



(51) International Patent Classification:

C09K 11/06 (2006.01) *C07C 15/38* (2006.01)
C07C 15/20 (2006.01) *H01L 51/50* (2006.01)

(21) International Application Number:

PCT/KR2014/005078

(22) International Filing Date:

10 June 2014 (10.06.2014)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

10-2013-0067043 12 June 2013 (12.06.2013) KR
10-2014-0060059 20 May 2014 (20.05.2014) KR

(71) Applicant: **SK CHEMICALS CO., LTD.** [KR/KR]; 310, Pangyo-ro, Bundang-gu, Seongnam-si, Gyeonggi-do 463-400 (KR).

(72) Inventors: **CHANG, Yu-Mi**; 102-1504, 69, Songjeong-ro (Nasan Apt., Gyeongandong), Gwangju-si, Gyeonggi-do 464-806 (KR). **LEE, Song**; 19, Dangsang-ro 50-gil (Dangsan-dong 6-ga), Yeongdeungpo-gu, Seoul 150-807 (KR). **JUN, Suk Woon**; 151-2305, 27, Jeongjacheon-ro 32beon-gil, Paldal-gu (Ggotmebeodeulmaeulkumgang Apt., Hwaseo-dong), Suwon-si, Gyeonggi-do 442-150 (KR). **PARK, Jeong Ho**; 121-504, 275, Dongpangyo-ro, Bundang-gu (Poongseong Simmiju Apt., Sampyeong-dong), Seongnam-si, Gyeonggi-do 463-891 (KR). **KANG, Ju-Sik**; 102-3103, 264, Dongtanbanseok-ro (Daewoo Purgio Apt., Seoku-dong), Hwaseong-si, Gyeonggi-do 445-170 (KR). **SHIN, Yong-Jun**; 114-2503, 100, Susaek-ro (DMC Raemian e-Pyeonhansesang Apt., Bukgajwa-dong),

Seodaemun-gu, Seoul 120-802 (KR). **YANG, Nam-choul**; 110-507, 91, Baumoe-ro (Woosung Apt., Yangjaedong), Seocho-gu, Seoul 137-793 (KR). **PARK, Jae-kyun**; 113-904, 120, Soseong-ro (Donga Poonglim Apt., Hagik-dong), Nam-gu, Incheon 402-873 (KR).

(74) Agent: **LEE, Soo Yeol**; 4th FL. Artspace Bldg., 13 Banpo-daero, 23-gil, Seocho-gu, Seoul 137-871 (KR).

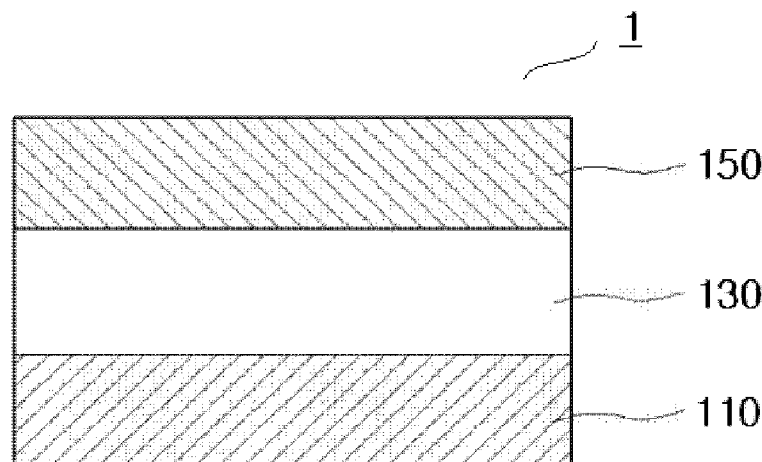
(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JP,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

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

Published:

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

(54) Title: COMPOUND FOR ORGANIC ELECTROLUMINESCENT DEVICE AND ORGANIC ELECTROLUMINESCENT DEVICE INCLUDING THE SAME



(57) Abstract: This invention relates to a compound for an organic electroluminescent device and to an organic electroluminescent device including the same. The present invention may provide a compound for an organic EL device which may be used as a host of a fluorescent light emitting layer with high electrical stability, high transport capacity of an electron and a hole, high efficiency and high colorimetric purity, and as an electron transport material or a hole transport material.



Description

Title of Invention: COMPOUND FOR ORGANIC ELECTROLUMINESCENT DEVICE AND ORGANIC ELECTROLUMINESCENT DEVICE INCLUDING THE SAME

Technical Field

- [1] The present invention relates to a compound for an organic electroluminescent device and an organic electroluminescent device including the same, and more particularly, to a compound for an organic electroluminescent device improving the light emission efficiency and an organic electroluminescent device including the same.

Background Art

- [2] Organic electroluminescent (EL) devices have a simpler structure, various processing advantages, higher brightness, superior viewing angle properties, quicker response rate, and a lower driving voltage compared to other flat panel displays such as liquid crystal displays (LCDs), plasma display panels (PDPs), field emission displays (FEDs), etc., and are thus being thoroughly developed so as to be utilized as light sources of flat panel displays such as wall-mountable TVs, etc. or backlight units of the displays, illuminators, advertisement boards and so on.
- [3] Typically, when a direct-current voltage is applied to an organic EL device, holes injected from an anode and electrons injected from a cathode recombine to form electron-hole pairs, namely, excitons. While the excitons return to a stable ground state, energy corresponding thereto is transferred to a light emitting material and is thereby converted into light.
- [4] In order to increase efficiency and stability of an organic EL device, since C. W. Tang et al. of Eastman Kodak Company made an organic EL device operating at low voltage by forming a tandem organic thin film between two opposite electrodes (C. W. Tang, S. A. Vanslyke, Applied Physics Letters, vol. 51, pp. 913, 1987), extensive and intensive research into organic materials for organic EL devices having a multilayered thin-film structure has been ongoing. The efficiency and lifetime of such a tandem organic EL device are closely related to the molecular structure of a material for the thin film. For example, quantum efficiency may greatly vary depending on the structure of the material for the thin film, particularly a host material, a hole transport layer material or an electron transport layer material. When thermal stability of the material decreases, the material may be crystallized at a high temperature or a driving temperature, undesirably shortening the lifetime of the device.
- [5] Hole transport materials for use in organic EL devices, which have been known to date, are problematic because thin films formed therefrom using vacuum deposition are

thermally and electrically unstable, and thus may rapidly crystallize due to heat generated upon device driving and also the film materials may change, undesirably deteriorating the light emission efficiency of the devices. Further, non-emission parts referred to as dark spots may increasingly occur, and the voltage may increase upon constant-current driving, undesirably damaging the devices.

- [6] The light emitting materials can be divided into a host and a light emitting materials (dopant). The light emitting materials can be divided into the fluorescent and the phosphorescent materials in accordance with the light emitting mechanism. Especially if the fluorescent light emitting materials are used, the fluorescent host materials are needed to satisfy both high efficiency and high colorimetric purity.

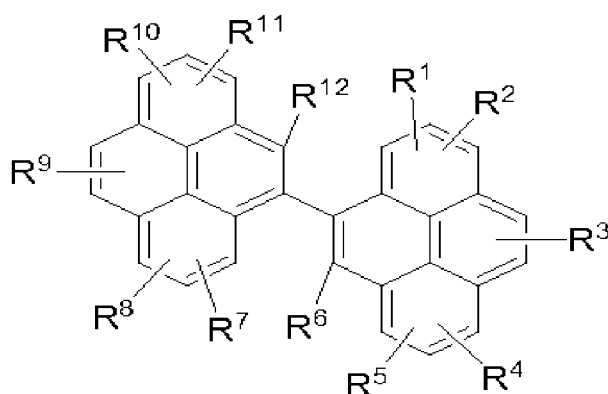
Disclosure of Invention

Technical Problem

- [7] Accordingly, an object of the present invention is to provide a compound for an organic EL device which may be used as a host of a fluorescent light emitting layer with high electrical stability, high transport capacity of an electron and a hole, high efficiency, and high colorimetric purity and an organic electroluminescent device including the same.
- [8] Another object of the present invention is to provide a compound for an organic EL device which may be used as an electron or a hole transport material and an organic electroluminescent device including the same.

Solution to Problem

- [9] In order to accomplish the above objects, an aspect of the present invention provides a compound for an organic EL device, as represented by Chemical Formula 1 below.
- [10] [Chemical Formula 1]
- [11]

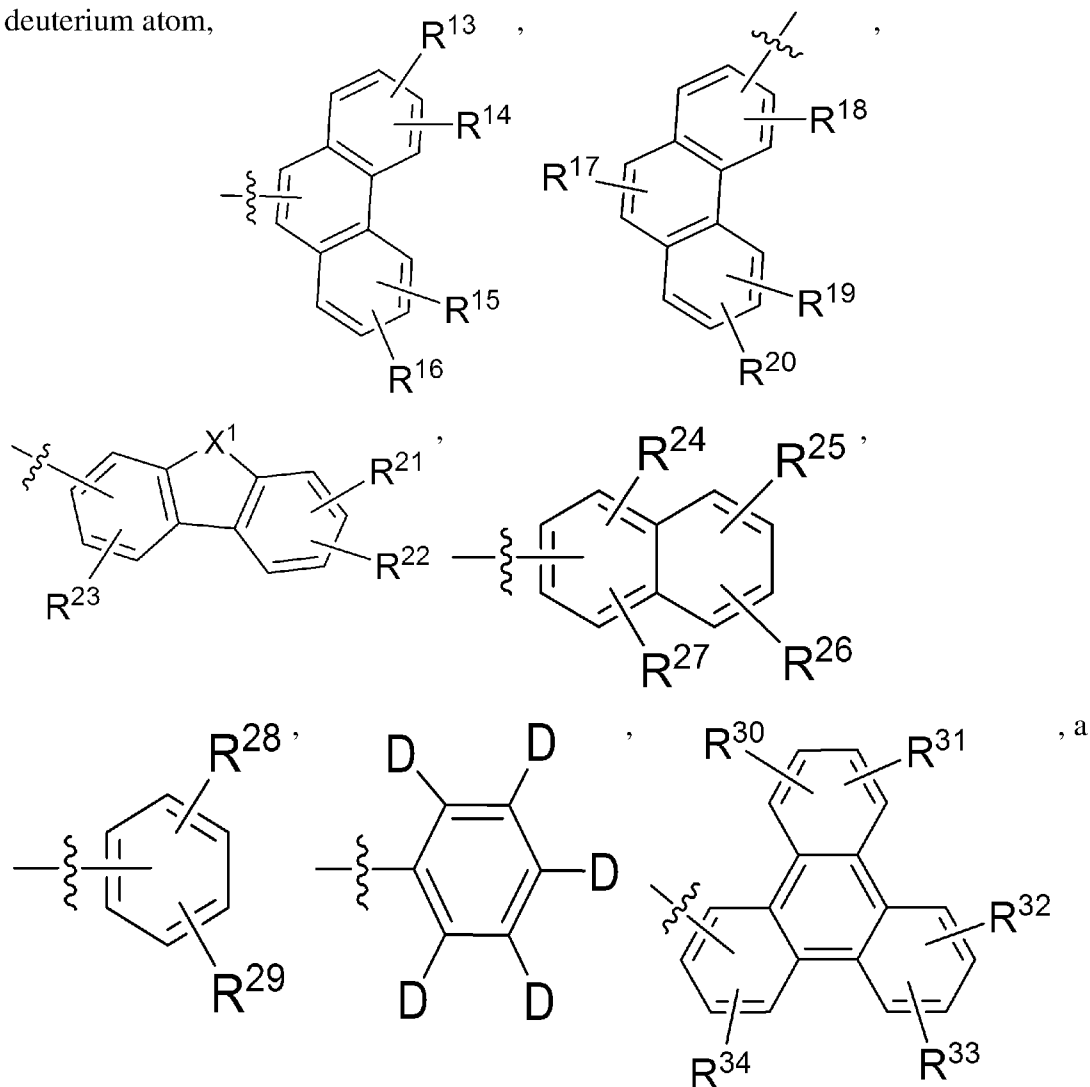


- [12] In Chemical Formula 1, R^1 to R^5 , and R^7 to R^{11} are identical to or different from each other, and R^1 to R^5 , and R^7 to R^{11} are each independently a hydrogen atom, a deuterium atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30

heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, or at least one of R¹ to R⁵, and R⁷ to R¹¹ is further coupled with a carbon atom adjacent to a carbon atom linked therewith to form a substituted or unsubstituted fused C3 to C30 cycloalkyl group, a substituted or unsubstituted fused C1 to C30 heterocycloalkyl group, a substituted or unsubstituted fused C6 to C30 aryl group, or a substituted or unsubstituted fused C1 to C30 heteroaryl group, and

- [13] R⁶ to R¹² are identical to or different from each other, and R⁶ to R¹² are each independently a hydrogen atom, a deuterium atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group.

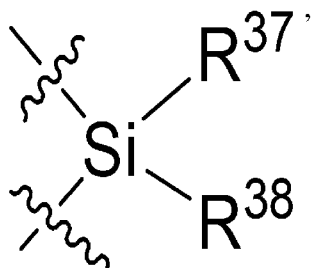
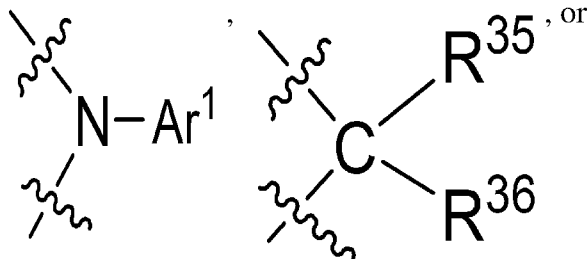
- [14] In a preferred embodiment of the present invention, R¹ to R¹² are identical to or different from each other, and R¹ to R¹² are each independently a hydrogen atom, a deuterium atom,



substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to

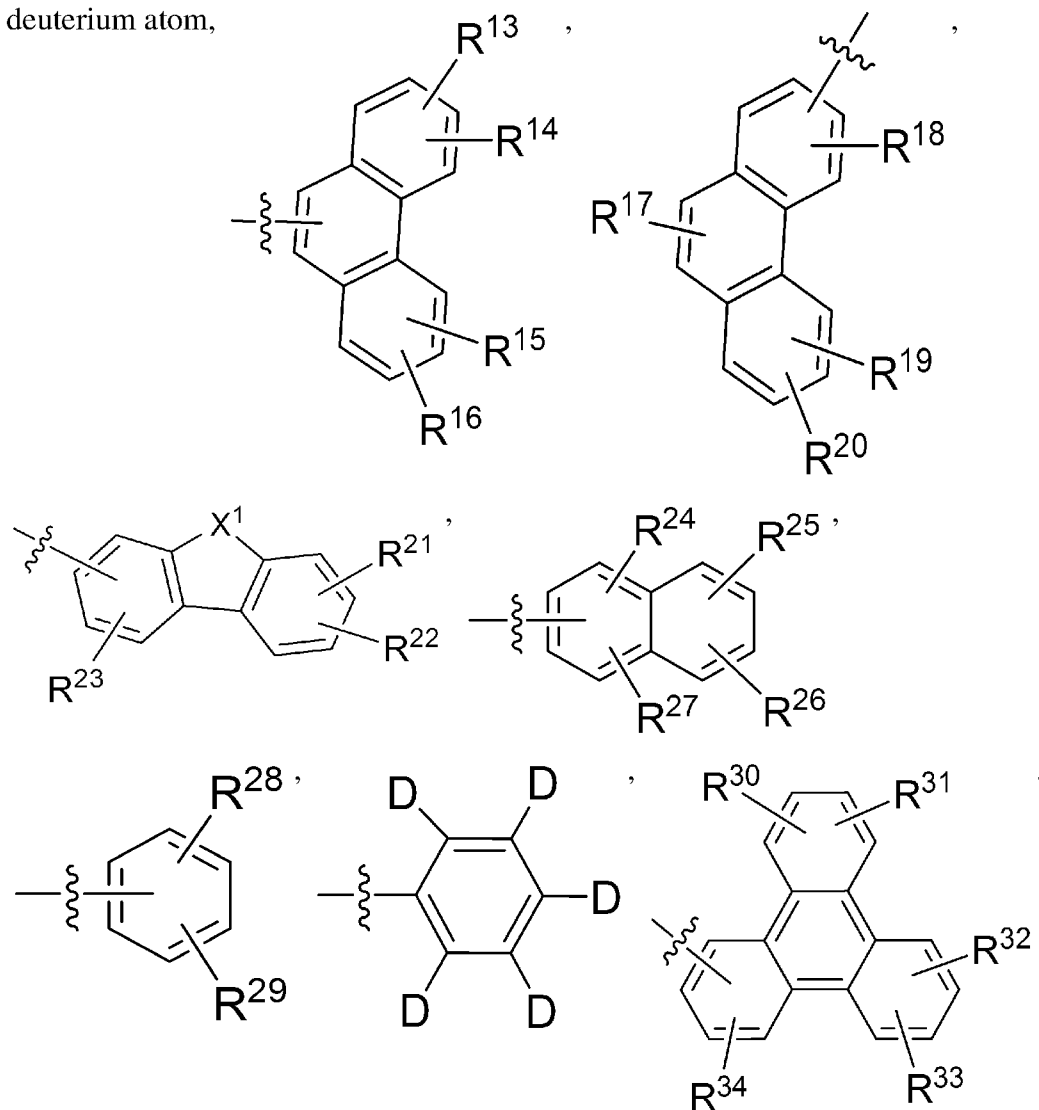
C30 cycloalkyl group, or a substituted or unsubstituted C1 to C30 heterocycloalkyl group,

- [15] X¹ is an oxygen atom, a sulfur atom,



- [16] Ar¹ is a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group,
- [17] R³⁵ to R³⁸ are identical to or different from each other, and R³⁵ to R³⁸ are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, or R³⁵ and R³⁶, and R³⁷ and R³⁸, respectively, are linked to form a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, together with a carbon atom or a silicon atom therebetween, and
- [18] R¹³ to R³⁴ are identical to or different from each other, and R¹³ to R³⁴ are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, or at least one of R¹³ to R³⁴ is further coupled with a carbon atom adjacent to a carbon atom linked therewith to form a substituted or unsubstituted fused C3 to C30 cycloalkyl group, a substituted or unsubstituted fused C1 to C30 heterocycloalkyl group, a substituted or unsubstituted fused C6 to C30 aryl group, or a substituted or unsubstituted fused C1 to C30 heteroaryl group.

- [19] In a preferred embodiment of the present invention, R^1 to R^{12} are identical to or different from each other, and R^1 to R^{12} are each independently a hydrogen atom, a deuterium atom,



- [20] X^1 is a oxygen atom, a sulfur atom, ,

- [21] or ,

- [22] Ar^1 is a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group,

- [23] R^{35} to R^{38} are identical to or different from each other, and R^{35} to R^{38} are each inde-

pendently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, or a substituted or unsubstituted C1 to C30 heterocycloalkyl group, and

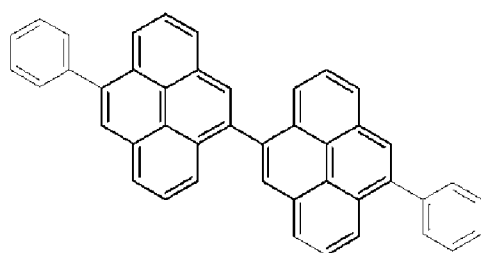
- [24] R^{13} to R^{34} are identical to or different from each other, and R^{13} to R^{34} are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group.

- [25] Examples of the substituted or unsubstituted C2 to C30 heteroaryl group may include a substituted or unsubstituted pyridinyl group, a substituted or unsubstituted pyrimidinyl group, a substituted or unsubstituted triazinyl group, a substituted or unsubstituted thiophenyl group, a substituted or unsubstituted pyrrolyl group, a substituted or unsubstituted benzothiophenyl group, a substituted or unsubstituted indolyl group, a substituted or unsubstituted imidazo[1,2-a]pyridinyl group, a substituted or unsubstituted benzimidazolyl group, a substituted or unsubstituted indazolyl group, a substituted or unsubstituted phenothiazinyl group, a substituted or unsubstituted phenazinyl group, a substituted or unsubstituted carbazolyl group, a substituted or unsubstituted dibenzothiophenyl group, a substituted or unsubstituted imidazolyl group, a substituted or unsubstituted triazolyl group, a substituted or unsubstituted tetrazolyl group, a substituted or unsubstituted oxadiazolyl group, a substituted or unsubstituted oxatriazolyl group, a substituted or unsubstituted thiatriazolyl group, a substituted or unsubstituted benzotriazolyl group, a substituted or unsubstituted pyrazinyl group, a substituted or unsubstituted pyridazinyl group, a substituted or unsubstituted purinyl group, a substituted or unsubstituted quinolinyl group, a substituted or unsubstituted isoquinolinyl group, a substituted or unsubstituted phthalazinyl group, a substituted or unsubstituted naphpyridinyl group, a substituted or unsubstituted quinoxalinyl group, a substituted or unsubstituted quinazolinyl group, a substituted or unsubstituted acridinyl group, or a substituted or unsubstituted phenanthrolinyl group. Preferably useful is a substituted or unsubstituted pyridinyl group, a substituted or unsubstituted pyrimidinyl group, a substituted or unsubstituted triazinyl group, a substituted or unsubstituted thiophenyl group, a substituted or unsubstituted pyrrolyl group, a substituted or unsubstituted benzothiophenyl group, a substituted or unsubstituted indolyl group, a substituted or unsubstituted imidazo[1,2-a]pyridinyl group, a substituted or unsubstituted benzimidazolyl group, a substituted or unsubstituted indazolyl group, a substituted or unsubstituted phenothiazinyl group, a substituted or unsubstituted phenazinyl group, a substituted or unsubstituted carbazolyl group, or a substituted or unsubstituted dibenzothiophenyl group.

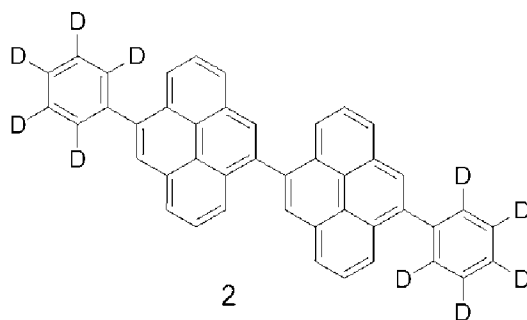
- [26]

[27] According to a preferred embodiment of the present invention, the compound for an organic EL device is any one selected from among Compounds 1 to 65 represented by the following chemical formulas.

