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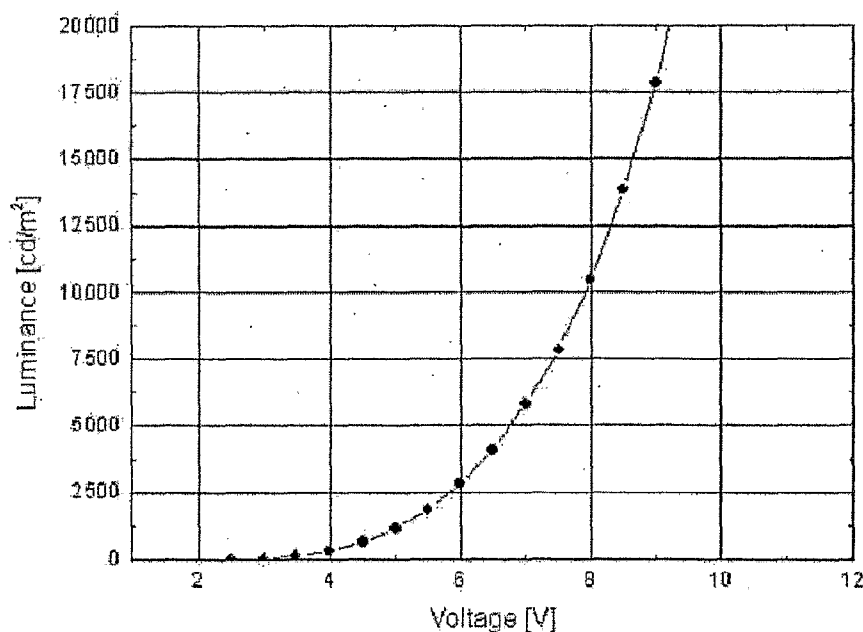
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[Continued on next page]

(54) Title: ORGANIC ELECTROLUMINESCENT COMPOUNDS AND DISPLAY DEVICE USING THE SAME AS AN ELECTROLUMINESCENT MATERIAL



(57) Abstract: The present invention relates to an organic electroluminescent compound represented by Chemical Formula 1 and an electroluminescent device containing the same as an electroluminescent material. The electroluminescent compound according to the present invention is advantageous in that it prominently lowers the driving voltage and considerably enhances the power efficiency when being used as a host material for an OLED device.

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Description

ELECTROLUMINESCENT COMPOUNDS AND ORGANIC ELECTROLUMINESCENT DEVICE USING THE SAME

Technical Field

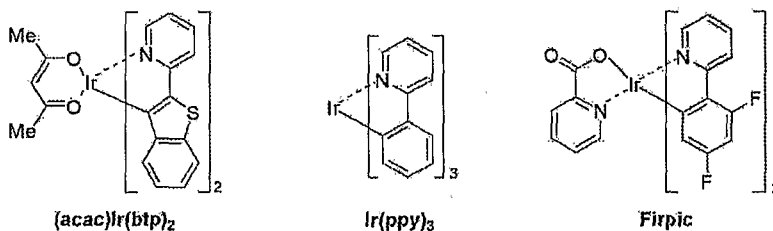
- [1] The present invention relates to an electroluminescent compound comprised of a metal complex, which shows excellent electrical conductivity and electroluminescent property with high efficiency, and an electroluminescent device comprising the same as a host material.

[2]

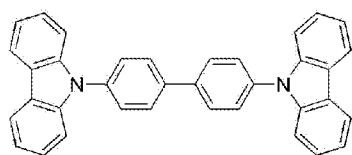
Background Art

- [3] The most important factor to determine luminous efficiency in an OLED is the electroluminescent characteristics of electroluminescent material. Though a fluorescent material has been widely used as an electroluminescent material up to the present, a development of phosphorescent material is one of the best solutions to improve luminous efficiency theoretically up to four times in view of electroluminescent mechanism.
- [4] Up to now, iridium(III) complexes are widely known as phosphorescent dopants, including (acac)Ir(btp)₂, Ir(ppy)₃ and Firpic, as the red, green and blue one, respectively. In particular, a lot of phosphorescent materials have been investigated in Japan and Europe and America, so that development of further improved phosphorescent materials is expected.

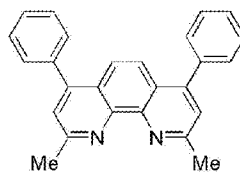
[5]



- [6] As a host material for phosphorescent light emitting material, CBP is most widely known up to the present, and OLEDs having high efficiency to which a hole blocking layer such as BCP and BAQ, etc. has been applied have been known. Pioneer (Japan) reported OLEDs having high efficiency using a BAQ derivative as the host.

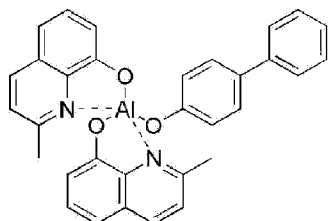


CBP

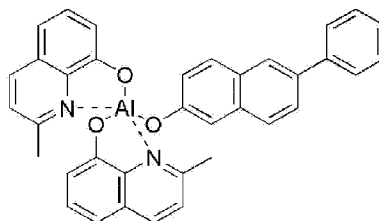


BCP

[8]



BAiq



BAiq DERIVATIVE

[9] Though the materials in prior art are advantageous in view of light emitting property, they have low glass transition temperature and very poor thermal stability, so that the materials tend to be changed during high temperature vacuum-vapor-deposition process. In addition, they are not satisfactory in terms of lifetime of an OLED device, so that development of host materials having better material stability and more excellent EL performance is required.

[10] According to the present invention, developed are metal complex materials exhibiting excellent material stability, excellent electrical conductivity and luminous property of high efficiency as compared to conventional materials. An aromatic ring containing a hetero atom or a side chain substituent hetero atom containing non-bonding electron pair has a property to readily coordinate to metal. Such a coordination shows very stable property in electrochemical aspect, which has been known widely. The present invention developed various ligands, prepared metal complexes having above-mentioned properties and applied them as host materials.

[11] A number of conventional complexes of such type have been researched since the middle of 1990's. However, those materials have been applied merely as an electroluminescent material, but rarely as a host material.

[12]

Disclosure of Invention

Technical Problem

[13] The object of the invention is to overcome the disadvantages as described above, and to provide mixed type ligand-metal complexes as electroluminescent materials, which are very excellent in luminous and physical properties as compared to conventional organic host materials or aluminum complexes. Another object of the

invention is to provide an electroluminescent device containing the electroluminescent compound thus prepared as a host material.

[14]

Technical Solution

[15] The present invention relates to an electroluminescent compound comprised represented by Chemical Formula 1 and an electroluminescent device containing the same as a host material.

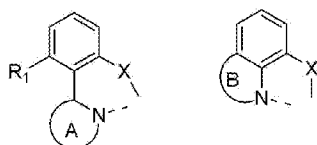
[16]

[17] [Chemical Formula 1]

[18] $L^1 L^2 M$

[19] In the formula, L^1 and L^2 are different each other, and selected from those represented by one of the following structural formulas:

[20]

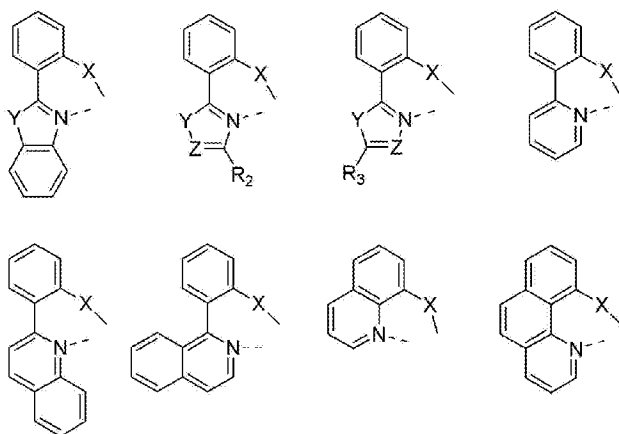


[21] wherein M is a divalent metal; X is O, S or Se; A ring is oxazole, thiazole, imidazole, oxadiazole, thiadiazole, benzoxazole, benzothiazole, benzimidazole, pyridine or quinoline, and the pyridine or quinoline may form a fused ring with R_1 via chemical bond, and said A ring may have additional substituent such as C1-C5 alkyl, or phenyl or naphthyl with or without substituent(s); B ring is pyridine or quinoline, and said B ring may have additional substituent such as C1-C5 alkyl, or phenyl or naphthyl with or without substituent(s); and R_1 independently represents hydrogen or C1-C5 alkyl.

