 8.55(1H, m)	504.60	504.14
	H28	δ = 6.47(1H, m), 6.58(1H, m), 7.25~7.33(3H, m), 7.41~7.52(8H, m), 7.58(2H, m), 7.79(2H, m), 7.94~7.98(3H, m), 8.45(1H, m), 8.55(1H, m)	490.62	490.15
TC-12	H4	δ = 7.25(1H, m), 7.33(2H, m), 7.41(2H, m), 7.5~7.52(6H, m), 7.79(4H, m), 7.94~7.98(2H, m), 8.05(1H, m), 8.45(1H, m), 8.55(1H, m), 8.63(1H, s)	503.62	503.15
	H34	δ = 7.09(1H, m), 7.25(1H, m), 7.33(2H, m), 7.5~7.52(2H, m), 7.69(1H, m), 7.94~7.98(2H, m), 8.05(1H, m), 8.45(1H, m), 8.55(1H, m)	340.40	340.07
	H77	δ = 7.25(1H, m), 7.33(2H, m), 7.5~7.57(3H, m), 7.68(2H, m), 7.79(2H, m), 7.94~7.98(2H, m), 8.05(1H, m), 8.42~8.45(2H, m), 8.55(1H, m), 8.7(1H, m), 9.24(1H, m)	426.53	426.12

[190]

[191] [Example 1-10] Manufacture of OLED's using organic electroluminescent compounds according to the present invention

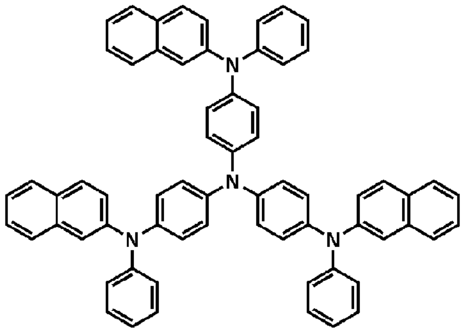
[192] OLED devices were manufactured by using the electroluminescent compounds according to the invention.

[193] First, a transparent electrode ITO thin film (15Ω/□) prepared from glass for OLED (produced by Samsung-Corning) was subjected to ultrasonic washing with trichloroethylene, acetone, ethanol and distilled water, sequentially, and stored in iso-propanol before use.

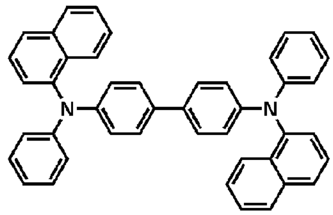
[194] Then, an ITO substrate was equipped in a substrate folder of a vacuum vapor-deposit device, and 4,4',4"-tris(N,N-(2-naphthyl)-phenylamino)triphenylamine (2-TNATA)(of which the chemical structure is shown below) was placed in a cell of the vacuum vapor-deposit device, which was then ventilated up to 10^{-6} torr of vacuum in the chamber. Electric current was applied to the cell to evaporate 2-TNATA, thereby providing vapor-deposit of a hole injection layer having 60 nm of thickness on the ITO substrate.

[195] Then, to another cell of the vacuum vapor-deposit device, charged was N,N'-bis(α-naphthyl)-N,N'-diphenyl-4,4'-diamine (NPB), and electric current was applied to the cell to evaporate NPB, thereby providing vapor-deposit of a hole transport layer of 20 nm of thickness on the hole injection layer.

[196]



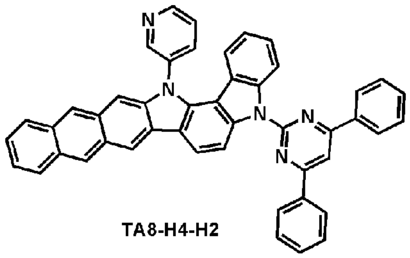
2-TNATA



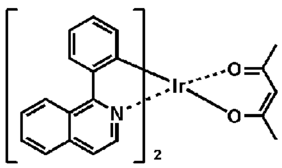
NPB

[197] To one cell of said vacuum vapor-deposit device, charged was a compound according to the present invention, which had been purified via vacuum sublimation under 10^{-6} torr (for example, Compound TA8-H4-H2), and an electroluminescent dopant (for example, compound $(piq)_2Ir(acac)$) to another cell, respectively. The two materials were evaporated at different rates to carry out doping in a concentration from 4 to 10 mol%, thereby vapor-depositing an electroluminescent layer having 30 nm of thickness on the hole transport layer.

