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(54) **ORGANIC COMPOUND AND ORGANIC LIGHT EMITTING DEVICE USING THE SAME**

ORGANISCHE VERBINDUNG UND ORGANISCHE LICHEMITTIERENDE VORRICHTUNG DAMIT
COMPOSE ORGANIQUE ET DISPOSITIF ELECTROLUMINESCENT ORGANIQUE UTILISANT CE
COMPOSE

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• **JAMES CASON, DONALD D. PHILLIPS: "THE**
SYNTEHSIS OF 1',9-DIMETHYL-1,2-
BENZANTHRACENE" JOURNAL OF ORGANIC
CHEMISTRY, vol. 17, no. 2, 29 February 1952
(1952-02-29), pages 298-312, XP002554453 DOI:
10.1021/jo01136a019

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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), which is incorporated herein by its entirety for reference.

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).

20 [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] EP 1 659 129 A1 relates to the technical problem of providing a coordination metal compound having properties suitable for being used in an organic electroluminescent device having great luminescence of emitted light and great storage stability under high temperature ([0010]). Specific compounds disclosed contain a spiro-substituted fluorene.

40 [0009] WO 2004/083160 A1 relates to oligocene compounds such as pentacene compounds that are suitable for being used as active constituents in semiconductor elements such as light-emitting diodes (page 1, lines 13-18; page 5, lines 26-28). Specific compounds disclosed contain a naphthalene moiety to which a non-aromatic ring is fused.

[0010] J. Cason et al. in J. Org. Chem., vol. 17, 1952, pages 298-312 describe the synthesis of a dimethyl-substituted benzantracene compound of which the possible carcinogenic properties are of interest. Compounds containing an anthracene substructure bearing a methyl group as a substituent in position 9, i.e. on the central benzene ring, are disclosed.

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Disclosure of Invention**Technical Problem**

50 [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.

55 **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 fused to a polycyclic aromatic hydrocarbon as a core

Advantageous Effects

[0013] According to the invention, a derivative having a structure in which at least one cycloalkane or polycycloalkane is directly fused to an anthracene as a core 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.

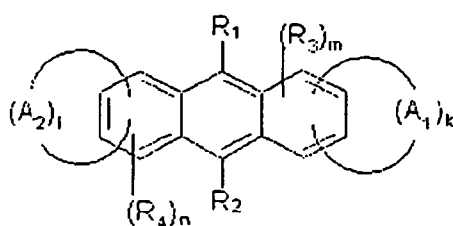
[Reference numerals]

[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 a compound of the following formula (1),



(1);

wherein

A₁ and A₂ each means a substituted or unsubstituted C₂₋₃₀ cycloalkane, or a substituted or unsubstituted C₅₋₅₀ polycycloalkane directly fused to a benzene ring of a polycyclic aromatic hydrocarbon;

R₁ to R₄ 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, a substituted or unsubstituted aryl group, a substituted or unsubstituted and mono- or diarylamine group and a substituted or unsubstituted aralkylamine group,

wherein 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, provided that R₁ and R₂ are not simultaneously a hydrogen atom;

k and 1 are an integer of 0 to 2 (provided that k+1 ≥ 1); and

m and n are an integer of 1 to 4.

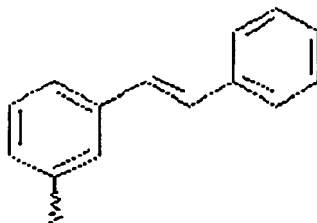
[0018] Furthermore, the present invention provides an organic light emitting device comprising, laminated successively, a first electrode, at least one organic layer, and a second electrode, wherein at least one layer of said at least one organic layer comprises at least one compound as defined hereinabove with reference to formula 1.

[0019] 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.

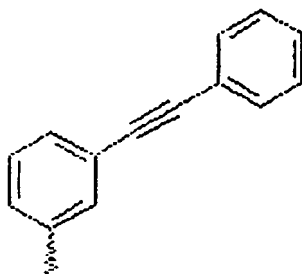
[0020] In the formula, the aryl group may be selected from the group consisting of a phenyl group, a biphenyl group, a terphenyl group, a benzyl group, a naphthyl group, an anthracenyl group, a tetracenyl group, a pentacenyl group, a perylenyl group and a coronenyl group and these may be monosubstituted, polysubstituted or unsubstituted.

[0021] 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.

[0022] 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.

[0023] 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.

[0024] 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.

[0025] In the formula (1), k and l are an integer of 0, 1 or 2 (provided that k + 1 ≥ 1); and m and n are an integer of 1 to 4.

[0026] In the case that k and l and u 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.

[0027] Unrestricted examples of substituents for the substituted cycloalkane or substituted bicycloalkane include a C₁₋₆ alkyl group.

Mode for the Invention

[0028] Hereinafter, the present invention will be described in more detail.

[0029] Polycyclic aromatic hydrocarbons such as anthracene, naphthalene, pyrene, rubrene and perylene can function 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.

[0030] As illustrated in the formula (1), the present invention is characterized by providing a derivative that has as a core the polycyclic aromatic hydrocarbon anthracene, in which sterically bulky cycloalkane or polycycloalkane is directly fused to the core

[0031] In the invention, polycycloalkane is preferably bicycloalkane.

[0032] According to the invention, the compound that has the polycyclic aromatic hydrocarbon anthracene as a core, in which a substituted or unsubstituted C₂₋₃₀ cycloalkane, or a substituted or unsubstituted C₅₋₅₀ polycycloalkane is directly fused to 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 compound according to the invention can emit blue, green and red

light by controlling the substituents introduced or the conjugation length.

[0033] The polycyclic aromatic hydrocarbon derivative according to the invention performs light absorption or light emission, thereby determining its main wavelength band.

[0034] On the other hand, a substituted or unsubstituted C₂₋₃₀ cycloalkane, or a substituted or unsubstituted C₅₋₅₀ bicycloalkane directly fused to the anthracene core can move the wavelength of the chromophore to a longer wavelength.

[0035] Since anthracene itself has amphoteric properties, holes or electrons can be selectively transported depending on the introduction of the substituents.

[0036] The cycloalkane or polycycloalkane fused to the anthracene can give a nonplanar structure (e.g., chair type) similar to an independent cycloalkane or polycycloalkane to the anthracene, 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.

[0037] Further, since the cycloalkane or polycycloalkane fused to the anthracene 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 anthracene 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.

[0038] 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).

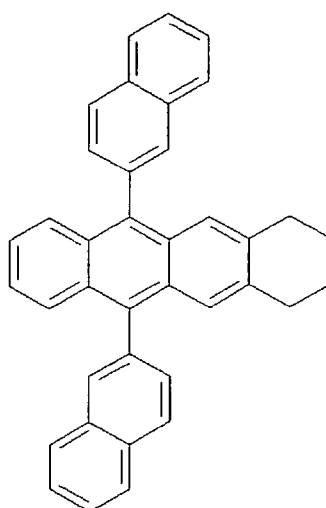
[0039] Therefore, the compound of the present invention can be used as a hole transporting material. Unlike an anthracene derivative disclosed in US Patent No. 6465115, a structure surrounded by cycloalkane or polycycloalkane is more electrochemically stable (cationic radical) and the energy level (HOMO) thereof can be optimized. Therefore, the compound of the present invention is improved in stability as the hole transporting material to thus attain a stable morphology and to facilitate hole injection.

[0040] The number of the cycloalkane or polycycloalkane fused to the polycyclic aromatic hydrocarbon is preferably 1 to 4.

[0041] The cycloalkane fused according to the invention has 2 to 30, preferably 3 to 8 carbon atoms.

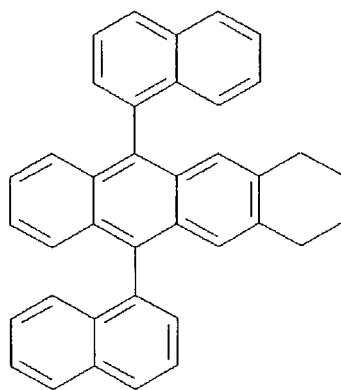
[0042] The polycycloalkane fused according to the invention has 5 to 50, preferably 5 to 25 carbon atoms.

