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(54) Title: NOVEL ORGANIC ELECTROLUMINESCENT COMPOUNDS AND ORGANIC ELECTROLUMINESCENT DE-VICE USING THE SAME

(57) Abstract: Provided are novel organic electroluminescent compounds and an organic electroluminescent device using the same. More particularly, the organic electroluminescent compound disclosed herein is represented by Chemical Formula 1. Since the organic electroluminescent compound disclosed herein exhibits good luminescent efficiency and life property, it may be used to manufacture OLED devices having very superior operation life.

Description

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

Technical Field

[1] The present invention relates to novel organic electroluminescent compounds and an organic electroluminescent device using the same. The organic electroluminescent compound according to the present invention is represented by Chemical Formula 1:

[2] [Chemical Formula 1]

[3]
$$R_{3}$$
 R_{1} R_{1} R_{1} R_{2} R_{1} R_{10} R_{11} R_{12} R_{15} R_{14} R_{15} R_{15}

Background Art

- [4] In general, the organic EL device commonly has a configuration of anode/hole injection layer (HIL)/hole transport layer (HTL)/emission material layer (EML)/electron transport layer (ETL)/electron injection layer (EIL)/cathode. Organic electroluminescent devices emitting blue, green or red light may be created depending on how to form the emission material layer.
- [5] In functional aspect, the electroluminescent materials may be divided into host materials and dopant materials. In general, an electroluminescent layer prepared by doping a dopant in a host is known to provide superior EL property. Recently, development of an organic EL device having high efficiency and long operation life is becoming an imminent task. Especially, considering the level of EL performance required for medium-to-large sized OLED panels, development of materials which are much superior to existing electroluminescent materials is urgently needed.
- [6] At present, CBP is the most widely known as a host material for a phosphorescent material. High-efficiency OLEDs using a hole blocking layer comprising BCP, BAlq, etc. are reported. High-performance OLEDs using BAlq derivatives as a host were

reported by Pioneer (Japan) and others.

- [8] Although these materials provide good electroluminescence characteristics, they are disadvantageous in that degradation may occur during the high-temperature deposition process in vacuum because of low glass transition temperature and poor thermal stability. Since the power efficiency of an OLED is given by (II/ voltage) current efficiency, the power efficiency is inversely proportional to the voltage. High power efficiency is required to reduce the power consumption of an OLED. Actually, OLEDs using phosphorescent materials provide much better current efficiency (cd/A) than those using fluorescent materials. However, when the existing materials such as BAlq, CBP, etc. are used as a host of the phosphorescent material, there is no significant advantage in power efficiency (lm/W) over the OLEDs using fluorescent materials because of high driving voltage.
- [9] Further, the OLED devices do not have satisfactory operation life. Therefore, development of more stable, higher-performance host materials is required.

Disclosure of Invention

Technical Problem

[10] Accordingly, an object of the present invention is to provide an organic electroluminescent compound having luminescence efficiency and device operation life improved over existing host materials and having superior backbone with appropriate color coordinates in order to solve the aforesaid problems. Another object of the present invention is to provide an organic electroluminescent device employing the organic electroluminescent compound as an electroluminescent material.

Solution to Problem

- The present invention relates to organic electroluminescent compounds represented by Chemical Formula (1), and an organic electroluminescent device using the same.

 The organic electroluminescent compounds according to the invention exhibit high luminous efficiency, and excellent color purity and life property of the material, so that OLED's with very excellent operation life can be manufactured therefrom.
- [12] [Chemical Formula 1]
- [13]

$$R_{3}$$
 R_{4}
 R_{4}
 R_{4}
 R_{5}
 R_{6}
 R_{6}

- [14] wherein
- [15] Ar₁ and Ar₂ independently represent a chemical bond, (C6-C40)arylene with or without substituent(s) or (C2-C40)heteroarylene with or without substituent(s);
- R₁ through R₁₆ independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), substituted or unsubstituted (C6-C30)aryl fused with one or more (C3-C30)cycloalkyl(s) with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s), 5- to 7-membered heterocycloalkyl with or without substituent(s), 5- to 7-membered heterocycloalkyl fused with one or more aromatic ring(s) with or without substituent(s), (C3-C30)cycloalkyl fused with one or more aromatic ring(s) with or without substituent(s), (C3-C30)cycloalkyl fused with one or more aromatic ring(s) with or without substituent(s), cyano, NR₂₁R₂₂, BR₂₃R₂₄, PR₂₅ R₂₆, P(=O)R₂₇R₂₈, R^aR^bR^cSi-, R^dY-, R^cC(=O)-, R^fC(=O)O-, (C6-C30)ar(C1-C30)alkyl with or without substituent(s), (C2-C30)alkenyl with or without substituent(s),

(C2-C30)alkynyl with or without substituent(s), R_{63} or R_{62} , R_{62} R_{62}

or each of them may be linked to an adjacent substituent via (C3-C30)alkylene or (C3-C30)alkenylene with or without a fused ring to form an alicylic ring, a mono- or polycyclic aromatic ring or a mono- or polycyclic heteroaromatic ring;

- [17] W represents $-(CR_{51}R_{52})_m$, $-(R_{51})C=C(R_{52})$, $-N(R_{53})$, -S, -O, $-Si(R_{54})(R_{55})$, $-P(R_{56})$, $-P(=O)(R_{57})$, -C(=O) or $-B(R_{58})$;
- [18] R_{51} through R_{58} and R_{61} through R_{63} are the same as R_1 through R_{16} ;
- [19] the heterocycloalkyl or heteroaryl may contain one or more heteroatom(s) selected from B, N, O, S, P(=O), Si and P;
- [20] R_{21} through R_{28} independently represent (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or (C3-C30)heteroaryl with or without substituent(s), the R^a , R^b , R^c , and R^d independently represent (C1-C30)alkyl

with or without substituent(s) or (C6-C30)aryl with or without substituent(s), the Y represents S or O, and the R^e and R^f represent (C1-C30)alkyl with or without substituent(s), (C1-C30)alkoxy with or without substituent(s), (C6-C30)aryl with or without substituent(s);

- [21] a and b represent an integer 0 or 2; and
- [22] m represents an integer 1 or 2.

[23]

- In the present invention, "alkyl", "alkoxy" and other substituents containing "alkyl" moiety include both linear and branched species. In the present invention, "cycloalkyl" includes both adamantyl with or without substituent(s) and (C7-C30)bicycloalkyl with or without substituent(s).
- [25] In the present invention, "aryl" means an organic radical derived from an aromatic hydrocarbon by the removal of one hydrogen atom, and may include a 4- to 7-membered, particularly 5- or 6-membered, single ring or fused ring, including a plurality of aryls linked by single bond(s). Specific examples include phenyl, naphthyl, biphenyl, anthryl, indenyl, fluorenyl, phenanthryl, triphenylenyl, pyrenyl, perylenyl, chrysenyl, naphthacenyl, fluoranthenyl, etc., but are not limited thereto. The naphthyl includes 1-naphthyl and 2-naphthyl, the anthryl includes 1-anthryl, 2-anthryl and 9-anthryl, and the fluorenyl includes 1-fluorenyl, 2-fluorenyl, 3-fluorenyl, 4-fluorenyl and 9-fluorenyl. In the present invention, "heteroaryl" means an aryl group containing 1 to 4 heteroatom(s) selected from B, N, O, S, P(=O), Si and P as aromatic ring backbone atom(s), other remaining aromatic ring backbone atoms being carbon. It may be 5- or 6-membered monocyclic heteroaryl or polycyclic heteroaryl resulting from condensation with a benzene ring, and may be partially saturated. Further, the heteroaryl includes more than one heteroaryls linked by single bond(s). The heteroaryl includes a divalent aryl group wherein the heteroatom(s) in the ring may be oxidized or quaternized to form, for example, an N-oxide or a quaternary salt. Specific examples include monocyclic heteroaryl such as furyl, thiophenyl, pyrrolyl, imidazolyl, pyrazolyl, thiazolyl, thiadiazolyl, isothiazolyl, isoxazolyl, oxazolyl, oxadiazolyl, triazinyl, tetrazinyl, triazolyl, tetrazolyl, furazanyl, pyridyl, pyrazinyl, pyrimidinyl, pyridazinyl, etc., polycyclic heteroaryl such as benzofuranyl, benzothiophenyl, isobenzofuranyl, benzimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenanthridinyl, benzodioxolyl, etc., an N-oxide thereof (e.g., pyridyl N-oxide, quinolyl N-oxide, etc.), a quaternary salt thereof, etc., but are not limited thereto.
- [26] The "(C1-C30)alkyl" groups described herein may include (C1-C20)alkyl or (C1-C10)alkyl and the "(C6-C30)aryl" groups include (C6-C20)aryl or (C6-C12)aryl.

