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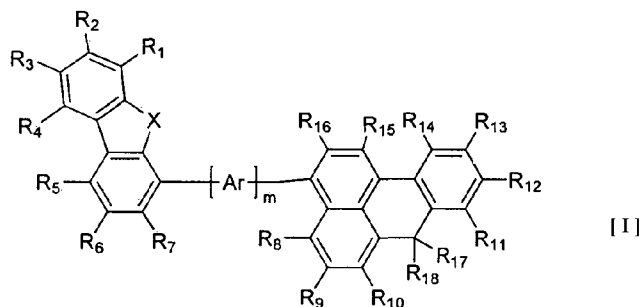
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(54) Title: NOVEL ORGANIC ELECTROLUMINESCENT COMPOUNDS AND ORGANIC ELECTROLUMINESCENT DEVICE USING THE SAME



(57) Abstract: Organic electroluminescent compounds of Chemical Formula 1 : wherein the variables R₁ to R₁₈, Ar, X and m are as defined in the specification. These compounds exhibit good luminous efficiency and excellent life property. As such, they may be used to manufacture OLED devices having very superior operation life and consuming less power due to improved power efficiency.

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.

Background Art

- [2] Among display devices, electroluminescent (EL) devices are advantageous in that they provide wide view angle, superior contrast and fast response rate as self-emissive display devices. In 1987, Eastman Kodak first developed an organic EL device using a low-molecular-weight aromatic diamine and aluminum complex as a substance for forming an electroluminescent layer [*Appl. Phys. Lett.* 51, 913, 1987].
- [3] In an organic EL device, when a charge is applied to an organic layer formed between an electron injection electrode (cathode) and a hole injection electrode (anode), an electron and a hole are paired and exciton is generated. Light is emitted by using electroluminescence (phosphorescence or fluorescence) in a state that the exciton is inactivated. The organic EL device emits polarization of light at voltage of about 10V and high brightness of about 100~10,000cd/m². The organic EL device has a feature in that light is emitted in a spectrum ranging from blue color to red color by simply selecting a fluorescent material. The organic EL device is advantageous in that it can be formed on a flexible transparent substrate such as plastic, is operable with relatively low voltage (10 V or lower) as compared to plasma display panels or inorganic EL displays, consumes less power, and provides excellent color.
- [4] In an organic EL device, the most important factor that determines its performance including luminescence efficiency and operation life is the electroluminescent material. Some requirements of the electroluminescent material include high electroluminescence quantum yield in solid state, high electron and hole mobility, resistance to decomposition during vacuum deposition, ability to form uniform film and stability.
- [5] Organic electroluminescent materials are generally classified into high-molecular materials and low-molecular materials. The low-molecular materials include metal complexes and thoroughly organic electroluminescent materials which do not contain metal, from the aspect of molecular structure. Such electroluminescent materials include chelate complexes such as tris(8-quinolinolato)aluminum complexes, coumarin derivatives, tetraphenylbutadiene derivatives, bis(styrylarylene) derivatives and oxadiazole derivatives. From those materials, it is reported that light emission of

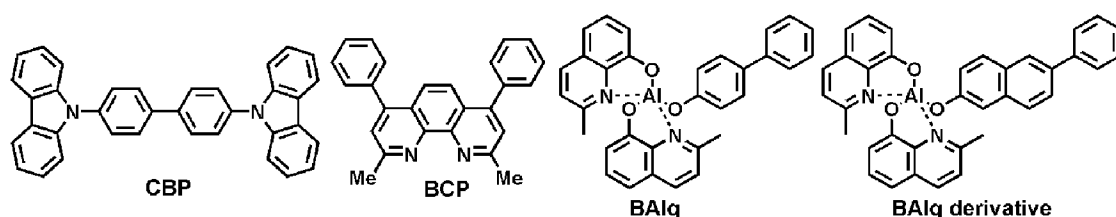
visible region from blue to red can be obtained.

- [6] Three electroluminescent materials (for red, green and blue) are employed to realize a full-colored organic light-emitting diode (OLED) display. The important issue is to develop red, green and blue electroluminescent materials with high efficiency and long life, in order to enhance the overall feature of the organic electroluminescent (EL) devices. From the aspect of function, the EL materials are classified into host materials and dopant materials. It is generally known that a device structure having the most excellent EL properties can be fabricated with an EL layer prepared by doping a dopant to a host. Recently, development of organic EL devices with high efficiency and long life comes to the fore as an urgent subject, and particularly urgent is development of a material with far better EL properties as compared to conventional EL materials as considering EL properties required for a medium to large sized OLED panel. From this point of view, development of host material is one of the most important issues to be settled. The desired properties for the host material (serving as a solvent and energy conveyer in solid state) are high purity and appropriate molecular weight to enable vapor-deposition in vacuo. In addition, glass transition temperature and thermal decomposition temperature should be high enough to ensure thermal stability. Further, the host material should have high electrochemical stability for providing long life. It is to be easy to form an amorphous thin film, with high adhesiveness to other adjacent materials but without interlayer migration.

- [7] When the organic EL device is fabricated by doping technology, transferring energy from host molecule to dopant in an excited state does not achieve 100% and a host material as well as dopant emits light. In particular, since the host material emits light in a range of wavelength having larger visibility than the dopant in case of a red light emitting device, color purity is deteriorated due to dull light emission of the host material. If the technology is actually applied, it is required to increase luminescence life and improve durability.

- [8] At present, CBP is most widely known as a host material for a phosphorescent material. High-efficiency OLEDs using a hole blocking layer comprising BCP, BAQ, etc. are reported. High-performance OLEDs using BAQ derivatives as a host were reported by Pioneer (Japan) and others.

[9]



- [10] 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 $(\pi / \text{voltage}) \times \text{current efficiency}$, 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 BA1q, 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. 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

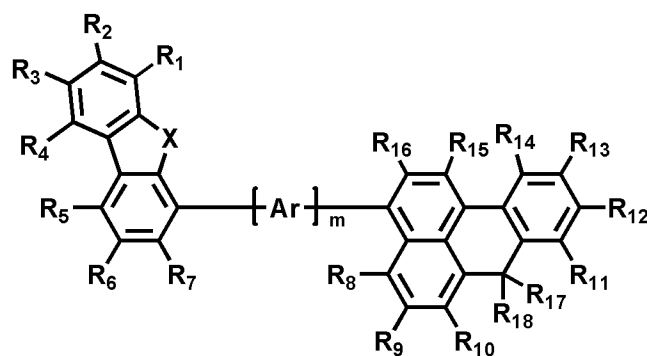
- [11] Accordingly, an object of the present invention is to provide an organic electroluminescent compound having luminescence efficiency and device operation life improved over existing materials and having superior backbone with appropriate color coordinates in order to solve the aforesaid problems.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

Solution to Problem

- [12] Provided are a novel organic electroluminescent compound represented by following Chemical Formula 1 and an organic electroluminescent device using the same. Since the organic electroluminescent compound according to the present invention exhibits good luminous efficiency and excellent life property compared to the existing host material, it may be used to manufacture OLED devices having very superior operation life and consuming less power due to improved power efficiency.

- [13] [Chemical Formula 1]

[14]



- [15] wherein

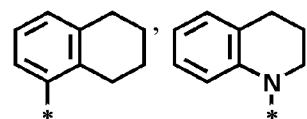
- [16] X represents $-C(R_{20}R_{21})$, $-N(R_{22})$ -, $-S$ -, $-O$ - or $-Si(R_{23}R_{24})$ -;
- [17] Ar represents (C6-C30)arylene with or without substituent(s) or (C3-C30)heteroarylene with or without substituent(s);
- [18] R_1 through R_{16} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s), 5- to 7-membered heterocycloalkyl 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), 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), (C6-C30)ar(C1-C30)alkyl with or without substituent(s), cyano, nitro, hydroxyl, $-NR_{31}$, R_{32} , $-BR_{33}R_{34}$, $-PR_{35}R_{36}$, $-P(=O)R_{37}R_{38}$, $-SiR_{39}R_{40}R_{41}$ or $-YR_{42}$, or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring, wherein a carbon atom of the alicyclic ring or the mono- or polycyclic aromatic ring may be substituted with one or more heteroatom(s) selected from nitrogen, oxygen and sulfur;
- [19] R_{17} , R_{18} and R_{20} through R_{24} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s) or 5- to 7-membered heterocycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring, wherein a carbon atom of the alicyclic ring or the mono- or polycyclic aromatic ring may be substituted with one or more heteroatom(s) selected from nitrogen, oxygen and sulfur;
- [20] R_{31} through R_{42} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s) or 5- to 7-membered heterocycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring, wherein a carbon atom of the alicyclic ring or the mono- or polycyclic aromatic ring may be substituted with one or more heteroatom(s) selected from nitrogen, oxygen and sulfur;
- [21] Y represents S or O;
- [22] m represents an integer from 0 to 3, and each Ar may be identical or different and

- may be linked to an adjacent substituent to form a ring, when m is 2 or greater; and
- [23] the heterocycloalkyl or heteroaryl includes one or more heteroatom(s) selected from B, N, O, S, P(=O), Si and P.
- [24]
- [25] In the present invention, "alkyl", "alkoxy" and other substituents containing "alkyl" moiety include both linear and branched species. In the present invention, the cycloalkyl includes polycyclic hydrocarbon ring such as adamantyl with or without substituent(s) or (C7-C30)bicycloalkyl with or without substituent(s) as well as a monocyclic hydrocarbon ring.
- [26] 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).
- [27] 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. The heteroaryl also includes heteroaryl groups having single bond therebetween.
- [28] 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, benzothienophenyl, isobenzofuranyl, benzimidazolyl, benzothiazolyl, benzoisothiazolyl, benzoisoxazolyl, benzoxazolyl, isoindolyl, indolyl, indazolyl, benzothiadiazolyl, quinolyl, isoquinolyl, cinnolinyl, quinazolinyl, quinoxalinyl, carbazolyl, phenanthridinyl, benzo-dioxolyl, etc., an N-oxide thereof (e.g., pyridyl N-oxide, quinolyl N-oxide, etc.), a quaternary salt thereof, etc., but are not limited thereto.
- [29] 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.