[22]

[23] In the Chemical Formula 1 as described above, the ligands L^1 and L^2 are different each other, and may be selected from those represented by one of the following structural formulas:

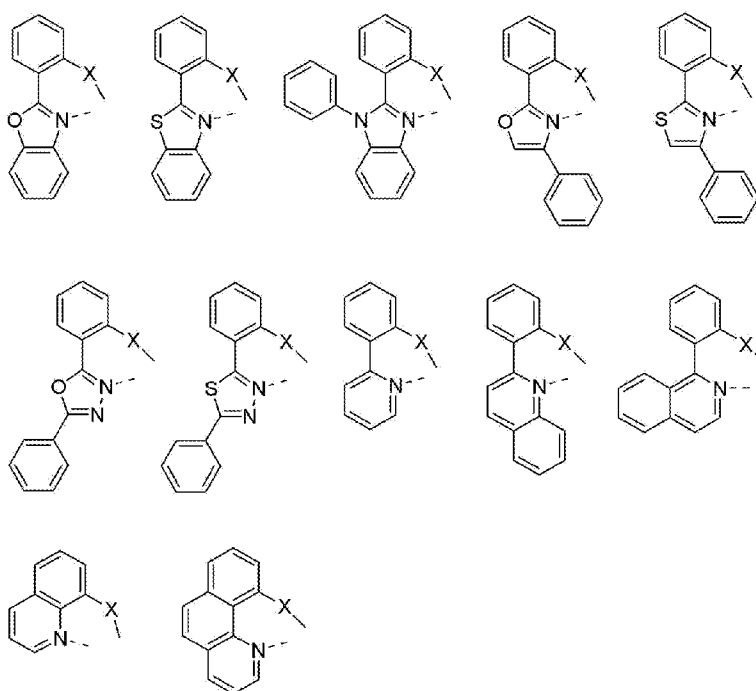
[24]



[25] wherein, M is divalent metal; X is O, S or Se; Y is O, S or N-R₄, Z is CH or N; R₂ and R₃ independently represent hydrogen, phenyl or naphthyl with or without substituent(s); and R₄ is C1-C5 alkyl, or phenyl or naphthyl with or without substituent(s).

[26] In Chemical Formula 1, M is preferably selected from Be, Zn, Mg, Cu and Ni, and the ligands L¹ and L² are preferably selected from those represented by one of the following structural formulas:

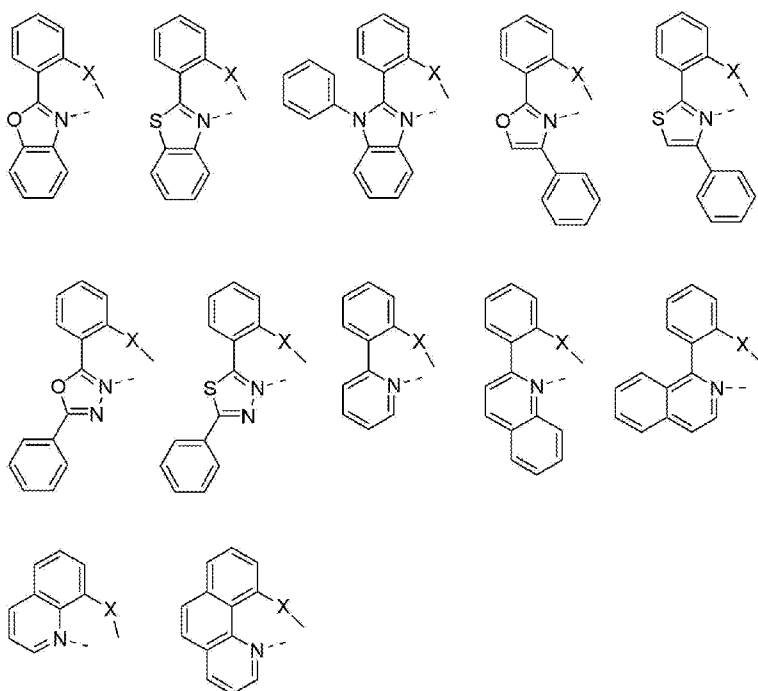
[27]



[28] wherein, X is O, S or Se.

[29] The ligands L¹ and L² of the electroluminescent compounds according to the present invention are exemplified as follows:

[30]

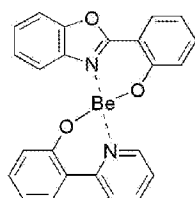


[31] wherein, X is O or S.

[32] Specifically, the electroluminescent compounds of Chemical Formula 1 according to the present invention may be exemplified as the compounds represented by one of the Chemical Formulas 1-1 through 1-18:

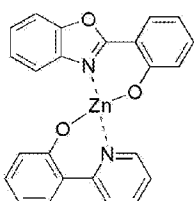
[33] [Chemical Formula 1-1]

[34]



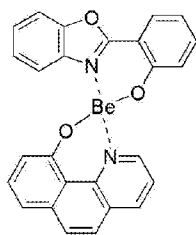
[35] [Chemical Formula 1-2]

[36]



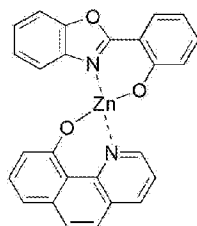
[37] [Chemical Formula 1-3]

[38]



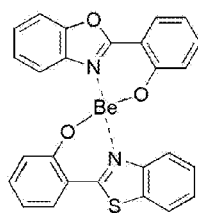
[39] [Chemical Formula 1-4]

[40]



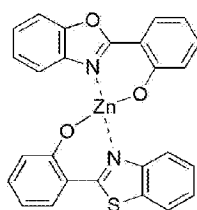
[41] [Chemical Formula 1-5]

[42]



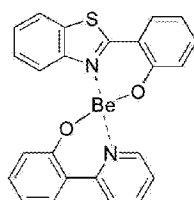
[43] [Chemical Formula 1-6]

[44]



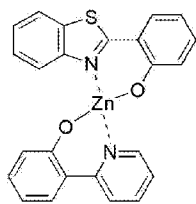
[45] [Chemical Formula 1-7]

[46]



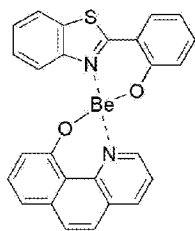
[47] [Chemical Formula 1-8]

[48]



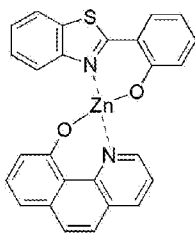
[49] [Chemical Formula 1-9]

[50]



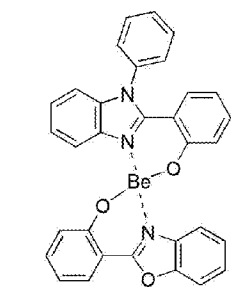
[51] [Chemical Formula 1-10]

[52]