The "(C3-C30)heteroaryl" groups include (C3-C20)heteroaryl or (C3-C12)heteroaryl and the "(C3-C30)cycloalkyl" groups include (C3-C20)cycloalkyl or (C3-C7)cycloalkyl. The "(C2-C30)alkenyl or alkynyl" group include (C2-C20)alkenyl or alkynyl, (C2-C10)alkenyl or alkynyl.

- [27] In the term 'substituted or unsubstituted (or with or without) substituent(s)' described herein, the term 'substituted' means having one or more substituent(s) independently selected from deuterium, halogen, (C1-C30)alkyl with or without halogen substituent(s), (C6-C30)aryl, (C3-C30)heteroaryl with or without (C6-C30)aryl substituent(s), a 5- to 7-membered heterocycloalkyl, a 5- to 7-membered heterocycloalkyl fused with one or more aromatic ring(s), (C3-C30)cycloalkyl, (C3-C30)cycloalkyl fused with one or more aromatic ring(s), tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, (C2-C30)alkenyl, $(C2-C30) alkynyl, \ cyano, \ carbazolyl, \ NR_{31}R_{32}, \ BR_{33}R_{34}, \ PR_{35}R_{36}, \ P(=O)R_{37}R_{38}, \\$ (C6-C30)ar(C1-C30)alkyl, (C1-C30)alkyl(C6-C30)aryl, (C1-C30)alkyloxy, (C1-C30)alkylthio, (C6-C30)aryloxy, (C6-C30)arylthio, (C1-C30)alkoxycarbonyl, (C1-C30)alkylcarbonyl, (C6-C30)arylcarbonyl, (C6-C30)aryloxycarbonyl, (C1-C30)alkoxycarbonyloxy, (C1-C30)alkylcarbonyloxy, (C6-C30)arylcarbonyloxy, (C6-C30) aryloxycarbonyloxy, carboxyl, nitro and hydroxyl; or that adjacent substituent(s) are linked together to form a ring; and the R₃₁ through R₃₈ independently represent (C1-C30)alkyl, (C6-C30)aryl or (C3-C30)heteroaryl.
- [28] The R₁ through R₁₆, R₂₁ through R₂₈, R₅₁ through R₅₈, and R₆₁ through R₆₃ are selected from hydrogen, deuterium, halogen, alkyl such as methyl, ethyl, propyl, butyl, pentyl, hexyl, ethylhexyl, heptyl, octyl, etc., aryl such as phenyl, naphthyl, fluorenyl, biphenyl, phenanthryl, terphenyl, pyrenyl, perylenyl, spirobifluorenyl, fluoranthenyl, chrysenyl, triphenylenyl, etc., aryl fused with one or more cycloalkyl such as 1,2-dihydroacenaphthyl, heteroaryl such as dibenzothiophenyl, dibenzofuryl, carbazolyl, pyridyl, furyl, thienyl, quinolyl, triazinyl, pyrimidinyl, pyridazinyl, quinoxalinyl, phenanthrolinyl, etc., heterocycloalkyl fused with one or more aromatic ring such as benzopyrrolidino, benzopiperidino, dibenzomorpholino, dibenzoazepino, etc., amino substituted by aryl such as phenyl, naphthyl, fluorenyl, biphenyl, phenanthryl, terphenyl, pyrenyl, perylenyl, spirobifluorenyl, fluoranthenyl, chrysenyl, triphenylenyl, etc. or heteroaryl such as dibenzothiophenyl, dibenzofuryl, carbazolyl, pyridyl, furyl, thienyl, quinolyl, triazinyl, pyrimidinyl, pyridazinyl, quinoxalinyl, phenanthrolinyl, etc., aryloxy such as biphenyloxy, etc., arylthio such as biphenylthio, etc., aralkyl such as biphenylmethyl, triphenylmethyl, etc.,, R_{63} or

 R_{62} , but are not limited thereto, and may be further substituted as shown in R_{61}

Chemical Formula 1.

[29] More specifically, the R_1 through R_{16} may be exemplified as following structures but are not limited thereto.

- [35] wherein
- [36] R₇₁ through R₁₃₆ independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl, (C6-C30)aryl, (C6-C30)aryl fused with one or more (C3-C30)cycloalkyl(s), (C3-C30)heteroaryl, 5- to 7-membered heterocycloalkyl, 5- to 7-membered heterocycloalkyl fused with one or more aromatic ring(s), (C3-C30)cycloalkyl, (C3-C30)cycloalkyl fused with one or more aromatic ring(s), cyano, amino, (C1-C30)alkylamino, (C6-C30)arylamino, NR₄₁R₄₂, BR₄₃R₄₄, PR₄₅R₄₆, P(=O)R₄₇R₄₈, tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, (C6-C30)arylcarbonyl, (C1-C30)alkylcarbonyl, (C1-C30)alkylcarbonyl, (C6-C30)arylcarbonyl, (C2-C30)alkenyl, (C2-C30)alkynyl, (C6-C30)aryloxycarbonyl, (C2-C30)aryloxycarbonyl, (C2-C30)aryloxycarbonyl, (C6-C30)aryloxycarbonyl, (C2-C30)aryloxycarbonyl, (C2-C30)aryloxycarbonyl,

(C1-C30)alkoxycarbonyloxy, (C1-C30)alkylcarbonyloxy, (C6-C30)arylcarbonyloxy, (C6-C30)aryloxycarbonyloxy, carboxyl, nitro or hydroxyl, or each of them may be linked to an adjacent substituent via (C3-C30)alkylene or (C3-C30)alkenylene with or without a fused ring to form an alicylic ring or a mono- or polycyclic aromatic ring, and

- [37] R_{41} through R_{48} independently represent (C1-C30)alkyl, (C6-C30)aryl or (C3-C30)heteroaryl.
- [38] The *- $(Ar_1)_{\overline{a}}Ar_2$ is exemplified as the following structures but is not limited thereto. a is the same as definition in Chemical Formula 1.

[44]

[49] The organic electroluminescent compound according to the present invention may be specifically exemplified as following compounds but is not limited thereto.

$$\begin{bmatrix} 50 \end{bmatrix}$$

$$\begin{bmatrix} N \\ N \\ N \\ N \end{bmatrix}$$

$$\begin{bmatrix} N \\ N \\ N \end{bmatrix}$$

[59]

[72]

[73]
$$\begin{array}{c} N \\ N \\ N \\ N \end{array}$$
 106
$$\begin{array}{c} N \\ N \\ N \end{array}$$
 107
$$\begin{array}{c} N \\ N \\ N \end{array}$$
 108
$$\begin{array}{c} N \\ N \\ N \end{array}$$
 109
$$\begin{array}{c} N \\ N \\ N \end{array}$$
 110

[74] The organic electroluminescent compound according to the present invention may be prepared as shown in following Reaction Scheme 1.