[0043] Specific examples of the compound represented by the formula (1) include, but are not limited to, the compounds represented by the following formulae (1-1) to (1-13):



(1-1);

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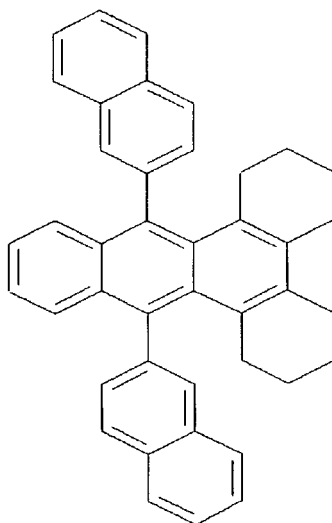


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(1-2);

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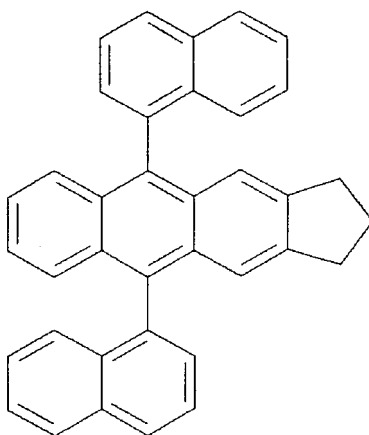
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(1-3);

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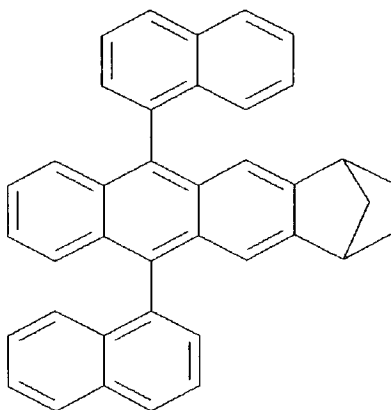
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(1-4);

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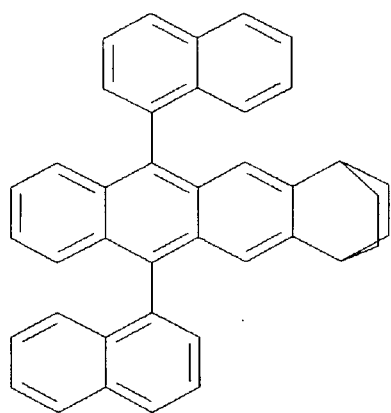


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(1-5);

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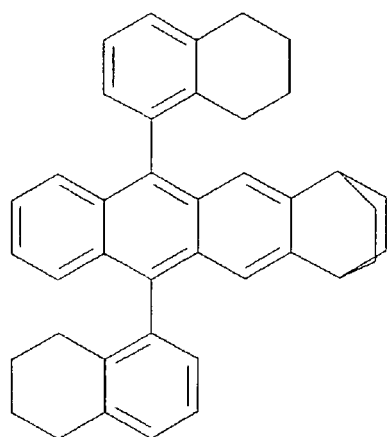


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(1-6);

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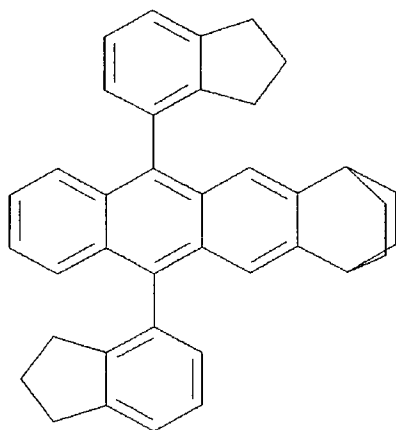
(1-7);

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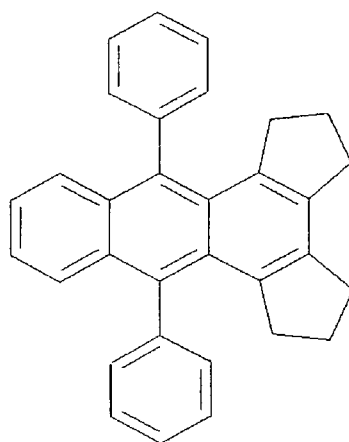


(1-8);

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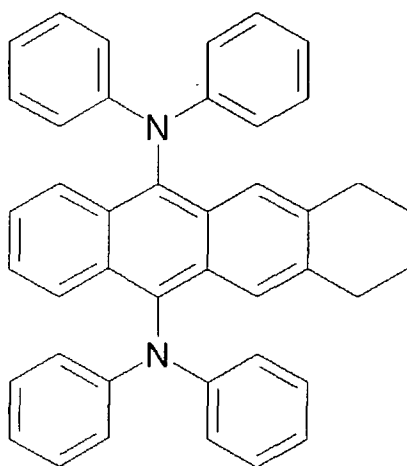
(1-9);

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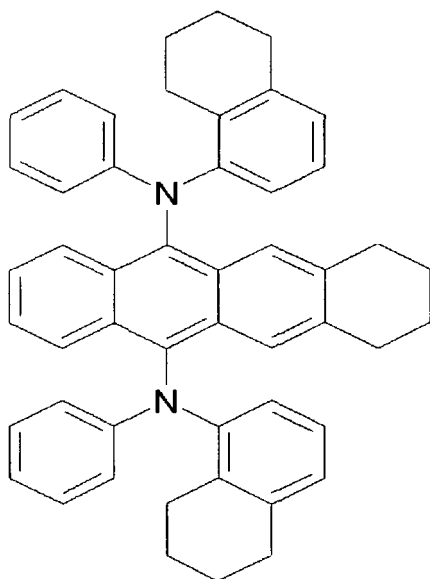
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(1-10);

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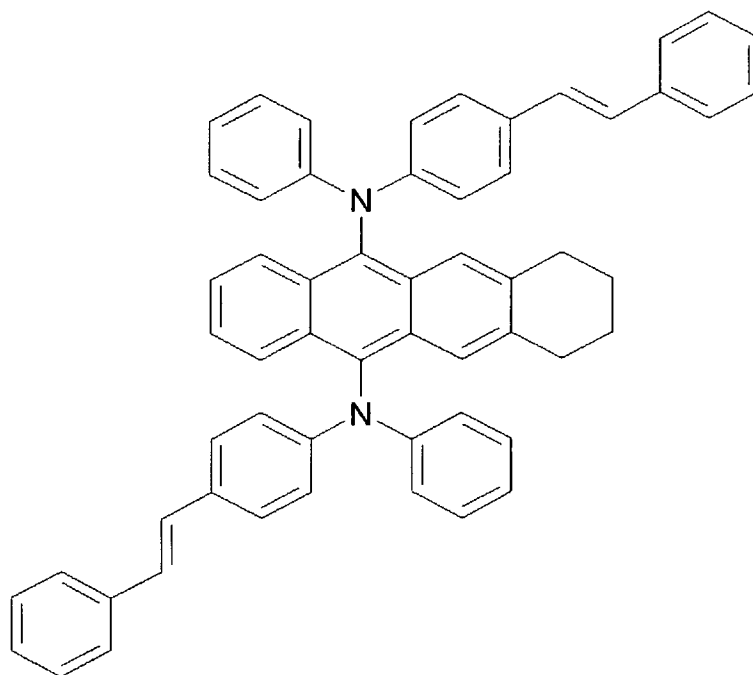
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(1-11);

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(1-12); and

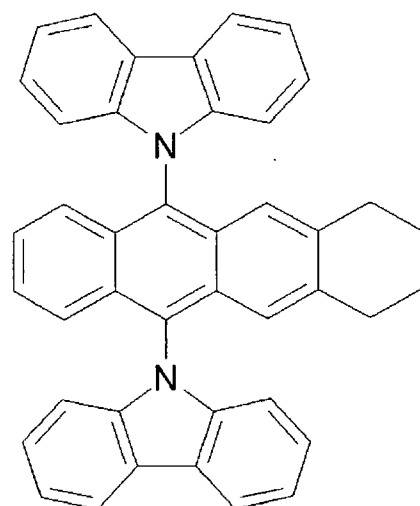
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(1-13)

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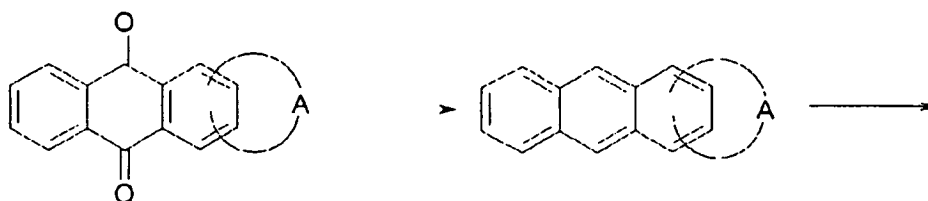
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[0044] In an example of the general production method of the compound of the formula (1), an anthraquinone derivative can be synthesized and reduced to anthracene by a general reduction reaction anthracene, and various substituents can be introduced into a general chemical reaction through a halogenation reaction including bromination at the 9- or 10-position of anthracene (e.g., Suzuki coupling reaction, amine reaction). The production method can be represented by the following reaction scheme A:

[Reaction scheme A]

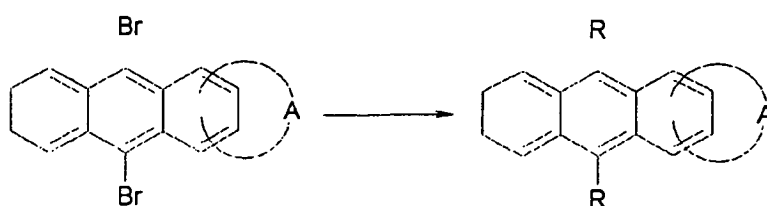
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[0045] The production method of the compounds of the formula (1) will be explained in more detail in Preparative Examples to be described below.