[198]



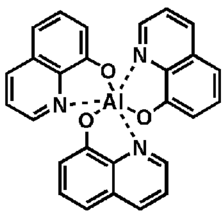
TA8-H4-H2



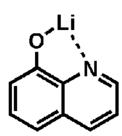
$(piq)_2Ir(acac)$

[199] Then, tris(8-hydroxyquinoline)aluminum (III) (Alq) [of which the structure is shown below] was vapor-deposited as an electron transport layer with a thickness of 20 nm, and lithium quinolate (Liq) was vapor-deposited as an electron injection layer with a thickness of 1 to 2 nm. Thereafter, an Al cathode was vapor-deposited with a thickness of 150 nm by using another vacuum vapor-deposit device to manufacture an OLED.

[200]



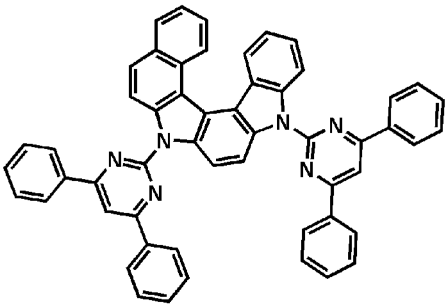
Alq



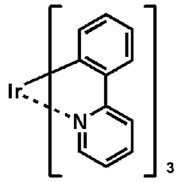
Liq

[201] [Example 11-20] Manufacture of OLED's by using electroluminescent compounds according to the present invention

[202] OLED's were manufactured according to the same procedure as for OLED s of Examples 1 to 10, but using compounds according to the present invention (for example: Compound TA4-H4-H4) as host material, and organic iridium complex $(Ir(ppy)_3)$ represented by the chemical formula below as electroluminescent dopant.

[203] 

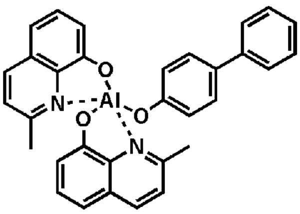
TA4-H4-H4



Ir(ppy)₃

[204] [Comparative Example 1 and 2] Manufacture of OLED's by using conventional electroluminescent material

[205] OLED's were manufactured according to the same procedure described in Examples 1 and 11, but another cell of the vacuum vapor-deposition device was charged with bis(2-methyl-8-quinolinato)(p-phenylphenolato)aluminum (III) (BAlq), instead of the electroluminescent compound according to the invention, as host material.

[206] 

BAlq

[207] The operation voltage and power efficiency of the OLED's manufactured from Examples 1 to 10 and Examples 11 to 20 (which comprises the organic electroluminescent compounds according to the present invention), and from Comparative Examples 1 and 2 (which comprises conventional electroluminescent compound) were measured at 1,000 cd/m^2, and the results are listed in Tables 3 and 4.

[208] As can be seen from Table 3 and Table 4, the organic electroluminescent compounds developed by the present invention exhibited superior properties in terms of device performances as compared to conventional materials.

[209] [Table 3]

[210]

	Host material			EL material	@ 1,000 cd/m^2		EL color
	Compound	Ar_1	Ar_2		Operation voltage (V)	Power Efficiency (lm/W)	
Ex.1	TA8	H4	H2	$(piq)_2Ir(acac)$	5.9	3.6	Red
Ex.2	TA33	Phenyl	H74	$(piq)_2Ir(acac)$	6.2	3.8	Red
Ex.3	TA45	H97	H69	$(piq)_2Ir(acac)$	4.9	5.1	Red
Ex.4	TA74	H12	H12	$(piq)_2Ir(acac)$	6.4	4.0	Red
Ex.5	TB27	H27	Phenyl	$(piq)_2Ir(acac)$	5.7	3.7	Red
Ex.6	TB40	H4	Phenyl	$(piq)_2Ir(acac)$	5.1	4.3	Red
Ex.7	TC1	H9	-	$(piq)_2Ir(acac)$	6.0	3.5	Red
Ex.8	TC6	H14	-	$(piq)_2Ir(acac)$	5.0	4.8	Red
Ex.9	TC9	H52	-	$(piq)_2Ir(acac)$	5.4	4.5	Red
Ex.10	TC12	H34	-	$(piq)_2Ir(acac)$	6.1	3.9	Red
Comp. Ex.1	BAlq			$(piq)_2Ir(acac)$	7.5	2.6	Red