[75] [76]

[Reaction Scheme 1]

$$\begin{bmatrix} 77 \end{bmatrix} \xrightarrow{R_{5}} \xrightarrow{R_{4}} \xrightarrow{R_{3}} \xrightarrow{R_{2}} \xrightarrow{R_{6}} \xrightarrow{R_{5}} \xrightarrow{R_{4}} \xrightarrow{R_{3}} \xrightarrow{R_{10}} \xrightarrow{R_{11}} \xrightarrow{R_{12}} \xrightarrow{R_{10}} \xrightarrow{R_{11}} \xrightarrow{R_{12}} \xrightarrow{R_{11}} \xrightarrow{R_{12}} \xrightarrow{R_{13}} \xrightarrow{R_{14}} \xrightarrow{R_{15}} \xrightarrow{R_{$$

[78] wherein

[79] R_1 through R_{16} , Ar_1 , Ar_2 , a and b are the same as definition in the Chemical Formula 1.

- [80] Provided is an organic electroluminescent device, which comprises a first electrode; a second electrode; and one or more organic layer(s) interposed between the first electrode and the second electrode, wherein the organic layer comprises one or more organic electroluminescent compound(s) represented by Chemical Formula 1. The organic electroluminescent compound is used as a host material of the electroluminescent layer.
- [81] In addition, the organic layer may include the electroluminescent layer, and the electroluminescent layer may further include one or more dopants besides one or more

organic electroluminescent compounds of Chemical Formula 1. The dopant applied to the organic electroluminescent device of the present invention is not specifically limited.

- [82] Preferably, the dopant applied to the organic electroluminescent device of the present invention may be selected from following Chemical Formula 2.
- [83] [Chemical Formula 2]
- [84] $M^1L^{101}L^{102}L^{103}$
- [85] wherein
- [86] M¹ is a metal selected from a group consisting of Group 7, Group 8, Group 9, Group 10, Group 11, Group 13, Group 14, Group 15 and Group 16 metals, and ligand L¹0¹, L¹0² and L¹0³ are independently selected from the following structures:

$$\begin{bmatrix} 87 \end{bmatrix}$$

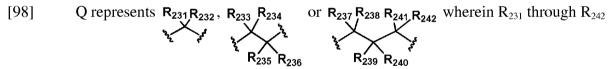
$$\begin{array}{c} R_{217} \\ R_{216} \\ R_{220} \\ R_{211} \\ R_{206} \\ R_{206}$$

$$\begin{bmatrix} 90 \end{bmatrix} \\ R_{211} \\ R_{208} \\ R_{208} \\ R_{207} \\ R_{208} \\ R_{209} \\ R_{209} \\ R_{200} \\ R_{2$$

[91] wherein

[92] R₂₀₁ through R₂₀₃ independently represent hydrogen, (C1-C30)alkyl with or without halogen substituent(s), (C6-C30)aryl with or without (C1-C30)alkyl substituent(s) or halogen;

- [93] R₂₀₄ through R₂₁₉ independently represent hydrogen, (C1-C30)alkyl with or without substituent(s), (C1-C30)alkoxy with or without substituent(s), (C3-C30)cycloalkyl with or without substituent(s), (C2-C30)alkenyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), mono- or di-(C1-C30)alkylamino with or without substituent(s), SF₅, tri(C1-C30)alkylsilyl with or without substituent(s), di(C1-C30)alkylc(C6-C30)arylsilyl with or without substituent(s), tri(C6-C30)arylsilyl with or without substituent(s), cyano or halogen;
- [94] R_{220} through R_{223} independently represent hydrogen, (C1-C30)alkyl with or without halogen substituent(s) or (C6-C30)aryl with or without (C1-C30)alkyl substituent(s);
- [95] R₂₂₄ and R₂₂₅ independently represent hydrogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or halogen, or R₂₂₄ and R₂₂₅ may be linked via (C3-C12)alkylene or (C3-C12)alkenylene with or without a fused to form an alicylic ring or a mono- or polycyclic aromatic ring;
- [96] R₂₂₆ represents (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C5-C30)heteroaryl with or without substituent(s) or halogen;
- [97] R_{227} through R_{229} independently represent hydrogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or halogen; and



independently represent hydrogen, (C1-C30)alkyl with or without halogen substituent(s), (C1-C30)alkoxy, halogen, (C6-C30)aryl with or without substituent(s), cyano, (C5-C30)cycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via alkylene or alkenylene to form a spiro ring or a fused ring, or may be linked to R_{207} or R_{208} via alkylene or alkenylene to form a saturated or unsaturated fused ring.

[99] The meaning of the electroluminescent layer may be a single layer as a layer where the light is emitted or may be a multiple layer where two or more layers are laminated. In the configuration of the present invention, when host-dopant are used in mixture, it is confirmed that the luminous efficiency are remarkably improved by the electroluminescent host of the present invention. It may be configured at doping concentration of 0.5 to 10wt%. Compared to other host materials, the electroluminescent host of the present invention has superior conductivity with respect to the hole and electron and excellent stability in material, thereby showing a characteristic of remarkably in-

creasing its life span as well as improving the luminous efficiency.

[100] The M¹ is selected from a group consisting of Ir, Pt, Pd, Rh, Re, Os, Tl, Pb, Bi, In, Sn, Sb, Te, Au and Ag. The dopant compounds of Chemical Formula 2 are exemplified by the compounds described in Korean Patent Application No. 10-2008-0112855, but are not limited thereto.

- [101] In the organic electronic device of the present invention, the organic layer may further include, in addition to the organic electroluminescent compound represented by Chemical Formula 1, one or more compound(s) selected from a group consisting of arylamine compounds and styrylarylamine compounds, at the same time. The arylamine compounds or styrylarylamine compounds are exemplified in Korean Patent Application No. 10-2008-0123276, 10-2008-0107606 or 10-2008-0118428, but are not limited thereto.
- [102] Further, in the organic electroluminescent device of the present invention, the organic layer may further include, in addition to the organic electroluminescent compound represented by Chemical Formula 1, one or more metal(s) selected from a group consisting of organic metals of Group 1, Group 2, 4th period and 5th period transition metals, lanthanide metals and d-transition elements or complex compound(s). The organic layer may include an electroluminescent layer and a charge generating layer.
- [103] Further, the organic layer may include, in addition to the organic electroluminescent compound of Chemical Formula 1, one or more organic electroluminescent layer(s) emitting blue, green or red light at the same time in order to embody a white-emitting organic electroluminescent device. The compound emitting blue, green or red light may be exemplified by the compounds described in Korean Patent Application No. 10-2008-0123276, 10-2008-0107606 or 10-2008-0118428, but are not limited thereto.
- In the organic electroluminescent device of the present invention, a layer (hereinafter referred to as "surface layer") selected from a chalcogenide layer, a metal halide layer and a metal oxide layer may be placed on the inner surface of one or both electrode(s) among the pair of electrodes. More specifically, a metal chalcogenide (including oxide) layer of silicon or aluminum may be placed on the anode surface of the electroluminescent medium layer, and a metal halide layer or metal oxide layer may be placed on the cathode surface of the electroluminescent medium layer. Operation stability may be attained therefrom.
- [105] The chalcogenide may be, for example, SiO_X ($1 \le x \le 2$), AlO_X ($1 \le x \le 1.5$), SiON, SiAlON, etc. The metal halide may be, for example, LiF, MgF_2 , CaF_2 , a rare earth metal fluoride, etc. The metal oxide may be, for example, Cs_2O , Li_2O , MgO, SrO, BaO, CaO, etc.
- [106] In the organic electroluminescent device according to the present invention, it is also preferable to arrange on at least one surface of the pair of electrodes thus manufactured

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. In that case, since the electron transport compound is reduced to an anion, injection and transport of electrons from the mixed region to an electroluminescent medium are facilitated. In addition, since the hole transport compound is oxidized to a cation, injection and transport of holes from the mixed region to an electroluminescent medium are facilitated. Preferable oxidative dopants include various Lewis acids and acceptor compounds. Preferable reductive dopants include alkali metals, alkali metal compounds, alkaline earth metals, rare-earth metals, and mixtures thereof.