[0046] On the other hand, the compound of the present invention 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.

[0047] 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.

[0048] 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).

[0049] 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.

[0050] 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").

[0051] 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).

[0052] In this case, the compound of the present invention may be also mixed with 0.1 to 99.0% by weight of an inorganic metal, inorganic salt, or a different organic material.

[0053] Hereinafter, the organic light emitting device according to the invention will be described.

[0054] 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.

[0055] 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.

[0056] 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.

[0057] 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.

[0058] the compound of the present invention substituted or unsubstituted C₅₋₅₀ polycycloalkane is directly fused to the core or is 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 compound of the present 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.

[0059] When the compound of the present 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.

[0060] When the compound of the present invention is used as a dopant, the compound 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.

[0061] Further, the compound of the present 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.

[0062] The compound of the present 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 compound may be contained in the hole transporting layer and/or electron transporting layer.

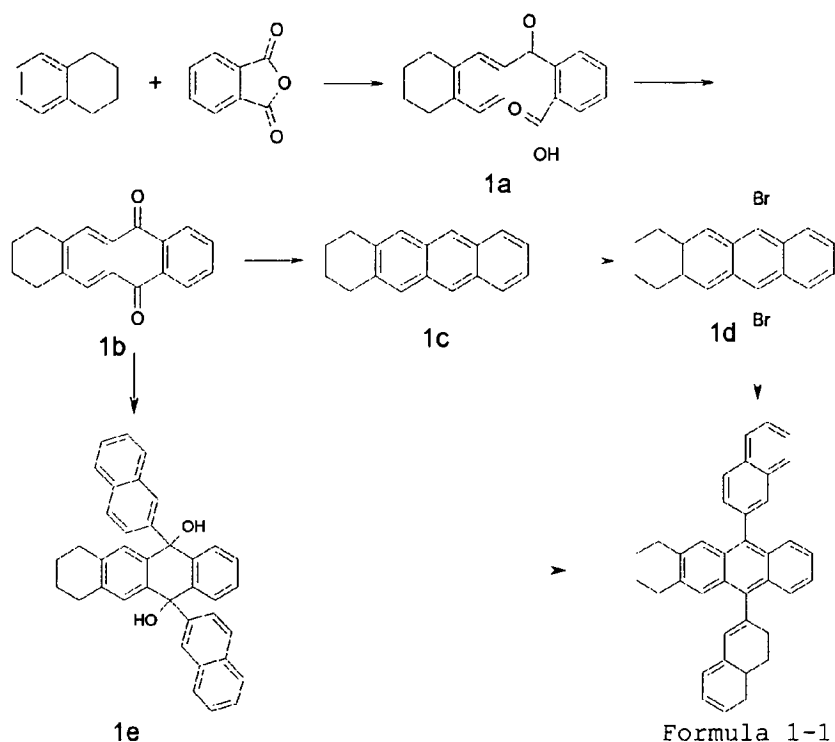
[0063] The organic light emitting device comprising the compound of the present invention can be enhanced in terms of the life span and the thermal stability. The reason is in that, by introducing a sterically bulky cycloalkyl group thereto, (1) a melting point and a glass transition temperature of the compound of the present invention 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.

[0064] 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 1-1

[0065]

[Reaction scheme 1]



(1) Synthesis of Compound 1a

[0066] Tetralin (50.5 mL, 371 mmol) and phthalic anhydride (50.0 g, 338 mmol) were dissolved in dichloromethane (60 mL), AlCl_3 was slowly added thereto at 0°C , and the mixture was stirred at 0°C for 30 minutes and was slowly warmed to normal temperature to proceed the reaction for 4 hours. The solution of the reaction mixture was poured into iced water, the organic phase was separated, and the water phase was twice extracted with dichloromethane. The organic phase was combined, dried on anhydrous MgSO_4 , filtered, and then concentrated under reduced pressure. The residue was recrystallized from dichloromethane and petroleum ether to obtain a compound of Formula 1a (84 g, 89%).

MS $[\text{M}+\text{H}]$ 281

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(2) Synthesis of Compound 1b

5 [0067] Compound 1a (10 g, 35 mmol) was dissolved in dichloromethane (30 mL), and SOCl_2 (3.9 mL, 53.4 mmol) was added thereto to proceed the reaction for 12 hours. The reaction mixture was concentrated under reduced pressure to remove SOCl_2 , and the residue was then dissolved in dichloromethane (30 mL). The solution was cooled to 0°C , AlCl_3 was slowly added thereto, and the mixture was warmed to normal temperature and then allowed to proceed the reaction for 3 hours. The reaction mixture was poured into iced water, the organic phase was separated, and the water phase was twice extracted with dichloromethane. The organic phase was combined, dried on anhydrous MgSO_4 , filtered, and then concentrated under reduced pressure. The residue was purified by column chromatography to obtain Compound 1b (3.0 g, 32%).
10 MS [M+H] 262

(3) Synthesis of Compound 1c

15 [0068] Compound 1b (4.0 g, 15 mmol) was put to glacial acetic acid (250 mL), HI (40 mL) was slowly added thereto, and the mixture was refluxed for 8 hours. After termination of the reaction, the mixture was cooled to normal temperature, and the reaction mixture was poured into an aqueous sodium thiosulfate solution, and then extracted from ethyl ether. The organic phase was dried on anhydrous MgSO_4 , filtered, and then concentrated under reduced pressure. The residue was purified by column chromatography to obtain Compound 1c (1.1 g, 31 %).
20 MS [M+H] 233

(4) Synthesis of Compound 1d

25 [0069] Compound 1c (1.5 g, 6.4 mmol) was dissolved in DMF (30 mL), and NBS (N-bromosuccinimide) (2.87 g, 16.1 mmol) was added thereto to proceed the reaction for 10 hours. The reaction mixture was poured into water, and extracted from dichloromethane. The organic phase was dried on anhydrous MgSO_4 , and then concentrated under reduced pressure. The residue was recrystallized from dichloromethane and ethanol to obtain Compound 1d (1.2 g, 47%).
MS [M] 390

(5) Synthesis of compound of Formula 1-1

30 [0070] Compound 1d (1.3 g, 2.5 mmol) was dissolved in THF (tetrahydrofuran), 2-naphthyl boronic acid (0.9 g, 5.0 mmol) and 4 M K_2CO_3 (2.56 mL) were sequentially added thereto, and the mixture was refluxed. After termination of the reaction, the organic phase was separated and the water phase was extracted from ethyl acetate. The organic phase was combined, dried on anhydrous MgSO_4 , filtered, and then concentrated under reduced pressure. The residue was purified by column chromatography and then recrystallized from ethyl acetate and ethanol to obtain a compound of Formula 1-1 (1.1 g, 87%).

35 [0071] $^1\text{H NMR}$ (500 MHz, CDCl_3) 8.08 (d, 2H), 8.05-8.02 (m, 2H), 7.98 (s, 2H), 7.96-7.92 (m, 2H), 7.68-7.58 (m, 8H), 7.42 (s, 2H), 7.25-7.22 (m, 2H), 2.81-2.76 (br, 4H), 1.78-1.73 (quintet, 4H); MS [M+H] 485

Preparative Example 2: Synthesis of compound of Formula 1-2

40 [0072] The same procedure as in Preparative Example 1 was used until the step of synthesizing Compound 1d. Further, in the same manner as in Preparative Example 1 except that 1-naphthyl boronic acid was used instead of 2-naphthyl boronic acid in the step of synthesizing the compound of Formula 1-1 from Compound 1d, the compound of Formula 1-2 was synthesized.

45 [0073] $^1\text{H NMR}$ (500 MHz, CDCl_3) 8.12-8.02 (m, 4H), 7.78-7.72 (m, 2H), 7.68-7.62 (m, 2H), 7.55-7.48 (m, 2H), 7.39-7.35 (m, 2H), 7.3-7.18 (m, 6H), 7.14-7.11 (m, 2H), 2.72-2.62 (q, 4H), 1.74-1.64 (m, 4H); MS [M+H] 485

50 [0074] Hereinbelow, Examples are presented, wherein the compounds prepared in the above Preparative Examples were applied in the organic light emitting devices.

Example 1

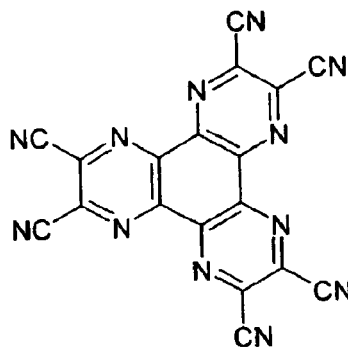
55 [0075] A glass substrate coated with the ITO (indium tin oxide) having a thickness of 1000 Å was ultrasonically washed in a distilled water in which a detergent was melted. The product manufactured by Fischer Co. was used as the detergent, and the distilled water was twice filtered with the filter 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.

[0076] Then, the substrate was washed for 5 minutes by using nitrogen plasma, and then transported to a vacuum deposition device.