[211] [Table 4]

[212]

	Host material			EL material	@ 1,000 cd/m^2		EL color
	Compound	Ar_1	Ar_2		Operation voltage (V)	Power Efficiency (lm/W)	
Ex.11	TA4	H4	H4	$Ir(ppy)_3$	5.4	14.2	Green
Ex.12	TA49	phenyl	H12	$Ir(ppy)_3$	5.7	14.9	Green
Ex.13	TA58	H47	Phenyl	$Ir(ppy)_3$	5.2	15.7	Green
Ex.14	TA84	H95	Phenyl	$Ir(ppy)_3$	5.1	16.1	Green
Ex.15	TB3	H79	H2	$Ir(ppy)_3$	6.4	13.8	Green
Ex.16	TB30	H96	H14	$Ir(ppy)_3$	6.5	13.5	Green
Ex.17	TB45	H59	H76	$Ir(ppy)_3$	5.5	15.9	Green
Ex.18	TC3	H94	-	$Ir(ppy)_3$	5.3	15.8	Green
Ex.19	TC4	H50	-	$Ir(ppy)_3$	5.6	14.7	Green
Ex.20	TC11	H28	-	$Ir(ppy)_3$	6.3	13.9	Green
Comp. Ex.2	BAlq			$Ir(ppy)_3$	7.8	8.4	Green

[213] As can be seen from Table 3, the compounds developed by the present invention showed excellent properties in terms of luminescent properties as compared to the conventional materials. The devices manufactured according to the present invention showed excellent current properties as compared to the device of Comparative Example 1 which was manufactured with conventional material, thereby providing operation voltage lowered by 1 V or more. They also showed higher current efficiency properties of at least 1.4 folds as compared to the device of Comparative Example 1, due to the remarkably improved luminous properties.

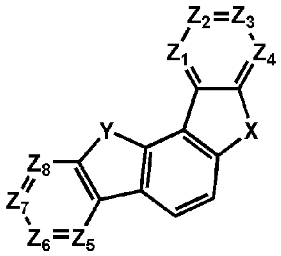
[214] As can be seen from Table 4, when the compounds developed by the present invention were used as host for green electroluminescence, the device showed, due to their excellent luminous properties, far higher power efficiency of at least 1.6 folds as compared to the device of Comparative Example 2. Excellent luminous properties were confirmed as compared to the conventional materials. Particularly, the device of Example 14 was operated at a lower voltage by 2.7 V as compared to that of Comparative Example 1, and the device of Example 17 showed 5.5 V of operation voltage and 15.9 lm/W of power efficiency at 1000 cd/m^2.

[215] Therefore, the devices employing the electroluminescent compounds according to the present invention as host material for emitting red or green light exhibited excellent luminous properties, with lowering the operation voltage, so that the device for emitting green light, in particular, induces increase of power efficiency by 5.1 to 7.7 lm/W to result in improvement in power consumption.

