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(54) **Organic compound and organic light emitting device using the same**

Organische Verbindung und organische lichtemittierende Vorrichtung damit

Composé organique et dispositif électroluminescent organique utilisant ce composé

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US-A- 5 968 675

• **LEPAGE YVES ET AL: "1,4,5,8,9,10-Hexaphenylanthracene", BULLETIN DE LA SOCIETE CHIMIQUE DE FRANCE, SOCIETE FRANCAISE DE CHIMIE. PARIS, FRANCE, no. 8, 1 January 1965 (1965-01-01), pages 2342-2344, XP008134080, ISSN: 0037-8968**

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Description**Technical Field**

5 **[0001]** The present invention relates to a new compound usable in an organic layer of an organic light emitting device and an organic light emitting device using the same.

[0002] The present application claims the benefit of Korean Patent Application No. 2005-0086501 (filed on September 15, 2005).

10 **Background Art**

[0003] In general, the term "organic light emitting phenomenon" refers to a phenomenon in which electric energy is converted to light energy by means of an organic material. Particularly, when an organic layer is disposed between an anode and a cathode and then a voltage is applied between both electrodes, holes from the anode and electrons from a cathode are injected into the organic layer, the holes and the electrons injected are combined together to form excitons. Further, when the excitons drop to a ground state, lights are emitted.

15 **[0004]** In addition to the above-described organic light emitting phenomenon in which light emission is made by recombining of charges injected from both electrodes, there is another mechanism in which holes and electrons are not injected from external electrodes but are generated by an amphoteric charge-generating layer under the application of alternating current voltage, as in the case of an inorganic thin film light emitting device, and the holes and electrons move to an organic thin film layer, resulting in light emission (Appl. Phys. Lett., 85(12), 2382-2384).

[0005] Since Pope, Kallman and Magnate have found electro-luminescence in anthracene single crystal in 1963, active research and development into OLEDs (Organic Light Emitting Devices) have been made up to now. Recently, organic light emitting devices have been used in various applied products such as flat panel display devices and lighting devices.

25 **[0006]** In order to manufacture more efficient organic light emitting devices, an attempt has been made to manufacture an organic layer in the device in the form of a multilayer structure instead of a monolayer structure. Most of currently used organic light emitting devices have a structure in which an organic layer and electrodes are deposited. The organic layer generally has a multilayer structure including a hole injecting layer, a hole transporting layer, a light emitting layer, an electron transporting layer and an electron injecting layer.

30 **[0007]** It is known that organic light emitting devices are characterized by high brightness, high efficiency, low drive voltage, color changeability, low cost, etc. However, in order to meet such characteristics, each layer forming an organic layer in a device (for example, a hole injecting layer, a hole transporting layer, a light emitting layer, an electron transporting layer and an electron injecting layer) must be formed of more stable and efficient materials.

35 **[0008]** JP 11 273860 A describes an organic electroluminescent element having high emission luminescence and superior stability. The electroluminescent organic compounds used in said element have a naphthalene substructure bearing at least two diaryl amino substituents, wherein the aryl groups preferably are biphenyl groups.

[0009] WO 2005/033118 AI discloses an OLED comprising compounds having a cycloalkane moiety that is directly fused to a naphthalene core.

40 **[0010]** US 5,968,675 A discloses an OLED comprising compounds in which a cycloalkane moiety is fused to a substituent of a naphthalene core.

Disclosure of Invention**Technical Problem**

45 **[0011]** The present inventors have attempted molecular design to solve problems caused by the intermolecular interaction of polycyclic aromatic hydrocarbon derivatives such as anthracene, naphthalene, pyrene, rubrene and perylene, which is capable of carrying out hole transportation, light emission and/or electron transportation in an organic light emitting device.

50 **Technical Solution**

[0012] Accordingly, it is an object of the present invention to provide a new organic compound having a structure in which at least one cycloalkane or polycycloalkane is directly linked to a polycyclic aromatic hydrocarbon as a core or is linked to a substituent thereof.

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Advantageous Effects

[0013] According to the invention, a derivative having a structure in which at least one cycloalkane or polycycloalkane is directly fused to a polycyclic aromatic hydrocarbon as a core or is fused to a substituent of the polycyclic aromatic hydrocarbon, can maximally decrease interaction between compounds by bulky cycloalkane or polycycloalkane moieties (steric protection), and can further exhibit induction effect and hyperconjugative effect.

[0014] Therefore, it is possible to efficiently exhibit a light-emitting color having a low reduction in light emitting efficiency and having high color purity due to a reduction in the interaction between compounds and it is also possible to enhance the life span, the efficiency and the thermal stability of a device and to drive it at low voltage when the compound according to the invention is used in an organic light emitting device.

Brief Description of the Drawings

[0015]

Figs. 1 to 5 are cross-sectional views illustrating a structure of a general organic light emitting device usable in the present invention.

[Reference numerals]

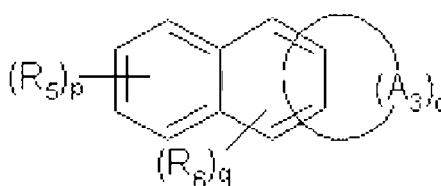
[0016]

- 1: substrate 2: anode
- 3: hole injecting layer 4: hole transporting layer
- 5: organic light emitting layer 6: electron transporting layer
- 7: cathode

Best Mode for Carrying Out the Invention

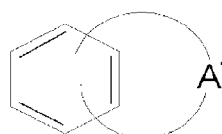
[0017] The present invention provides an organic light emitting device comprising a first electrode, at least one organic layer, and a second electrode, laminated successively, in which at least one layer of the organic layer has a polycyclic aromatic hydrocarbon as a core and comprises at least one of a derivative in which an unsubstituted or C₁₋₆-alkyl-substituted C₂₋₃₀ cycloalkane, or an unsubstituted or C₁₋₆-alkyl-substituted C₅₋₅₀ polycycloalkane is fused to a substituent of the polycyclic aromatic hydrocarbon as the core.

[0018] Still furthermore, the present invention provides a compound of the following formula (2) which are capable of carrying out at least one function of a light emitting material, a hole transporting material and an electron transporting material:



(2)

wherein



means an unsubstituted or C₁₋₆-alkyl-substituted C₂₋₃₀ cycloalkane, or an unsubstituted or C₁₋₆-alkyl-substituted C₅₋₅₀

polycycloalkane directly fused to a benzene ring of a polycyclic aromatic hydrocarbon (wherein A' means A₃); and the substituents R₅ to R₆ are the same or different from each other and are each selected from the group consisting of a hydrogen, a halogen, a nitrile group (-CN), a nitro group (-NO₂), a sulfonyl group (-SO₂R'), a sulfoxide group (-SOR'), a sulfonamide group (-SO₂NR'₂), a sulfonate group (-SO₃R'), a trifluoromethyl group (-CF₃), an ester group (-COOR'), an amide group (-CONHR' or -CONR'R"), a substituted or unsubstituted and linear or branched C₁₋₁₂ alkoxy group, a substituted or unsubstituted and aromatic or nonaromatic heterocyclic group, and a substituted or unsubstituted aryl group, two R's may form a fused ring, or two R's may linearly linked to each other to form a polycyclic aromatic hydrocarbon derivative as a polymer, provided that R₁ and R₂ are not simultaneously a hydrogen atom.

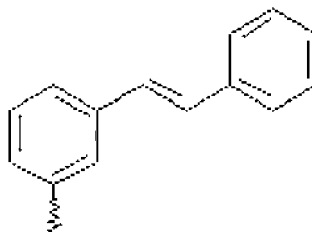
[0019] In this case, R' and R" are each selected from the group consisting of a substituted or unsubstituted C₁₋₆₀ alkyl group, a substituted or unsubstituted aryl group and a substituted or unsubstituted 5-7 membered heterocyclic group.

[0020] In R' and R", the C₁₋₆₀ alkyl group, the aryl group and the heterocyclic group each may be substituted with one or more optional group selected from one or more amine group, an amide group, an ether group and an ester group.

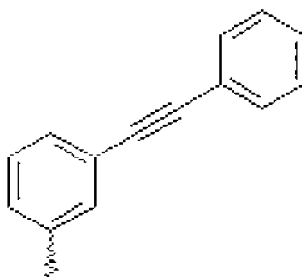
[0021] In the formula, the aryl group may be selected from the group consisting of a phenyl group, a biphenyl group, a terphenyl group, a benzyl group, a naphthyl group, an anthracenyl group, a tetracenyl group, a pentacenyl group, a perylenyl group and a coronenyl group and these may be monosubstituted, polysubstituted or unsubstituted.

[0022] In this case, when the substituent is a substituted aryl group, particularly a substituted phenyl group, it may contain a double bond or triple bond.

[0023] Examples of the substituted aryl group include a stilbenyl group of



and an acetylenyl group of



, and the substituted aryl group is preferably substituted at the 9-position of an anthracene core.

[0024] Examples of the aromatic heterocyclic group in the formula include groups derived from thiophene, furan, pyrrole, imidazole, thiazole, oxazole, oxadiazole, thiadiazole, triazole, pyridine, pyridazine, pyrazine, quinoline and isoquinoline.

[0025] Examples of the C₁₋₂₀ aliphatic hydrocarbon group in the formula include an alkyl group such as a methyl group, an ethyl group, n-propyl group, an isopropyl group, n-butyl group, a sec-butyl group, an isobutyl group, a tert-butyl group, a pentyl group, a hexyl group; an alkenyl group having a double bond, such as a styryl group; and an alkynyl group having a triple bond, such as an acetylene group.

[0026] In the formula (2), o is an integer of 1 or 2; and p and q are an integer of 1 to 4.