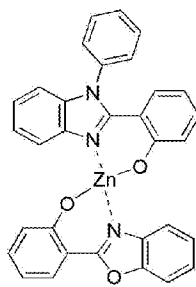
[53] [Chemical Formula 1-11]

[54]



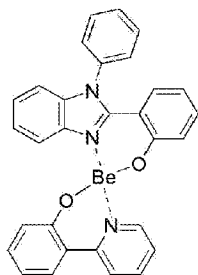
[55] [Chemical Formula 1-12]

[56]



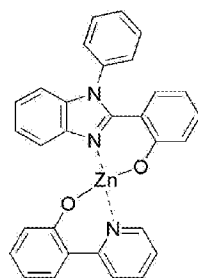
[57] [Chemical Formula 1-13]

[58]



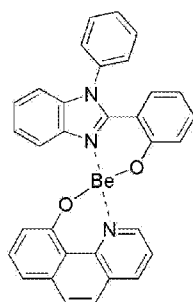
[59] [Chemical Formula 1-14]

[60]



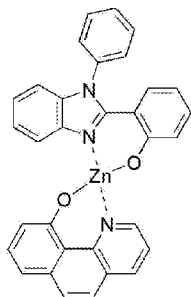
[61] [Chemical Formula 1-15]

[62]



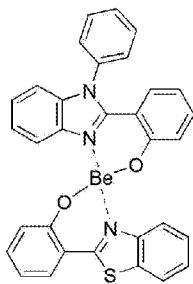
[63] [Chemical Formula 1-16]

[64]



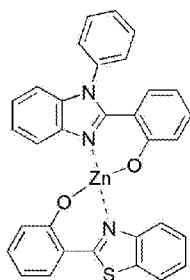
[65] [Chemical Formula 1-17]

[66]



[67] [Chemical Formula 1-18]

[68]



[69]

Brief Description of the Drawings

[70]

[71] Fig. 1 EL spectrum of the OLED device prepared according to Comparative Example 1

[72] Fig. 2 Luminance-applied voltage characteristic of the OLED device prepared according to Comparative Example 1

[73] Fig. 3 Luminous efficiency-luminance characteristic of the OLED device prepared according to Comparative Example 1

[74] Fig. 4 Luminance-applied voltage characteristic of the OLED device prepared according to Example 1

[75] Fig. 5 Luminous efficiency-luminance characteristic of the OLED device prepared according to Example 1

[76]

[77] Other and further objects, features and advantages of the invention will appear more fully from the following description.

[78]

[79]

Mode for the Invention

[80] The present invention is further described with respect to the electroluminescent compounds according to the present invention, a process for preparing the same and

the electroluminescent properties of the device employing the same, by referring to representative compounds according to the present invention, which are provided for illustration only and are not intended to be limiting in any way.

[81] [Preparation Example 1] Compound of Chemical Formula 1-1

[82] In 50 mL of methanol, 2-pyridin-2-yl-phenol (1.0 g, 5.84 mmol) was dissolved, and 10 mL of aqueous 1M sodium hydroxide solution was added thereto. To the mixed solution, a solution of beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol) in 10 mL of aqueous methanol (methanol 7 mL: water 3 mL) was added dropwise, and the resultant mixture was stirred at ambient temperature for 2 hours. After completing the stirring, 2-hydroxy-phenyl benzoxazole (1.54 g, 7.30 mmol) dissolved in 50 mL of methanol was slowly added. The reaction solution was then stirred at ambient temperature for 2 hours. The temperature of the solution was raised to 50°C, and the solution was stirred for 10 hours.

[83] After completion of the stirring, the precipitate produced was filtered, washed with water (50 mL) and acetone (50 mL), and dried to obtain the title compound, Compound (1-1) (0.80 g, 2.04 mmol, yield: 34%).

[84] MS/FAB: 391(found), 391.43(calculated)

[85] EA: C 73.55%, H 4.59%, N 7.05%, O 12.41%

[86] [Preparation Example 2] Compound of Chemical Formula 1-2

[87] In 50 mL of methanol, 2-pyridin-2-yl-phenol (1.0 g, 5.84 mmol) was dissolved, and 10 mL of aqueous 1M sodium hydroxide solution was added thereto. To the mixed solution, zinc acetate (0.95 g, 5.18 mmol) dissolved in methanol (10 mL) was added dropwise, and the resultant mixture was stirred at ambient temperature for 2 hours. After completing the stirring, 2-hydroxy-phenyl benzoxazole (1.50 g, 7.10 mmol) dissolved in 50 mL of methanol was slowly added. The reaction mixture was then stirred at ambient temperature for 10 hours.

[88] After completion of the stirring, the precipitate produced was filtered, washed with water (50 mL) and acetone (50 mL), and dried to obtain the title compound, Compound (1-2) (0.72 g, 1.61 mmol, yield: 27%).

[89] MS/FAB: 447(found), 447.79(calculated)

[90] EA: C 64.22%, H 4.01%, N 6.05%, O 10.95%

[91] [Preparation Example 3] Compound of Chemical Formula 1-3

[92] The same procedure as Preparation Example 1 was carried out by using 2-hydroxy-phenyl benzoxazole (1.23 g, 5.82 mmol), 10-hydroxybenzo[h]quinoline (1.48 g, 7.58 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-3) (0.35 g, 0.84 mmol, yield: 14%).

[93] MS/FAB: 415(found), 415.46(calculated)

[94] EA: C 75.02%, H 4.27%, N 6.64%, O 11.65%

- [95] [Preparation Example 4] Compound of Chemical Formula 1-4
- [96] The same procedure as Preparation Example 2 was carried out by using 2-hydroxy-phenyl benzoxazole (1.23 g, 5.82 mmol), 10-hydroxybenzo[*h*]quinoline (1.48 g, 7.58 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-4) (0.52 g, 1.10 mmol, yield: 19%).
- [97] MS/FAB: 471(found), 471.81(calculated)
- [98] EA: C 66.08%, H 3.79%, N 5.84%, O 10.30%
- [99] [Preparation Example 5] Compound of Chemical Formula 1-5
- [100] The same procedure as Preparation Example 1 was carried out by using 2-hydroxy-phenyl benzoxazole (1.23 g, 5.82 mmol), 2-hydroxy-phenyl benzothiazole (1.72 g, 7.57 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-5) (0.96 g, 2.15 mmol, yield: 37%).
- [101] MS/FAB: 447(found), 447.52(calculated)
- [102] EA: C 69.68%, H 4.01%, N 6.16%, O 10.85% S 7.05%
- [103] [Preparation Example 6] Compound of Chemical Formula 1-6
- [104] The same procedure as Preparation Example 2 was carried out by using 2-hydroxy-phenyl benzoxazole (1.23 g, 5.82 mmol), 2-hydroxy-phenyl benzothiazole (1.72 g, 7.57 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-6) (1.36 g, 2.70 mmol, yield: 46%).
- [105] MS/FAB: 503(found), 503.88(calculated)
- [106] EA: C 61.88%, H 3.54%, N 5.46%, O 9.73%, S 6.26%
- [107] [Preparation Example 7] Compound of Chemical Formula 1-7
- [108] The same procedure as Preparation Example 1 was carried out by using 2-hydroxy-phenyl benzothiazole (1.32 g, 5.80 mmol), 2-pyridine-2-yl-phenol (1.30 g, 7.59 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-7) (0.59 g, 1.45 mmol, yield: 25%).
- [109] MS/FAB: 407(found), 407.50(calculated)
- [110] EA: C 70.64%, H 4.35%, N 6.76%, O 7.96%, S 7.75%
- [111] [Preparation Example 8] Compound of Chemical Formula 1-8
- [112] The same procedure as Preparation Example 2 was carried out by using 2-hydroxy-phenyl benzothiazole (1.32 g, 5.80 mmol), 2-pyridine-2-yl-phenol (1.30 g, 7.59 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-8) (0.83 g, 1.79 mmol, yield: 31%).
- [113] MS/FAB: 463(found), 463.86(calculated)
- [114] EA: C 62.04%, H 3.82%, N 5.98%, O 7.02%, S 6.83%
- [115] [Preparation Example 9] Compound of Chemical Formula 1-9
- [116] The same procedure as Preparation Example 1 was carried out by using 2-hydroxy-phenyl benzothiazole (1.32 g, 5.80 mmol), 10-hydroxybenzo[*h*]quinoline

(1.48 g, 7.58 mmol) instead of 2-hydroxy-phenyl benzoxazole, and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-9) (0.98 g, 2.27 mmol, yield: 39%).

