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**Okuda et al.**(10) **Pub. No.: US 2011/0017984 A1**(43) **Pub. Date: Jan. 27, 2011**(54) **METAL COMPLEX COMPOUND AND  
ORGANIC ELECTROLUMINESCENT  
DEVICE USING SAME**No. 10/565,274, filed on Jan. 20, 2006, now Pat. No.  
7,667,228, filed as application No. PCT/JP2004/  
010687 on Jul. 21, 2004.(75) Inventors: **Fumio Okuda**, Sodegaura-shi (JP);  
**Toshihiro Iwakuma**, Sodegaura-shi  
(JP); **Keiko Yamamichi**,  
Sodegaura-shi (JP); **Chishio**  
**Hosokawa**, Sodegaura-shi (JP)(30) **Foreign Application Priority Data**

Jul. 22, 2003 (JP) ..... 2003-199995

**Publication Classification**(51) **Int. Cl.****H01L 51/54** (2006.01)**C07F 15/00** (2006.01)(52) **U.S. Cl.** ..... **257/40**; 546/4; 257/E51.026(57) **ABSTRACT**

Correspondence Address:

**STEPTOE & JOHNSON LLP**  
**1330 CONNECTICUT AVENUE, N.W.**  
**WASHINGTON, DC 20036 (US)**(73) Assignee: **Idemitsu Kosan Co., Ltd.**,  
Chiyoda-ku (JP)(21) Appl. No.: **12/923,633**(22) Filed: **Sep. 30, 2010****Related U.S. Application Data**(63) Continuation of application No. 12/656,892, filed on  
Feb. 18, 2010, which is a continuation of applicationA metal complex compound having a special structure con-  
taining metals such as iridium. An organic electrolumines-  
cence device which comprises at least one organic thin film  
layer sandwiched between a pair of electrode consisting of an  
anode and a cathode, wherein the organic thin film layer  
comprises the above metal complex compound, which emits  
light by applying an electric voltage between the pair of  
electrode. An organic EL device employing the novel metal  
complex compound emits various phosphorous lights includ-  
ing blue light having an enhanced current efficiency and  
prolonged lifetime.

# METAL COMPLEX COMPOUND AND ORGANIC ELECTROLUMINESCENT DEVICE USING SAME

## TECHNICAL FIELD

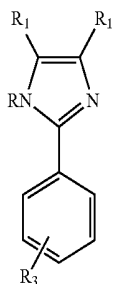
[0001] The present invention relates to a novel metal complex compound and an organic electroluminescence device using the compound. Particularly, the present invention relates to an organic electroluminescence device ("electroluminescence" will be referred to as "EL", hereinafter) having excellent efficiency of light emission and prolonged lifetime, and to a metal complex compound realizing it.

## BACKGROUND ART

[0002] The organic EL devices have been expected to be applied to color wide screen image display devices replacing liquid crystal display devices, and have been intensively developed. Recently, although displays using the organic EL devices have now been used in practical applications, full-color image display devices using the same are still in the course of development because they lack in sufficient light emitting property. Very high efficiency green organic light emitting devices based on electrophosphorescence employing ortho metalized iridium complex (fac-tris(2-phenylpyridine) iridium) as a phosphorus light emitting material for improving properties of the organic EL device are proposed. (refer to, for example, D. F. O'Brien and M. A. Baldo et al "Improved energy transferring electrophosphorescent devices" Applied Physics letters Vol. 74 No. 3, pp 442-444, Jan. 18, 1999; and M. A. Baldo et al "Very high-efficiency green organic light emitting devices based on electrophosphorescence" Applied Physics letters Vol. 75 No. 1, pp-4-6, Jul. 5, 1999).

[0003] Because the current organic EL devices employing the phosphorus photoluminescence are limited to emitting only green light, coverage as the color display devices is narrow. Therefore, it has been demanded to develop organic EL devices which emit light of different colors from green with improved light emission property. Regarding particularly with EL devices which emit blue light, those having an external quantum yield exceeding 5% is not reported yet. Accordingly, an improvement in the EL devices which emit blue light, if possible, enables the display devices to display full colors or white light resultantly advancing toward practical use of phosphorus light EL device greatly.

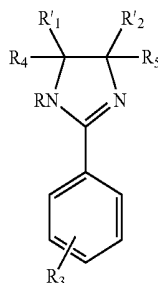
[0004] Further, although International PCT Patent Publication No. WO 02/15645 discloses following structures of ligands (A) and (B):



(A)

-continued

(B)



wherein  $R_1$  to  $R_5$  each independently represents a hydrogen atom, a halogen atom, an alkyl group, an aromatic group and an arylene group; and  $R_1'$  and  $R_2'$  an aromatic group, which may bond each other;

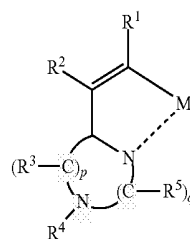
any practical synthesis example of real complex with the use of the ligands is not described.

## DISCLOSURE OF THE INVENTION

[0005] The present invention has been made to overcome the above problems and has an object of providing an organic EL device having an enhanced efficiency of light emission and prolonged lifetime, and an object of providing a metal complex compound realizing it.

[0006] As a result of intensive researches and studies to achieve the above object by the present inventors, it was found that the iridium complex proposed in the former patent literature neither generates nor isolates stably in a case where R is H in the above ligands (A) and (B) and that it is important for stably isolating the iridium complex to replace an atom on a side of N without forming a coordinate bond with a metal to an atom except a hydrogen atom. Then, the inventors designed ligands having various kinds of substituent on N, and succeeded in synthesizing iridium complex for the first time. Further, it was found that an employment of a metal complex compound having a partial structure represented by a following general formula (I) provides the EL device achieving an external quantum yield of 8% and exhibits an enhanced efficiency of light emission not only in blue region but also about various phosphorus photoluminescence and prolonged lifetime, resultantly completing the present invention.

[0007] Namely, the present invention provides a metal complex compound having a partial structure represented by a following general formula (I):



(I)

wherein  $R^1$  to  $R^5$  each independently represents a hydrogen atom, a cyano group, a nitro group, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon

atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms or a substituted or unsubstituted aromatic group having 1 to 30 carbon atoms; and a couple of  $R^1$  and  $R^2$ , a couple of  $R^2$  and  $R^3$ , a couple of  $R^3$  and  $R^4$  and a couple of  $R^4$  and  $R^5$  may bond each other to form a ring structure;

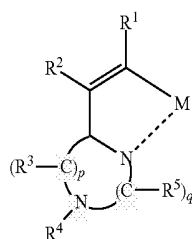
p and q each independently represents an integer of 0 to 3; p+q being 2 or 3; further, when p is an integer of 2 or greater, plural of  $R^3$  may bond each other to form a ring structure; when q is an integer of 2 or greater, plural of  $R^5$  may bond each other to form a ring structure; and

M represents any one metal atom selected from iridium (Ir) atom, rhodium (Rh) atom, platinum (Pt) atom or palladium (Pd) atom.

[0008] Further, the present invention provides an organic EL device which comprises at least one organic thin film layer sandwiched between a pair of electrode consisting of an anode and a cathode, wherein the organic thin film layer comprises the above metal complex compound, which emits light by applying an electric voltage between the pair of electrode.

#### THE PREFERRED EMBODIMENT TO CARRY OUT THE INVENTION

[0009] The present invention provides a metal complex compound having a partial structure represented by a following general formula (I):



[0010] In the general formula (I),  $R^1$  to  $R^5$  each independently represents a hydrogen atom, a cyano group, a nitro group atom, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms or a substituted or unsubstituted aromatic group having 1 to 30 carbon atoms; and a couple of  $R^1$  and  $R^2$ , a couple of  $R^2$  and  $R^3$ , a couple of  $R^3$  and  $R^4$  and a couple of  $R^4$  and  $R^5$  may bond each other to form a ring structure.

[0011] Examples of the halogen atom include fluorine atom, chlorine atom, bromine atom and iodine atom.

[0012] Examples of the alkyl group described above include methyl group, ethyl group, propyl group, isopropyl group, n-butyl group, s-butyl group, isobutyl group, t-butyl group, n-pentyl group, n-hexyl group, n-heptyl group, n-octyl group, etc.

[0013] The alkoxy group is expressed as —OY, wherein Y represents the same as the foregoing description about the alkyl group.

[0014] Examples of the alkylsilyl group include trimethylsilyl group, t-butyl dimethylsilyl group, etc.

[0015] Examples of the acyl group include acetyl group, propionyl group, butyryl group, isobutyryl group, etc.

[0016] Examples of the above aromatic group include benzene, naphthalene, anthracene, phenanthrene, pyrene, coronene, biphenyl, terphenyl, pyrrole, furan, thiophene, benzothienophene, oxadiazoline, diphenylanthracene, indoline, carbazole, pyridine, benzoquinone, fluoranthene, acenaphthofluoranthene, etc.

[0017] Further, examples of the substituent for those groups include cyano group, hydroxyl group, nitro group, halogen atom, substituted or unsubstituted alkyl group, substituted or unsubstituted amino group, substituted or unsubstituted alkoxy group, substituted or unsubstituted alkylsilyl group, substituted or unsubstituted acyl group, substituted or unsubstituted aromatic group, substituted or unsubstituted alkenyl group, a substituted or unsubstituted cycloalkyl group, substituted or unsubstituted heterocyclic group, substituted or unsubstituted arylalkyl group, a substituted or unsubstituted aryloxy group, substituted or unsubstituted alkoxycarbonyl group, carboxyl group, etc.

[0018] Examples of the ring structure formed by bonding  $R^1$  and  $R^2$ ,  $R^3$  and  $R^4$ , or  $R^4$  and  $R^5$  each independently include benzene, pyridine, naphthalene, benzothiazole, quinoline, etc.