[107] Further, a white-emitting electroluminescent device having two or more electroluminescent layers may be manufactured by employing a reductive dopant layer as a charge generating layer.

Advantageous Effects of Invention

[108] Since the organic electroluminescent compound according to the present invention exhibits good luminous efficiency and excellent life property, it may be used to manufacture OLED devices having very superior operation life.

Brief Description of Drawings

- [109] The present invention is further described with respect to organic electroluminescent compounds according to the present invention, processes for preparing the same, and luminescence properties of devices employing the same. However, the following examples are provided for illustrative purposes only and they are not intended to limit the scope of the present invention.
- [111] [Preparation Example 1] Preparation of Compound 1
- [113] After 2-(2-aminophenyl)benzimidazole (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50 mL), the mixture was heated with stirring for 20 hours. After the reaction temperature was lowered to room temperature, a produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound 1 (4.2 g, 14.22 mmol, 71.10 %).
- [114] [Preparation Example 2] Preparation of Compound 41
- [115]

[110]

- [116] Preparation of Compound **2-1**
- 2,4-dibromo-6-methyl-1,3,5-triazin (20 g) was dissolved in THF (200 mL), and phenylmagnesium bromide (79.08 mL, 237.25 mmol, 3.0M in ethyl ether) was slowly added thereto at 0°C. 5 hours later, distilled water was slowly added. After extracting with EA and washing with distilled water, the extract was dried with magnesium sulfate and distilled under reduced pressure. Recrystallization using EA and methanol gave Compound **2-1** (16 g, 64.70 mmol, 81.90 %).
- [118] Preparation of Compound 2-2
- [119] Compound **2-2** (12.6 g, 45.60 mmol, 70.5 %) was obtained by using Compound **2-1** with reference to Journal of organic chemistry vol. 29, pages 678-681, 1963.
- [120] <u>Preparation of Compound 2-3</u>
- [121] Compound **2-3** (6.7 g, 25.60 mmol, 56.3 %) was obtained by using Compound **2-2** with reference to Journal of organic chemistry vol. 29, pages 678-681, 1963.
- [122] <u>Preparation of Compound 41</u>
- [123] After Compound **2-3** (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50 mL), the mixture was heated with stirring for 20 hours. After lowering reaction temperature to room temperature, the produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound **41** (4.8 g, 10.66 mmol, 53.3 %).
- [124] [Preparation Example 3] Preparation of Compound **86**
- [125] $Br \longrightarrow OH \longrightarrow NH_{2} \longrightarrow NH_{2}N \longrightarrow$
- [126] Preparation of Compound **3-1**
- 2-amino-5-bromobenzoic acid0 (20 g, 92.57 mmol), 1,2-diaminobenzene (10 g, 92.57 mmol), and polyphosphoric acid (100 mL) were mixed and the mixture was stirred at 250 °C for 5 hours. After cooling to 100 °C and slowly adding distilled water thereto, a produced solid was filtered under reduced pressure. NaOH aqueous solution was stirred with the produced solid. When the resultant mixture was neutralized, filtering under reduced pressure followed by recrystallization using methanol gave

Compound **3-1** (11 g, 38.17 mmol, 41.24 %).

- [128] Preparation of Compound 3-2
- [129] After Compound **3-1** (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50 mL), the mixture was heated with stirring for 20 hours. After lowering reaction temperature to room temperature, the produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound **3-2** (4.3 g, 11.49 mmol, 57.0 %).
- [130] Preparation of Compound 86
- [131] Compound **3-2** (4 g, 10.68 mmol), carbazole (1.78 g, 10.68 mmol), Pd(Oac)₂ (0.11 g, 0.53 mmol), P(t-bu)₃ (0.13 mL, 1.06 mmol, 50 % in toluene), NaOt-bu (3.08 g, 32.06 mmol), and toluene (100 mL) were mixted under reflux. 4 hours later, the reaction temperature was lowered to room temperature and distilled water was slowly added thereto. After extracting with EA and drying with magnesium sulfate, distillation under reduced pressure followed by column separation gave Compound **86** (2.6 g, 5.64 mmol, 52.86 %).
- [132] [Preparation Example 4] Preparation of Compound 90

[133]

$$OH$$
 OH
 H_2N
 Br
 H_2N
 H_2

- [134] Preparation of Compound 4-1
- 2-amino-4,5-dibromobenzoic acid (20 g, 92.57 mmol), 1,2-diaminobenzene (10 g, 92.57 mmol), and polyphosphoric acid (100 mL) were mixed and stirred at 250 °C for 5 hours. After cooling at 100 °C, distilled water was slowly added thereto, the produced solid was filtered under reduced pressure. NaOH aqueous solution was stirred with solid. When the resultant mixture was neutralized, filtering under reduced pressure followed by recrystallization using methanol gave Compound **4-1** (17.2 g, 46.86 mmol, 50.62 %).
- [136] Preparation of Compound 4-2
- [137] After Compound **4-1** (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50 mL), the mixture was heated with stirring for 20 hours. When the reaction temperature was lowered to room temperature, the produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound **4-2** (4.7 g, 10.37 mmol, 51.65 %).
- [138] Preparation of Compound 90
- [139] Compound **4-2** (4 g, 8.82 mmol), penylboronic acid (3.22 g, 26.48 mmol), Pd(PPh₃)₄ (0.5 g, 0.44 mmol), 2M K₂CO₃ (15 mL), toluene (100 mL), and ethanol (50 mL) were

mixed and stirred under reflux. 10 hours later, the reaction temperature was lowered to room temperature and distilled water was slowly added thereto. After extracting with EA and drying with magnesium sulfate, distillation under reduced pressure followed by column separation gave Compound **90** (2.3 g, 5.13 mmol, 58.26 %).

[140] [Preparation Example 5] Preparation of Compound 97

- [142] Preparation of Compound 5-1
- 2-amino-3,5-dibromobenzoic acid (20 g, 92.57 mmol), 1,2-diaminobenzene (10 g, 92.57 mmol), and polyphosphoric acid 100 mL were mixed and stirred at 250 °C for 5 hours. After cooling at 100 °C, distilled water was slowly added thereto, the produced solid was filtered under reduced pressure. NaOH aqueous solution was stirred with solid. When the resultant mixture was neutralized, filtering under reduced pressure followed by recrystallization using methanol gave Compound **5-1** (13.5 g, 36.78 mmol, 39.72 %).
- [144] <u>Preparation of Compound 5-2</u>
- [145] After Compound **5-1** (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50 mL), the mixture was heated with stirring for 20 hours. When the reaction temperature was lowered to room temperature, the produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound **5-2** (4.5 g, 9.93 mmol, 49.45 %).
- [146] <u>Preparation of Compound 97</u>
- [147] Compound **5-2** (4 g, 10.68 mmol), carbazole (1.78 g, 10.68 mmol), Pd(Oac)₂ (0.11 g, 0.53 mmol), P(t-bu)₃ (0.13 mL, 1.06 mmol, 50 % in toluene), NaOt-bu (3.08 g, 32.06 mmol), and toluene (100 mL) were mixed and stirred under reflux. 4 hours later, the reaction temperature was lowered to room temperature and distilled water was slowly added thereto. After extracting with EA and drying with magnesium sulfate, distillation under reduced pressure followed by column separation gave Compound **97** 3.2 g(5.11 mmol, 47.9 %).
- [148] [Preparation Example 6] Preparation of Compound **101**
- [149]

[141]

$$CI \stackrel{=N}{\underset{6-1}{\overset{N}{\longrightarrow}}} CI \stackrel{=N}{\underset{6-2}{\overset{N}{\longrightarrow}}} O \stackrel{N}{\underset{N}{\longrightarrow}} O \stackrel{N}{\underset$$