- [30] In the term 'substituted or unsubstituted (or with or without) substituent(s)' described herein, the term 'substituted' means that the unsubstituted substituent is further substituted with substituent(s). The substituents of Ar, R₁ through R₁₆, R₁₇, R₁₈, R₂₀ through R₂₄ and R₃₁ through R₄₂ may be further substituted by one or more substituent(s) selected from the group consisting of 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, (C6-C30)cycloalkyl fused with one or more aromatic ring(s), R^aR^bR^cSi-, (C2-C30)alkenyl, (C2-C30)alkynyl, cyano, carbazolyl, -NR^dR^e, -BR^fR^g, -PR^hRⁱ, -P(=O)R^jR^k, (C6-C30)ar(C1-C30)alkyl, (C1-C30)alkyl(C6-C30)aryl, R^lZ-, R^mC(=O)-, R^mC(=O)O-, carboxyl, nitro and hydroxyl, wherein R^a through R^l independently represent (C1-C30)alkyl, (C6-C30)aryl or (C3-C30)heteroaryl; Z represents S or O; and R^m represents (C1-C30)alkyl, (C1-C30)alkoxy, (C6-C30)aryl or (C6-C30)aryloxy.
- [31] The X represents -C(R₂₀R₂₁), -N(R₂₂)-, -S-, -O- or -Si(R₂₃R₂₄)-;
- [32] Ar represents (C6-C30)arylene with or without substituent(s) or (C3-C30)heteroarylene with or without substituent(s);
- [33] R₁ through R₁₆ independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl 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), 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), cyano, -NR₃₁R₃₂, -BR₃₃R₃₄ or -SiR₃₉R₄₀R₄₁, or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring;
- [34] R₁₇, R₁₈ and R₂₀ through R₂₄ independently represent hydrogen, deuterium, (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), or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring; and
- [35] R₃₁ through R₃₄ and R₃₉ through R₄₁ independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without

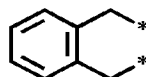
[36] More specifically, the R₁ through R₇ independently represent hydrogen, fluorine, t-butyl, cyclohexyl, diphenylamino, N-carbazolyl, diphenylmethylsilyl, triphenylsilyl, triphenylenyl, N-phenyl-carbazole-3-yl, diphenyltriazinyl, , ,



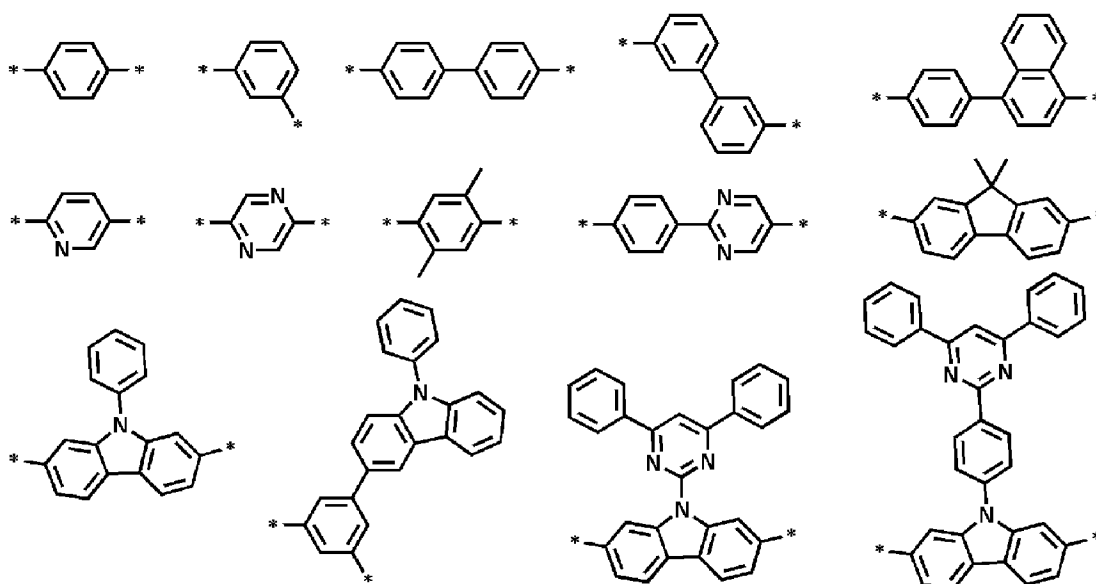
Chemical structure of 2-(4-phenylphenyl)-4-phenyl-1H-imidazole, showing a central imidazole ring substituted with three phenyl groups.

adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring;

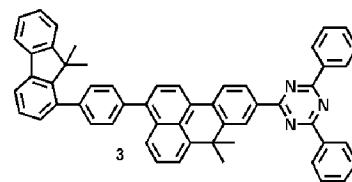
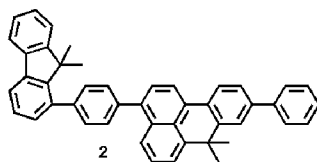
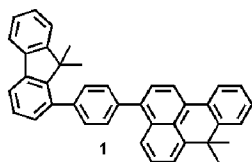
[38] R₁₇ and R₁₈ independently represent methyl, or each of them may be linked to an adjacent substituent via C4 alkylene or  to form a ring; and