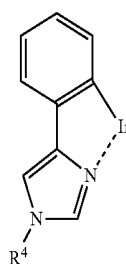
[0019] It is preferable that  $R^1$  to  $R^5$  each independently represents a hydrogen atom, a cyano group, a nitro group, a fluorine atom, a trifluoromethyl group, a dimethylamino group, a methoxy group, a t-butyl group, a trimethylsilyl group and an acetyl group.

[0020] In the general formula (I), p and q each independently represents an integer of 0 to 3 (preferably 0 to 2); p+q being 2 or 3; further, when p is an integer of 2 or greater, plural of  $R^3$  may bond each other to form a ring structure; when q is an integer of 2 or greater, plural of  $R^5$  may bond each other to form a ring structure.

[0021] Examples of the ring structure formed by plural of  $R^3$  and plural of  $R^5$  each independently include benzene, pyridine, etc.

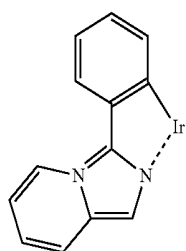
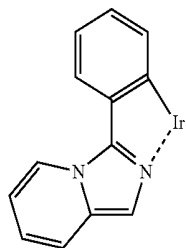
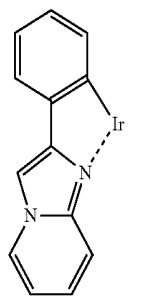
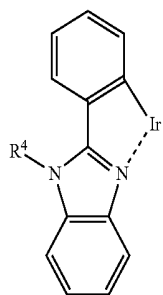
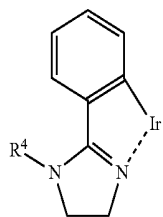
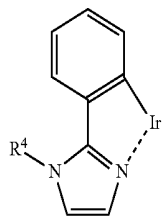
[0022] In the general formula (I), M represents any one metal atom selected from iridium (Ir) atom, rhodium (Rh) atom, platinum (Pt) atom or palladium (Pd) atom; while Ir and Pt are preferable and Ir is more preferable.

[0023] Further, it is preferable that the partial structure represented by general formula (I) is expressed by any one of (i) to (vii) or (i') to (vii') below, while (i) to (iii) being further preferable.



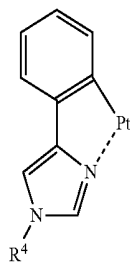
(i)

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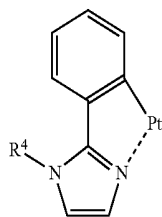


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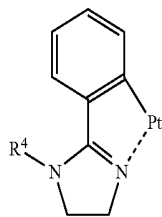
(ii)



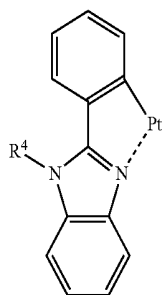
(iii)



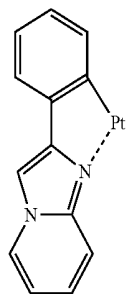
(iv)



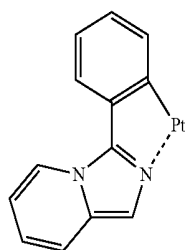
(v)



(vi)



(vii)



(i')

(ii')

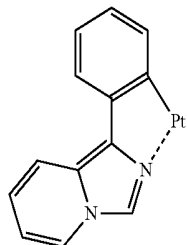
(iii')

(iv')

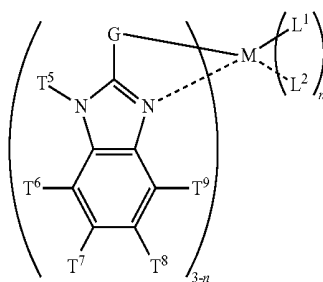
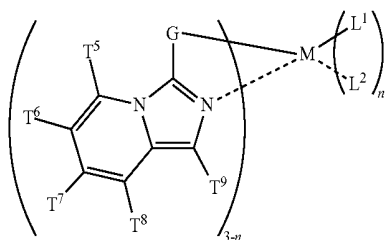
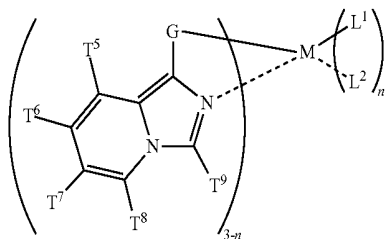
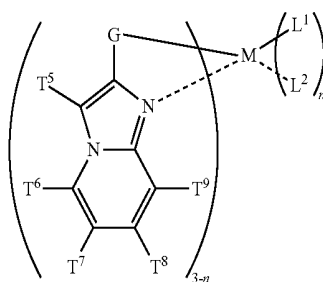
(v')

(vi')

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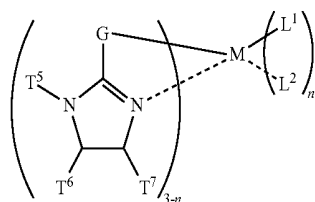
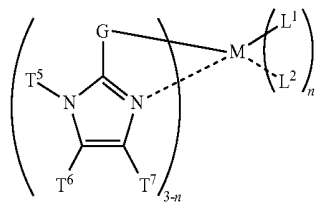
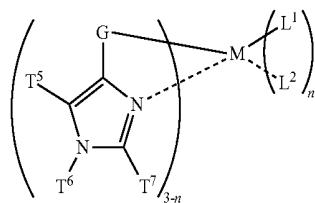


[0024] Furthermore, it is preferable that the metal complex compound of the present invention has basic skeletal structure expressed by following general formulae 1 to 7 and 1' to 7'.



(vii')

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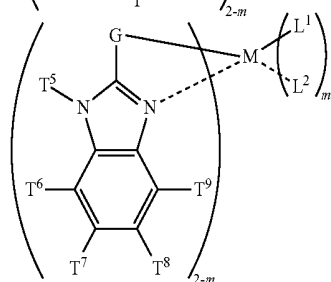
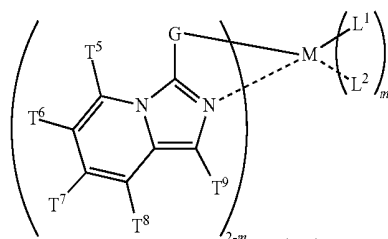
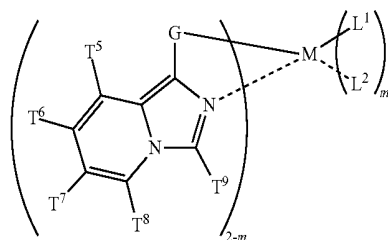
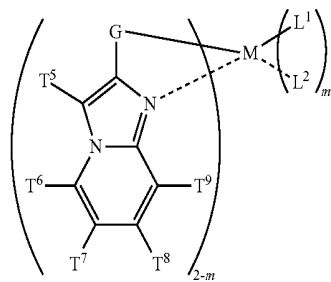


1

2

3

4



5

6

7

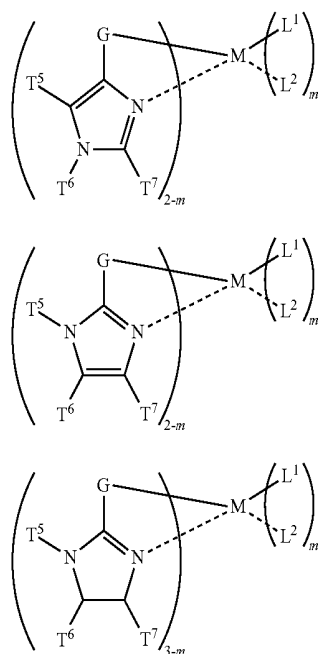
1'

2'

3'

4'

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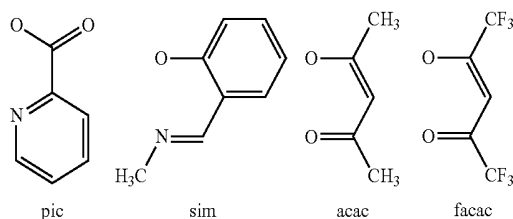
**[0025]** In the general formulae 1 to 7 and 1' to 7',  $T^5$  to  $T^9$  each independently represents a hydrogen atom, a cyano group, a nitro group atom, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms or a substituted or unsubstituted aromatic group having 1 to 30 carbon atom. Further, a couple of  $T^5$  and  $T^6$ , a couple of  $T^6$  and  $T^7$ , a couple of  $T^7$  and  $T^8$  and a couple of  $T^8$  and  $T^9$  may bond each other to form a ring structure.

**[0026]** Examples of the above halogen atom, alkyl group, alkoxy group, alkylsilyl group, acyl group, aromatic group, these substituents, and these preferable examples are the same as explained about  $R^1$  to  $R^5$  in the general formula (I).

**[0027]** Moreover, examples of the ring structure formed by bonding the couple of  $T^5$  and  $T^6$ , the couple of  $T^6$  and  $T^7$ , the couple of  $T^7$  and  $T^8$  and the couple of  $T^8$  and  $T^9$  each independently include benzene, pyridine, etc.