- [150] Preparation of Compound 6-1
- [151] Compound **6-2** (17.8 g, 112.97 mmol, 72.6 %) was obtained by using 5-chloro-2-methylpyrimidine (20 g, 155.57 mmol) with reference to Journal of organic chemistry vol. 29, pages 678-681, 1963.
- [152] Preparation of Compound **6-2**
- [153] Compound **6-2** (8.9 g, 62.44 mmol, 55.28 %) was obtained by using Compound **6-1** with reference to Journal of organic chemistry vol. 29, pages 678-681, 1963.
- [154] <u>Preparation of Compound 6-3</u>
- [155] After Compound **6-2** (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50 mL), the mixture was heated with stirring for 20 hours. When the reaction temperature was lowered to room temperature, the produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound **6-3** (3.7 g, 9.69 mmol, 48.68 %).
- [156] Preparation of Compound **101**
- [157] Compound **6-3** (5 g, 13.09 mmol), 2,6-diphenylpyridine-4-boronic acid (3.6 g, 13.09 mmol), Pd(PPh₃)₄ (0.7 g, 0.65 mmol), 2M K₂CO₃ (20 mL), toluene (100 mL), and ethanol (40 mL) were mixed and stirred under reflux. 12 hours later, the reaction temperature was lowered to room temperature and distilled water was slowly added thereto. After extracting with EA and drying with magnesium sulfate, distillation under reduced pressure followed by column separation gave Compound **101** (3.5 g, 6.06 mmol, 46.36 %).
- [158] [Preparation Example 7] Preparation of Compound **106**

[160] After 2-(2-aminophenyl)benzimidazole (4.18 g, 20.0 mmol) and benzaldehyde (2.3 g, 22.0 mmol) were dissolved in nitrobenzene (50mL), the mixture was heated with stirring for 20 hours. When the reaction temperature was lowered to room temperature, the produced yellow solid was filtered. Washing with ethyl ether and drying gave Compound **106** (4.2 g, 14.22 mmol, 71.10 %).

Organic electroluminescent Compounds 1 to 110 were prepared according to Preparation Examples 1 to 7 and Table 1 shows ¹H NMR and MS/FAB of the prepared organic electroluminescent compounds.

[162] [Table 1]

[163]

| Cmpd. | ¹H NMR(CDCI _{3r} 200 MHz) | MS/FAB | |
|---------|--|--------|------------|
| Cilipu. | H MWIR(CDCI3, 200 WIHZ) | found | calculated |
| 1 | δ = 7.22(2H, m), 7.41(1H, m), 7.51(2H, m), 7.58~7.59(2H, m), 7.83~7.84(2H, m), 8.16(1H, m), 8.28(2H, m), 8.56(1H, m) | 295.34 | 295.11 |
| 4 | $\delta = 7.22 \sim 7.25(3 \text{H, m}), 7.33(1 \text{H, m}), 7.45 \sim 7.5(3 \text{H, m}), 7.58 \sim 7.59(4 \text{H, m}), 7.69(1 \text{H, m}), 7.77(1 \text{H, m}), 7.83 \sim 7.87(3 \text{H, m}), 7.94(1 \text{H, m}), 8.16(1 \text{H, m}), 8.55 \sim 8.56(2 \text{H, m})$ | 460.53 | 460.17 |
| 7 | δ = 7.22(2H, m), 7.42(1H, m), 7.49(1H, m), 7.58~7.63(3H, m), 7.72(1H, m), 7.83~7.84(2H, m), 7.92(1H, m), 8.16(1H, m), 8.56(1H, m), 8.97(1H, m) | 346.38 | 346.12 |
| 13 | $\delta = 7.22(2H, m), 7.41(2H, m), 7.51~7.52(8H, m), 7.58~7.59(2H, m), 7.66(3H, m), 7.83~7.84(2H, m), 8.16(1H, m), 8.56(1H, m)$ | 447.53 | 447.17 |
| 19 | δ = 7.22(2H, m), 7.37(6H, m), 7.46~7.59(13H, m), 7.83~7.89(4H, m), 8.16(1H, m), 8.56(1H, m) | 553.73 | 553.20 |
| 28 | $\delta = 7.22(2H, m)$, $7.53\sim7.59(4H, m)$, $7.83\sim7.84(2H, m)$, $8.01(1H, m)$, $8.16\sim8.18(2H, m)$, $8.56(1H, m)$ | 352.41 | 352.08 |

| 32 | $\delta = 1.69(6H, s), 6.94(1H, s), 7.22~7.3(6H, m), 7.58~7.59(2H, m), 7.83~7.84(2H, m), 8.16(1H, m), 8.56(1H, m)$ | 361.44 | 361.16 |
|----|--|--------|--------|
| 34 | δ = 7(1H, m), 7.22~7.26(3H, m), 7.51(1H, m), 7.58~7.59(2H, m), 7.83~7.88(4H, m), 8.16(1H, m), 8.5(1H, m), 8.56(1H, m), 8.81(2H, m) | | 372.14 |
| 40 | δ = 7.22(2H, m), 7.47(2H, m), 7.54~7.59(6H, m), 7.83~7.84(2H, m), 8.05(2H, m), 8.16(1H, m), 8.3(4H, m), 8.56(1H, m) | 448.52 | 448.17 |
| 41 | δ = 7.22(2H, m), 7.41(2H, m), 7.51(4H, m), 7.58~7.59(2H, m), 7.83~7.84(2H, m), 8.16(1H, m), 8.28(4H, m), 8.56(1H, m) | 450.49 | 450.16 |
| 45 | $\delta = 7.22(2H, m), 7.41~7.59(10H, m), 7.83~7.84(2H, m), 8.11~8.16(2H, m), 8.3(2H, m), 8.56(2H, m)$ | 448.52 | 448.17 |
| 48 | $\delta = 7.22 \sim 7.25 (4H, m), 7.47 (2H, m), 7.54 \sim 7.59 (6H, m), 7.83 \sim 7.85 (4H, m), 8.16 \sim 8.2 (3H, m), 8.3 (4H, m), 8.56 (1H, m)$ | 524.61 | 524.20 |
| 54 | δ = 7.22(2H, m), 7.41(2H, m), 7.51~7.52(8H, m), 7.58~7.59(2H, m), 7.66(3H, m), 7.83~7.84(2H, m), 8.16(1H, m), 8.56(1H, m), 9.48(2H, m) | 525.60 | 525.20 |
| 60 | $\delta = 6.41(1H, m), 6.68(1H, m), 7.1~7.11(2H, m), 7.22(2H, m),$ $7.41~7.44(2H, m), 7.51~7.52(4H, m), 7.58~7.59(2H, m),$ $7.83~7.84(2H, m), 8.16(1H, m), 8.56(1H, m), 9.48(2H, m)$ | | 488.17 |
| 65 | $\delta = 7.22 \sim 7.33(5H, m), 7.5(1H, m), 7.58 \sim 7.68(5H, m),$ | 460.53 | 460.17 |