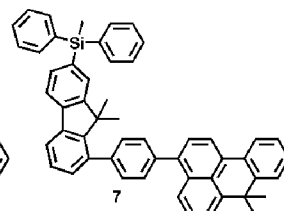
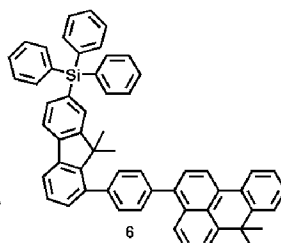
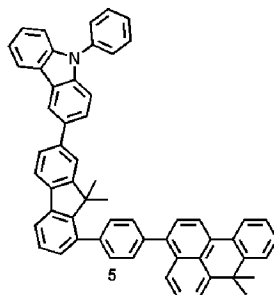
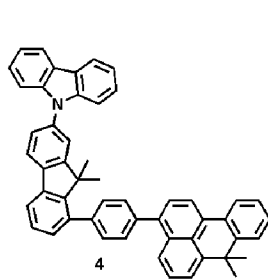
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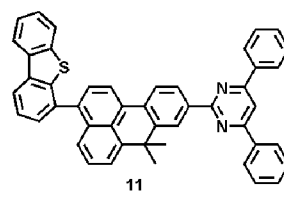
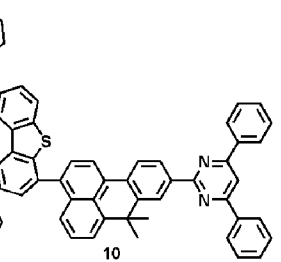
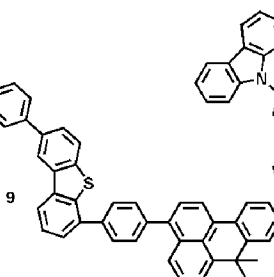
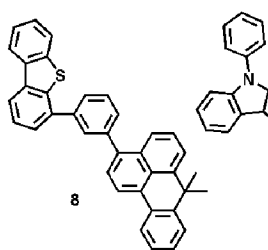
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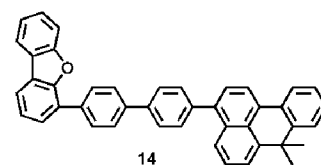
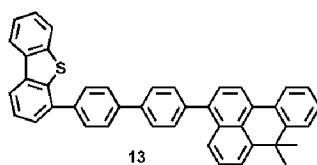
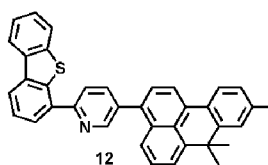
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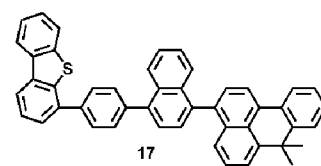
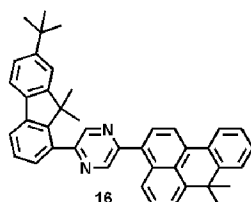
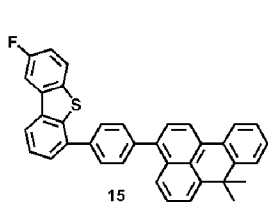
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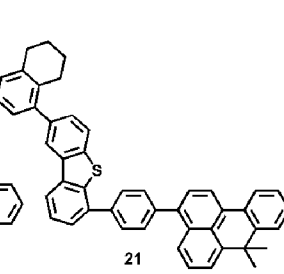
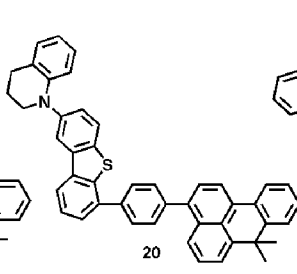
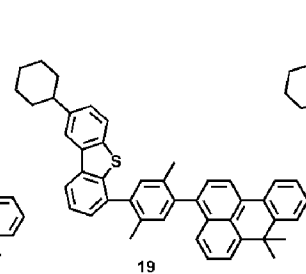
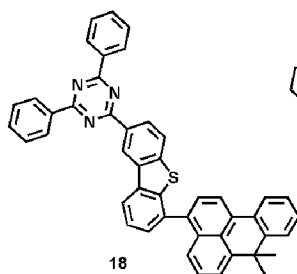
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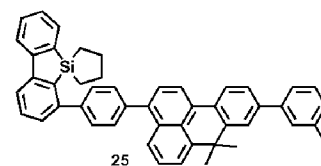
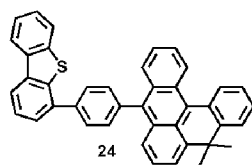
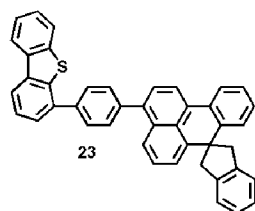
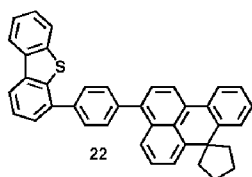
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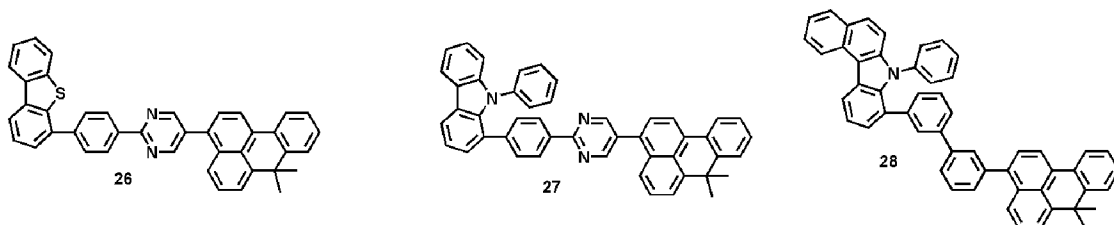
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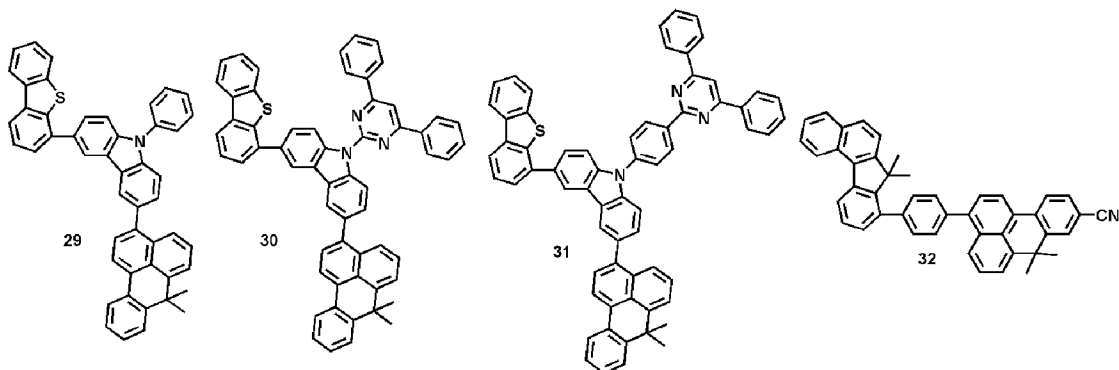
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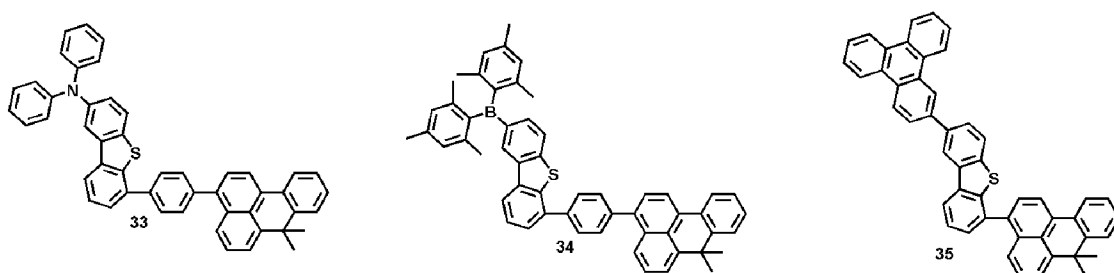
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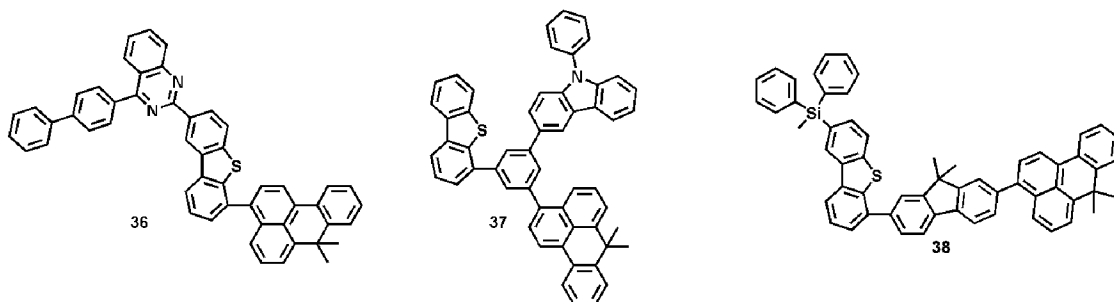
[51]



[52]



[53]

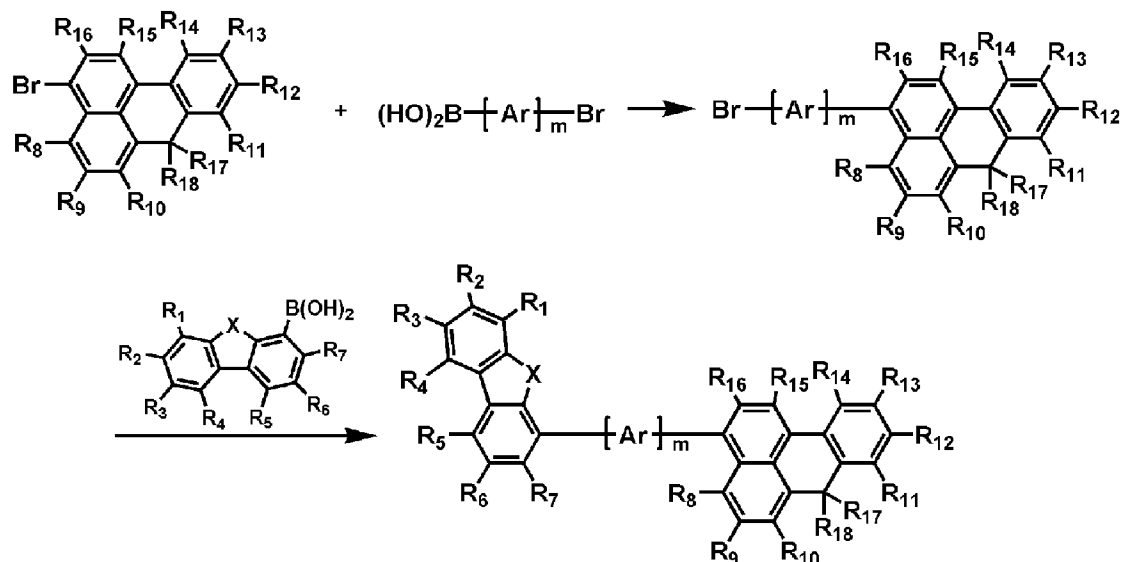


[54]

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

[56] [Scheme 1]

[57]



[58] wherein

[59] R_1 through R_{18} , X , Ar and m are the same as defined in Chemical Formula 1.

[60] 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 layer comprises an electroluminescent layer, in which the organic electroluminescent compounds of Chemical Formula 1 are used as a host material.

[61] When the organic electroluminescent compounds of Chemical Formula 1 are used as the host, one or more dopant is included. The dopant used in the organic electroluminescent device of the present invention is not particularly limited, but may be selected from the compounds represented by Chemical Formula 2:

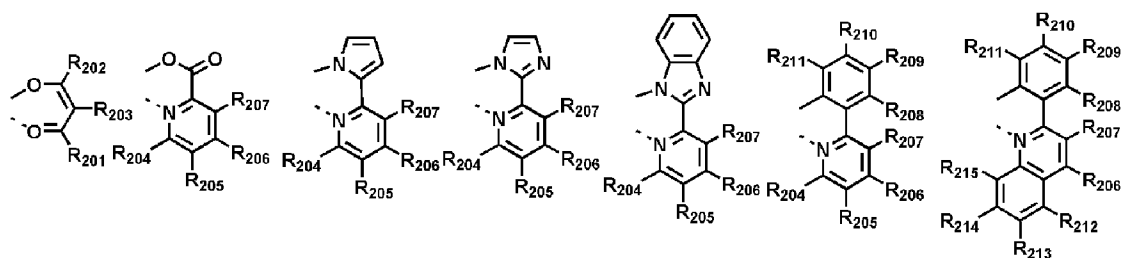
[62] [Chemical Formula 2]

[63] $M^1 L^{101} L^{102} L^{103}$

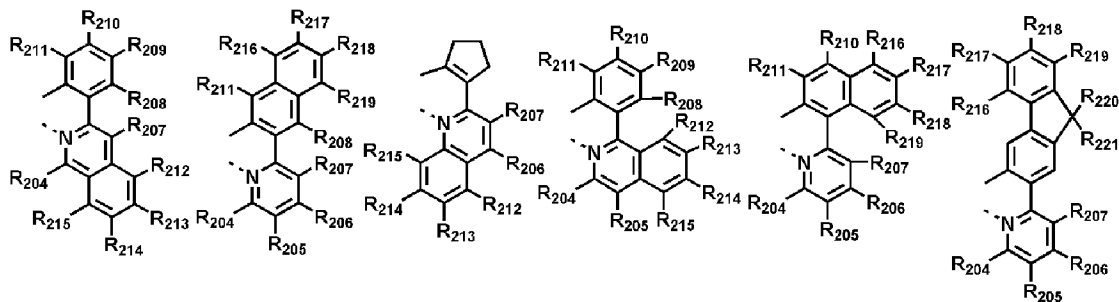
[64] wherein

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

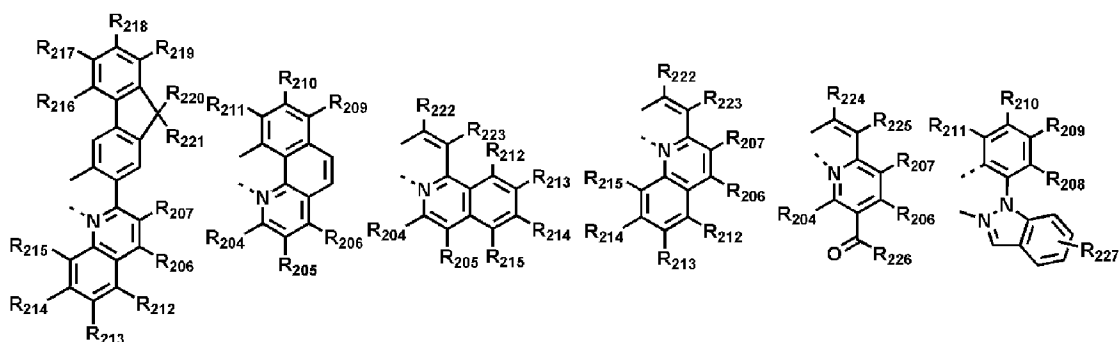
[66]