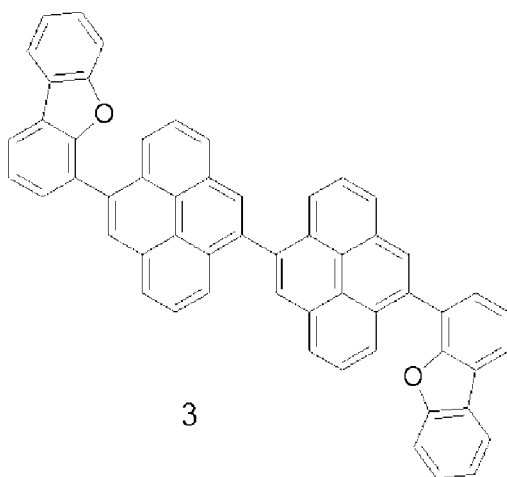
[28]



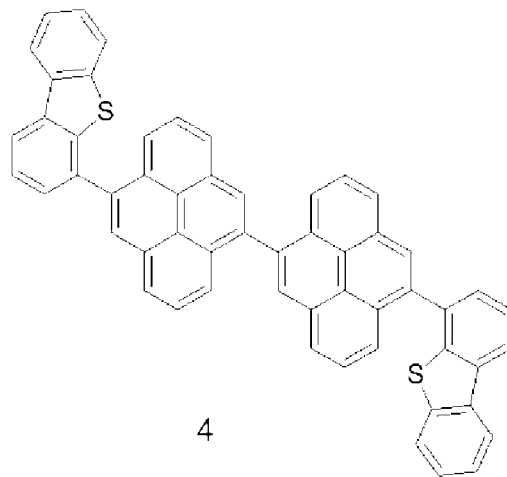
1



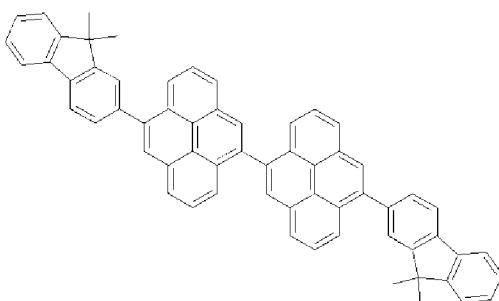
2



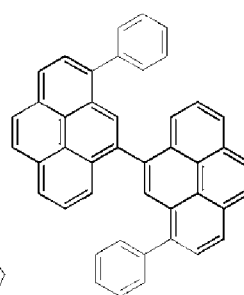
3



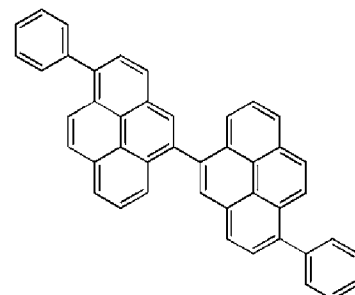
4



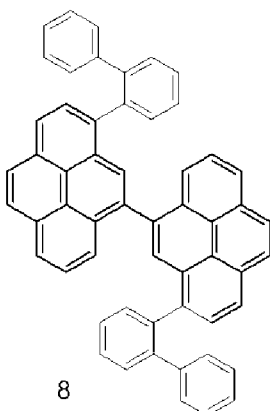
5



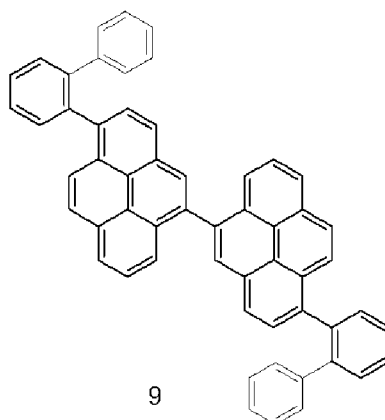
6



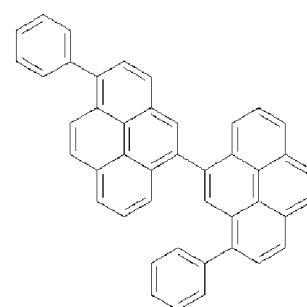
7



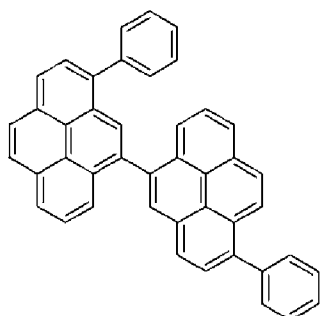
8



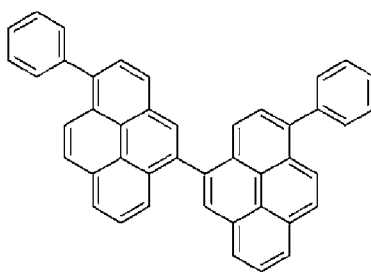
9



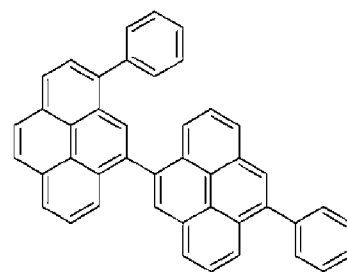
10



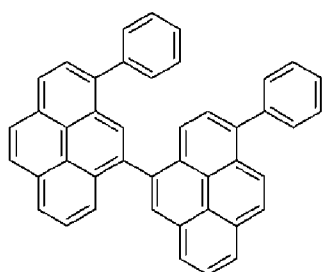
11



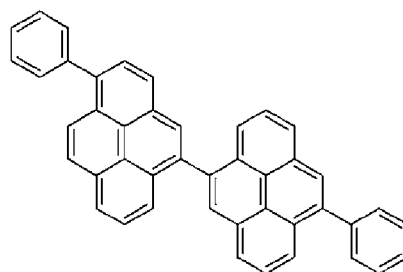
12



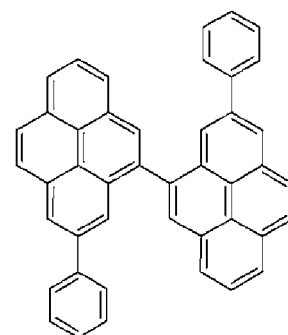
13



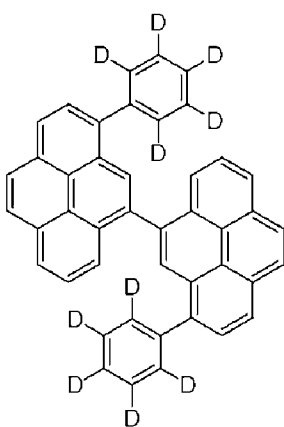
14



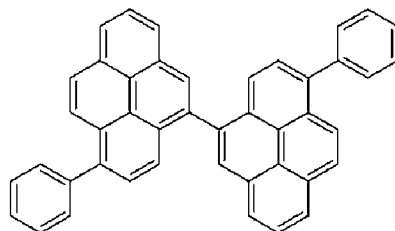
15



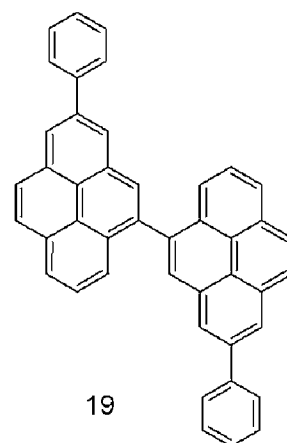
16



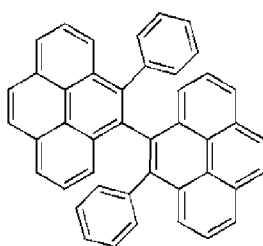
17



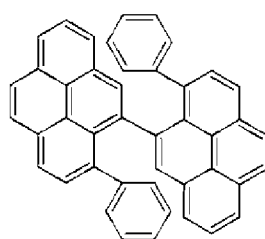
18



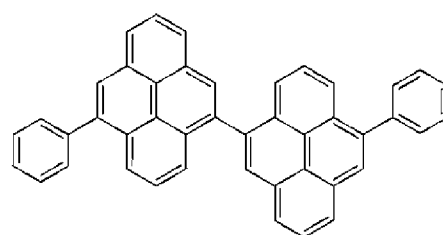
19



20

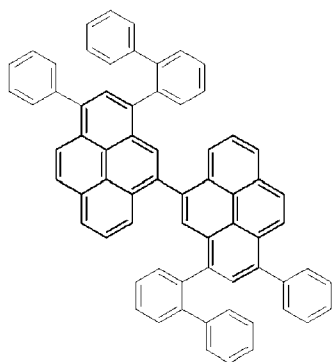


21

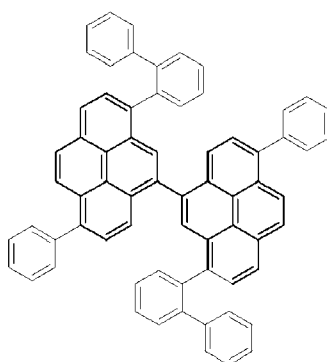


22

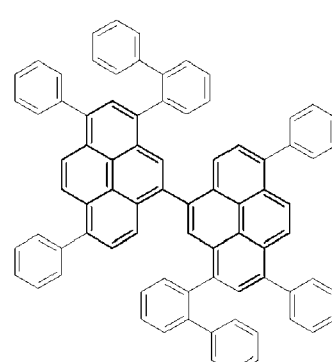
[30]



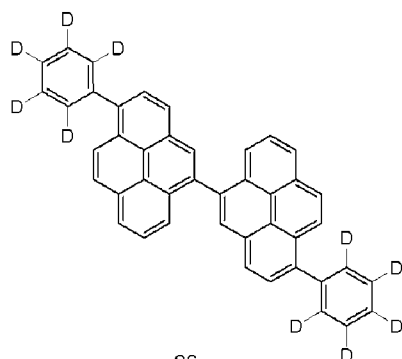
23



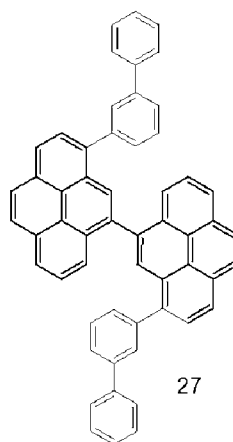
24



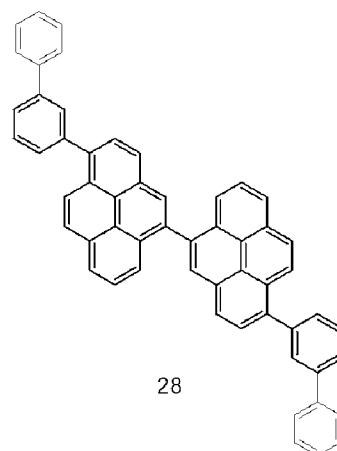
25



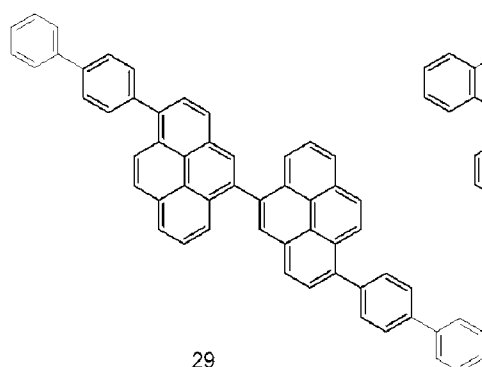
26



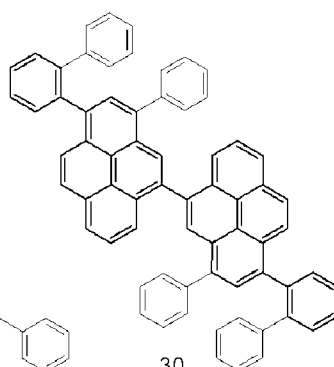
27



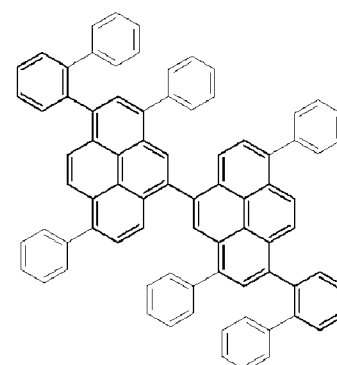
28



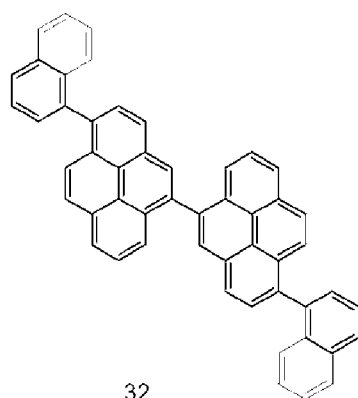
29



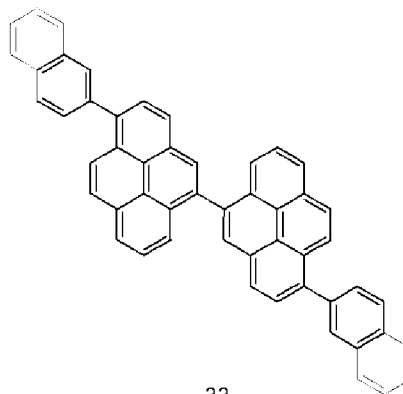
30



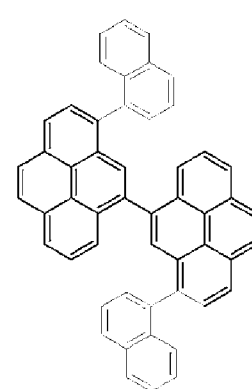
31



32

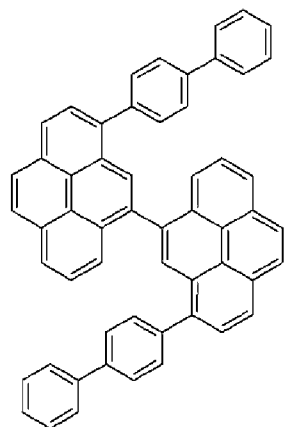


33

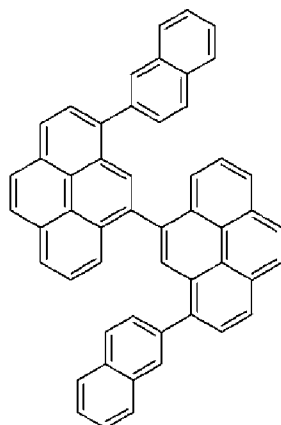


34

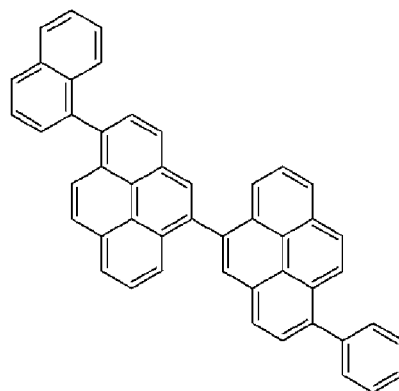
[31]



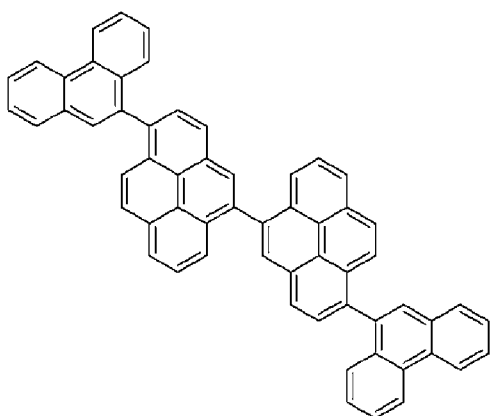
35



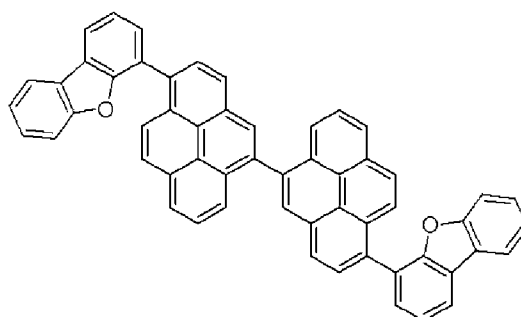
36



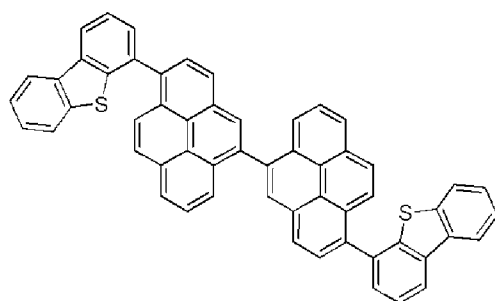
37



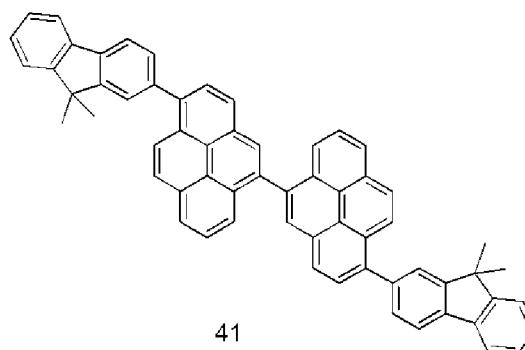
38



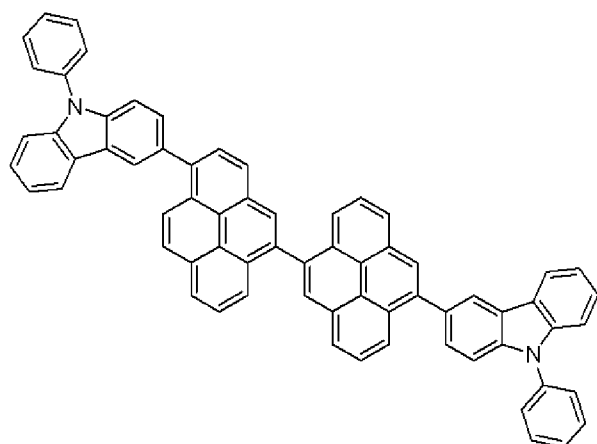
39



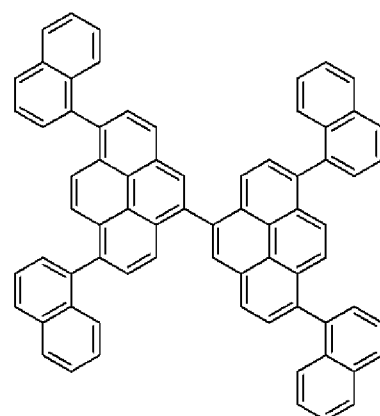
40



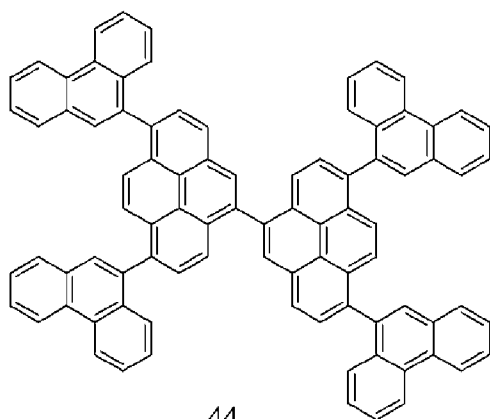
41



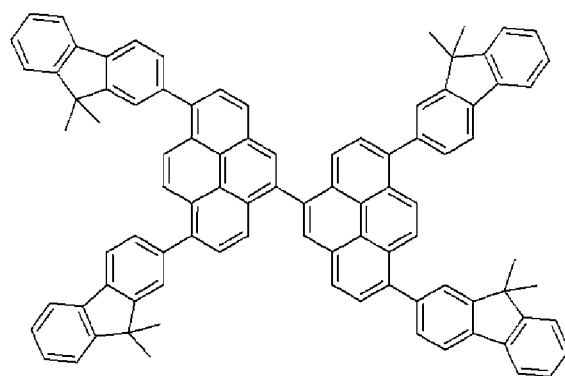
42



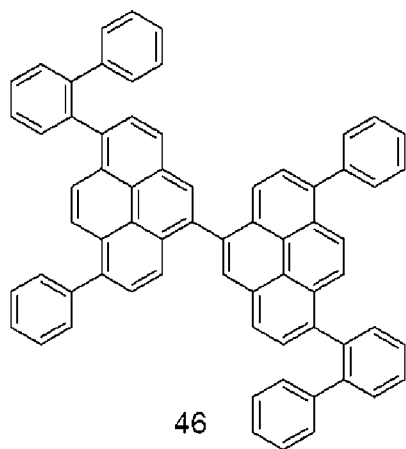
43



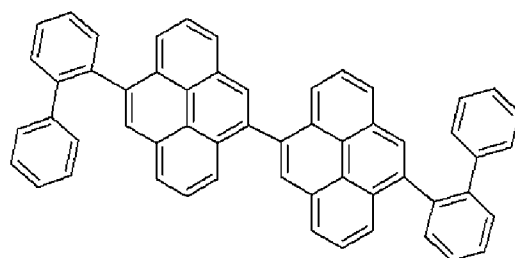
44



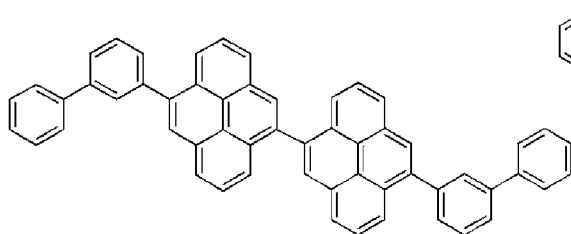
45



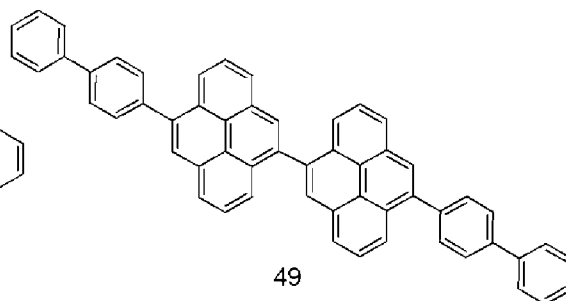
46



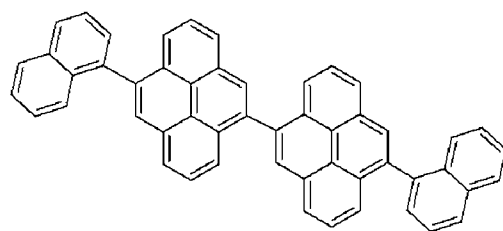
47



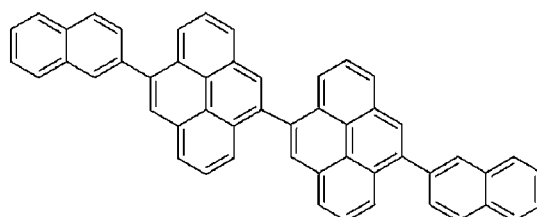
48



49

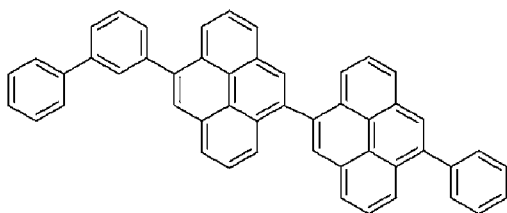


50

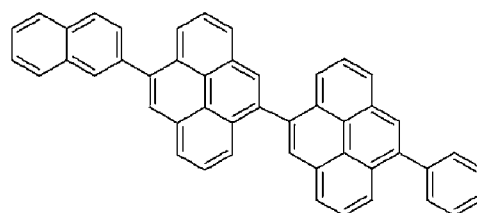


51

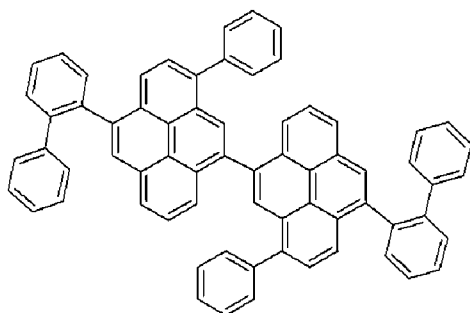
[32]