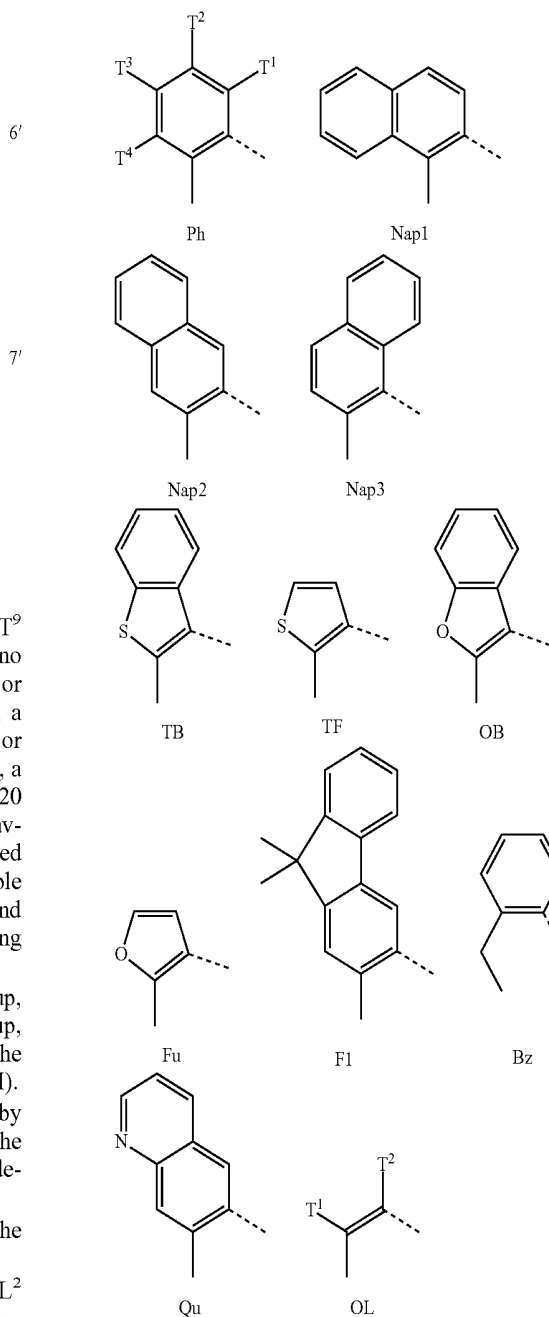
**[0028]** In the general formulae 1 to 7 and 1' to 7', M is the same as the forgoing description.

**[0029]** In the general formulae 1 to 7 and 1' to 7',  $L^1$  and  $L^2$  are each expressed by any one of the following structures:



**[0030]** In the general formulae 1 to 7 and 1' to 7', n represents an integer of 0 to 2, preferably 0 or 1, m represents an integer of 0 or 1.

**[0031]** In the general formulae 1 to 7 and 1' to 7', G is a group expressed by any one of groups below.



**[0032]** In the above groups, a dotted line “.....” represents a covalent bond with M.

**[0033]**  $T^1$  to  $T^4$  in the above Ph and OL each may independently represents a hydrogen atom, a cyano group, a nitro group, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms

or a substituted or unsubstituted aromatic group having 1 to 30 carbon atom. Examples of those groups, their substituents and those preferable examples are the same as explained about R<sup>1</sup> to R<sup>5</sup> in the general formula (I).

**[0034]** Further, examples of the substituent forming the ring structure by bonding the couple of V and T<sup>2</sup>, the couple of T<sup>2</sup> and T<sup>3</sup> or the couple of T<sup>3</sup> and T<sup>4</sup> in the Ph include a divalent group expressed by any one of groups below, while BL, MES1, MES2, PS1 and PS2 being preferable.



BL



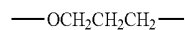
PL



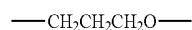
MEE1



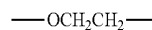
MEE2



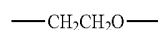
PA1



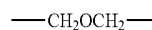
PA2



EA1



EA2



ME



AT



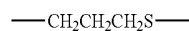
MES1



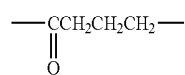
MES2



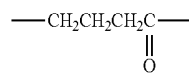
PS1



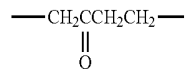
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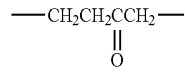
BAL1



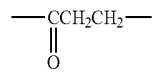
BAL2



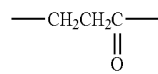
MEK1



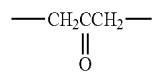
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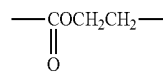
PAL1



PAL2

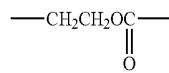


MMK

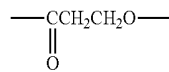


EES1

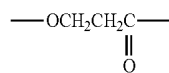
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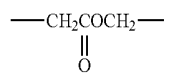
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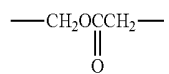
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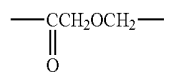
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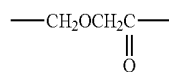
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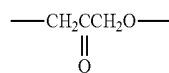
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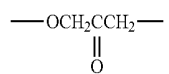
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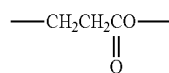
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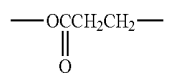
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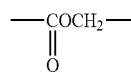
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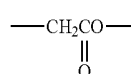
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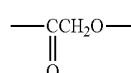
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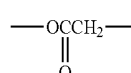
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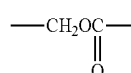
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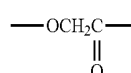
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EE2



MS1

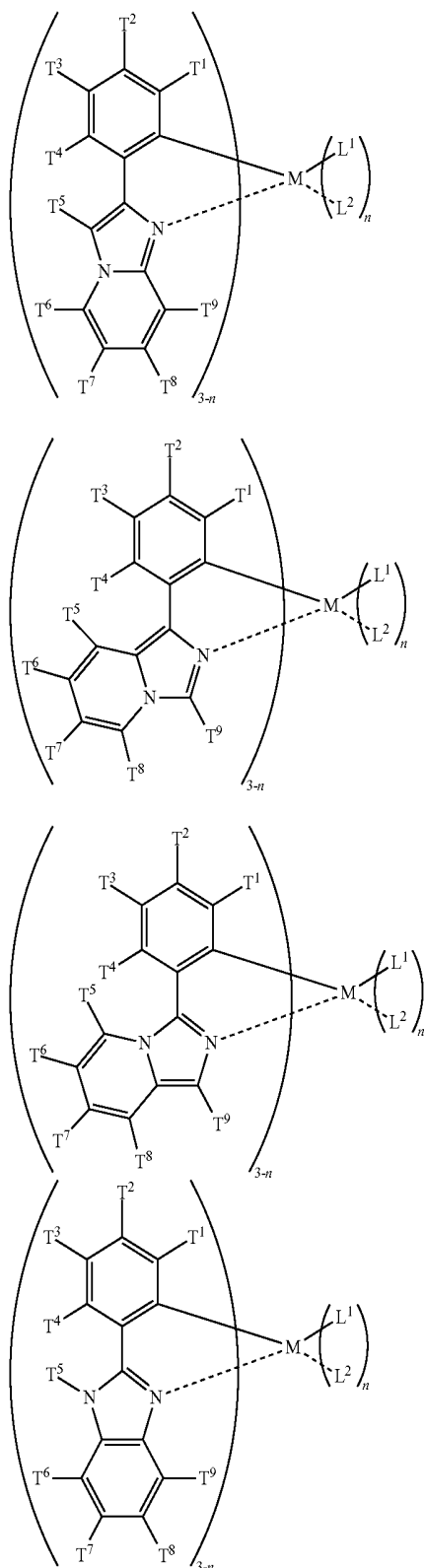


MS2

**[0035]** However, the group with a smaller number of superscript among T<sup>1</sup> to T<sup>4</sup> bonds to the left of the divalent group and the group with a greater number superscript among T<sup>1</sup> to T<sup>4</sup> bonds to the right of the divalent group.

**[0036]** Specific examples of the metal complex compound having any one basic skeletal structure among the general formulae 1' to 7' will be shown in Tables below, though not limited thereto.

**[0037]** In the Tables below, T<sup>1</sup> to T<sup>9</sup>, L<sup>1</sup> and L<sup>2</sup> (in the cases of the basic skeletal structures 1 to 4 and 1' to 4') or T<sup>1</sup> to T<sup>7</sup>, L<sup>1</sup> and L<sup>2</sup> (in the cases of the basic skeletal structures 5 to 7 and 5' to 7') are described within the columns righter to the basic skeletal structures.



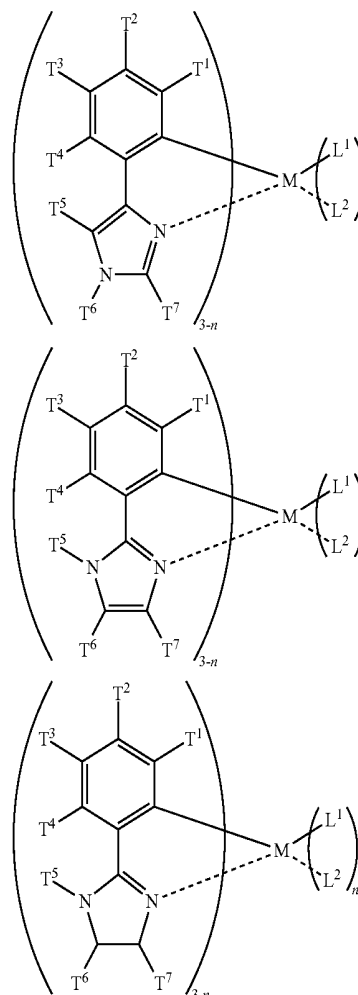
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**[0038]** Further in the Tables below, “BBS” means Basic Skeletal Structure, and “BS” means Skeletal Structure.

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**[0039]** The metal complex compound of the present invention is preferably a material for a light emitting element and in particular, more preferably a material for the organic EL device.

**[0040]** The present invention also provides an organic EL device which comprises at least one organic thin film layer sandwiched between a pair of electrode consisting of an anode and a cathode, wherein the organic thin film layer comprises the above metal complex compound of the present invention, which emits light by applying an electric voltage between the pair of electrode.