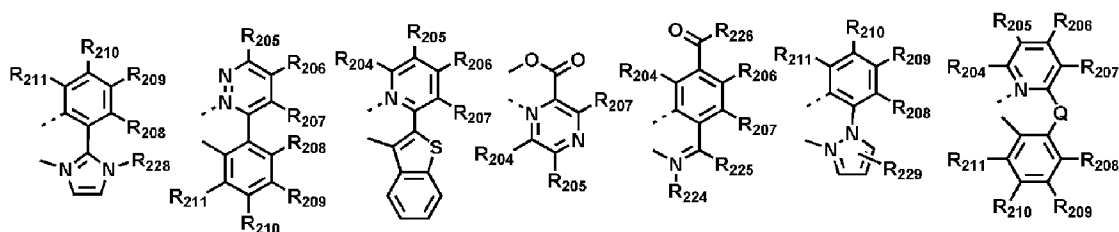
[67]



[68]



[69]



[70] wherein

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

[72] R₂₀₄ through R₂₁₉ independently represent hydrogen, deuterium, (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), 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), cyano or halogen;

[73] R₂₂₀ through R₂₂₃ independently represent hydrogen, deuterium, (C1-C30)alkyl with or without halogen substituent(s) or (C6-C30)aryl with or without (C1-C30)alkyl substituent(s);

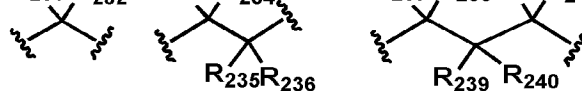
[74] R₂₂₄ and R₂₂₅ independently represent hydrogen, deuterium, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s) or halogen, or R₂₂₄ and R₂₂₅ may be linked via (C3-C12)alkylene or (C3-C12)alkenylene with or without a

fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring;

[75] R_{226} 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;

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

[77] Q represents $R_{231}R_{232}$, $R_{233}R_{234}$ or $R_{237}R_{238}R_{241}R_{242}$, wherein R_{231} through R_{242}

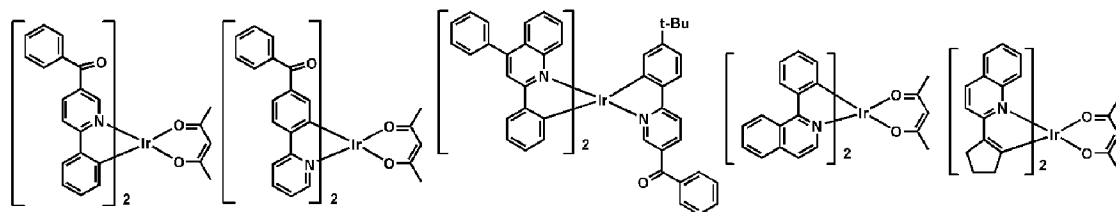


R_{242} independently represent hydrogen, deuterium, (C1-C30)alkyl with or without halogen substituent(s), (C1-C30)alkoxy, halogen, (C6-C30)aryl with or without substituent(s), cyano or (C5-C30)cycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via alkylene 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.

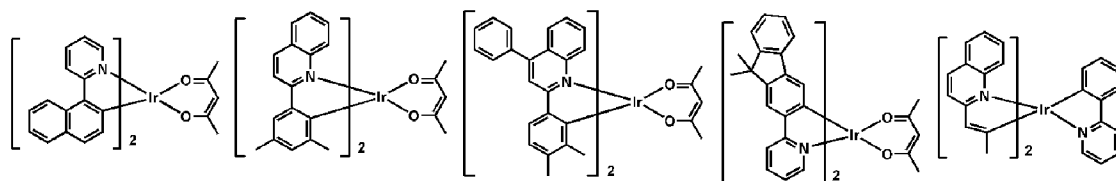
[78]

[79] The dopant compounds of Chemical Formula 2 may be exemplified as Compounds having following structures but are not limited thereto:

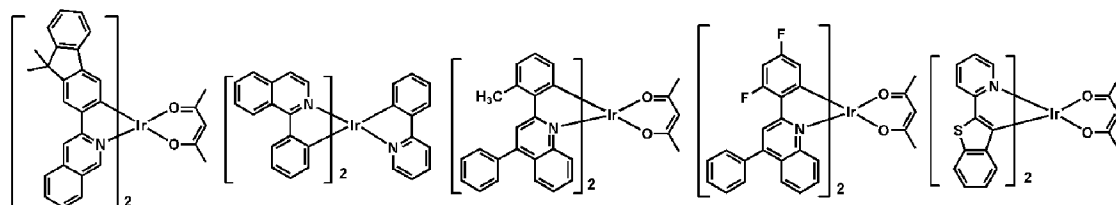
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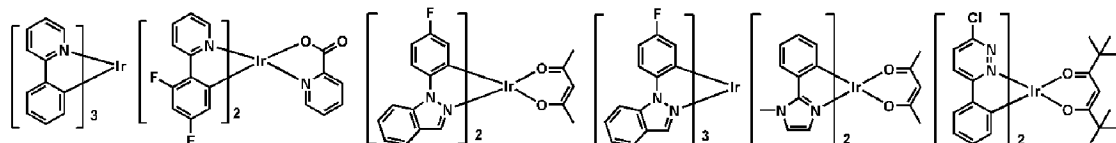
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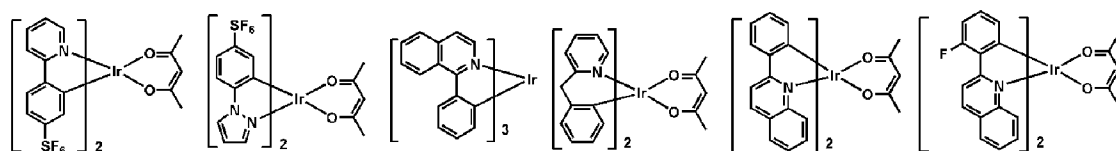
[82]



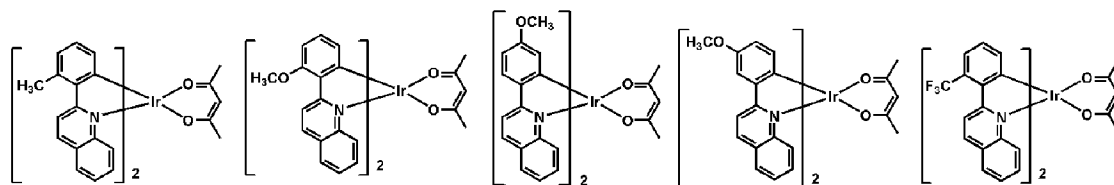
[83]



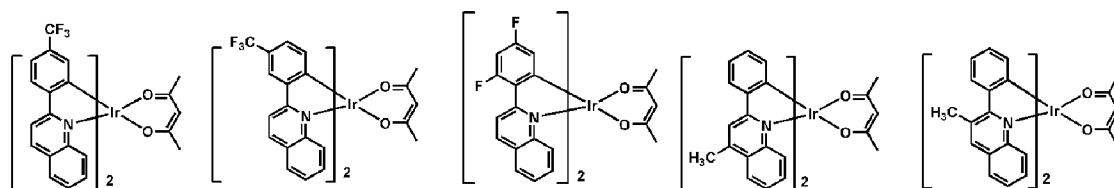
[84]



[85]



[86]



[87]

[88]

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 the 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.

[89]

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 the 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.

[90]

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.

[91]

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.

[92]

The chalcogenide may be, for example, SiO_x ($1 = x = 2$), AlO_x ($1 = x = 1.5$), SiON ,

SiAlON, etc. The metal halide may be, for example, LiF, MgF₂, CaF₂, a rare earth metal fluoride, etc. The metal oxide may be, for example, Cs₂O, Li₂O, MgO, SrO, BaO, CaO, etc.

- [93] 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. 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

- [94] 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.

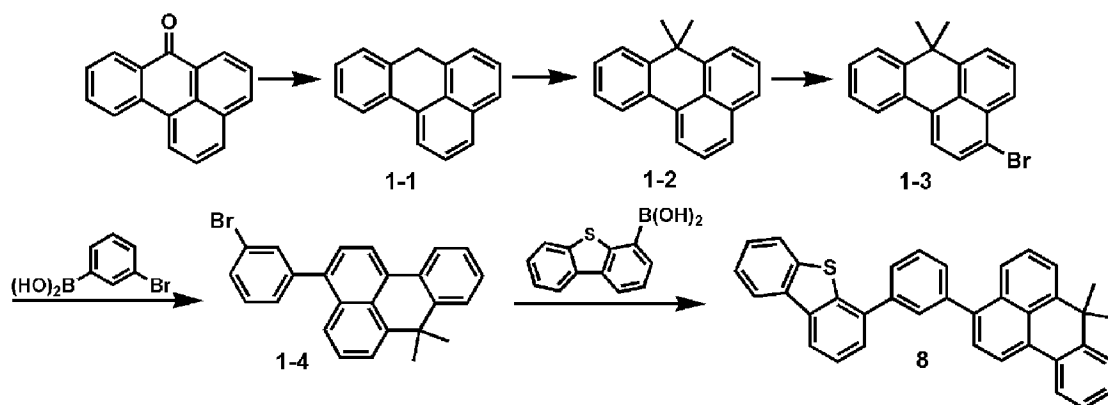
Mode for the Invention

- [95] 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.