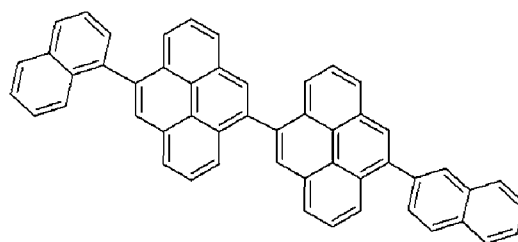
52



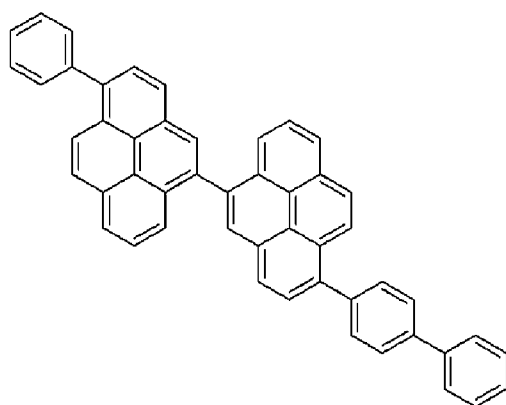
53



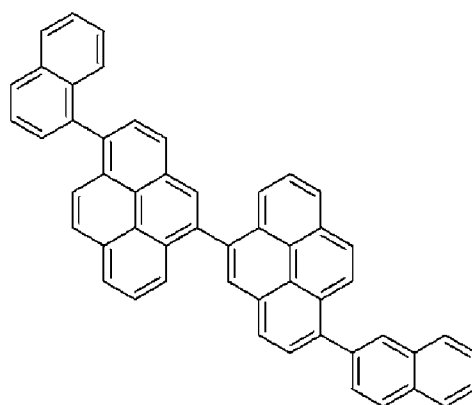
54



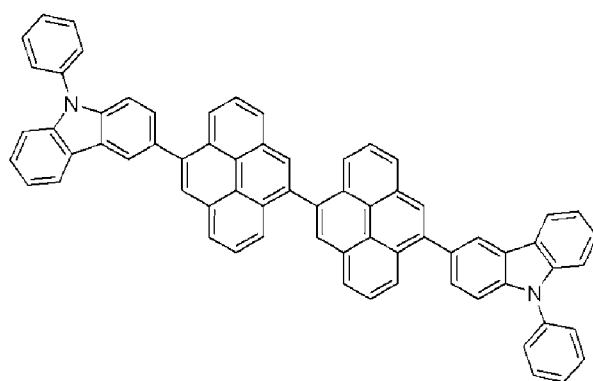
55



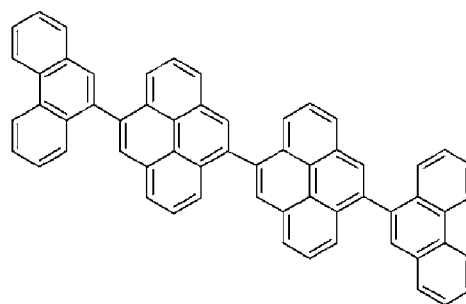
56



57

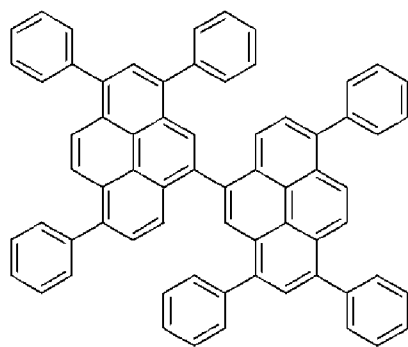


58

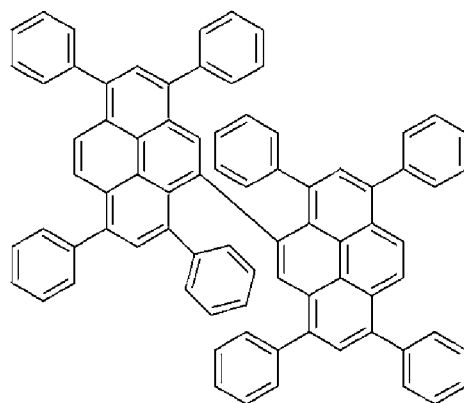


59

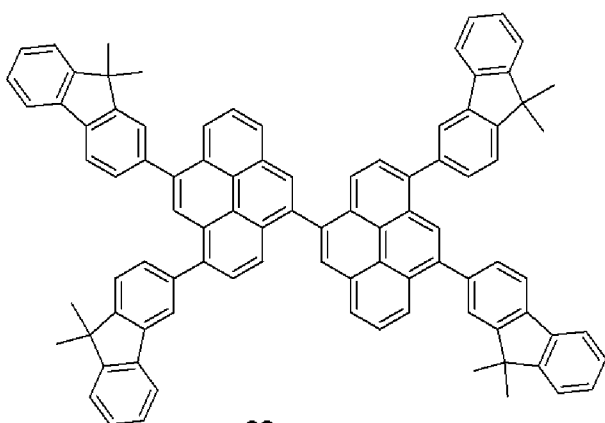
[33]



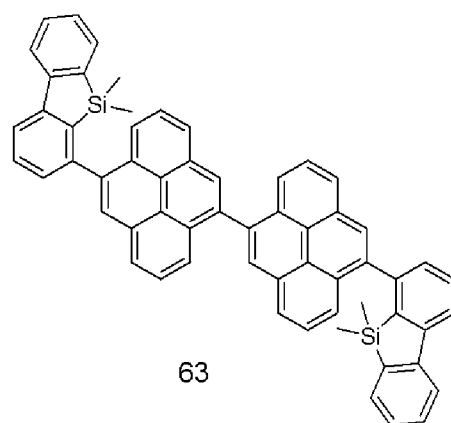
60



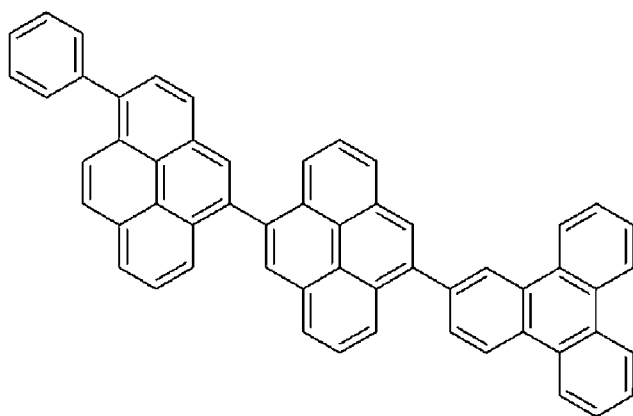
61



62

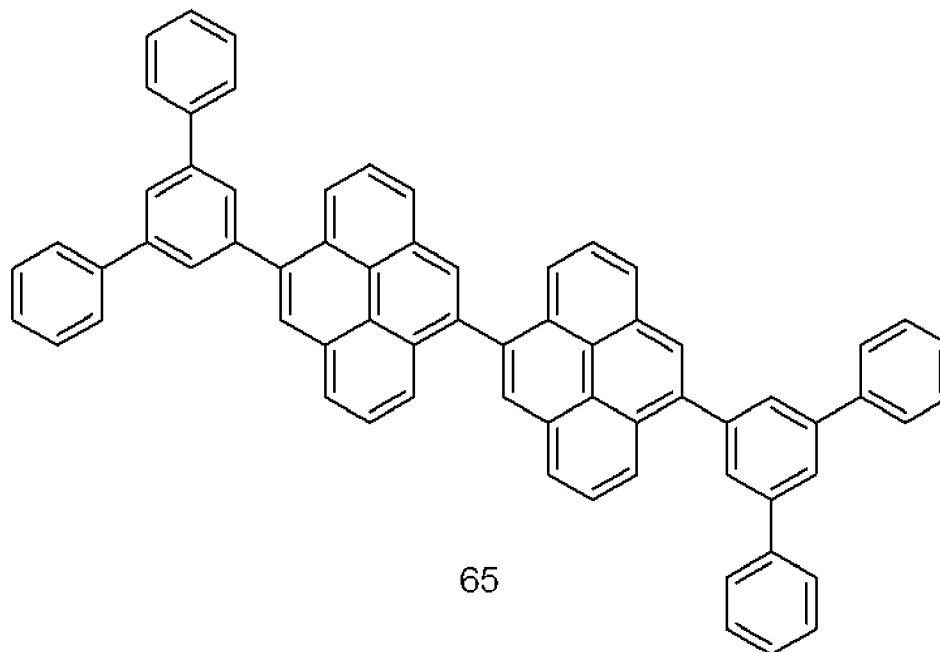


63



64

[34]



[35] According to an embodiment of the present invention, an organic electroluminescent (EL) device including the compound for an organic EL device according to the present invention may be provided.

[36] According to an embodiment of the present invention, an organic EL device may include a first electrode, a second electrode, and a single organic layer or a plurality of organic layers between the first electrode and the second electrode, and one or more organic layers selected from among the single organic layer or the plurality of organic layers may include the compound for an organic EL device according to the present invention.

[37] According to an embodiment of the present invention, the single organic layer or the plurality of organic layers may include a light emitting layer.

[38] According to an embodiment of the present invention, the plurality of organic layers may include a light emitting layer, and the plurality of organic layers may further include one or more selected from among an electron injection layer, an electron transport layer, a hole blocking layer, an electron blocking layer, a hole transport layer and a hole injection layer.

[39] According to an embodiment of the present invention, the light emitting layer may include a host and a dopant.

[40]

Advantageous Effects of Invention

[41] The present invention may provide a compound for an organic EL device which may be used as a host of a fluorescent light emitting layer with high electrical stability, high transport capacity of an electron and a hole, high efficiency and high colorimetric

purity, and an organic electroluminescent device including the same.

- [42] The present invention may also provide a compound for an organic EL device which may be used as an electron transport material or a hole transport material, and an organic electroluminescent device including the same.

Brief Description of Drawings

- [43] The above and other objects, features and advantages of the present invention will be more clearly understood from the following detailed description taken in conjunction with the accompanying drawings, in which:
- [44] FIG. 1 is a cross-sectional view illustrating an organic EL device according to an embodiment of the present invention; and
- [45] FIG. 2 is a cross-sectional view illustrating an organic EL device according to another embodiment of the present invention.

Mode for the Invention

- [46] The present invention may be variously modified, and may have a variety of embodiments, and is intended to illustrate specific embodiments. However, the following description does not limit the present invention to specific embodiments, and should be understood to include all variations, equivalents or substitutions within the spirit and scope of the present invention. Furthermore, in the description of the present invention, when it is determined that the detailed description of the related art would obscure the gist of the present invention, the description thereof will be omitted.
- [47] Also, in the following description, the terms “first,” “second” and the like are used to differentiate a certain component from other components, but the configuration of such components should not be construed to be limited by the terms. For example, a first component may be referred to as a second component, and a second component may be referred to as a first component, within the scope of the present invention.
- [48] Also, when any one component is mentioned to be “formed” or “stacked” on another component, it may be directly attached to the entire surface or one surface of another component, or a further component may be additionally interposed therebetween.
- [49] Unless otherwise stated, the singular expression includes a plural expression. In this application, the terms “include” and “have” are used to designate the presence of features, numbers, steps, operations, components, parts or combinations thereof described in the specification, not intending to exclude the presence or additional possibility of one or more different features, numbers, steps, operations, components, parts or combinations thereof are not excluded.
- [50] As used herein, unless otherwise defined, the term “valence bond” means a single bond, a double bond or a triple bond.
- [51] As used herein, unless otherwise defined, the term “substituted” means that at least

one hydrogen on a substituent or a compound is substituted with deuterium, a halogen group, a hydroxyl group, an amino group, a C1 to C30 amine group, a nitro group, a silyl group, a C1 to C30 alkyl group, a C1 to C30 alkylsilyl group, a C3 to C30 cycloalkyl group, a C1 to C30 heterocycloalkyl group, a C6 to C30 aryl group, a C1 to C30 heteroaryl group, a C1 to C20 alkoxy group, a C1 to C10 trifluoroalkyl group or a cyano group.

- [52] Further, among the halogen group, the hydroxyl group, the amino group, the C1 to C30 amine group, the C3 to C30 silyl group, the C1 to C30 alkyl group, the C1 to C30 alkylsilyl group, the C3 to C30 cycloalkyl group, the C6 to C30 aryl group, the C1 to C20 alkoxy group, the C1 to C10 trifluoroalkyl group or the cyano group, which is substituted, two adjacent substituents may be fused to form a ring.
- [53] As used herein, unless otherwise defined, the term “hetero” means a functional group containing 1 ~ 4 heteroatoms selected from the group consisting of N, O, S and P, the remainder being carbon.
- [54] As used herein, unless otherwise defined, the term “combination thereof” means that two or more substituents are coupled with each other by a linker or two or more substituents are condensed to each other.
- [55] As used herein, unless otherwise defined, the term “hydrogen” means hydrogen, deuterium or tritium.
- [56] As used herein, unless otherwise defined, the term “alkyl group” means an aliphatic hydrocarbon group.
- [57] The alkyl group may be a “saturated alkyl group” without any double bond or triple bond.
- [58] The alkyl group may be an “unsaturated alkyl group” with at least one double bond or triple bond.
- [59] The term “alkenylene group” means a functional group having at least one carbon-carbon double bond between at least two carbon atoms, and the term “alkynylene group” means a functional group having at least one carbon-carbon triple bond between at least two carbon atoms. The alkyl group may be branched, linear or cyclic, regardless of whether it is saturated or unsaturated.
- [60] The alkyl group may be a C1 to C30 alkyl group, preferably a C1 to C20 alkyl, more preferably a C1 to C10 alkyl group, and much more preferably a C1 to C6 alkyl group.
- [61] For example, a C1 to C4 alkyl group indicates an alkyl chain containing 1 ~ 4 carbon atoms, particularly an alkyl chain which is selected from the group consisting of methyl, ethyl, propyl, iso-propyl, n-butyl, iso-butyl, sec-butyl and t-butyl.
- [62] Specific examples of the alkyl group include a methyl group, an ethyl group, a propyl group, an isopropyl group, a butyl group, an isobutyl group, a t-butyl group, a pentyl group, a hexyl group, an ethenyl group, a propenyl group, a butenyl group, a cy-

- clopropyl group, a cyclobutyl group, a cyclopentyl group, a cyclohexyl group, etc.
- [63] The “amine group” includes an arylamine group, an alkylamine group, an arylalkylamine group, or an alkylarylamine group.
- [64] The term “cycloalkyl group” refers to a monocyclic or fused-ring polycyclic (i.e., rings which share adjacent pairs of carbon atoms) functional group.
- [65] The term “heterocycloalkyl group” means a cycloalkyl group containing 1 ~ 4 heteroatoms selected from the group consisting of N, O, S and P, the remainder being carbon. In the case where the heterocycloalkyl group is a fused ring, at least one ring may contain 1 ~ 4 heteroatoms.
- [66] The term “aromatic group” means a cyclic functional group where all ring atoms have p-orbitals, and these p-orbitals form conjugation. Specific examples thereof include an aryl group and a heteroaryl group.
- [67] The term “aryl group” refers to a monocyclic or fused-ring polycyclic (i.e., rings which share adjacent pairs of carbon atoms) functional group.
- [68] The term “heteroaryl group” means an aryl group containing 1 ~ 4 heteroatoms selected from the group consisting of N, O, S and P, the remainder being carbon. In the case where the heteroalkyl group is a fused ring, at least one ring may contain 1 ~ 4 heteroatoms.
- [69] In the aryl group and the heteroaryl group, the number of ring atoms is the sum of the number of carbons and the number of non-carbon atoms.
- [70] When alkyl and aryl are used in combination as in “alkylaryl group” or “arylalkyl group,” “alkyl” and “aryl” respectively have the meanings as above.
- [71] The term “arylalkyl group” means an aryl substituted alkyl radical such as benzyl, and is incorporated in the alkyl group.
- [72] The term “alkylaryl group” means an alkyl substituted aryl radical, and is incorporated in the aryl group.
- [73] Below is a description of embodiments of the present invention with reference to the appended drawings, wherein the same or similar components are designated by the same reference numerals and the overlapping description thereof is omitted.
- [74] With reference to FIGS. 1 and 2, according to an embodiment of the present invention, an organic EL device 1 including the compound for an organic EL device according to the present invention may be provided.
- [75] According to another embodiment of the present invention, an organic EL device includes a first electrode 110, a second electrode 150, and a single organic layer or a plurality of organic layers 130 between the first electrode and the second electrode, and one or more organic layers selected from among the single organic layer or the plurality of organic layers 130 may include the compound for an organic EL device according to the present invention.

- [76] As such, the single organic layer or the plurality of organic layers 130 may include a light emitting layer 134.
- [77] The plurality of organic layers 130 include a light emitting layer 134, and the plurality of organic layers 130 may further include one or more selected from among an electron injection layer 131, an electron transport layer 132, a hole blocking layer 133, an electron blocking layer 135, a hole transport layer 136 and a hole injection layer 137.
- [78] The light emitting layer 134 may include a host and a dopant.
- [79] The organic EL device is preferably supported by a transparent substrate. The material for the transparent substrate is not particularly limited so long as it has good mechanical strength, thermal stability and transparency. Specific examples thereof may include glass, a transparent plastic film, etc.
- [80] The anode material of the organic EL device according to the present invention may include a metal, an alloy, an electrically conductive compound or a mixture thereof, having a work function of 4 eV or more. Specific examples thereof may include Au metal or a transparent conductive material such as CuI, ITO (indium tin oxide), SnO₂ and ZnO. The thickness of the anode film is preferably set to 10 ~ 200 nm.
- [81] The cathode material of the organic EL device according to the present invention may include a metal, an alloy, an electrically conductive compound or a mixture thereof, having a work function of less than 4 eV. Specific examples thereof may include Na, a Na-K alloy, calcium, magnesium, lithium, a lithium alloy, indium, aluminum, a magnesium alloy, or an aluminum alloy. In addition, aluminum/AlO₂, aluminum/lithium, magnesium/silver or magnesium/indium may be used. The thickness of the cathode film is preferably set to 10 ~ 200 nm.
- [82] In order to increase light emission efficiency of the organic EL device, one or more electrodes preferably have a light transmittance of 10% or more. The sheet resistance of the electrodes is preferably hundreds of Ω/mm or less. The thickness of the electrodes falls in the range of 10 nm ~ 1 μm , and preferably 10 ~ 400 nm. Such electrodes may be manufactured in the form of a thin film using the above electrode material via vapor deposition such as chemical vapor deposition (CVD), physical vapor deposition (PVD) or the like, or sputtering.
- [83] When the compound for an organic EL device according to the present invention is used so as to be adapted for the purposes of the present invention, a hole transport material, a hole injection material, a light emitting layer material, a host material for a light emitting layer, an electron transport material, and an electron injection material, which are known, may be used alone in each organic layer, or may be used in selective combination with the compound for an organic EL device according to the present invention.

- [84] Examples of the hole transport material may include porphyrin compound derivatives including N,N-dicarbazoyl-3,5-benzene (mCP), poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS), N,N'-di(1-naphthyl)-N,N'-diphenylbenzidine (NPD), N,N'-diphenyl-N,N'-di(3-methylphenyl)-4,4'-diaminobiphenyl (TPD), N,N'-diphenyl-N,N'-dinaphthyl-4,4'-diaminobiphenyl, N,N,N',N'-tetra-p-tolyl-4,4'-diaminobiphenyl, N,N,N',N'-tetraphenyl-4,4'-diaminobiphenyl, 1,10,15,20-tetraphenyl-21H,23H-porphyrin copper(II), etc., triarylamine derivatives including polymers having an aromatic tertiary amine in the main chain or side chain thereof, 1,1-bis(4-di-p-tolylaminophenyl)cyclohexane, N,N,N-tri(p-tolyl)amine and 4,4',4'-tris[N-(3-methylphenyl)-N-phenylamino]triphenylamine, carbazole derivatives including N-phenylcarbazole and polyvinylcarbazole, phthalocyanine derivatives including metal-free phthalocyanine and copper phthalocyanine, starburst amine derivatives, enaminestilbene-based derivatives, aromatic tertiary amine-containing styrylamine compound derivatives, polysilane, etc.
- [85] Examples of the electron transport material may include diphenylphosphine oxide-4-(triphenylsilyl)phenyl (TSPO1), Alq₃, 2,5-diaryl sylol derivatives (PyPySPyPy), per-fluorinated compounds (PF-6P), octasubstituted cyclooctatetraene compounds (COTs), etc.
- [86] In the organic EL device according to the present invention, an electron injection layer, an electron transport layer, a hole transport layer and a hole injection layer may be provided in the form of a single layer containing one or more kinds of the above compound, or may be provided in the form of a plurality of stacked layers containing different kinds of compounds.
- [87] The light emitting material may include, for example, photoluminescent fluorescent materials, fluorescent brighteners, laser dyes, organic scintillators and fluorescence analysis reagents. Specific examples thereof include carbazole-based compounds, phosphine oxide-based compounds, carbazole-based phosphine oxide compounds, polyaromatic compounds including bis((3,5-difluoro-4-cyanophenyl)pyridine)iridium picolinate (FCNlRpic), tris(8-hydroxyquinoline) aluminum (Alq₃), anthracene, phenanthrene, pyrene, chrysene, perylene, coronene, rubrene and quinacridone, oligophenylene compounds including quaterphenyl, scintillators for liquid scintillation including 1,4-bis(2-methylstyryl)benzene, 1,4-bis(4-methylstyryl)benzene, 1,4-bis(4-methyl-5-phenyl-2-oxazolyl)benzene, 1,4-bis(5-phenyl-2-oxazolyl)benzene, 2,5-bis(5-t-butyl-2-benzoxazolyl)thiophene, 1,4-diphenyl-1,3-butadiene, 1,6-diphenyl-1,3,5-hexatriene and 1,1,4,4-tetraphenyl-1,3-butadiene, metal complexes of oxine derivatives, coumarine dyes, dicyanomethylenepyran dyes, di-

cyanomethylenethiopyran dyes, polymethine dyes, oxobenzanthracene dyes, xanthene dyes, carbostyryl dyes, perylene dyes, oxazine compounds, stilbene derivatives, spiro compounds, oxadiazole compounds, etc.

[88] Each layer of the organic EL device according to the present invention may be provided in the form of a thin film using a known process such as vacuum deposition, spin coating or casting, or may be manufactured using each layer material. The thickness of each layer is not particularly limited, but may be appropriately set depending on the material properties, and may be typically determined in the range of 2 ~ 5,000 nm.

[89] Because the compound for an organic EL device according to the present invention may be subjected to vacuum deposition, a thin film formation process is simple and a uniform thin film which does not substantially have pin holes may be easily obtained.

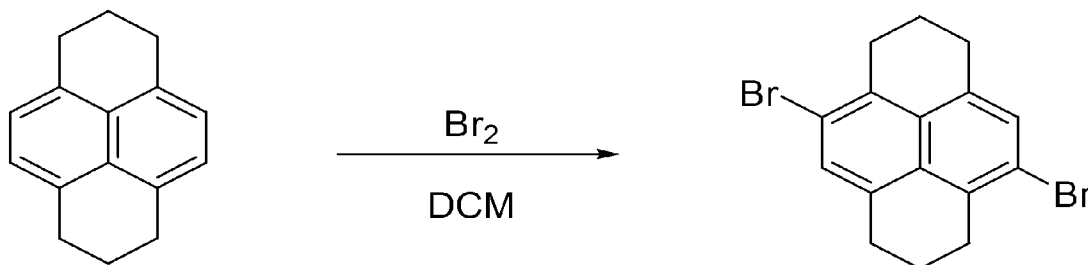
[90]

[91] [Example]

[92] A better understanding of the present invention regarding the synthesis of the compound for an organic EL device and the manufacture of the organic EL device including the same may be obtained through the following examples which are set forth to illustrate, but are not to be construed as limiting, the present invention.

[93] Preparation Example 1. Synthesis of Intermediate 1
(4,9-dibromo-1,2,3,6,7,8-hexahydropyrene)

[94]

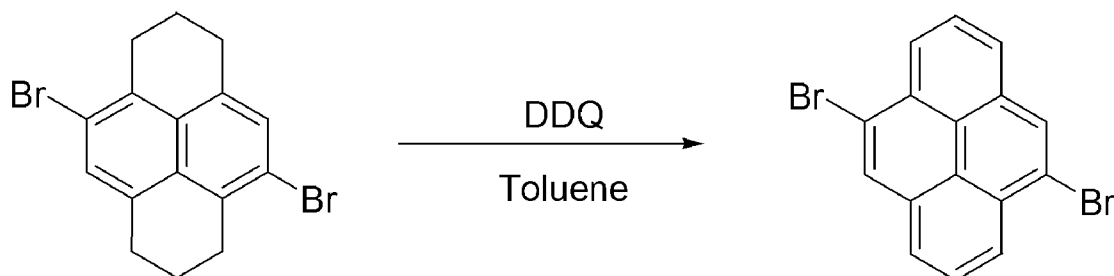


[95] In a 500mL round-bottom three-neck flask, 10.0 g of 1,2,3,6,7,8-hexahydropyrene, and 200ml of dichloromethane(DCM) were placed, and 7.8g of bromine was slowly dropped, with stirring at room temperature. After completion of the dropping, additional stirring was performed at room temperature for 3 hr. After completion of the reaction, the extracted solid products was obtained through vacuum filtration, and recrystallized from dichloromethane, and then washed with n-hexane, thus obtaining 9.4 g of Intermediate 1 (yield 53%).

[96] ^1H NMR (CDCl_3 , 600 MHz) δ 7.39 (s, 2H), 3.07 (t, 4H), 2.98 (t, 4H), 2.04-2.00(m, 4H)

[97] Preparation Example 2. Synthesis of Intermediate 2 (4,9-dibromopyrene)

[98]

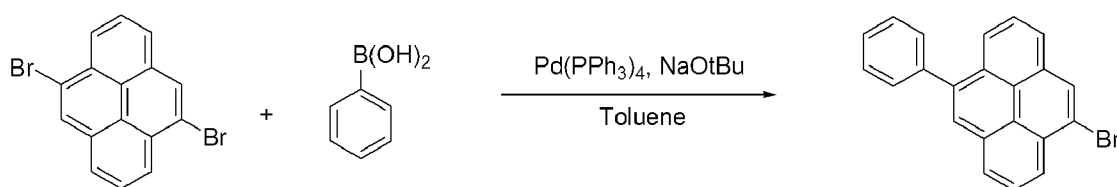


[99] In a 1L round-bottom three-neck flask in a nitrogen atmosphere, 9.4 g of Intermediate 1, 25.1 g of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone(DDQ) and 550 ml of toluene were placed, and refluxed for 5 hr. The reaction solution was cooled, filtered with silica gel, concentrated and then subjected to column chromatography with a solvent mixture of dichloromethane and n-hexane, thus obtaining 6.6 g of Intermediate 2 (yield 71%).

