Title: NOVEL ORGANIC ELECTROLUMINESCENT COMPOUND AND ORGANIC ELECTROLUMINESCENT DEVICE COMPRISING THE SAME

Abstract: The present disclosure relates to a novel organic electroluminescent compound and an organic electroluminescent device comprising the same. The organic electroluminescent compound of the present disclosure has excellent hole transport ability, and thus can be used for a hole transport layer. By comprising the organic electroluminescent compound of the present disclosure, an organic electroluminescent device showing improved current efficiency, improved power efficiency, and long lifespan can be provided.
Description

Title of Invention: NOVEL ORGANIC ELECTROLUMINESCENT COMPOUND AND ORGANIC ELECTROLUMINESCENT DEVICE COMPRISING THE SAME

Technical Field

[1] The present disclosure relates to a novel organic electroluminescent compound and an organic electroluminescent device comprising the same.

Background Art

[2] An electroluminescent (EL) device is a self-light-emitting device which has advantages in that it provides a wider viewing angle, a greater contrast ratio, and a faster response time. An organic EL device was first developed by Eastman Kodak, by using small aromatic diamine molecules and aluminum complexes as materials to form a light-emitting layer [Appl. Phys. Lett. 51, 913, 1987].

[3] The organic EL device converts electric energy into light when electricity is applied to an organic light-emitting material(s). Generally, the organic EL device has a structure comprising an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer of the organic EL device comprises a hole injection layer, a hole transport layer, a light-emitting layer (comprising a host material and a dopant material), an electron transport layer, an electron injection layer, etc. Depending on its function, materials for forming the organic layer can be classified as a hole injection material, a hole transport material, a light-emitting material, an electron transport material, an electron injection material, etc. When a voltage is applied to the organic EL device, holes and electrons are injected from an anode and a cathode, respectively, to the light-emitting layer. Excitons having high energy are formed by recombinations between the holes and the electrons, the energy puts the organic light-emitting compound in an excited state, and the decay of the excited state results in a relaxation of the energy level into a ground state, accompanied by light-emission.

[4] The most important factor determining luminous efficiency in the organic EL device is light-emitting materials. The light-emitting material needs to have high quantum efficiency, high electron mobility, and high hole mobility. Furthermore, the light-emitting layer formed by the light-emitting material needs to be uniform and stable. Depending on colors visualized by light-emission, the light-emitting materials can be classified as a blue-, green-, or red-emitting material, and can additionally include a yellow- or orange-emitting material. Depending on the excited state, the light-emitting material can be classified as fluorescent materials (singlet state) and phosphorescent
materials (triplet state). Fluorescent materials have been widely used for the organic EL device. However, since phosphorescent materials enhance luminous efficiency by four (4) times compared to fluorescent materials and can reduce power consumption to have longer lifespan, development of phosphorescent light-emitting materials are widely being researched.

[5] Iridium(III) complexes have been widely known as phosphorescent materials, including bis(2-(2'-benzothienyl)-pyridinato-N,C-3')iridium(acetylacetonate) ((acac)Ir(btp)2), tris(2-phenylpyridine)iridium (Ir(ppy)3) and bis(4,6-difluorophenylpyridinato-N,C2)picolinate iridium (Firpic) as red-, green- and blue-emitting materials, respectively.

[6] The light-emitting material can be prepared by combining a host material with a dopant to improve color purity, luminous efficiency, and stability. The host materials greatly influence the efficiency and performance of the EL device when using a host material/dopant system as the light emitting material, and thus their selection is important. At present, 4,4'-N,N'-dicarbazol-biphenyl (CBP) is the most widely known host material for phosphorescent materials. Recently, Pioneer (Japan) et al., developed a high performance organic EL device using bathocuproine (BCP) and aluminum(III)bis(2-methyl-8-quinolinate)(4-phenylphenolato) (BAIq) etc., as host materials, which were known as hole blocking materials.

[7] Although these phosphorescent host materials provide good light-emitting characteristics, they have the following disadvantages: (1) Due to their low glass transition temperature and poor thermal stability, their degradation may occur during a high-temperature deposition process in a vacuum. (2) The power efficiency of the organic EL device is given by [(π/voltage) x current efficiency], and the power efficiency is inversely proportional to the voltage. Although the organic EL device comprising phosphorescent host materials provides higher current efficiency (cd/A) than one comprising fluorescent materials, a significantly high driving voltage is necessary. Thus, there is no merit in terms of power efficiency (lm/W). (3) Furthermore, the operational lifespan of the organic EL device is short, and luminous efficiency is still required to be improved.

[8] Meanwhile, copper phthalocyanine (CuPc), 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (NPB), N,N'-diphenyl-N,N'-bis(3-methylphenyl)-(1,1-biphenyl)-4,4'-diamine (TPD), 4,4',4''-tris(3-methylphenylphenylamino)triphenylamine (MTDATA), etc., were used as a hole injection and transport material for an organic EL device. However, the organic EL device using these materials is problematic in quantum efficiency and lifespan. It is due to thermal stress occurring between an anode and a hole injection layer, when the organic EL device is driven under high current. Thermal stress sig-
significantly reduces the lifespan of the device. Furthermore, since the organic material used in the hole injection layer has very high hole mobility, the hole-electron charge balance may be broken and quantum efficiency (cd/A) may decrease.

In order to prevent the decrease of quantum efficiency and enhance luminous efficiency, the holes and the electrons should recombine within the light-emitting layer. For such improvements of luminous characteristics of the organic EL device, it is important to develop a hole transport material and an electron transport material as well as a host material and a dopant material. Accordingly, there is a growing interest in organic compounds efficiently transporting holes and electrons from electrodes to the light-emitting layer.

Korean Patent Application Laying-open Nos. 10-2012-0014913 and 10-2012-0047706 disclose, respectively, fluorene derivatives as a hole transport compound, and fused heterocyclic derivatives as a hole injection and transport compound or an electron injection and transport compound. However, it is necessary to develop organic compounds having better current and power efficiencies than those of the above references.

**Disclosure of Invention**

**Technical Problem**

The objective of the present disclosure is to provide an organic electroluminescent compound having good hole transport ability, and an organic electroluminescent device comprising the organic electroluminescent compound of the present disclosure in a hole transport layer and having improved current and power efficiencies and long lifespan.

**Solution to Problem**

The present inventors found that the above objective can be achieved by an organic electroluminescent compound represented by the following formula 1.

```
Ar2
  \N-\L2-\L1-\R4 (R7)c
  \Ar1

[R5]a
  \X
```

(1)

wherein

- \( L_1 \) represents a single bond, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (5- to 30-membered)heteroarylene;
- \( L_2 \) represents a single bond, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (5- to 30-membered)heteroarylene;
Art and Ar₂, each independently, represent a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl;

X represents -O-, -S-, -C(Ri)(R₂)-, or -N(R₃)-;

R₁ to R₅, each independently, represent hydrogen, deuterium, a halogen, a cyano, a carboxy, a nitro, a hydroxy, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl; or R₁ and R₂ may be linked with each other to form a (3- to 30-membered), mono- or polycyclic, alicyclic or aromatic ring, whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur;

R₄ to R₆, each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (5- to 30-membered)heteroaryl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl(Cl-C30)alkyl, -N(R₁₀)(Rn), -Si(R₁₂)(R₁₃)(R₁₄), -S(Si₃), -O(R₁₆), a cyano, a nitro, or a hydroxy; or may be linked to an adjacent substituent(s) to form a (3- to 30-membered), mono- or polycyclic, alicyclic or aromatic ring, whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur;

R₁₀ to R₁₆, each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (5- to 30-membered)heteroaryl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked to an adjacent substituent(s) to form a (3- to 30-membered), mono- or polycyclic, alicyclic or aromatic ring, whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen and sulfur;

the heteroaryl(ene) and the heterocycloalkyl, each independently, contain at least one hetero atom selected from B, N, O, S, P(=0), Si, and P;

a and b, each independently, represent an integer of 1 to 4; where a or b is an integer of 2 or more, each of R₅ or each of R₆ may be the same or different;

c represents an integer of 1 or 2; and where c is 2, each of R₇ may be the same or different.