| | 7.79~7.84(4H, m), 7.94(1H, m), 8.12~8.16(2H, m), | | |
|----|---|--------|--------|
| | 8.55~8.56(2H, m) | | |
| | $\delta = 7.22 \sim 7.33(7H, m), 7.5(1H, m), 7.58 \sim 7.68(5H, m),$ | | |
| 67 | 7.79~7.85(6H, m), 7.94(1H, m), 8.12~8.16(2H, m), | 536.62 | 536.20 |
| | 8.55~8.56(2H, m) | | |
| | $\delta = 7.22 \sim 7.25(6H, m), 7.41(2H, m), 7.51 \sim 7.52(8H, m),$ | | |
| 70 | 7.58~7.59(2H, m), 7.83~7.85(6H, m), 8.16(1H, m), 8.56(1H, | 602.69 | 602.22 |
| | m) | | |
| | $\delta = 7.22 \sim 7.24(3H, m), 7.37(6H, m), 7.46(6H, m),$ | | |
| 72 | 7.55~7.59(6H, m), 7.7(1H, m), 7.83~7.84(2H, m), 8.16(1H, m), | 632.80 | 632.22 |
| | 8.24(2H, m), 8.56(1H, m), 8.67(1H, m) | | |
| | $\delta = 7.22 \sim 7.25(3H, m), 7.33(1H, m), 7.58 \sim 7.68(8H, m),$ | | |
| 78 | 7.79~7.84(4H, m), 7.94(1H, m), 8.16(2H, m), 8.54~8.56(3H, | 510.59 | 510.18 |
| | m) | | |
| | $\delta = 7.22(2H, m), 7.41(4H, m), 7.51(8H, m), 7.58~7.59(2H, m),$ | | |
| 84 | 7.68~7.69(3H, m), 7.77~7.87(7H, m), 8(1H, m), 8.16~8.18(2H, | 923.03 | 922.33 |
| | m), 8.28(8H, m), 8.56(1H, m) | | |
| | δ = 7.22~7.33(5H, m), 7.41(1H, m), 7.5~7.51(3H, m), | | |
| 86 | 7.59~7.63(2H, m), 7.94~7.98(2H, m), 8.06~8.16(3H, m), | 460.53 | 460.17 |
| | 8.28(2H, m), 8.55~8.56(2H, m) | | |
| 90 | δ = 7.22(2H, m), 7.41(3H, m), 7.51(6H, m), 7.59(1H, m), | 447.53 | 447.17 |

| | 7.79(4H, m), 8.12(1H, s), 8.28(2H, m), 8.29(1H, s), 8.56(1H, m) | | |
|-----|---|--------|--------|
| 97 | δ = 7.22~7.33(8H, m), 7.41(1H, m), 7.5~7.51(4H, m), 7.59~7.63(3H, m), 7.94(2H, m), 8.05~8.12(4H, m), 8.28(2H, m), 8.55~8.56(3H, m) | | 625.23 |
| 100 | δ = 7.22(2H, m), 7.41(2H, m), 7.51~7.52(8H, m), 7.59(1H, m), 7.66~7.67(5H, m), 7.84(1H, m), 8.01(1H, m), 8.16(2H, m), 8.56(1H, m), 9.48(2H, m) | | 575.21 |
| 104 | δ = 7.22(2H, m), 7.39~7.41(5H, m), 7.51(4H, m), 7.59(1H, m), 7.91(3H, m), 8.28~8.31(6H, m), 8.56(1H, m), 9.48(2H, m) | 628.68 | 628.21 |
| 105 | δ = 7.22(2H, m), 7.28(1H, m), 7.41(2H, m), 7.51(4H, m), 7.59(1H, m), 7.67(1H, m), 8.28(4H, m), 8.56(1H, m), 8.63(2H, m), 9.48(2H, m) | | 632.19 |
| 106 | δ = 7.22~7.25(8H, m), 7.58~7.59(4H, m), 7.83~7.85(8H, m), 8.16(2H, m), 8.56(2H, m) | 588.66 | 588.21 |
| 107 | $\delta = 7.22 \sim 7.25(8H, m), 7.59(2H, m), 7.67(4H, m),$ $7.83 \sim 7.85(6H, m), 8.16(4H, m), 8.54 \sim 8.56(4H, m)$ | | 688.24 |
| 108 | δ = 7.22~7.25(8H, m), 7.41(4H, m), 7.51(8H, m), 7.59(2H, m), 7.79~7.85(12H, m), 8.12(2H, s), 8.29(2H, s), 8.56(2H, m) | 893.04 | 892.33 |
| 109 | $\delta = 7.22(6H, m), 7.58\sim7.59(6H, m), 7.66(3H, m),$ $7.83\sim7.84(6H, m), 8.16(3H, m), 8.56(3H, m)$ | 729.79 | 729.24 |

| | 7.79(4H, m), 8.12(1H, s), 8.28(2H, m), 8.29(1H, s), 8.56(1H, | | |
|-----|---|--------|--------|
| | m) | | |
| | δ = 7.22~7.33(8H, m), 7.41(1H, m), 7.5~7.51(4H, m), | | |
| 97 | 7.59~7.63(3H, m), 7.94(2H, m), 8.05~8.12(4H, m), 8.28(2H, | 625.72 | 625.23 |
| | m), 8.55~8.56(3H, m) | | |
| | δ = 7.22(2H, m), 7.41(2H, m), 7.51~7.52(8H, m), 7.59(1H, m), | | |
| 100 | 7.66~7.67(5H, m), 7.84(1H, m), 8.01(1H, m), 8.16(2H, m), | 575.66 | 575.21 |
| | 8.56(1H, m), 9.48(2H, m) | | |
| 104 | δ = 7.22(2H, m), 7.39~7.41(5H, m), 7.51(4H, m), 7.59(1H, m), | 628.68 | 628.21 |
| 107 | 7.91(3H, m), 8.28~8.31(6H, m), 8.56(1H, m), 9.48(2H, m) | 020.00 | 020.21 |
| | δ = 7.22(2H, m), 7.28(1H, m), 7.41(2H, m), 7.51(4H, m), | | |
| 105 | 7.59(1H, m), 7.67(1H, m), 8.28(4H, m), 8.56(1H, m), 8.63(2H, | 632.64 | 632.19 |
| | m), 9.48(2H, m) | | |
| 106 | $\delta = 7.22 \sim 7.25(8H, m), 7.58 \sim 7.59(4H, m), 7.83 \sim 7.85(8H, m),$ | 588.66 | 588.21 |
| | 8.16(2H, m), 8.56(2H, m) | 300.00 | 300.21 |
| 107 | $\delta = 7.22 \sim 7.25(8H, m), 7.59(2H, m), 7.67(4H, m),$ | 688.78 | 688.24 |
| 107 | 7.83~7.85(6H, m), 8.16(4H, m), 8.54~8.56(4H, m) | 000.70 | |
| 100 | δ = 7.22~7.25(8H, m), 7.41(4H, m), 7.51(8H, m), 7.59(2H, m), | | 902.22 |
| 108 | 7.79~7.85(12H, m), 8.12(2H, s), 8.29(2H, s), 8.56(2H, m) | 893.04 | 892.33 |
| | $\delta = 7.22(6H, m), 7.58\sim7.59(6H, m), 7.66(3H, m),$ | | 729.24 |
| 109 | 7.83~7.84(6H, m), 8.16(3H, m), 8.56(3H, m) | 729.79 | |
| | | | |

[171]

| 110 | δ = 1.72(6H, s), 7.22(4H, m), 7.58~7.63(6H, m), 7.77(2H, m), 7.83~7.84(4H, m), 7.93(2H, m), 8.16(2H, m), 8.56(2H, m) | | 628.24 |
|-----|--|--|--------|
| | | | |

[172]

[173] [Example 1] Manufacture of OLED device using the organic electroluminescent

compound according to the present invention

[174] An OLED device was manufactured using the electroluminescent material according to the present invention.

- [175] First, a transparent electrode ITO thin film $(15\Omega/\Box)$ obtained from a glass for OLED (produced by Samsung Corning) was subjected to ultrasonic washing with trichloroethylene, acetone, ethanol and distilled water, sequentially, and stored in isopropanol before use.
- Then, an ITO substrate was equipped in a substrate folder of a vacuum vapor deposition apparatus, and 4,4',4"-tris(N,N-(2-naphthyl)-phenylamino)triphenylamine (2-TNATA) was placed in a cell of the vacuum vapor deposition apparatus, which was then ventilated up to 10-6 torr of vacuum in the chamber. Then, electric current was applied to the cell to evaporate 2-TNATA, thereby forming a hole injection layer having a thickness of 60 nm on the ITO substrate.
- [177] Then, *N*,*N*'-bis(a-naphthyl)-*N*,*N*'-diphenyl-4,4'-diamine (NPB) was placed in another cell of the vacuum vapor deposition apparatus, and electric current was applied to the cell to evaporate NPB, thereby forming a hole transport layer having a thickness of 20 nm on the hole injection layer.
- [178] After forming the hole injection layer and the hole transport layer, an electroluminescent layer was formed thereon as follows. Compound 41 was placed in a cell of a vacuum vapor deposition apparatus as host, and Compound Ir(ppy)₃ having a following structure was placed in another cell as a dopant. The two materials were evaporated at different rates such that an electroluminescent layer having a thickness of 30 nm was vapor-deposited on the hole transport layer at 4 to 10 wt%.