[0027] In the case that o, p, q, are an integer of 2 or more, there are substituted at several positions of the aromatic ring with not only same substituents but also different substituents.

[0028] Unrestricted examples of substituents for the substituted cycloalkane or substituted bicycloalkane include a C₁₋₆ alkyl group.

Mode for the Invention

[0029] Hereinafter, the present invention will be described in more detail.

[0030] Polycyclic aromatic hydrocarbons such as anthracene, naphthalene, pyrene, rubrene and perylene can a func-

tion as a chromophore. In particular, an organic compound having anthracene as a core is widely used for a hole transporting material, a light emitting material (including a dopant), an electron transporting material, etc. in an organic electronic device such as an organic light emitting device.

[0031] As illustrated in the formula (2), the present invention is characterized by providing a derivative that has as a core the polycyclic aromatic hydrocarbon such as anthracene, naphthalene, pyrene, rubrene and perylene, in which sterically bulky cycloalkane or polycycloalkane is directly fused to the core or is fused to a substituent of the core.

[0032] According to the invention, the derivative that has the polycyclic aromatic hydrocarbon as a core, in which a substituted or unsubstituted C_{2-30} cycloalkane, or a substituted or unsubstituted C_{5-50} polycycloalkane is directly fused to the core or is fused to a substituent of the core, can be used as a light emitting material and as a light emitting host or a light emitting dopant in an organic light emitting device. In particular, the polycyclic aromatic hydrocarbon derivative according to the invention can emit blue, green and red light by controlling the substituents introduced or the conjugation length.

[0033] Examples of the polycyclic aromatic hydrocarbon derivative according to the invention include compounds of the formula (2).

[0034] The polycyclic aromatic hydrocarbon derivative according to the invention performs light absorption or light emission, thereby determining its main wavelength band.

[0035] On the other hand, an unsubstituted or C_{1-6} -alkyl-substituted C_{2-30} cycloalkane, or an unsubstituted or C_{1-6} -alkyl-substituted C_{5-50} bicycloalkane directly fused to the polycyclic aromatic hydrocarbon core can move the wavelength of the chromophore to a longer wavelength.

[0036] Since anthracene itself has amphoteric properties, holes or electrons can be selectively transported depending on the introduction of the substituents.

[0037] The cycloalkane or polycycloalkane fused to the polycyclic aromatic hydrocarbon can give a nonplanar structure (e.g., chair type) similar to an independent cycloalkane or polycycloalkane to the polycyclic aromatic hydrocarbon, unlike a flat aromatic ring. Therefore, by further exhibiting amorphous characteristics, a device can be prevented from breakdown that occurs due to crystallization caused by Joule heat generated upon operation of an organic electronic device such as an organic light emitting device.

[0038] Further, since the cycloalkane or polycycloalkane fused to the polycyclic aromatic hydrocarbon is relatively sterically bulky, a melting point and a glass transition temperature of the compound can be increased; the compound has a strong molecular structure and thus has high quantum efficiency; and quenching effects and adverse effects generated by the intermolecular interaction, such as deterioration in color purity caused by the broad light emission band, can be reduced to enhance characteristics of the molecule itself, by subjecting to a steric hindrance due to a bulky molecular structure. Further, the polycyclic aromatic hydrocarbon can improve a function as a dopant capable of inhibiting the intermolecular interaction between the hosts by the introduction of sterically bulky cycloalkane or polycycloalkane into a molecule.

[0039] In particular, in a structure in which the aromatic core is surrounded by cycloalkane or polycycloalkane framework, the electronic density of the aromatic core is varied due to an inductive effect and hyperconjugative effect of the cycloalkane or polycycloalkane framework, thereby greatly stabilizing cation radicals. Specifically, the polycyclic aromatic hydrocarbon has p-type behavior stronger than that of the core itself because of the cycloalkane or polycycloalkane framework. Further, from electrochemical oxidation measurements, it can be confirmed that the more the number of cycloalkane or polycycloalkane framework, the easier the oxidation and the more stable the cation radical (see J. Am. Chem. Soc. 1998, 120, 6012-6018 and Tetrahedron Letters (1997), 38 (19), 3427-3430).

[0040] Therefore, the polycyclic aromatic hydrocarbon to which the cycloalkane or polycycloalkane is directly fused can be used as a hole transporting material. Unlike an anthracene derivative disclosed in US Patent No. 6465115, a structure surrounded by cycloalkane or polycycloalkane is more electrochemically stable (cationic radical) and the energy level (HOMO) thereof can be optimized. Therefore, the polycyclic aromatic hydrocarbon is improved in stability as the hole transporting material to thus attain a stable morphology and to facilitate hole injection.

[0041] The number of the cycloalkane or polycycloalkane fused to the polycyclic aromatic hydrocarbon is preferably 1 to 4.

[0042] The cycloalkane fused according to the invention has 2 to 30, preferably 3 to 8 carbon atoms.

[0043] The polycycloalkane fused according to the invention has 5 to 50, preferably 5 to 25 carbon atoms.

[0044] The polycyclic aromatic hydrocarbon as the core in the invention may be a derivative that is substituted with at least one substituent (R) such as R_5 to R_6 , described in the formula (2).

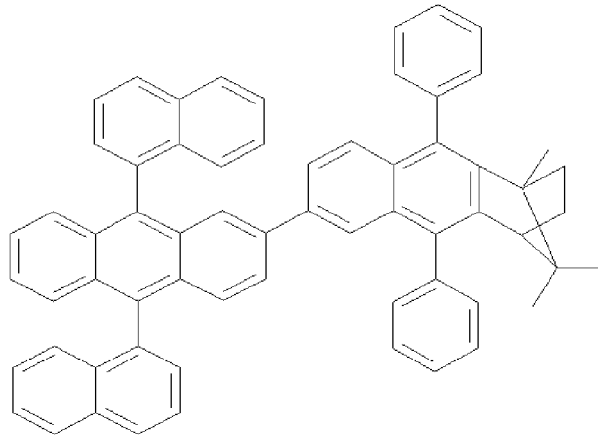
[0045] On the other hand, when an unsubstituted or C_{1-6} -alkyl-substituted C_{2-30} cycloalkane, or an unsubstituted or C_{1-6} -alkyl-substituted C_{5-50} polycycloalkane is fused to the substituent of the core of the polycyclic aromatic hydrocarbon, a benzene ring is preferably contained in the substituent moieties fused.

[0046] Specific examples of the compound represented by the formula (2) include, but are not limited to, the compounds represented by the following formulae (2-1) to (2-6):

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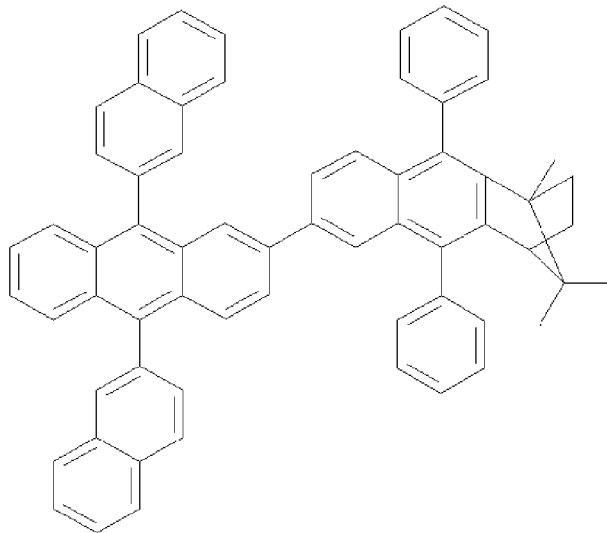
(2-1);

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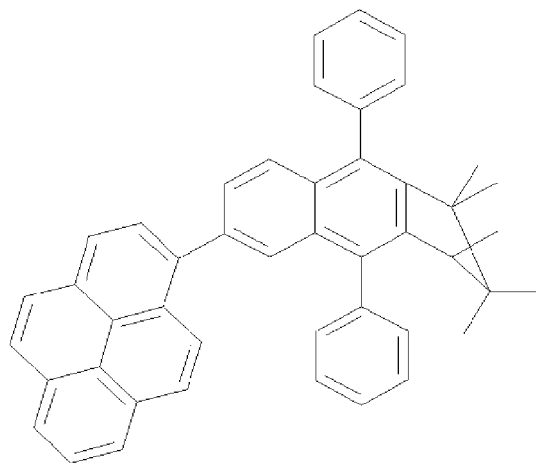
(2-2);

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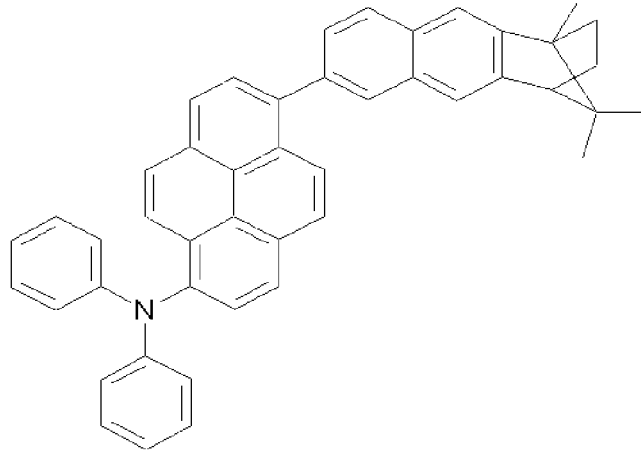


(2-3);