[96]

[97] [Preparation Example 1] Preparation of Compound 8

[98]



[99] Preparation of Compound 1-1

[100] After 7H-benzo[de]anthracen-7-one (40.0g, 0.17mol) was dissolved in diethyl ether (1000mL), AlCl_3 (28g, 0.21mol) was slowly added thereto. After stirring the mixture for 15 minutes, the mixture was cooled to 0°C and lithium aluminum hydride (LAH) (10g, 0.26mol) was slowly added thereto. After stirring the mixture under reflux for 1 hour, the mixture was slowly cooled to room temperature upon completion of the reaction. EA was slowly added to the mixture until the bubble stopped. After adding 6M HCl (100mL), the mixture was extracted with distilled water and ethyl acetate. After drying an organic layer with MgSO_4 and removing solvent by a rotary type evaporator, Compound 1-1 (36.0g, 95%) was obtained by purification via column chromatography using dichloro methane and hexane as a developing solvent.

[101] Preparation of Compound 1-2

[102] After Compound 1-1 (36.0g, 0.16mol) was dissolved in DMSO (420mL), sodium tert-butoxide (113.0g, 1.2mol) was added at room temperature and stirred at 70°C for 15 minutes. Methyl iodide (90 mL, 1.4mol) was slowly added thereto and stirred for 1 hour. Upon completion of the reaction, the reaction mixture was cooled at room temperature and distilled water was added thereto. After stirring the mixture for 20 minutes, a solid was produced and filtered. Compound 1-2 (26g, 63%) was obtained by recrystallizing the solid with methanol and acetone.

[103] Preparation of Compound 1-3

[104] Compound 1-2 (20g, 90mmol) was dissolved in DMF (300mL), and N-bromosuccinimide (16g, 90mmol) was slowly added thereto. The mixture was stirred at room temperature for one day. Upon completion of the reaction, the mixture was extracted with distilled water and EA. After drying an organic layer with MgSO_4 and removing solvent by a rotary type evaporator, Compound 1-3 (26g, 91%) was obtained by purification via column chromatography using dichloro methane and hexane as a developing solvent.

[105] Preparation of Compound 1-4

[106] After Compound 1-3 (26g, 80.5mmol), 3-bromophenylboronic acid (19.4g, 96.6mmol), $\text{Pd}(\text{PPh}_3)_4$ (4.6g, 4.03mmol) and Na_2CO_3 (12.8, 120.8mmol) were dissolved in toluen/ethanol/distilled water (400mL/100mL/80mL), the mixture was stirred at 100°C. Upon completion of the reaction, the reaction mixture was extracted with distilled water and EA. After drying an organic layer with MgSO_4 and removing solvent by a rotary type evaporator, Compound 1-4 (24g, 75%) was obtained by purification via column chromatography using dichloro methane and hexane as a developing solvent.

[107] Preparation of Compound 8

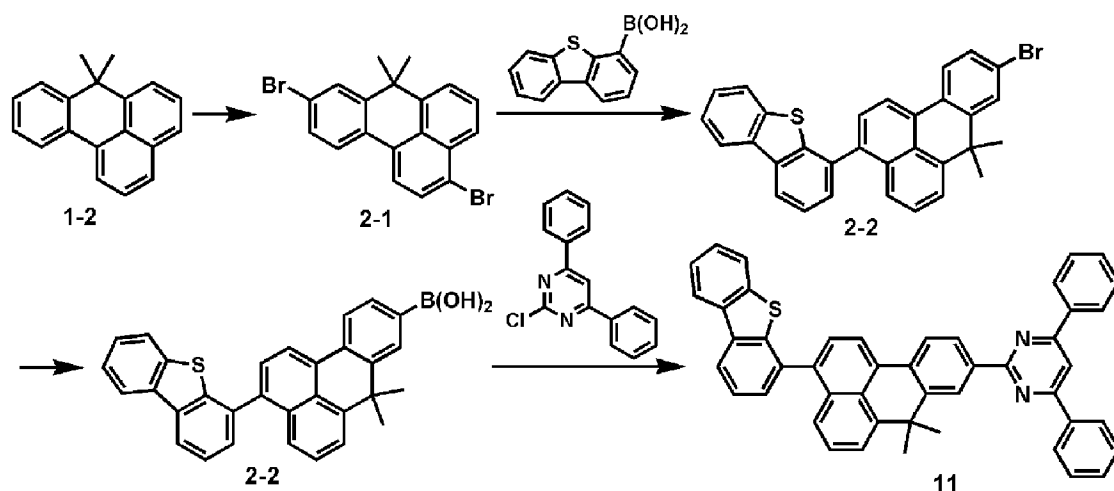
[108] After Compound 1-4 (24g, 60.1mmol), dibenzo[b,d]thiophen-4-ylboronic acid

(16.4g, 72.12mmol), $\text{Pd}(\text{PPh}_3)_4$ (3.4g, 3.0mmol) and Na_2CO_3 (7.7g, 72.12mmol) were dissolved in toluen/ethanol/distilled water (300mL/60mL/50mL), the mixture was stirred at 100°C. Upon completion of the reaction, the reaction mixture was extracted with distilled water and EA. After drying an organic layer with MgSO_4 and removing solvent by a rotary type evaporator, Compound **8** (26g, 86%) was obtained by purification via column chromatography using dichloro methane and hexane as a developing solvent.

[109]

[110] [Preparation Example 2] Preparation of Compound **11**

[111]

[112] Preparation of Compound **2-1**

[113] After Compound **1-2** (15g, 0.06 mol) was dissolved in THF (300mL), the mixture was slowly added to Br_2 (7mL, 0.13mol) dropwise. After stirring the mixture for 12 hours at room temperature, the mixture was extracted with distilled water and EA. After drying an organic layer with MgSO_4 and removing solvent by a rotary type evaporator, Compound **2-1** (13g, 44%) was obtained by purification via column chromatography using dichloro methane and hexane as a developing solvent.

[114] Preparation of Compound **2-2**

[115] After Compound **2-1** (16g, 44mmol), dibenzo[b,d]thiophen-4-ylboronic acid 5g (22mmol), $\text{Pd}(\text{PPh}_3)_4$ 1g (0.88mmol) and Na_2CO_3 (6.9g, 66mmol) were dissolved in toluen/ethanol (100mL/50mL), the mixture was stirred at 100°C for 12 hours. Upon completion of the reaction, the mixture was extracted with distilled water and EA. After drying an organic layer with MgSO_4 and removing solvent by a rotary type evaporator, Compound **2-2** (5g, 45 %) was obtained by purification via column chromatography using dichloro methane and hexane as a developing solvent.

[116] Preparation of Compound **2-3**

[117] After Compound **2-2** (5g, 9.9mmol) was dissolved in THF (100mL), the mixture was cooled to -78°C, and n-BuLi (4.4mL, 2.5M in hexane, 10.9mmol) was slowly added

thereto. After stirring the mixture for 1 hour, triisopropylborate (2.7mL, 12.9 mmol) was slowly added to the mixture. After slowly raising the temperature, the mixture was stirred at room temperature for one day. Upon completion of the reaction, the reaction mixture was quenched with 2M HCl solution, and extracted with EA/H₂O. After removing moisture with MgSO₄ and performing distillation under reduced pressure, Compound **2-3** (3.2g, 68%) was obtained by column(MC/Hexane) separation.

[118] Preparation of Compound **11**

[119] After Compound **2-3** (3.2g, 6.8mmol), 2-chloro-4,6-diphenylpyrimidine (1.8g, 5.7mmol), Pd(PPh₃)₄ (0.4g, 0.29mmol) and K₂CO₃ (3.1g, 17.1mmol) were dissolved in toluen/ethanol (40mL/20mL), the mixture was stirred at 120°C for 12 hours. Upon completion of the reaction, the mixture was extracted with EA/H₂O. After removing moisture with MgSO₄ and performing distillation under reduced pressure, Compound **11** (3g, 65%) was obtained by column(MC/Hexane) separation.

[120] Organic electroluminescent compounds **1** to **38** were prepared according to the procedure of Preparation Examples 1 and 2. ¹H NMR and MS/FAB data of thus prepared organic electroluminescent compounds are given in Table 1.

[121] Table 1

[Table 1]

[Table]

Com p.	¹ H NMR(CDCl ₃ , 200 MHz)	MS/FAB	
		found	calculate d
1	δ = 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.25~7.44(11H, m), 7.53~7.55(2H, m), 7.71(1H, m), 7.83~7.87(2H, m), 7.98~8(2H, m), 8.39(1H, m)	512.68	512.25
2	δ = 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.07(1H, m), 7.25~7.28(5H, m), 7.38~7.44(4H, m), 7.51~7.55(6H, m), 7.77(1H, m), 7.83~7.92(3H, m), 7.98~8(2H, m), 8.39(1H, m)	588.78	588.28
3	δ = 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.25~7.28(5H, m), 7.38~7.44(5H, m), 7.51~7.55(6H, m), 7.67(1H, m), 7.77(1H, m), 7.83~7.92(3H, m), 7.98~8(2H, m), 8.28(4H, m), 8.39(1H, m)	743.93	743.33
4	δ = 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.17(1H, m), 7.23~7.42(13H, m), 7.5~7.53(2H, m), 7.63(1H, m), 7.71(1H, m), 7.83~7.87(2H, m), 7.94~8(3H, m), 8.12(1H, m), 8.39(1H, m), 8.55(1H, m)	677.87	677.31
5	δ = 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.25(4H, m), 7.29(1H, m), 7.33(2H, m), 7.36~7.45(12H, m), 7.71~7.77(3H, m), 7.83(1H, m), 7.93~8(4H, m), 8.12(1H, m), 8.18(1H, m), 8.39(1H, m)	753.97	753.34
6	δ = 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.25(4H, m), 7.33~7.46(17H, m), 7.53~7.55(4H, m), 7.66~7.71(2H, m), 7.83(2H, m), 7.97~8(3H, m), 8.39(1H, m)	771.07	770.34
7	δ = 0.66(3H, s), 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.25(4H, m), 7.33~7.46(13H, m), 7.53~7.55(3H, m), 7.66~7.71(2H, m), 7.83(2H, m), 7.97~8(3H, m), 8.39(1H, m)	709.00	708.32
8	δ = 1.85(6H, s), 7(1H, m), 7.33~7.42(4H, m), 7.48~7.58(6H, m), 7.7~7.71(2H, m), 7.98~8(3H, m), 8.2(1H, m), 8.39~8.45(3H, m)	502.67	502.18
9	δ = 1.85(6H, s), 7(1H, m), 7.25~7.5(13H, m),	743.95	743.26