[100] $^1\text{H NMR}(600\text{MHz}, \text{CDCl}_3)$: δ 8.62 (d, 2H), 8.45 (s, 2H), 8.18 (d, 2H), 8.10 (t, 2H)

[101] Preparation Example 3. Synthesis of Intermediate 3 (4-bromo-9-phenylpyrene)

[102]

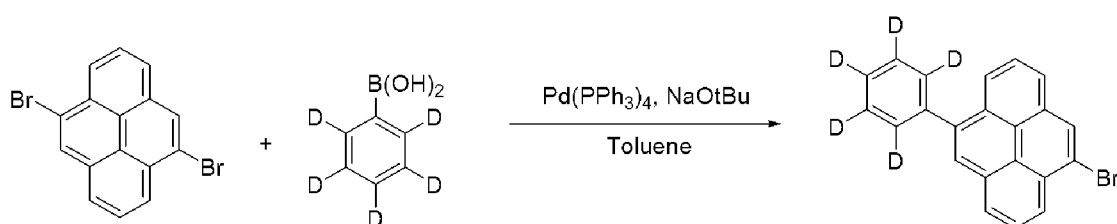


[103] In a 250 ml round-bottom three-neck flask in a nitrogen atmosphere, 6.6 g of Intermediate 2, 2.2 g of phenylboronic acid, 0.6g of tetrakis(triphenylphosphine)palladium(0), 5.2g of sodium tert-butoxide and 66 ml of toluene were placed, and stirred at 75 °C for 12 hr. The reaction solution was cooled, filtered with silica gel, concentrated and then subjected to column chromatography with a solvent mixture of dichloromethane and n-hexane, thus obtaining 4.1 g of Intermediate 3 (yield 63%).

[104] $^1\text{H NMR}(600\text{MHz}, \text{CDCl}_3)$: δ 8.58 (d, 1H), 8.44 (s, 1H), 8.22 (d, 2H), 8.11-8.07 (m, 2H), 8.02 (s, 1H), 7.93 (t, 1H), 7.66 (d, 2H), 7.57 (t, 2H), 7.52 (t, 1H)

[105] Preparation Example 4. Synthesis of Intermediate 4 (4-bromo-9-phenyl(d_5)pyrene)

[106]



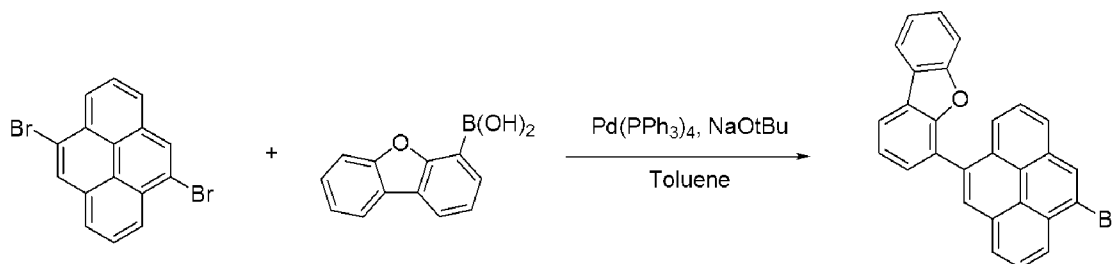
[107] In a 250 ml round-bottom three-neck flask in a nitrogen atmosphere, 6.6 g of Intermediate 2, 2.3 g of phenylboronic acid(d_5), 0.6g of tetrakis(triphenylphosphine)palladium(0), 5.2g of sodium tert-butoxide and 66 ml of toluene were placed, and stirred at 75 °C for 12 hr. The reaction solution was cooled,

filtered with silica gel, concentrated and then subjected to column chromatography with a solvent mixture of dichloromethane and n-hexane, thus obtaining 3.8 g of Intermediate 4 (yield 58%).

[108] ^1H NMR(600MHz, CDCl_3): δ 8.58 (d, 1H), 8.44 (s, 1H), 8.22 (d, 2H), 8.11-8.07 (m, 2H), 8.02 (s, 1H), 7.93 (t, 1H)

[109] Preparation Example 5. Synthesis of Intermediate 5
(4-bromo-(9-dibenzofuranyl)pyrene)

[110]

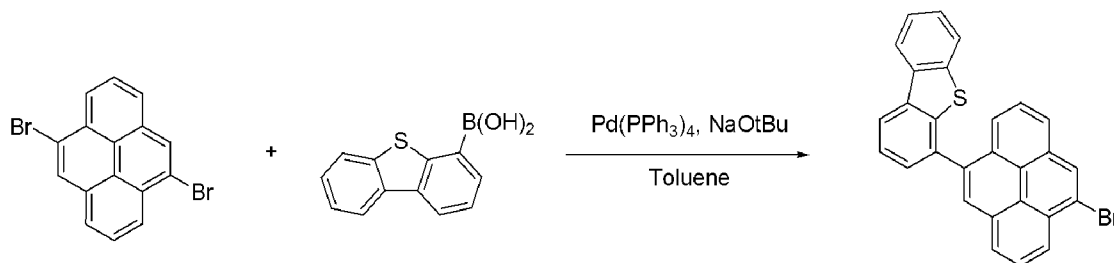


[111] In a 250 ml round-bottom three-neck flask in a nitrogen atmosphere, 6.6 g of Intermediate 2, 3.9 g of 4-(dibenzofuranyl)boronic acid, 0.6g of tetrakis(triphenylphosphine)palladium(0), 5.2g of sodium tert-butoxide and 66 ml of toluene were placed, and stirred at 80 °C for 16 hr. The reaction solution was cooled, filtered with silica gel, concentrated, thus obtaining 5.0 g of Intermediate 5 (yield 62%).

[112] ^1H NMR(600MHz, CDCl_3): δ 8.65 (d, 1H), 8.50 (s, 1H), 8.31 (d, 1H), 8.26 (s, 1H), 8.15-8.12 (m, 3H), 8.05 (d, 1H), 8.03 (d, 1H), 7.90 (t, 1H), 7.69 (d, 1H), 7.56 (t, 1H), 7.40-7.37 (m, 3H)

[113] Preparation Example 6. Synthesis of Intermediate 6
(4-bromo-9-dibenzothiophenylpyrene)

[114]

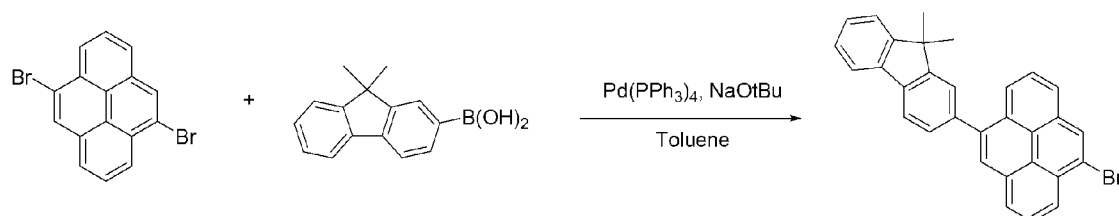


[115] In a 250 ml round-bottom three-neck flask in a nitrogen atmosphere, 6.6 g of Intermediate 2, 4.2 g of 4-dibenzothiophenylboronic acid, 0.6g of tetrakis(triphenylphosphine)palladium(0), 5.2g of sodium tert-butoxide and 66 ml of toluene were placed, and stirred at 80 °C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, thus obtaining 5.8 g of Intermediate 6 (yield 70%).

[116] ^1H NMR (600MHz, CDCl_3): δ 8.60 (d, 1H), 8.47 (s, 1H), 8.25 (d, 2H), 8.15-8.09 (m, 4H), 8.04 (s, 1H), 7.96 (t, 1H), 7.87-7.84 (m, 1H), 7.50-7.45 (m, 4H)

[117] Preparation Example 7. Synthesis of Intermediate 7
(4-bromo-9-(9,9-dimethyl-9H-fluoren-2-yl)pyrene)

[118]

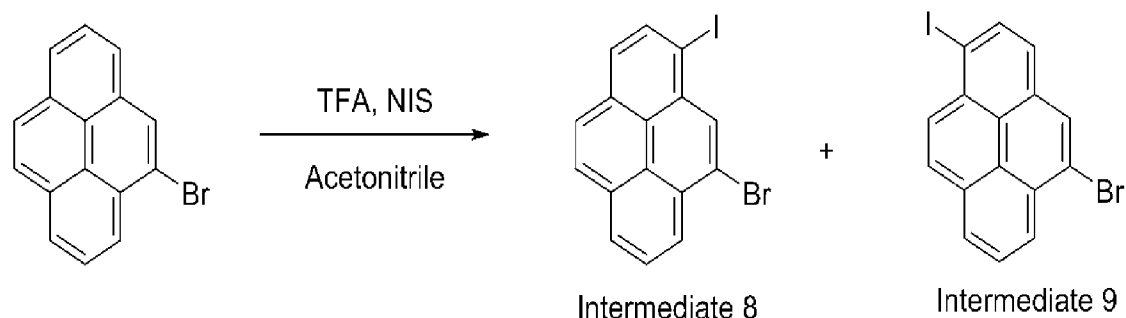


[119] In a 250 ml round-bottom three-neck flask in a nitrogen atmosphere, 6.6 g of Intermediate 2, 4.4 g of 9,9-dimethyl-9H-fluoren-2-yl boronic acid, 0.6g of tetrakis(triphenylphosphine)palladium(0), 5.2g of sodium tert-butoxide and 66 ml of toluene were placed, and stirred at 90°C for 12 hr. The reaction solution was cooled, filtered with silica gel, concentrated, thus obtaining 5.4 g of Intermediate 7 (yield 63%).

[120] ¹H NMR(600MHz, CDCl₃): δ 8.61 (d, 1H), 8.49 (s, 1H), 8.32 (d, 1H), 8.28 (d, 1H), 8.16-8.12 (m, 3H), 7.98 (t, 1H), 7.90 (d, 1H), 7.82 (d, 1H), 7.72 (s, 1H), 7.64-7.63 (m, 1H), 7.50 (d, 1H), 7.40-7.37 (m, 2H), 1.58 (s, 6H)

[121] Preparation Example 8. Synthesis of Intermediate 8, 9 (4-bromo-6-iodopyrene, 4-bromo-8-iodopyrene)

[122]



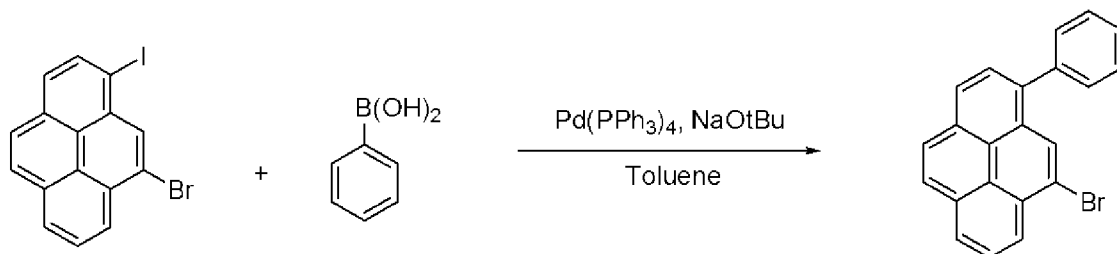
[123] In a 500 ml round-bottom three-neck flask in a nitrogen atmosphere, 28.2 g of 4-bromopyrene, 3.4 g of trifluoroacetic acid, 22.4 g of NIS (N-Iodosuccinimide) and 400 ml of acetonitrile were placed, and refluxed for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography using a solvent of n-hexane, thus obtaining 14.0 g of Intermediate 8, and 12.1g of Intermediate 9 (yield 64%).

[124] Intermediate 8: ¹H NMR(600MHz, CDCl₃): δ 8.70 (s, 1H), 8.64 (d, 1H), 8.50 (d, 1H), 8.27 (d, 1H), 8.13-8.09 (m, 2H), 8.03 (d, 1H), 7.90 (d, 1H)

[125] Intermediate 9: ¹H NMR(600MHz, CDCl₃): δ 8.62 (d, 1H), 8.51 (d, 1H), 8.38 (s, 1H), 8.31 (d, 1H), 8.29 (d, 1H), 8.16 (d, 1H), 8.12 (t, 1H), 7.81 (d, 1H)

[126] Preparation Example 9. Synthesis of Intermediate 10 (4-bromo-6-phenylpyrene)

[127]

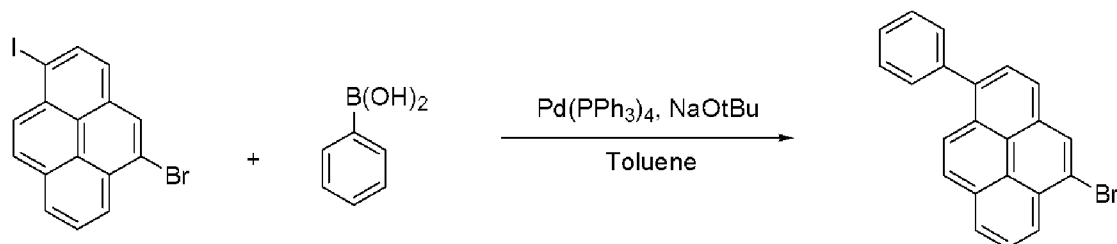


[128] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 6.2 g of Intermediate 8, 1.8 g of phenylboronic acid, 0.5 g of tetrakis(triphenylphosphine)palladium(0), 4.4 g of sodium tert-butoxide and 60 ml of toluene were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent mixture of dichloromethane and n-hexane, thus obtaining 3.6 g of Intermediate 10 (yield 68%).

[129] $^1\text{H NMR}$ (600MHz, CDCl_3): δ 8.61 (d, 1H), 8.46 (s, 1H), 8.23 (d, 1H), 8.18 (d, 1H), 8.16 (d, 1H), 8.10 (t, 1H) 7.99 (d, 2H), 7.61 (d, 2H), 7.56 (t, 2H), 7.49 (t, 1H)

[130] Preparation Example 10. Synthesis of Intermediate 11 (4-bromo-8-phenylpyrene)

[131]

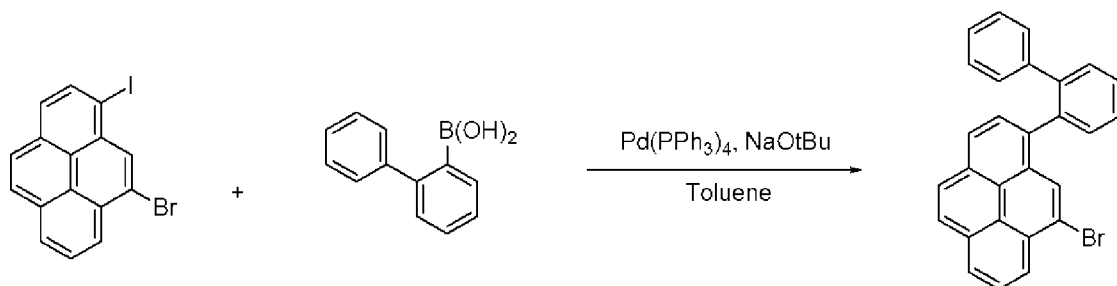


[132] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 8.0 g of Intermediate 9, 2.3 g of phenylboronic acid, 0.6 g of tetrakis(triphenylphosphine)palladium(0), 5.7 g of sodium tert-butoxide and 80 ml of toluene were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of n-hexane, thus obtaining 5.3 g of Intermediate 11 (yield 75%).

[133] $^1\text{H NMR}$ (600MHz, CDCl_3): δ 8.58 (d, 1H), 8.51 (s, 1H), 8.26-8.24 (m, 2H), 8.11-8.08 (m, 3H), 7.98 (d, 1H), 7.62-7.58 (m, 4H), 7.51 (t, 1H)

[134] Preparation Example 11. Synthesis of Intermediate 12 (4-bromo-6-(2-biphenyl)pyrene)

[135]

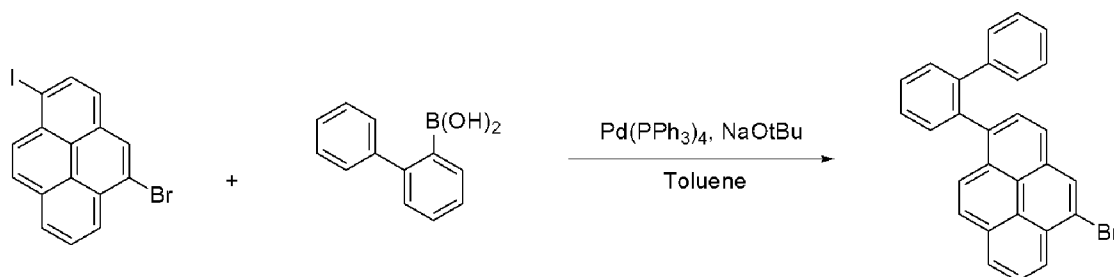


[136] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 4.1 g of Intermediate 8, 2.0 g of 2-biphenylboronic acid, 0.3 g of tetrakis(triphenylphosphine)palladium(0), 2.9 g of sodium tert-butoxide and 40 ml of toluene were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of n-hexane, thus obtaining 3.0 g of Intermediate 12 (yield 70%).

[137] ¹H NMR(600MHz, CDCl₃): δ 8.57 (d, 1H), 8.37 (s, 1H), 8.22 (d, 1H), 8.06 (t, 1H), 7.97-7.94 (m, 3H), 7.72 (d, 1H), 7.61-7.56 (m, 2H), 7.52-7.51 (m, 2H), 7.05-7.03 (m, 2H), 6.95-6.93 (m, 3H)

[138] Preparation Example 12. Synthesis of Intermediate 13
(4-bromo-8-(2-biphenyl)pyrene)

[139]

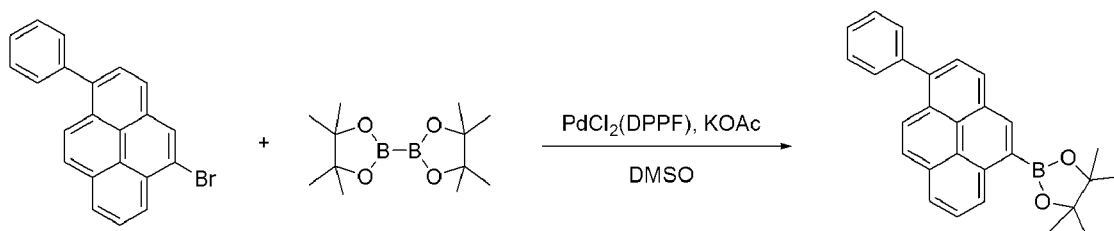


[140] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 4.1 g of Intermediate 9, 2.0 g of biphenylboronic acid, 0.3 g of tetrakis(triphenylphosphine)palladium(0), 2.9 g of sodium tert-butoxide and 40 ml of toluene were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 2.7 g of Intermediate 13 (yield 63%).

[141] ¹H NMR(600MHz, CDCl₃): δ 8.52 (d, 1H), 8.28 (s, 1H), 8.21 (d, 1H), 8.08-8.01 (m, 4H), 7.73 (d, 1H), 7.63-7.58 (m, 2H), 7.54-7.52 (m, 2H), 7.06-7.04 (m, 2H), 6.96-6.94 (m, 3H)

[142] Preparation Example 13. Synthesis of Intermediate 14
(8-phenyl-4-(pinacolatoboron-yl)pyrene)

[143]

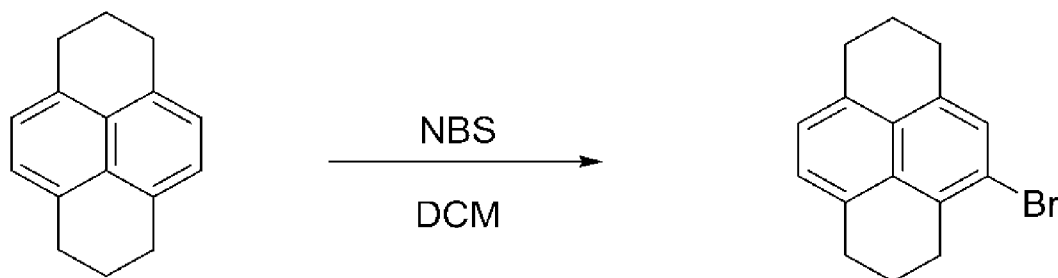


[144] In a 100 mL round-bottom three-neck flask in a nitrogen atmosphere, 2.0 g of Intermediate 11, 1.6 g of bis(pinacolato)diboron, 0.1 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 1.6 g of potassium

acetate and 20 ml of DMSO were placed, and stirred at 90°C for 12 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.2 g of Intermediate 14 (yield 53%).

[145] Preparation Example 14. Synthesis of Intermediate 15
(4-bromo-1,2,3,6,7,8-hexahydropyrene)

[146]

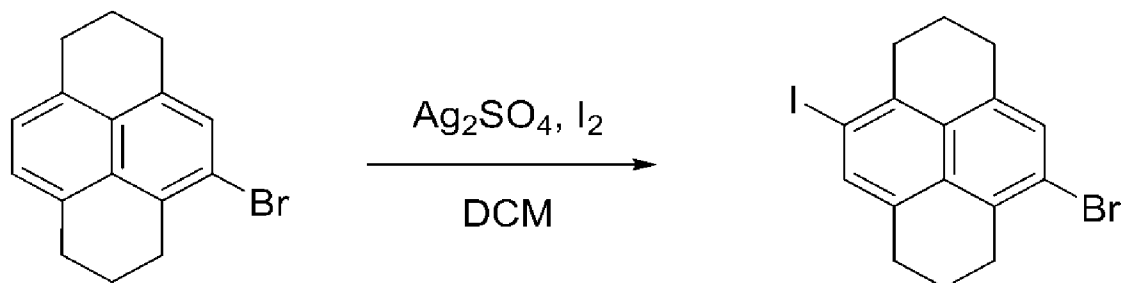


[147] In a 2 L round-bottom three-neck flask in a nitrogen atmosphere, 25.0 g of 1,2,3,6,7,8-hexahydropyrene, 250 ml of dichloromethane(DCM), 875 ml of acetonitrile and 19.2g of NBS(N-bromosuccinimide) were placed, and stirred at room temperature for 24 hr. After completion of the reaction, the extracted solid products was obtaining through vaccum filtration, and washed with methanol, thus obtaining 25.0 g of Intermediate 15 (yield 73%).

[148] ^1H NMR(600MHz, CDCl_3): δ 7.35 (s, 1H), 7.16-7.11 (m, 2H), 3.09 (t, 2H), 3.06-3.01 (m, 6H), 2.04-2.02 (m, 4H)

[149] Preparation Example 15. Synthesis of Intermediate 16
(4-bromo-9-iodo-1,2,3,6,7,8-hexahydropyrene)

[150]



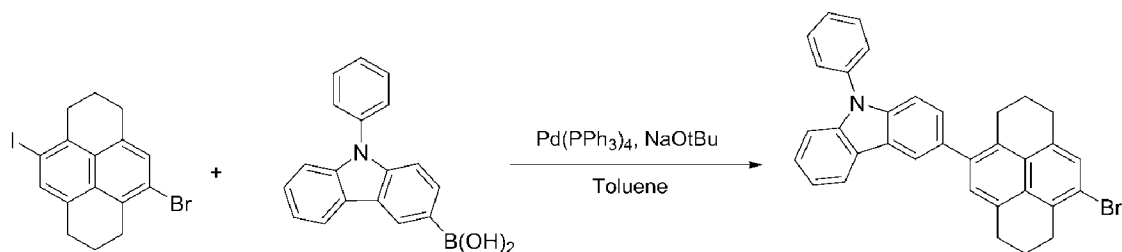
[151] In a 2 L round-bottom three-neck flask in a nitrogen atmosphere, 28.3 g of Intermediate 15, 33.8g of silver sulfate, 27.5g of iodine(I_2) and 1000 ml of dichloromethane(DCM) were placed, and stirred at room temperature for 24 hr. After completion of the reaction, The reaction solution was filtered and vaccum concentrated, thus obtaining 18.8 g of Intermediate 16 (yield 46%).