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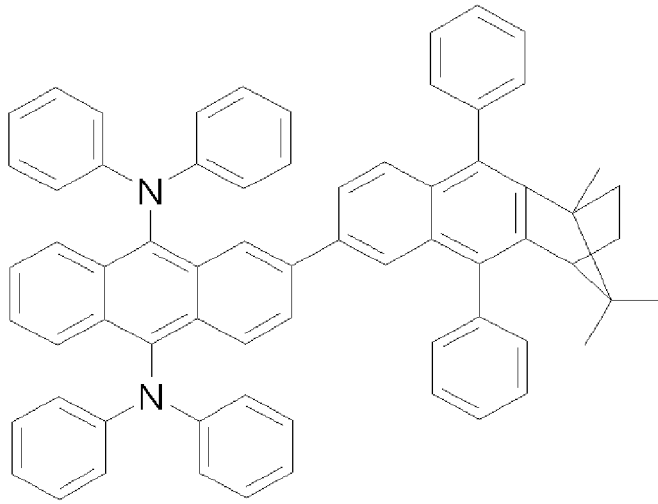
(2-4);

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(2-5);

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and

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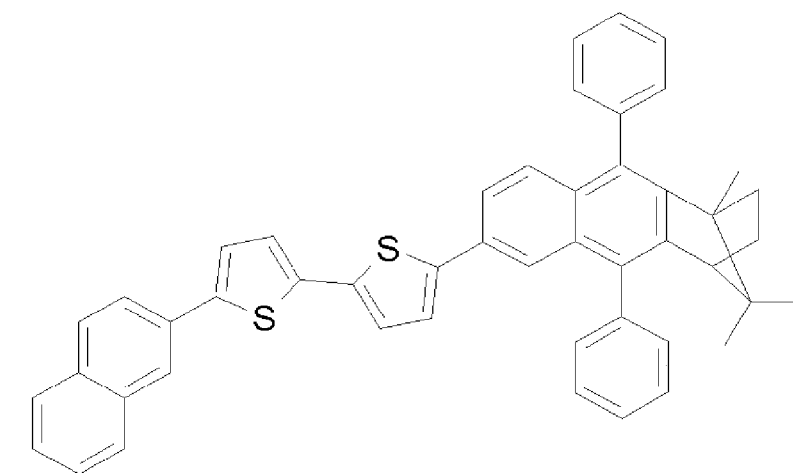
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(2-6)

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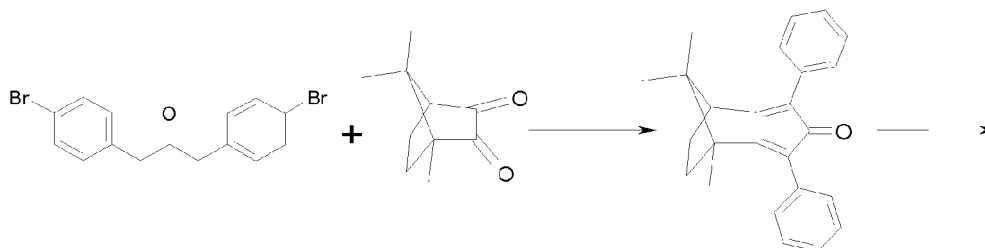
[0047] In an example of the general production method of the compound of the formula (2), the maximum number of the reaction site through a general fused cyclization can be 3 and various derivatives can be prepared by a general chemical reaction. Specifically, various fused ring compounds can be synthesized by the introduction of various dichito (e.g., camphorquinone) derivatives as starting materials.

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[0048] The production method can be represented by the following reaction scheme B:

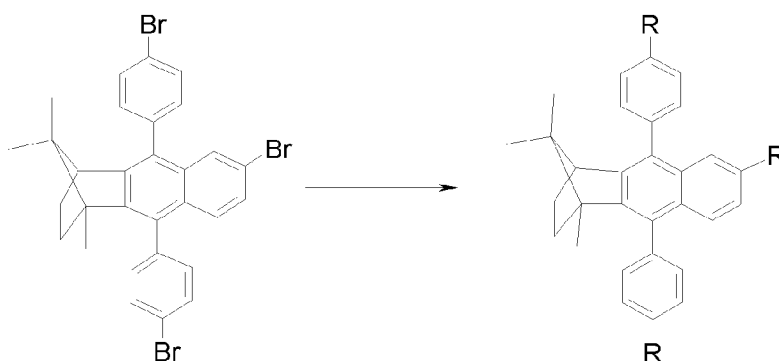
[Reaction scheme B]

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[0049] The production method of the compounds of the formulae (2) will be explained in more detail in Preparative Examples to be described below.

[0050] On the other hand, the derivative that has the polycyclic aromatic hydrocarbon as a core, in which an unsubstituted or C₁₋₆-alkyl-substituted C₂₋₃₀ cycloalkane, or a substituted or an unsubstituted or C₁₋₆-alkyl-substituted C₅₋₅₀ polycycloalkane is directly fused to the core or is fused to a substituent of the core, can carry out a function as a charge carrier extracting, injecting or transporting material. In this case, the charge carrier may be holes or electrons.

[0051] The organic electronic device requiring hole transportation between electrodes and an organic layer usually comprises two or more electrodes and one or more organic layer interposed therebetween. The organic electronic device can be largely classified into two types according to its operational principle as follows.

[0052] One type is an organic electronic device having a configuration in which an exciton is formed in an organic layer by energy flow from external energy into the device and the exciton is separated into an electron and a hole, the electron and the hole formed are used as a current source (voltage source). Examples of this type of the organic electronic device include an organic solar cell and a sensor such as an organic photoconductor (OPC).

[0053] The other type is an electronic device operated by a hole and/or electron directly injected into a semiconductive organic layer forming an interface with an electrode by applying a voltage to two or more electrodes. Examples of this type of the electronic device include an organic light emitting device carrying out light emission by simultaneously injecting an electron and a hole from two electrodes and an organic transistor having a switch function in which holes formed in an organic layer are transported from a source electrode (hereinafter referred to as a "source") to a drain electrode (hereinafter referred to as a "drain") by a voltage applied to a diode or gate.

[0054] In order to improve the device performance of the organic electronic device requiring hole transportation between the electrodes and the organic layer, it is important to enhance hole injection and extraction efficiency between the electrodes and the organic layer, and/or to efficiently transport holes formed in the organic layer to an electrode or other organic layers. To this end, the improvement in the device performance of most electronic devices has been attempted by forming at least one of an organic layer primarily required, which a main reaction takes place (for example, in the case of an organic solar cell, an organic layer forming an electron and a hole by photons from an external light source and in the case of an organic transistor, an organic layer forming a hole by a voltage applied to a gate), and an additional organic layer such as a charge injecting organic layer (hereinafter referred to as a "charge injecting layer"), a charge extracting organic layer (hereinafter referred to as a "charge extracting layer") and a charge transporting organic layer (hereinafter referred to as a "charge transporting layer").

[0055] Therefore, the charge carrier extracting, injecting or transporting material according to the invention can be used in an organic layer of an organic electronic device such as an organic light emitting diode, an organic solar cell, an organic transistor and an organic photoconductor (OPC).

[0056] In this case, according to the invention, the derivative that has the polycyclic aromatic hydrocarbon as a core, in which an unsubstituted or C₁₋₆-alkyl-substituted C₂₋₃₀ cycloalkane, or an unsubstituted or C₁₋₆-alkyl-substituted C₅₋₅₀ polycycloalkane is directly fused to the core or is fused to a substituent of the core, may be also mixed with 0.1 to 99.0% by weight of an inorganic metal, inorganic salt, or a different organic material.

[0057] Hereinafter, the organic light emitting device according to the invention will be described.

[0058] The organic light emitting device has a structure comprising a substrate, an anode, a cathode and at least one organic layer interposed between the anode and the cathode. The organic layers interposed between the anode and the cathode, can be further subdivided according to functions, if necessary, to thus increase the number of the organic layer, and to the contrary, one layer can have various functions to thus decrease the number of the organic layer.

[0059] Preferably, the organic light emitting device according to the invention may have a structure comprising a substrate, an anode, a hole injecting layer, a hole transporting layer, a light emitting layer, an electron transporting layer and a cathode, sequentially stacked from bottom to top in this order. Further, if desired, a hole blocking layer may be interposed between the electron transporting layer and the light emitting layer in order to prevent holes from moving into the electron transporting layer.

[0060] Examples of a structure of the organic light emitting device are shown in Figs. 1 to 5, but are not limited thereto. In Fig. 1, the organic layers are divided into four portions. Fig. 2 shows an example of the light emitting layer simultaneously performing functions as the electron transporting layer and the light emitting layer. Fig. 3 shows an example of a hole transporting layer simultaneously performing functions of hole injection and hole transportation. Fig. 4 shows an example of a light emitting layer simultaneously performing three functions as a hole injecting layer, a hole transporting layer and a light emitting layer. Fig. 5 shows an example of a light emitting layer simultaneously performing functions as a hole injecting layer, a hole transporting layer, an electron transporting layer and a light emitting layer.

[0061] In the organic light emitting device according to the invention, each layer may be in the form of a thin film and the thin film may be formed by a conventional production method according to the materials used. For example, the thin film may be formed by CVD (chemical vapor deposition), EB (electron beam vapor deposition), thermal vapor deposition, sputtering, or thermal evaporation in high vacuum, or alternatively by spin-coating, roll-coating, screen-printing, dip-coating, doctor-blading, inkjet printing or thermal transfer after dissolving the derivative in a solution.

[0062] According to the invention, the derivative that has the polycyclic aromatic hydrocarbon as a core, in which an unsubstituted or C₁₋₆-alkyl-substituted C₂₋₃₀ cycloalkane, or an unsubstituted or C₁₋₆-alkyl-substituted C₅₋₅₀ polycycloalkane is directly fused to the core or is fused to a substituent of the core, may be used as a light emitting material in the organic light emitting device having the above-mentioned structure, or as a light emitting host or dopant for excited energy movement, for assisting light emission of other dopants. The polycyclic aromatic hydrocarbon derivative according to the invention may be used in combination of two or more types, and in combination with other light emitting dyes within the range of not damaging the performance of the invention.