	7.58~7.63(4H, m), 7.71~7.77(2H, m), 7.86(1H, m), 7.98~8(5H, m), 8.12(1H, m), 8.18~8.2(2H, m), 8.39~8.41(2H, m)		
10	δ = 1.85(6H, s), 7(1H, m), 7.25~7.33(3H, m), 7.41~7.51(9H, m), 7.58~7.67(3H, m), 7.77~7.79(5H, m), 7.92~8(6H, m), 8.12(1H, m), 8.2(1H, m), 8.23(1H, s), 8.39~8.41(2H, m), 8.55(1H, m)	822.03	821.29
11	δ = 1.85(6H, s), 7(1H, m), 7.41~7.42(3H, m), 7.5~7.52(6H, m), 7.58(1H, m), 7.67(1H, m), 7.77~7.79(5H, m), 7.92(1H, m), 7.98~8(3H, m), 8.2(1H, m), 8.23(1H, s), 8.39~8.45(3H, m)	656.84	656.23
12	δ = 1.85(6H, s), 2.34(3H, s), 7(1H, m), 7.11(1H, m), 7.23(1H, m), 7.42(1H, m), 7.5~7.52(2H, m), 7.59~7.61(2H, m), 7.69(1H, m), 7.98~8.03(4H, m), 8.31(1H, m), 8.39~8.47(3H, m), 8.78(1H, m)	517.68	517.19
13	δ = 1.85(6H, s), 7(1H, m), 7.25(8H, m), 7.33~7.42(4H, m), 7.5~7.52(2H, m), 7.58(1H, m), 7.71(1H, m), 7.98~8(3H, m), 8.2(1H, m), 8.39~8.45(3H, m)	578.76	578.21
14	δ = 1.85(6H, s), 7(1H, m), 7.25(8H, m), 7.32~7.42(7H, m), 7.66~7.71(2H, m), 7.81~7.89(3H, m), 7.98~8(2H, m), 8.39(1H, m)	562.70	562.23
15	δ = 1.85(6H, s), 7(1H, m), 7.19~7.25(5H, m), 7.33~7.42(4H, m), 7.49(1H, m), 7.58(1H, m), 7.71(1H, m), 7.96~8(3H, m), 8.2(1H, m), 8.39~8.41(2H, m)	520.66	520.17
16	δ = 1.35(9H, s), 1.72(6H, s), 1.85(6H, s), 7(1H, m), 7.33~7.44(6H, m), 7.53~7.58(2H, m), 7.71(1H, m), 7.79~7.83(2H, m), 7.98~8(2H, m), 8.39(1H, m), 8.79(2H, s)	570.76	570.30
17	δ = 1.85(6H, s), 7(1H, m), 7.25(4H, m), 7.33~7.42(4H, m), 7.5~7.58(5H, m), 7.71(1H, m), 7.98~8.01(5H, m), 8.2(1H, m), 8.39~8.45(3H, m), 8.55(2H, m)	628.82	628.22
18	δ = 1.85(6H, s), 7(1H, m), 7.33~7.42(6H, m), 7.51(4H, m), 7.58(1H, m), 7.71(1H, m), 7.8(1H, m), 7.86(1H, m), 7.98~8(3H, m), 8.2(1H, m), 8.28(4H, m), 8.39~8.41(2H, m)	657.82	657.22

19	$\delta = 1.48(6H, m), 1.73(4H, m), 1.85(6H, s), 2.59(6H, s), 2.72(1H, m), 7(1H, m), 7.33\sim 7.42(5H, m), 7.58(1H, m), 7.68\sim 7.71(2H, m), 7.73(2H, s), 7.9(1H, m), 7.98\sim 8(2H, m), 8.2(1H, m), 8.39\sim 8.41(2H, m)$	612.86	612.29
20	$\delta = 1.85(6H, s), 1.96(2H, m), 2.76(2H, m), 3.06(2H, m), 6.55(1H, m), 6.72(1H, m), 6.83(1H, m), 7\sim 7.07(3H, m), 7.25(4H, m), 7.33\sim 7.42(5H, m), 7.58(1H, m), 7.71\sim 7.76(2H, m), 7.98\sim 8(2H, m), 8.2(1H, m), 8.39\sim 8.41(2H, m)$	633.84	633.25
21	$\delta = 1.72(4H, m), 1.85(6H, s), 2.74(4H, m), 6.88(1H, m), 6.98\sim 7(2H, m), 7.15(1H, m), 7.25(4H, m), 7.33\sim 7.42(4H, m), 7.58(1H, m), 7.71(1H, m), 7.86(1H, m), 7.98\sim 8(4H, m), 8.2(1H, m), 8.39\sim 8.41(2H, m)$	632.85	632.22
22	$\delta = 1.51(4H, m), 2.11(4H, m), 7(1H, m), 7.25(4H, m), 7.33\sim 7.42(4H, m), 7.5\sim 7.52(2H, m), 7.58(1H, m), 7.71(1H, m), 7.98\sim 8(3H, m), 8.2(1H, m), 8.39\sim 8.45(3H, m)$	528.70	528.19
23	$\delta = 3.51(4H, s), 7(1H, m), 7.2\sim 7.25(8H, m), 7.33\sim 7.42(4H, m), 7.5\sim 7.52(2H, m), 7.58(1H, m), 7.71(1H, m), 7.98\sim 8(3H, m), 8.2(1H, m), 8.39\sim 8.45(3H, m)$	576.75	576.19
24	$\delta = 1.85(6H, s), 7.17(1H, m), 7.25\sim 7.26(5H, m), 7.33\sim 7.39(5H, m), 7.5\sim 7.52(2H, m), 7.58(1H, m), 7.71\sim 7.75(2H, m), 7.91(2H, m), 7.98(1H, m), 8.2(1H, m), 8.41\sim 8.45(2H, m)$	552.73	552.19
25	$\delta = 1.3(4H, m), 1.45(4H, m), 1.85(6H, s), 2.34(3H, s), 7(1H, m), 7.07(1H, m), 7.19\sim 7.25(5H, m), 7.33\sim 7.42(4H, m), 7.52(1H, m), 7.61\sim 7.67(2H, m), 7.77\sim 7.92(6H, m), 7.98\sim 8(2H, m), 8.39(1H, m)$	644.92	622.29
26	$\delta = 1.85(6H, s), 7(1H, m), 7.25(2H, m), 7.33\sim 7.42(4H, m), 7.5\sim 7.52(2H, m), 7.58(1H, m), 7.71(1H, m), 7.85(2H, m), 7.98\sim 8(3H, m), 8.2(1H, m), 8.39\sim 8.45(3H, m), 9.26(2H, m)$	580.74	580.20
27	$\delta = 1.85(6H, s), 7(1H, m), 7.25(3H, m), 7.33\sim 7.5(9H, m), 7.58(2H, m), 7.71(1H, m), 7.85\sim 7.87(3H, m), 7.94\sim 8(3H, m), 8.08(1H, m), 8.39(1H, m), 8.55(1H, m), 9.26(2H, m)$	639.79	639.27
28	$\delta = 1.85(6H, s), 7(1H, m), 7.33\sim 7.5(12H, m), 7.57\sim 7.58(4H, m), 7.67\sim 7.71(5H, m), 7.87(1H, m),$	687.87	687.29

	7.94~8(4H, m), 8.08(1H, m), 8.16(1H, m), 8.39(1H, m), 8.54(1H, m)		
29	δ = 1.85(6H, s), 7(1H, m), 7.33~7.52(9H, m), 7.58(3H, m), 7.69~7.77(4H, m), 7.87(1H, m), 7.98~8(4H, m), 8.18~8.2(2H, m), 8.39~8.45(3H, m)	667.86	667.23
30	δ = 1.85(6H, s), 7(1H, m), 7.33~7.42(6H, m), 7.5~7.52(6H, m), 7.58(1H, m), 7.69~7.79(8H, m), 7.87(1H, m), 7.98~8(4H, m), 8.18~8.2(2H, m), 8.39~8.45(3H, m), 8.63(1H, s)	822.03	821.29
31	δ = 1.85(6H, s), 7(1H, m), 7.33~7.42(6H, m), 7.5~7.52(6H, m), 7.58(1H, m), 7.68~7.79(12H, m), 7.87(1H, m), 7.98~8(4H, m), 8.18~8.2(2H, m), 8.23(1H, s), 8.39~8.45(3H, m)	898.12	897.32
32	δ = 1.78(6H, s), 1.85(6H, s), 7(1H, m), 7.14(1H, m), 7.25(4H, m), 7.42(1H, m), 7.49~7.54(4H, m), 7.64(1H, m), 7.89(1H, m), 7.98~8.09(6H, m), 8.39(1H, m), 8.52(1H, m)	587.75	587.26
33	δ = 1.85(6H, s), 6.63(4H, m), 6.81~6.86(3H, m), 7(1H, m), 7.2~7.25(8H, m), 7.33~7.42(5H, m), 7.58(1H, m), 7.71~7.73(2H, m), 7.98~8(2H, m), 8.2(1H, m), 8.39~8.41(2H, m)	669.87	669.25
34	δ = 1.85(6H, s), 2.34(18H, s), 6.91(4H, m), 7(1H, m), 7.25(4H, m), 7.33~7.47(5H, m), 7.58(1H, m), 7.71(1H, m), 7.94~8(4H, m), 8.2(1H, m), 8.39~8.41(2H, m)	750.84	750.35
35	δ = 1.85(6H, s), 7(1H, m), 7.33~7.42(4H, m), 7.58(1H, m), 7.71(1H, m), 7.82~7.88(5H, m), 7.98~8.04(5H, m), 8.12(2H, m), 8.18~8.2(2H, m), 8.39~8.41(2H, m), 8.93(2H, m), 9.15(1H, m)	652.84	652.22
36	δ = 1.85(6H, s), 7(1H, m), 7.33~7.42(5H, m), 7.51~7.52(4H, m), 7.58(2H, m), 7.71(1H, m), 7.8~7.86(6H, m), 7.98~8(3H, m), 8.16~8.2(2H, m), 8.3(2H, m), 8.39~8.41(2H, m)	706.89	706.24
37	δ = 1.85(6H, s), 7(1H, m), 7.25(1H, m), 7.33~7.52(10H, m), 7.58(3H, m), 7.66~7.77(6H, m), 7.87(1H, m), 7.94~8(4H, m), 8.2(1H, m), 8.39~8.45(3H, m), 8.55(1H, m)	743.95	743.26
38	δ = 0.66(3H, s), 1.72(6H, s), 1.85(6H, s), 7(1H, m),	815.15	814.31