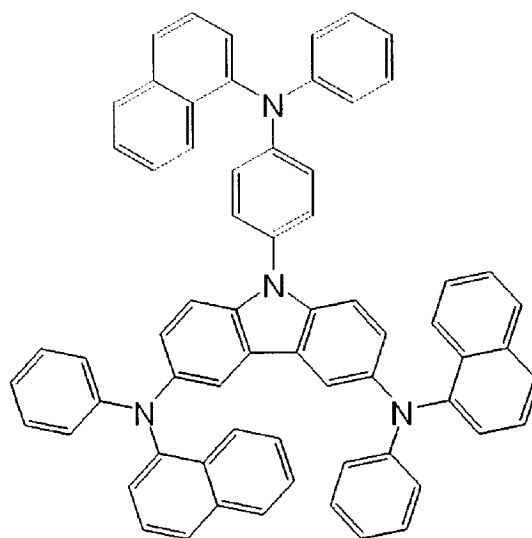
[0077] Hexanitride hexaazatriphenylene of the following Formula 4 was thermally vacuum deposited on the ITO transparent electrode to a thickness of 80 Å to form a hole injection layer.

[Formula 4]



[0078] 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]

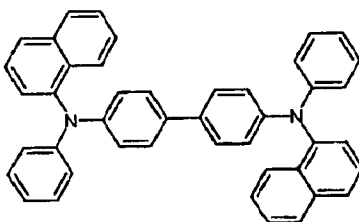


[0079] A layer (300 Å) formed of NPB of the following Formula 6, which is capable of transporting holes, was formed on the layer formed of the compound of the Formula 5 by vacuum deposition.

[Formula 6]

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[0080] 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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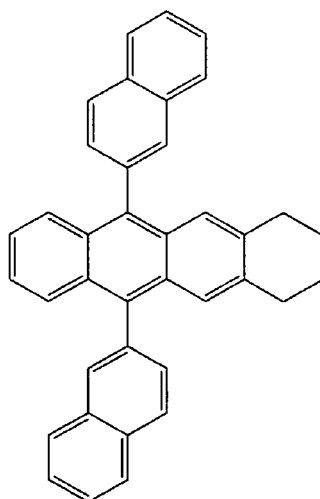
[Formula 1-1]

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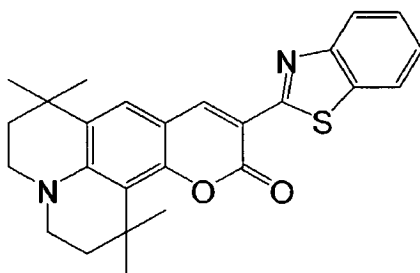
host

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[Formula 7]

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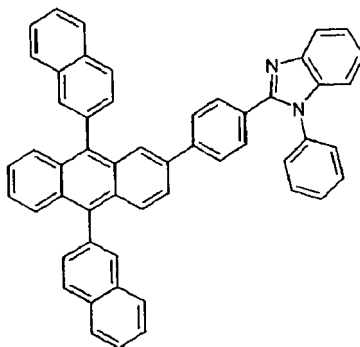


dopant

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[0081] 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.

[Formula 8]



[0082] 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 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.

[0083] 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 2 to 4

[0084] In the same manner as in Example 1 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

[0085] In the same manner as in Example 1 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.

Table 1

Example	Host	Dopant(concentration%)	Voltage V)	Emission color	Luminous efficiency(cd/A)
Example 1	Formula 1-1	Formula 7(2%)	5.8	Green	6.6
Example2	Formula 1-1	None	6.0	Blue	1.7
Example3	Formula 1-2	Formula 7 (2%)	6.3	Green	6.5
Example4	Formula 1-2	None	6.2	Blue	1.4
Comparative Example1	9,10-(2-Naphthyl)anthracene	None	6.5	Blue	1.2

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

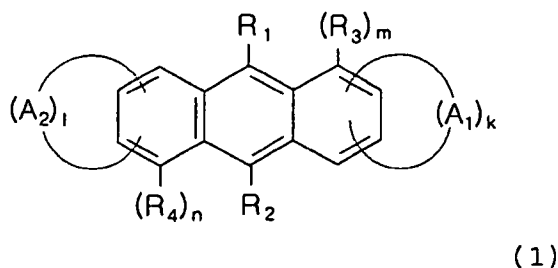
[0086] As shown in Table 1, if the compound according to the present invention is applied to an organic light emitting device, it is possible to drive the device at low voltage and to enhance the life span.

[0087] 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 (1):



wherein

A₁ and A₂ each means a substituted or unsubstituted C₂₋₃₀ cycloalkane, or a substituted or unsubstituted C₅₋₅₀ polycycloalkane directly fused to a benzene ring of a polycyclic aromatic hydrocarbon;

R₁ to R₄ 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''), a substituted or unsubstituted and linear or branched C₁₋₁₂ alkoxy group, a substituted or unsubstituted and aromatic or nonaromatic heterocyclic group, a substituted or unsubstituted aryl group, a substituted or unsubstituted and mono- or diarylamine group and a substituted or unsubstituted aralkylamine group,

wherein 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,

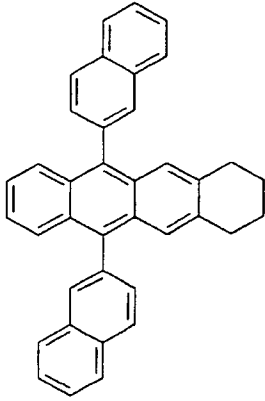
provided that R₁ and R₂ are not simultaneously a hydrogen atom;

k and l are an integer of 0 to 2 (provided that k+l ≥ 1); and

m and n are an integer of 1 to 4.

2. The compound according to claim 1, wherein the compound represented by the formula (1) is selected from the group consisting of the compounds represented by the following formulae (1-1) to (1-13):

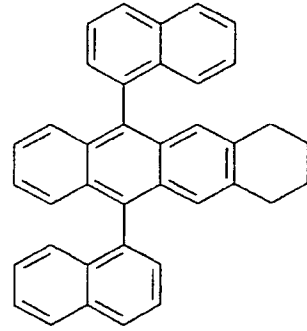
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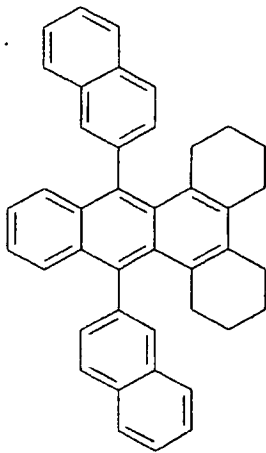
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(1-1)



(1-2)

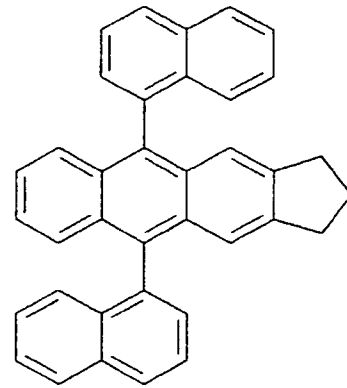
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(1-3)



(1-4)

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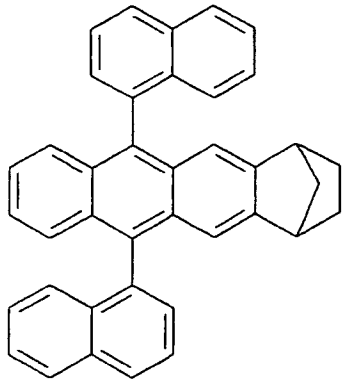
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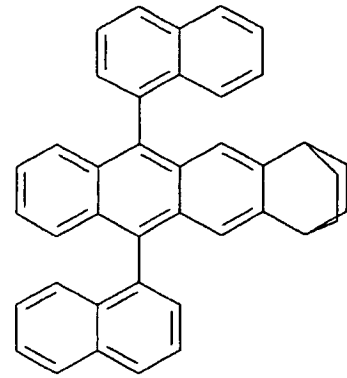
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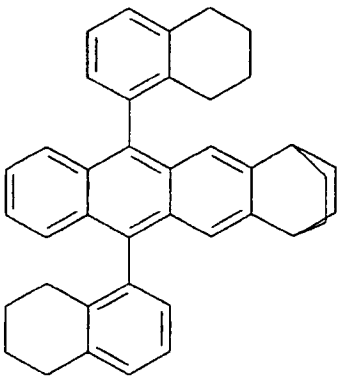
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(1-5)



(1-6)