**[0041]** With regard to the amount of the metal complex compound of the present invention contained in the organic thin film layer, it is usually 0.1 to 100% by weight, preferably 1 to 30% by weight of total mass of the light emitting layer.

**[0042]** It is preferable for the organic EL device of the present invention that the light emitting layer comprises the metal complex compound of the present invention. Further, the light emitting layer is usually formed to a thin film by means of vapor deposition process or coating process, however, it is preferable that the layer comprising the metal complex compound of the present invention is formed into film by coating process because it simplifies the production process.

**[0043]** In the organic EL device of the present invention, a monolayer-type organic thin layer consists of a light emitting layer, which comprises the metal complex compound of the present invention. Typical examples of the construction of the organic EL device include (an anode/a hole injecting layer (a hole transporting layer)/a light emitting layer/a cathode); (an anode/a light emitting layer/an electron injecting layer (an electron transporting layer)/a cathode); and (an anode/a hole injecting layer (a hole transporting layer)/a light emitting layer/an electron injecting layer (an electron transporting layer)/a cathode).

**[0044]** The anode in the organic EL device covers a role of injecting holes into a hole injecting layer, a hole transporting layer or into a light emitting layer, and as the material for the anode, metals, alloys, metal oxides, electroconductive compounds, or these mixtures may be employable. Specific examples of the material for the anode include electroconductive metal oxides such as tin oxide, zinc oxide, indium oxide, indium tin oxide (ITO), etc.; metals such as gold, silver, chromium, nickel, etc.; mixtures or laminated materials of these electroconductive metal oxide and metals; inorganic electroconductive substance such as copper iodide, copper sulfide, etc.; organic electroconductive materials such as polyaniline, polythiophene, polypyrrole, etc.; and laminated materials of the above materials with ITO; preferably are the electroconductive metal oxides. Particularly, it is preferable to employ ITO from viewpoints such as productivity, enhanced electroconductivity, transparency, etc. Regarding with a film thickness of the anode, it is possible to be appropriately selected depending on the material.

**[0045]** With regard to the cathode, it covers a role of injecting electrons into an electron injecting layer, an electron transporting layer or into a light emitting layer. Specific examples of the material for the cathode include alkali metals (for example, Li, Na, K, etc.) and their fluoride or oxide, alkaline earth metals (for example, Mg, Ca, etc.) and their fluoride or oxide, gold, silver, lead, aluminum, sodium-potassium alloy or sodium-potassium mixed metals, lithium-aluminum alloy or lithium-aluminum mixed metals, magnesium-silver alloy or the magnesium-silver mixed metals, or rare earth metals such as indium, ytterbium, etc. Among those, preferable examples are aluminum, lithium-aluminum alloy or lithium-aluminum mixed metals, magnesium-silver alloy or magnesium-silver mixed metals, etc. The cathode may be a monolayer structure of the above material, and may be a laminated structure of the layer containing the above material. For example, the laminated structure such as aluminum/lithium fluoride, aluminum/lithium oxide or the like is preferable. Regarding with a film thickness of the cathode, it is possible to be appropriately selected depending on the material.

**[0046]** It may be appropriate that the hole injecting layer and the hole transporting layer of the organic EL device of the present invention have any function of injecting holes from the anode, transporting holes, or barrier the electrons injected from the cathode. Specific examples include carbazole derivatives, triazole derivatives, oxazole derivatives, oxadiazole derivatives, imidazole derivatives, polyarylethane derivatives, pyrazoline derivatives, pyrazolone derivatives, phenylenediamine derivatives, arylamine derivatives, amino substituted chalcone derivatives, styryl anthracene derivatives, fluorenone derivatives, hydrazone derivatives, stilbene derivatives, silazane derivatives, aromatic tertiary amine compounds, styryl amine compound, aromaticdimethylidene-based compounds, porphyrin-based compounds, polysilane-based compounds, poly(N-vinyl carbazole) derivatives, aniline-based copolymer; electroconductive

polymer oligomer such as thiophene oligomer, polythiophene, etc.; organosilane derivatives, metal complex compound of the present invention, etc. The hole injecting layer and the hole transporting layer may be composed of single layer comprising one or more kind of these hole injecting materials and those hole transporting materials or may be laminated with themselves or a layer comprising another kind of compound.

[0047] It may be appropriate that the electron injecting layer and the electron transporting layer of the organic EL device of the present invention have any function of injecting electrons from the cathode, transporting electrons, or barriering the holes injected from the anode. Specific examples include triazole derivatives, oxazole derivatives, oxadiazole derivatives, imidazole derivatives, fluorenone derivatives, anthraquinodimethane derivatives, anthrone derivatives, diphenylchinone derivatives, thiopyrandioxide derivatives, carbodiimide derivatives, fluorenylidene methane derivatives, distyrylpyrazine derivatives; aromatic ring tetracarboxylic acid anhydride such as naphthalene, perylene, etc.; phthalocyanine derivatives, various metal complexes represented by metal complexes of 8-quinolinol derivatives or metal complexes having benzoxazole or benzothiazole as ligand; organosilane derivatives, metal complex compound of the present invention, etc. The electron injecting layer may be composed of single layer comprising one or more kind of these electron injecting materials or may be laminated with an electron injecting layer comprising another kind of compound.

[0048] It is preferable that the light emitting layer in the organic EL device of the present invention has functions capable of injecting holes from the anode or the hole injecting layer when an electric field is applied, of injecting electrons from the cathode or the electron injecting layer, of mobilizing the injected electric charges (electrons and holes) by means of the electric field, and of providing a space for recombination of the electrons and holes thereby urging the light emission. It is preferable for the organic EL device of the present invention that the light emitting layer at least comprises the metal complex compound of the present invention, and it may comprise a host material which employs the metal complex compound as a guest material. Examples of the above host material include such as those having a carbazole skeleton, those having a diarylamine skeleton, those having a pyridine skeleton, those having a pyrazine skeleton, those having a triazine skeleton, those having an arylsilane skeleton, etc. It is preferable that T1 (energy level in the minimum triplet excitation state) of the host material is larger than T1 level of the guest material. The host material may be either a low molecular weight compound or a high molecular weight compound. Further, the light emitting layer in which the above light emitting materials are doped into the above host materials can be formed by co-deposition of the host materials and the light emitting materials such as the above metal complex compound, etc.

[0049] In the organic EL device of the present invention, although a process for forming each layers are not particularly specified, various kinds of process such as a vacuum deposition process, a LB process, a resistance heating deposition process, an electron beam process, a sputtering process, a molecular lamination process, a coating process (a spin coating process, a casting process, a dip coating process), an ink-jet process, a printing process are employable and the coating process of applying the materials over a substrate is preferable in the present invention.

[0050] In the above coating process, preparing a coating solution by dissolving the metal complex compound of the present invention into a solvent, and by applying the coating solution over the surface of a predetermined layer (or, electrode), followed by drying may form the organic thin film layer. In the coating solution, a resin may be contained either by dissolved in a solvent or by dispersing into the solvent. Regarding with the resin, both non-conjugate high polymer (for example, polyvinylcarbazole) and conjugate high polymer (for example, polyolefin-based high polymer) are employable. Specific examples include polyvinylchloride, polycarbonate, polystyrene, polymethyl methacrylate, polybutylmethacrylate, polyester, polysulfone, polyphenylene oxide, polybutadiene, poly (N-vinyl carbazole), hydrocarbon resin, ketone resin, phenoxy resin, polyamide, ethyl cellulose, vinyl acetate, ABS resin, polyurethane, melamine resin, unsaturated polyester resin, alkyd resin, epoxide resin, silicone resin, etc.

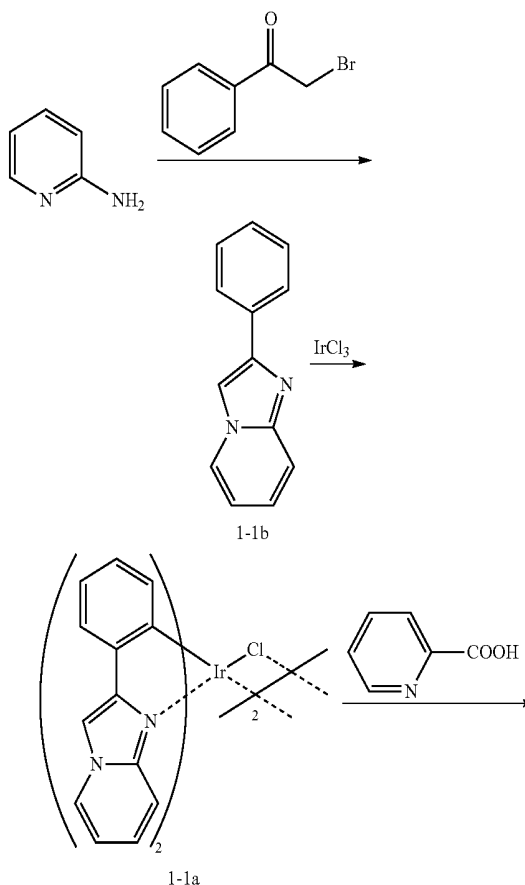
## EXAMPLES

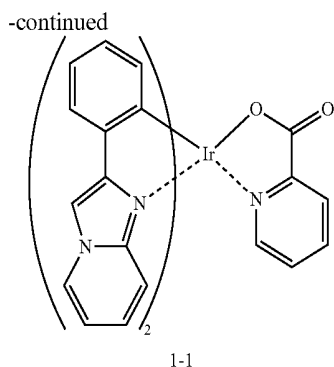
[0051] The present invention will be described in more detail by reference to the following examples. However, it should be noted that these examples are only illustrative and not intended to limit the invention thereto.