[0063] When the polycyclic aromatic hydrocarbon derivative according to the invention is used as a dopant having an energy band gap smaller than a host forming a light emitting layer, the excitons generated on a host are transported to

a dopant, thereby emitting light having high efficiency.

[0064] When the polycyclic aromatic hydrocarbon derivative according to the invention is used as a dopant, the derivative may be doped in the whole or part of the layer containing it, and may be doped uniformly or doped to have a concentration distribution in the direction of the film thickness thereof. The doping amount of the compound is preferably 10^{-3} to 15% by weight, more preferably 0.1 to 10% by weight relative to the host material.

[0065] Further, the polycyclic aromatic hydrocarbon derivative according to the invention may have, in addition to the above-mentioned light emitting properties, other properties necessary for an organic layer of an organic light emitting device, such as hole injecting, hole transporting, electron transporting and electron injecting properties.

[0066] The polycyclic aromatic hydrocarbon derivative according to the invention is preferably contained in a light emitting layer of an organic light emitting device. When a hole transporting layer and/or electron transporting layer have (has) a function as a light emitting layer without separately forming the light emitting layer, the derivative may be contained in the hole transporting layer and/or electron transporting layer.

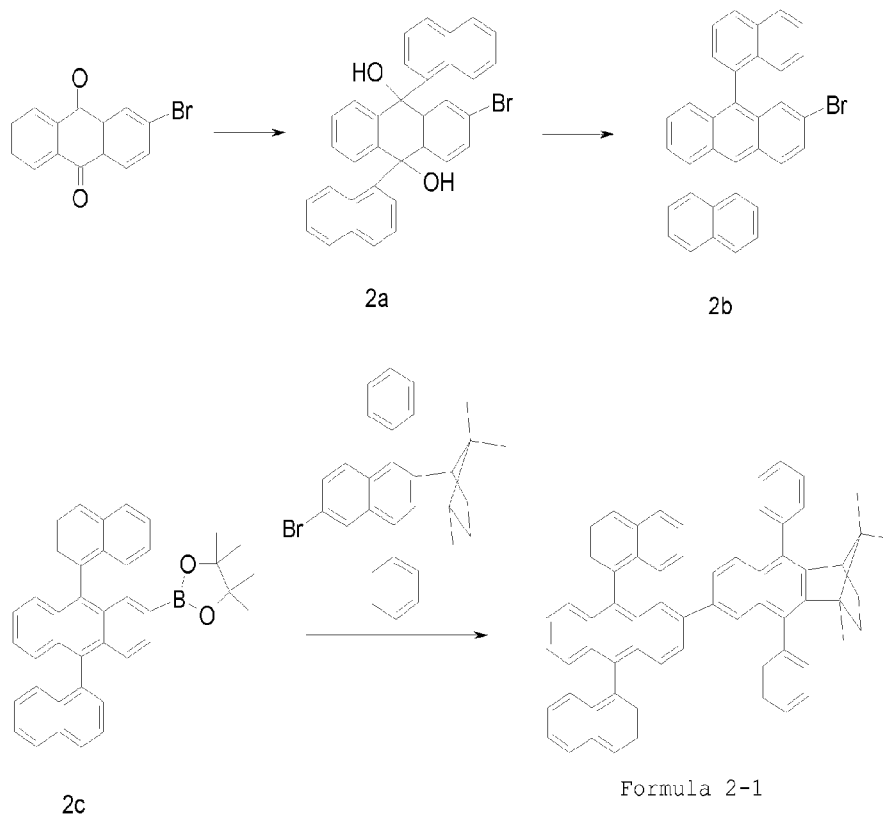
[0067] The organic light emitting device comprising the polycyclic aromatic hydrocarbon derivative according to the invention can be enhanced in terms of the life span and the thermal stability. The reason is in that, by introducing a sterically bulky cycloalkyl group thereto, (1) a melting point and a glass transition temperature of the polycyclic aromatic hydrocarbon derivative can be increased to enhance thermal stability; and (2) by further exhibiting amorphous characteristics, a device can be prevented from breakdown that occurs due to crystallization caused by Joule heat generated upon operation of an organic light emitting device.

[0068] The following Preparative Examples and Examples are presented for the purpose of giving better understanding of the present invention. However, the following Preparative Examples and Examples are presented simply for the purpose of giving better understanding of the present invention, and thus the present invention is not limited thereto.

Preparative Example 1 Synthesis of compound of Formula 2-1

[0069]

[Reaction scheme 2]



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(1) Synthesis of Compound 2a

(2-Bromo-9,10-di-naphthalen-1-yl-9,10-dihydro-anthracene-9,10-diol)

5 **[0070]** 5-Bromo-1,2,3,4-tetrahydro-naphthalene (13.7 mL, 88.0 mmol) was dissolved in anhydrous THF (tetrahydrofuran) (100 mL), the solution was maintained at -78°C with stirring, and n-BuLi (42.6 mL, 106 mmol) was slowly added dropwise to the solution. After 30 minutes, 2-bromo-9,10-anthraquinone (10.2 g, 35.5 mmol) was added thereto, and the mixture was stirred. After 2 hours, the reaction mixture was washed with a NH₄Cl solution, and further twice with distilled water, and then water was removed in anhydrous MgSO₄. The solvent was removed with a rotary evaporator.
10 The residue was recrystallized from diethyl ether and petroleum ether to obtain Compound 2a (8.7 g, 45%). Analysis results of this compound are as follows.

[0071] ¹H NMR (500 MHz, CDCl₃) 7.78 (dd, 4H), 7.38 (dd, 4H), 6.82 (dd, 2H), 6.73 (dd, 2H), 6.46 (dd, 2H), 2.60 (t, 4H), 2.37 (t, 4H), 1.64 (m, 8H); MS [M+1-H₂O] 526

15 (2) Synthesis of Compound 2b (2-Bromo-9,10-di-naphthalen-1-yl-anthracene)

[0072] 2-Bromo-9,10-di-naphthalen-1-yl-9,10-dihydro-anthracene-9,10-diol (8.74 g, 16.1 mmol) was dissolved in glacial acetic acid (100 mL), the solution was stirred, KI (2.67 g, 16.1 mmol) and NaPO₂H₂ (17.1 g, 161 mmol) were added thereto, and the mixture was refluxed. As the reaction proceeded, the reactants started to be molten therein, and after
20 2 hours, white precipitates were generated to complete the reaction. Glacial acetic acid was filtered off, the precipitate was dispersed in ethanol, and H₂O was added thereto to generate the precipitates, which were further filtered to obtain a white solid compound 2b (7.5 g, 92%). Analysis results of this compound are as follows.

MS [M+1] 510

25 (3) Synthesis of Compound 2c

(2-(9,10-Di-naphthalen-1-yl-anthracen-2-yl)-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane)

[0073] Compound 2a (3 g, 5.9 mmol) was dissolved in anhydrous THF (tetrahydrofuran) (30 mL), the solution was maintained at -78°C with stirring, and n-BuLi (3.1 mL, 7.7 mmol) was slowly added dropwise to the solution. After 30
30 minutes, 2-isopropoxy-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane (1.6 mL, 7.7 mmol) was added thereto, and the mixture was stirred. After 1 hour, an aqueous NH₄Cl solution was added thereto, and the mixture was extracted from ethyl acetate, and further washed twice with distilled water, and then water was removed in anhydrous MgSO₄. The solvent was removed with a rotary evaporator. The residue was recrystallized from diethyl ether and petroleum ether to obtain
35 Compound 2c (1.7 g, 52%).

(4) Synthesis of compound of Formula 2-1:

[0074] Compound 2c (1.7 g, 3.06 mmol) was dissolved in THF (20 mL), and Compound 3b (1.57 g, 3.36 mmol) was added to the solution. Pd(PPh₃)₄ (176 mg, 0.15 mmol), and an aqueous 2 MK₂CO₃ solution (6.12 mL, 12.2 mmol) were sequentially added thereto, and the mixture was refluxed with stirring. After 2 hours, THF (tetrahydrofuran) was added to the solution, and the mixture was extracted from ether, and further washed twice with distilled water. Water was removed from the solution in anhydrous MgSO₄. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography to obtain a white solid. The solid was recrystallized from diethyl ether and petroleum
45 ether and filtered under reduced pressure to obtain a white compound of Formula 2-1 (1.0 g, 39%).