Advantageous Effects of Invention
The organic electroluminescent compound of the present disclosure has excellent hole transport ability. Thus, by comprising the organic electroluminescent compound of the present disclosure in a hole transport layer, an organic electroluminescent device shows increased current density and lowered driving voltage, thereby providing increased current and power efficiencies and long lifespan.

**Mode for the Invention**

Hereinafter, the present disclosure will be described in detail. However, the following description is intended to explain the present disclosure, and is not meant in any way to restrict the scope of the present disclosure.

The present disclosure provides the organic electroluminescent compound of formula 1 above, an organic electroluminescent material comprising the same, and an organic electroluminescent device comprising the material.

Herein, 
"(C1-C30)alkyl(ene)" indicates a linear or branched alkyl(ene) having 1 to 30, preferably 1 to 20, and more preferably 1 to 10 carbon atoms, and includes methyl, ethyl, n-propyl, isopropyl, n-butyl, isobutyl, tert-butyl, etc. 
"(C2-C30) alkenyl" indicates a linear or branched alkenyl having 2 to 30, preferably 2 to 20, and more preferably 2 to 10 carbon atoms and includes vinyl, 1-propenyl, 2-propenyl, 1-butenyl, 2-butenyl, 3-butenyl, 2-methylbut-2-enyl, etc. 
"(C2-C30)alkynyl" indicates a linear or branched alkenyl having 2 to 30, preferably 2 to 20, and more preferably 2 to 10 carbon atoms and includes ethynyl, 1-propynyl, 2-propynyl, 1-butynyl, 2-butylnyl, 3-butylnyl, 1-methylpent-2-ynyl, etc. 
"(C3-C30)cycloalkyl" indicates a mono- or polycyclic hydrocarbon having 3 to 30, preferably 3 to 20, and more preferably 3 to 7 carbon atoms and includes cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, etc. 
"(3- to 7-membered) heterocycloalkyl" indicates a cycloalkyl having 3 to 7, preferably 5 to 7 ring backbone atoms including at least one hetero atom selected from B, N, O, S, P(=0), Si, and P, preferably O, S, and N, and includes tetrahydrofuran, pyrrolidine, thiolan, tetrahydropyran, etc. Furthermore, 
"(C6-C30)aryl(ene)" indicates a monocyclic or fused ring derived from an aromatic hydrocarbon and having 6 to 30, preferably 6 to 20, and more preferably 6 to 15 ring backbone carbon atoms, and includes phenyl, biphenyl, terphenyl, naphthyl, fluorenyl, phenanthrenyl, anthracenyl, indenyl, triphenylphenyl, pyrenyl, tetracenyl, perylenyl, chrysennyl, naphthacenyl, fluoranthenyl, etc. 
"(3- to 30-membered) heteroaryl(ene)" indicates an aryl group having 3 to 30, preferably 3 to 20, and more preferably 3 to 15 ring backbone atoms including at least one, preferably 1 to 4, hetero atom selected from the group consisting of B, N, O, S, P(=0), Si, and P; may be a monocyclic ring, or a fused ring condensed with at least one benzene ring; may be partially saturated; may be one formed by linking at least one heteroaryl or aryl group to a heteroaryl group via a single bond(s); and includes a
monocyclic ring-type heteroaryl such as furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiodiazolyl, isoazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, etc., and a fused ring-type heteroarylen such as benzofuranyl, benzothiophenyl, isobenzofuranyl, dibenzofuranyl, dibenzothiophenyl, benzoimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quininazolyl, quinoxalinyl, carbazolyl, phenoxazinyl, phenanthridinyl, benzodioxolyl, etc. Furthermore, "halogen" includes F, Cl, Br, and I.

Herein, "substituted" in the expression, "substituted or unsubstituted," means that a hydrogen atom in a certain functional group is replaced with another atom or group, i.e., a substituent. In formula 1 of the present disclosure, the substituents of the substituted alkyl, the substituted cycloalkyl, the substituted cycloalkenyl, the substituted heterocycloalkyl, the substituted aryl(ene) and the substituted heteroarylen(ene) in Li, L₂, A₁, A₂, R₁ to R₇, and R₁₀ to R₁₆, each independently, are at least one selected from the group consisting of deuterium, a halogen, a cyano, a carboxy, a nitro, a hydroxy, a (Cl-C30)alkyl, a halo(Cl-C30)alkyl, a (C2-C30)alkenyl, a (C2-C30)alkynyl, a (Cl-C30)alkoxy, a (Cl-C30)alkylthio, a (C3-C30)cycloalkyl, a (C3-C30)cycloalkenyl, a (3- to 7-membered) heterocycloalkyl, a (C6-C30)aryloxy, a (C6-C30)arylmthio, a (3- to 30-membered) heteroaryl unsubstituted or substituted with a (C6-C30)aryl, a (C6-C30)aryl unsubstituted or substituted with a (3- to 30-membered) heteroaryl, a tri(Cl-C30)alkylsilyl, a tri(C6-C30)arylsilyl, a di(Cl-C30)alkyl(C6-C30)arylsilyl, a (Cl-C30)alkyldi(C6-C30)arylsilyl, an amino, a mono- or di(Cl-C30)alkylamino, a mono- or di(C6-C30)arylamino, a (Cl-C30)alkylcarbonyl, a (C6-C30)arylcarbonyl, a (C6-C30)arylcrotonyl, a di(Cl-C30)alkylcarbonyl, a (Cl-C30)alkyl(C6-C30)arylcrotonyl, a (C6-C30)aryl(Cl-C30)alkyl, and a (C1-C30)alkyl(C6-C30)aryl.

In formula 1, Li and L₂, each independently, represent preferably, a single bond, a substituted or unsubstituted (C6-C20)arylene, or a substituted or unsubstituted (5- to 20-membered) heteroarylene; and more preferably, a single bond, a substituted or unsubstituted (C6-C15)arylene, or a substituted or unsubstituted (5- to 15-membered) nitrogen-containing heteroarylene. Specifically, Li and L₂, each independently, may be selected from a single bond, a substituted or unsubstituted phenyl, a substituted or unsubstituted naphthyl, a substituted or unsubstituted biphenyl, a substituted or unsubstituted terphenyl, a substituted or unsubstituted pyridyl, a substituted or unsubstituted pyrimidinyl, a substituted or unsubstituted triazinyl, and a substituted or unsubstituted fluorenyl. The substituent of Li and L₂ may be selected from a (Cl-C10)alkyl, a mono-
or di(C6-C18)arylamino, and a (C6-C18)aryl.