[117] MS/FAB: 431(found), 431.52(calculated)

[118] EA: C 72.22%, H 4.10%, N 6.40%, O 7.62%, S 7.33%

[119] [Preparation Example 10] Compound of Chemical Formula 1-10

[120] The same procedure as Preparation Example 4 was carried out by using 2-hydroxy-phenyl benzothiazole (1.32 g, 5.80 mmol), 10-hydroxybenzo[*h*]quinoline (1.48 g, 7.58 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-10) (1.22 g, 2.50 mmol, yield: 43%).

[121] MS/FAB: 487(found), 487.88(calculated)

[122] EA: C 63.93%, H 3.65%, N 5.64%, O 6.70%, S 6.44%

[123] [Preparation Example 11] Compound of Chemical Formula 1-11

[124] The same procedure as Preparation Example 1 was carried out by using 2-hydroxy-phenyl benzoxazole (1.23 g, 5.82 mmol), 2-(1-phenyl-1H-benzoimidazol-2-yl)-phenol (2.17 g, 7.58 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-11) (0.56 g, 1.11 mmol, yield: 19%).

[125] MS/FAB: 506(found), 506.57(calculated)

[126] EA: C 75.67%, H 4.50%, N 8.20%, O 9.68%

[127] [Preparation Example 12] Compound of Chemical Formula 1-12

[128] The same procedure as Preparation Example 2 was carried out by using 2-hydroxy-phenyl benzoxazole (1.23 g, 5.82 mmol), 2-(1-phenyl-1H-benzoimidazol-2-yl)-phenol (2.17 g, 7.58 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-12) (0.72 g, 1.28 mmol, yield: 22%).

[129] MS/FAB: 562(found), 562.93(calculated)

[130] EA: C 68.16%, H 4.05%, N 7.36%, O 8.68%

[131] [Preparation Example 13] Compound of Chemical Formula 1-13

[132] The same procedure as Preparation Example 1 was carried out by using 2-(1-phenyl-1H-benzoimidazol-2-yl)phenol (1.67 g, 5.83 mmol), 2-pyridin-2-yl-phenol (1.30 g, 7.59 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-13) (0.84 g, 1.80 mmol, yield: 31%).

[133] MS/FAB: 466(found), 466.55(calculated)

[134] EA: C 77.08%, H 4.87%, N 8.90%, O 6.98%

[135] [Preparation Example 14] Compound of Chemical Formula 1-14

[136] The same procedure as Preparation Example 2 was carried out by using 2-(1-phenyl-1H-benzimidazol-2-yl)-phenol (1.67 g, 5.83 mmol),

2-pyridine-2-yl-phenol (1.30 g, 7.59 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-14) (0.88 g, 1.68 mmol, yield: 29%).

[137] MS/FAB: 522(found), 522.91(calculated)

[138] EA: C 68.81%, H 4.33%, N 7.92%, O 6.32%

[139] [Preparation Example 15] Compound of Chemical Formula 1-15

[140] The same procedure as Preparation Example 1 was carried out by using 2-(1-phenyl-1H-benzoimidazol-2-yl)-phenol (1.67 g, 5.83 mmol), 10-hydroxybenzo[h]quinoline (1.50 g, 7.68 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-15) (0.26 g, 0.53 mmol, yield: 9%).

[141] MS/FAB: 490(found), 490.57(calculated)

[142] EA: C 78.20%, H 4.68%, N 8.42%, O 6.70%

[143] [Preparation Example 16] Compound of Chemical Formula 1-16

[144] The same procedure as Preparation Example 2 was carried out by using 2-(1-phenyl-1H-benzimidazol-2-yl)-phenol (1.67 g, 5.83 mmol), 10-hydroxybenzo[h]quinoline (1.50 g, 7.68 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-16) (0.42 g, 0.77 mmol, yield: 13%).

[145] MS/FAB: 546(found), 546.93(calculated)

[146] EA: C 70.13%, H 4.16%, N 7.58%, O 5.98%

[147] [Preparation Example 17] Compound of Chemical Formula 1-17

[148] The same procedure as Preparation Example 1 was carried out by using 2-hydroxy-phenyl benzothiazole (1.32 g, 5.80 mmol), 2-(1-phenyl-1H-benzoimidazol-2-yl)-phenol (2.17 g, 7.58 mmol) and beryllium sulfate tetrahydrate (1.05 g, 5.93 mmol), to obtain the title compound, Compound (1-17) (0.64 g, 1.22 mmol, yield: 21%).

[149] MS/FAB: 522(found), 522.64(calculated)

[150] EA: C 73.42%, H 4.34%, N 7.97%, O 6.25%, S 6.04%

[151] [Preparation Example 18] Compound of Chemical Formula 1-18

[152] The same procedure as Preparation Example 2 was carried out by using 2-hydroxy-phenyl benzothiazole (1.32 g, 5.80 mmol), 2-(1-phenyl-1H-benzimidazol-2-yl)-phenol (2.17 g, 7.58 mmol) and zinc acetate (0.95 g, 5.18 mmol), to obtain the title compound, Compound (1-18) (0.94 g, 1.62 mmol, yield: 28%).

[153] MS/FAB: 578(found), 578.99(calculated)

[154] EA: C 66.22%, H 3.94%, N 7.16%, O 5.70%, S 5.49%

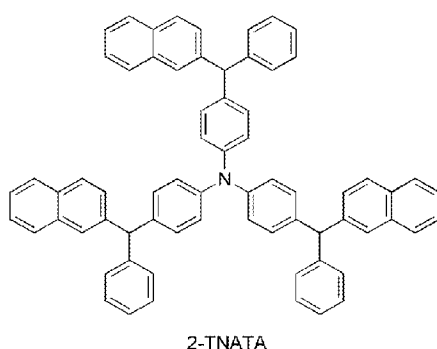
[155] [Example 1 - 18] Manufacture of OLED device by using the compounds according to the present invention

[156] OLED devices having the structure employing the host materials according to the present invention were manufactured.

[157] First, a transparent electrode ITO thin film ($15 \Omega/\square$) obtained from a glass for OLED was subjected to ultrasonic washing with trichloroethylene, acetone, ethanol and distilled water, subsequently, and stored in isopronanol before use.

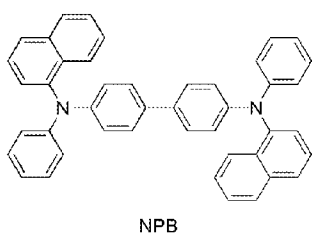
[158] Then, an ITO substrate was equipped in a substrate folder of vacuum vapor-deposit device, and 4,4',4''-tris(N,N-(2-naphthyl)-phenylamino)triphenylamine (2-TNATA) represented by following structural formula was placed in a cell of the vacuum vapor-deposit device, which was then ventilated up to 10^{-6} torr of vacuum in the chamber. Electric current was applied to the cell to evaporate 2-TNATA to vapor-deposit a hole injection layer having 40 nm of thickness on the ITO substrate.