	7.33~7.46(12H, m), 7.55~7.63(6H, m), 7.71~7.77(3H, m), 7.93~8(4H, m), 8.06~8.08(2H, m), 8.2(1H, m), 8.39~8.41(2H, m)		
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- [122] [Example 1] Manufacture of OLED device using the organic electroluminescent compound according to the present invention
- [123] An OLED device was manufactured using the electroluminescent material according to the present invention. First, a transparent electrode ITO thin film ($15 \Omega/\square$) 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.
- [124] 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.
- [125] Then, *N,N'*-bis(α -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.
- [126] After forming the hole injection layer and the hole transport layer, an electroluminescent layer was formed thereon as follows. Compound **8** was placed in a cell of a vacuum vapor deposition apparatus as a host, and (piq)₂Ir(acac) [bis-(1-phenylisoquinolyl)iridium(III)acetylacetonate] 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 through doping at 4 to 10 wt%.
- [127] Subsequently, tris(8-hydroxyquinoline)-aluminum(III) (Alq) was vapor-deposited with a thickness of 20 nm as an electron transport layer on the electroluminescent 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.
- [128] Each compound used in the OLED was purified by vacuum sublimation at 10^{-6} torr.
- [129] As a result, it was confirmed that current of 16.5 mA/cm² flows at voltage of 6.2 V and a red light of 1060 cd/m² was emitted.
- [130] [Example 2] Manufacture of OLED device using organic electroluminescent

compounds according to the present invention

[131] An OLED device was manufactured as in Example 1 except that Compound **12** was added as a host material on the electroluminescent layer.

[132] As a result, it was confirmed that current of 16.0 mA/cm² flows at voltage of 6.3 V and a red light of 1120 cd/m² was emitted.

[133] [Example 3] Manufacture of OLED device using organic electroluminescent compounds according to the present invention

[134] An OLED device was manufactured as in Example 1 except that Compound **37** was added as a host material on the electroluminescent layer.

[135] As a result, it was confirmed that current of 17.5 mA/cm² flows at voltage of 6.5 V and a red light of 1100 cd/m² was emitted.

[136] [Comparative Example 1]

[137] An OLED device 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 as a host material at one cell of the vacuum vapor deposition apparatus, (piq)₂Ir(acac) [bis-(1-phenylisoquinolyl)iridium(III)acetylacetonate] as a dopant, and bis(2-methyl-8-quinolinato)(*p*-phenylphenolato)aluminum(III) (BALq) as a hole blocking layer were used.

[138] As a result, it was confirmed that current of 15.3 mA/cm² flows at voltage of 7.5 V and a red light of 1000 cd/m² was emitted.

[139] 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 and improving power consumption.

Industrial Applicability

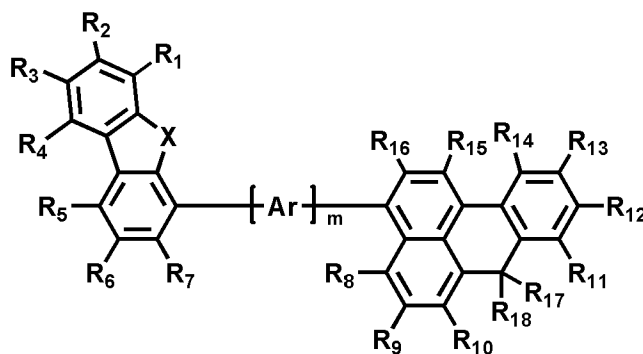
[140] Since the organic electroluminescent compound according to the present invention exhibits good luminous efficiency and excellent life property, it may be used to manufacture OLED devices having very superior operation life.

Claims

[Claim 1]

An organic electroluminescent compound represented by Chemical Formula 1:

[Chemical Formula 1]



wherein

X represents $-C(R_{20}R_{21})$, $-N(R_{22})$, $-S$, $-O$ or $-Si(R_{23}R_{24})$;

Ar represents (C6-C30)arylene with or without substituent(s) or (C3-C30)heteroarylene with or without substituent(s);

R_1 through R_{16} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s), 5- to 7-membered heterocycloalkyl 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), 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), (C6-C30)ar(C1-C30)alkyl with or without substituent(s), cyano, nitro, hydroxyl, $-NR_{31}R_{32}$, $-BR_{33}R_{34}$, $-PR_{35}R_{36}$, $-P(=O)R_{37}R_{38}$, $-SiR_{39}R_{40}R_{41}$ or $-YR_{42}$, or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring, wherein a carbon atom of the alicyclic ring or the mono- or polycyclic aromatic ring may be substituted with one or more heteroatom(s) selected from nitrogen, oxygen and sulfur;
 R_{17} , R_{18} and R_{20} through R_{24} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with

or without substituent(s) or 5- to 7-membered heterocycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring, wherein a carbon atom of the alicyclic ring or the mono- or polycyclic aromatic ring may be substituted with one or more heteroatom(s) selected from nitrogen, oxygen and sulfur;

R₃₁ through R₄₂ independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s) or 5- to 7-membered heterocycloalkyl with or without substituent(s), or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring, wherein a carbon atom of the alicyclic ring or the mono- or polycyclic aromatic ring may be substituted with one or more heteroatom(s) selected from nitrogen, oxygen and sulfur;

Y represents S or O;

m represents an integer from 0 to 3, and each Ar may be identical or different and may be linked to an adjacent substituent to form a ring, when m is 2 or greater; and

the heterocycloalkyl or heteroaryl includes one or more heteroatom(s) selected from B, N, O, S, P(=O), Si and P.

[Claim 2]

The organic electroluminescent compound according to claim 1, wherein the substituent of Ar, R₁ through R₁₆, R₁₇, R₁₈, R₂₀ through R₂₄ and R₃₁ through R₄₂ may be further substituted by one or more substituent(s) selected from the group consisting of 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, (C6-C30)cycloalkyl fused with one or more aromatic ring(s), R^aR^bR^cSi-, (C2-C30)alkenyl, (C2-C30)alkynyl, cyano, carbazolyl, -NR^dR^e, -BR^fR^g, -PR^hRⁱ, -P(=O)R^jR^k, (C6-C30)ar(C1-C30)alkyl, (C1-C30)alkyl(C6-C30)aryl, R^lZ-, R^mC(=O)-, R^mC(=O)O-, carboxyl, nitro and hydroxyl, wherein R^a through R^l independently represent

(C1-C30)alkyl, (C6-C30)aryl or (C3-C30)heteroaryl; Z represents S or O; and R^m represents (C1-C30)alkyl, (C1-C30)alkoxy, (C6-C30)aryl or (C6-C30)aryloxy.

[Claim 3]

The organic electroluminescent compound according to claim 1, wherein X represents $-C(R_{20}R_{21})$, $-N(R_{22})-$, $-S-$, $-O-$ or $-Si(R_{23}R_{24})-$;

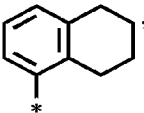
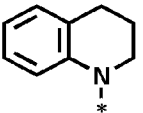
Ar represents (C6-C30)arylene with or without substituent(s) or (C3-C30)heteroarylene with or without substituent(s);

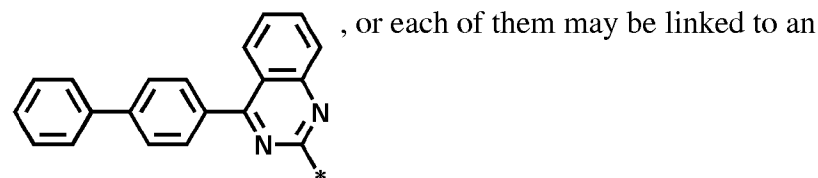
R_1 through R_{16} independently represent hydrogen, deuterium, halogen, (C1-C30)alkyl with or without substituent(s), (C6-C30)aryl with or without substituent(s), (C3-C30)heteroaryl with or without substituent(s), substituted or unsubstituted (C6-C30)aryl fused with one or more (C3-C30)cycloalkyl(s) with or without substituent(s), 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), cyano, $-NR_{31}R_{32}$, $-BR_{33}R_{34}$ or $-SiR_{39}R_{40}R_{41}$, or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring;

R_{17} , R_{18} and R_{20} through R_{24} independently represent hydrogen, deuterium, (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), or each of them may be linked to an adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring; and

R_{31} through R_{34} and R_{39} through R_{41} independently represent hydrogen, deuterium, halogen, (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).