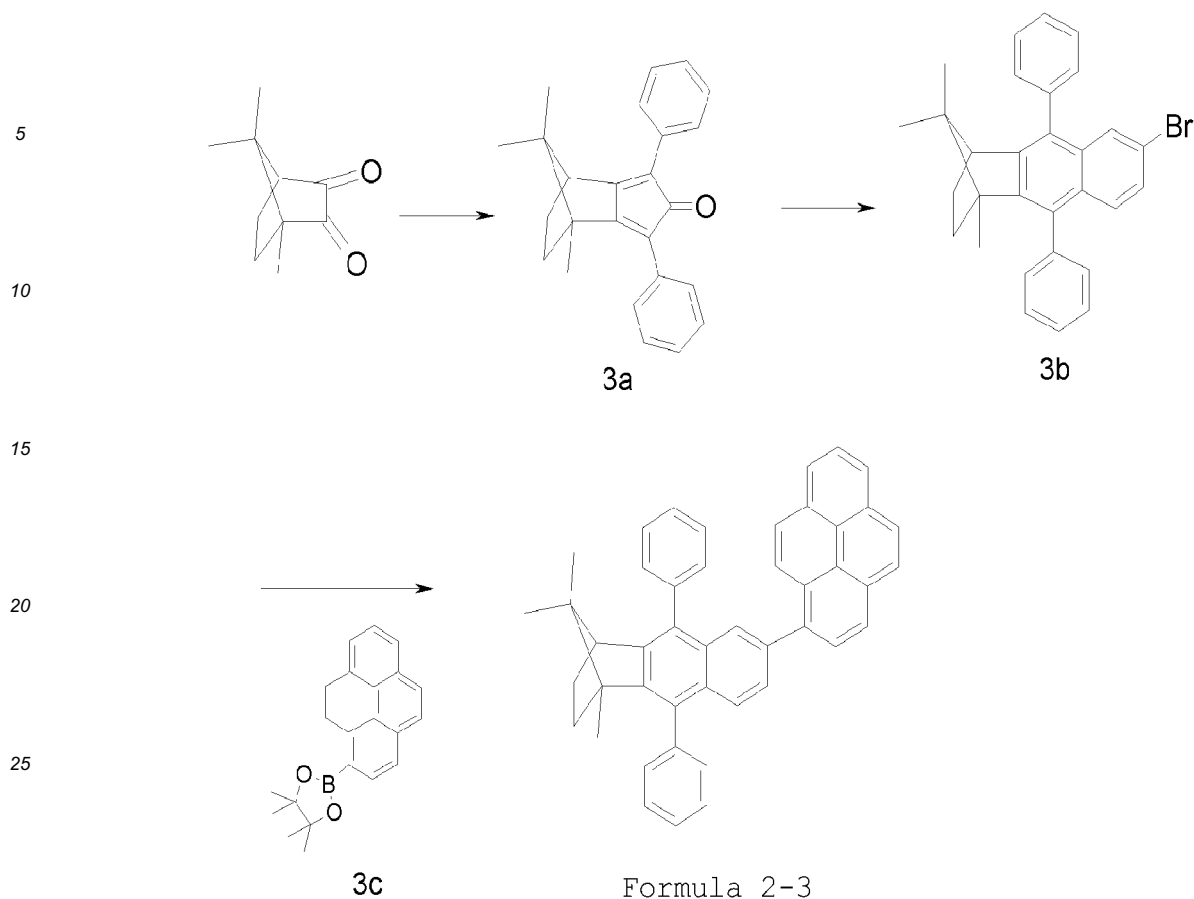
MS [M+1] 817

Preparative Example 2 : Synthesis of compound of Formula 2-3

50 **[0075]**

[Reaction scheme 3]

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(1) Synthesis of Compound 3a

(4,8,8-Trimethyl-1,3-diphenyl-4,5,6,7-tetrahydro-4,7-methano-inden-2-one)

35 **[0076]** DL-camphorquinone (10 g, 60 mmol) and diphenyl acetone (12.7 g, 60 mmol) were added to triethylene glycol (50 mL), the mixture was slightly heated to be molten, benzyl trimethylammonium hydroxide in methanol (40%) (6.5 mL, 14.3 mmol) was added thereto, and the mixture was heated to 120°C and stirred. After the reaction proceeded, the mixture turned red, and after 24 hours and thus completion of the reaction, H₂O was added thereto, and the mixture was extracted from ethyl acetate. Water was removed from the solution in anhydrous MgSO₄. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography to obtain a red oily compound 3a (10 g, 49%). MS [M+1] 341

(2) Synthesis of Compound 3b

45 **[0077]** Compound 3a (10 g, 29 mmol) and 5-bromoanthranilic acid (6.89 g, 31.9 mmol) were dissolved in 1,2-dichloroethane (100 mL), isoamyl nitrate (6.1 mL, 43.5 mmol) was added to the solution, and the mixture was refluxed at 90°C. After 1 hour, and thus completion of the reaction, H₂O was added thereto, and the mixture was extracted from ethyl acetate. Water was removed from the solution in anhydrous MgSO₄. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography to obtain a transparent oily compound 3b (6.7 g, 49%). MS [M+1] 468

(3) Synthesis of Compound 3c (4,4,5,5-Tetramethyl-2-pyren-1-yl-[1,3,2] dioxaborolane)

55 **[0078]** 2-Bromo-pyrene (5 g, 17.8 mmol) was dissolved in anhydrous THF (100 mL), the solution was maintained at -78°C with stirring, and n-BuLi (9.7 mL, 23.2 mmol) was slowly added dropwise to the solution. After 30 minutes, 2-isopropoxy-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane (4.8 mL, 23.1 mmol) was added thereto and the mixture was stirred. After 1 hour, an aqueous NH₄Cl solution was added thereto, and the mixture was extracted from ethyl acetate, and further washed twice with distilled water, and then water was removed from the solution in anhydrous MgSO₄. The

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solvent was removed with a rotary evaporator to obtain a transparent oily mixed compound 3c (6.0 g, 99%).
MS [M+1] 329

(4) Synthesis of compound of Formula 2-3

[0079] Compound 3c (2.4 g, 7.3 mmol) was dissolved in THF (30 mL), and Compound 3b (3.4 g, 7.3 mmol) was added to the solution. Pd(PPh₃)₄ (421 mg, 0.365 mmol) and an aqueous 2 M K₂CO₃ solution (14.6 mL, 29.2 mmol) were sequentially added thereto, and the mixture was refluxed with stirring. After 2 hours, THF was added to the solution, and the mixture was extracted from ether. Water was removed from the solution in anhydrous MgSO₄. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography to obtain a white solid. The solid was recrystallized from methanol and H₂O, and filtered under reduced pressure to obtain a white Compound of Formula 2-3 (2.5 g, 58%).

MS [M+1] 589

[0080] Hereinbelow, Examples are presented, wherein the compounds prepared in the above Preparative Examples were applied in the organic light emitting devices.

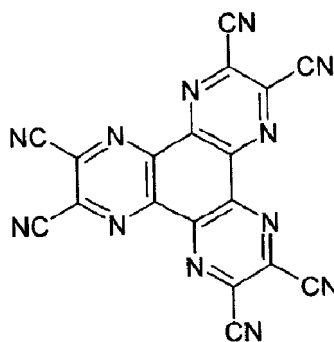
Reference Example

[0081] A glass substrate coated with the ITO (indium tin oxide) having a thickness of 1000 Å was ultrasonically washed in a distilled water in which a detergent was melted. The product manufactured by Fischer Co. was used as the detergent, and the distilled water was twice filtered with the filter manufactured by Millipore Co. After washing the glass substrate for 30 minutes, the glass substrate was further ultrasonically washed in the distilled water for 10 minutes, which was repeated twice. After washing, the glass substrate was sequentially ultrasonically washed in an isopropyl alcohol solvent, an acetone solvent, and a methanol solvent, dried, and then transported to a plasma cleaner.

[0082] Then, the substrate was washed for 5 minutes by using nitrogen plasma, and then transported to a vacuum deposition device.

[0083] Hexanitride hexaazatriphenylene of the following Formula 4 was thermally vacuum deposited on the ITO transparent electrode to a thickness of 80 Å to form a hole injection layer.

[Formula 4]



[0084] A layer (80 Å) formed of the compound of the following Formula 5, which is capable of injecting and transporting holes, was formed on the layer formed of the compound of the Formula 4 by vacuum deposition.

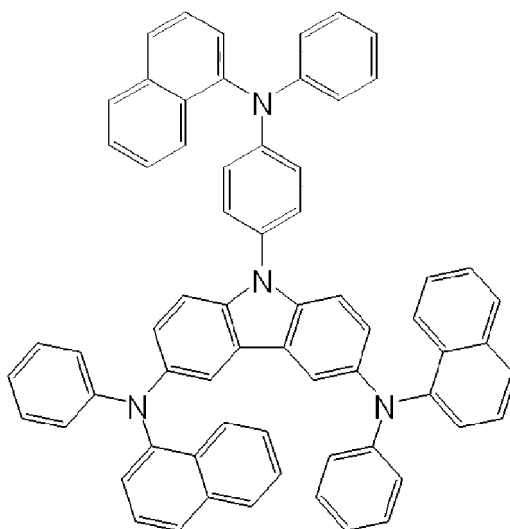
[Formula 5]

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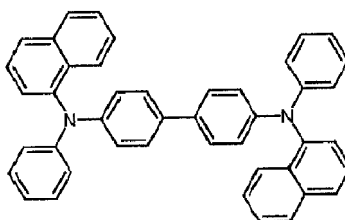
[0085] A layer (300 Å) formed of NPB of the following Formula 6, which is capable of transporting holes, was formed on the layer formed of the compound of the Formula 5 by vacuum deposition.

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[Formula 6]

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[0086] The compound of the Formula 7 as a green dopant was co-deposited at a concentration of 2% on the layer formed of the Formula 6 with the compound of the following Formula 1-1 as a light emitting host, to form a light emitting layer having a thickness of 300 Å.

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[Formula 1-1]

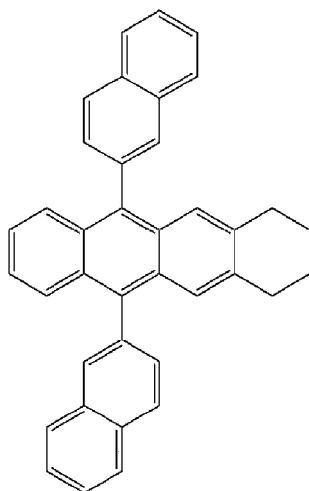
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host



[Formula 7]

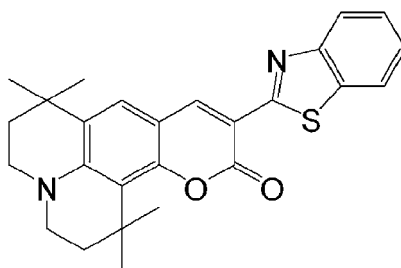
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dopant

[0087] The compound of the following Formula 8, which is capable of injecting and transporting electron, was vacuum deposited on the light emitting layer to a thickness of 200 Å to complete the film formation of an organic layer.