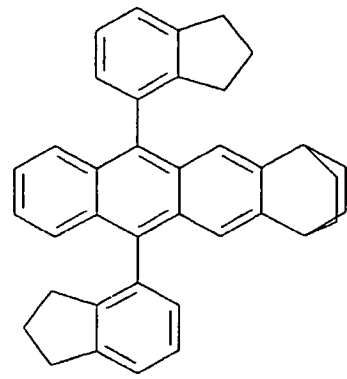
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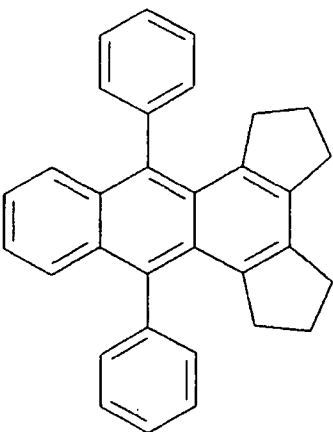
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(1-7)



(1-8)

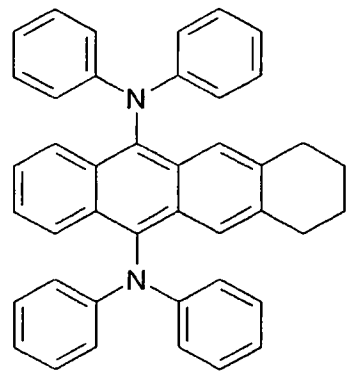
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(1-9)

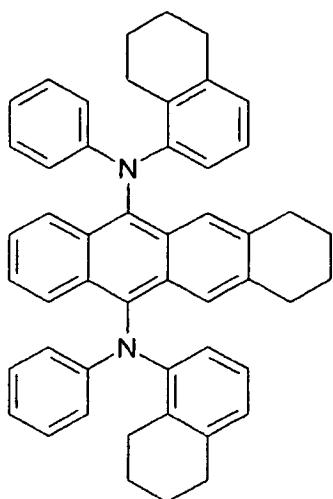


(1-10)

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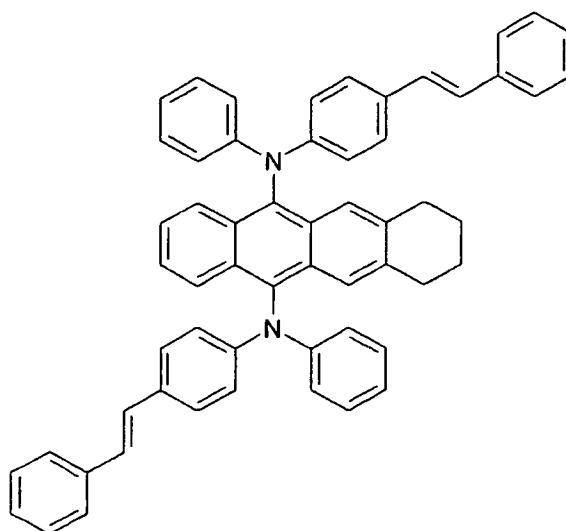
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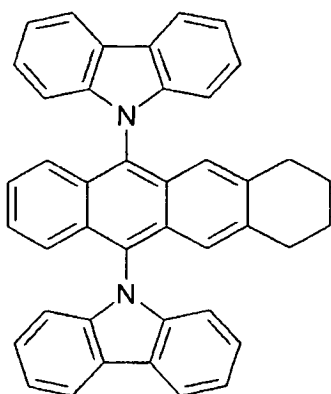
(1-11)



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(1-12)

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(1-13)

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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.

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

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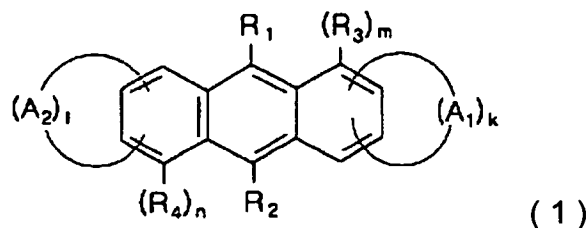
6. The organic light emitting device according to claim 5, wherein the number of the cycloalkane or polycycloalkane fused is 1 to 4.

7. The organic light emitting device according to claim 5 or claim 6, wherein the polycycloalkane is a bicycloalkane.

8. The organic light emitting device according to any of claims 7 to 9, wherein the organic layer containing the at least one compound as defined in claim 1 or claim 2 is mixed with 0.1 to 99.0% by weight of an inorganic metal, inorganic salt, or a different organic material.

Patentansprüche

1. Verbindung der nachstehenden Formel (1):



worin

15 A_1 bis A_2 jeweils substituiertes oder unsubstituiertes C_{2-30} -Cycloalkan oder substituiertes oder unsubstituiertes C_{5-50} -Polycycloalkan, das direkt mit einem Benzolring eines polycyclischen aromatischen Kohlenwasserstoffs kondensiert ist, bedeuten;

20 R_1 bis R_4 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 C_{1-12} -Alkoxygruppe, einer substituierten oder unsubstituierten und aromatischen oder nichtaromatischen heterocyclischen Gruppe, einer substituierten oder unsubstituierten Arylgruppe, einer substituierten oder unsubstituierten Mono- oder Diarylamingruppe und einer substituierten oder unsubstituierten Aralkylamingruppe ausgewählt sind,

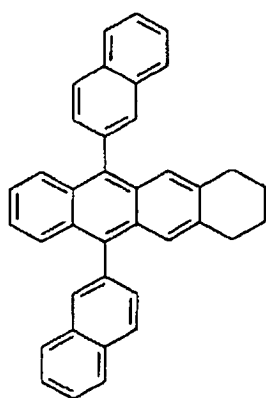
25 worin R' und R'' jeweils aus der Gruppe bestehend aus einer substituierten oder unsubstituierten C_{1-60} -Alkylgruppe, einer substituierten oder unsubstituierten Arylgruppe und einer substituierten oder unsubstituierten, 5- bis 7-gliedrigen, heterocyclischen Gruppe ausgewählt sind,

vorausgesetzt, dass R_1 und R_2 nicht gleichzeitig ein Wasserstoffatom sind;

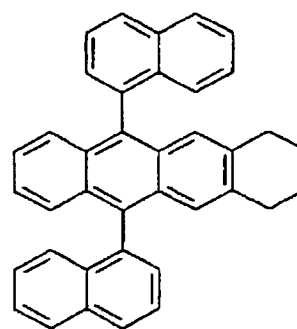
30 k und l eine ganze Zahl von 0 bis 2 sind (vorausgesetzt, dass $k + l \geq 1$); und

m und n eine ganze Zahl von 1 bis 4 sind.

2. Verbindung gemäss Anspruch 1, wobei die Verbindung der Formel (1) aus der Gruppe bestehend aus den Verbindungen der nachstehenden Formeln (1-1) bis (1-13) ausgewählt ist:



(1-1)

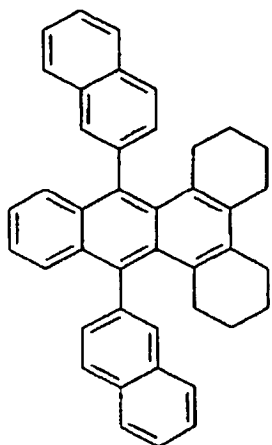


(1-2)

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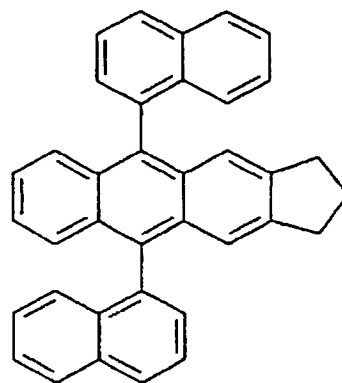
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(1-3)

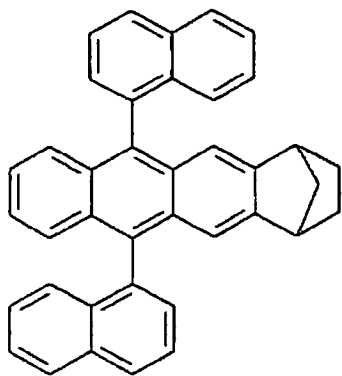
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(1-4)

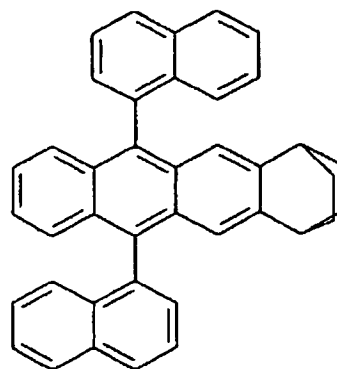
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(1-5)

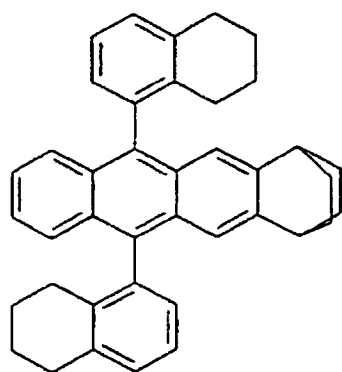
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(1-6)