[31] In formula 1, Ar1 and Ar2, each independently, represent preferably, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered) heteroaryl; and more preferably, a substituted or unsubstituted (C6-C15)aryl, or a substituted or unsubstituted (5- to 15-membered) nitrogen-containing heteroaryl. Specifically, Ar1 and Ar2, each independently, may be selected from a substituted or unsubstituted phenyl, a substituted or unsubstituted naphthyl, a substituted or unsubstituted biphenyl, a substituted or unsubstituted terphenyl, a substituted or unsubstituted phenanthrenyl, a substituted or unsubstituted anthracenyl, a substituted or unsubstituted triphenylenyl, a substituted or unsubstituted fluorenyl, a substituted or unsubstituted benzofluorenyl, a substituted or unsubstituted pyridyl, a substituted or unsubstituted pyrimidinyl, a substituted or unsubstituted triazinyl, a substituted or unsubstituted quinolyl, a substituted or unsubstituted isoquinolyl, a substituted or unsubstituted quinazolinyl, a substituted or unsubstituted quinoxalinyl, and a substituted or unsubstituted phenanthridinyl. The substituent of Ar1 and Ar2 may be selected from a (Cl-C10)alkyl, a mono- or di(C6-C18)arylamino, and a (C6-C18)aryl.

[32] In formula 1, X represents -O-, -S-, -C(R0(R2))- or -N(R3)-. R1 to R3, each independently, represent preferably, a substituted or unsubstituted (Cl-C20)alkyl, or a substituted or unsubstituted (C6-C20)aryl; and more preferably, a substituted or unsubstituted (Cl-C10)alkyl, or a substituted or unsubstituted (C6-C15)aryl. Specifically, X may represent -O-, -S-, or -C(Ri)(Rj)-.

[33] In formula 1, R4 represents preferably, a substituted or unsubstituted (Cl-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered) heteroaryl; and more preferably, a substituted or unsubstituted (Cl-C10)alkyl, a substituted or unsubstituted (C6-C15)aryl, or a substituted or unsubstituted (5- to 15-membered) nitrogen-containing heteroaryl. Specifically, R4 may be selected from a substituted or unsubstituted (Cl-C10)alkyl, a substituted or unsubstituted phenyl, a substituted or unsubstituted biphenyl, a substituted or unsubstituted terphenyl, a substituted or unsubstituted naphthyl, a substituted or unsubstituted phenanthrenyl, a substituted or unsubstituted anthracenyl, a substituted or unsubstituted fluorenyl, a substituted or unsubstituted pyridyl, and a substituted or unsubstituted pyrimidinyl. The substituent of R4 may be selected from a (Cl-C10)alkyl, a mono- or di(C6-C18)arylamino, and a (C6-C18)aryl.

[34] In formula 1, R5 to R7, each independently, represent preferably, hydrogen, a substituted or unsubstituted (Cl-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, a substituted or unsubstituted (5- to 20-membered) heteroaryl, or -N(Ri)(Rj); and more preferably hydrogen, a substituted or unsubstituted (Cl-C10)alkyl, a substituted or unsubstituted (C6-C15)aryl, a substituted or unsubstituted (5- to 15-membered) nitrogen-
containing heteroaryl, or \(-\text{N}(R_i)\)\(_n\). \(R_i\) to \(R_{11}\), each independently, represent preferably, a substituted or unsubstituted \((C6-C20)\)aryl; and more preferably, a substituted or unsubstituted \((C6-C15)\)aryl.

According to one embodiment of the present disclosure, in formula 1, \(L_i\) and \(L_{2}\), each independently, may represent a single bond, a substituted or unsubstituted \((C6-C20)\)arylene, or a substituted or unsubstituted \((5\text{-}20\text{-}membered)\)heteroarylene; \(A_{ri}\) and \(A_{r2}\), each independently, may represent a substituted or unsubstituted \((C6-C20)\)aryl, or a substituted or unsubstituted \((5\text{-}20\text{-}membered)\)heteroaryl; \(R_i\) to \(R_3\), each independently, may represent a substituted or unsubstituted \((Cl-C20)\)alkyl, or a substituted or unsubstituted \((C6-C20)\)aryl; \(R_4\) may represent a substituted or unsubstituted \((Cl-C20)\)alkyl, \(R_5\) to \(R_7\), each independently, may represent hydrogen, a substituted or unsubstituted \((Cl-C20)\)alkyl, a substituted or unsubstituted \((C6-C20)\)aryl, a substituted or unsubstituted \((5\text{-}20\text{-}membered)\)heteroaryl, or \(-\text{N}(R_i)\)\(_n\); and \(R_{i0}\) to \(R_{11}\), each independently, may represent a substituted or unsubstituted \((C6-C20)\)aryl.

According to another embodiment of the present disclosure, in formula 1, \(L_i\) and \(L_{2}\), each independently, may represent a single bond, a substituted or unsubstituted \((C6-C15)\)arylene, or a substituted or unsubstituted \((5\text{-}15\text{-}membered)\) nitrogen-containing heteroarylene; \(A_{ri}\) and \(A_{r2}\), each independently, may represent a substituted or unsubstituted \((C6-C15)\)aryl, or a substituted or unsubstituted \((5\text{-}15\text{-}membered)\) nitrogen-containing heteroaryl; \(R_1\) to \(R_3\), each independently, may represent a substituted or unsubstituted \((Cl-C15)\)alkyl, or a substituted or unsubstituted \((C6-C15)\)aryl; \(R_4\) may represent a substituted or unsubstituted \((Cl-C15)\)alkyl, a substituted or unsubstituted \((C6-C15)\)aryl, or a substituted or unsubstituted \((5\text{-}15\text{-}membered)\) nitrogen-containing heteroaryl; \(R_5\) to \(R_7\), each independently, may represent hydrogen, a substituted or unsubstituted \((Cl-C15)\)alkyl, a substituted or unsubstituted \((C6-C15)\)aryl, a substituted or unsubstituted \((5\text{-}15\text{-}membered)\) nitrogen-containing heteroaryl, or \(-\text{N}(R_i)\)\(_i\); and \(R_{i0}\) to \(R_{11}\), each independently, may represent a substituted or unsubstituted \((C6-C15)\)aryl.

According to another embodiment of the present disclosure, in formula 1, \(X\) may represent \(-0\text{-}, \text{-S-}, \text{-C(Ri)(R_2)-}\); and \(R_4\) may represent a substituted or unsubstituted \((C6-C20)\)aryl, or a substituted or unsubstituted \((5\text{-}20\text{-}membered)\)heteroaryl.

According to another embodiment of the present disclosure, in formula 1, \(L_i\) and \(L_{2}\), each independently, may represent a single bond or a \((C6-C20)\)arylene; \(X\) may represent \(-0\text{-}, \text{-S-}, \text{-C(Ri)(R_2)-}\); and \(R_4\) may represent a substituted or unsubstituted \((C6-C20)\)aryl.

The compound of formula 1 can be selected from the following, but is not limited
thereto:

[40]

[41]

[42]

[43]

[44]

[45]

[46]
The organic electroluminescent compound of the present disclosure can be prepared by a synthetic method known to one skilled in the art. For example, it can be prepared according to the following reaction scheme 1.