### Example 1

#### Synthesis of Metal Complex Compound 1-1

[0052] The route for synthesis of Metal complex Compound 1-1 is illustrated as the following.





[0053] In the above route, the structural formula of Intermediate 1-1a expresses a dimer configuration.

#### (1) Synthesis of Intermediate 1-1b

[0054] Placing 2-aminopyridine in an amount of 3.5 g (36 mmol),  $\alpha$ -bromoacetophenone in an amount of 7.2 g (36 mmol) and sodium hydrogen carbonate in an amount of 3.6 g (43 mmol) into a flask, the resultant mixture reacted among 120 milliliter of ethanol for 4 hours at the room temperature and subsequently for 2 hours under refluxing. Separating insoluble by filtration, the resultant filtrate was concentrated. Extracting with the use of methylene chloride in an amount of 150 milliliter, the resultant extract was washed three times using 200 milliliter of water. After drying an organic layer with the use of magnesium sulfide and removing the solvent, brown crystals were obtained. Refining the crystals by means of silicagel column (hexane/methylene chloride), 6.3 g of 2-phenylimidazo[1,2-a]pyridine Intermediate 1-1b as white crystals was obtained (yield: 90%). The white crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum. The measurement result is shown as follows:

[0055]  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  7.8-8.3 (m, 4H),  $\delta$  7.0-8.3 (m, 5H),  $\delta$  0.6-6.9 (m, 1H)

#### (2) Synthesis of Intermediate 1-1a

[0056] Placing Intermediate 1-1b in an amount of 5.0 g (25.7 mmol) and  $\text{IrCl}_3$  hydrate (available from Strem Chemicals, Inc.) in an amount of 1.9 g (6.4 mmol) into a flask, replacing the atmosphere with argon gas, and after pouring 2-ethoxyethanol in an amount of 40 milliliter, the resultant mixture was reacted for 15 hours under refluxing. A resultant yellow precipitation was separated by filtration, followed by washing twice with the use of ethanol in an amount of 5 milliliter. Further, it was dissolved in 150 milliliter of methylene chloride, and the resultant solution was washed with the use of HCl aqueous solution, followed by washing three times with the use of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and as a result, 1.39 g of Intermediate 1-1a as yellow crystals was obtained (yield: 35%).

#### (3) Synthesis of Metal Complex Compound 1-1

[0057] Placing Intermediate 1-1a in an amount of 1.39 g (1.13 mmol) and 2-pyridinecarboxylic acid in an amount of 0.55 g (4.52 mmol) into a flask, replacing the atmosphere with argon gas, and after pouring 1,2-dichloroethane in an amount of 20 milliliter, the resultant mixture was reacted for 17 hours under refluxing. Separating the resultant yellow precipitation, dissolving the precipitation into 400 milliliter of methylene

chloride, it was washed three times using 150 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and then, washing the resultant mixture with using a small amount of methylene chloride, 0.85 g of Metal complex Compound 1-1 as yellow crystals was obtained (yield: 54%). The yellow crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum and from the result in accordance with Field Desorption Mass Spectrum (FD-MS) analysis. The measurement result is shown as follows:

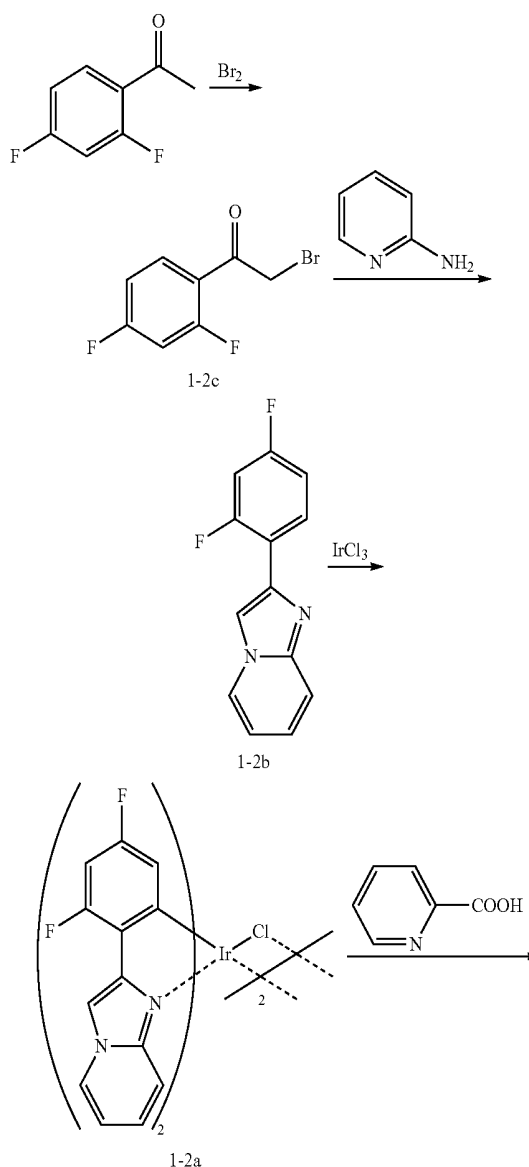
[0058] FD-MS:  $m/z=701$

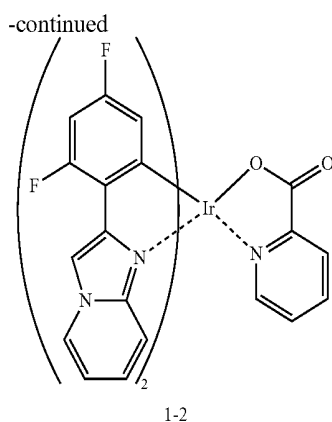
[0059] Further, by measuring phosphorus light (methylene chloride solution) of the resultant Metal complex Compound 1-1, it was found that  $\lambda_{\text{max}}$  (wave length of peak light emission intensity) of phosphorus light was 580 nm.

#### Example 2

##### Synthesis of Metal Complex Compound 1-2

[0060] The route of synthesis of Metal complex Compound 1-2 is illustrated in the following.





[0061] In the above route, the structural formula of Intermediate 1-1a expresses a dimer configuration.

#### (1) Synthesis of Intermediate 1-2c

[0062] While cooling acetic acid solution prepared by dissolving 25 g (160.1 mmol) of 2,4-difluorophenyl acetophenone in an amount of 50 milliliter down to 10° C. or cooler, 25.5 g (160.1 mmol) of bromine was dripped and the resultant solution reacted for 7 hours. Throwing the resultant solution into 300 milliliter of water, the solution was extracted with the use of methylene chloride. After drying an organic layer with the use of magnesium sulfide, the solvent was removed. Refining the resultant residues by means of silica column (hexane), 23.4 g of  $\alpha$ -bromo-2,4-difluorophenyl acetophenone Intermediate 1-2c as brown oil was obtained (yield: 62%). The brown oil was confirmed as the aimed compound from <sup>1</sup>H-NMR spectrum. The measurement result is shown as follows:

[0063] <sup>1</sup>H-NMR (CDCl<sub>3</sub>):  $\delta$  7.87-8.14 (m, 1H),  $\delta$  6.8-7.13 (m, 2H),  $\delta$  4.49 (d, 2H)

#### (2) Synthesis of Intermediate Product 1-2b

[0064] Placing 2-aminopyridine in an amount of 3.3 g (35.5 mmol), Intermediate 1-2c in an amount of 8.4 g (35.5 mmol) and sodium hydrogen carbonate in an amount of 3.6 g (43 mmol) into a flask, the resultant mixture reacted among 120 milliliter of ethanol for 4 hours at the room temperature and subsequently for 2 hours under refluxing. Separating insolubles by filtration, the resultant filtrate was concentrated. Extracting with the use of dichloromethane in an amount of 150 milliliter, the resultant extract was washed three times using 200 milliliter of water. After drying an organic layer with the use of magnesium sulfide and removing the solvent, brown crystals were obtained. Refining the crystals by means of silicagel column (hexane/methylene chloride), 7.3 g of 2-(2',4'-difluorophenyl)imidazo[1,2-a]pyridine Intermediate 1-2b was obtained (yield: 89%). The brown crystals were confirmed as the aimed compound from <sup>1</sup>H-NMR spectrum. The measurement result is shown as follows:

[0065] <sup>1</sup>H-NMR (CDCl<sub>3</sub>):  $\delta$  7.9-8.45 (m, 3H),  $\delta$  7.5-7.7 (m, 1H),  $\delta$  6.7-7.28 (m, 4H)

#### (3) Synthesis of Intermediate 1-2a

[0066] Placing Intermediate 1-2b in an amount of 4.7 g (20.6 mmol) and IrCl<sub>3</sub> hydrate (available from Strem Chemicals, Inc.) in an amount of 1.53 g (5.1 mmol) into a flask, replacing the atmosphere with argon gas, and after pouring

2-ethoxyethanol in an amount of 25 milliliter, the resultant mixture was reacted for 15 hours under refluxing. A resultant pale yellow precipitation was separated by filtration, followed by washing twice with the use of ethanol in an amount of 5 milliliter. Further, it was dissolved in 150 milliliter of methylene chloride, and the resultant solution was washed three times with the use of HCl aqueous solution, followed by washing twice with the use of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and as a result, 1.39 g of Intermediate 1-2a as yellow crystals was obtained (yield: 35%).