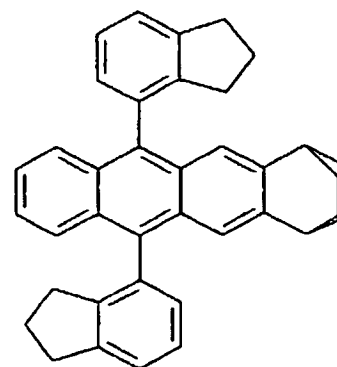
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(1-7)

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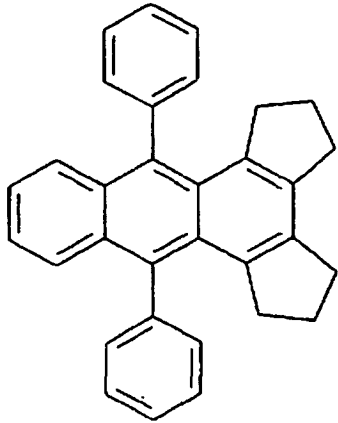
(1-8)

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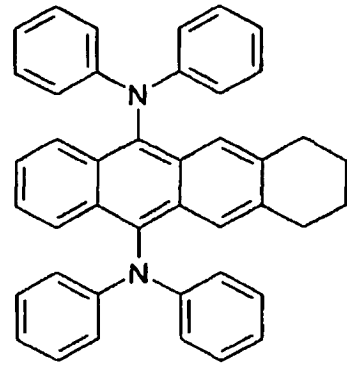
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(1-9)

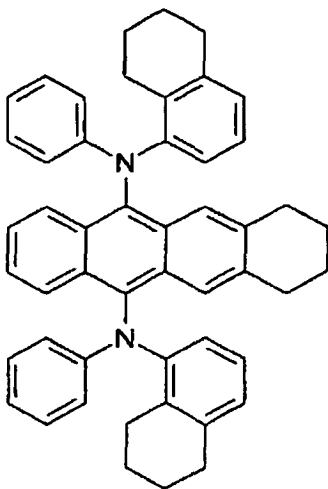
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(1-10)

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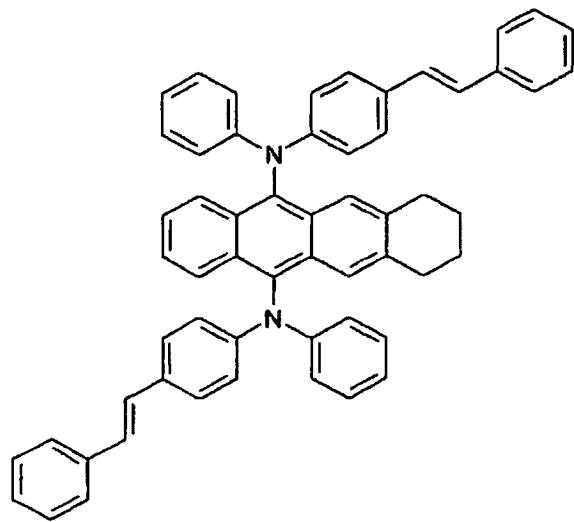
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(1-11)

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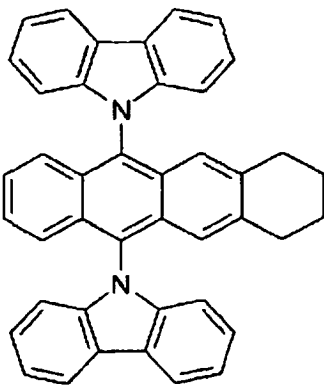
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(1-12)

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(1-13)

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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.

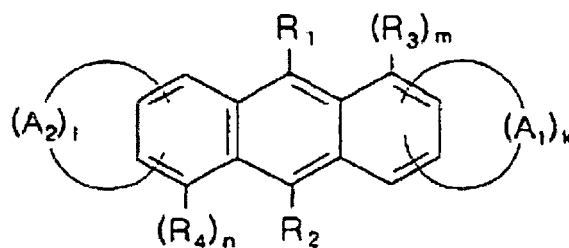
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4. Verbindung gemäß Anspruch 1 oder Anspruch 2, wobei die Verbindung mit 0,1 bis 99,0 Gew.% eines anorganischen Metalls, anorganischen Salzes oder eines unterschiedlichen organischen Materials vermischt ist.

5. Organische Licht-emittierende Vorrichtung, umfassend in nacheinander laminiertes Form eine erste Elektrode, mindestens eine organische Schicht, und eine zweite Elektrode, wobei mindestens eine Schicht der mindestens einen organischen Schicht mindestens eine der in Anspruch 1 oder Anspruch 2 definierten Verbindungen umfasst.
6. Organische Licht-emittierende Vorrichtung gemäss Anspruch 5, wobei die Zahl der kondensierten Cycloalkane oder Polycycloalkane 1 bis 4 ist.
7. Organische Licht-emittierende Vorrichtung gemäss Anspruch 5 oder Anspruch 6, wobei das Polycycloalkan Bicycloalkan ist.
8. Organische Licht-emittierende Vorrichtung gemäss irgendeinem der Ansprüche 7 bis 9, wobei die organische Schicht, die die mindestens eine in Anspruch 1 oder Anspruch 2 definierte Verbindung enthält, mit 0,1 bis 99,0 Gew. % eines anorganischen Metalls, anorganischen Salzes oder eines unterschiedlichen organischen Materials vermischt ist.

Revendications

1. composé de la formule (1) suivante :



(1)

dans laquelle

A_1 et A_2 désignent chacun un cycloalcane en C_{2-30} substitué ou non substitué, ou un polycycloalcane en C_{1-50} substitué ou non substitué directement condensé à un cycle benzénique d'un hydrocarbure polycyclique aromatique ; R_1 à R_4 sont choisis chacun dans le groupe constitué par 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 C_{1-12} linéaire ou ramifié, substitué ou non substitué, un groupe hétérocyclique aromatique ou non aromatique et substitué ou non substitué, un groupe aryle substitué ou non substitué, un groupe mono ou diarylamine et substitué ou non substitué et un groupe aralkylamine substitué ou non substitué,

dans laquelle R' et R'' sont choisis chacun dans le groupe constitué par un groupe alkyle en C_{1-60} substitué ou non substitué, un groupe aryle substitué ou non substitué et un groupe hétérocyclique de 5 à 7 chaînons substitué ou non substitué,

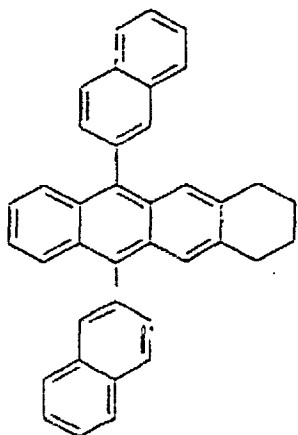
à condition que R_1 et R_2 ne soient pas simultanément un atome d'hydrogène ;

k et l sont un nombre entier de 0 à 2 (à condition que $k+l \geq 1$) ; et

m et n sont un nombre entier de 1 à 4.

2. Composé selon la revendication 1, dans lequel le composé représenté par la formule (1) est choisi dans le groupe constitué des composés représentés par les formules (1-1) à (1-13) suivantes :

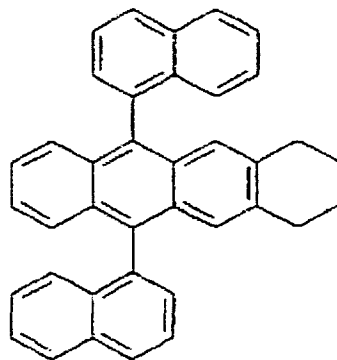
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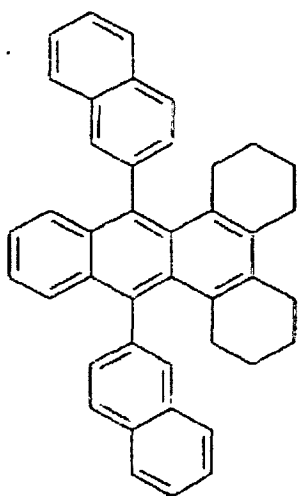
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(1-1)



(1-2)

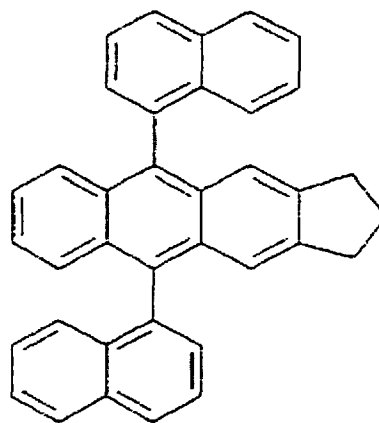
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(1-3)



(1-4)