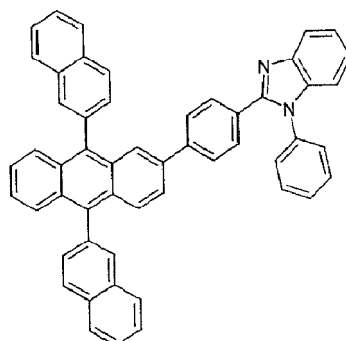
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[Formula 8]

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[0088] Lithium fluoride (LiF) having a thickness of about 12 Å and aluminum having a thickness of 2500 Å were sequentially vacuum deposited on the electron injecting and transporting layer to form a cathode. During the above step, the vacuum deposition rate of the organic compounds was maintained at 0.3 to 0.8 Å/sec, and the vacuum deposition

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rate of lithium fluoride and the vacuum deposition rate of aluminum were maintained at 0.3 Å/sec and 1.5 to 2.5 Å/sec, respectively.

[0089] 100 mA/cm² of forward current was run on thus prepared organic light emitting device to form an electric field of 5.8 V. At this time, for emission color, a spectrum having a brightness of 6500 nit which corresponds to x = 0.262 and y = 0.590 based on a 1931 CIE color coordinate was observed. Upon application of a constant DC at a current density of 100 mA/cm², a time taken until the luminance was lowered to 50% of the initial luminance (L_{0.5}) was 420 hours.

Examples 1 to 2

[0090] In the same manner as in Reference Example except that upon formation of the light emitting layer, the hosts and the dopants as described in Table 1 were used, organic light emitting devices were prepared. The results of the tests on the performances of the organic light emitting device as prepared in each of Examples are shown in Table 1.

Comparative Example 1

In the same manner as in Reference Example except that upon formation of the light emitting layer, 9,10-(2-naphthyl)anthracene was used as a host, an organic light emitting device was prepared.

[0091]

Table 1

Example	Host	Dopant(concentration%)	Voltage*(V)	Emission color	Luminous efficiency(cd/A)
Reference Example	Formula 1-1	Formula 7(2%)	5.8	Green	6.6
Example 1	Formula 2-2	Formula 7 (2%)	6.9	Green	6.5
Example 2	Formula 2-2	None	6.8	Blue	1.9
Comparative Example1	9,10-(2-Naphthyl)anthracene	None	6.5	Blue	1.2

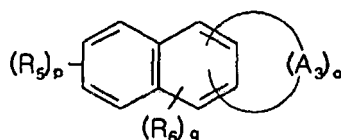
* Voltage was measured at a current density of 100 mA/cm².

[0092] As shown in Table 1, if the compound according to the present invention is applied to an organic light emitting device, it is possible to drive the device at low voltage and to enhance the life span.

[0093] The compound according to the present invention, to which various dopants are applied, can emit blue, green or red light, and in particular, provide a high efficiency light emitting material with excellent thermal stability. Further, the compound according to the present invention is used in the light emitting host in the organic light emitting device, it is possible to enhance the life span of the device and to drive the device at low voltage.

Claims

1. A compound of the following formula (2):



wherein

A₃ means a C₂₋₃₀ cycloalkane, which is unsubstituted or substituted with a C₁₋₆ alkyl group, or a C₅₋₅₀ bicycloalkane, which is unsubstituted or substituted with a C₁₋₆ alkyl group, directly fused to a benzene ring of a polycyclic aromatic hydrocarbon;

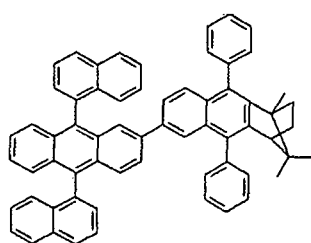
R₅ and R₆ are each selected from the group consisting of a hydrogen, a halogen, a nitrile group (-CN), a nitro group (-NO₂), a sulfonyl group (-SO₂R'), a sulfoxide group (-SOR'), a sulfonamide group (-SO₂NR'₂), a sulfonate group (-SO₃R'), a trifluoromethyl group (-CF₃), an ester group (-COOR'), an amide group (-CONHR' or -CONR'R"), a substituted or unsubstituted and linear or branched C₁₋₁₂ alkoxy group, a substituted or unsubstituted and linear or branched C₁₋₂₀ aliphatic hydrocarbon group, a substituted or unsubstituted and aromatic or nonaromatic heterocyclic group, a substituted or unsubstituted aryl group,

wherein R¹ and R" are each selected from the group consisting of a substituted or unsubstituted C₁₋₆₀ alkyl group, a substituted or unsubstituted aryl group and a substituted or unsubstituted 5-7 membered heterocyclic group;

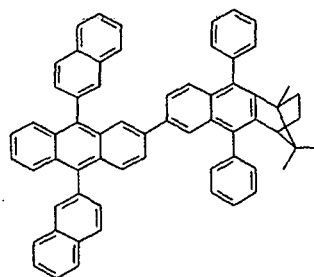
o is an integer of 1 to 2; and

p and q are an integer of 1 to 4.

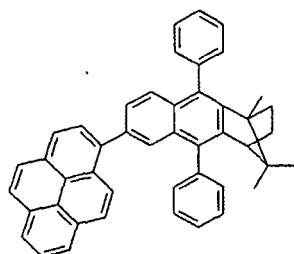
2. The compound according to claim 1, wherein the compound represented by the formula (2) is selected from the group consisting of the compounds represented by the following formulae (2-1) to (2-6):



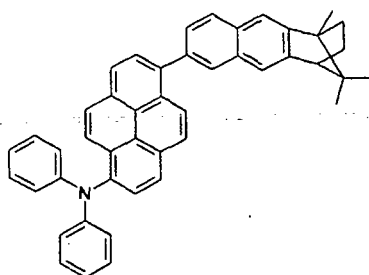
(2-1)



(2-2);

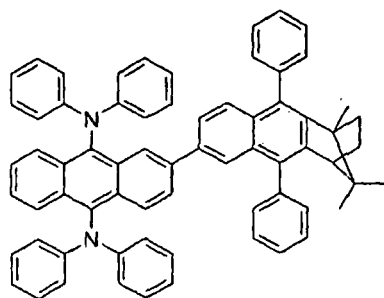


(2-3)



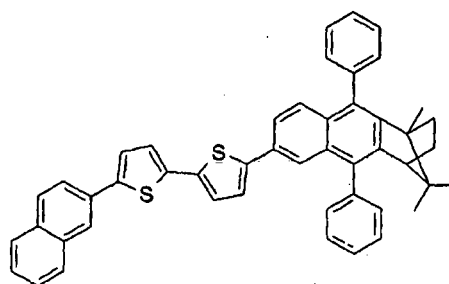
(2-4)

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(2-5)

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(2-6)

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3. The compound according to claim 1 or claim 2, wherein the compound performs at least one of any functions among light emission, hole injection, hole transporting, and electron transporting in an organic electronic device.

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4. The compound according to claim 1 or claim 2, wherein the compound is mixed with 0.1 to 99.0% by weight of an inorganic metal, inorganic salt, or a different organic material.

5. An organic light emitting device comprising a first electrode, at least one organic layer, and a second electrode, laminated successively, wherein at least one layer of organic layers comprises a compound of formula (2) as defined in claim 1 or claim 2.

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6. The organic light emitting device according to claim 5, wherein the number of the cycloalkane or bicycloalkane fused in the compound of formula (2) as defined in claim 1 or claim 2 is 1 to 2.

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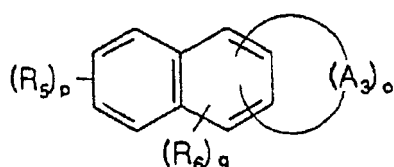
7. The organic light emitting device according to claim 5 or claim 6, wherein the organic layer containing the compound is mixed with 0.1 to 99.0% by weight of an inorganic metal, inorganic salt, or a different organic material.

Patentansprüche

35

1. Verbindung der nachstehenden Formel (2):

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(2)

45

worin

A₃ ein C₂₋₃₀-Cycloalkan, das unsubstituiert oder mit einer C₁₋₆-Alkylgruppe substituiert ist, oder ein C₅₋₅₀-Bicycloalkan, das unsubstituiert oder mit einer C₁₋₆-Alkylgruppe substituiert ist, die direkt mit einem Benzolring eines polycyclischen aromatischen Kohlenwasserstoffs kondensiert ist, bedeutet;

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R₅ und R₆ jeweils aus der Gruppe bestehend aus Wasserstoff, einem Halogen, einer Nitrilgruppe (-CN), einer Nitrogruppe (-NO₂), einer Sulfonylgruppe (-SO₂R'), einer Sulfoxidgruppe (-SOR'), einer Sulfonamidgruppe (-SO₂NR'₂), einer Sulfonatgruppe (-SO₃R'), einer Trifluormethylgruppe (-CF₃), einer Estergruppe (-COOR'), einer Amidgruppe (-CONHR' oder -CONR'R''), einer substituierten oder unsubstituierten und geradkettigen oder verzweigten C₁₋₁₂-Alkoxygruppe, einer substituierten oder unsubstituierten und geradkettigen oder verzweigten C₁₋₂₀-aliphatischen Kohlenwasserstoffgruppe, einer substituierten oder unsubstituierten und aromatischen oder nichtaromatischen heterocyclischen Gruppe, einer substituierten oder unsubstituierten Arylgruppe ausgewählt sind,

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wobei R' und R'' jeweils aus der Gruppe bestehend aus einer substituierten oder unsubstituierten C₁₋₆₀-Al-

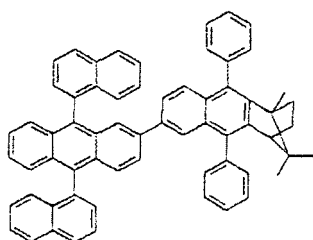
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kylgruppe, einer substituierten oder unsubstituierten Arylgruppe und einer substituierten oder unsubstituierten 5- bis 7-gliedrigen heterocyclischen Gruppe ausgewählt sind;
o eine ganze Zahl von 1 bis 2 ist; und
p und q eine ganze Zahl von 1 bis 4 sind.