[Claim 4]

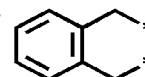
The organic electroluminescent compound according to claim 3, wherein R_1 through R_7 independently represent hydrogen, fluorine, t-butyl, cyclohexyl, diphenylamino, N-carbazolyl, diphenylmethylsilyl, triphenylsilyl, triphenylenyl, N-phenyl-carbazole-3-yl, diphenyl-triazinyl, , , dimesitylboranyl or



adjacent substituent via substituted or unsubstituted (C3-C30)alkylene or substituted or unsubstituted (C3-C30)alkenylene with or without a fused ring to form an alicyclic ring or a mono- or polycyclic aromatic ring;

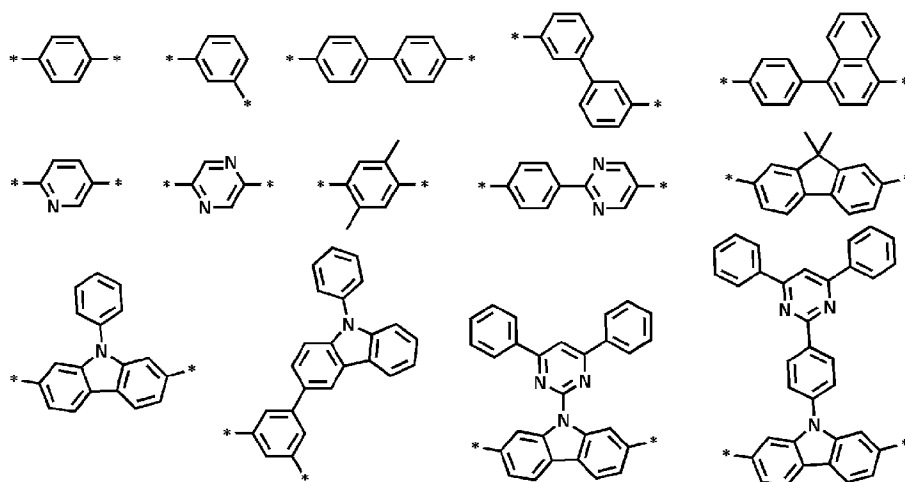
R₈ through R₁₆ independently represent hydrogen, methyl, phenyl, cyano, pyrimidyl or triazolyl, and the phenyl, pyrimidyl or triazolyl of R₈ through R₁₆ may be further substituted with one or more substituent(s) selected from methyl and phenyl;

R₁₇ and R₁₈ independently represent methyl, or each of them may be linked to an adjacent substituent via C4 alkylene or



to form a ring; and

$\ast - \text{Ar} - \ast$ is selected from the following structures:



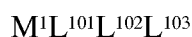
[Claim 5]

An organic electroluminescent device comprising the organic electroluminescent compound according to any of claims 1 to 4.

[Claim 6]

The organic electroluminescent device according to claim 5, 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) according to any of claims 1 to 4 and one or more host(s) represented Chemical Formula 2:

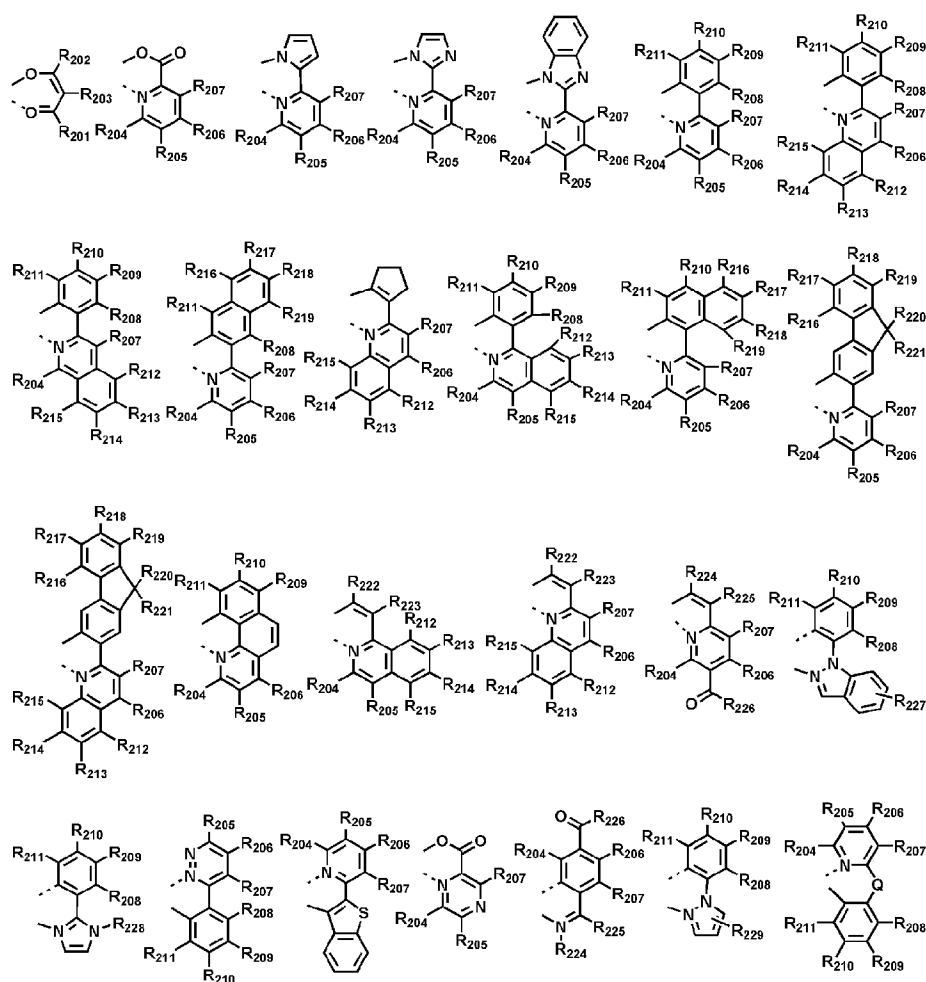
[Chemical Formula 2]



wherein

M¹ is a metal selected from the group consisting of Group 7, Group 8, Group 9, Group 10, Group 11, Group 13, Group 15 and Group 16 metals, and ligands L¹⁰¹, L¹⁰² and L¹⁰³ are independently selected from

the structures:



wherein

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

R₂₀₄ through R₂₁₉ independently represent hydrogen, deuterium, (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), 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), cyano or halogen;

R₂₂₀ through R₂₂₃ independently represent hydrogen, deuterium, (C1-C30)alkyl with or without halogen substituent(s) or (C6-C30)aryl

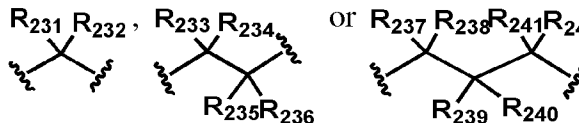
with or without (C1-C30)alkyl substituent(s);

R_{224} and R_{225} independently represent hydrogen, deuterium, (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 ring to form an alicyclic ring or a mono- or polycyclic aromatic ring;

R_{226} 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;

R_{227} through R_{229} independently represent hydrogen, deuterium, (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



R_{231} through R_{242} independently represent hydrogen, deuterium, (C1-C30)alkyl with or without halogen substituent(s), (C1-C30)alkoxy, halogen, (C6-C30)aryl with or without substituent(s), cyano or (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 7] The organic electroluminescent device according to claim 6, wherein the organic layer further comprises one or more amine compound(s) selected from the group consisting of arylamine compounds and styrylarylamine compounds.

[Claim 8] The organic electroluminescent device according to claim 6, wherein the organic layer further comprises one or more metal(s) selected from the group consisting of organic metals of Group 1, Group 2, 4th period and 5th period transition metals, lanthanide metals and d-transition elements.

[Claim 9] The organic electroluminescent device according to claim 6, wherein the organic layer comprises an electroluminescent layer and a charge generating layer.

[Claim 10] The organic electroluminescent device according to claim 6, which is a white-light emitting organic electroluminescent device wherein the organic layer further comprises one or more organic electroluminescent layer(s) emitting blue, red or green light.

INTERNATIONAL SEARCH REPORT

International application No.

PCT/KR2011/001918

A. CLASSIFICATION OF SUBJECT MATTER

Int. Cl.

C07C 13/66 (2006.01) *C07D 307/91* (2006.01) *C07F 7/08* (2006.01)
C07D 209/86 (2006.01) *C07D 333/76* (2006.01) *C09K 11/06* (2006.01)
C07D 239/26 (2006.01) *C07D 409/02* (2006.01) *H01L 51/54* (2006.01)
C07D 251/24 (2006.01) *C07F 5/02* (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)

STN CAS Online: Registry, CAPLUS – substructure search based on Chemical Formula 1

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	JP 2009-001499 A (MITSUI CHEMICALS INC.; IDEMITSU KOSAN CO LTD) 8 January 2009 Abstract, paragraphs [0055]-[0070]	
A	JP 2002-110356 A (MITSUI CHEMICALS INC) 12 April 2002 Abstract, paragraphs [0018]-[0060]	
A	JP 2001-267075 A (MITSUI CHEMICALS INC) 28 September 2001 Abstract, paragraphs [0017]-[0046]	
A	JP 2005-113071 A (TOYO INK MFG CO LTD) 28 April 2005 Abstract, paragraphs [0082]-[0088], page 28 - compound 105	



Further documents are listed in the continuation of Box C



See patent family annex

* Special categories of cited documents:	
"A" document defining the general state of the art which is not considered to be of particular relevance	"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
"E" earlier application or patent but published on or after the international filing date	"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
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"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
"O" document referring to an oral disclosure, use, exhibition or other means	"&" document member of the same patent family
"P" document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search
10 May 2011

Date of mailing of the international search report
12 MAY 2011

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INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No.

PCT/KR2011/001918

This Annex lists the known "A" publication level 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.

Patent Document Cited in Search Report		Patent Family Member
JP	2009001499	NONE
JP	2002110356	NONE
JP	2001267075	NONE
JP	2005113071	NONE
Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001.		
END OF ANNEX		