[159]



[160] Then, to another cell of the vacuum vapor-deposit device, charged was N,N'-bis(α -naphthyl)-N,N'-diphenyl-4,4'-diamine (NPB), and electric current was applied to the cell to evaporate NPB to vapor-deposit a hole transport layer of 20 nm of thickness on the hole injection layer.

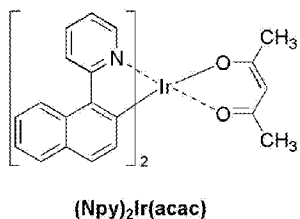
[161]



[162]

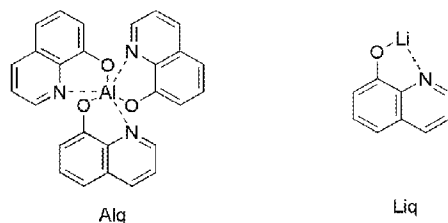
[163] After forming the hole injection layer and hole transport layer, an electroluminescent layer was vapor-deposited thereon as follows. In one cell of the vacuum vapor-deposit device, charged was a compound selected from Compounds 1-1 through 1-18 which was purified via sublimation in vacuo under 10^{-6} torr, as a host material, and in another cell, charged was $(\text{NPy})_2\text{Ir}(\text{acac})$. The two materials were evaporated at different rates to give doping of 4~10 mol%, to vapor-deposit light emitting layer having 30 nm of thickness on the hole transport layer.

[164]



[165] Then, tris(8-hydroxyquinoline)aluminum(III) (Alq) represented by following structural formula was vapor-deposited as an electron transport layer in a thickness of 20 nm, and lithium quinolate (Liq) represented by following structural formula was vapor-deposited as an electron injection layer in a thickness of 1 to 2 nm. Thereafter, an Al cathode was vapor-deposited in a thickness of 150 nm by using another vapor-deposit device to manufacture an OLED.

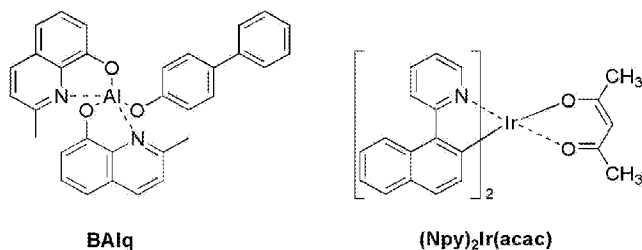
[166]



[167] [Comparative Example 1]

[168] An OLED device was made according to the same procedure as described in Example 1, but bis(2-methyl-8-quinolino)(p-phenylphenolato)aluminum(III) (BAIq) was charged to another cell in the vacuum vapor-deposit device as a light emitting host material, while (NPy)₂Ir(acac) was charged as a light emitting material in still another cell, and the two materials were evaporated at different rates to give doping of 4~10 mol%, to vapor-deposit a light emitting layer having 30 nm of thickness on said hole transport layer.

[169]



[170] [Example 19]

[171] Confirmation of OLED properties

[172] The luminous efficiency and power efficiency of each OLED device containing the electroluminescent compound according to the present invention prepared from one of Examples 1-18 and the conventional electroluminescent compound prepared from

Comparative Example 1 were measured at $1,000 \text{ cd/m}^2$, of which the results are shown in Table 1.

[173] From the Table showing the light emitting properties of the complexes developed by the present invention, it is found that the complexes developed by the present invention exhibit excellent properties in terms of performances as compared to conventional material.

[174] Table 1

	Host material	EL material	Driving voltage @ $1,000 \text{ cd/m}^2$	Luminous Efficiency (cd/A) @ $1,000 \text{ cd/m}^2$	Power efficiency (lm/W) @ $1,000 \text{ cd/m}^2$	Color Coordinate (x, y)
Ex. 1	1-1	(NPY) ₂ Ir(acac)	5.24	6.60	3.95	(0.677, 0.322)
Ex. 2	1-2	(NPY) ₂ Ir(acac)	5.20	6.54	3.95	(0.677, 0.322)
Ex. 3	1-3	(NPY) ₂ Ir(acac)	5.26	6.27	3.74	(0.677, 0.322)
Ex. 4	1-4	(NPY) ₂ Ir(acac)	5.21	6.57	3.96	(0.677, 0.322)
Ex. 5	1-5	(NPY) ₂ Ir(acac)	5.31	5.80	3.43	(0.674, 0.325)
Ex. 6	1-6	(NPY) ₂ Ir(acac)	5.23	6.40	3.84	(0.677, 0.322)
Ex. 7	1-7	(NPY) ₂ Ir(acac)	5.57	5.78	3.26	(0.675, 0.324)
Ex. 8	1-8	(NPY) ₂ Ir(acac)	6.00	5.84	3.06	(0.676, 0.323)
Ex. 9	1-9	(NPY) ₂ Ir(acac)	4.85	6.40	4.14	(0.677, 0.322)
Ex. 10	1-10	(NPY) ₂ Ir(acac)	4.80	6.29	4.11	(0.677, 0.321)
Ex. 11	1-11	(NPY) ₂ Ir(acac)	4.90	6.45	4.13	(0.677, 0.321)
Ex. 12	1-12	(NPY) ₂ Ir(acac)	4.79	6.51	4.27	(0.677, 0.321)
Ex. 13	1-13	(NPY) ₂ Ir(acac)	5.22	6.55	3.94	(0.677, 0.322)
Ex. 14	1-14	(NPY) ₂ Ir(acac)	4.86	6.67	4.31	(0.676, 0.322)
Ex. 15	1-15	(NPY) ₂ Ir(acac)	5.20	6.10	3.68	(0.677, 0.322)
Ex. 16	1-16	(NPY) ₂ Ir(acac)	4.81	6.24	4.07	(0.677, 0.321)
Ex. 17	1-17	(NPY) ₂ Ir(acac)	5.30	6.36	3.77	(0.677, 0.322)
Ex. 18	1-18	(NPY) ₂ Ir(acac)	4.85	5.52	3.57	(0.677, 0.322)
Comp. Ex. 1	BAIq	(NPY) ₂ Ir(acac)	7.49	6.16	2.58	(0.677, 0.321)

[175] As can be seen from the Table, when the electroluminescent material according to the present invention is applied as a host, the EL performance is noticeably improved as a rule.

[176] Fig. 1, an EL spectrum of Comparative Example 1 wherein (NPY)₂Ir(acac) compound (emitting orange-red light) was used as an electroluminescent material and BAIq as a host material, shows maximum EL peak at about 624 nm. From Fig. 2 showing luminance-applied voltage characteristic of Comparative Example 1, it is confirmed that driving voltage of the device of Comparative Example 1 is about 5 V, and the driving voltage at $1,000 \text{ cd/m}^2$ (standard of Table 1) was 7.49 V. From Fig. 3

which shows luminous efficiency-luminance characteristic of Comparative Example 1 and Table 1, it is confirmed that the device of Comparative Example 1 showed luminous efficiency of about 6.16 cd/A at the luminance of about 1,000 cd/m², and color coordinates of (0.677,0.321).

[177] As can be seen from Fig. 4 which shows luminance-applied voltage characteristic of the OLED device prepared according to Example 14, the device of Example 14 employing the electroluminescent compound according to the present invention showed driving voltage of about 3 V, and luminance of about 1,000 cd/m² at about 4.86 V; the result shows decrease of driving voltage by at least 2.6 V as compared to the device of Comparative Example 1.

[178] Further, as can be seen from Fig. 5 which shows luminous efficiency-luminance characteristic of the device according to Example 14, it showed luminous efficiency of about 6.67 cd/A at 1,000 cd/m² of luminance; which shows higher luminous efficiency by about 0.5 cd/A as compared to the device of Comparative Example 1 at the same luminance.