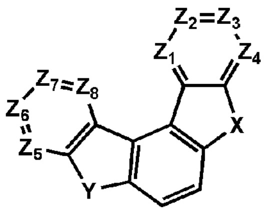
Claims

[Claim 1] An organic electroluminescent compound represented by one of Chemical Formulas 1 to 5:

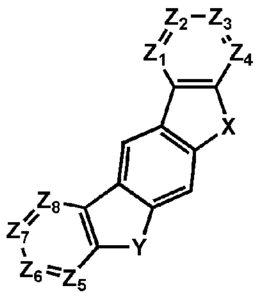
[Chemical Formula 1]



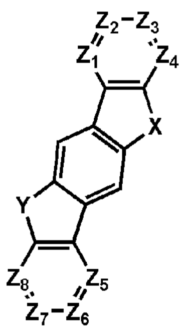
[Chemical Formula 2]



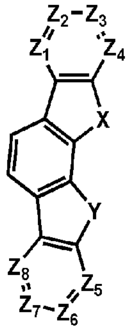
[Chemical Formula 3]



[Chemical Formula 4]



[Chemical Formula 5]



wherein,

X and Y are independently selected from $N(Ar_1)$, O and S, wherein Ar_1 may be different from one another, and Ar_1 may be represented as Ar_1 or Ar_2 where there are two or more Ar_1 groups;

Z_1 through Z_8 are independently selected from $C(Ar_3)$ and N, wherein Ar_3 may be different from one another, and adjacent Ar_3 groups may be linked together to form a ring;

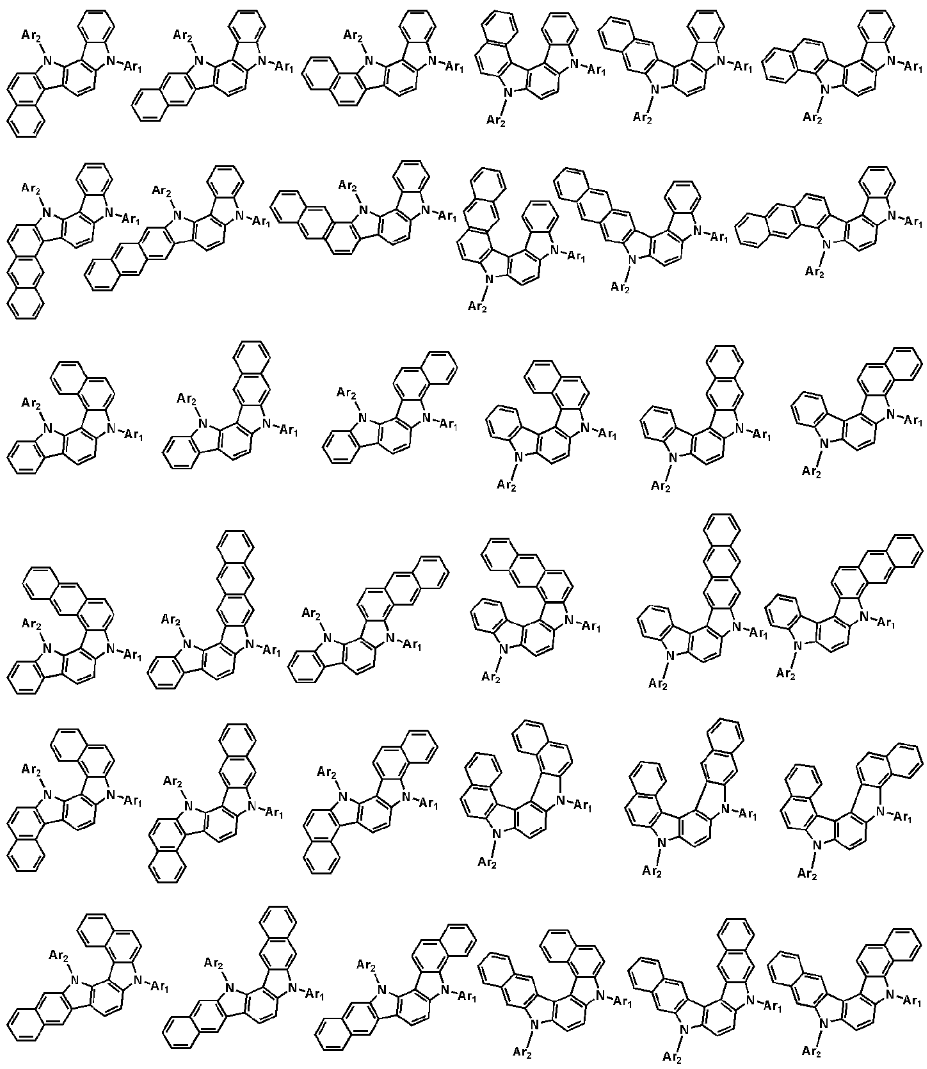
Ar_1 and Ar_2 are independently selected from (C1-C60)alkyl, (C3-C60)cycloalkyl, 5- or 6-membered heterocycloalkyl containing one or more heteroatom(s) selected from N, O, S, Si and P, (C7-C60)bicycloalkyl, adamantyl, (C2-C60)alkenyl, (C2-C60)alkynyl, (C6-C60)aryl and (C3-C60)heteroaryl;