#### (4) Synthesis of Metal Complex compound 1-2

[0067] Placing Intermediate 1-2a in an amount of 1.39 g (1.13 mmol) and 2-picolinic acid in an amount of 0.55 g (4.52 mmol) into a flask, the atmosphere was replaced with argon gas. Pouring 20 milliliter of 1,2-dichloroethane into the resultant solution, it was reacted for 17 hours under refluxing. Separating the resultant yellow precipitation, dissolving the precipitation into 400 milliliter of methylene chloride, it was washed three times using 150 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and then, washing the resultant mixture using a small amount of methylene chloride, 0.85 g of Metal complex Compound 1-2 as yellow crystals was obtained (yield: 54%). The yellow crystals were confirmed as the aimed compound from <sup>1</sup>H-NMR spectrum and from the result in accordance with FD-MS analysis. The measurement result is shown as follows:

[0068] <sup>1</sup>H-NMR (CDCl<sub>3</sub>):  $\delta$  7.84-8.30 (m, 7H),  $\delta$  7.2-7.47 (m, 2H),  $\delta$  6.7-7.0 (m, 3H),  $\delta$  6.2-6.6 (m, 2H),  $\delta$  5.44-5.88 (m, 4H)

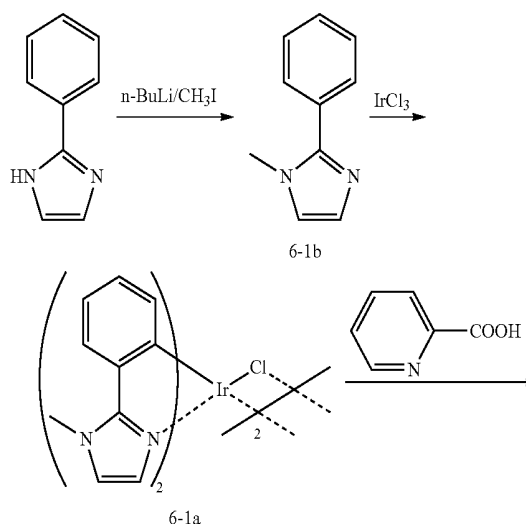
[0069] FD-MS: m/z=773

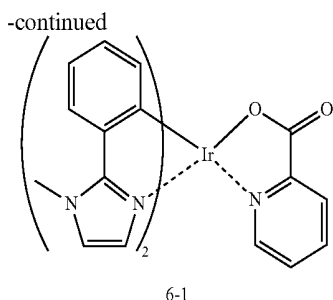
[0070] Further, by measuring phosphorus light (methylene chloride solution) of the resultant Metal complex Compound 1-2, it was found that  $\lambda$  max of phosphorus light was 529 nm.

### Example 3

#### Synthesis of Metal Complex Compound 6-1

[0071] The route for synthesis of Metal complex Compound 6-1 is illustrated in the following.





[0072] In the above route, the structural formula of Intermediate 6-1a expresses a dimer configuration.

#### (1) Synthesis of Intermediate 6-1b

[0073] Placing 2-phenylimidazole in an amount of 8.6 g (60 mmol) into a flask having a dropping funnel, and after replacing the atmosphere with argon gas, 180 milliliter of tetrahydrofuran was added. Under cooling with ice, n-butyllithium of 1.56 mol/liter in an amount of 39.1 milliliter (61 mmol) was dripped down into the solution spending 30 minutes and subsequently, 8.6 g (61 mmol) of methyl iodide dissolved into 10 milliliter of tetrahydrofuran was dripped down. After termination of dripping down, the resultant solution was reacted at the room temperature for 3 hours. Concentrating the reacted solution and extracting the resultant solid using 150 milliliter of methylene chloride, it was washed three times using 150 milliliter of water. After drying an organic layer with the use of magnesium sulfate, the solvent was removed. Refining the crystals by means of silicagel column (hexane/methylene chloride), 6.1 g of 1-methyl-2-phenylimidazole Intermediate 6-1b as white crystals was obtained (yield: 69%). The white crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum. The measurement result is shown as follows:

[0074]  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  7.29-7.67 (m, 5H),  $\delta$  6.93-7.10 (m, 2H),  $\delta$  3.69 (s, 3H)

#### (2) Synthesis of Intermediate 6-1a

[0075] Placing Intermediate 6-1b in an amount of 4.1 g (26.2 mmol) and  $\text{IrCl}_3$  hydrate (available from Strem Chemicals, Inc.) in an amount of 1.95 g (6.5 mmol) into a flask, replacing the atmosphere with argon gas, and after pouring 2-ethoxyethanol in an amount of 30 milliliter, the resultant mixture was reacted for 11 hours under refluxing. A resultant yellow precipitation was separated by filtration, followed by washing twice with the use of ethanol in an amount of 5 milliliter. Further, it was dissolved in 600 milliliter of methylene chloride, and the resultant solution was washed three times using 200 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and as a result, 1.35 g of Intermediate 6-1a as pale yellow crystals was obtained (yield: 38%). The pale yellow crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum. The measurement result is shown as follows:

[0076]  $^1\text{H-NMR}$  ( $\text{CD}_2\text{Cl}_2$ ):  $\delta$  7.26-7.42 (m, 2H),  $\delta$  6.47-6.94 (m, 3H),  $\delta$  6.0-6.09 (m, 1H),  $\delta$  4.13 (s, 3H)

#### (3) Synthesis of Metal Complex Compound 6-1

[0077] Placing Intermediate 6-1a in an amount of 1.32 g (1.21 mmol) and 2-picolinic acid in an amount of 0.59 g (4.87 mmol) into a flask, the atmosphere was replaced with argon

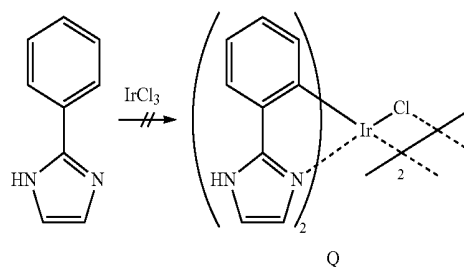
gas. Pouring 15 milliliter of 1,2-dichloroethane into the resultant solution, it was reacted for 8 hours under refluxing. Separating the resultant yellow precipitation, dissolving the precipitation into 200 milliliter of methylene chloride, it was washed 4 times using 150 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and further, re-crystallized from methylene chloride/hexane. As a result 1.17 g of Metal complex Compound 6-1 as yellow crystals was obtained (yield: 78%). The yellow crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum. The measurement result is shown as follows:

[0078]  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  8.1-8.2 (m, 1H),  $\delta$  7.75-7.90 (m, 2H),  $\delta$  7.2-7.51 (m, 3H),  $\delta$  6.3-7.0 (m, 9H),  $\delta$  6.13 (d, 1H),  $\delta$  4.06 (s, 3H)

[0079] Further, by measuring phosphorus light (methylene chloride solution) of the resultant Metal complex Compound 6-1, it was found that  $\lambda_{\text{max}}$  of phosphorus light was 562 nm.

#### Comparative Example 1

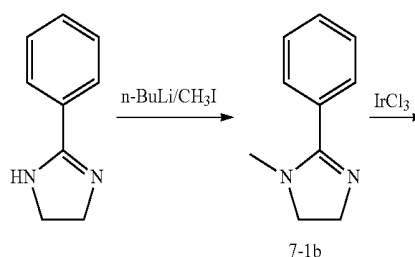
[0080] Placing 4-phenylimidazole in an amount of 3.8 g (26.3 mmol) and  $\text{IrCl}_3$  hydrate (available from Strem Chemicals, Inc.) in an amount of 1.96 g (6.6 mmol) into a flask, the atmosphere was replaced with argon gas. Adding 30 milliliter of 2-ethoxyethanol, the resultant solution reacted for 18 hours under refluxing and as a result, a homogeneous blackish brown solution was prepared without any precipitate. Distilling the solvent away, the resultant solution was processed and a black solid was obtained, however, it was not identified as an aimed Ir metal complex compound (Q below). Comparing with Example 3, when a hydrogen atom exists at N position of imidazole as illustrated below, it was understood that any substituent such as a methyl group is necessary because synthesizing Ir complex is difficult.



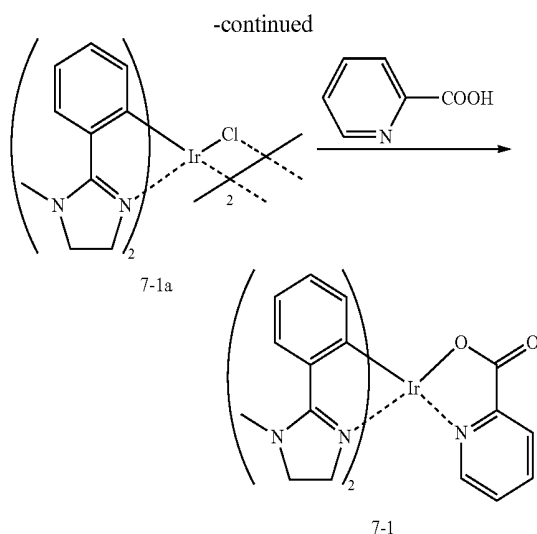
#### Example 4

##### Synthesis of Metal Complex Compound 7-1

[0081] The route for synthesis of Metal complex Compound 7-1 is illustrated in the following.







[0082] In the above route, the structural formula of Intermediate 7-1a expresses a dimer configuration.