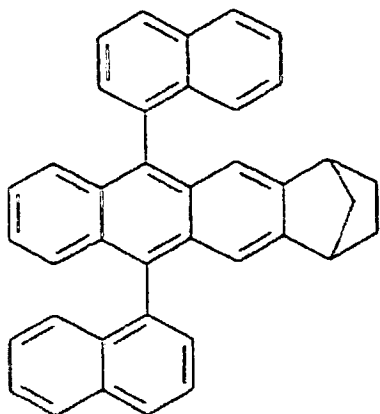
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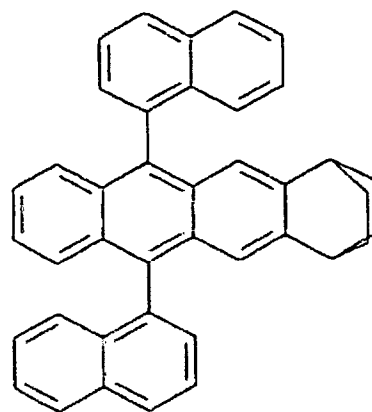
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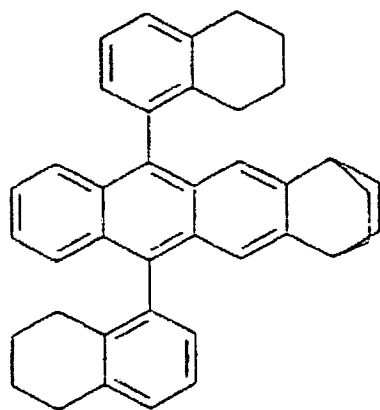
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(1-5)



(1-6)

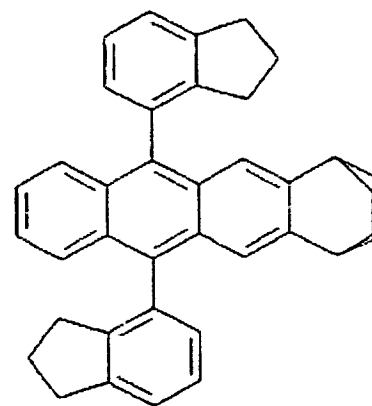
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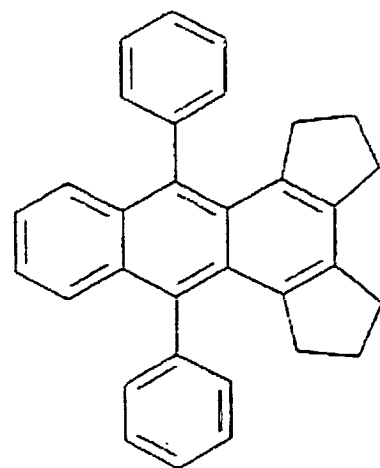
(1-7)



(1-8)

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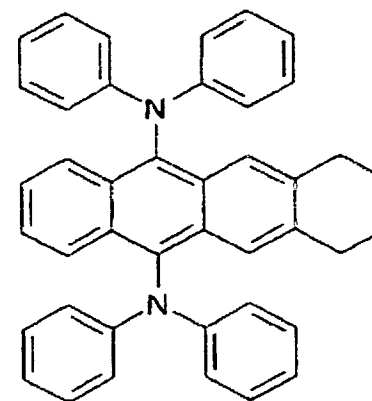
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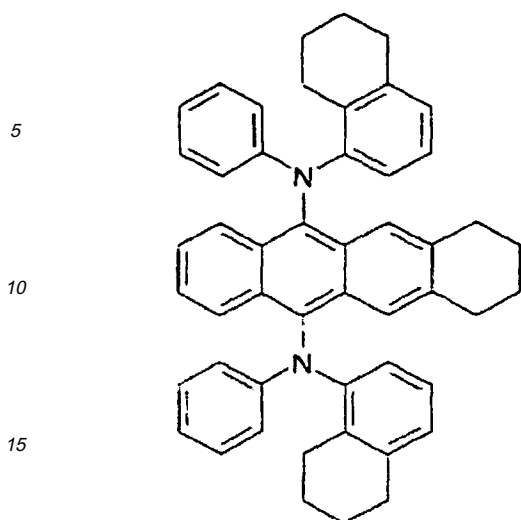
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(1-9)

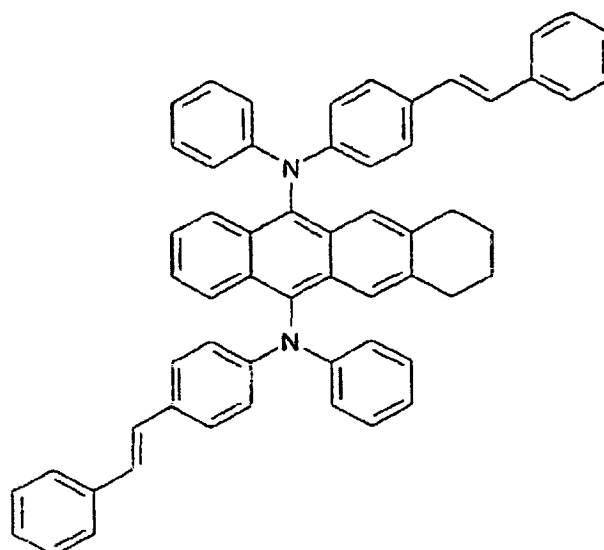


(1-10)

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(1-11)



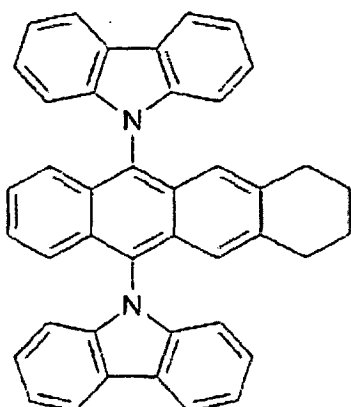
(1-12)

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(1-13)

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3. Composé selon la revendication 1 ou la revendication 2, dans lequel le composé réalise au moins l'une quelconque des fonctions parmi l'émission de lumière, l'injection de trous, le transport de trou, et le transport d'électrons dans un dispositif électronique organique.
 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 minéral, ou d'un matériau organique différent.
 5. Dispositif électroluminescent organique comprenant, successivement stratifiées, une première électrode, au moins une couche organique, et une deuxième électrode, dans lequel au moins une couche de ladite au moins une couche organique comprend au moins un composé 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 polycycloalcane(s) condensé(s) est de 1 à 4.
 7. Dispositif électroluminescent organique selon la revendication 5 ou la revendication 6, dans lequel le polycycloalcane est un bicycloalcane.