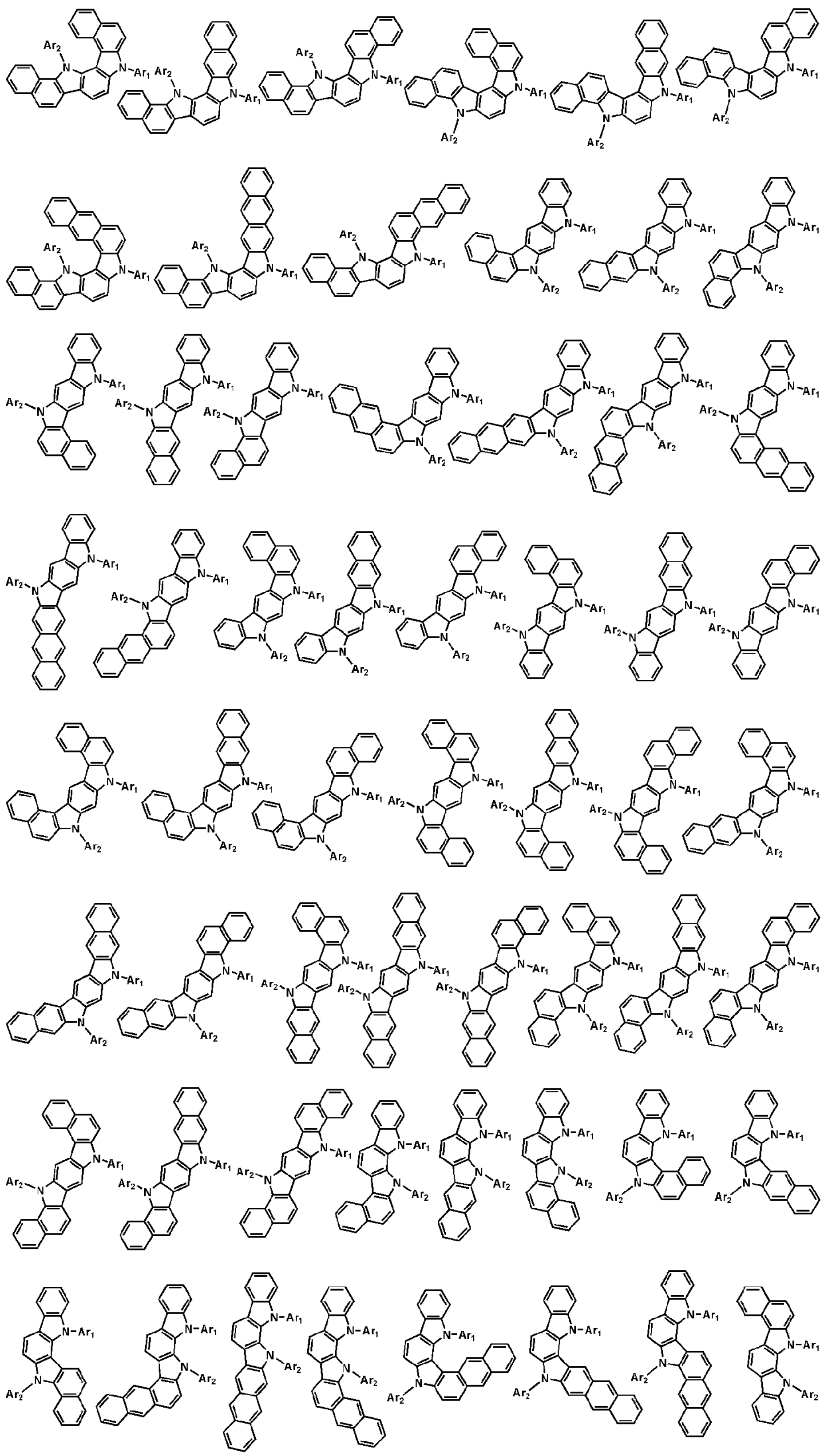
Ar_3 are independently selected from hydrogen, (C1-C60)alkyl, halogen, cyano, (C3-C60)cycloalkyl, 5- or 6-membered heterocycloalkyl containing one or more heteroatom(s) selected from N, O, S, Si and P, (C7-C60)bicycloalkyl, adamantyl, (C2-C60)alkenyl, (C2-C60)alkynyl, (C6-C60)aryl, (C1-C60)alkoxy, (C6-C60)aryloxy, (C3-C60)heteroaryl, (C6-C60)arylthio, (C1-C60)alkylthio, mono- or di(C1-C30)alkylamino, mono- or di(C6-C30)arylamino, tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, mono- or di(C6-C30)arylboranyl, mono- or di(C1-C60)alkylboranyl, nitro and hydroxyl; and