[152] ^1H NMR(600MHz, CDCl_3): δ 7.65 (s, 1H), 7.39 (s, 1H), 3.08-2.95 (m, 8H), 2.03-1.99 (m, 4H)

[153] Preparation Example 16. Synthesis of Intermediate 17

(3-(9-bromo-1,2,3,6,7,8-hexahydropyrene-4-yl)-9-phenyl-9H-carbazole)

[154]



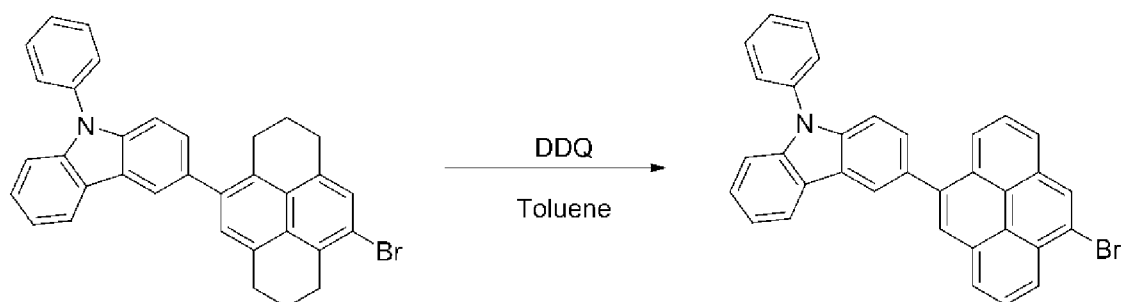
[155] In a 250 mL round-bottom three-neck flask in a nitrogen atmosphere, 10.0 g of Intermediate 16, 7.0g of 9-phenyl-9H-carbazol-3-ylboronic acid, 0.8g of tetrakis(triphenylphosphine)palladium(0), 7.0 g of sodium tert-butoxide and 140 ml of toluene were placed, and stirred at 60°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 4.3 g of Intermediate 17 (yield 33%).

[156] ¹H NMR(600MHz, CDCl₃): δ 8.14-8.12 (m, 2H), 7.65-7.60 (m, 4H), 7.49-7.41 (m, 6H), 7.32-7.28 (m, 2H) , 3.14 (t, 2H), 3.09-3.05 (m, 6H), 2.11-2.07 (m, 2H), 1.95-1.91 (m, 2H)

[157] Preparation Example 17. Synthesis of Intermediate 18

(3-(9-bromopyrene-4-yl)-9-phenyl-9H-carbazole)

[158]



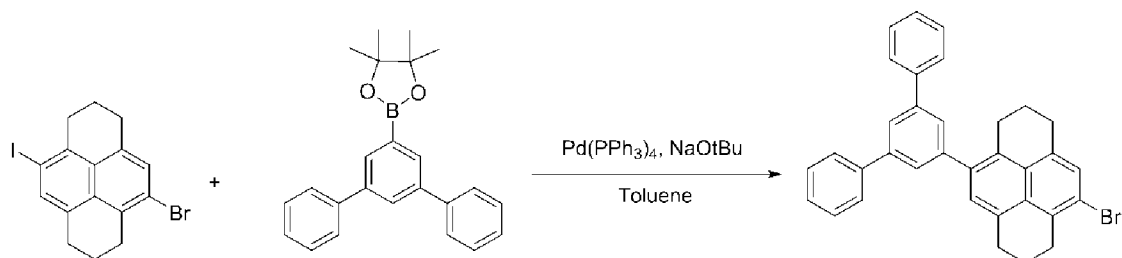
[159] In a 250 mL round-bottom three-neck flask in a nitrogen atmosphere, 4.3 g of Intermediate 17, 7.4g of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone(DDQ) and 200 ml of toluene were placed, and refluxed for 2 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 3.1 g of Intermediate 18 (yield 72%).

[160] ¹H NMR(600MHz, CDCl₃): δ 8.62 (d, 1H), 8.49 (s, 2H), 8.42 (s, 1H) , 8.35 (d, 1H) , 8.29 (d, 1H) , 8.18-8.12 (m, 4H), 7.96 (t, 1H) , 7.70-7.66 (m, 5H) , 7.59 (d, 1H) , 7.52-7.44 (m, 3H) , 7.31 (t, 1H)

[161] Preparation Example 18. Synthesis of Intermediate 19

(4-bromo-9-([1,1':3',1''-tertphenyl]-5'-yl)-1,2,3,6,7,8-hexahydropyrene)

[162]

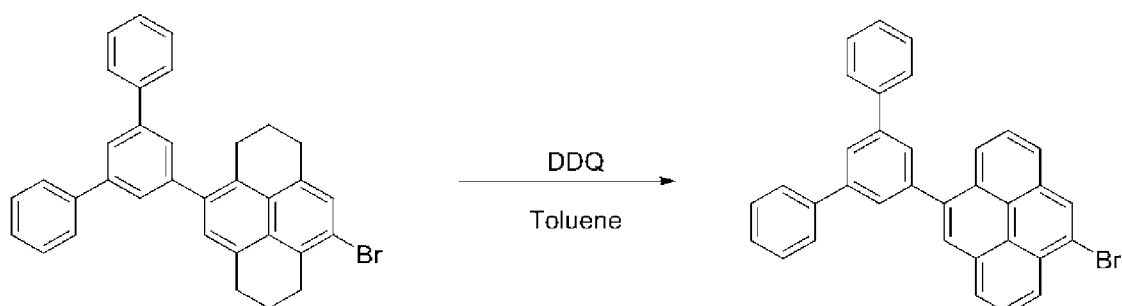


[163] In a 100 mL round-bottom three-neck flask in a nitrogen atmosphere, 5.0 g of Intermediate 16, 4.3g of 1,3-diphenyl-5-phenyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, 0.4g of tetrakis(triphenylphosphine)palladium(0), 3.5 g of sodium tert-butoxide and 70 ml of toluene were placed, and stirred at 60°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 3.5 g of Intermediate 19 (yield 56%).

[164] ^1H NMR(600MHz, CDCl_3): δ 7.81 (s, 1H), 7.70 (d, 4H), 7.59 (d, 2H), 7.47 (t, 4H), 7.42 (s, 1H), 7.38 (t, 2H), 7.29 (s, 1H), 3.13 (t, 2H), 3.09-3.05 (m, 6H), 2.10-2.07 (m, 2H), 1.97-1.94 (m, 2H)

[165] Preparation Example 19. Synthesis of Intermediate 20
(4-bromo-9-([1,1':3',1''-tertphenyl]-5'-yl)pyrene)

[166]

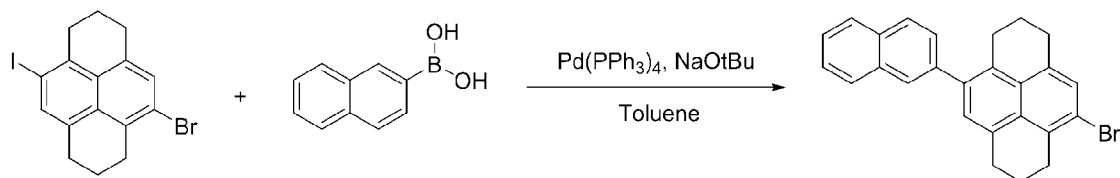


[167] In a 250 mL round-bottom three-neck flask in a nitrogen atmosphere, 7.0 g of Intermediate 19, 12.3g of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone(DDQ) and 300 ml of toluene were placed, and refluxed for 12 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 4.6 g of Intermediate 20 (yield 67%).

[168] ^1H NMR(600MHz, CDCl_3): δ 8.62 (d, 1H), 8.49 (s, 1H), 8.36 (d, 1H), 8.27 (d, 1H), 8.16-8.12 (m, 3H), 8.00-7.96 (m, 2H), 7.88-7.87 (m, 2H), 7.76 (d, 4H), 7.49 (t, 4H), 7.40 (t, 2H)

[169] Preparation Example 20. Synthesis of Intermediate 21
(4-bromo-9-naphthyl-hexahydropyrene)

[170]

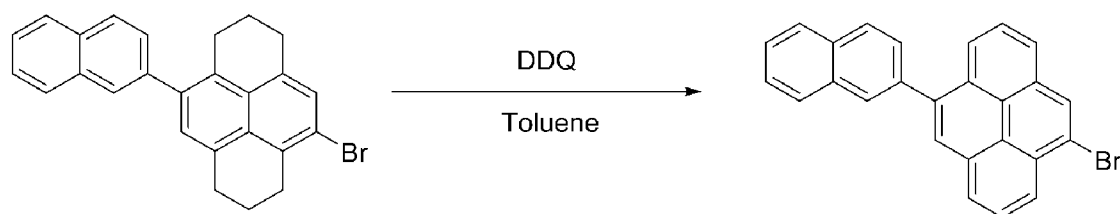


[171] In a 100 mL round-bottom three-neck flask in a nitrogen atmosphere, 9.8 g of Intermediate 16, 4.1 g of naphthylboronic acid, 1.1 g of tetrakis(triphenylphosphine)palladium(0), 6.8 g of sodium tert-butoxide and 200 ml of toluene were placed, and stirred at 60°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 5.2 g of Intermediate 21 (yield 53%).

[172] ¹H NMR(600MHz, CDCl₃): δ 7.90-7.86 (m, 3H), 7.82 (s, 1H), 7.53-7.49 (m, 3H), 7.42 (s, 1H), 7.27 (s, 1H), 3.14 (t, 2H), 3.07-3.04 (m, 4H), 3.01 (t, 2H), 2.11-2.07 (m, 2H), 1.93-1.90 (m, 2H)

[173] Preparation Example 21. Synthesis of Intermediate 22 (4-bromo-9-naphthylpyrene)

[174]

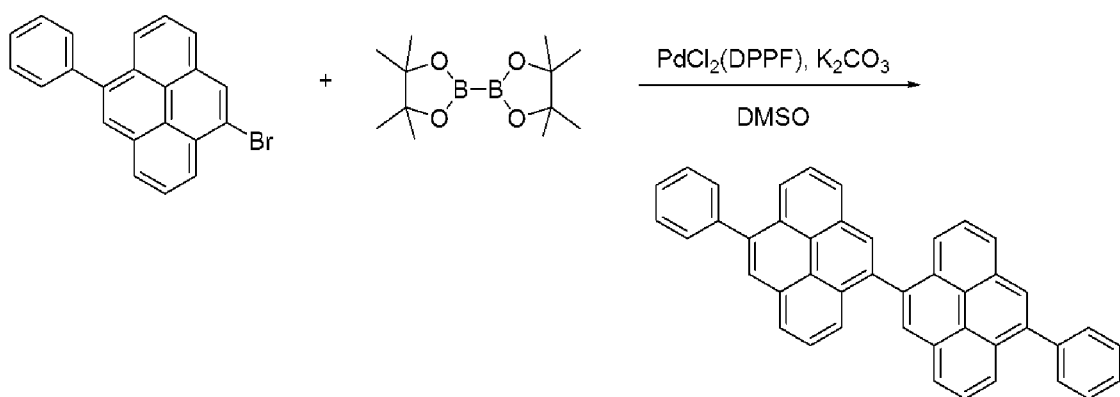


[175] In a 1 L round-bottom three-neck flask in a nitrogen atmosphere, 5.2 g of Intermediate 21, 12.3 g of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone(DDQ) and 350 ml of toluene were placed, and refluxed for 5 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 4.8 g of Intermediate 22 (yield 94%).

[176] ¹H NMR(600MHz, CDCl₃): δ 8.62 (d, 1H), 8.49 (s, 1H), 8.28 (d, 1H), 8.25 (d, 1H), 8.16-8.12 (m, 4H), 8.03 (d, 1H), 7.98-7.94 (m, 3H), 7.78 (d, 1H), 7.58-7.57 (m, 2H)

[177] Example 1. Synthesis of Compound 1

[178]



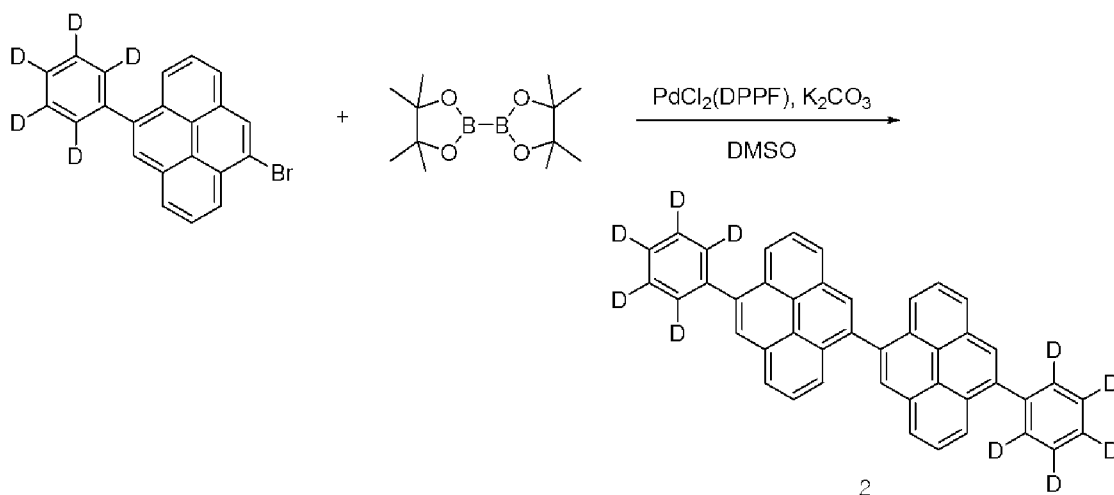
[179] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 4.1 g of Intermediate 3, 1.5 g of bis(pinacolato)diboron, 0.3 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 4.8 g of potassium carbonate and 40 ml of DMSO were placed, and stirred at 80°C for 12 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.6 g of Compound 1 (yield 49%).

[180] ^1H NMR(600MHz, CDCl_3): δ 8.35 (s, 2H), 8.30 (t, 4H), 8.21 (d, 2H), 8.12 (s, 2H), 8.04 (t, 2H), 7.87 (d, 2H), 7.80 (t, 2H), 7.75 (d, 4H), 7.61 (t, 4H), 7.54 (t, 2H)

[181] MS (ESI): $[\text{M}+\text{H}]^+$ 555

[182] Example 2. Synthesis of Compound 2

[183]



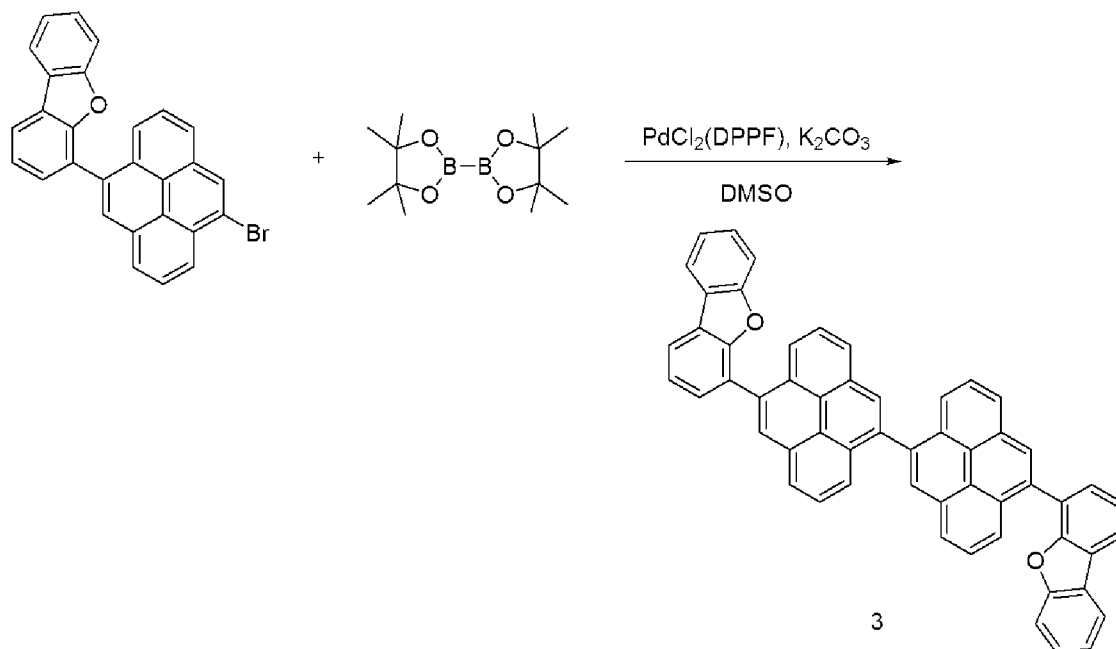
[184] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 3.8 g of Intermediate 4, 1.3 g of bis(pinacolato)diboron, 0.2 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 4.4 g of potassium carbonate and 40 ml of DMSO were placed, and stirred at 80°C for 12 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.6 g of Compound 2 (yield 54%).

[185] ^1H NMR(600MHz, CDCl_3): δ 8.35 (s, 2H), 8.30 (t, 4H), 8.21 (d, 2H), 8.12 (s, 2H), 8.04 (t, 2H), 7.87 (d, 2H), 7.80 (t, 2H)

[186] MS (ESI): $[\text{M}+\text{H}]^+$ 565

[187] Example 3. Synthesis of Compound 3

[188]



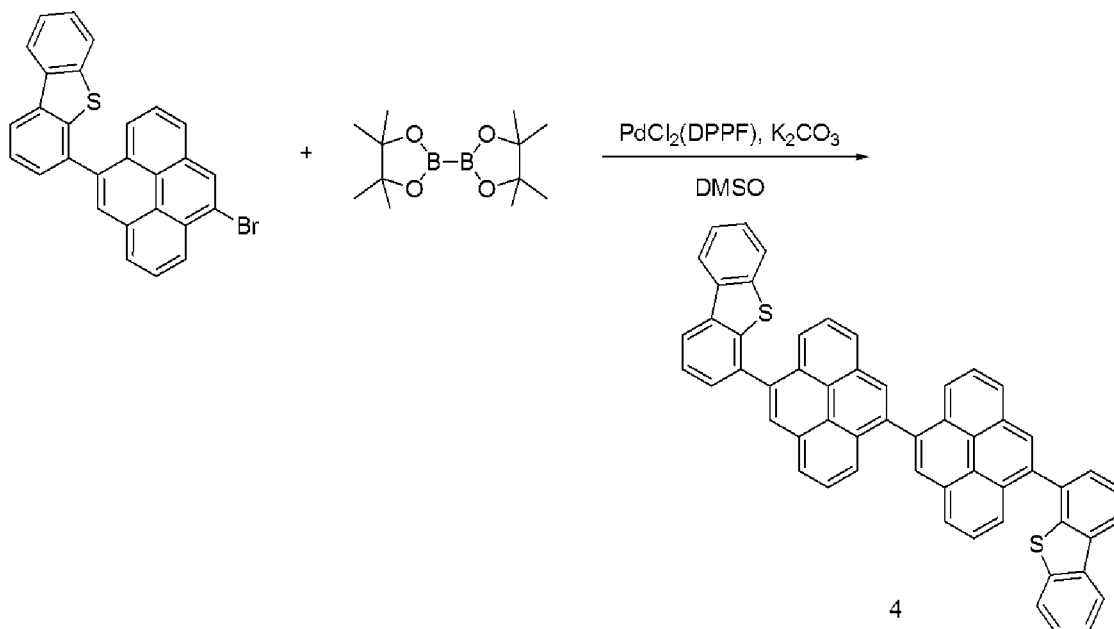
[189] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 5.0 g of Intermediate 5, 1.4 g of bis(pinacolato)diboron, 0.2 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 4.6 g of potassium carbonate and 40 ml of DMSO were placed, and stirred at 80°C for 24 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 2.4 g of Compound 3 (yield 58%).

[190] ^1H NMR(600MHz, CDCl_3): δ 8.54 (s, 2H), 8.50 (d, 2H), 8.44-8.42 (m, 4H), 8.38 (d, 2H), 8.28 (d, 2H), 8.08 (t, 2H), 7.96-7.92 (m, 4H), 7.83-7.80 (m, 4H), 7.69 (t, 2H), 7.54 (d, 2H), 7.49 (t, 2H), 7.48-7.43 (m, 2H)

[191] MS (ESI): $[\text{M}+\text{H}]^+$ 735

[192] Example 4. Synthesis of Compound 4

[193]



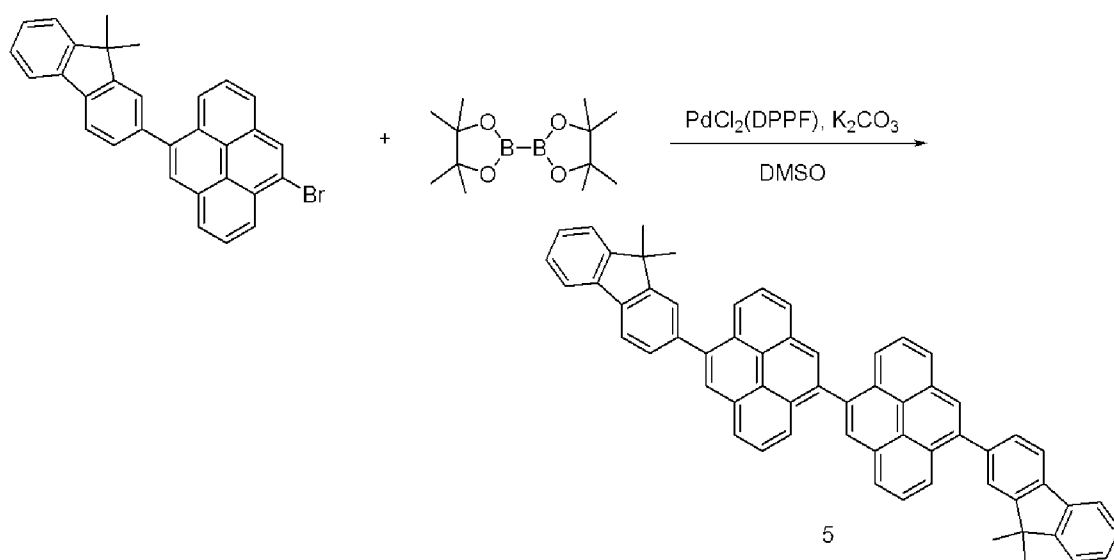
[194] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 5.8 g of Intermediate 6, 1.6 g of bis(pinacolato)diboron, 0.3 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 5.3 g of potassium carbonate and 40 ml of DMSO were placed, and stirred at 80°C for 24 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 2.0 g of Compound 4 (yield 41%).

[195] ^1H NMR(600MHz, CDCl_3): δ 8.41 (s, 2H), 8.37 (t, 4H), 8.29 (d, 2H), 8.19 (s, 2H), 8.13-8.07 (m, 6H), 7.91 (d, 2H), 7.85-7.83 (m, 4H), 7.49-7.44 (m, 8H)

[196] MS (ESI): $[\text{M}+\text{H}]^+$ 767

[197] Example 5. Synthesis of Compound 5

[198]



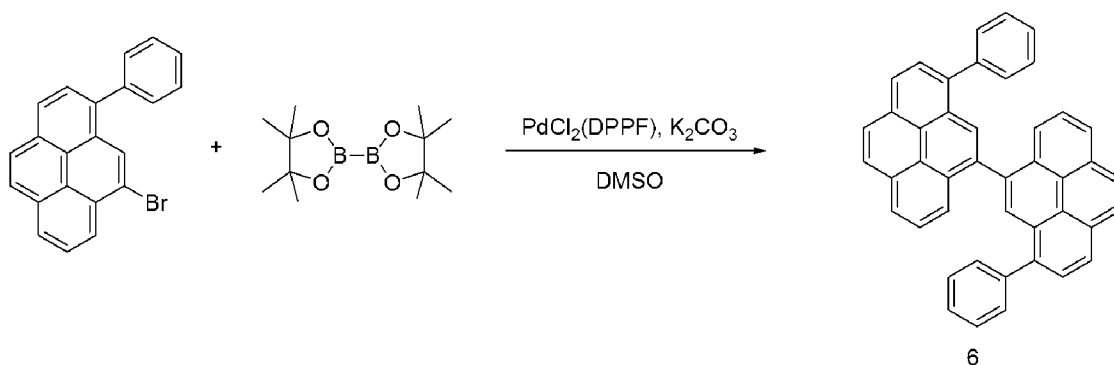
[199] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 5.4 g of Intermediate 7, 1.5 g of bis(pinacolato)diboron, 0.3 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 4.8 g of potassium carbonate and 40 ml of DMSO were placed, and stirred at 80°C for 24 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 2.2 g of Compound 5 (yield 49%).