[179] With respect to power efficiency which is considered important in a practical panel, since the term voltage is included in the denominator in Formula 1 below, the device having lowered driving voltage becomes far advantageous in terms of power consumption:

[180]
$$\text{Power efficiency (lm/W)} = (\pi \times \text{luminance}) / (\text{current density} \times \text{voltage}) \text{-----(1)}$$

[181] As can be seen from Table 1 above, the device employing an electroluminescent compound according to the present invention as the host material lowers the driving voltage to induce increase of power efficiency by 0.5 ~ 2.0 lm/W, thereby improving the power consumption.

[182]

Industrial Applicability

[183] When the electroluminescent compounds according to the present invention are employed in OLED devices as a host material, driving voltage is noticeably lowered and power efficiency is considerably increased. Thus, the compounds in the present invention are suitable for an OLED material in next generation, and expected to greatly contribute for the development of large size display adopted OLED.

[184]

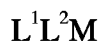
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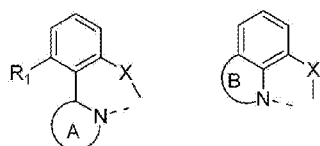
Claims

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

[Chemical Formula 1]

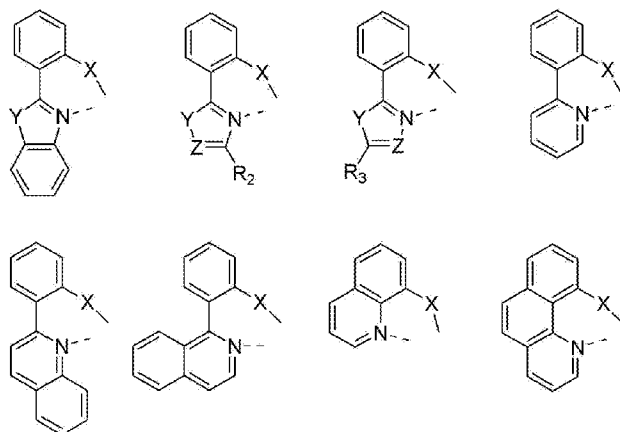


wherein, L^1 and L^2 are different each other, and selected from those represented by one of the following structural formulas:



wherein, M is a divalent metal; X is O, S or Se; A ring is oxazole, thiazole, imidazole, oxadiazole, thiadiazole, benzoxazole, benzothiazole, benzimidazole, pyridine or quinoline, and the pyridine or quinoline may form a fused ring with R_1 via chemical bond, and said A ring may have additional substituent such as C1-C5 alkyl, or phenyl or naphthyl with or without substituent(s); B ring is pyridine or quinoline, and said B ring may have additional substituent such as C1-C5 alkyl, or phenyl or naphthyl with or without substituent(s); and R_1 independently represents hydrogen or C1-C5 alkyl.

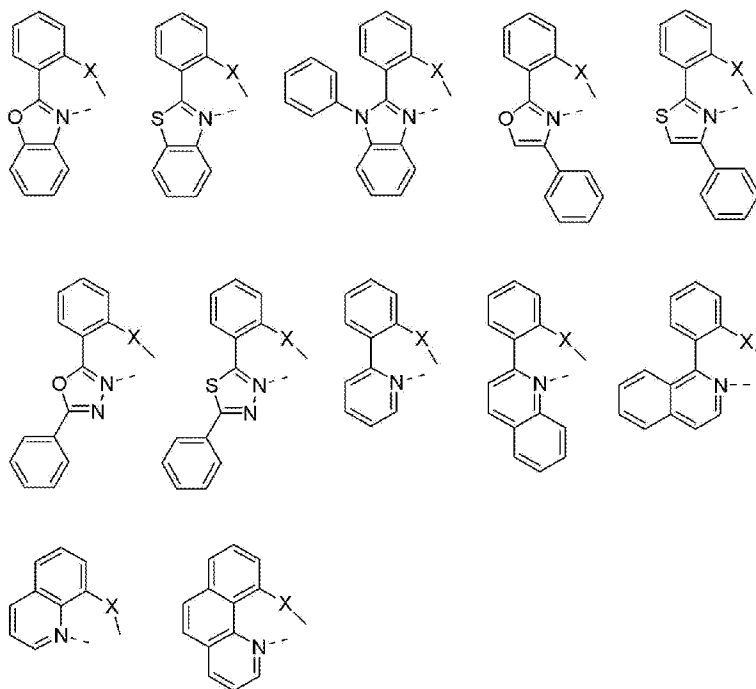
[2] An electroluminescent compound according to claim 1, wherein the ligands L^1 and L^2 are different each other, and selected from those represented by one of the following structural formulas:



wherein, M is divalent metal; X is O, S or Se; Y is O, S or $N-R_4$, Z is CH or N; R_2 and R_3 independently represent hydrogen, phenyl or naphthyl with or without substituent(s); and R_4 is C1-C5 alkyl, or phenyl or naphthyl with or without substituent(s).

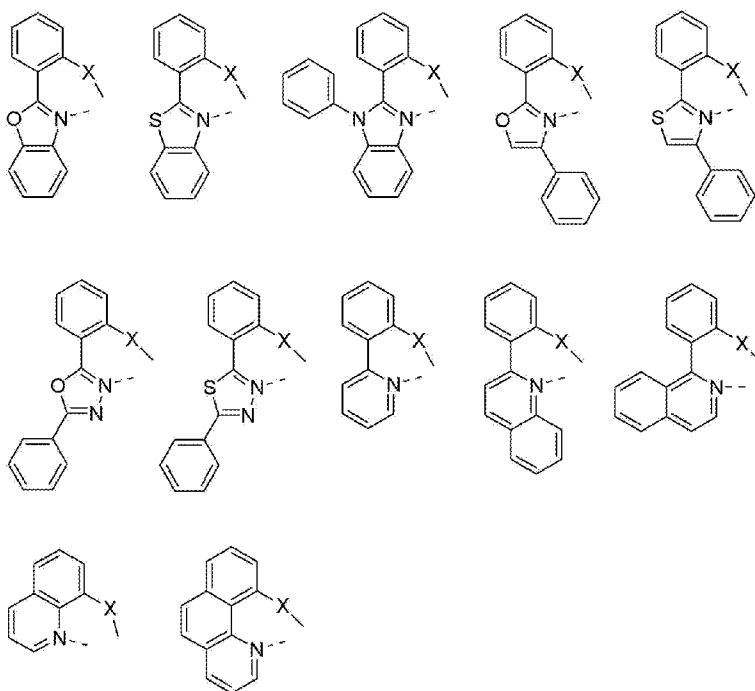
[3] An electroluminescent compound according to claim 1, wherein M is selected from Be, Zn, Mg, Cu and Ni.

- [4] An electroluminescent compound according to claim 1, wherein the ligands L^1 and L^2 are different each other and selected from those represented by one of the following structural formulas:



wherein, X is O, S or Se.

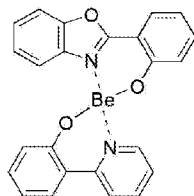
- [5] An electroluminescent compound according to claim 4, wherein the ligands L^1 and L^2 are different each other, and selected from those represented by one of the following structural formulas:



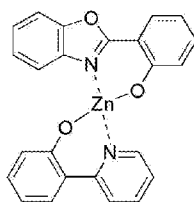
wherein, X is O or S.