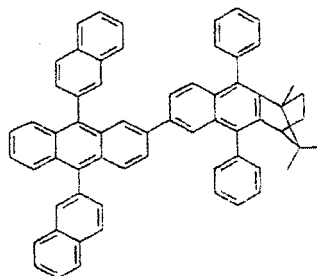
- 5
2. Verbindung gemäß Anspruch 1, wobei die Verbindung der Formel (2) aus der Gruppe bestehend aus den Verbindungen der nachstehenden Formeln (2-1) bis (2-6) ausgewählt ist:

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(2-1)

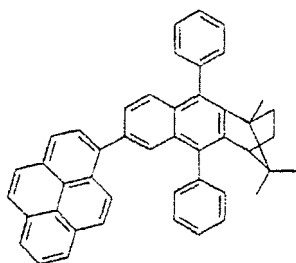


(2-2);

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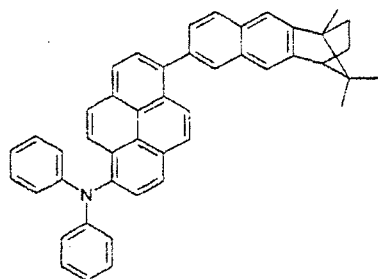
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(2-3)

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(2-4)

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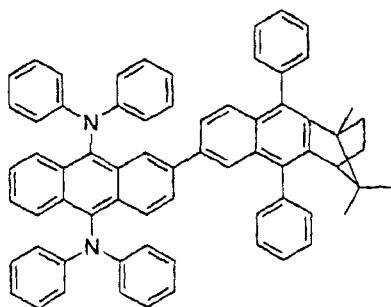
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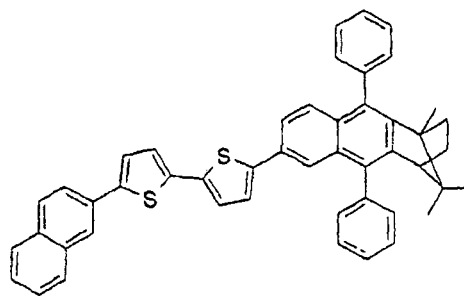
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(2-5)



(2-6)

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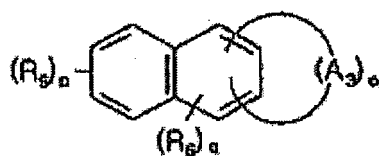
3. Verbindung gemäß Anspruch 1 oder Anspruch 2, wobei die Verbindung mindestens eine der Funktionen aus Lichtemission, Lochinjektion, Lochtransport und Elektronentransport in einer organischen elektronischen Vorrichtung ausübt.
4. Verbindung gemäß Anspruch 1 oder Anspruch 2, wobei die Verbindung mit 0,1 bis 99,0 Gew. % eines anorganischen Metalls, anorganischen Salzes oder eines unterschiedlichen organischen Materials vermischt ist.
5. Organische Licht-emittierende Vorrichtung, umfassend in nacheinander laminierte Form eine erste Elektrode, mindestens eine organische Schicht, und eine zweite Elektrode, wobei mindestens eine Schicht der organischen Schichten eine Verbindung gemäß Formel (2), wie in Anspruch 1 oder Anspruch 2 definiert, umfasst.
6. Organische Licht-emittierende Vorrichtung gemäß Anspruch 5, wobei die Anzahl der kondensierten Cycloalkane oder Bicycloalkane in der Verbindung gemäß Formel (2), wie in Anspruch 1 oder Anspruch 2 definiert, 1 bis 2 beträgt.
7. Organische Licht-emittierende Vorrichtung gemäß Anspruch 5 oder Anspruch 6, wobei die organische Schicht, die die Verbindung enthält, mit 0,1 bis 99,0 Gew. % eines anorganischen Metalls, anorganischen Salzes oder eines unterschiedlichen organischen Materials vermischt ist.

Revendications

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1. Composé de la formule (2) suivants :

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(2)

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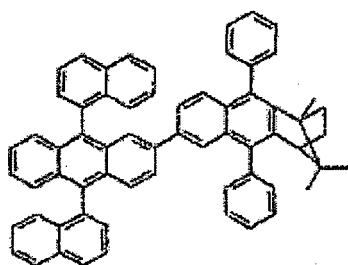
dans laquelle

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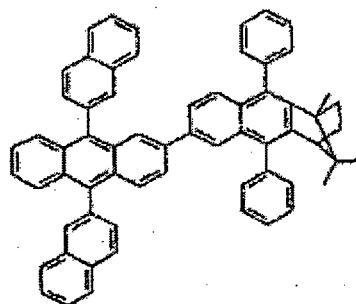
A₃ signifie un cycloalcane en C₂₋₃₀, qui est non substitué ou substitué avec un groupe alkyle en C₁₋₆, ou un bicycloalcane en C₅₋₅₀, qui est non substitué ou substitué avec un groupe alkyle en C₁₋₆, directement condensé à un cycle benzénique d'un hydrocarbure polycyclique aromatique ;
 R₅ et R₆ sont choisis chacun parmi le groupe consistant en un atome d'hydrogène, un atome d'halogène, un groupe nitrile (-CN), un groupe nitro (-NO₂), un groupe sulfonyle (-SO₂R'), un groupe sulfoxyde (-SOR'), un groupe sulfonamide (-SO₂NR'₂), un groupe sulfonate (-SO₃R'), un groupe trifluorométhyle (-CF₃), un groupe ester (-COOR'), un groupe amide (-CONHR' ou -CONR'R''), un groupe alcoxy en C₁₋₁₂ substitué ou non substitué et linéaire ou ramifié, un groupe hydrocarbure aliphatique en C₁₋₂₀ substitué ou non substitué et linéaire ou

ramifié, un groupe hétérocyclique substitué ou non substitué et aromatique ou non aromatique, un groupe aryle substitué ou non substitué, dans laquelle R' et R'' sont choisis chacun parmi le groupe consistant en un groupe alkyle en C₁₋₆₀ substitué ou non substitué, un groupe aryle substitué ou non substitué et un groupe hétérocyclique de 5 à 7 chaînons substitué ou non substitué ;
 o est un entier de 1 à 2 ; et
 p et q sont un entier de 1 à 4.

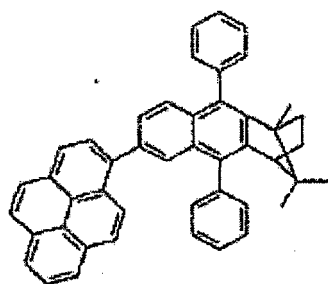
2. Composé selon la revendication 1, dans lequel le composé représenté par la formule (2) est choisi parmi le groupe consistant en les composés représentés par les formules (2-1) à (2-6) suivantes :



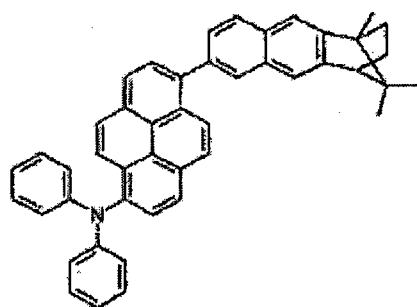
(2-1)



(2-2)

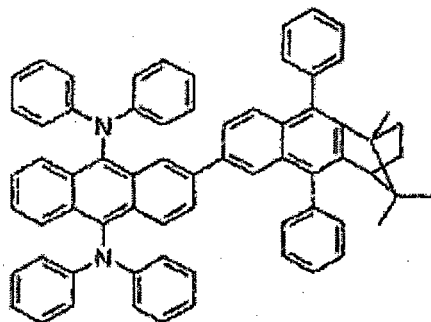


(2-3)



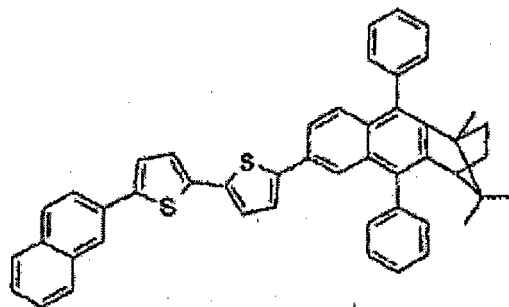
(2-4)

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(2-5)

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(2-6)

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3. Composé selon la revendication 1 ou la revendication 2, dans lequel le composé réalise au moins l'une de quelques fonctions parmi une émission de lumière, une injection de trous, un transport de trous, et un transport d'électrons dans un dispositif électronique organique.

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4. Composé selon la revendication 1 ou la revendication 2, dans lequel le composé est mélangé à 0,1 à 99,0% en poids d'un métal inorganique, d'un sel inorganique, ou d'un matériau organique différent.

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5. Dispositif électroluminescent organique comprenant une première électrode, au moins une couche organique, et une deuxième électrode, successivement stratifiées, dans lequel au moins une couche parmi les couches organiques comprend un composé de formule (2) tel que défini selon la revendication 1 ou la revendication 2.

6. Dispositif électroluminescent organique selon la revendication 5, dans lequel le nombre de cycloalcane(s) ou de bicycloalcane(s) condensé(s) dans le composé de formule (2) tel que défini selon la revendication 1 ou la revendication 2 est 1 à 2.