[Reaction Scheme 1]
In the above reaction scheme 1, X, L₁, L₂, Ar₁, Ar₂, R₄ to R₇, a, b, and c are as defined in formula 1 above, and Hal represents a halogen.

According to another aspect of the present disclosure, an organic electroluminescent material comprising the organic electroluminescent compound of formula 1, and an organic electroluminescent device comprising the material are provided. The material may consist of the organic electroluminescent compound of the present disclosure. Otherwise, the material may further comprise a conventional compound(s) which has been comprised in an organic electroluminescent material, in addition to the compound of the present disclosure. The organic electroluminescent device of the present disclosure may comprise a first electrode, a second electrode, and at least one organic layer disposed between the first and second electrodes. The organic layer may comprise at least one organic electroluminescent compound of formula 1.

One of the first and second electrodes may be an anode, and the other may be a cathode. The organic layer may comprise a light-emitting layer, and may further comprise at least one layer selected from a hole injection layer, a hole transport layer, an electron transport layer, an electron injection layer, an interlayer, and a hole blocking layer. The organic electroluminescent compound of formula 1 of the present disclosure may be comprised in a hole transport layer.

When used in the hole transport layer, the organic electroluminescent compound of the present disclosure may be comprised therein as a hole transport material. When used in the light-emitting layer, the organic electroluminescent compound of the present disclosure may be comprised therein as a host material.

The organic electroluminescent device comprising the organic electroluminescent compound of the present disclosure may further comprise at least one host compound other than the organic electroluminescent compound of the present disclosure. Furthermore, the organic electroluminescent device may further comprise at least one dopant.

Where the organic electroluminescent compound of the present disclosure is comprised as a host material (a first host material) in a light-emitting layer, another compound may be comprised as a second host material. The weight ratio between the first host material and the second host material is in the range of 1:99 to 99:1.

The second host material may be from any of the known phosphorescent host materials. The material selected from the group consisting of the compounds of formulae 6 to 8 below is preferable as the second host material in view of luminous efficiency.

\[ H-(Cz-L₄)_{n}M \] (6)

\[ H-(Cz)_{r}L_{q}^{*}M \] (7)
Wherein, \( C_z \) represents the following structure:

\[
R_2^1 \text{ to } R_2^4, \text{ each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (3- to 30-membered)heteroaryl or } R_{25}^i R_{27}, \text{ each independently, represent a substituted or unsubstituted (Cl-C30)alkyl, or a substituted or unsubstituted (C6-C30)aryl; } L_4 \text{ represents a single bond, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (5- to 30-membered)heteroarylene; } M \text{ represents a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl; } Y_1 \text{ and } Y_2, \text{ each independently, represent } -0-, -S-, -N(R_3^i)- \text{ or } -C(R_{32})(R_{33})-, \text{ provided that } Y_1 \text{ and } Y_2 \text{ do not simultaneously exist; } R_{33}^i \text{ to } R_{33}^j, \text{ each independently, represent a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl; } R_{32} \text{ and } R_{33}^i \text{ may be the same or different; } h \text{ and } i, \text{ each independently, represent an integer of } 1 \text{ to } 3; j, k, o \text{ and } p, \text{ each independently, represent an integer of } 0 \text{ to } 4; \text{ and where } h, i, j, k, o \text{ or } p \text{ is an integer of } 2 \text{ or more, each of } (Cz-L_4), \text{ each of } (Cz), \text{ each of } R_{21}, \text{ each of } R_{22}, \text{ each of } R_{23} \text{ or each of } R_{24} \text{ may be the same or different.}
\]

Specifically, the second host material includes the following:
The dopant for the organic electroluminescent device of the present disclosure is preferably at least one phosphorescent dopant. The phosphorescent dopant for the organic electroluminescent device of the present disclosure is not limited, but may be preferably selected from metallated complex compounds of iridium (Ir), osmium (Os), copper (Cu) or platinum (Pt), more preferably selected from ortho-metallated complex compounds of iridium (Ir), osmium (Os), copper (Cu) or platinum (Pt), and even more preferably ortho-metallated iridium complex compounds.

The phosphorescent dopant may be preferably selected from the group consisting of compounds represented by the following formulae 9 to 11.

wherein L is selected from the following structures:

R_{110} represents hydrogen, or a substituted or unsubstituted (Cl-C30)alkyl; R_{i0} to R_{109} and R_{111} to R_{123}, each independently, represent hydrogen, deuterium, a halogen, a (Cl-C30)alkyl unsubstituted or substituted with a halogen, a cyano, a substituted or un-
substituted (Cl-C30)alkoxy, or a substituted or unsubstituted (C3-C30)cycloalkyl, or R
120 to R 1 2 3 may be linked to an adjacent substituent(s) to form a fused ring, e.g.
quiline; R 1 2 4 to R 1 2 7, each independently, represent hydrogen, deuterium, a halogen, a
substituted or unsubstituted (Cl-C30)alkyl, or a substituted or unsubstituted
(C6-C30)aryl; where R 1 2 4 to R 1 2 7 are aryl, they may be linked to an adjacent sub-
stituent(s) to form a fused ring, e.g. fluorene, benzofuran or benzo thiophene; R 2 0 1 to R
2 1 1, each independently, represent hydrogen, deuterium, a halogen, a (Cl-C30)alkyl un-
substituted or substituted with a halogen, or a substituted or unsubstituted
(C6-C30)aryl, or R 2 0 8 to R 2 1 1 may be linked to an adjacent substituent(s) to form a sub-
tituted or unsubstituted (3- to 30-membered), mono- or polycyclic, alicyclic or
aromatic or heteroaromatic ring, e.g. fluorene, dibenzothiophene, or dibenzofuran; o
and p, each independently, represent an integer of 1 to 3; where o or p is an integer of 2
or more, each of R 1 6, o may be the same or different; and q represents an integer of 1 to
3.

[98] Specifically, the phosphorescent dopant material includes the following:

[99]  

[100]  

[101]  

[102]
According to additional aspect of the present disclosure, a mixture or composition for preparing an organic electroluminescent device is provided. The mixture or composition comprises the compound of the present disclosure. The mixture or composition may be a mixture or composition for preparing a light-emitting layer or a hole transport layer of an organic electroluminescent device. The mixture or composition may further comprise a conventional compound(s) which has been comprised for an organic electroluminescent device, in addition to the compound of the present disclosure.

The organic electroluminescent device of the present disclosure may comprise a first electrode, a second electrode, and at least one organic layer disposed between the first and second electrodes. The organic layer may comprise a light-emitting layer, which may comprise the mixture or composition for preparing an organic electroluminescent device of the present disclosure.

The organic electroluminescent device of the present disclosure comprises the compound of formula 1 in the organic layer. The organic electroluminescent device of the present disclosure may further comprise at least one compound selected from the group consisting of arylamine-based compounds and styrylarylamine-based compounds.

In the organic electroluminescent device of the present disclosure, the organic layer may further comprise, in addition to the compound of formula 1, at least one metal selected from the group consisting of metals of Group 1, metals of Group 2, transition metals of the 4th period, transition metals of the 5th period, lanthanides and organic metals of the d-transition elements of the Periodic Table, or at least one complex compound comprising the metal.