- [6] An electroluminescent compound according to claim 5, which is selected from the compounds represented by one of Chemical Formulas 1-1 through 1-18:

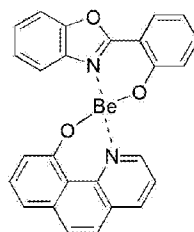
[Chemical Formula 1-1]



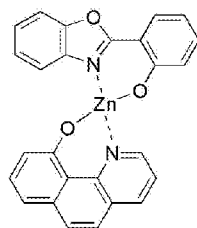
[Chemical Formula 1-2]



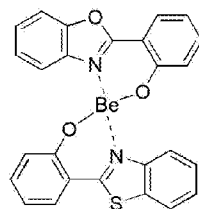
[Chemical Formula 1-3]



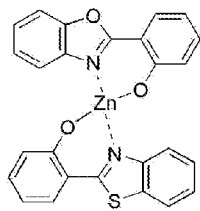
[Chemical Formula 1-4]



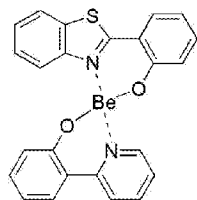
[Chemical Formula 1-5]



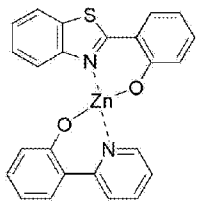
[Chemical Formula 1-6]



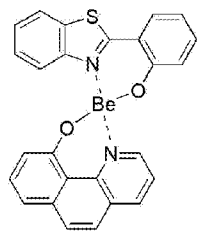
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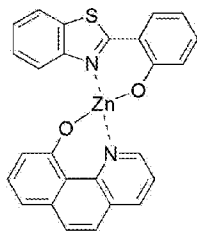
[Chemical Formula 1-8]



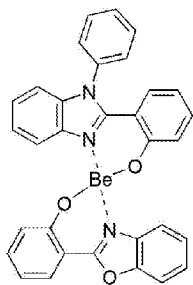
[Chemical Formula 1-9]



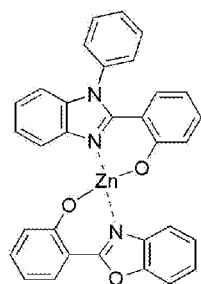
[Chemical Formula 1-10]



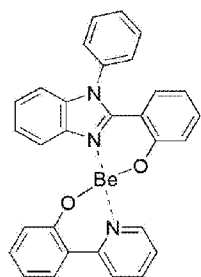
[Chemical Formula 1-11]



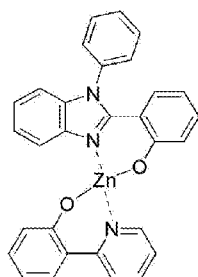
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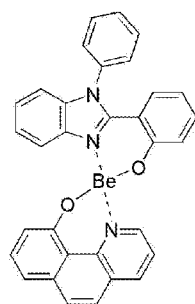
[Chemical Formula 1-13]



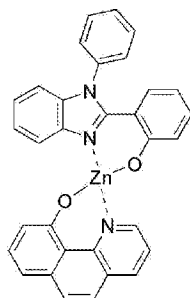
[Chemical Formula 1-14]



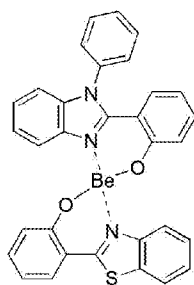
[Chemical Formula 1-15]



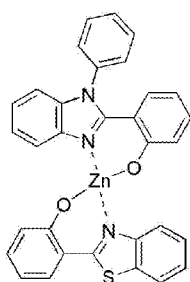
[Chemical Formula 1-16]



[Chemical Formula 1-17]



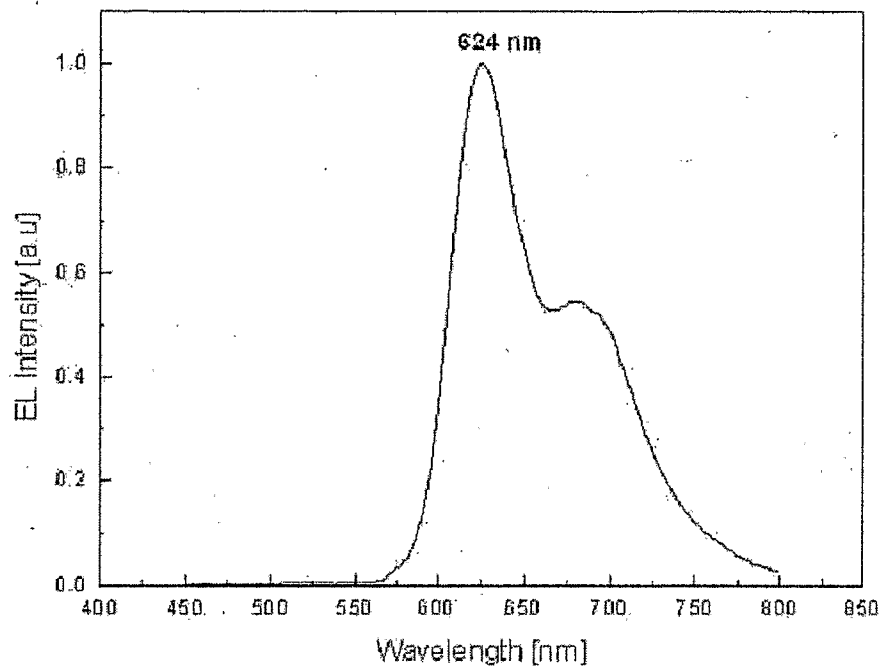
[Chemical Formula 1-18]



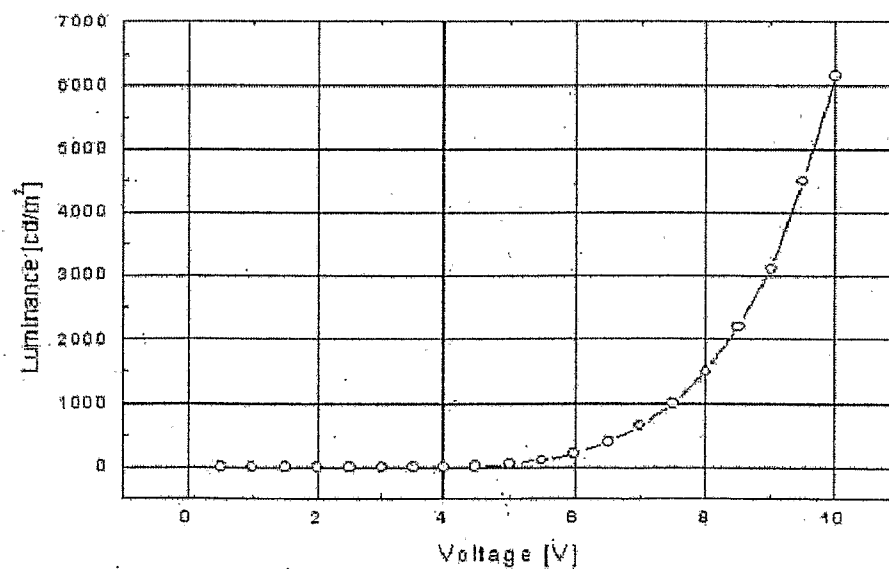
- [7] An electroluminescent device comprising an electroluminescent compound according to any one of claims 1 to 6.
- [8] An electroluminescent device according to claim 7, in which the electroluminescent compound is used as a host material in an emitting layer.