#### (1) Synthesis of Intermediate 7-1b

[0083] Placing 2-phenylimidazole in an amount of 8.9 g (60.8 mmol) into a flask having a dropping funnel, and after replacing the atmosphere with argon gas, 210 milliliter of tetrahydrofuran was added. Under cooling with ice, n-butyllithium of 1.56 mol/liter in an amount of 39.3 milliliter (61.2 mmol) was dripped down into the solution spending 30 minutes and subsequently, 8.7 g (61.3 mmol) of methyl iodide dissolved into 10 milliliter of tetrahydrofuran was dripped down. After termination of dripping down, the resultant solution was reacted at the room temperature for 3 hours. Concentrating the reacted solution and extracting the resultant solid using 150 milliliter of methylene chloride, it was washed three times using 150 milliliter of water. After drying an organic layer with the use of magnesium sulfate, the solvent was removed. Refining the crystals by means of silicagel column (hexane/methylene chloride), 8.0 g of 1-methyl-2-phenylimidazo Intermediate 7-1b as white crystals was obtained (yield: 83%). The white crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum. The measurement result is shown as follows:

[0084]  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  7.33-7.60 (m, 5H),  $\delta$  3.27-3.98 (m, 4H),  $\delta$  2.76 (s, 3H)

#### (2) Synthesis of Intermediate 7-1a

[0085] Placing Intermediate 7-1b in an amount of 4.4 g (27.5 mmol) and  $\text{IrCl}_3$  hydrate (available from Strem Chemicals, Inc.) in an amount of 2.1 g (6.9 mmol) into a flask, the atmosphere was replaced with argon gas. Pouring 30 milliliter of 2-ethoxyethanol into the resultant solution, it was reacted for 16 hours under refluxing. A resultant yellow precipitation was separated by filtration, followed by washing twice with the use of ethanol in an amount of 5 milliliter. Further, it was dissolved in 200 milliliter of methylene chloride, and the resultant solution was washed 4 times using 200 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and as a result, 2.1 g of Intermediate 7-1a as orange crystals was obtained (yield: 57%). The orange crystals were confirmed as the aimed compound from  $^1\text{H-NMR}$  spectrum. The measurement result is shown as follows:

[0086]  $^1\text{H-NMR}$  ( $\text{DMSO-d}_6$ ):  $\delta$  7.51-7.61 (m, 1H),  $\delta$  6.69-6.97 (m, 3H),  $\delta$  3.60-4.1 (m, 4H),  $\delta$  3.33 (s, 3H)

#### (3) Synthesis of Metal Complex Compound 7-1

[0087] Placing Intermediate 7-1a in an amount of 1.95 g (1.78 mmol) and 2-picolinic acid in an amount of 0.88 g (7.14 mmol) into a flask, the atmosphere was replaced with argon gas. Pouring 20 milliliter of 1,2-dichloroethane into the resultant solution, it was reacted for 17 hours under refluxing. Removing the solvent from the reacted solution and dissolving the resultant brown solid using 150 milliliter of methylene chloride, it was washed 5 times using 200 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and further, refined by means of silica column (methylene chloride/hexane). Intermediate 7-1 as brown crystals in an amount of 1.2 g was obtained (yield: 53%). It was confirmed in accordance with FD-MS that the brown crystals were the aimed compound. The measurement result is shown as follows:

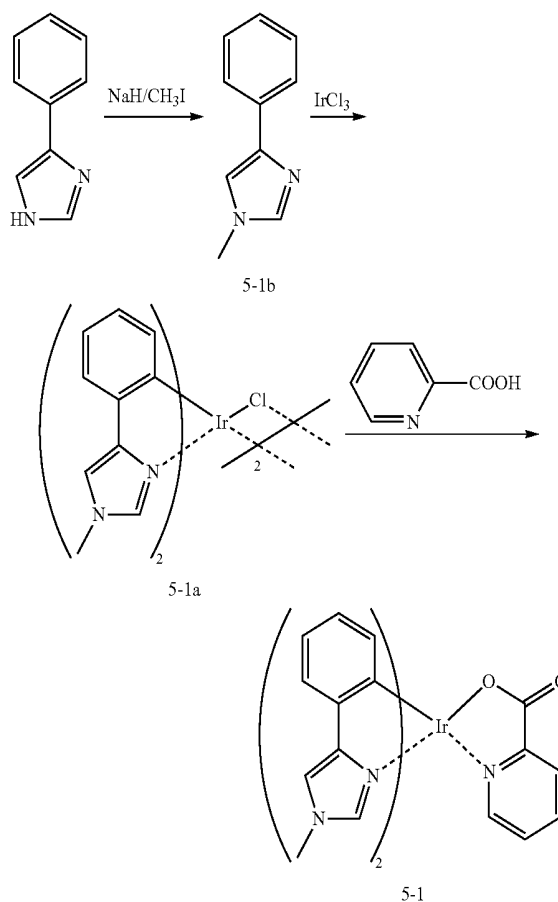
[0088] FD-MS:  $m/z$ =632

[0089] Further, by measuring phosphorus light (methylene chloride solution) of the resultant Metal complex Compound 7-1, it was found that  $\lambda_{\text{max}}$  of phosphorus light was 562 nm

#### Example 5

##### Synthesis of Metal Complex Compound 5-1

[0090] The route for synthesis of Metal complex Compound 5-1 is illustrated in the following.



## (1) Synthesis of Intermediate 5-1b

**[0091]** Placing 4-phenylimidazole in an amount of 9.6 g (67 mmol) into a flask having a dropping funnel, and after replacing the atmosphere with argon gas, 50 milliliter of dimethylsulfoxide was added. Adding 2.8 g (60% in oil, 70 mmol equivalent) of NaH little by little into the solution and after achieving the addition of entire amount, the resultant solution was heated for 2 hours at a temperature of 80° C. Subsequently, 9.6 g (68 mmol) of methyl iodide dissolved into 15 milliliter of methylsulfoxide was dripped down and the resultant solution was heated again for further 15 hours at the temperature of 80° C.

**[0092]** Throwing the resultant solution into 200 milliliter of water, the solution was extracted using 200 milliliter of ethylene chloride. After separating an organic layer, it was washed 5 times using 200 milliliter of water, and it was dried with the use of magnesium sulfate. After concentrating the solution, refining the resultant pale brown solids by means of silicagel column (methylene chloride), 5.5 g of 1-methyl-4-phenylimidazo Intermediate 5-1b as white crystals was obtained (yield: 52%).

## (2) Synthesis of Intermediate 5-1a

**[0093]** Placing Intermediate 5-1b in an amount of 3.0 g (18.9 mmol) and  $\text{IrCl}_3$  hydrate (available from Strem Chemicals, Inc.) in an amount of 1.41 g (4.7 mmol) into a flask, the atmosphere was replaced with argon gas. Pouring 15 milliliter of 2-ethoxyethanol into the resultant solution, it was reacted for 13 hours under refluxing. A resultant white precipitation was separated by filtration, followed by washing twice with the use of ethanol in an amount of 5 milliliter. Further, it was dissolved in 500 milliliter of methylene chloride, and the resultant solution was washed 3 times using 150 milliliter of water. After drying the resultant solution with the use of magnesium sulfate, the solvent was distilled away and as a result, 1.77 g of Intermediate 5-1a as white crystals was obtained (yield: 69%).

## (3) Synthesis of Metal Complex Compound 5-1

**[0094]** Placing Intermediate 5-1a in an amount of 1.38 g (1.27 mmol) and 2-picolinic acid in an amount of 0.62 g (5.1 mmol) into a flask, the atmosphere was replaced with argon gas. Pouring 20 milliliter of 1,2-dichloroethane into the resultant solution, it was reacted for 12 hours under refluxing. Separating the resultant yellow precipitation, dissolving the precipitation into 300 milliliter of methylene chloride, it was washed 4 times using 200 milliliter of water. After drying the solution with the use of magnesium sulfate, the solvent was distilled away. Resultant yellow crystals were refined with silicagel column (methylene chloride/methanol). Intermediate 5-1 as pale yellow crystals in an amount of 0.4 g was obtained (yield: 26%).

**[0095]** Further, by measuring phosphorus light (methylene chloride solution) of the resultant Metal complex Compound 5-1, it was found that  $\lambda_{\text{max}}$  of phosphorus light was 453 nm.

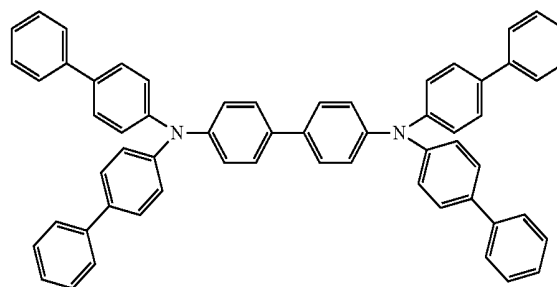
## Example 6

## Fabrication of Organic EL Device

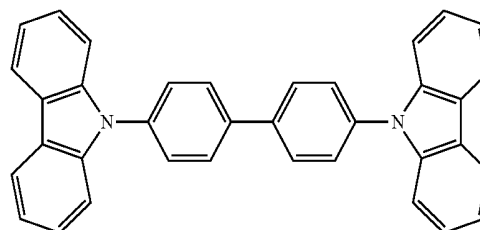
**[0096]** A glass substrate of 25 mm×75 mm×1.1 mm thickness having an ITO transparent electrode was cleaned by application of ultrasonic wave in isopropyl alcohol for 5 minutes and then by exposure to ozone generated by ultraviolet light for 30 minutes. The cleaned substrate having the transparent electrode lines was attached to a substrate holder, and on the surface of the cleaned substrate at the side having

the transparent electrode, a film of 4,4'-bis [N-(4-biphenyl)-N-(4-biphenyl)amino]biphenyl below having a thickness of 40 nm was formed so that the formed film covered the transparent electrode. The formed film worked as the hole transporting layer. Further, a host material (CBP) below together with adding a photo luminescent Ir-Metal Complex Compound 1-1 as a dopant were vapor deposited obtaining a film thickness of 30 nm on the formed film. The formed film worked as a light emitting layer. A concentration of Compound 1-1 in the light emitting layer was 5% by weight. On the light emitting layer, a film of (1,1-bisphenyl)-4-olate)bis (2-methyl-8-quinolinolato) aluminum (BALq) below having a thickness of 10 nm was formed. The formed film of BALq worked as the hole barrier layer. On the film formed above, a film of aluminum complex of 8-hydroxyquinoline (Alq) having a thickness of 30 nm was formed. The film of Alq worked as the electron injecting layer. Subsequently, lithium fluoride (LiF) being alkali metal halide was vapor deposited up to 0.15 nm in thickness and then, aluminum was vapor deposited up to 150 nm in thickness. The Al/LiF worked as a cathode.