In addition, the organic electroluminescent device of the present disclosure may emit white light by further comprising at least one light-emitting layer, which comprises a blue electroluminescent compound, a red electroluminescent compound or a green electroluminescent compound known in the field, besides the compound of the present disclosure. If necessary, it may further comprise an orange light-emitting layer or a yellow light-emitting layer.

In the organic electroluminescent device of the present disclosure, preferably, at least one layer (hereinafter, "a surface layer") may be placed on an inner surface(s) of one or
both electrode(s), selected from a chalcogenide layer, a metal halide layer and a metal oxide layer. Specifically, a chalcogenide (includes oxides) layer of silicon or aluminum is preferably placed on an anode surface of an electroluminescent medium layer, and a metal halide layer or a metal oxide layer is preferably placed on a cathode surface of an electroluminescent medium layer. Such a surface layer provides operation stability for the organic electroluminescent device. Preferably, the chalcogenide includes SiO_x (1<X<2), AlO_x (1≤X<1.5), SiON, SiAlON, etc.; the metal halide includes LiF, MgF_2, CaF_2, a rare earth metal fluoride, etc.; and the metal oxide includes Cs_2O, Li_2O, MgO, SrO, BaO, CaO, etc.

[117] In the organic electroluminescent device of the present disclosure, a mixed region of an electron transport compound and a reductive dopant, or a mixed region of a hole transport compound and an oxidative dopant may be placed on at least one surface of a pair of electrodes. In this case, the electron transport compound is reduced to an anion, and thus it becomes easier to inject and transport electrons from the mixed region to an electroluminescent medium. Furthermore, the hole transport compound is oxidized to a cation, and thus it becomes easier to inject and transport holes from the mixed region to the electroluminescent medium. Preferably, the oxidative dopant includes various Lewis acids and acceptor compounds, and the reductive dopant includes alkali metals, alkali metal compounds, alkaline earth metals, rare-earth metals, and mixtures thereof. A reductive dopant layer may be employed as a charge generating layer to prepare an electroluminescent device having two or more light-emitting layers and emitting white light.

[118] In order to form each layer of the organic electroluminescent device of the present disclosure, dry film-forming methods such as vacuum evaporation, sputtering, plasma and ion plating methods, or wet film-forming methods such as ink jet printing, nozzle printing, slot coating, spin coating, dip coating, and flow coating methods can be used.

[119] When using a wet film-forming method, a thin film can be formed by dissolving or diffusing materials forming each layer into any suitable solvent such as ethanol, chloroform, tetrahydrofuran, dioxane, etc. The solvent can be any solvent where the materials forming each layer can be dissolved or diffused, and where there are no problems in film-formation capability.

[120] Hereinafter, the compound of the present disclosure, the preparation method of the compound, and the luminescent properties of the device will be explained in detail with reference to the following examples.

[121]

[122] Example 1: Preparation of compound C-3
Preparation of compound 1-1

After introducing 1,2-dibromobenzene 31g (130mmol), 4-dibenzofuran boronic acid 25g (120mmol), palladium tetrakis(triphenylphosphine) [Pd(PPh₃)₄] 4.1g (3.54mmol), sodium carbonate 31g (295mmol), toluene 600mL and ethanol 150mL into a reaction vessel, distilled water 150mL was added thereto. The mixture was stirred for 6 hours at 120°C. After the completion of the reaction, the mixture was washed with distilled water, and extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed therefrom by a rotary evaporator. The products were purified by column chromatography to obtain compound 1-1 (22g, 59%).

Preparation of compounds 1-2 and 1-3

After introducing compound 1-1, 22g (69mmol) and tetrahydrofuran 250mL into a reaction vessel, the mixture was cooled to -78°C under nitrogen atmosphere, and n-butyl lithium 33mL (2.5M, 83mmol) was then dropped slowly thereto. The mixture was stirred for 2 hours at -78°C, and 4-bromobenzophenone dissolved in tetrahydrofuran 250 mL was then dropped slowly thereto. After the dropping, the mixture was warmed slowly to room temperature, and then additionally stirred for 30 minutes. After adding ammonium chloride aqueous solution to the reaction mixture to terminate the reaction, the mixture was extracted with ethyl acetate. The organic layer was dried with magnesium sulfate, and the solvent was then removed by a rotary evaporator to obtain compound 1-2. After adding acetic acid 700 mL and HCl 0.5 mL to the obtained compound 1-2, the mixture was stirred at 120°C overnight. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound 1-3 (22g, 65%).

Preparation of compound C-3

[128]
After introducing compound 1-3, 8 g (16.41mmol), 4-(naphthalen-2-yl)-N-phenylaniline 4.8 g (16.41 mmol), palladium(II) acetate [Pd(OAc)₂] 0.15 g (0.66 mmol), tri-t-butyl phosphine [P(tBu)₃] 0.8 mL (50%, 1.64 mmol), sodium tert-butoxide (NaOtBu) 2.4 g (24.62 mmol) and o-xylene 80 mL into a reaction vessel, the mixture was under reflux for 2 hours. The reaction mixture was cooled to room temperature, and then filtered. The obtained solids were washed with methylene chloride (MC). The filtrate was distilled under reduced pressure, and purified by column chromatography to obtain compound C-3 (5.9 g, 51%).

Example 2: Preparation of compound C-1

After introducing compound 1-3, 6 g (12.31 mmol), di([l,l'-biphenyl]-4-yl)amine 4 g (12.31 mmol), palladium(II) acetate 0.11 g (0.50 mmol), tri-t-butyl phosphine 0.5 mL (50%, 1.00 mmol), sodium tert-butoxide 1.8 g (18.47 mmol) and o-xylene 62 mL into a reaction vessel, the mixture was under reflux for 2 hours. The reaction mixture was cooled to room temperature, and then filtered. The obtained solids were washed with methylene chloride (MC). The filtrate was distilled under reduced pressure, and purified by column chromatography to obtain compound C-1 (1.7 g, 19%).

Example 3: Preparation of compound C-25

After introducing compound 1-3, 7 g (14.36 mmol), (4-([l,l'-biphenyl]-4-yl(phenyl)amino)boronic acid 6.3 g (17.23 mmol), palladium tetrakis(triphenylphosphine) 0.5 g (0.43 mmol), sodium carbonate 3.8 g (35.90 mmol), toluene 72 mL and ethanol 18 mL into a reaction vessel, distilled water 18 mL was added thereto. The mixture was stirred for 6 hours at 120°C. After the completion of the reaction, the mixture was washed with distilled water, and extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound C-25 (25.2 g, 50%).