[200] ¹H NMR(600MHz, CDCl₃): δ 8.40 (t, 4H), 8.31 (d, 2H), 8.24 (d, 2H), 8.20 (s, 2H), 8.06 (t, 2H), 7.95 (d, 2H), 7.89 (d, 2H), 7.86 (d, 2H), 7.83-7.81 (m, 4H), 7.75-7.73 (m, 2H), 7.52 (d, 2H), 7.43-7.39 (m, 4H), 1.63 (s, 12H)

[201] MS (ESI): [M+H]⁺ 787

[202] Example 6. Synthesis of Compound 6

[203]



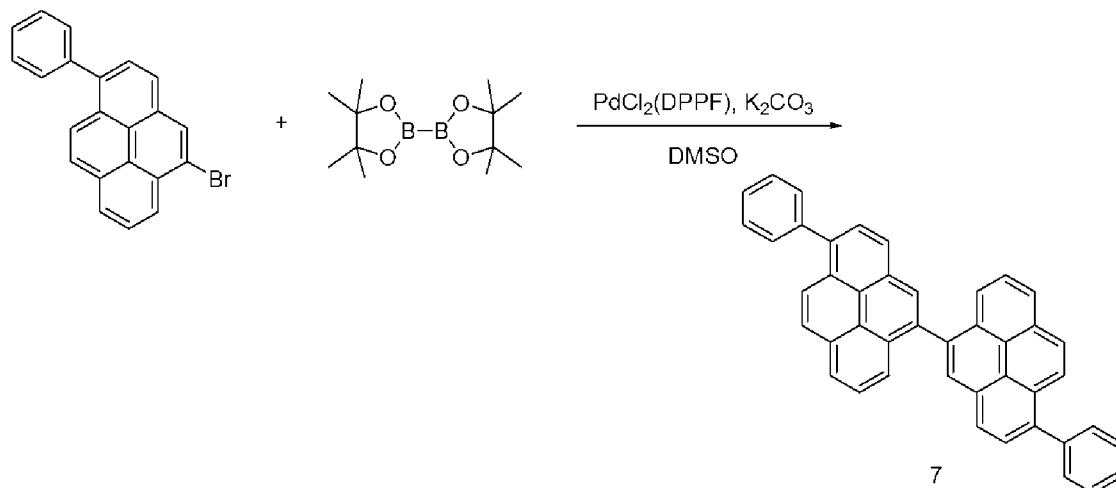
[204] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 2.5 g of Intermediate 10, 0.9 g of bis(pinacolato)diboron, 0.2 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 2.9 g of potassium carbonate and 25 ml of DMSO were placed, and stirred at 80°C for 12 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.1 g of Compound 6 (yield 55%).

[205] ¹H NMR(600MHz, CDCl₃): δ 8.32 (s, 2H), 8.29-8.25 (m, 4H), 8.10-8.05 (m, 4H), 7.84 (d, 2H), 7.76-7.74 (m, 4H), 7.69 (d, 4H), 7.43 (t, 4H), 7.33 (t, 2H)

[206] MS (ESI): [M+H]⁺ 555

[207] Example 7. Synthesis of Compound 7

[208]



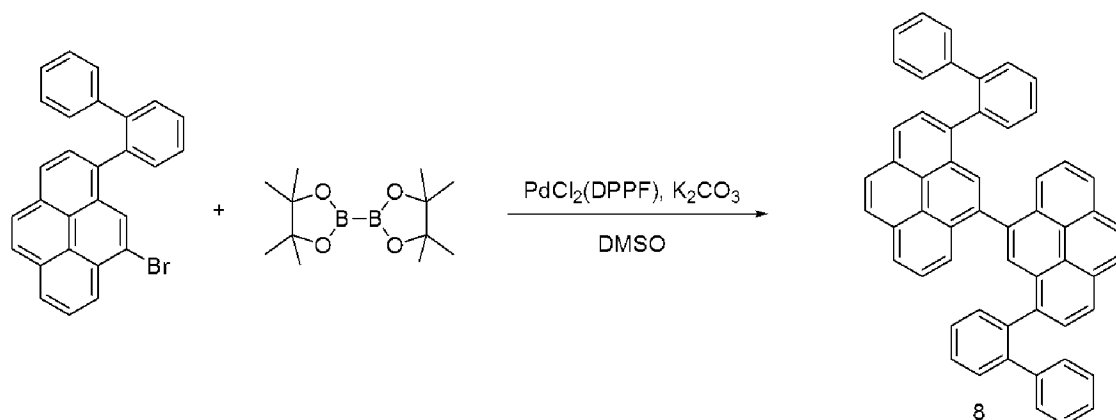
[209] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 3.3 g of Intermediate 11, 1.2 g of bis(pinacolato)diboron, 0.2 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 3.8 g of potassium carbonate and 35 ml of DMSO were placed, and stirred at 80°C for 12 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.5 g of Compound 7 (yield 60%).

[210] ¹H NMR(600MHz, CDCl₃): δ 8.34 (s, 2H), 8.29 (d, 2H), 8.18 (d, 2H), 8.16-8.14 (m, 4H), 8.03 (d, 2H), 7.79 (d, 2H), 7.76 (t, 2H), 7.63 (d, 4H), 7.59 (t, 4H), 7.51 (t, 2H)

[211] MS (ESI): [M+H]⁺ 555

[212] Example 8. Synthesis of Compound 8

[213]



[214] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 3.0 g of Intermediate 12, 1.2 g of bis(pinacolato)diboron, 0.1 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 2.9 g of potassium carbonate and 30 ml of DMSO were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to

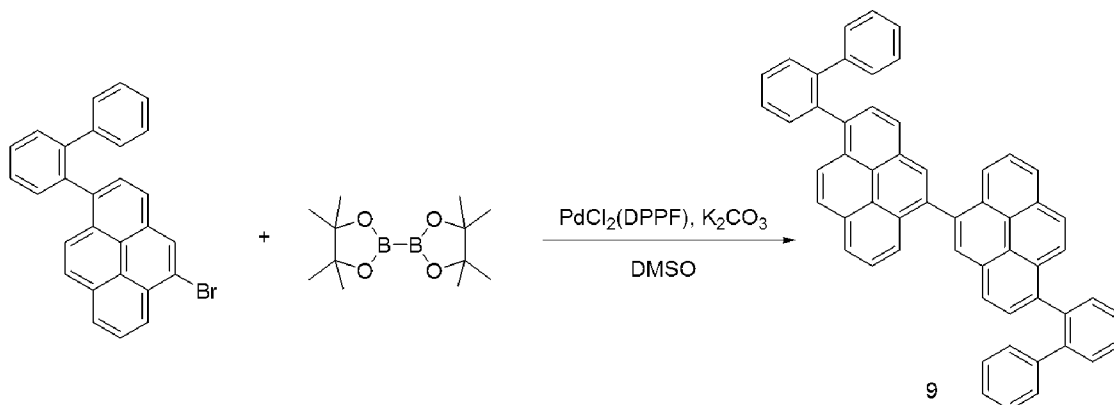
column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.3 g of Compound 8 (yield 52%).

[215] ^1H NMR(600MHz, CDCl_3): δ 8.23 (d, 2H), 8.11-8.03 (m, 8H), 7.79-7.73 (m, 4H), 7.65-7.54 (m, 10H), 7.17-7.13 (m, 4H), 7.03-6.99 (m, 6H)

[216] MS (ESI): $[\text{M}+\text{H}]^+$ 707

[217] Example 9. Synthesis of Compound 9

[218]



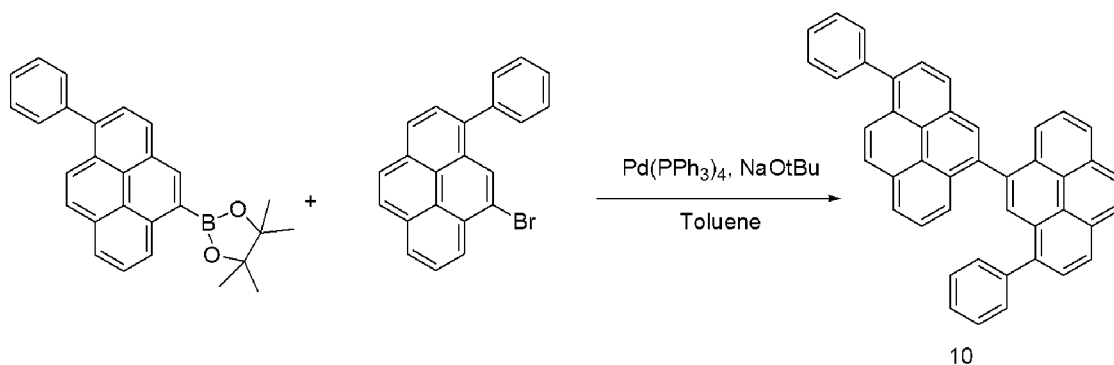
[219] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 2.7 g of Intermediate 13, 0.8 g of bis(pinacolato)diboron, 0.1 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 2.6 g of potassium carbonate and 30 ml of DMSO were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.0 g of Compound 9 (yield 45%).

[220] ^1H NMR(600MHz, CDCl_3): δ 8.13 (d, 2H), 8.09-7.96 (m, 6H), 7.75-7.69 (m, 4H), 7.63-7.51 (m, 8H), 7.45-7.32 (m, 4H), 7.15-7.12 (m, 4H), 7.07-7.01 (m, 6H)

[221] MS (ESI) : $[\text{M}+\text{H}]^+$ 707

[222] Example 10. Synthesis of Compound 10

[223]



[224] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 1.2 g of Intermediate 14, 1.1 g of Intermediate 10, 0.1 g of tetrakis(triphenylphosphine)palladium(0), 0.9 g of sodium tert-butoxide and 12 ml of

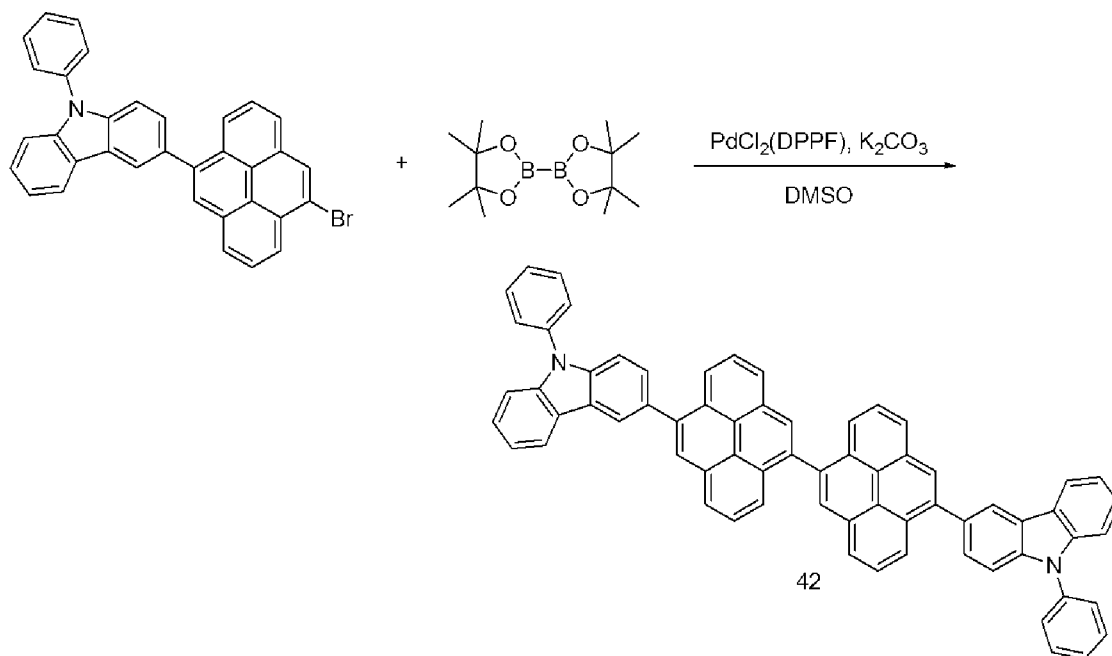
toluene were placed, and stirred at 90°C for 24 hr. The reaction solution was cooled, filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.1 g of Compound 10 (yield 66%).

[225] ^1H NMR(600MHz, CDCl_3): δ 8.41 (s, 1H), 8.33 (d, 1H), 8.26-8.19 (m, 6H), 8.15 (d, 1H), 8.09-8.06 (m, 2H), 8.03 (d, 1H), 7.83-7.76 (m, 4H), 7.68-7.65 (m, 4H), 7.59 (t, 2H), 7.51 (t, 1H), 7.43 (t, 2H), 7.33 (t, 1H)

[226] MS (ESI) : $[\text{M}+\text{H}]^+$ 555

[227] Example 11. Synthesis of Compound 42

[228]



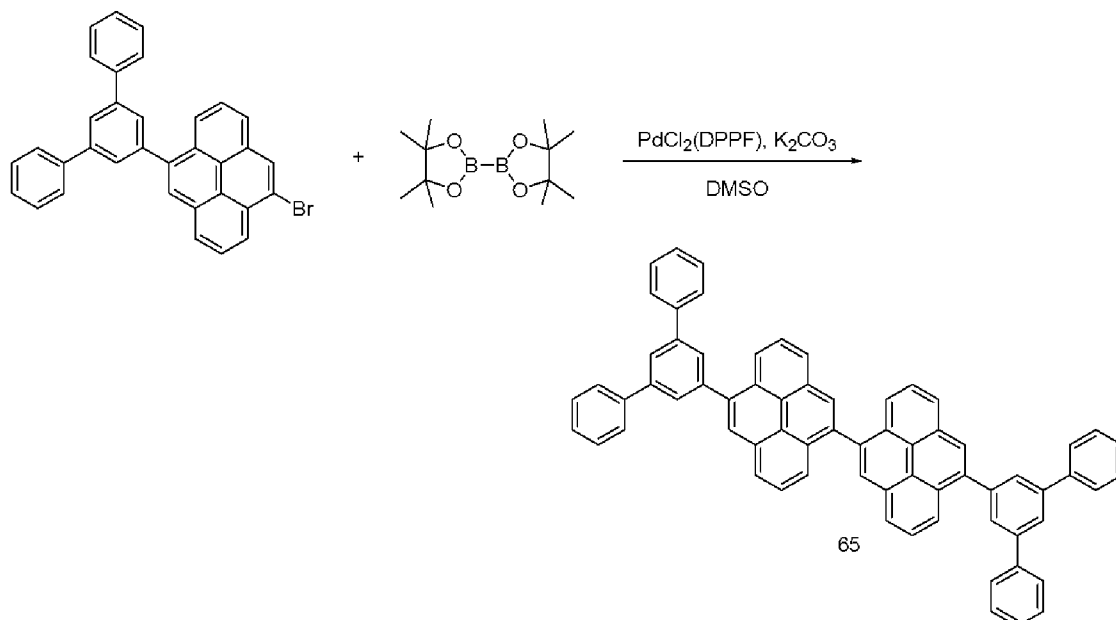
[229] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 2.7 g of Intermediate 18, 0.9 g of bis(pinacolato)diboron, 0.2 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 2.2 g of potassium carbonate and 40 ml of DMSO were placed, and stirred at 80°C for 4 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.4 g of Compound 42 (yield 62%).

[230] ^1H NMR(600MHz, CDCl_3): δ 8.53 (s, 2H), 8.43 (d, 2H), 8.40 (s, 2H), 8.31 (d, 2H), 8.25-8.22 (m, 6H), 8.06 (t, 2H), 7.91 (d, 2H), 7.84-7.80 (m, 4H), 7.72-7.67 (m, 8H), 7.64 (d, 2H), 7.54-7.46 (m, 6H), 7.34 (t, 2H)

[231] MS (ESI) : $[\text{M}+\text{H}]^+$ 885

[232] Example 12. Synthesis of Compound 65

[233]



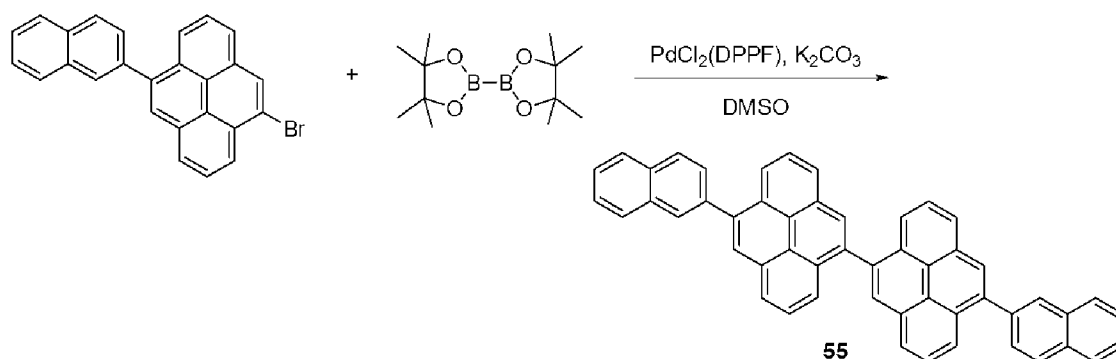
[234] In a 100 ml round-bottom three-neck flask in a nitrogen atmosphere, 3.0 g of Intermediate 20, 1.0 g of bis(pinacolato)diboron, 0.2 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 2.4 g of potassium carbonate and 43 ml of DMSO were placed, and stirred at 80°C for 4 hr. The reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to column chromatography with a solvent of mixture of dichloromethane and n-hexane, thus obtaining 1.2 g of Compound 65 (yield 47%).

[235] ^1H NMR(600MHz, CDCl_3): δ 8.45 (d, 2H), 8.39 (s, 2H), 8.32 (d, 2H), 8.25-8.24 (m, 4H), 8.07 (t, 2H), 8.00-7.98 (m, 6H), 7.90 (d, 2H), 7.84-7.80 (m, 10H), 7.52 (t, 8H), 7.42 (t, 4H)

[236] MS (ESI) : $[\text{M}+\text{H}]^+$ 859

[237] Example 13. Synthesis of Compound 55

[238]



[239] In a 250 ml round-bottom three-neck flask in a nitrogen atmosphere, 4.7 g of Intermediate 22, 2.1 g of bis(pinacolato)diboron, 0.3 g of [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (II), 4.8 g of potassium carbonate and 120 ml of DMSO were placed, and stirred at 80°C for 20 hr. The

reaction solution was cooled and then extracted with dichloromethane and water, after which the organic layer was filtered with silica gel, concentrated, and then subjected to recrystallization with a solvent of toluene, thus obtaining 1.9 g of Compound 55 (yield 50%).

[240] ^1H NMR(600MHz, CDCl_3): NMR analysis of Compound 13 could not be performed, because Compound 13 was not soluble in NMR solvent.

[241] MS (ESI) : $[\text{M}+\text{H}]^+$ 655

[242]

[243] Device Example 1. Manufacture of organic EL device including Compound 1 as host

[244] A glass substrate coated with an ITO (indium tin oxide) thin film having a thickness of 100 nm was ultrasonically washed with an isopropyl alcohol solvent, dried, placed in a plasma cleaning system so that the substrate was cleaned using oxygen plasma for 5 min, and then transferred into a vacuum deposition system.

[245] The ITO transparent electrode thus prepared was used as an anode, and DNTPD [N,N'-diphenyl-N,N'-bis-[4-(phenyl-m-tolylamino)-phenyl]-biphenyl-4,4'-diamine] was vacuum deposited on the ITO substrate, thus forming a hole injection layer having a thickness of 40 nm. Subsequently, NPB [N,N'-bis(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine] as a hole injection layer was deposited to a thickness of 30 nm, thus forming the hole transport layer, and DPP [N1,N1,N6,N6-tetraphenylpyrene-1,6-diamine] as a dopant, was deposited to 0.1nm/sec of deposition speed of compound 1 and 0.003nm/sec of deposition speed of DPP, and 3 % of deposition speed rate of DPP was deposited to a thickness of 25 nm on the hole transport layer, thus forming a light emitting layer.

[246] Thereafter, an electron transport layer was formed to a thickness of 25 nm depositing Alq_3 on the light emitting layer, and 2 nm thick Liq [lithium quinolate] and 100 nm thick Al were sequentially vacuum deposited on the electron transport layer to form a cathode, thereby manufacturing an organic EL device.

[247] At this time, deposition speed of materials was 0.1nm/sec of organic compound 1, DNTPD, NPB and Alq_3 , 0.01 nm/sec of lithium fluoride and 0.5nm/sec of alluminium.

[248] Device Example 2. Manufacture of organic EL device including Compound 2 as host

[249] An organic EL device was manufactured in the same manner as in Device Example 1, with the exception that Compound 2 was used instead of Compound 1 in Device Example 2.

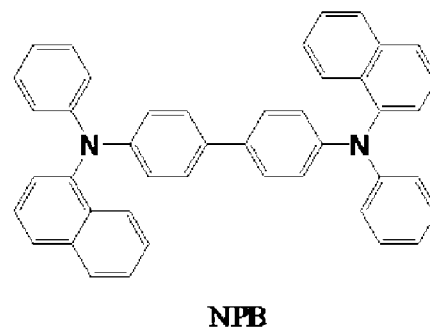
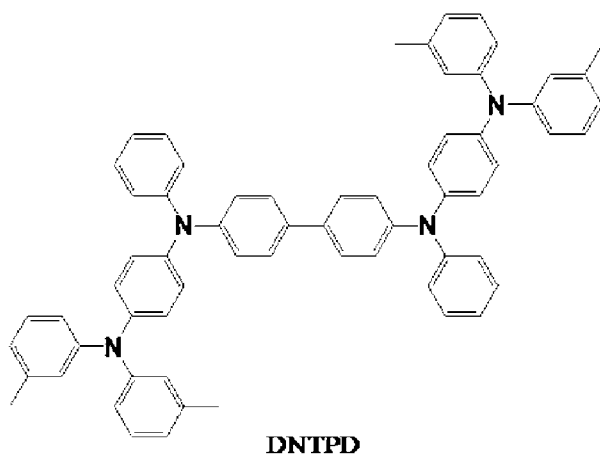
[250] Device Example 3. Manufacture of organic EL device including Compound 3 as host

[251] An organic EL device was manufactured in the same manner as in Device Example 1, with the exception that Compound 3 was used instead of Compound 1 in Device Example 3.

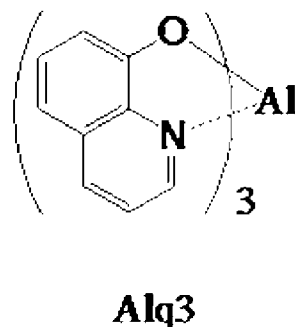
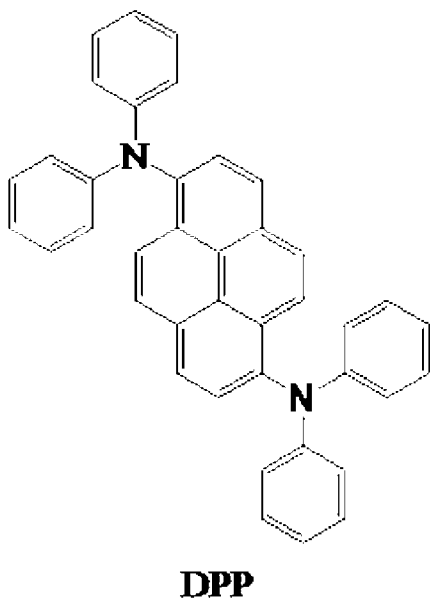
[252] Device Example 4. Manufacture of organic EL device including Compound 4 as host

- [253] An organic EL device was manufactured in the same manner as in Device Example 1, with the exception that Compound 4 was used instead of Compound 1 in Device Example 4.
- [254] Device Example 5. Manufacture of organic EL device including Compound 5 as host
- [255] An organic EL device was manufactured in the same manner as in Device Example 1, with the exception that Compound 5 was used instead of Compound 1 in Device Example 5.
- [256] Device Example 6. Manufacture of organic EL device including Compound 6 as hole transport layer
- [257] An organic EL device was manufactured in the same manner as in Device Example 1, with the exception that Compound 6 was used instead of Compound 1 in Device Example 6.
- [258]
- [259] The chemical formulas of DNTPD, NPB, DPP and Alq₃ used in the examples are represented below.