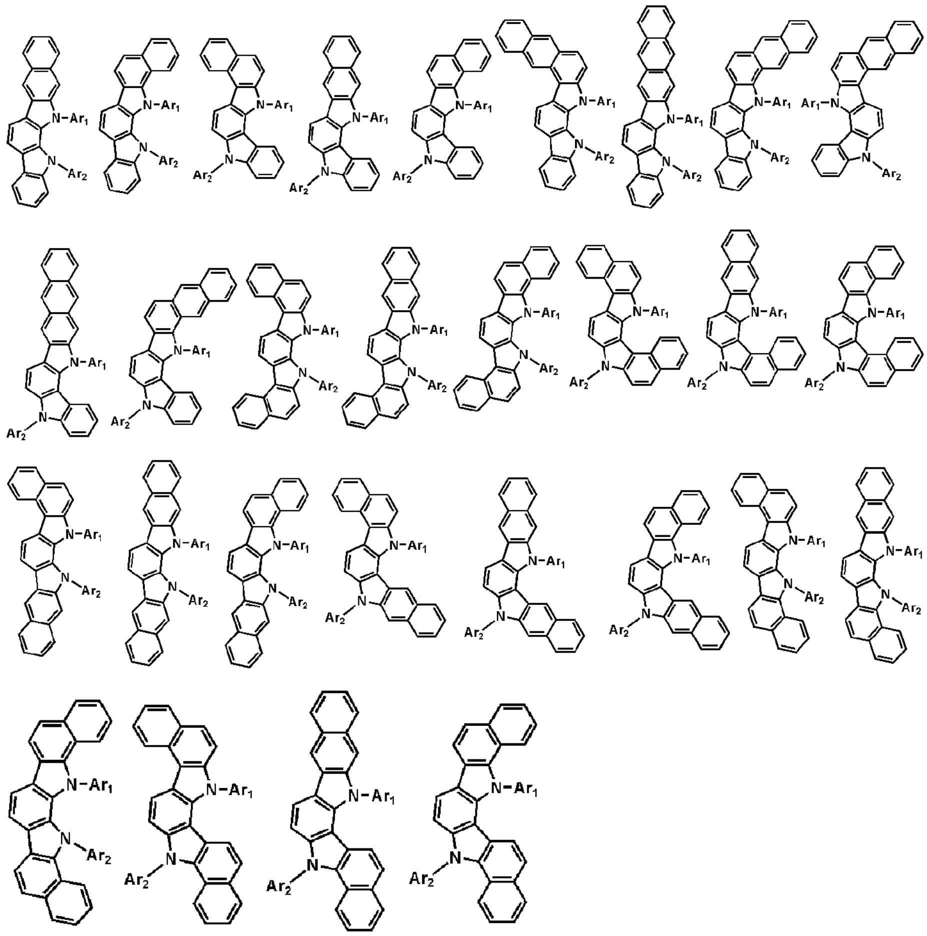
the alkyl, cycloalkyl, heterocycloalkyl, bicycloalkyl, adamantyl, alkenyl, alkynyl, aryl, alkoxy, aryloxy, heteroaryl, arylthio, alkylthio, alkylamino, arylamino, trialkylsilyl, dialkylarylsilyl, triarylsilyl, arylboranyl or alkylboranyl of Ar_1 through Ar_3 may be further substituted by one or more substituent(s) selected from a group consisting of (C1-C60)alkyl, halogen, cyano, (C3-C60)cycloalkyl, 5- or 6-membered heterocycloalkyl containing one or more heteroatom(s) selected from N, O, S, Si and P, (C7-C60)bicycloalkyl, adamantyl, (C2-C60)alkenyl, (C2-C60)alkynyl, (C6-C60)aryl, (C1-C60)alkoxy, (C6-C60)aryloxy, (C6-C60)aryl substituted by $P(=O)R_aR_b$ [R_a and R_b independently represent (C1-C60)alkyl or (C6-C60)aryl], (C3-C60)heteroaryl, (C3-C60)heteroaryl subsitituted by (C6-C60)aryl, (C3-C60)heteroaryl substituted by (C1-C60)alkyl, (C6-C60)ar(C1-C60)alkyl, (C6-C60)arylthio, (C1-C60)alkylthio, mono- or di(C1-C30)alkylamino, mono- or di(C6-C30)arylamino, tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, mono- or di(C6-C30)arylboranyl, mono- or di(C1-C60)alkylboranyl, nitro and hydroxyl,