Example 4: Preparation of compound C-38

After introducing compound 1-3, 7 g (14.36 mmol), 6-(2-naphthyl)quinolylboronic acid 5.3 g (17.23 mmol), palladium(II) acetate [Pd(OAc)₂] 0.2 g (0.66 mmol), tri-t-butyl phosphine [P(tBu)₃] 0.8 mL (50%, 1.64 mmol), sodium tert-butoxide (NaOtBu) 2.4 g (24.62 mmol) and o-xylene 80 mL into a reaction vessel, the mixture was under reflux for 2 hours. The reaction mixture was cooled to room temperature, and then filtered. The obtained solids were washed with methylene chloride (MC). The filtrate was distilled under reduced pressure, and purified by column chromatography to obtain compound C-38 (5.9 g, 51%).
After introducing dibenzo[b,d]thiophen-4-yl boronic acid 30g (132mmol), l-bromo-2-iodobenzene 74g (263mmol), palladium tetrakis(triphenylphosphine) 7.6g (6.5mmol), potassium carbonate 36.3g (263mmol), toluene 900mL and ethanol 130mL into a reaction vessel, the mixture was stirred for 12 hours at 120°C. After cooling the reaction mixture to room temperature, the cooled mixture was diluted with ethyl acetate, washed with distilled water, and then dried with anhydrous magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound 2-1 (29g, 56%).

Preparation of compound 2-2

After dissolving compound 2-1, 29.2g (86.1mmol) into tetrahydrofuran 500mL, n-butyl lithium 51.6mL (2.5 M, in hexane) was added slowly thereto at -78°C. After 1 hour, (4-chlorophenyl)(phenyl)methanone 22.4g (103mmol) dissolved in tetrahydrofuran 100mL was added slowly to the mixture. The mixture was warmed to room temperature, and then stirred for 12 hours. After the completion of the reaction, the mixture was washed with distilled water, extracted with ethyl acetate, and then dried with magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound 2-2 (28g, 68%).

Preparation of compound 2-3

After introducing compound 2-2, 28g (58.7mmol), hydrochloric acid 0.24mL (2.93mmol) and acetic acid 600mL into a reaction vessel, the mixture was stirred for 12 hours at 130°C. After the completion of the reaction, the mixture was extracted with methylene chloride, and then dried with magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound 2-3 (13g, 48%).

Preparation of compound C-38

After introducing compound 2-3, 7g (15.2 mmol), 4-(naphthalen-2-yl)-N-phenylaniline 4.9g (16.8mmol), tris(dibenzylindeneacetone)dipalladium(0) [Pd2(dba)3] 0.7g (7.6mmol), S-Phos (2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl) 0.75g (18.3 mmol), sodium tert-butoxide 3.66g (38.1mmol) and o-xylene 100mL into a reaction vessel, the mixture was
stirred for 1 hour at 180°C, and then cooled to room temperature. The cooled mixture was diluted with ethyl acetate, washed several times with water, and then dried with anhydrous magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound C-38 (1.8g, 16%).

[149]

Example 5: Preparation of compound C-36

After introducing compound 2-3, 6g (13.1mmol), di([l,r-biphenyl]-4-yl)amine 4.62g (14.4 mmol), tris(dibenzylideneacetone)dipalladium(0) 0.6g (0.65mmol), S-Phos 0.64g (1.57mmol), sodium tert-butoxide 3.14g (32.7mmol) and o-xylene 90mL into a reaction vessel, the mixture was stirred for 1 hour at 180°C, and then cooled to room temperature. The cooled mixture was diluted with ethyl acetate, washed with distilled water, and then dried with anhydrous magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound C-36 (3.0g, 31%).

[150]

Example 6: Preparation of compound C-ll

After introducing compound 1-3, 7.3 g (15.07 mmol), 9,9-dimethyl-N-phenyl-9H-fluoren-2-amine 4.3 g (15.07 mmol), palladium(II) acetate 0.13 g (0.60 mmol), tri-t-butyl phosphine 0.7 mL (50%, 1.51 mmol), sodium tert-butoxide 2.2 g (22.61 mmol) and o-xylene 75 mL into a reaction vessel, the mixture was under reflux for 2 hours. The reaction mixture was cooled to room temperature, and then filtered. The obtained solids were washed with methylene chloride. The filtrate was distilled under reduced pressure, and then purified by column chromatography to obtain compound C-ll (4g, 38%).

[152]

Example 7: Preparation of compound C-98

[157]

Preparation of compound 3-3

After introducing compound 1-1 (10g, 30.9 mmol) and tetrahydrofuran 125 mL into a reaction vessel, the mixture was cooled to -78°C under nitrogen atmosphere, and n-butyl lithium 13mL(2.5M, 34.0mmol) was then dropped slowly thereto. The mixture
was stirred for 1 hour at -78°C, and 3-bromobenzophenone (8.4g, 32.4mmol) dissolved in tetrahydrofuran 40 mL was then dropped slowly thereto. After the dropping, the mixture was warmed slowly to room temperature, and then additionally stirred for 16 hours. After adding ammonium chloride aqueous solution into the reaction mixture to terminate the reaction, the mixture was extracted with ethyl acetate. The extracted organic layer was dried with magnesium sulfate, and the solvent was removed therefrom by a rotary evaporator to obtain compound 3-2. After adding acetic acid 200 mL and HCl 0.3 mL to the obtained compound 3-2, the mixture was stirred at 120°C overnight. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound 3-3 (12g, 80%).

Preparation of compound C-98

After introducing compound 1-3 (5.5g, 11.2mmol), bisbibiphenylamine (3.6g, 11.2mmol), palladium acetate (0.1g, 0.45mmol), S-Phos (0.4g, 1.12mmol), sodium tert-butoxide (2.7g, 28.2mmol) and toluene 60mL into a reaction vessel, the mixture was under reflux for 1 hour. After the completion of the reaction, the mixture was washed with distilled water, and then extracted with methylene chloride (MC). The extracted organic layer was dried with magnesium sulfate. After removing the solvent by a rotary evaporator, the products were purified by column chromatography to obtain compound C-98 (7g, 86%).

The physical properties of compounds prepared in Examples 1 to 7 are shown in Table 1 below.

<table>
<thead>
<tr>
<th>Compound</th>
<th>UV (in toluene) (nm)</th>
<th>PL (in toluene) (nm)</th>
<th>Melting Point (°C)</th>
<th>MS/EIMS Found</th>
<th>Calculated</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-3</td>
<td>386</td>
<td>405</td>
<td>258</td>
<td>701.85</td>
<td>701.27</td>
</tr>
<tr>
<td>C-1</td>
<td>384</td>
<td>397</td>
<td>240</td>
<td>727.89</td>
<td>707.29</td>
</tr>
<tr>
<td>C-25</td>
<td>378</td>
<td>397</td>
<td>161</td>
<td>727.89</td>
<td>727.29</td>
</tr>
<tr>
<td>C-38</td>
<td>380</td>
<td>405</td>
<td>289</td>
<td>718.25</td>
<td>717.25</td>
</tr>
<tr>
<td>C-36</td>
<td>374</td>
<td>393</td>
<td>242</td>
<td>744.26</td>
<td>743.26</td>
</tr>
<tr>
<td>C-11</td>
<td>378</td>
<td>389</td>
<td>153</td>
<td>691.86</td>
<td>691.29</td>
</tr>
<tr>
<td>C-98</td>
<td>360</td>
<td>392</td>
<td>282</td>
<td>727.89</td>
<td>727.29</td>
</tr>
</tbody>
</table>