[260]



[261]



[262]

[263] Evaluation of properties of organic EL device[264] The properties of the organic EL devices in the manufactured Device Examples 1 to 6, were evaluated at a brightness of 2000 cd/m², and the results are shown in Table 1 below.

[265] Table 1

[Table 1]

	Host material	Current density(mA/cm ²)	Brightness efficiency(cd/A)	Color coordinatesCIE (x,y)
Device Examples 1	Compound 1	43.48	4.6	0.15,0.18
Device Examples 2	Compound 2	44.43	4.5	0.15,0.18
Device Examples 3	Compound 3	44.49	4.5	0.15,0.18
Device Examples 4	Compound 4	47.62	4.2	0.15,0.18
Device Examples 5	Compound 5	46.51	4.3	0.15,0.18
Device Examples 6	Compound 6	45.46	4.4	0.15,0.18

- [266] The organic EL devices in the manufactured Device Examples 1 to 6, while a voltage was increased from 0 V to 10 V, current of each unit device was measured using a current-voltage meter (Keithley 2635A Source Meter), and the measured current value was divided by the area, thus obtaining current density.
- [267] In the manufactured organic EL devices, while a voltage was increased from 0 V to 10 V, the brightness was measured using a brightness meter (Minolta CS-2000), and the measured brightness value was divided by the current value, thus obtaining brightness efficiency. Also, the color coordinates were measured using a brightness meter (Minolta CS-2000).
- [268] According to the table 1, as is apparent from the results of manufacturing organic EL devices using the compound 1 to 6 according to the present invention as the material for the host, exhibited superior properties.
- [269] Although the preferred embodiments of the present invention have been disclosed for illustrative purposes, those skilled in the art will appreciate that various modifications, additions and substitutions are possible, without departing from the scope and spirit of the invention as disclosed in the accompanying claims.
- [270]

Industrial Applicability

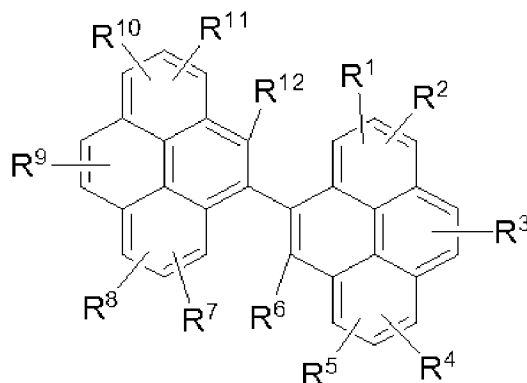
- [271] The present invention may provide a compound for an organic EL device which may be used as a host of a fluorescent light emitting layer with high electrical stability, high transport capacity of an electron and a hole, high efficiency and high colorimetric purity, and an organic electroluminescent device including the same.
- [272] The present invention may also provide a compound for an organic EL device which may be used as an electron transport material or a hole transport material, and an organic electroluminescent device including the same.

Claims

[Claim 1]

A compound for an organic electroluminescent device, represented by Chemical Formula 1 below:

[Chemical Formula 1]

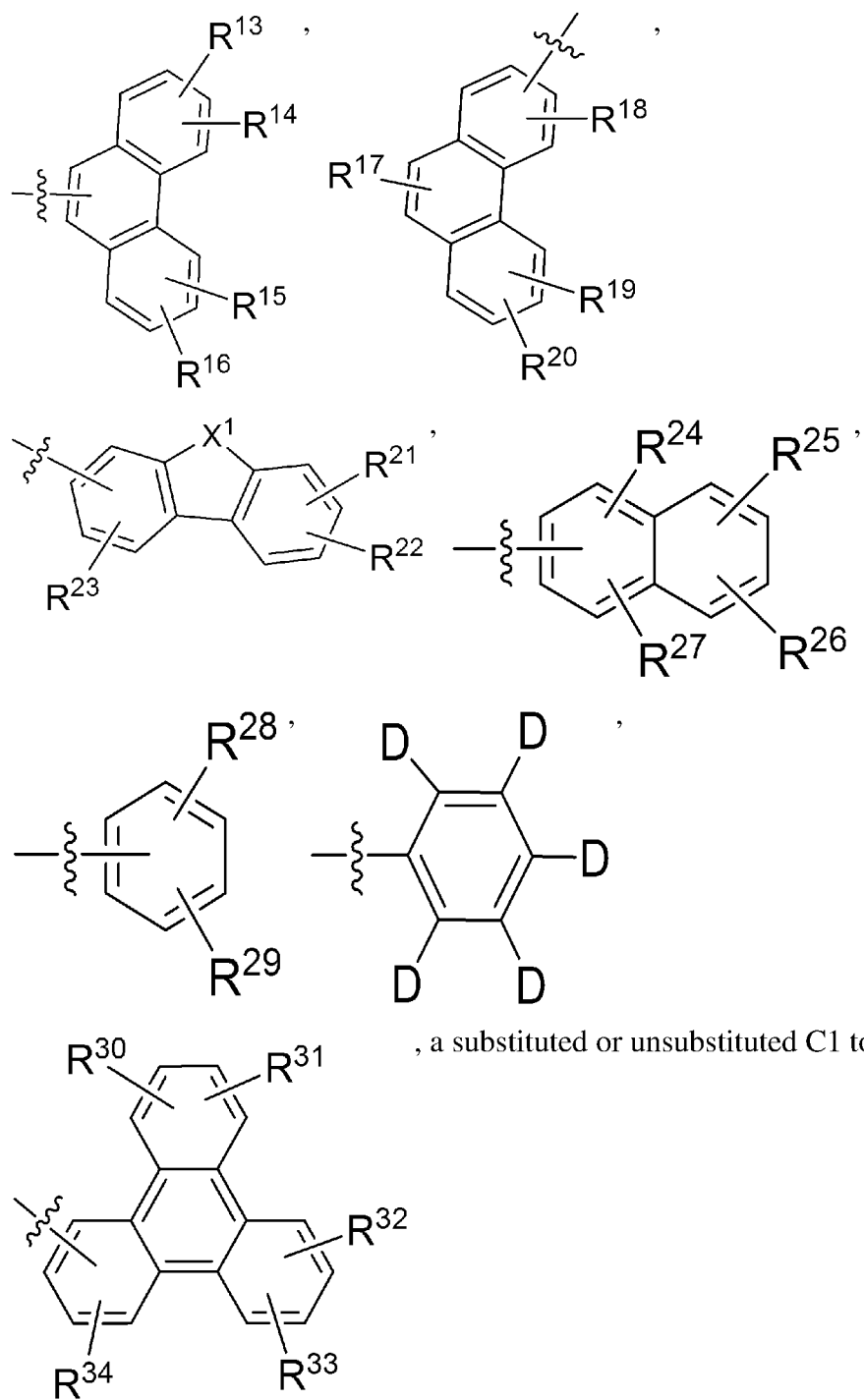


wherein R^1 to R^5 , and R^7 to R^{11} are identical to or different from each other, and R^1 to R^5 , and R^7 to R^{11} are each independently a hydrogen atom, a deuterium atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, or at least one of R^1 to R^5 , and R^7 to R^{11} is further coupled with a carbon atom adjacent to a carbon atom linked therewith to form a substituted or unsubstituted fused C3 to C30 cycloalkyl group, a substituted or unsubstituted fused C1 to C30 heterocycloalkyl group, a substituted or unsubstituted fused C6 to C30 aryl group, or a substituted or unsubstituted fused C1 to C30 heteroaryl group, and

R^6 to R^{12} are identical to or different from each other, and R^6 to R^{12} are each independently a hydrogen atom, a deuterium atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group.

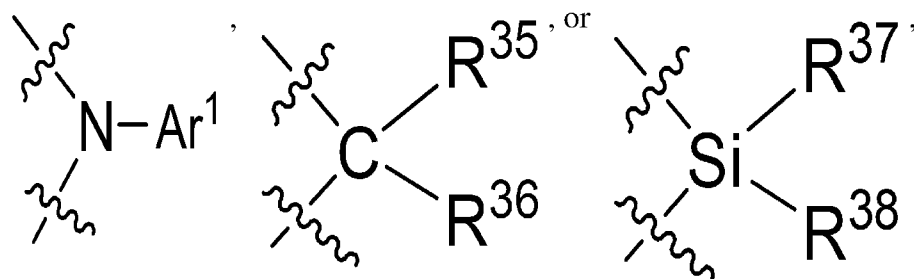
[Claim 2]

The compound of claim 1, wherein R^1 to R^{12} are identical to or different from each other, and R^1 to R^{12} are each independently a hydrogen atom, a deuterium atom,



C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, or a substituted or unsubstituted C1 to C30 heterocycloalkyl group,

X¹ is an oxygen atom, a sulfur atom,



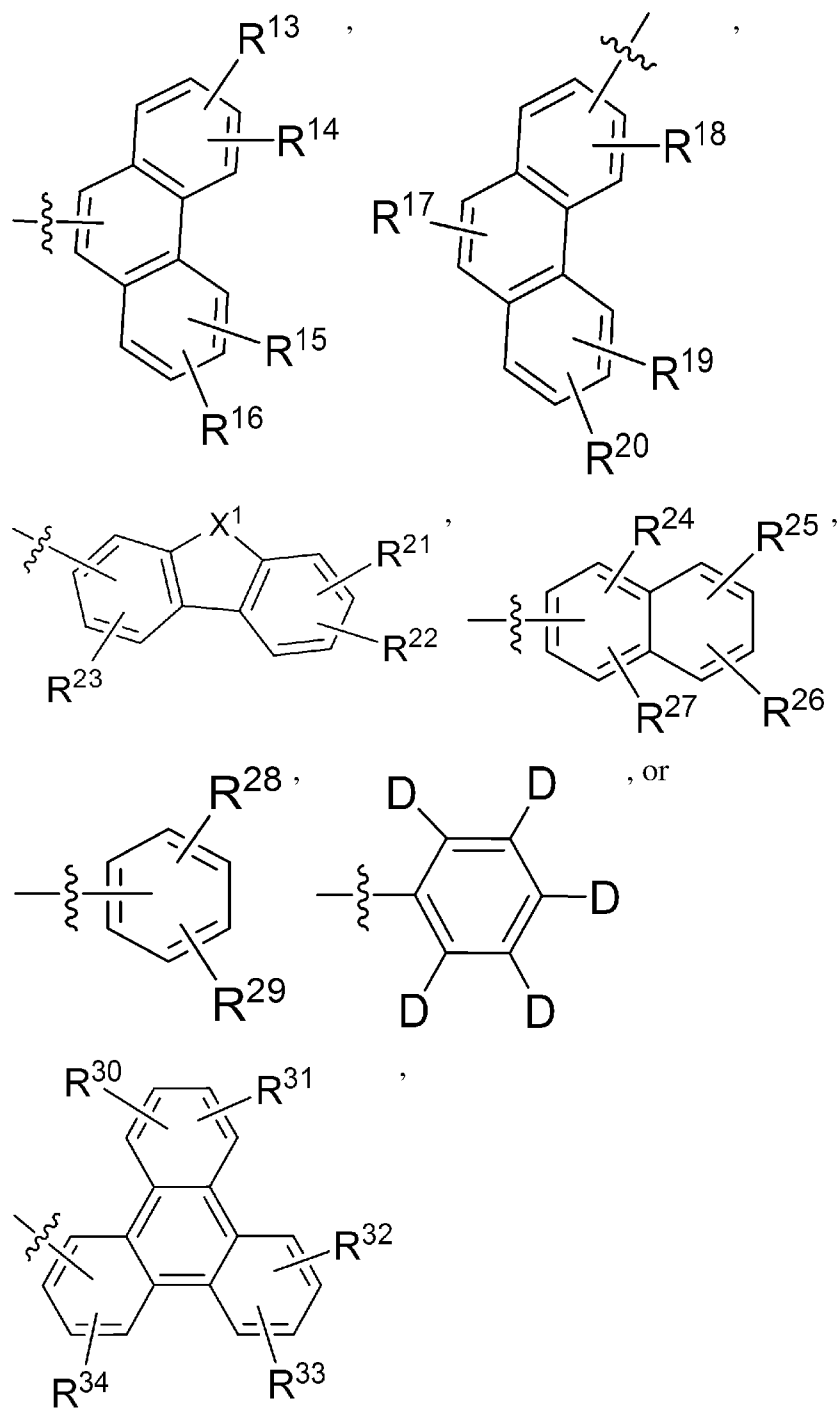
Ar¹ is a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group,

R³⁵ to R³⁸ are identical to or different from each other, and R³⁵ to R³⁸ are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, or R³⁵ and R³⁶, and R³⁷ and R³⁸, respectively, are linked to form a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, together with a carbon atom or a silicon atom therebetween, and

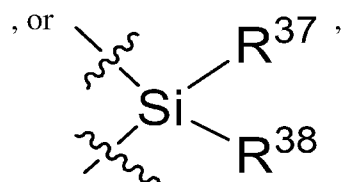
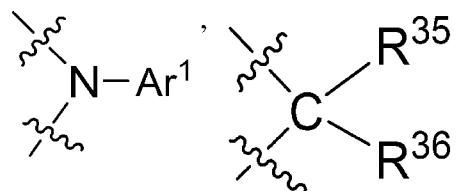
R¹³ to R³⁴ are identical to or different from each other, and R¹³ to R³⁴ are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group, or at least one of R¹³ to R³⁴ is further coupled with a carbon atom adjacent to a carbon atom linked therewith to form a substituted or unsubstituted fused C3 to C30 cycloalkyl group, a substituted or unsubstituted fused C1 to C30 heterocycloalkyl group, a substituted or unsubstituted fused C6 to C30 aryl group, or a substituted or unsubstituted fused C1 to C30 heteroaryl group.

[Claim 3]

The compound of claim 1, wherein R¹ to R¹² are identical to or different from each other, and R¹ to R¹² are each independently a hydrogen atom, a deuterium atom,



X^1 is a oxygen atom, a sulfur atom,



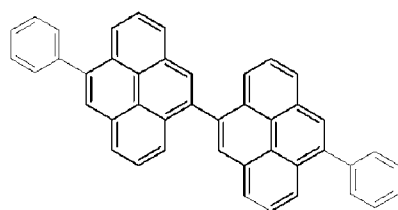
Ar¹ is a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group,

R³⁵ to R³⁸ are identical to or different from each other, and R³⁵ to R³⁸ are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, or a substituted or unsubstituted C1 to C30 heterocycloalkyl group, and

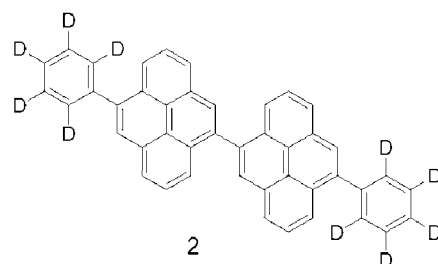
R¹³ to R³⁴ are identical to or different from each other, and R¹³ to R³⁴ are each independently a hydrogen atom, a substituted or unsubstituted C1 to C30 alkyl group, a substituted or unsubstituted C3 to C30 cycloalkyl group, a substituted or unsubstituted C1 to C30 heterocycloalkyl group, a substituted or unsubstituted C6 to C30 aryl group, or a substituted or unsubstituted C1 to C30 heteroaryl group.

[Claim 4]

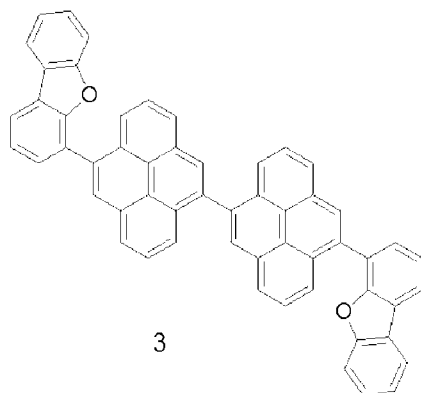
The compound of claim 1, which is any one selected from among Compounds 1 to 65 represented by the following chemical formulas:



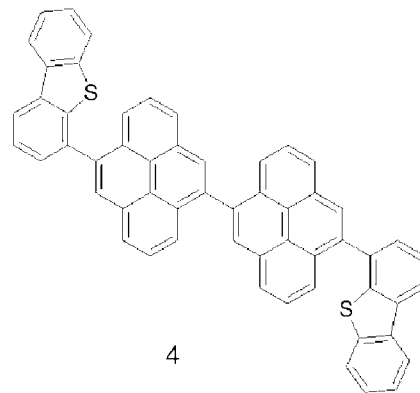
1



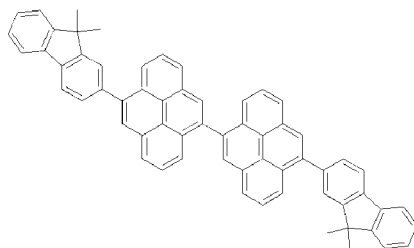
2



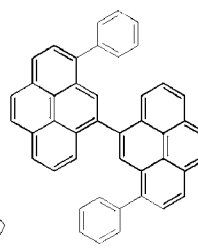
3



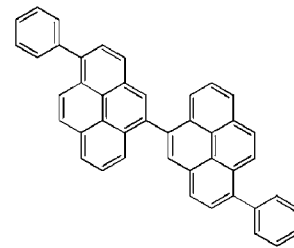
4



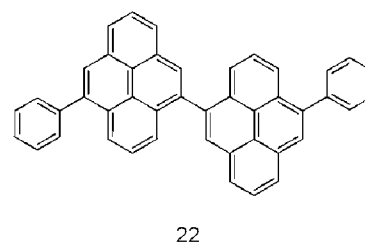
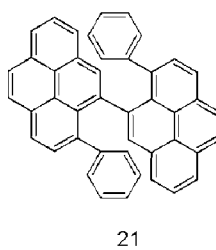
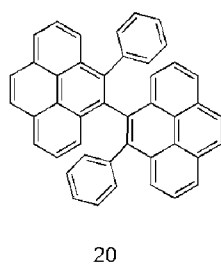
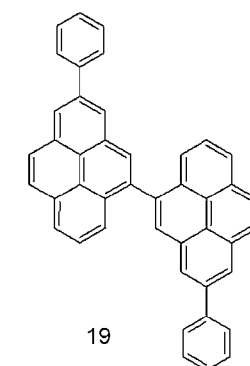
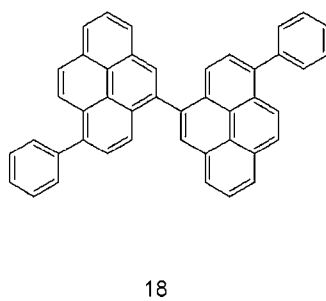
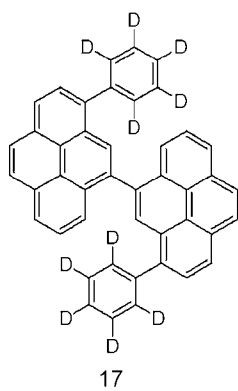
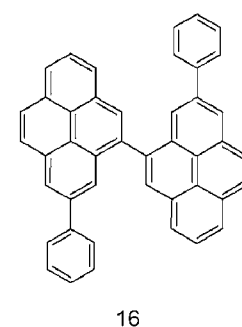
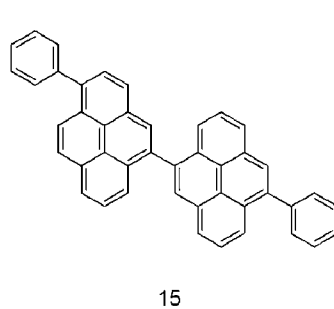
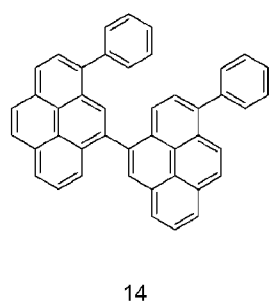
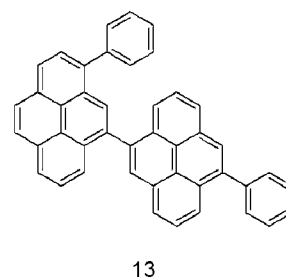
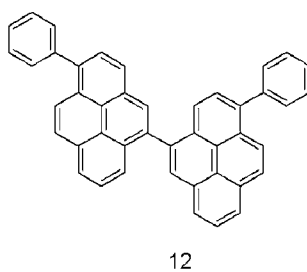
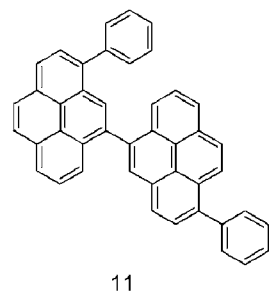
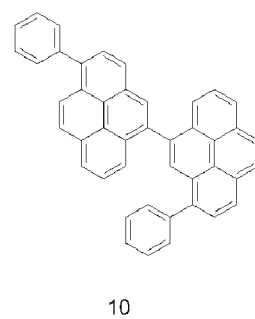
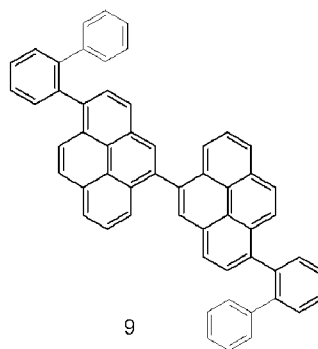
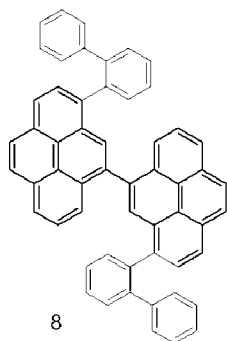
5