**[0097]** An organic EL device was fabricated in the manner described above. The device fabricated above was examined by feeding electric current. Yellowish green light was emitted at a luminance of 103  $\text{cd/m}^2$  under a voltage of 6.7 V and a current density of 2.79  $\text{mA/cm}^2$ . The CIE chromaticity coordinates were (0.347, 0.494), and the current efficiency was 3.7  $\text{cd/A}$ . Additionally,  $\lambda_{\text{max}}$  of light emission was 533 nm.



4,4'-bis[N-(4-biphenyl)-N-(4-biphenyl)amino]biphenyl

**[0098]**

CBP

## INDUSTRIAL APPLICABILITY

**[0099]** As described above in detail, the organic EL device employing the novel metal complex compound of the present invention emits various phosphorous light including blue light having an enhanced current efficiency and prolonged lifetime. Accordingly, the present invention is applicable for a field such as various display devices, display panels, backlights, illuminating light sources, beacon lights, signboards, and interior designs, particularly suitable as display device for color displays.

## LENGTHY TABLES

The patent application contains a lengthy table section. A copy of the table is available in electronic form from the USPTO web site (<http://seqdata.uspto.gov/?pageRequest=docDetail&DocID=US20110017984A1>). An electronic copy of the table will also be available from the USPTO upon request and payment of the fee set forth in 37 CFR 1.19(b)(3).

1.-8. (canceled)

9. A metal complex compound comprising a structure which comprises a metal atom selected from the group consisting of Ir, Rh and Pt, a first ring structure and a second ring structure which bonds to the first ring structure via a carbon to carbon single bond, wherein

the first ring structure comprises a five-membered or six-membered ring structure constituted by carbon atoms and two nitrogen atoms, one of two nitrogen atoms coordinating to the metal atom, and the other nitrogen atom which does not coordinate to the metal atom is substituted by a group selected from the group consisting of a cyano group, a nitro group, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms, and a substituted or unsubstituted aromatic group having 1 to 30 carbon atoms;

the carbon atoms constituting the first ring structure other than the carbon atom which bonds to the second ring structure are each optionally substituted by a group selected from the group consisting of a cyano group, a nitro group, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms, and a substituted or unsubstituted aromatic group having 1 to 30 carbon atoms;

a pair of substituents optionally bond to each other to form a ring structure; and

the second ring structure comprises an aromatic ring constituted by only carbon atoms or a combination of carbon atoms and one heteroatom selected from the group consisting of nitrogen, oxygen and sulfur;

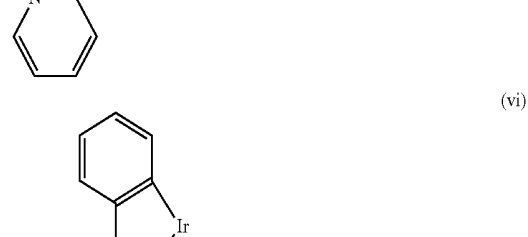
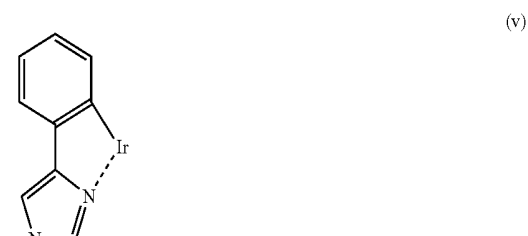
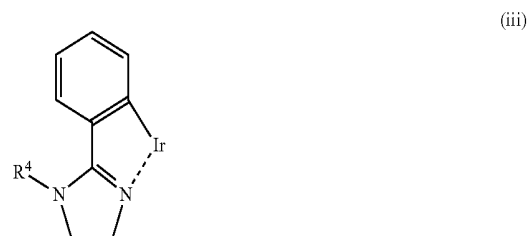
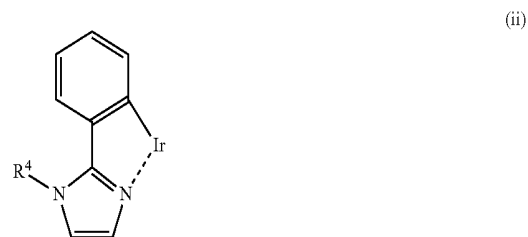
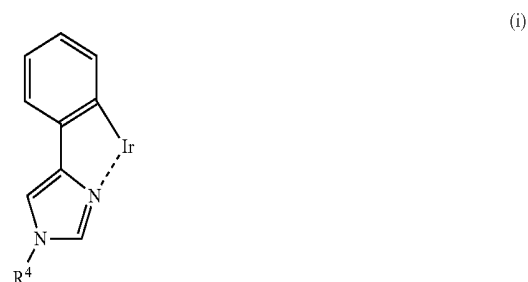
with the proviso that when the first ring structure is a five-membered ring which bonds to the second ring structure via the carbon atom between two nitrogen atoms, substituents on two carbon atoms do not bond to each other to form a ring structure, and

when the first ring structure is a five-membered ring which bonds to the second ring structure via the carbon atom between two nitrogen atoms, the second ring structure is not substituted with phenyl.

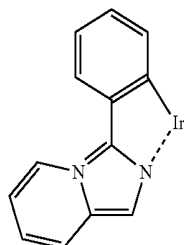
10. The metal complex compound according to claim 9, which is a material for an light emitting element.

11. The metal complex compound according to claim 9, wherein the structure comprising the metal atom, the first ring

structure and the second ring structure is represented by any one of formulae (i) to (iii) and (v) to (vii):



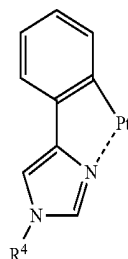
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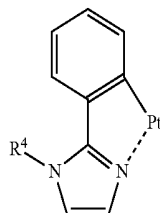
(vii)

wherein  $R^4$  is a group selected from the group consisting of a cyano group, a nitro group, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms, and a substituted or unsubstituted aromatic group having 1 to 30 carbon atoms.

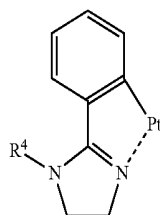
**12.** The metal complex compound according to claim 9, wherein the structure comprising the metal atom, the first ring structure and the second ring structure is represented by any one of formulae (i') to (iii') and (v') to (vii'):



(i')

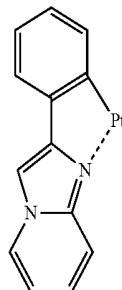


(ii')

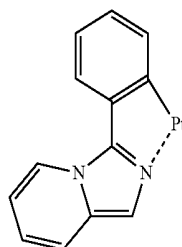


(iii')

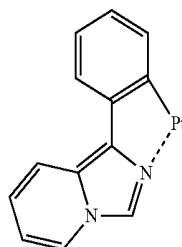
-continued



(v')



(vi')



(vii')

wherein  $R^4$  is a group selected from the group consisting of a cyano group, a nitro group, a halogen atom, a substituted or unsubstituted alkyl group having 1 to 20 carbon atoms, a substituted or unsubstituted amino group, a substituted or unsubstituted alkoxy group having 1 to 20 carbon atoms, a substituted or unsubstituted alkylsilyl group having 1 to 20 carbon atoms, a substituted or unsubstituted acyl group having 1 to 20 carbon atoms, and a substituted or unsubstituted aromatic group having 1 to 30 carbon atoms.

**13.** The metal complex compound according to claim 9, wherein the second ring structure is the aromatic ring structure selected from the group consisting of benzene, pyridine, naphthalene, benzothiazole, quinoline, thiazole, furan, benzofuran and 9,9-dimethylfluorene.

**14.** An organic electroluminescence device which comprises at least one organic thin film layer sandwiched between a pair of electrode consisting of an anode and a cathode, wherein the organic thin film layer comprises the metal complex compound according to claim 9 which emits light by applying an electric voltage between the pair of electrode.

**15.** The organic electroluminescence device according to claim 14, wherein said light emitting layer comprises said metal complex compound.

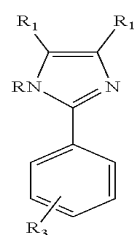
**16.** The organic electroluminescence device according to claim 14, wherein said organic thin film layer comprising the metal complex compound is formed by coating process.

\* \* \* \* \*

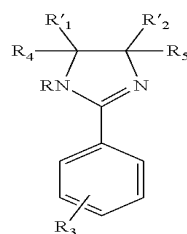
专利名称(译)	金属配合物和使用它的有机电致发光器件		
公开(公告)号	<a href="#">US20110017984A1</a>	公开(公告)日	2011-01-27
申请号	US12/923633	申请日	2010-09-30
申请(专利权)人(译)	出光兴产股份有限公司.		
当前申请(专利权)人(译)	出光兴产股份有限公司.		
[标]发明人	OKUDA FUMIO IWAKUMA TOSHIHIRO YAMAMICHI KEIKO HOSOKAWA CHISHIO		
发明人	OKUDA, FUMIO IWAKUMA, TOSHIHIRO YAMAMICHI, KEIKO HOSOKAWA, CHISHIO		
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# 摘要(译)

一种金属配位化合物，具有含铍等金属的特殊结构。一种有机电致发光器件，其包括夹在由阳极和阴极组成的一对电极之间的至少一个有机薄膜层，其中所述有机薄膜层包含上述金属络合物，其通过在所述电极之间施加电压而发光。一对电极。采用该新型金属配位化合物的有机EL器件发射各种磷光，包括具有提高的电流效率和延长的寿命的蓝光。



(A)



(B)