- [180] Subsequently, bis(2-methyl-8-quinolinato)(*p*-phenylphenolato)aluminum(III) (BAlq) was vapor-deposited with a thickness of 5 nm as an hole blocking layer on the electro-luminescent layer and tris(8-hydroxyquinoline)-aluminum(III) (Alq) was vapor-deposited with a thickness of 20 nm as an electron transport layer. Then, after vapor-depositing lithium quinolate (Liq) of a following structure with a thickness of 1 to 2 nm as an electron injection layer, an Al cathode having a thickness of 150 nm was formed using another vacuum vapor deposition apparatus to manufacture an OLED.
- [181] Each compound used in the OLED was purified by vacuum sublimation at 10-6 torr.
- [182] [Example 2] Manufacture of OLED using the organic electroluminescent compounds

of the present invention

[183] An OLED was manufactured as in Example 1 except that the hole blocking layer is not used

- [184] [Example 3] Manufacture of OLED using the organic electroluminescent compounds of the present invention
- [185] An OLED was manufactured as in Example 2 except for using Compound **78** as host in the electroluminescent layer and (piq)₂Ir(acac) as dopant.

[186]
$$\begin{array}{c} & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

- [187] [Comparative Example 1] Electroluminescent properties of the OLED device using conventional electroluminescent material
- [188] An OLED was manufactured in the same manner as Example 1 except that 4,4'-Bis(carbazol-9-yl)-biphenyl (CBP) instead of the compounds of the present invention was used as host material in a cell of the vacuum vapor deposition apparatus.
- [189] [Comparative Example 2] Electroluminescent properties of the OLED device using conventional electroluminescent material
- [190] An OLED was manufactured in the same manner as Example 3 except that 4,4'-bis(carbazol-9-yl)biphenyl (CBP) instead of the compounds of the present invention was used as host material in a cell of the vacuum vapor deposition apparatus and Bis(2-methyl-8-quinolinato)(p-phenyl-phenolato)aluminum(III) (BAlq) is used as the hole blocking layer.
- [191] Luminous efficiency of the OLED devices including the organic electroluminescent compound according to the present invention manufactured in Examples 1 to 3 and Comparative Examples 1 and 2 and the conventional electroluminescent compound was measured at 1,000 cd/m². The result is given in Table 2.
- [192] [Table 2]
- [193]

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| No. | | Host | Dopant | Hole blocking layer | Driving voltage(V) @1,000 cd/m² | Power efficiency(lm/W) @1,000 cd/m² | Color |
|---|----|------|----------------|---------------------------|--|---|-------|
| | 1 | 7 | Ir(ppy)₃ | BAlq | 6.8 | 16.9 | green |
| | 2 | 41 | Ir(ppy)₃ | BAlq | 6.6 | 17.5 | green |
| Example 1 | 3 | 50 | Ir(ppy)₃ | BAlq | 6.6 | 17.6 | green |
| | 4 | 74 | Ir(ppy)₃ | BAlq | 6.9 | 16.7 | green |
| | 5 | 89 | Ir(ppy)₃ | BAlq | 6.9 | 16.7 | green |
| | 11 | 48 | Ir(ppy)₃ | - | 6.5 | 16.6 | green |
| | 12 | 51 | Ir(ppy)₃ | - | 6.3 | 17.9 | green |
| Example 2 | 13 | 64 | Ir(ppy)₃ | - | 6.2 | 18.2 | green |
| | 14 | 70 | Ir(ppy)₃ | - | 6.3 | 18.1 | green |
| | 15 | 102 | Ir(ppy)₃ | - | 6.4 | 17.6 | green |
| | 16 | 78 | (piq)₂Ir(acac) | - | 6.2 | 5.0 | red |
| l | 17 | 81 | (piq)₂Ir(acac) | - | 6.0 | 5.3 | red |
| Example 3 | 18 | 82 | (piq)₂Ir(acac) | - | 6.1 | 5.1 | red |
| | 19 | 100 | (piq)₂Ir(acac) | - | 5.8 | 5.5 | red |
| | 20 | 106 | (piq)₂Ir(acac) | - | 5.9 | 5.3 | red |
| Comparative Example1 Comparative Example2 | | СВР | Ir(ppy)₃ | BAlq | 7.5 | 10.5 | green |
| | | СВР | (piq)₂Ir(acac) | BAlq | 7.5 | 2.6 | red |

[194] As shown in Table 2, the organic electroluminescent compounds according to the present invention have excellent properties compared with the conventional material. In addition, the device using the organic electroluminescent compound according to the present invention as host material has excellent electroluminescent properties and drops driving voltage, thereby increasing power efficiency to 1.7~3.2 lm/W and improving power consumption.

Claims

[Claim 1] An organic electroluminescent compound represented by Chemical Formula 1:

$$R_{3}$$
 R_{4}
 R_{4}
 R_{5}
 R_{6}
 R_{6}
 R_{6}
 R_{6}
 R_{6}
 R_{6}
 R_{6}
 R_{7}
 R_{10}
 R_{11}
 R_{9}
 R_{10}
 R_{11}
 R_{12}
 R_{12}
 R_{13}
 R_{16}
 R_{14}
 R_{15}
 R_{15}

wherein

 Ar_1 and Ar_2 independently represent a chemical bond, (C6-C40)arylene with or without substituent(s) or (C2-C40)heteroarylene with or without substituent(s);

R₁ through R₁₆ independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), substituted or unsubstituted (C6-C30)aryl fused with one or more (C3-C30)cycloalkyl(s) with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s), 5- to 7-membered heterocycloalkyl with or without substituent(s), 5- to 7-membered heterocycloalkyl fused with one or more aromatic ring(s) with or without substituent(s), (C3-C30)cycloalkyl with or without substituent(s), (C3-C30)cycloalkyl fused with one or more aromatic ring(s) with or without substituent(s), cyano, NR₂₁R₂₂, BR₂₃R₂₄, PR₂₅R₂₆, P(=O)R₂₇R₂₈, R^aR^bR^cSi-, R^dY-, R^cC(=O)-, R^fC(=O)O-, (C6-C30)ar(C1-C30)alkyl with or without substituent(s), (C2-C30)alkynyl with or without substituent(s),

$$R_{61}$$
 or R_{62} or each of them may be linked to R_{61}

an adjacent substituent via (C3-C30)alkylene or (C3-C30)alkenylene with or without a fused ring to form an alicylic ring, a mono- or polycyclic aromatic ring or a mono- or polycyclic heteroaromatic ring;

> W represents $-(CR_{51}R_{52})_m$, $-(R_{51})C=C(R_{52})$, $-N(R_{53})$, -S, -O, $-Si(R_{54})$ (R_{55}) -, $-P(R_{56})$ -, $-P(=O)(R_{57})$ -, -C(=O)- or $-B(R_{58})$ -; R_{51} through R_{58} and R_{61} through R_{63} are the same as R_1 through R_{16} ; the heterocycloalkyl or heteroaryl may contain one or more heteroatom(s) selected from B, N, O, S, P(=O), Si and P; R₂₁ through R₂₈ independently represent (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or (C3-C30)heteroaryl with or without substituent(s), the Ra, Rb, Rc, and R ^d independently represent (C1-C30)alkyl with or without substituent(s) or (C6-C30) aryl with or without substituent(s), the Y represents S or O, and the Re and Rf represent (C1-C30) alkyl with or without substituent(s), (C1-C30)alkoxy with or without substituent(s), (C6-C30)aryl with or without substituent(s) or (C6-C30)aryloxy with or without substituent(s); a and b represent an integer 0 or 2; and

m represents an integer 1 or 2.