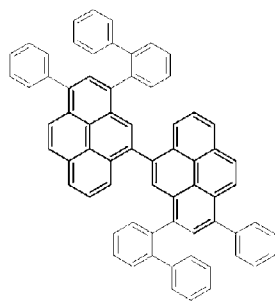


6

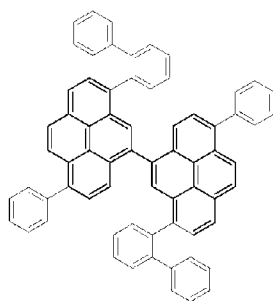


7

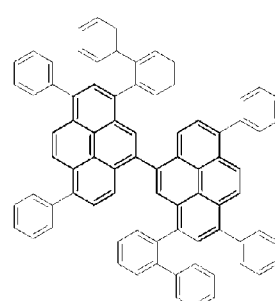




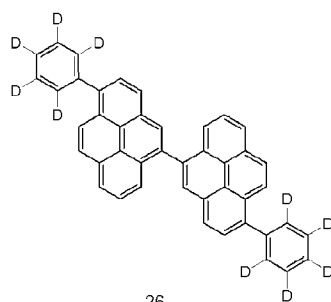
23



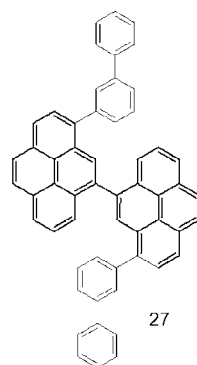
24



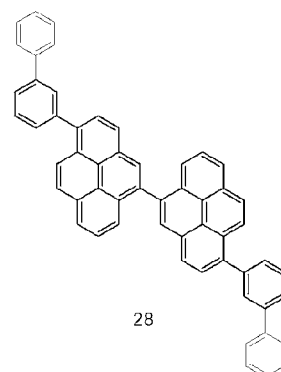
25



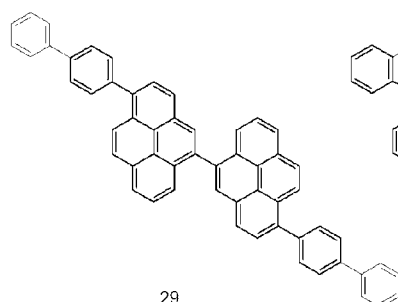
26



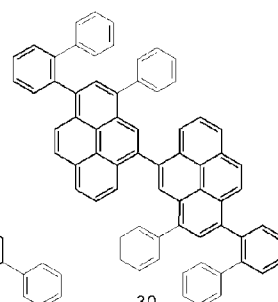
27



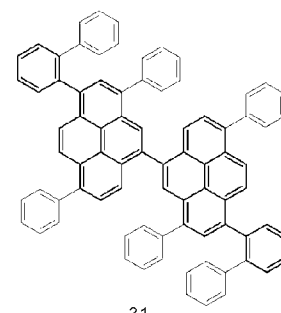
28



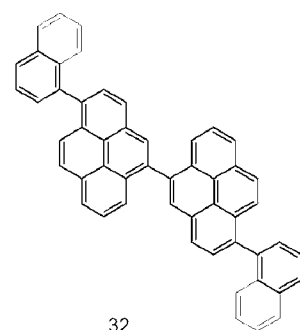
29



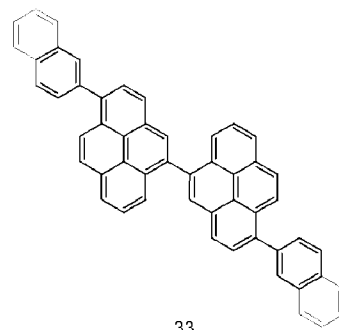
30



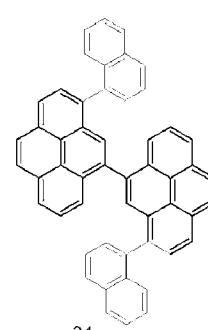
31



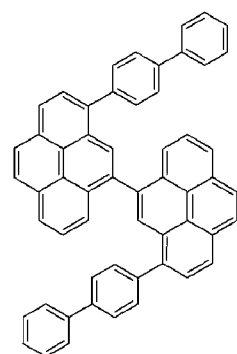
32



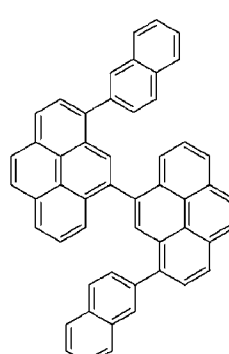
33



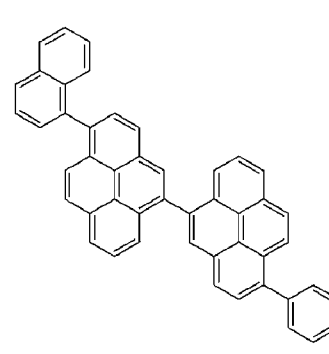
34



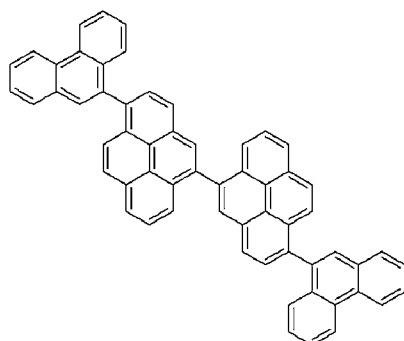
35



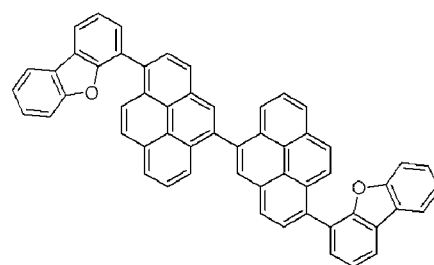
36



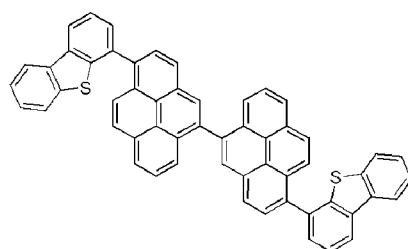
37



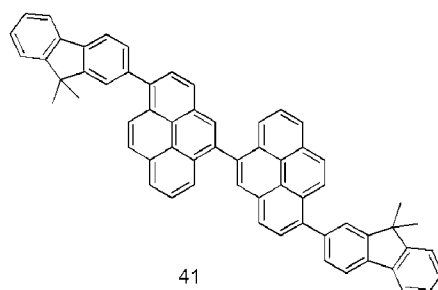
38



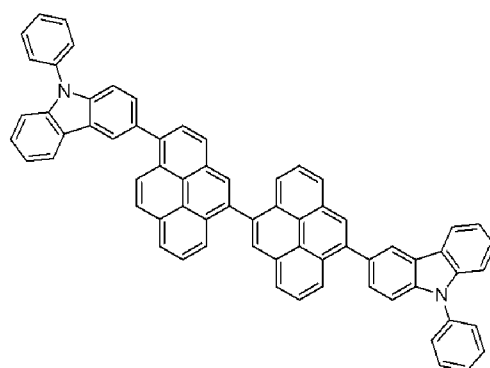
39



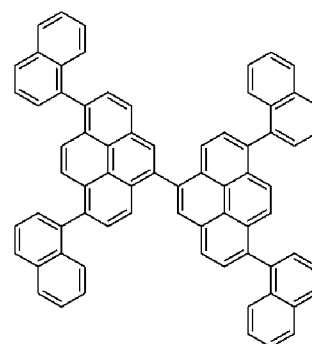
40



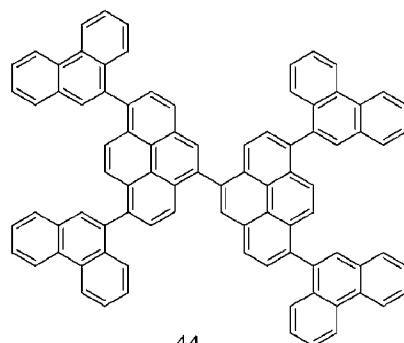
41



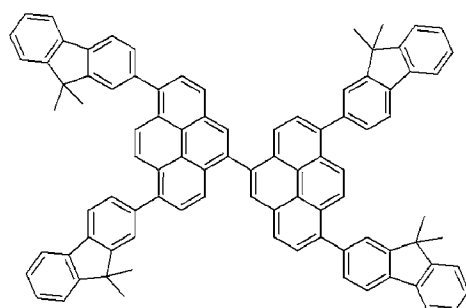
42



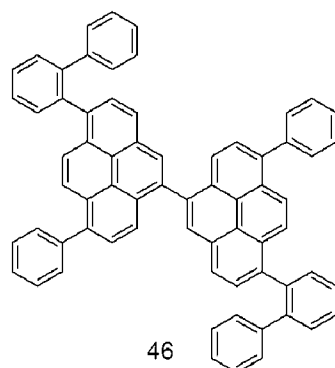
43



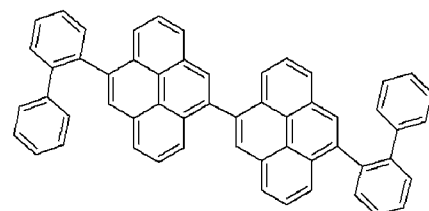
44



45

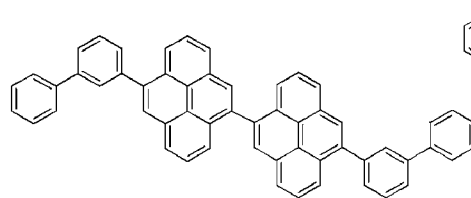


46

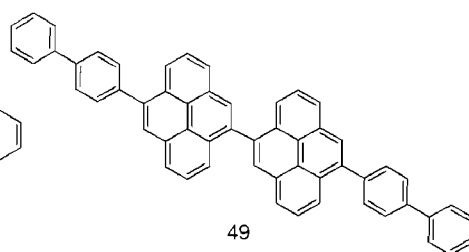


47

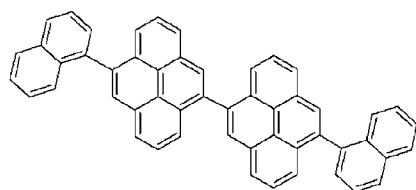
50



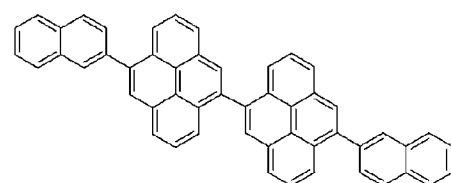
48



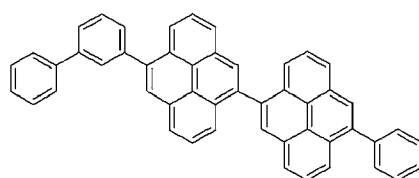
49



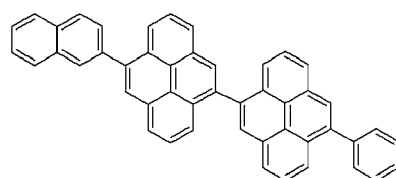
50



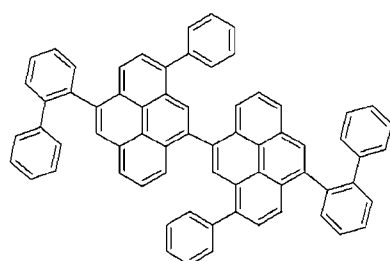
51



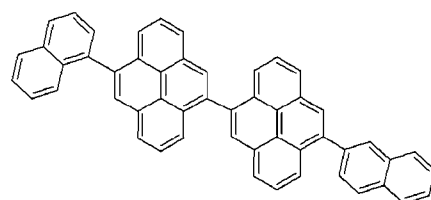
52



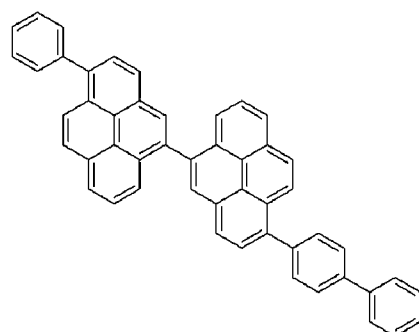
53



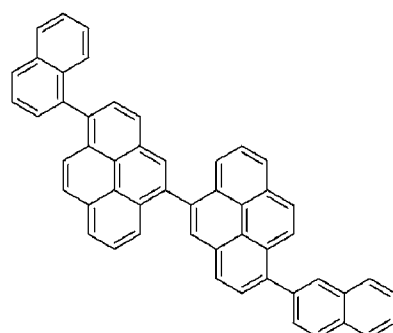
54



55

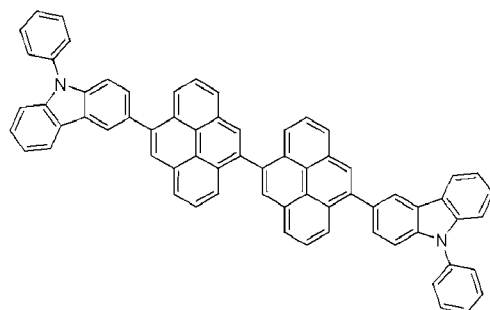


56

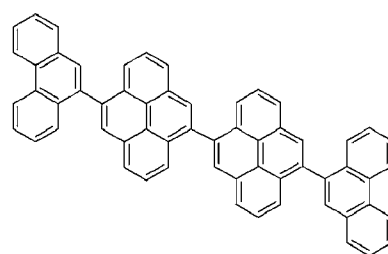


57

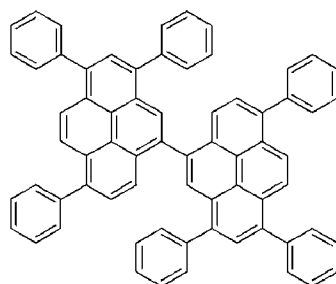
51



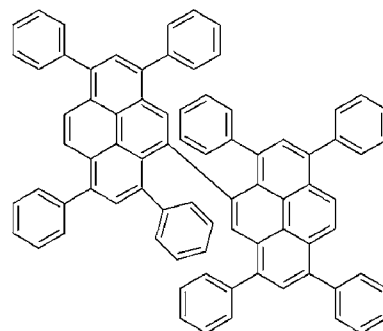
58



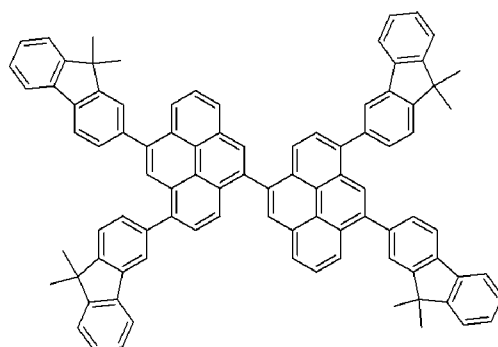
59



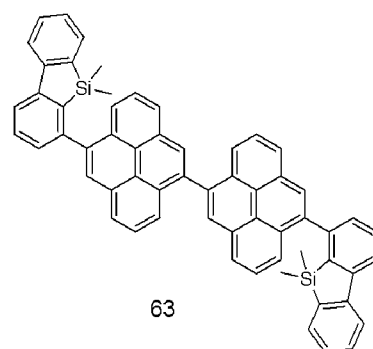
60



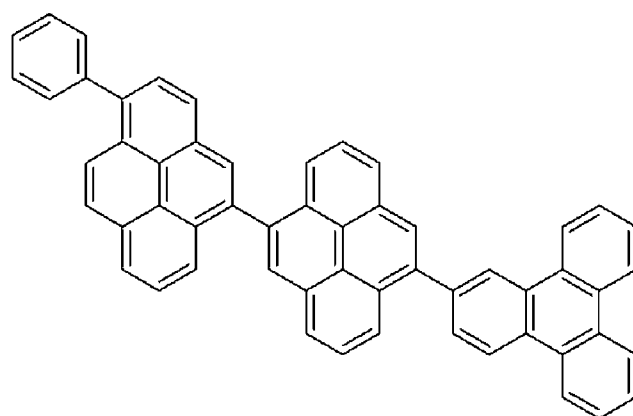
61



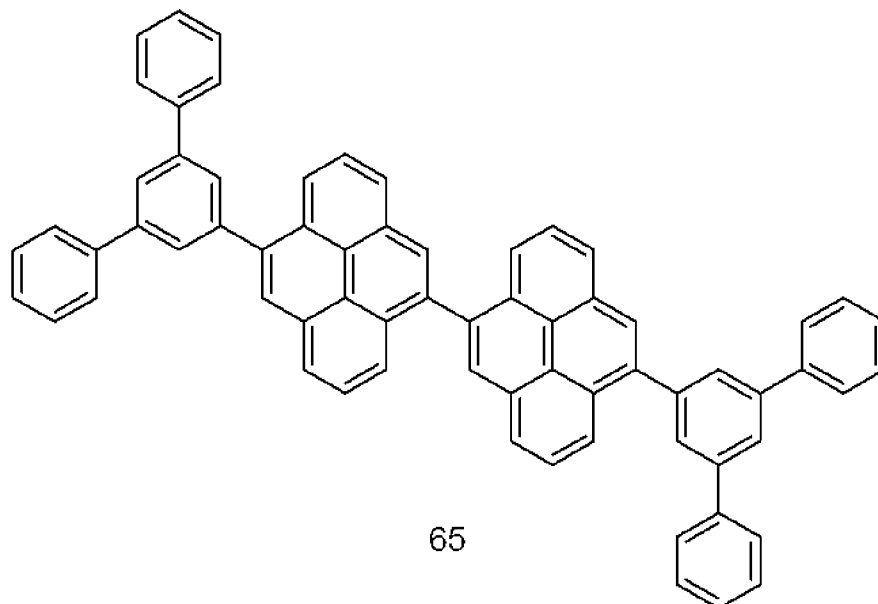
62



63

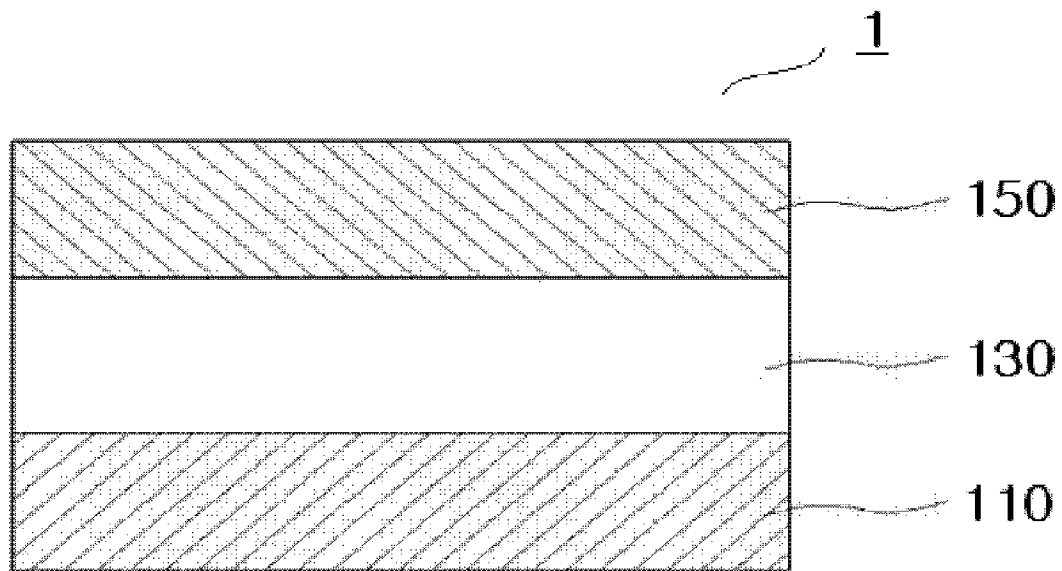


64

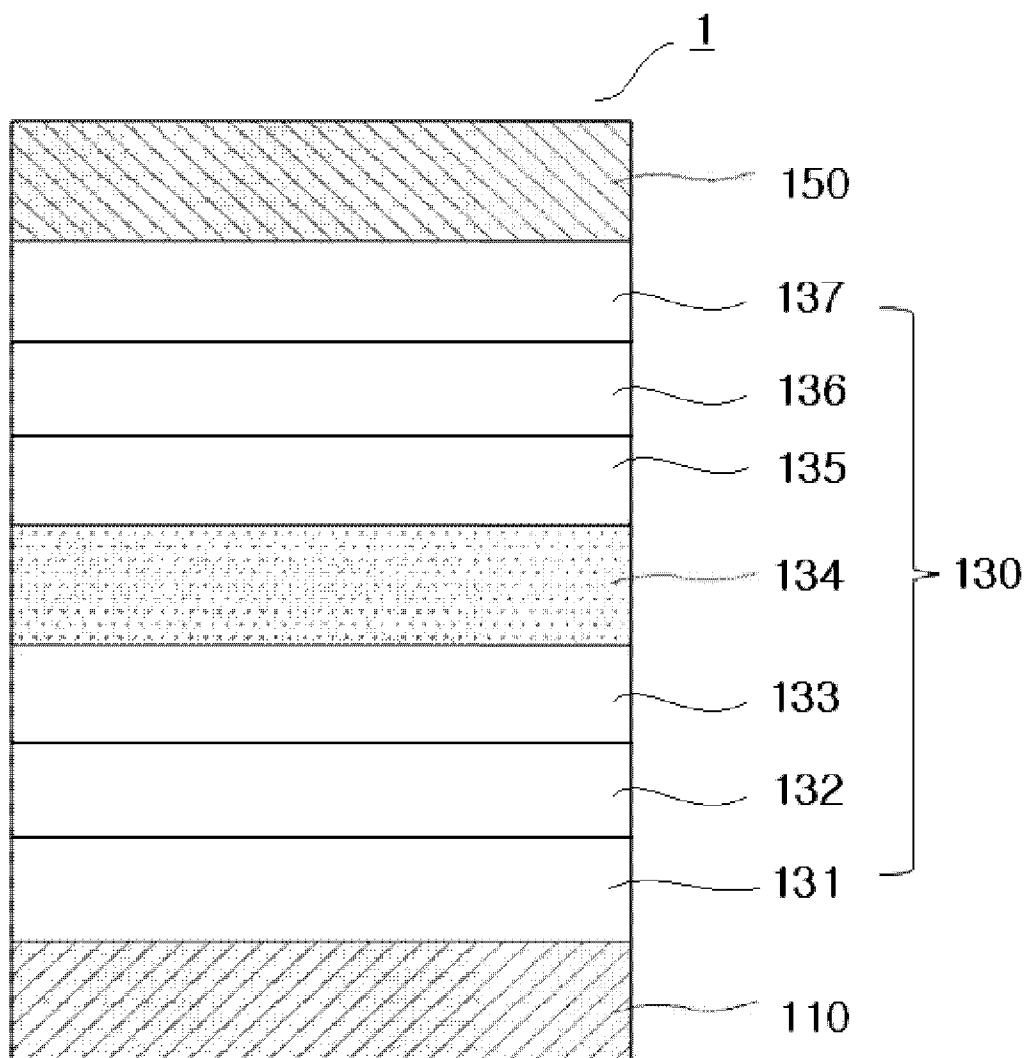


- [Claim 5] An organic electroluminescent device, including the compound which is any one selected from among claim 1 to 4.
- [Claim 6] An organic electroluminescent device, comprising a first electrode, a second electrode, and a single organic layer or a plurality of organic layers between the first electrode and the second electrode, wherein one or more organic layers selected from among the single organic layer or the plurality of organic layers include the compound which is any one selected from among claim 1 to 4.
- [Claim 7] The organic electroluminescent device of claim 6, wherein the single organic layer or the plurality of organic layers include a light emitting layer.
- [Claim 8] The organic electroluminescent device of claim 6, wherein the plurality of organic layers include a light emitting layer, and the plurality of organic layers further include one or more selected from among an electron injection layer, an electron transport layer, a hole blocking layer, an electron blocking layer, a hole transport layer and a hole injection layer.
- [Claim 9] The organic electroluminescent device of claim 7, wherein the light emitting layer includes a host and a dopant.

[Fig. 1]



[Fig. 2]



INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2014/005078**A. CLASSIFICATION OF SUBJECT MATTER****C09K 11/06(2006.01)i, C07C 15/20(2006.01)i, C07C 15/38(2006.01)i, H01L 51/50(2006.01)i**

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)

C09K 11/06; C07C 15/38; H01L 29/786; H01L 51/30; C07C 15/00; H01L 51/50; C07C 15/62; C07C 15/20

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

Korean utility models and applications for utility models

Japanese utility models and applications for utility models

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

eKOMPASS(KIPO internal) & Keywords: Organic Electroluminescent Device, OLED, pyrene.

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	JP 2009-070987 A (MITSUI CHEMICALS INC) 02 April 2009	1-4
Y	See general formula (1-c), compound 65.	5-9
Y	KR 10-2004-0034349 A (NATIONAL TSING HUA UNIVERSITY) 28 April 2004 See general formula (I) and (II).	5-9
A	WO 2011-077691 A1 (IDEMITSU KOSAN CO., LTD.) 30 June 2011 See formula (1).	1-9
A	WO 2011-030493 A1 (CANON KABUSHIKI KAISHA) 17 March 2011 See general formula (1).	1-9
A	WO 2007-004364 A1 (IDEMITSU KOSAN CO., LTD.) 11 January 2007 See general formula (1) and [0025]-[0045].	1-9

☐ 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

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

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

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

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

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

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

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

"&" document member of the same patent family

Date of the actual completion of the international search

30 September 2014 (30.09.2014)

Date of mailing of the international search report

30 September 2014 (30.09.2014)

Name and mailing address of the ISA/KR

International Application Division
Korean Intellectual Property Office
189 Cheongsu-ro, Seo-gu, Daejeon Metropolitan City, 302-701,
Republic of Korea

Facsimile No. +82-42-472-7140

Authorized officer

OH, Se Zu

Telephone No. +82-42-481-5596



INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No.

PCT/KR2014/005078

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
JP 2009-070987 A	02/04/2009	JP 5134322 B2	30/01/2013
KR 10-2004-0034349 A	28/04/2004	JP 03-848296 B2	22/11/2006
		JP 2004-139957 A	13/05/2004
		TW 593624 A	21/06/2004
		TW 593624 B	21/06/2004
		US 2004-0076852 A1	22/04/2004
		US 6861163 B2	01/03/2005
WO 2011-077691 A1	30/06/2011	CN 102473848 A	23/05/2012
		EP 2518787 A1	31/10/2012
		JP 0201-1077691 A1	30/06/2011
		KR 10-2012-0113655 A	15/10/2012
		TW 201134790 A	16/10/2011
		US 2012-0187826 A1	26/07/2012
WO 2011-030493 A1	17/03/2011	JP 2011-057651A	24/03/2011
		US 2012-0168736 A1	05/07/2012
WO 2007-004364 A1	11/01/2007	CN 101213161 A0	02/07/2008
		EP 1905754 A1	02/04/2008
		JP 2007-015961A	25/01/2007
		KR 10-2008-0027332 A	26/03/2008
		TW 200702322 A	16/01/2007
		US 2008-0124571 A1	29/05/2008
		US 7585574 B2	08/09/2009