excluding the case where both X and Y are $N(Ar_1)$ and all of Z_1 through Z_8 are $C(Ar_3)$.

[Claim 2] The organic electroluminescent compound according to claim 1, which is selected from the following compounds:



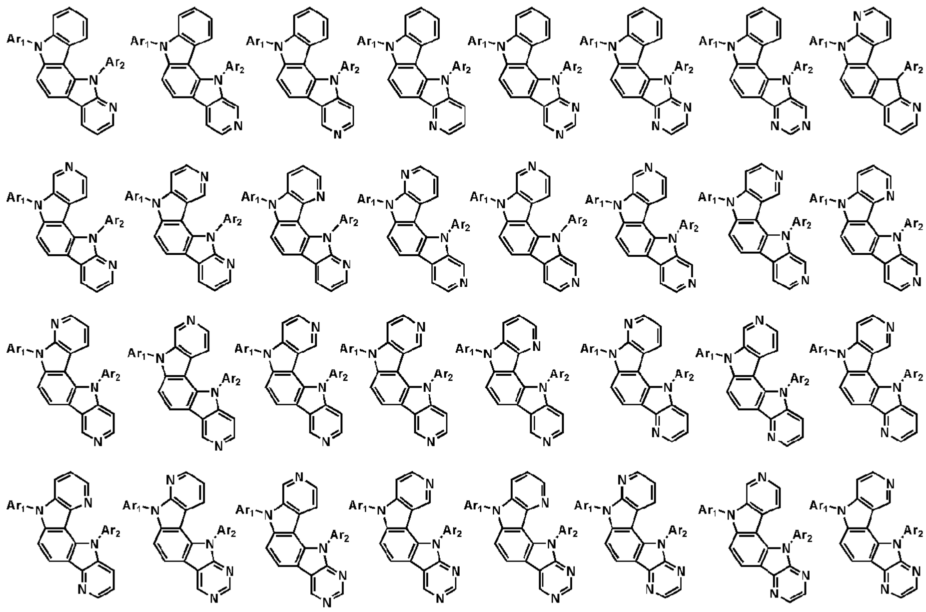


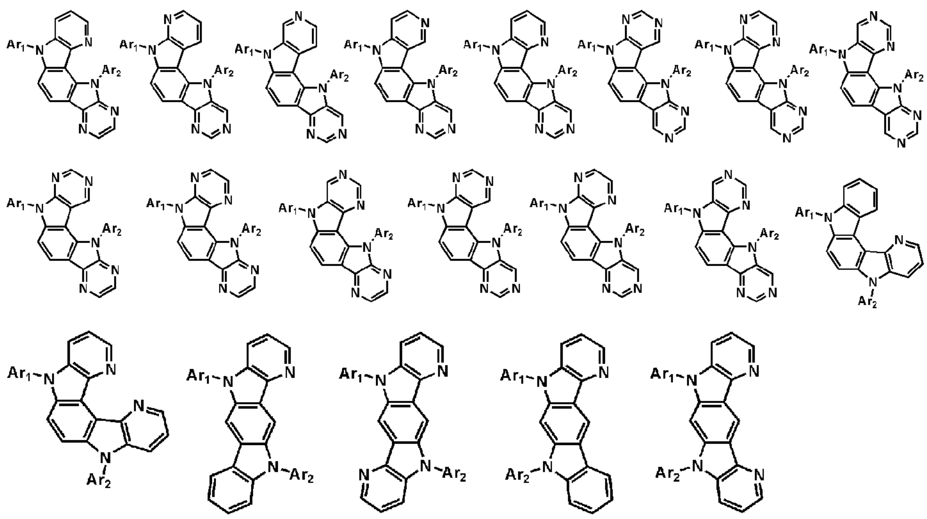


wherein,

Ar_1 and Ar_2 are defined as in claim 1.

[Claim 3] The organic electroluminescent compound according to claim 1, which is selected from the following compounds:

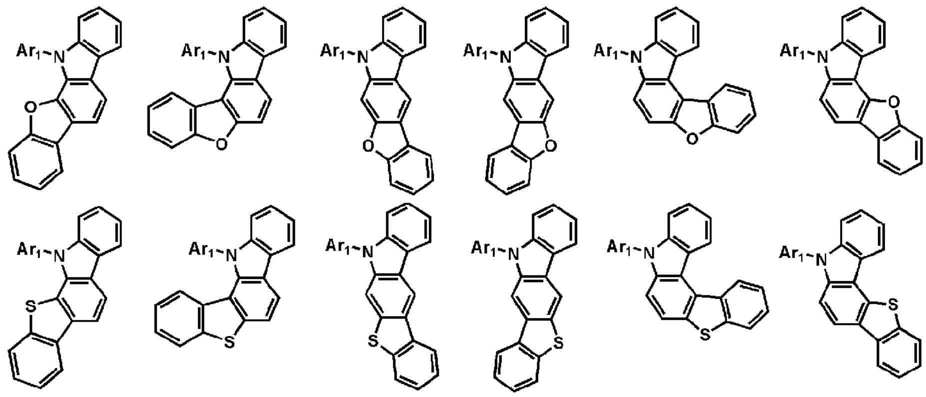




wherein,

Ar_1 and Ar_2 are defined as in claim 1.

[Claim 4] The organic electroluminescent compound according to claim 1, which is selected form the following compounds:



wherein,

Ar_1 is defined as in claim 1.

[Claim 5] An organic electroluminescent device comprising the organic electroluminescent compound according to any one of claims 1 to 4.

[Claim 6] The organic electroluminescent device according to claim 5, which comprises a first electrode; a second electrode; and one or more organic layer(s) interposed between the first electrode and the second electrode, wherein the organic layer comprises one or more organic electroluminescent compound(s) according to any one of claims 1 to 4 and one or more phosphorescent dopant(s).

[Claim 7] The organic electroluminescent device according to claim 6, wherein the organic layer further comprises one or more amine compound(s) selected from a group consisting of arylamine compounds and styrylarylamine compounds.

[Claim 8] The organic electroluminescent device according to claim 6, wherein the organic layer further comprises one or more metal(s) selected from a group consisting of organic metals of Group 1, Group 2, 4th period and 5th period transition metals, lanthanide metals and d-transition elements, or complex(es) formed therefrom.

[Claim 9] The organic electroluminescent device according to claim 6, wherein the organic layer comprises an electroluminescent layer and a charge generating layer.

[Claim 10] The organic electroluminescent device according to claim 6, which is a white light-emitting organic electroluminescent device wherein the organic layer simultaneously comprises one or more organic electroluminescent layer(s) emitting blue, red or green light.