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8. Dispositif électroluminescent organique selon l'une quelconque des revendications 7 à 9, dans lequel la couche organique contenant le au moins un composé tel que défini selon la revendication 1 ou la revendication 2 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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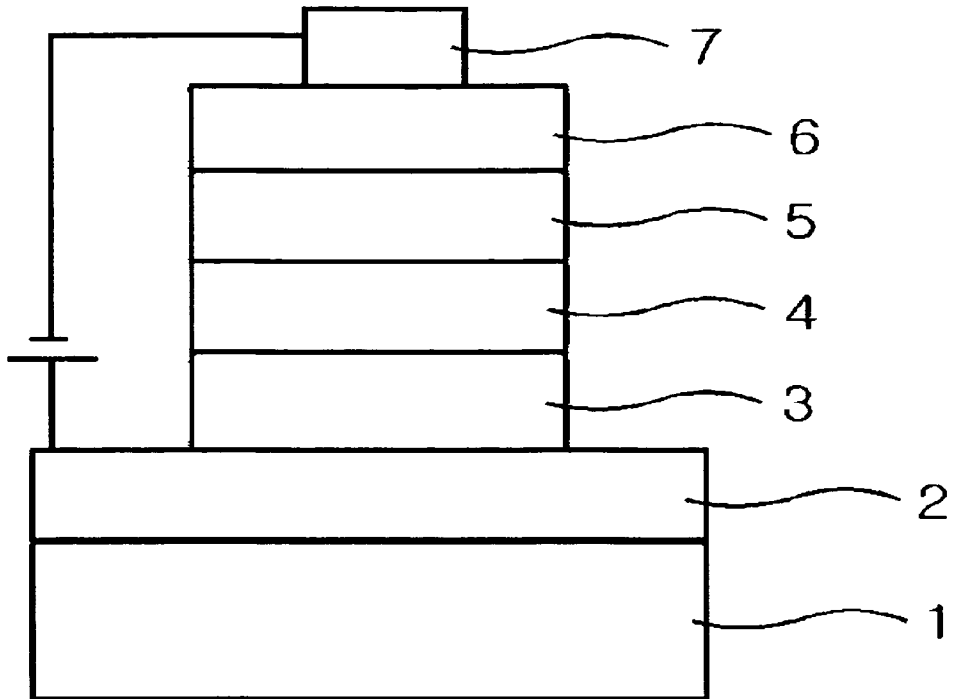
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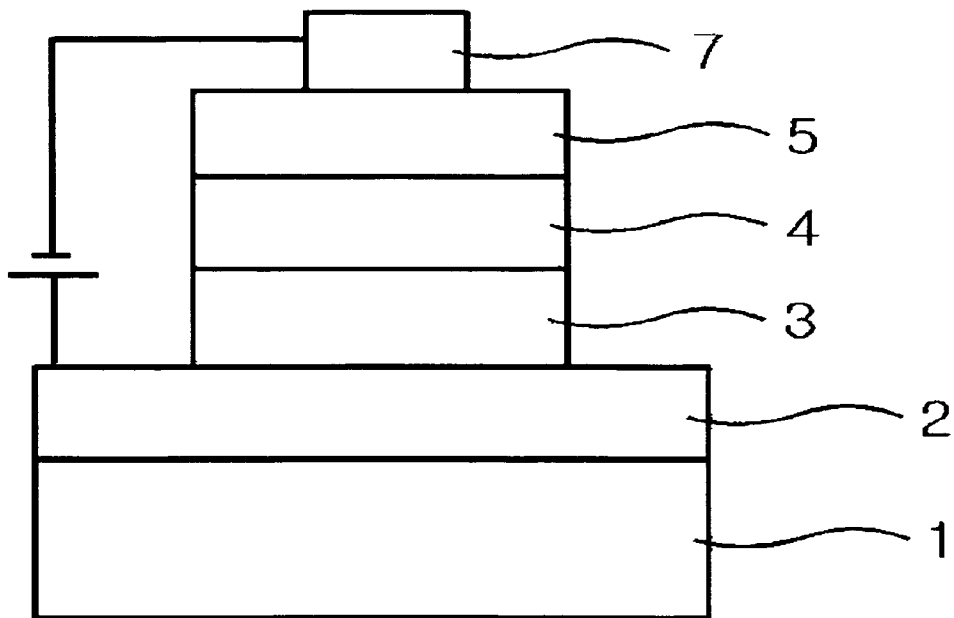
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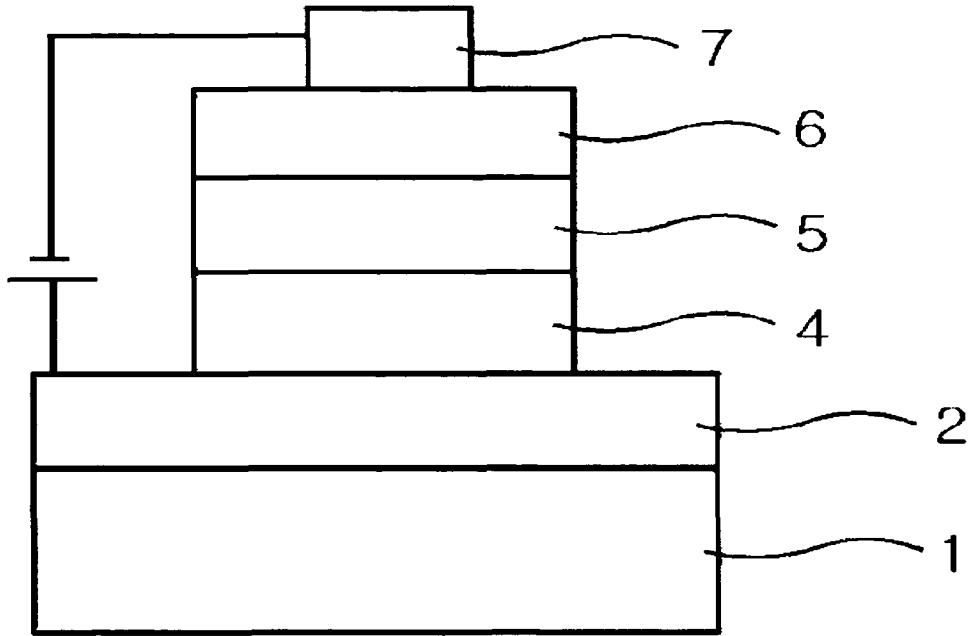
[Fig. 1]



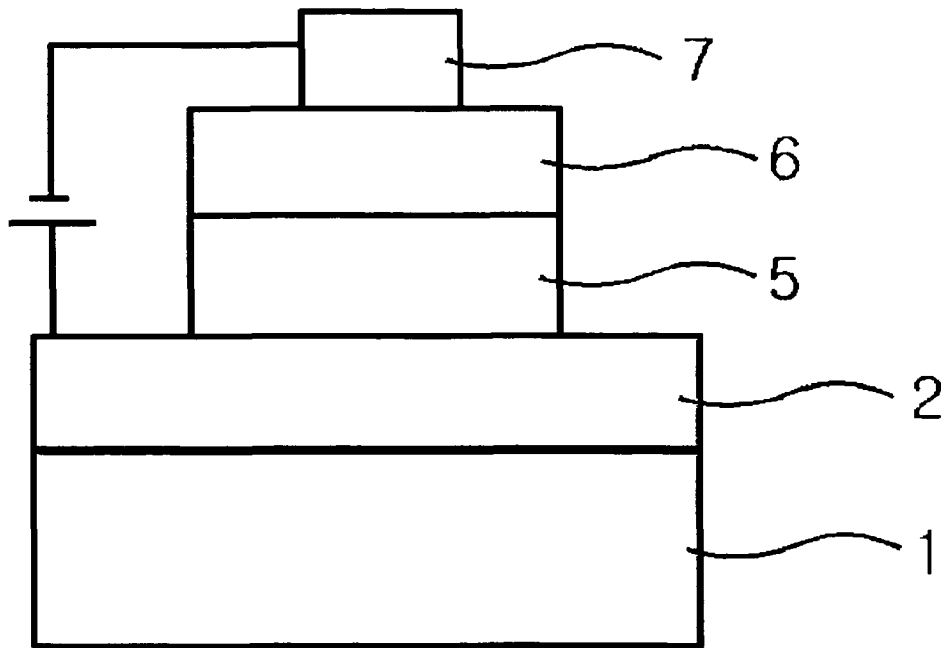
[Fig. 2]



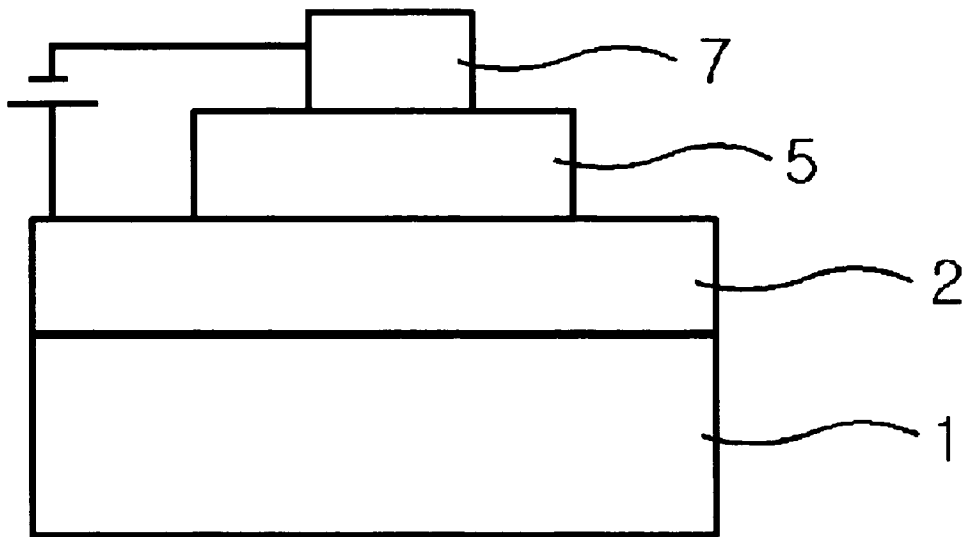
[Fig. 3]



[Fig. 4]



[Fig. 5]



REFERENCES CITED IN THE DESCRIPTION

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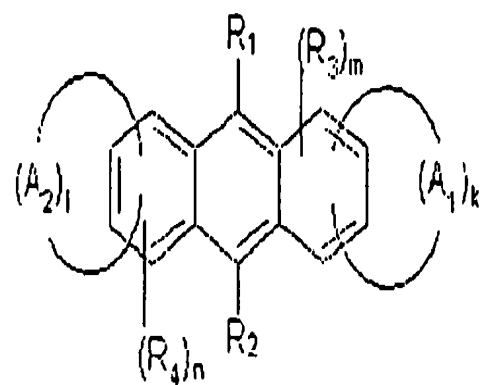
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专利名称(译)	有机化合物和使用其的有机发光器件		
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[标]申请(专利权)人(译)	乐金化学股份有限公司		
申请(专利权)人(译)	LG化学有限公司.		
当前申请(专利权)人(译)	LG化学有限公司.		
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发明人	KIM, KONG-KYEOM HONG, SUNG-KIL JANG, HYE-YOUNG JEONG, DONG-SEOB,		
IPC分类号	C09K11/06		
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优先权	1020050086501 2005-09-15 KR		
其他公开文献	EP1943323A4 EP1943323A1		
外部链接	Espacenet		

摘要(译)

多环芳烃化合物本发明涉及多环芳烃化合物，其中取代或未取代的C2-30环烷烃，或取代或未取代的C5-50多环烷烃与所述多环芳烃的取代基稠合，如式(3)所示。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。



(1);