Device Example 11 OLED using the compound of the present disclosure

OLED was produced using the compound of the present disclosure as follows. A transparent electrode indium tin oxide (ITO) thin film (10 Ω/sq) on a glass substrate for an organic light-emitting diode (OLED) (Geomatec) was subjected to an ultrasonic
washing with acetone and isopropanol, sequentially, and was then stored in isopropanol. The ITO substrate was then mounted on a substrate holder of a vacuum vapor depositing apparatus. N',N' - ([1,1'-biphenyl]-4,4'-diyl)bis(N-1-(naphthalen-1-yl)-N4,N4'-diphenylbenzene-1,4-diamine) was introduced into a cell of said vacuum vapor depositing apparatus, and then the pressure in the chamber of said apparatus was controlled to 10^-6 torr. Thereafter, an electric current was applied to the cell to evaporate the above introduced material, thereby forming a hole injection layer having a thickness of 60 nm on the ITO substrate. Compound C-25 was then introduced into another cell of said vacuum vapor depositing apparatus, and evaporated by applying electric current to the cell, thereby forming a hole transport layer having a thickness of 20 nm on the hole injection layer. Thereafter, compound H-1 was introduced into one cell of the vacuum vapor depositing apparatus as a host material, and compound D-1 was introduced into another cell as a dopant. The two materials were evaporated at different rates, so that the dopant was deposited in a doping amount of 15 wt% based on the total amount of the host and dopant to form a light-emitting layer having a thickness of 30 nm on the hole transport layer.

2-(4-(9,10-di(naphthalen-2-yl)anthracen-2-yl)phenyl)-1-phenyl-1H-benzo[1]imidazole was then introduced into one cell, and lithium quinolate was introduced into another cell. The two materials were evaporated at the same rate, so that they were respectively deposited in a doping amount of 50 wt% to form an electron transport layer having a thickness of 30 nm on the light-emitting layer. After depositing lithium quinolate as an electron injection layer having a thickness of 2 nm on the electron transport layer, an Al cathode having a thickness of 150 nm was then deposited by another vacuum vapor deposition apparatus on the electron injection layer. Thus, an OLED was produced. All the materials used for producing the OLED were those purified by vacuum sublimation at 10^-6 torr. The produced OLED showed green emission having a luminance of 1,300 cd/m^2 and a current density of 2.7 mA/cm^2.

[168] **Device Example 21: OLED using the compound of the present disclosure**

[169] OLED was produced in the same manner as in Device Example 1, except that compound C-1 was used to form a hole transport layer having a thickness of 20 nm; and after introducing compound H-2 as a host material and compound D-78 as a dopant into the two cells of the vacuum vapor depositing apparatus, respectively, the two materials were evaporated at different rates, so that the dopant was deposited in a doping amount of 3 wt% based on the total amount of the host and dopant to form a light-emitting layer having a thickness of 30 nm on the hole transport layer. The produced OLED showed red emission having a luminance of 1,500 cd/m^2 and a current density of 10.2 mA/cm^2.
Device Example 3: OLED using the compound of the present disclosure

OLED was produced in the same manner as in Device Example 1, except that compound C-3 was used to form a hole transport layer, and compound H-3 and compound D-3 shown in the below table were used as a host material and a dopant, respectively. The produced OLED showed blue emission having a luminance of 900 cd/m² and a current density of 17.3 mA/cm².

Device Example 4: OLED using the compound of the present disclosure

OLED was produced in the same manner as in Device Example 1, except that compound C-36 was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed green emission having a luminance of 800 cd/m² and a current density of 1.7 mA/cm².

Device Example 5: OLED using the compound of the present disclosure

OLED was produced in the same manner as in Device Example 1, except that compound C-98 was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed green emission having a luminance of 1,100 cd/m² and a current density of 2.3 mA/cm².

Device Example 6: OLED using the compound of the present disclosure

OLED was produced in the same manner as in Device Example 2, except that compound C-11 was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed red emission having a luminance of 1,000 cd/m² and a current density of 6.3 mA/cm².

Comparative Device Example 1: OLED using conventional compounds

OLED was produced in the same manner as in Device Example 1, except that N,N'-di(4-biphenyl)-N,N'-di(4-biphenyl)-4,4'-diaminobiphenyl was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed green emission having a luminance of 10,000 cd/m² and a current density of 26.5 mA/cm².

Comparative Device Example 2: OLED using conventional compounds

OLED was produced in the same manner as in Device Example 3, except that N,N'-di(4-biphenyl)-N,N'-di(4-biphenyl)-4,4'-diaminobiphenyl was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed blue emission having a luminance of 4,000 cd/m² and a current density of 108.1 mA/cm².

Comparative Device Example 3: OLED using conventional compounds

OLED was produced in the same manner as in Device Example 2, except that
N,N'-di(4-biphenyl)-N,N'-di(4-biphenyl)-4,4'-diaminobiphenyl was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed red emission having a luminance of 8,000 cd/m² and a current density of 102.6 mA/cm².

[Comparative Device Example 4]

OLED was produced in the same manner as in Device Example 1, except that N,N-di([1,1'-biphenyl]-4-yl)-7,7-dimethyl-7H-fluoreno[4,3-b]benzofuran-9-amine (HT-1) was used to form a hole transport layer having a thickness of 20 nm. The produced OLED showed green emission having a luminance of 7,000 cd/m² and a current density of 17.2 mA/cm².

As confirmed by the Device Examples, the organic electroluminescent compound of the present disclosure has better luminous characteristics than the conventional compounds. The organic electroluminescent device of the present disclosure shows excellences in luminous efficiency, especially current and power efficiencies, and lifespan by using the organic electroluminescent compound of the present disclosure.
Claims

[Claim 1] An organic electroluminescent compound represented by the following formula 1:

$$\text{(1)}$$

wherein

$L_i$ represents a single bond, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (5- to 30-membered)heteroarylene;

$L_2$ represents a single bond, a substituted or unsubstituted (C6-C30)arylene, or a substituted or unsubstituted (5- to 30-membered)heteroarylene;

$A_{r1}$ and $A_{r2}$, each independently, represent a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl;

$X$ represents -0-, -S-, -C(R$_1$)(R$_2$)-, or -N(R$_3$)-;

$R_i$ to $R_3$, each independently, represent hydrogen, deuterium, a halogen, a cyano, a carboxy, a nitro, a hydroxy, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (C3-C30)cycloalkenyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl, or a substituted or unsubstituted (5- to 30-membered)heteroaryl; or $R_i$ and $R_2$ may be linked with each other to form a (3- to 30-membered), mono- or polycyclic, alicyclic or aromatic ring, whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur;

$R_4$ to $R_7$, each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (5- to 30-membered)heteroaryl, a substituted or unsubstituted (C3-C30)cycloalkyl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, a substituted or unsubstituted (C6-C30)aryl(Cl-C30)alkyl, -N(R$_{10}$)(Rn), -Si(R$_{12}$)(R$_{14}$)(Ri$_4$), -S(R$_{15}$), -
0(Ri)₆, a cyano, a nitro, or a hydroxy; or may be linked to an adjacent substituent(s) to form a (3- to 30-membered), mono- or polycyclic, alicyclic or aromatic ring, whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur; Rio to R₁₆, each independently, represent hydrogen, deuterium, a halogen, a substituted or unsubstituted (Cl-C30)alkyl, a substituted or unsubstituted (C6-C30)aryl, a substituted or unsubstituted (5- to 30-membered)heteroaryl, a substituted or unsubstituted (3- to 7-membered)heterocycloalkyl, or a substituted or unsubstituted (C3-C30)cycloalkyl; or may be linked to an adjacent substituent(s) to form a (3- to 30-membered), mono- or polycyclic, alicyclic or aromatic ring, whose carbon atom(s) may be replaced with at least one hetero atom selected from nitrogen, oxygen, and sulfur; the heteroaryl(ene) and the heterocycloalkyl, each independently, contain at least one hetero atom selected from B, N, O, S, P(=0), Si, and P;

a and b, each independently, represent an integer of 1 to 4; where a or b is an integer of 2 or more, each of R₅ or each of R₆ may be the same or different;

c represents an integer of 1 or 2; and where c is 2, each of R₇ may be the same or different.