[Claim 2]

The organic electroluminescent compound according to claim 1, wherein the substituent of R_1 through R_{16} , R_{21} through R_{28} , R_{51} through R_{58} and R_{61} through R_{63} is further substituted by one or more substituent(s) selected from a group consisting of hydrogen, deuterium, halogen, (C1-C30)alkyl with or without halogen substituent(s), (C6-C30)aryl, (C3-C30)heteroaryl with or without (C6-C30)aryl substituent(s), 5- to 7-membered heterocycloalkyl, 5- to 7-membered heterocycloalkyl fused with one or more aromatic ring(s), (C3-C30)cycloalkyl, (C3-C30)cycloalkyl fused with one or more aromatic ring(s), tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, (C2-C30)alkenyl, (C2-C30)alkynyl, cyano, carbazolyl, NR₃₁R₃₂, BR₃₃R $_{34}$, $PR_{35}R_{36}$, $P(=O)R_{37}R_{38}$, (C6-C30)ar(C1-C30)alkyl, (C1-C30)alkyl(C6-C30)aryl, (C1-C30)alkyloxy, (C1-C30)alkylthio, (C6-C30) aryloxy, (C6-C30) arylthio, (C1-C30) alkoxycarbonyl, (C1-C30)alkylcarbonyl, (C6-C30)arylcarbonyl, (C6-C30)aryloxycarbonyl, (C1-C30)alkoxycarbonyloxy, (C1-C30)alkylcarbonyloxy, (C6-C30)arylcarbonyloxy, (C6-C30)aryloxycarbonyloxy, carboxyl, nitro and hydroxyl, or is linked to an adjacent substituent to form a ring, and R₃₁ through R₃₈ independently represent (C1-C30)alkyl, (C6-C30)aryl or (C3-C30)heteroaryl.

[Claim 3]

The organic electroluminescent compound according to claim 1, wherein R_1 through R_{16} are selected from the following structures:

wherein

 R_{71} through R_{136} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl, (C6-C30)aryl, (C6-C30)aryl fused with one or more (C3-C30)cycloalkyl(s), (C3-C30)heteroaryl, 5- to 7-membered heterocycloalkyl, 5- to 7-membered heterocycloalkyl fused with one or more aromatic ring(s),(C3-C30)cycloalkyl, (C3-C30)cycloalkyl fused with one or more aromatic ring(s), cyano, amino, (C1-C30)alkylamino, (C6-C30) arylamino, NR₄₁R₄₂, BR₄₃R₄₄, PR₄₅R₄₆, P(=0)R₄₇R₄₈, tri(C1-C30)alkylsilyl, di(C1-C30)alkyl(C6-C30)arylsilyl, tri(C6-C30)arylsilyl, (C6-C30)ar(C1-C30)alkyl, (C1-C30)alkyloxy, (C1-C30)alkylthio, (C6-C30)aryloxy, (C6-C30)arylthio, (C1-C30)alkoxycarbonyl, (C1-C30)alkylcarbonyl, (C6-C30)arylcarbonyl, (C2-C30)alkenyl, (C2-C30)alkynyl, (C6-C30)aryloxycarbonyl, (C1-C30)alkoxycarbonyloxy, (C1-C30)alkylcarbonyloxy, (C6-C30)arylcarbonyloxy, (C6-C30)aryloxycarbonyloxy, carboxyl, nitro or hydroxyl, or each of them may be linked to an adjacent substituent via (C3-C30)alkylene or (C3-C30) alkenylene with or without a fused ring to form an alicylic ring or a mono- or polycyclic aromatic ring, and

 R_{41} through R_{48} independently represent (C1-C30)alkyl, (C6-C30)aryl or (C3-C30)heteroaryl.

[Claim 4]

The organic electroluminescent compound according to claim 1, wherein $*-(Ar_1)_{\overline{a}}Ar_2-|$ is selected from the following structures:

[Claim 5]

The organic electroluminescent compound according to claim 1, which is selected from the following structures:

[Claim 6]

An organic electroluminescent device comprising the organic electroluminescent compound according to any of claims 1 to 5.

[Claim 7]

The organic electroluminescent device according to claim 6, which comprises a first electrode; a second electrode; and one or more organic layer(s) interposed between the first electrode and the second electrode, wherein the organic layer comprises one or more organic electroluminescent compound(s) and one or more dopant(s) represented by Chemical Formula 2:

[Chemical Formula 2]

 $M^1L^{101}L^{102}L^{103}$

wherein

 M^1 is a metal selected from a group consisting of Group 7, Group 8, Group 9, Group 10, Group 11, Group 13, Group 14, Group 15 and Group 16 metals, and ligand L^{101} , L^{102} and L^{103} are independently selected from the following structures:

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$$\begin{array}{c} R_{217} \\ R_{216} \\ R_{221} \\ R_{221} \\ R_{205} \\ R_{206} \\ R_{213} \\ R_{214} \\ R_{213} \\ R_{214} \\ R_{213} \\ R_{214} \\ R_{215} \\ R_{215} \\ R_{216} \\ R_{206} \\$$

wherein

 R_{201} through R_{203} independently represent hydrogen, (C1-C30)alkyl with or without halogen substituent(s), (C6-C30)aryl with or without (C1-C30)alkyl substituent(s) or halogen;

 R_{204} through R_{219} independently represent hydrogen, (C1-C30)alkyl with or without substituent(s), (C1-C30)alkoxy with or without substituent(s), (C2-C30)alkenyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), mono- or di-(C1-C30)alkylamino with or without substituent(s), mono- or di-(C6-C30)arylamino with or without substituent(s), sF₅, tri(C1-C30)alkylsilyl with or without substituent(s), di(C1-C30)alkyl(C6-C30)arylsilyl with or without substituent(s), tri(C6-C30)arylsilyl with or without substituent(s), tri(C6-C30)arylsilyl with or without substituent(s), cyano or halogen; R_{220} through R_{223} independently represent hydrogen, (C1-C30)alkyl with or without halogen substituent(s) or (C6-C30)aryl with or without (C1-C30)alkyl substituent(s);

 R_{224} and R_{225} independently represent hydrogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or halogen, or R_{224} and R_{225} may be linked via (C3-C12)alkylene or (C3-C12)alkenylene with or without a fused to form an alicylic ring or a mono- or polycyclic aromatic ring;

R₂₂₆ represents (C1-C30)alkyl swith or without substituent(s), (C6-C30)aryl with or without substituent(s), (C5-C30)heteroaryl with or without substituent(s) or halogen;

 R_{227} through R_{229} independently represent hydrogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or halogen; and

Q represents
$$R_{231}R_{232}$$
, R_{233} R_{234} or R_{237} R_{238} R_{241} R_{242} wherein R_{231} R_{235} R_{236} R_{239} R_{240}

through R_{242} independently represent hydrogen, (C1-C30)alkyl with or without halogen substituent(s), (C1-C30)alkoxy, halogen, (C6-C30)aryl with or without substituent(s), cyano, (C5-C30)cycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via alkylene or alkenylene to form a spiro ring or a fused ring, or may be linked to R_{207} or R_{208} via alkylene or alkenylene to form a saturated or unsaturated fused ring.

[Claim 8]

The organic electroluminescent device according to claim 7, wherein the organic layer further comprises one or more amine compound(s) selected from a group consisting of arylamine compounds and styry-larylamine compounds, or one or more metal(s) selected from a group consisting of organic metals of Group 1, Group 2, 4th period and 5th period transition metals, lanthanide metals and d-transition elements or complex compound(s).

[Claim 9]

The organic electroluminescent device according to claim 7, wherein the organic layer comprises an electroluminescent layer and a charge generating layer.

[Claim 10]

The organic electroluminescent device according to claim 7, which is a white light-emitting organic electroluminescent device wherein the organic layer comprises one or more organic compound layer(s) emitting red, green or blue light at the same time.