【DRAWINGS】

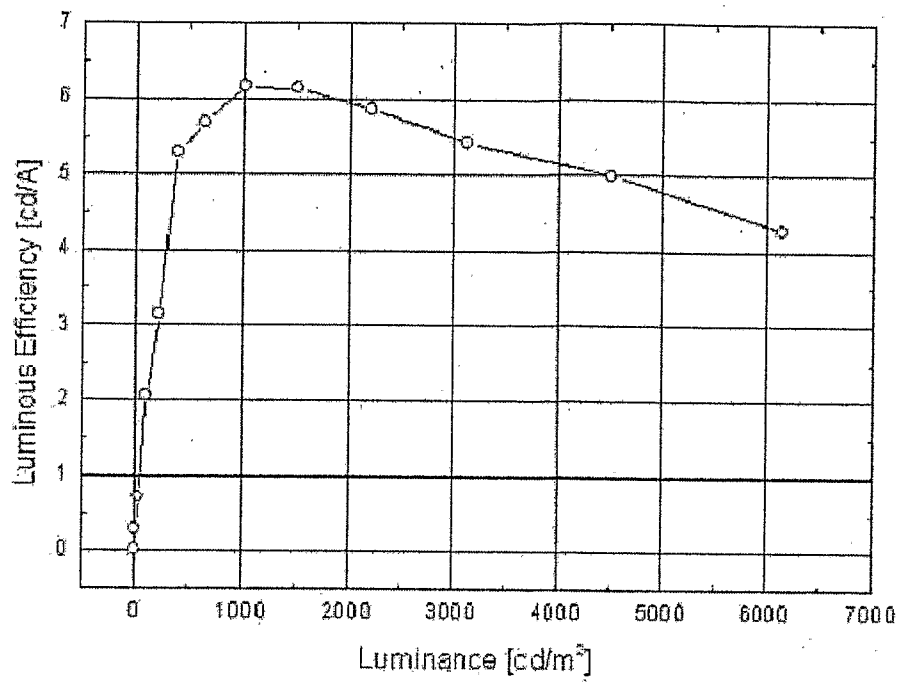
【Figure 1】



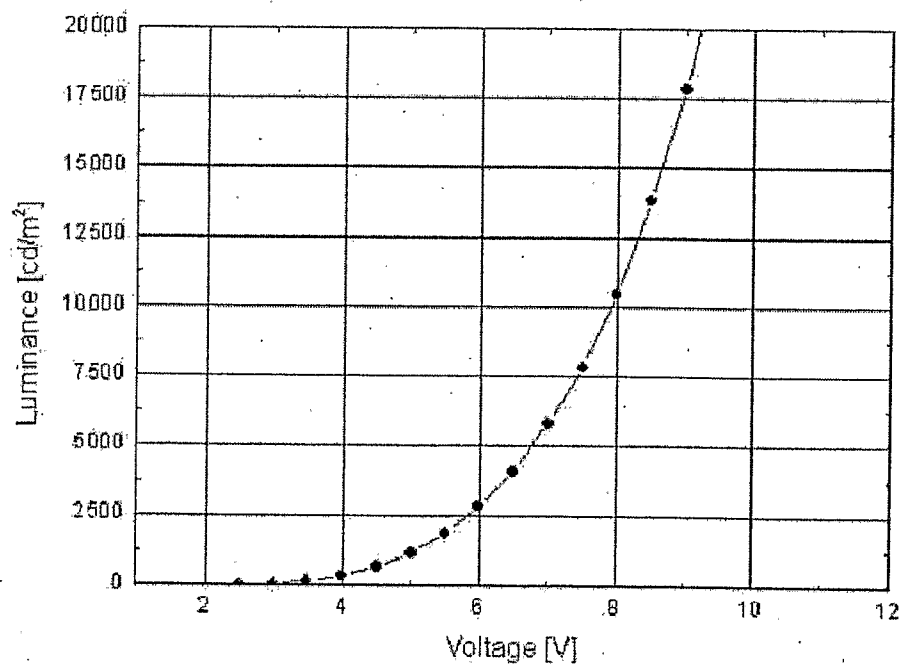
【Figure 2】



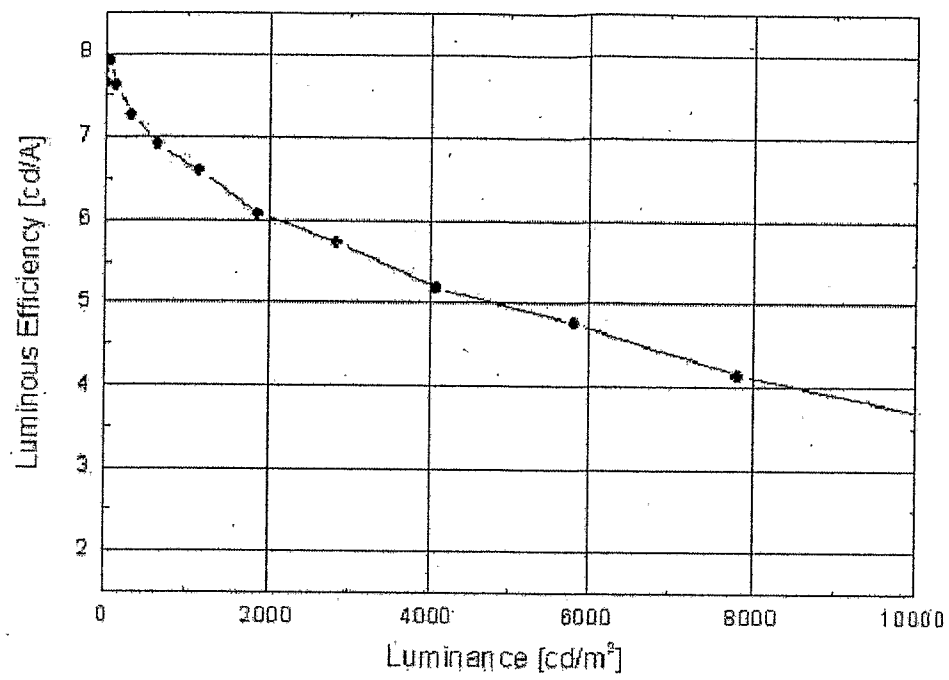
[Figure 3]



[Figure 4]



[Figure 5]



INTERNATIONAL SEARCH REPORT

International application No.
PCT/KR2007/000423**A. CLASSIFICATION OF SUBJECT MATTER****C09K 11/06(2006.01)i**

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)

IPC8 C09K 11/06

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)

eKIPASS, USPAT, PAJ, CA(STN)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	JP 2005-2101 A (SEMICONDUCTOR ENERGY LAB. CO., LTD) 06 January 2005 See abstract, claims, formula(1)	1-8
A	US 6936716 B1 (LIN) 30 August 2005 See abstract, claims, formula (I)	1-8
A	JP 2003-252888 A (MITSUBISHI CHEMICALS CORP) 10 September 2003 See the whole document	1-8
A	JP 2003-192691 A (MITSUBISHI CHEMICALS CORP) 09 July 2003 See the whole document	1-8
A	JP 2005-163036 A (CHI MEI ELECTRONICS CORP et al.) 23 June 2005 See the whole document	1-8

☐ Further documents are listed in the continuation of Box C.☒ See patent family annex.

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"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

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Date of the actual completion of the international search

09 MAY 2007 (09.05.2007)

Date of mailing of the international search report

09 MAY 2007 (09.05.2007)

Name and mailing address of the ISA/KR

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Facsimile No. 82-42-472-7140

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SOHN, Chang Ho

Telephone No. 82-42-481-8398



INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No.

PCT/KR2007/000423

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
JP17002101	06.01.2005	CN1609101A KR2004099161A US2004230061AA US2005033054AA US6998492BB	27.04.2005 26.11.2004 18.11.2004 10.02.2005 14.02.2006
US6936716B1	30.08.2005	None	
JP15252888	10.09.2003	None	
JP15192691	09.07.2003	None	
JP17163036	23.06.2005	TW245068B US2005116626AA US7193088BB	11.12.2005 02.06.2005 20.03.2007

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摘要(译)

本发明涉及由化学式1表示的有机电致发光化合物和包含其作为电致发光材料的电致发光器件。根据本发明的电致发光化合物的优点在于，当其用作OLED器件的主体材料时，其显著降低了驱动电压并显著提高了功率效率。