[Claim 2]

The organic electroluminescent compound according to claim 1, wherein Li and L₂, each independently, represent a single bond, a substituted or unsubstituted (C6-C20)arylene, or a substituted or unsubstituted (5- to 20-membered)heteroarylene; Ar₁ and Ar₂, each independently, represent a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl; R₁ to R₃, each independently, represent a substituted or unsubstituted (Cl-C20)alkyl, or a substituted or unsubstituted (C6-C20)aryl; R₄ represents a substituted or unsubstituted (Cl-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted (5- to 20-membered)heteroaryl; R₅ to R₇, each independently, represent hydrogen, a substituted or unsubstituted (Cl-C20)alkyl, a substituted or unsubstituted (C6-C20)aryl, a substituted or unsubstituted (5- to 20-membered)heteroaryl, or -N(Rio)(Rn); and R₁₁ to R₁₁, each independently, represent a substituted or unsubstituted (C6-C20)aryl.

[Claim 3]

The organic electroluminescent compound according to claim 1, wherein X represents -0-, -S-, or -C(Ri)(R₂); and R₄ represents a sub-
stituted or unsubstituted (C6-C20)aryl, or a substituted or unsubstituted
(5- to 20-membered)heteroaryl.

[Claim 4] The organic electroluminescent compound according to claim 1,
wherein the substituents of the substituted alkyl, the substituted cy-
cloalkyl, the substituted cycloalkenyl, the substituted heterocycloalkyl,
the substituted aryln(ene) and the substituted heteroaryln(ene) in \( L_1 \), \( L_2 \),
\( \text{Ari} \), \( \text{Ar}_2 \), \( \text{R}_1 \) to \( \text{R}_7 \), and \( \text{R}_{10} \) to \( \text{R}_{16} \), each independently, are at least one
selected from the group consisting of deuterium, a halogen, a cyano, a
carboxy, a nitro, a hydroxy, a (Cl-C30)alkyl, a halo(Cl-C30)alkyl, a
(C2-C30)alkenyl, a (C2-C30)alkynyl, a (Cl-C30)alkoxy, a
(Cl-C30)alkythio, a (C3-C30)cycloalkyl, a (C3-C30)cycloalkenyl, a
(3- to 7-membered)heterocycloalkyl, a (C6-C30)aryloxy, a
(C6-C30)arylthio, a (3- to 30-membered)heteroaryl unsubstituted or
substituted with a (C6-C30)aryl, a (C6-C30)aryl unsubstituted or sub-
stituted with a (3- to 30-membered)heteroaryl, a tri(Cl-C30)alkylsilyl,
a tri(C6-C30)arylsilyl, a di(Cl-C30)alkyl(Cl-C30)arylsilyl, a
(C1-C30)alkyldi(C6-C30)arylsilyl, an amino, a mono- or
di(Cl-C30)alkylamino, a mono- or di(C6-C30)arylamino, a
(Cl-C30)alkyl(Cl-C30)arylamino, a (Cl-C30)alkylcarbonyl, a
(Cl-C30)alkoxy carbonyl, a (C6-C30)arylcarbonyl, a
di(C6-C30)arylboronyl, a di(Cl-C30)alkylboronyl, a
(Cl-C30)alkyl(Cl-C30)aryl boronyl, a (C6-C30)aryl(Cl-C30)alkyl, and
a (C1-C30) alkyl(Cl-C30)aryl.

[Claim 5] The organic electroluminescent compound according to claim 1,
wherein the compound of formula 1 is selected from the group
consisting of:
[Claim 6] An organic electroluminescent device comprising the organic electrolu-
minescent compound according to claim 1.
A. CLASSIFICATION OF SUBJECT MATTER

C09K 11/06 (2006.01)  C07D 333/76 (2006.01)  C07D 307/91 (2006.01)  C07D 209/94 (2006.01)  C07C 211/54 (2006.01)
C07D 405/12 (2006.01)  C07D 405/04 (2006.01)  C07D 409/04 (2006.01)  C07D 409/12 (2006.01)  C07D 239/74 (2006.01)
C07D 215/12 (2006.01)  H01L 51/54 (2006.01)

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

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

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

REGISTRY, CAPLUS: Sub-structure search based on formulae (1).

ESPACENET: Inventor + applicant search

C. DOCUMENTS CONSIDERED TO BE RELEVANT

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<th>Category*</th>
<th>Citation of document, with indication, where appropriate, of the relevant passages</th>
<th>Relevant to claim No.</th>
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<td>Documents are listed in the continuation of Box C</td>
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[X] Further documents are listed in the continuation of Box C  [X] See patent family annex

* Special categories of cited documents:
  "A" document defining the general state of the art which is not considered to be of particular relevance
  "E" earlier application or patent but published on or after the international filing date
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  "O" document referring to an oral disclosure, use, exhibition or other means
  "P" document published prior to the international filing date but later than the priority date claimed
  "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
  "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
  "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
  "&" document member of the same patent family

Date of the actual completion of the international search
8 December 2014

Date of mailing of the international search report
08 December 2014

Name and mailing address of the ISA/AU

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Authorised officer

Marc Kloth
AUSTRALIAN PATENT OFFICE
(ISO 9001 Quality Certified Service)
Telephone No. +61 3 9935 9609

Form PCT/ISA/210 (fifth sheet) (July 2009)
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<td>WO 2010/137601 A1 (SEMICONDUCTOR ENERGY LABORATORY CO., LTD.) 02 December 2010 see abstract; page 4, paragraph [0015], formula (GI); and examples on pages 17-24 cited in the application</td>
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<td>WO 2010/083872 A2 (MERCK PATENT GMBH) 29 July 2010 see abstract; examples on pages 10-19 cited in the application</td>
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<td>SARAGI T.P.I. et al, &quot;Light responsive amorphous organic field-effect transistor based on spiro-linked compound&quot;, Optical Materials, 2007, 29, 879-884 see abstract; and page 880, figure 1, compound a</td>
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<td>EP 2096108 A1 (GRACEL DISPLAY INC.) 02 September 2009 see abstract; table 1, pages 196-200, compounds 2245-2310; and table 2, pages 329-334, compounds 4621-4686</td>
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<td>EP 2108690 A1 (GRACEL DISPLAY INC.) 14 October 2009 see abstract; table 1, pages 170-194, compounds 1050-1315; and table 2, pages 311-337, compounds 2368-2651</td>
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This Annex lists known patent family members relating to the patent documents cited in the above-mentioned international search report. The Australian Patent Office is in no way liable for these particulars which are merely given for the purpose of information.

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End of Annex

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

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