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7. Dispositif électroluminescent organique selon la revendication 5 ou la revendication 6, dans lequel la couche organique contenant le composé est mélangée à 0,1 à 99,0% en poids d'un métal inorganique, d'un sel inorganique, ou d'un matériau organique différent.

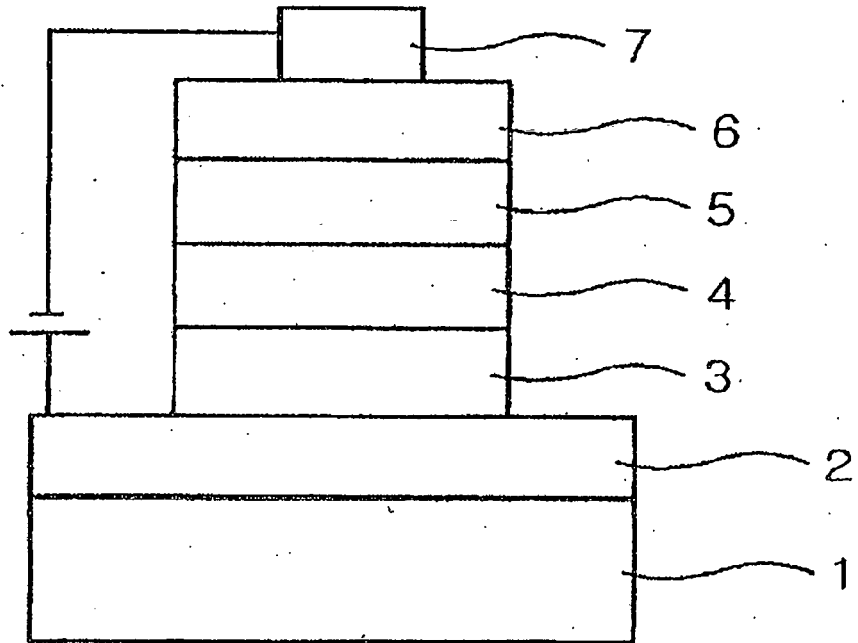
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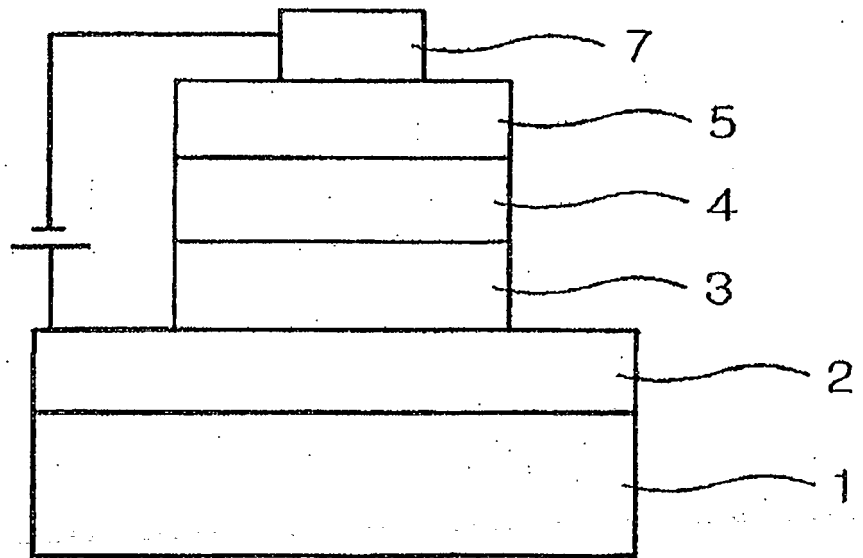
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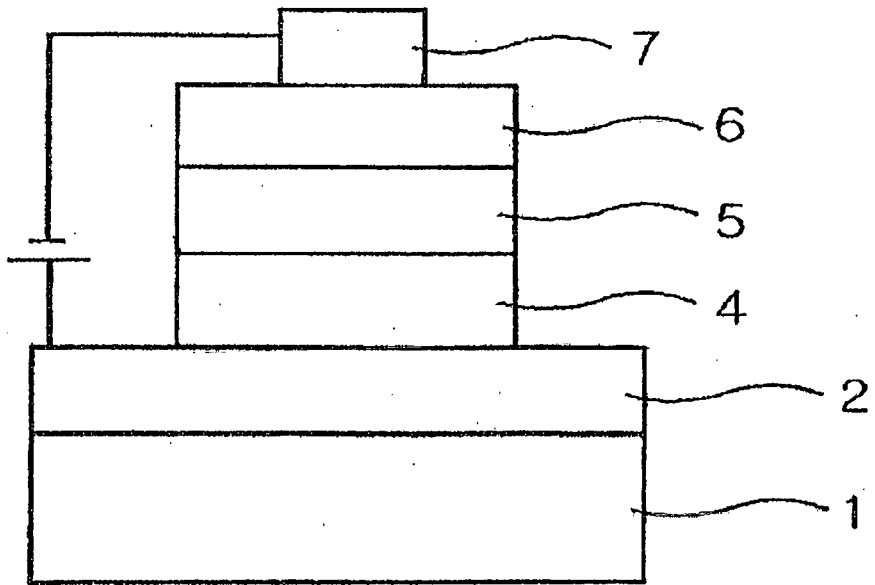
[Fig. 1]



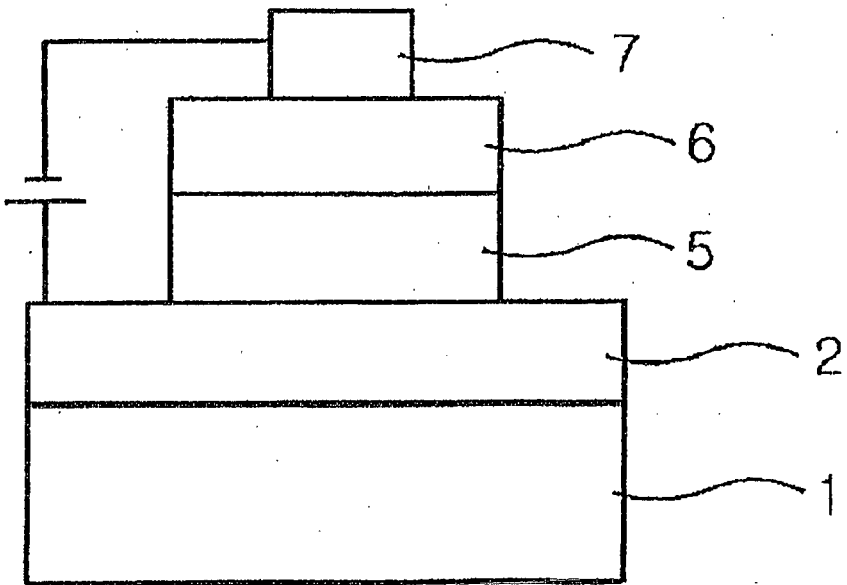
[Fig. 2]



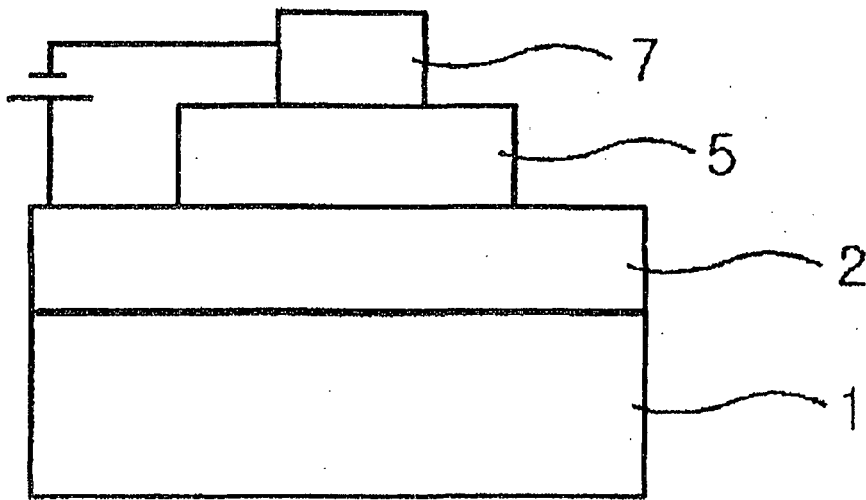
[Fig. 3]



[Fig. 4]



[Fig. 5]



REFERENCES CITED IN THE DESCRIPTION

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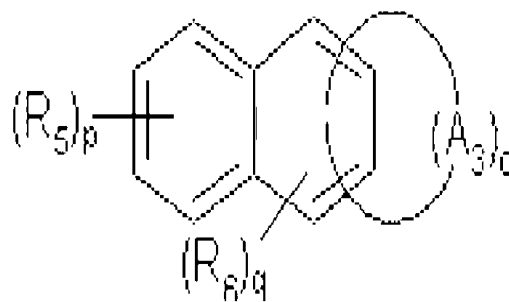
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专利名称(译)	有机化合物和使用其的有机发光器件		
公开(公告)号	EP2316905B1	公开(公告)日	2014-02-26
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发明人	KIM, KONG KYEOM HONG, SUNG-KIL JANG, HYE-YOUNG, JEONG, DONG-SEOB		
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优先权	1020050086501 2005-09-15 KR		
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外部链接	Espacenet		

摘要(译)

本发明提供一种多环芳烃化合物，其中取代或未取代的C2-30环烷烃，或取代或未取代的C5-50多环烷烃直接稠合到所述多环芳烃的多环芳烃的苯环上，如式所示(2)。此外，本发明涉及一种有机发光器件，其包括依次层叠的第一电极，至少一个有机层和第二电极，其中至少一个有机层包含所述多环芳烃化合物。



(2)